DIGITAL TECHNOLOGIES FOR SUSTAINABILITY IN THE EUROPEAN CHEMICAL INDUSTRY

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cefic

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FOREWORD

Today, the European chemical industry is at a crossroads. We support the goals of the European Green Deal and Europe's ambition to become climate neutral by 2050. Yet, implementing the Green Deal agenda represents a so-called 'double twin' transition for our sector. We need to become climate neutral, circular, innovate towards safe and sustainable chemicals, and digitalise our industry. And we must do it all while remaining competitive in the global market to keep a thriving chemical industry in Europe. This requires a massive effort from our industry and all connected value chains. Additional investments and new solutions will be necessary to undergo this unprecedented change.

Digitalisation holds the key to implementing many objectives of the European Green Deal. It has the power to entirely change the way our industry innovates, sources, produces, collaborates across ecosystems, and develops new business models. It opens up many new business opportunities for our sector.

This Report takes a closer look at concrete examples of how digital technologies, including artificial intelligence (AI), blockchain, and robotics can play a role in achieving sustainability goals in our sector.

From using real-time Internet of Things (IoT)-sensor data to monitor production parameters and reveal patterns for greater energy and resource efficiency, to deploying artificial intelligence for predictive maintenance and asset optimisation, the opportunities are endless. High performance and, in the future, quantum computers as well as predictive modelling, will play an increasingly decisive role in the innovation process. Digital passports will enable completely new opportunities for a circular economy.

These opportunities inevitably bring many challenges for the industry to overcome, which this Report highlights as well. For example, common data sharing standards will need to emerge, and new skills to implement digital solutions must be developed.

Get inspired and be part of this exciting journey!

Sincerely yours,

Dr. Martin Brudermüller
President, European Chemical Industry Council (Cefic)

PREFACE

The European chemical industry is fully committed to contributing to the European Green Deal. Chemical companies in Europe are not only working on their own sustainability objectives, but also providing innovative solutions that serve as enablers for many downstream industries to reach their own. The chemical industry's sustainability journey is often referred to as the 'quadruple challenge' or the 'double twin transition': a circular and climate-neutral economy, Safe and Sustainable-by-Design chemicals, and concurrent digital transition. Given the closely connected nature of these objectives, it is surprising to see a lack of clarity around many of the key components required to achieve them, such as in how the transitions interrelate on a practical level, which technologies to apply, collaboration across the ecosystem, regulatory frameworks, and roadmaps of where to start.

In its more than 150 years of history, the chemical industry has continuously evolved and implemented innovations in many technological fields, including digital technologies. For example, for many years, the industry has used digital, highly automated process control systems within its production plants that run 24/7. Digitalisation in the chemical industry is therefore nothing new. However, enormous opportunities exist beyond basic digitalisation — a journey that is just beginning for most players.

This Report considers how the industry can bring together the challenges it faces around the double twin transition, the opportunities transformation creates, and the capabilities it already has access to. Essentially, it aims to answer one central question: how can digital technologies enable European chemical companies to reach their sustainability objectives? The conclusions of this Report are therefore highly relevant for the industry, individual companies, and policymakers alike.

An additional challenge the sector faces today is the energy crisis. Focusing on the double twin transition helps mitigate this mid-term issue by enabling greater energy and material efficiency, as well as delivering mid- and long-term benefits as we move towards 2050.

We are optimistic that accelerated adoption of digital technologies, in conjunction with greater collaboration, the industry's proven ability to continuously improve and innovate, and the support of the European Union, national, and local governments, can and will unlock the power of digitalisation to deliver the green future that we all desire.

Dr. Daniel Witthaut
Executive Director Innovation
Cefic

Dr. Michael Kolk
Managing Partner
Arthur D. Little

EXECUTIVE SUMMARY

This Report focuses on how digital technologies can help the European chemical industry accelerate the journey to sustainability.

Arthur D. Little and the European Chemical Industry Council (Cefic) joined forces to prepare this Report, which summarises the views of digital technology experts from within and outside the chemical industry. Recommendations from this Report are based on the result of 15 individual interviews with senior digital and sustainability experts (e.g., chief digital officers or chief sustainability officers) as well as a survey of more than 70 experts from 50 companies that are broad representatives of the chemical industry in terms of type of business, size, and region. To add cross-industry perspectives, the study also took into account input from more than 10 globally recognised digital technology experts outside the chemical industry.

The Report highlights various use cases that demonstrate how leading companies in the chemical industry are developing and applying the latest digital technologies, including artificial intelligence and blockchain.[1] Advanced digital technologies are already widely applied across the value chain, from research and development to customer-facing aspects. From the industry perspective, it is clear that there is still a lot of unleveraged potential for digital technologies to further accelerate the achievement of the sustainability objectives described in Chapter 1.

Chapter 2 begins by exploring where along the chemicals value chain digital technologies can make the greatest contribution to achieving sustainability across the fields of greenhouse gas (GHG) reduction, circularity, health, safety, and environment. Although digital technologies can contribute to a great extent across all sustainability objectives, five priorities emerged as the most prominent for both large and small companies: (1) process design and production for climate and circularity objectives, (2) sustainability assessment, (3) enabling materials and chemicals circularity through tracking and tracing, (4) sustainable product design, and (5) safe and efficient logistics and distribution. Clearly, much wider and more intensive implementation will be required to accelerate the green and digital transition across these and other priorities. For example, the survey also showed that the number of chemical companies exploiting big data in production is expected to double in the coming years.

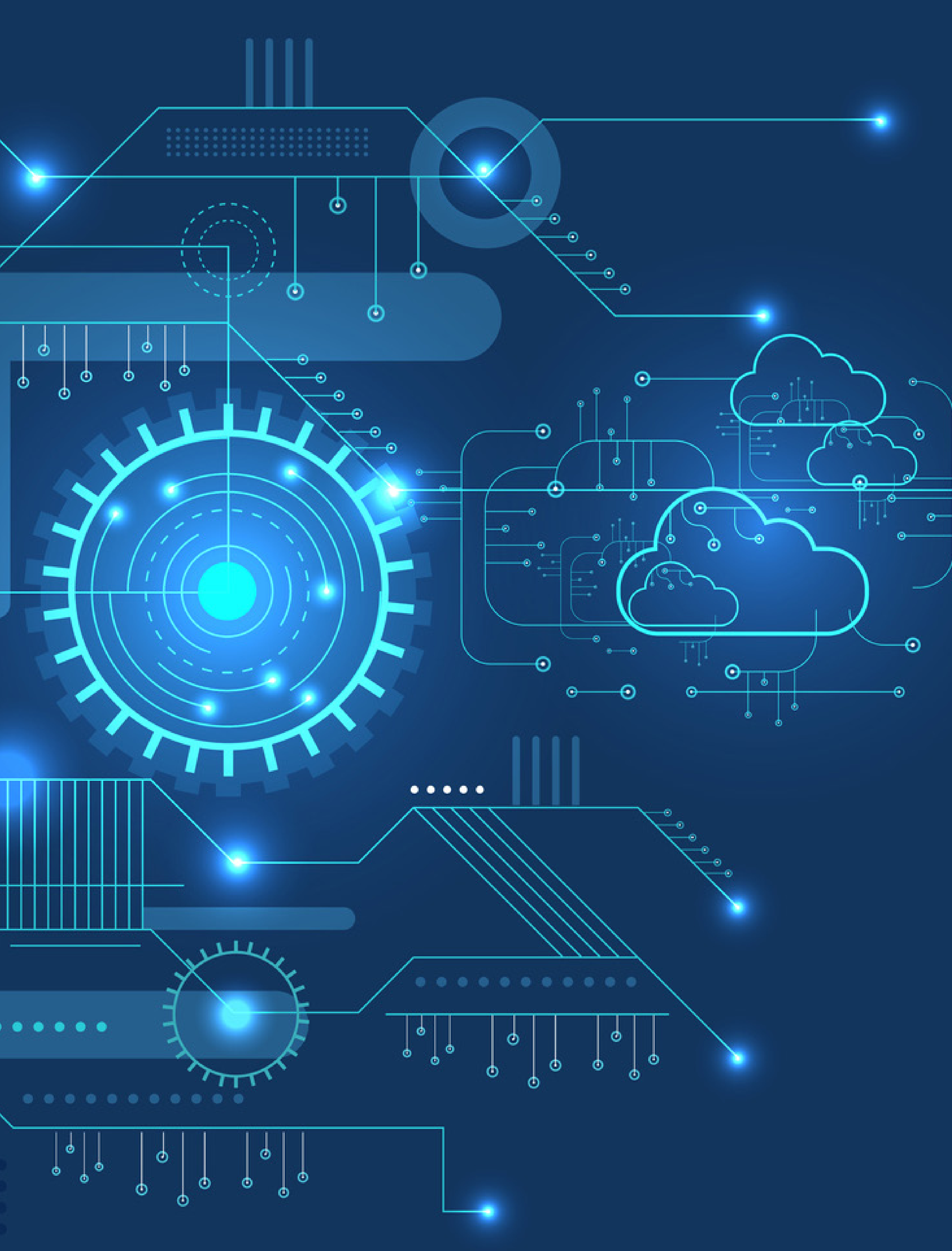
A wide variety of state-of-the-art digital technologies are already being used to address sustainability needs. These technologies can be clustered into four areas: (1) modelling and analytics, (2) internal and external data sharing, (3) enabling infrastructure, and (4) automation/limited human involvement. Most of these technologies are applied across the whole value chain, and our survey confirmed that all digital technologies are expected to increase significantly in importance in the coming years. The Report also shares a set of inspiring current chemical industry use cases for these technologies.

1 In addition to the illustrative use cases included in this Report, new examples from chemical companies regarding applications of digital technologies for sustainability in the European chemical industry will be regularly published on ChemistryCan, which promotes contributions of the chemical sector as a solution provider for a sustainable society.

Chapter 3 considers the range of technological, financial, human capital, and organisational challenges that needs to be overcome to further drive and accelerate implementation of digital technologies in the chemical sector. For example, technological challenges include data availability, interoperability, standardisation, IT infrastructure, and technology readiness. Costs and investments are also key issues. With regards to human capital, the industry needs to further develop the digital capabilities of its existing employees as well as hire new experts. Certainly, there is a 'war for digital talent,' but chemical companies also experience high interest from digital experts, given the major impact their work has on sustainability goals versus, for example, the big tech giants. Overcoming these challenges will deliver not only sustainability but also other business benefits, such as efficiency, effectiveness, innovativeness, and competitiveness.

In the final section of the Report, we draw some conclusions about the steps the chemical industry and the EU institutions need to take for a successful journey towards a green and digital Europe. These include:

- **Adopting an industry ecosystem perspective.** Since the double twin transition does not only affect the chemical industry, broad collaboration with the chemical value chain and across ecosystems is key to further success. Large and leading companies will continue their digitalisation journeys, but leaders need to exchange knowledge with other players, including smaller companies or non-EU partners, to ensure the whole value chain is digitalised. Bottlenecks in the collective digitalisation journey should be anticipated, and companies can address these by sharing best practices, adopting ecosystem thinking, and deciding what can be done better collectively.
- **Increased emphasis on data management and data sharing.** Reliable data is among a company's most vital assets. The industry has collected data extensively for many years but is still at an early stage in terms of data usage. Future-ready data governance and data management capabilities are needed, including IT infrastructure that enables data transparency, sovereignty, provenance, interoperability, and cybersecurity. Data sharing in a secure form, both internally within companies and externally with other value chain players, is one of the keys to driving sustainability. The industry, together with suppliers and customers, could accelerate efforts to establish standards in sustainability-related data collection, sharing, and reporting. Cybersecurity is increasingly important to ensure safe data sharing within unstructured networks.
- **Driving digital innovation and targeted investment.** The green and digital transition brings massive changes, prompting the need to explore new business models and anticipate major disruptions. The industry's innovation capacity and substantial investments in digital technologies are essential to drive the double twin transition. To further stimulate deployment of digital technologies and foster related collaborations, appropriate risk-sharing measures for the chemical sector may need to be considered. The industry should also take actions to attract necessary digital talents and develop internal capabilities.
- **Working actively with the EU institutions.** To complement the chemical industry's ongoing efforts, support from policymakers is needed. The industry should therefore play a more active role in working with the EU institutions and provide input for the development of EU digital standards, policies, and regulations. Efforts should aim at facilitating the chemical industry's required digitalisation journey, including the use of digital technologies under the ongoing EU legislative initiatives (e.g., Data Act, AI Act) and suggesting options to policymakers on how to harmonise regulations and remove obstacles.



1. THE EUROPEAN CHEMICAL INDUSTRY EN ROUTE TOWARDS THE EU GREEN DEAL GOALS

SUSTAINABLE DEVELOPMENT & THE EUROPEAN POLICY LANDSCAPE

The United Nations (UN) Sustainable Development Goals[2] and the European Green Deal[3] aim to achieve a climate-neutral, pollution-free, sustainable, circular, and inclusive economy by 2050. Major elements of the Green Deal with direct impact on the chemical industry include:

- The European Climate Law.[4]
- The new Circular Economy Action Plan.[5]
- The Zero Pollution Ambition[6] pillar, in particular the Chemicals Strategy for Sustainability[7] and the related Safe and Sustainable-by-Design[8] approach.

THE EUROPEAN CHEMICAL INDUSTRY & ITS TRANSFORMATION

Through its upstream positioning, the chemical industry has a significant impact on practically all value chains (including energy, transport, housing, electronics, etc.), resulting in a pivotal enabling role for the realisation of the European Green Deal ambitions.

With over 1.2 million workers, €499 billion annual turnover, and €9.4 billion of research and innovation (R&I) investments in 2020, the European chemical industry is a wealth-generating sector of the economy and an important contributor to building a sustainable future for Europe. As a major energy and resource intensive industry, the EU27 chemical industry has reduced its energy consumption by 21% and its greenhouse gas emissions (scope 1) by nearly 54% since 1990, while the production index has increased by 49% over the same period.[9]

The EU's ambitious climate and circularity targets as well as health, safety, and environment objectives, including the Chemicals Strategy for Sustainability, call for significant transformations in the chemical industry, which, combined with the need for digital modernisation, will require a double twin transition of the chemical value chain.

The successful development and deployment of a diverse portfolio of advanced technologies in the chemical sector will be essential to improve its own performance as well as to deliver solutions of utmost importance to help achieve the European Green Deal objectives (see Figure 1).

The European chemical industry has the ambition to become climate neutral by 2050. Main priorities towards this objective involve major transformations in the production of chemicals, including:

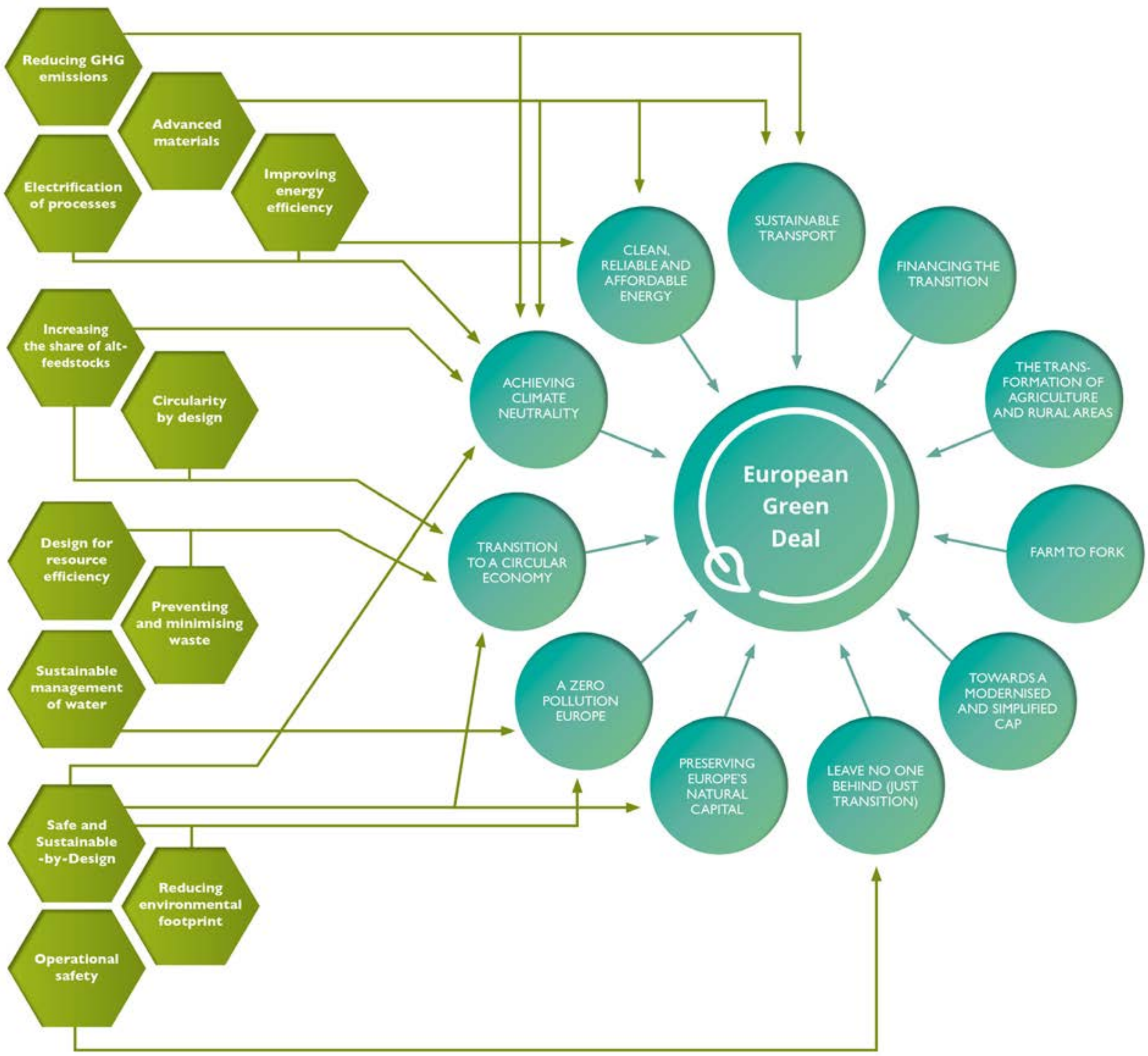
2 "Sustainable Development Goals." United Nations, accessed February 2023.
3 "The European Green Deal." European Commission, COM 640, 2019.
4 "The European Climate Law." European Union Regulation 2021/1119.
5 "A New Circular Economy Action Plan for a Cleaner and More Competitive Europe." European Commission, COM 98, 2020.
6 "Pathway to a Healthy Planet for All EU Action Plan: 'Towards Zero Pollution for Air, Water and Soil.'" European Commission, COM 400, 2021.
7 "Chemicals Strategy for Sustainability: Towards a Toxic-Free Environment." European Commission, COM 667, 2020.
8 "Strategic Research and Innovation Plan (SRIP) for Chemicals and Materials." European Commission, DOI: 10.2777/876851, 2020.
9 "2022 Facts and Figures of the European Chemical Industry." Cefic, 2022.

- The integration of climate-neutral energy, in particular through electrification, including:
  - Indirect electrification for heat (low and high temperature) and steam generation or upgrade.
  - Direct electrification of chemical processes, in particular through electrochemical processes.
  - Utilisation of alternative energy forms.
- The utilisation of alternative carbon feedstocks contributing to carbon circularity, including:
  - Waste, including plastic waste through chemical recycling.
  - Captured CO_2 (and CO from industrial waste gases).
  - Biomass from sustainable resources.
- The production of hydrogen with a reduced carbon footprint for existing and anticipated additional high future needs of hydrogen as feedstock in the chemical industry, as well as future utilisation of hydrogen as an energy carrier.
- Process efficiency, including process intensification and advanced separation technologies.

These priorities require the development of new process technologies, and their combination will be essential to reach the established objectives.

Carbon capture and storage are additional options to contribute to the climate, while more sustainable transport and logistics will contribute to reduce scope 3 GHG emissions at the sector level.

Figure 1. Priorities of the chemical sector to progress towards the European Green Deal objectives



Source: CEFIC

The chemical industry is a provider of advanced materials crucial for the development and transformation of many sectors, including electricity production, energy storage, transport, and electronics. As such, R&I for improved functionality and performance of chemicals and materials remain critical priorities for the chemical industry, alongside contributing to the circular economy, implementing the Chemicals Strategy for Sustainability, and meeting climate objectives. The transition from a linear to a circular economy requires the chemical industry to rethink the design of products taking into account the full value chains, using alternative feedstock (waste, bio-based resources, CO_2) and considering products' end-of-life while ensuring safety for workers, consumers, and the environment.

Beyond the technical transformation of its production supported by research and development, the European chemical industry will also need to rethink its role and develop new business models across ecosystems to build a circular economy. In this context, the EU chemical industry sees Safe and Sustainable-by-Design as a process to accelerate widespread market uptake of new and alternative chemical products and technologies that deliver greater consumer confidence in their safety, environmental and societal benefits, and advance the transition towards a circular economy and climate-neutral society.

Advanced tools that support decision-making from the product and process design phase through to production and along the whole value chain are key enabling priorities for the transition of the chemical sector towards more sustainable products. Digital technologies are therefore expected to play an essential enabling role in the transformation of the chemical industry, be critical for the development of the circular economy, and be instrumental in transforming the portfolio of solutions from the chemical sector through increased data sharing.

This Report identifies where and how digital technologies are expected to contribute the most to the major sustainability objectives and defines key priorities for a beneficial implementation of digital technologies in the EU chemical industry (see the Appendix for details on the methodology).

2. EXPERIENCE DIGITAL SOLUTIONS ACCELERATING THE CHEMICAL INDUSTRY'S GREEN TRANSITION

DIGITALISATION AS INTEGRAL PART OF CHEMICAL INDUSTRY EXCELLENCE

In general, digital transformation (or digitalisation) is a journey relevant for every industry. Modern and emerging digital technologies can help streamline workflows across disciplines, improve operational efficiency, become more agile, resilient, and sustainable, explore new business models and revenue streams, save time and costs, and meet customer expectations. Digital transformation frequently involves information technology (IT) infrastructure modernisation, more extensive use of data and analytics, and implementation of technologies such as AI, big data, Internet of Things (IoT), robotics, virtual and augmented reality (VR/AR), blockchain, and many others.

Digital transformation goes beyond simply adopting digital tools and digitalising processes. Leveraging the potential of digital technologies for innovation should be an integral part of corporate strategies. This also requires a cultural shift that alters operational norms, boosts employees' motivation and skill set, and ensures that the entire workforce has a suitable mindset, attitude, and behaviour. Becoming even more customer-centric is another benefit of digitalisation, enabling greater focus on customers' needs, enhancing customer experience, bringing greater transparency, convenience, and flexibility, and delivering new products and services faster and at a lower price.

Digital transformation is among the top priorities of the European Union,[10] driven by its ability to help address many economic and societal challenges, create opportunities for sustainability and prosperity, and empower businesses and citizens. A new wave of technological innovation is on its way to deliver transformative solutions in the face of global challenges[11] that include the UN Sustainable Development Goals. This technological innovation builds upon cutting-edge scientific discoveries, engineering advances and disruptive technologies such as advanced materials, industrial biotechnology, nanotechnology, renewable energy, AI, blockchain, IoT, robotic systems, cloud services, and quantum computing, which are already creating impactful market applications.

As Europe embarks on its transition towards the Green Deal objectives and digital transformation,[12] the energy-intensive industries have an important role to play in this great challenge and opportunity of our times[13] and are expected to make a major transformative change in terms of sustainable development, circular economy, and digital modernisation.[14]

10 "2030 Digital Compass: The European Way for the Digital Decade." European Commission, COM 118, 2021.
11 "A New European Innovation Agenda." European Commission, COM 332, 2022.
12 "Shaping Europe's Digital Future." European Commission, COM 67, 2020.
13 "A New Industrial Strategy for Europe." European Commission, COM 102, 2020.
14 "2022 Strategic Foresight Report." European Commission, COM 289, 2022.

Sustainable development of the chemical industry is a necessity today and requires a series of joint efforts, new strategies to mobilise the essential means for implementation, and a sustained commitment to overall sustainability goal.[15] Nowadays, more and more companies in the chemical industry are linking their sustainability strategies to digital transformation due to a growing belief that digital technologies can be a sustainability game changer. Indeed, chemical firms increasingly use digital technologies to facilitate sustainability progress in areas such as energy and resource optimisation, reduction of GHG emissions, and to enable a more circular economy.[16]

Digitalisation, sustainability, and the concept of a circular economy are of central importance to the trends, disruptive changes, and opportunities for growth in the chemical sector up to 2030 and beyond. Surging demand for sustainable innovation, products, and services presents chemical companies with possibilities to build new green offerings with the help of digital technologies, address changing customer needs, and develop new business models with fundamentally different patterns of product and material flows. However, these massive challenges also require a more complex cultural shift, new ways of thinking, and a willingness to embrace disruption of today's business models. All in all, focus on sustainability and circularity in the chemical industry clearly will continue to intensify over the coming years, and digitalisation certainly has an important role to play.

In the past years, many impressive digital initiatives have been integrated into companies' strategic agendas and have allowed early adopters in the chemical industry to experience positive impacts on their sustainability goals. These are typically large global corporations that invested heavily in the digitalisation of their operations. However, the majority of smaller, regional and local chemical companies still lag behind in their digital transformation journey due to a lack of adequate budget, knowledge, and expertise as well as C-level ownership. Research of a few years back[17] showed that the predominant part of chemical companies were then still at the beginning of their journey to digitalise main business functions, and their spending on digitalisation was less than half than, for example, in the telecommunication and IT industry, but more than double compared to sectors like discrete manufacturing. Nonetheless, inspired by the success of the most advanced and digitally more mature industries (e.g., tech sector, financial services, automotive industry), the entire chemical industry has geared up for change and has notably increased its digitalisation rate to become faster, innovative, responsive, and efficient by adopting digital technologies, without deviating its focus from safety of operations.

The new digital age has obviously started to play a prominent role in the chemical industry, and chemical companies have been focusing particularly on how digital technologies can help create a more sustainable future at the company level as well as industry-wide. However, the existing and new challenges ahead of the chemical sector will continue to yield opportunities for broader implementation of digital technologies and drive digital transformation of every segment in the chemical value chain. The chemical industry will also expand its value creation spectrum and increase its role as a supplier of innovative and sustainable solutions for the environment and other industries.

"Our growth strategy is enabled by digital to drive productivity, accelerate sustainability performance for a thriving planet, and to optimise insights for new business model innovations."

Alexa Dembek, Chief Technology & Sustainability Officer, DuPont

15 "Transition Pathway for the Chemical Industry." European Commission Directorate-General for Internal Market, Industry, Entrepreneurship and SMEs, 2023.
16 "Chemistry 4.0: Growth Through Innovation in a Transforming World." Deloitte and German Chemical Industry Association (VCI), 2017.
17 Kolk, Michael, et al. "Innovating in the Digital Age." Arthur D. Little, *Prism*, 2018.

APPLYING DIGITAL TECHNOLOGIES TO REINFORCE SUSTAINABLE DEVELOPMENT ACROSS VALUE CHAIN

In this section, we consider top current priorities for applying digital technologies to address sustainability issues along the chemical value chain. According to our survey, many chemical companies have already deployed digital technologies or are planning to implement them in a variety of roles across the value chain, as shown in Figure 2.

In fact, digital technologies can contribute significantly to all sustainability objectives, especially to GHG reduction in production, as well as health, safety, and environment. The concept of circularity enabled by digital technologies is also gaining momentum in the chemical industry, and more and more focus is being placed on energy and feedstock management. Furthermore, R&I activities can also benefit from modern digital technologies. The chemical industry is already making considerable efforts to apply digital technologies for sustainability in the entire value chain. However, wider and more intensive implementation will be required to accelerate the double twin transition.

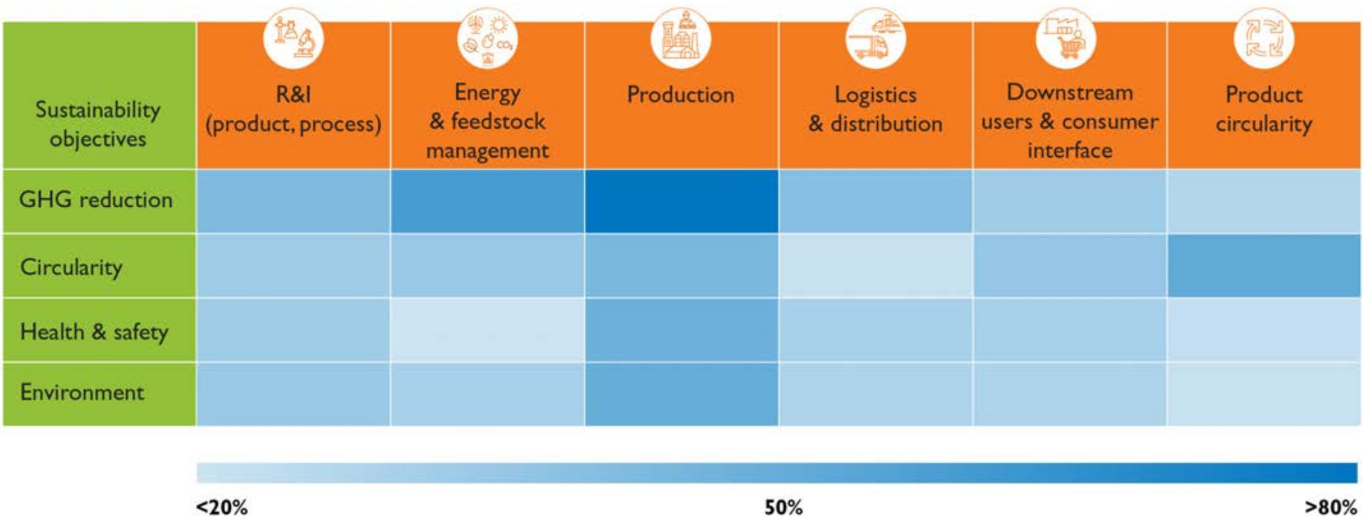
More specifically, we asked the chemical companies we surveyed to indicate what type of digital technologies and combinations thereof they currently use, or are considering for use in the near future, to address sustainability issues in the chemical value chain and related ecosystems. Based on the responses from both large and small chemical companies, Figure 3 represents the top five most prominent sustainability-related priorities in the chemical sector where implementation of digital technologies is expected to have a major impact.

1) Process design & production for climate & circularity objectives

Reaching the ambitious EU climate and circularity objectives calls for disruptive changes in types of energy sources (e.g., green electricity replacing fossil fuels) and feedstock (e.g., waste, CO_2, bio-based resources). Such far-reaching modifications imply design and development of advanced chemical processes, efficient production management, predictive maintenance, and asset optimisation activities.

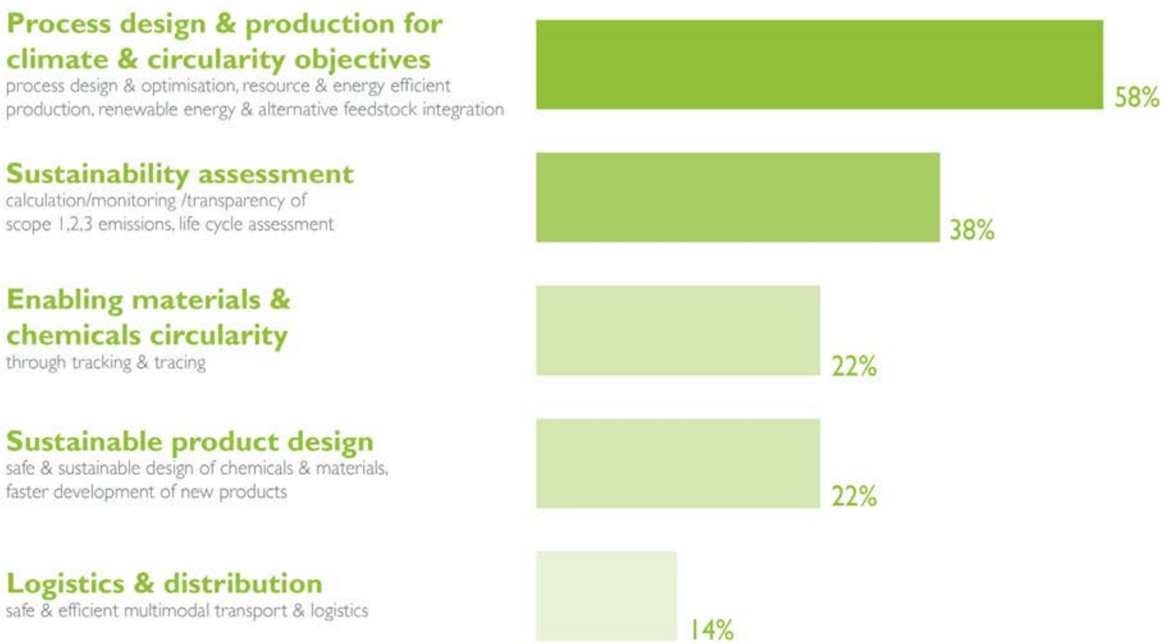
Among 58% of the chemical companies that responded to the survey, predominantly for large and medium-sized enterprises, process design and optimisation in production represent the highest sustainability priorities to be addressed with digital technologies. The survey also revealed that, whereas conventional data modelling and simulation techniques continue to be widely applied, the number of chemical companies exploiting big data in production is expected to double in the coming years. Indeed, real-time data generated by numerous advanced

Figure 2. Intensity of chemical companies' priorities in the value chain for current and future application of digital technologies to meet sustainability objectives



Source: CEFIC

Figure 3. Top 5 sustainability priorities for implementing digital technologies in the chemical industry



Source: CEFIC

sensors and IoT-enabled devices integrated into physical equipment is a very valuable asset. It allows monitoring of actual production parameters, reveals patterns to help achieve greater energy and resource efficiency, detects production anomalies, and improves product quality. (For an example, see "Lanxess employs an analytics platform supporting automation of its global production plants" on page 37.)

The number of chemical companies that employ AI-supported digital twins fed with current operational data also continues to grow and will surpass the 50% mark before long. This combination of digital technologies allows earlier recognition of possible equipment failures and can help avoid time-consuming interventions. (For an example, see "Shell uses a digital twin solution to manage its intensive assets portfolio," on page 28.) Thanks to AI-driven predictive maintenance and asset management systems, plants' downtime can be reduced and potential risks mitigated to preserve safety and operational efficiency.

2) Sustainability assessment

Meeting the climate goals demands systematic evaluation of carbon footprints at product and company levels, including scope 1, 2, and 3 emissions. In addition, the concept of sustainable development requires an evaluation of the existing portfolio of products across multiple criteria. Chemical companies are therefore actively searching for new tools to improve availability and transparency of relevant data in the chemical value chain and related ecosystems. Also, design and development of new products and processes entail advanced modelling and sustainability assessment tools to support decision-making from early-stage research onwards, including toxicity assessment.

Among survey respondents, 38% (mostly large and medium-sized enterprises) prioritised using digital technologies to approach these sustainability challenges.

"At the start of our digital transformation journey we saw immediate opportunities to optimise our assets and create value via improved data acquisition, analysis, and visualisation. This gives us better insights into how we are running assets and can improve resources and energy efficiency, production rate, and output quality. Digital technologies will help us run operations much more efficiently."

Philip Pyman, Vice President, Digital Transformation, LyondellBasell

BASF drives standardised calculation of product carbon footprints in the chemical industry

BASF strives to improve transparency on CO_2 emissions in the value chain and has developed a digital solution to automatically calculate the carbon footprint of around 45,000 sales products in its portfolio. The calculation method follows general standards for lifecycle assessments and is recognised by the German Chemical Industry Association (VCI) with the Responsible Care Award for digitalisation. The algorithm is based on several dynamic input factors, such as process emissions data collected from multiple BASF production plants and high-quality average information derived from various sources on purchased raw materials and energy demand. The calculation covers product-related greenhouse gas emissions generated from extraction of resources up to the factory gate. This digital solution is specific to its sector and has been certified by TÜV Rheinland. It creates increased transparency around CO_2 emissions and represents a powerful tool to collect and report product-specific data that forms the basis for Digital Product Passports. This solution has been transformed into marketable software for the standardised calculation of product-related CO_2 emissions and is offered by various licensees to other interested industry players.

In fact, digital solutions can support the sustainability assessment in the design phase, improve transparency in the value chain, and automatically calculate product carbon footprints. In particular, the survey confirms that the usage of big data and data sharing platforms will continue to grow in importance, as will advanced analytics, modelling, and simulation tools.

Several tools exist to automatically calculate carbon footprints of chemical products. For instance, BASF has developed a digital solution for a standardised calculation of product-related CO_2 emissions to improve transparency in the value chain (see “BASF drives standardised calculation of product carbon footprints in the chemical industry”). Also, to quantify the contribution of its products to sustainability, Solvay has designed a fact-based and future-oriented sustainable portfolio management tool, along with a detailed guide explaining how it is implemented in practice and how the outcomes are translated into actions.[18] In addition, Smart Freight Center together with Cefic have designed a method to compute GHG emissions from transport and logistics activities directly related to the chemical industry supply chain.[19] Such guidelines, combined with efficient data sharing mechanisms among relevant stakeholders, can support chemical companies in gaining knowledge about the scope 1, 2, and 3 emissions, which is important to take steps to reduce environmental impact, drive long-term sustainability growth, and provide true sustainable solutions to customers.

3) Enabling materials & chemicals circularity

It is both a challenge and an opportunity for chemical companies to take into account all aspects of the circular economy over the entire product lifecycle, including the feedstock considered for the production of chemicals and extending over all subsequent steps to the product’s end-of-life. Increasing number of chemical companies are focusing on the entire lifecycle’s importance to sustainability, and it is clear that digital technologies are indispensable for tracking and tracing materials and products for circularity.

With the introduction of the concept of a Digital Product Passport[20] as a key element for enhancing the traceability of products and their components to promote circularity in the EU, much broader collaboration will be required to ensure external data sharing among the value chain participants. In the survey, chemical companies indicate their intention to explore blockchain technology as a possible option for sharing data relevant to products’ circularity and end-to-end traceability across the value chain. (For an example, see “Eastman traces certified recycled content across the value chain with blockchain technology,” on page 33.) Blockchain will surely have its place in addressing specific challenges requiring its

18 “Solvay Sustainable Portfolio Management Guide.” Solvay, accessed February 2023.
19 “Calculating GHG Transport and Logistics Emissions for the European Chemical Industry.” Cefic and Smart Freight Centre, 2021.
20 “Making Sustainable Products the Norm in Europe.” European Commission Directorate-General for Environment, 2022.

"There is a trade-off between transparency and traceability. Blockchain technology can provide the right level of transparency to the involved stakeholders without sharing sensitive information. However, blockchain should not be seen as a wonder technology which solves every problem related to traceability."

Christian Buenger, Senior Economist I Digitalisation, Digital Transformation & Digital Advocacy, German Chemical Industry Association (VCI)

distinctive features, however, the chemical industry also needs to examine alternative solutions for data sharing in future ecosystems, as blockchain technology will not suit every use case.

4) Sustainable product design

Exploration of product structure-property relationships, greater product safety and sustainability, and improved product performance are key considerations for the chemical industry. The basic principle behind improving functionality and performance of chemicals, materials, products, processes, or services is the aim to considerably improve performance in at least one of the sustainability dimensions, without significant negative impacts on the other dimensions compared to existing solutions. While laboratory experiments clearly remain a necessity, computer modelling and simulation can facilitate R&I activities and greatly complement lab work. In fact, 75% of the surveyed companies that listed product design among their top sustainability priorities already apply advanced computational techniques to better understand what happens during lab experiments and bring to light alternative solutions that may not have been considered. This number covers chemical companies of all sizes and is expected to increase even further in the coming years.

The adoption of AI and machine learning capabilities further streamlines R&I activities, allowing for faster product design, more effective replacement of hazardous materials, AI-driven predictive toxicology (see "AI-empowered toxicity assessment"), and shorter time to market for new solutions (see, for example, "Dow harnesses the power of digitalisation to reimagine product design with AI" on page 26). Over 65% of the survey respondents that focus on sustainable product design already leverage historical knowledge to train machine learning algorithms on comprehensive datasets containing several decades of aggregated information, such as chemical formulations. Hereafter, machine learning can consider various parameters and carry out virtual testing on potential new formulations, so that researchers only run the physical experiments with the highest probability of a successful outcome.

AI-empowered toxicity assessment

The recent development and application of AI-based toxicity prediction models is an emerging concept in the chemical industry. The EU's regulatory toxicology often requires expensive and time-consuming testing of thousands of chemicals and results in the increased use of laboratory animals. Intelligent computational toxicology techniques gain considerable attention with their ability to predict chemical toxicity in an adequate and reliable manner, thus limiting the current paradigm of toxicity assessment that is heavily dependent on animal testing. The new frontier of AI-driven predictive toxicology offers promising alternative methods with non-animal testing strategies. It puts experiments into a useful framework based on known structures of chemical substances, including quantitative structure-activity relationships and complex physiological AI models simulating the behaviour and effects of chemicals in a sequence of events, leading to a solid and robust predictive toxicity assessment. The European Commission established a tracking system[21] that monitors the progress of such novel methods for testing chemicals towards regulatory acceptance, including within the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) regulation, and ensures their swift adoption for regulatory use.

21 "TSAR — Tracking System for Alternative methods towards Regulatory acceptance." European Commission, accessed February 2023.

Future possibilities include autonomous robotic systems that define and run plausible experiments by themselves while researchers concentrate on other added-value tasks. Such examples demonstrate the benefits of digital technological advancements to facilitate people's work while illustrating the continued need for human judgment.

Powerful computing technologies, namely supercomputing and ultimately quantum computing, are also expected to eventually bring dramatic benefits to R&I and change the way new products are developed in the chemical industry. (For an example, see "BASF boosts innovative power with a supercomputer" on page 28.) A number of large, global chemical companies are already exploring the possibility of using supercomputing and quantum computing to model complex systems such as molecules and polymers at a far greater precision level. For example, these technologies enable a search for the most suitable molecular designs or structures to accomplish specific tasks or achieve required effects to be performed in a matter of minutes rather than months. A single molecule can then be synthesised in a lab, further cutting the time it takes to launch new products. The survey indicates that the number of companies aiming to pursue high-performance computing technologies will at least double within the next few years.

5) Logistics & distribution

Chemical transport and logistic processes need to meet demanding company-specific and legal requirements on safety, quality, and security regarding the goods transported, the equipment used, and the people involved. In transport and logistics, digital solutions can enable secure and accurate data sharing (see, for example, "ECLIC — a multi-stakeholder chemical logistics platform" on page 23), help reduce operational costs, increase efficiency of resources, and foster modal shifts.

With the help of digital technologies, business processes can be optimised to pave the way towards real-time planning and steering, more sustainability, and more end-to-end transparency. Digital solutions may also bring early and proactive detection of risks and support rapid interventions. For authorities, digitised transport and logistics allow for highly efficient, system-based supervision and enforcement.

Alongside conventional modelling and simulation techniques, AI-empowered solutions are being considered for smarter and sustainable supply chain management. AI and machine learning–based tools can analyse structured and unstructured operational data from disparate systems (e.g., actual sales, demand planning and forecasts, sales opportunities, shipping methods, and schedules) and deliver accurate predictions when product stock is low, enabling smarter inventory decisions. This brings greater visibility and transparency across the complex supply chain with numerous production plants, distribution sites, and warehousing locations worldwide.

Thanks to integrated smart contracts, many standard business operations can be further streamlined, such as product sales, payment flows, shipments, regulatory compliance, and customs activities. IoT solutions are also commonly used in logistics processes to ensure the right transportation conditions (e.g., temperature, humidity), facilitate real-time tracking and monitoring of the transported goods, and bring more transparency to the communication process.

ECLIC — A multi-stakeholder chemical logistics platform

The European Chemical Logistics Information Council (ECLIC)[22] is an organisation that facilitates digital collaboration around sector-specific digital use cases. It represents a community of chemical companies and logistics service providers that work together and exchange transport and logistics data via trustful data sharing platforms-as-a-service. ECLIC has over 50 subscribed companies (e.g., Covestro, Evonik, BASF) and industry associations (e.g., essenscia, European Chemical Transport Association, European Federation of Tank Cleaning Organisations) as members, allowing chemical logistics actors to effectively work together digitally across an end-to-end chemical logistics network. Through secure data sharing, ECLIC aims to transform current manual and paper-driven logistics processes into more integrated, collaborative, electronic, and real-time processes.

DIVERSITY & IMPACT OF DIGITAL TECHNOLOGIES FOR SUSTAINABILITY IN THE CHEMICAL SECTOR

In this section, we consider the range and diversity of digital technologies and their combinations that are expected to contribute the most to the sustainability objectives in the chemicals industry — today and in the future.

The availability of high-quality data is a key starting point and essential element for the digital transformation that is already profoundly reshaping the chemical sector. Reliable data is among a company's most vital assets, since data translates into indispensable knowledge for informed and substantiated decision-making, improved problem solving, and greater understanding of business dynamics — all of which have a tremendous impact on long-term success. Data availability also delivers business and commercial benefits, such as cost reduction, faster time to market, and other competitive advantages. Therefore, it is important to utilise the right tools to make data as accurate as possible, create a standardised data architecture to ensure effective data governance and interoperability, and implement suitable digital technologies to fully leverage the large amount of data available.

When it comes to the circular economy and sustainable development, data quality, provenance, interoperability, and exchange play increasingly important roles. The right way to share relevant data across multiple players in the chemical value chain is currently a much-discussed topic. There is a need to develop a sector approach for collaborative work and establish common data sharing standards, which are as open as possible and as closed as necessary, to ensure that the chemical industry tackles sustainability across the entire value chain and other relevant industries.

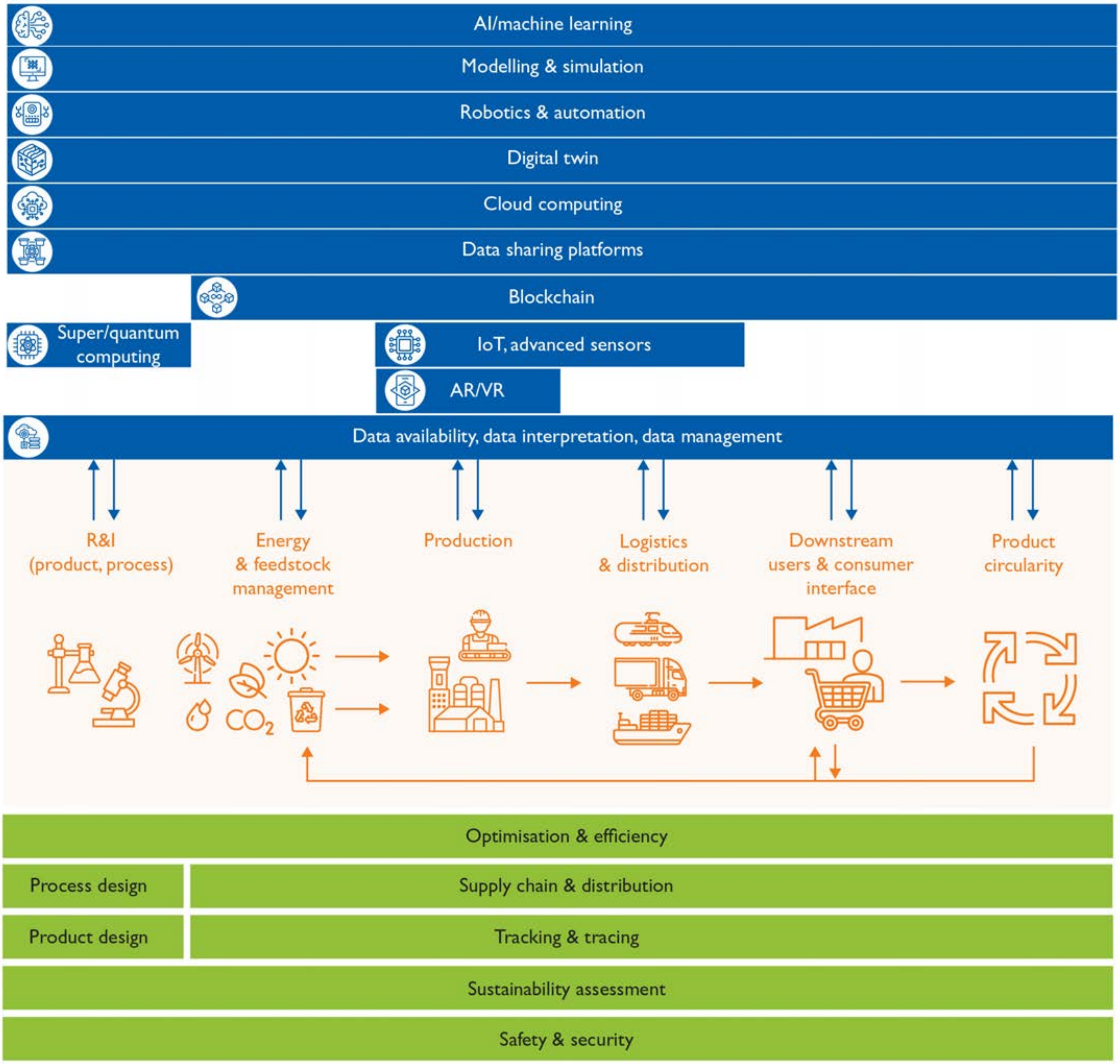
Data-driven digital transformation enables the chemical industry to use a broad range of modern digital technologies to help achieve sustainability goals (see Figure 4).
These include modelling and simulation techniques, AI and machine learning, digital twins, robotics and automation, cloud computing, data sharing platforms, and blockchain technology, which are already intensively used across the chemical value chain and related ecosystems, while applications of immersive technologies (AR/VR) and IoT integration are now primarily concentrated around production. Emerging high-performance computational capabilities, such as supercomputing and quantum computing, are currently showing the biggest technological progress towards digitalisation of R&I, with a potential to perform computationally intensive tasks in other fields like supply chain optimisation as well. The chemical industry has notably

"Big parts of the chemical industry are still at a relatively early stage when it comes to data usage. Until recently, the true value of data was often misinterpreted or not valued highly enough by chemical companies as a strategic asset."

Joerg Purwien, Head of Digital Labs, Evonik

22 "European Chemical Logistics Information Council." ECLIC, accessed February 2023.

Figure 4. Digital technologies and their current applications to address sustainability priorities in the chemical value chain and related ecosystems



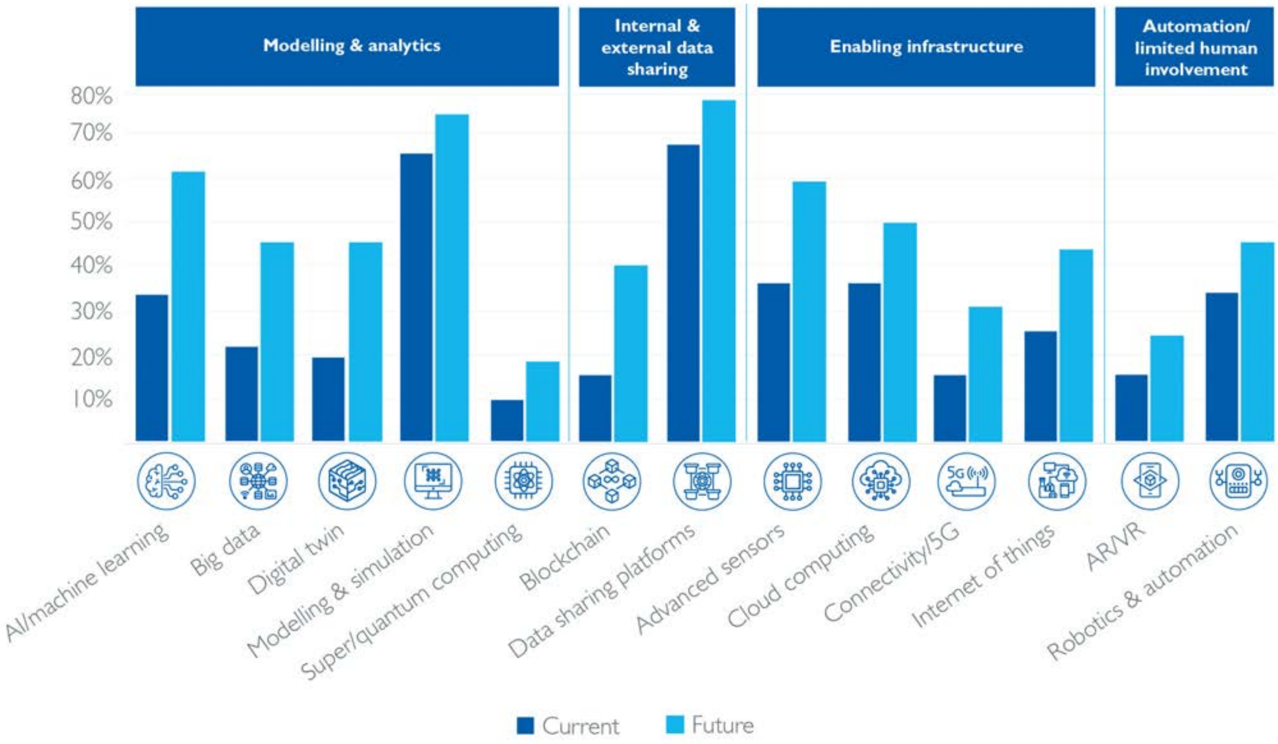
Source: CEFIC

increased its digitalisation rate to become more innovative, faster, more efficient, and sustainable, although much remains to be done.

Our survey confirmed that all digital technologies will increase in importance in the coming years (see Figure 5) and will positively contribute in terms of sustainable development of the chemical sector, especially AI and machine learning (+82%), big data (+110%), digital twin (+130%), and blockchain (+150%), while modelling and simulation techniques, and data sharing platforms will generally remain the most utilised digital technologies.

In the following sections, we look in more detail at how these technologies are currently being used in the chemical sector.

Figure 5. Digital technologies currently used and planned to be used in the future by chemical companies (%) in the context of the double twin transition



Source: CEFIC

MODELLING & ANALYTICS

Evolution of modelling & simulation in the big data era

Reliable data and advanced analytics are at the heart of a successful digital transformation. Various tools and techniques for performing data analysis offer chemical companies an opportunity to take advantage of the extensive data collected from their own businesses. Data analytics represents a process of scrutinising, cleansing, and modelling data to identify trends, extract valuable insights, and draw conclusions. Over a period of one year, this cumulative information can easily exceed hundreds of terabytes and will continue to grow progressively. Chemical companies have therefore been required to invest heavily in data capture and storage technology. With advanced modelling and simulation techniques, the chemical industry possesses the capability of leveraging this big data and using it to its fullest potential.

The chemical industry is already highly data-driven. For example, in R&I alone, data may include insights on complex structure-property relationships of chemical substances and performance of chemical formulations, multiple test series and measurements, analysis results, research reports, scientific papers, and patents. With growing amounts of high-quality data combined with advanced modelling and simulation tools, chemical companies can speed up innovation cycles and reach the market considerably faster.

In addition, production plants contribute huge volumes of data through environmental measurements performed every few seconds, such as temperature, pressure, flow rate, energy, emissions, performance status, and other parameters. This data is generated by thousands of equipment elements fitted with advanced sensors and wireless devices. By leveraging big data, chemical companies can not only monitor production parameters in real-time while respecting strict health and safety requirements, but also identify patterns to optimise efficiency and increase yield. Moreover, with data-driven predictive maintenance and asset management systems in place, companies can perform corrective interventions in a timely manner and reduce downtime for in-service equipment.

Besides the asset data, chemical companies also need to manage product portfolio information, including related documentation, product variants, batch details, packaging, environmental properties, stock levels, and real-time pricing as well as market and competitor monitoring. Furthermore, countless interactions with suppliers and customers create a lot of transactional data covering order history, sizes, prices, contracts and shipping details, custom clearances, utilisation of products, customer behaviour and preferences, emails, call recordings, and much more. By harnessing the power of big data extracted from multiple sources and predictive analytics, chemical companies can forecast changes in customers' behaviour and increase accuracy of demand planning. Moreover, digital solutions based on data shared in the transport and logistics ecosystem will bring more resilience in the supply chain and enable proactive planning and steering at the company level.

Our survey showed that over 70% of the chemical companies already exploit conventional data modelling and simulation techniques, yet only 20% take advantage of big data analytics. In the coming years, the chemical sector is expected to face a steep learning curve, and the uptake of big data analytics will at least double. Indeed, applying big data and advanced analytics is increasingly moving from being optional towards being a key prerequisite for continued success. Chemical companies must follow this increasingly important transformational path. Sustainability-related challenges and transformations bring the importance of this innovation engine into even sharper focus.

Next to big data analytics, implementation of AI and digital twins in new ways to create safer and more sustainable products and processes is gaining momentum in the chemical sector. The following sections look more closely at these digital technologies, which are critical enablers for attaining the sustainability goals in the chemical industry.

Revolutionising the chemical sector with artificial intelligence

In the chemical industry, widespread adoption of AI promises to transform operations and bring significant benefits in terms of safety, quality, productivity, cost efficiency, and growth. It also presents a major opportunity for chemical companies to contribute to the long-term sustainability goals, develop circular economy concepts, and reduce overall environmental footprint. Combining AI with existing experience and expertise offers the potential to generate competitive advantage, innovate faster, and defend against challenges from new market entrants.

Up until now, chemical companies have primarily applied rather standard methods and human intelligence to extract value from their massive amounts of raw data. The next step in deriving valuable insights more efficiently is to broadly incorporate advanced analytics techniques from data mining, predictive modelling, AI, and machine learning. According to recent research, the vast majority (over 95%) of large companies in the chemical industry have at least introduced an AI-driven strategy.[23] Our study reveals that over 60% of the chemical

Dow harnesses the power of digitalisation to reimagine product design with AI

With the ambition to accelerate innovation and deliver more sustainable products and practices, Dow is transforming its product development processes and bringing smarter solutions to the market faster. In particular, by combining expertise in sustainable material science with AI and machine learning, Dow has introduced an intelligence capability to predict product formulation properties and simulate processes faster. Thanks to the more efficient use of scientific and digital tools, this predictive intelligence allows a typically several months' long, laborious product development process to be sped up by reducing the material discovery phase to a matter of minutes and limiting the number of necessary lab trials to only the most promising candidates. This capability will further push boundaries by forecasting trends and customer needs through historical data, predictive mathematical models, automated work processes, and scale of applications. This predictive intelligence is a flagship digitalisation initiative that was recognised as a cutting-edge application of emerging technologies and represents an important milestone within the company's broader digitalisation vision and sustainable development strategy.

23 "Artificial Intelligence and Blockchain: Insights and Actions for the Chemical Industry." Accenture, 2019.

DuPont transitions from analogue to digital operation with a digital twin

To further improve operational efficiency, increase productivity, and create a safer work environment at production sites, DuPont has built a digital twin solution that provides operators and collaborators with an opportunity to visualise physical assets and their technical specifics through real-time data fed into an advanced monitoring tool. This unique interactive virtual model of a production plant is easy to navigate, scale up, and access remotely from any location and any device. This digital twin brings a variety of existing systems in use together in a single point of truth, facilitates data sharing, and makes teamwork more straightforward. As a result, many engineering activities such as asset management, planning for maintenance and repairs, simulated workflows, material procurement, and process hazard evaluation have been streamlined, ultimately limiting risks, increasing operational efficiency, and lowering costs.

companies are currently in the pilot or early adoption phase. Nevertheless, these are still isolated examples, typically driven by individual business units rather than large transformational programmes. Bringing a broader perspective into cross-business governance and scaling up will enable chemical companies, and the industry as a whole, to fully benefit and get more value from AI applications and investments. This especially applies to small and medium-sized companies (SMEs).

Our survey shows that AI capabilities have the potential to improve every aspect of the chemical value chain and contribute significantly to attaining sustainability objectives. Currently, several AI applications are rapidly evolving in the chemical industry, especially in product design, allowing smarter solutions to be brought to the market faster as well as enhancing predictive maintenance and optimisation in production operations.

These examples can be found among best practices from many leading companies in the chemical sector, including Dow (see "Dow harnesses the power of digitalisation to reimagine product design with AI,"page 26) and Shell (see "Shell uses a digital twin solution to manage its intensive assets portfolio," page 28).

Digital twin — when the chemical value chain meets its digital replica

Digital twin is another fascinating technology that is gaining traction rapidly. Digital twins have become ubiquitous at all stages of manufacturing, since regular flow of data from connected IoT sensors can be exploited to supervise products throughout their entire lifecycle, from design phase to finished goods and use in the real world. Through digital twins, businesses can also gain valuable insights about the quality and performance of their products, identify potential faults, and troubleshoot at a distance.

Likewise, companies in the chemical industry can benefit considerably from digital twin adoption. With large amounts of data available to simulate likely performance outcomes, digital twins enable more effective research and design of products, significantly reducing the process timeline and providing insights that help companies make necessary product refinements before starting production. The potential for using new raw materials and renewable energy can also be quickly evaluated. In the manufacturing process, digital twins monitor production sites and help achieve greater efficiency by reducing equipment downtime and increasing production capacity.

Digital twins also allow for remote commissioning of products that are already in use, and once products reach end-of-life, it is possible to determine which product components can be recycled. Across the entire value chain, digital twins support sustainability trends in the chemical industry.

Shell uses a digital twin solution to manage its intensive assets portfolio

Shell seeks to further accelerate its digital transformation by implementing digital twins to support lifecycle management across its global portfolio of assets. Connected IoT sensors collect real-time data from physical equipment and feed the corresponding digital twin with relevant information about the current operational conditions, reducing the necessity for physical inspections in hard-to-reach areas and offering the ability to perform structural assessments from anywhere and at any time. This increases operational safety and efficiency by enabling remote control, automation, and significantly improved collaboration. Data and models are coupled with interactive contextualised visualisations that make it possible to simulate operations, optimise maintenance, and drive proactive interventions. Digital twins embed AI technology such as predictive maintenance, which improves energy efficiency of production facilities and industrial processes. It also flags more accurately when equipment may fail and reduces unnecessary pre-emptive part replacement. Shell deploys digital twins across its conventional and new energies assets. Over 15,000 pieces of equipment are currently monitored by machine learning models across Shell's refining and chemical facilities, as well as in its upstream and integrated gas assets.

Having a digital twin is not always a prerequisite, and not every product is complex enough to require an intense and regular flow of sensor data. However, large-scale products or production initiatives with a high degree of complexity can certainly benefit digital twin adoption. According to our survey, more than 45% of chemical companies have begun to experiment with the use of digital twins and focus on improving at least one part of a larger process as a starting point. Use cases from DuPont (see "DuPont transitions from analogue to digital operation with a digital twin," see page 27) and Shell (see "Shell uses a digital twin solution to manage its intensive assets portfolio") illustrate how chemical companies can put digital twins into practice.

Catch the wave of the future with supercomputing

Supercomputing has shown some of the biggest technological progress towards digitalisation of R&I in the chemical sector. Compared to ordinary computers, a supercomputer can efficiently solve extremely complicated or data-intensive problems by concentrating the computational power of multiple, parallel computers operating at the same time. Supercomputers that achieve top computing power with several thousands of processors will play a key part in meeting future challenges. In the chemical industry, supercomputing power allows companies to further increase innovation strength by exploiting previously unknown molecular designs and encouraging completely new research approaches.

BASF boosts innovative power with a supercomputer

Taking advantage of all the opportunities digital technological progress has to offer, especially with regard to the accelerated sustainability transition and faster innovation, BASF explores the potential of supercomputing, currently the most powerful computing technology used for industrial chemical research. The deployed supercomputing capacity allows R&D experts to run complex simulations that were once deemed impossible. For instance, intricate modelling of molecular processes and materials with specific properties and functionalities that help to increase their sustainability performance can now be carried out within a few minutes, while covering a vast range of simulation parameters without the need for crude approximations. Supercomputing is also used in industrial catalyst research, aiming to increase efficiency and sustainability by decreasing input of raw materials and thus generating less waste. This form of high-performance computing offers researchers the prospect of surprising discoveries and innovative products to be launched within a much shorter time frame.

This can substantially accelerate time to market for new products and help address sustainability in an authentic and meaningful way. Among the chemical giants, BASF is the first to explore the potential of supercomputing capabilities (see "BASF boosts innovative power with a supercomputer," page 28).

Glimpse of the forthcoming quantum computing technology

Another emerging technology — quantum computing — is ideally suited to tackle issues relevant to the chemical industry. Although quantum computing is currently in its infancy and there are still major technical challenges to overcome, technological advancements are reported regularly, and the chemical industry is well-positioned to be an early beneficiary of its computational capabilities.

Quantum computing harnesses the laws of quantum mechanics, operating in several states at once, to be able to perform rapidly growing numbers of calculations simultaneously. Molecules are quantum mechanical systems themselves, and the mechanisms that are at work in molecular interactions involve exponentially increasing levels of complexity. Molecular simulation therefore lends itself well to quantum computing solutions, at least in theory. This gives an advantage to the chemical industry compared to other sectors with demanding computational needs.

Quantum computing could ultimately have many momentous applications in the chemical industry, such as digitally designing molecules and solid materials with enhanced properties, defining shapes of proteins to make better active ingredients, and discovering more effective formulations by modelling how ingredients affect chemical processes or how complex mixtures behave. Chemical companies that are able to exploit the potential of quantum computing would be able to develop new sustainable products at much lower cost and in record time. There is an emerging trend among chemical companies (e.g., Covestro, Dow, Evonik, and many others) to seek collaborations with key quantum computing developers and other players with a view to piloting first use cases within the chemical sector. To date, the particular focus has been placed on the development of new programmes and algorithms that could be deployed to exploit the above opportunities when powerful enough devices become accessible.

INTERNAL & EXTERNAL DATA SHARING

Amplify access to data & internal data sharing practices

Digital transformation trends suggest that internal data sharing and collaboration will become increasingly important for chemical companies' success and ability to reach business goals in the coming years. By prioritising data sharing and data management as business necessities, chemical companies can unlock their full potential and access systematic, data-driven insights to make more informed decisions.

Modern data sharing platforms allow data from multiple sources to be stored in flexible data lakes and available software enables data engineers to automate the most time-consuming and labour-intensive aspects of data sharing, such as cleaning and standardising data. The ability to easily access a unique data repository with accurate and up-to-date datasets available in usable formats, actionable data analytics, and multiple applications for various business purposes allow authorised users within a company to operate more efficiently and effectively, without any particular technical knowledge or coding experience. Data sharing platforms are not only highly flexible and easy to use, but also safe and secure, as it is possible to set preferred access limits and keep data transfers between different departments under control, for instance, to prevent data breaches or to respect legal arrangements.

According to our survey, around 70% of chemical companies either already experience benefits of internal data sharing (e.g., Clariant) or are currently in the process of setting up the required IT infrastructure. More and more chemical companies prefer cloud-based data sharing platforms over on-premise infrastructures to transfer required data into the right hands at greater speed, enabling teams to break through data access barriers and achieve both extreme scalability and data security. In any case, once data sharing is made user-friendly and secure, it will become the norm and data will circulate seamlessly across a company.

"Having a single data integration platform aids data governance and makes data available inside the company by providing each authorised user with required data in usable formats as well as access to data visualisation tools and self-service analytics."

Dominik de la Rosa, IT Manager Data Integration, Clariant SE

Data ecosystem vision & external data sharing

When it comes to external data sharing, most chemical companies are still reluctant to share data across the value chain, mainly due to technological challenges, associated cybersecurity risks, and the clear necessity to preserve competitive advantage. However, chemical companies also realise that in order to progress with the green transition, they must go beyond carbon-neutral operations within company boundaries and account for other indirect emissions that occur throughout the value chain. To establish true end-to-end visibility, as well as innovations along the value chain, both upstream and downstream players must collaborate, share relevant data, and adopt common data sharing platforms. Moreover, customers increasingly demand more transparency regarding products' provenance and authenticity; therefore, in several instances multiple stakeholders are already working jointly on data sharing solutions to create complete digital records along the chemical value chain. Much broader collaboration on external data sharing in the sector is expected in order to address various sustainability aspects, especially with Digital Product Passports becoming the norm for all EU-regulated products. This requires products to be tagged, identified, and linked to data relevant to their circularity and end-to-end traceability across the value chain.

For collaboration on external data sharing to be successful, chemical industry players need to work together to solve important policy, standardisation, and technological issues. Players must build mutual trust, identify the right data sharing mechanisms, deploy secure technologies, and establish industry-wide standards. The potential of collaborative business networks to accelerate the green transition can be illustrated by Catena-X,[24] the first standardised, open, and scalable data ecosystem for the automotive industry (see "Catena-X — a data ecosystem for the automotive industry"). Similar to Catena-X, the chemical sector could form an interoperable network and establish uniform digital standards to ensure seamless and secure data exchange, thus linking multiple players into the end-to-end value chain. It is also important to take into account the organisational and infrastructure readiness of all stakeholders and ensure participation of smaller players as well as larger ones. Data sharing must be user-friendly for all members of the value chain and require only relevant and necessary information. This type of collaboration will be the basis to enable new digital business models in the future and achieve a circular economy at scale.

Catena-X — A data ecosystem for the automotive industry

Catena-X is the first open and collaborative data ecosystem for the automotive industry of the future, connecting automotive manufacturers, suppliers, service providers, and other players into end-to-end value chains in a trustworthy and secure fashion. Catena-X makes use of the Eclipse foundation, which provides standards for building peer-to-peer data exchange solutions under the EU-sponsored Gaia-X data governance framework. Access to the Catena-X infrastructure is non-discriminatory, all participants have equal rights, retain sovereign control over their data, and decide individually which partners are involved in the data exchange and under which conditions. The Catena-X standardised global data exchange provides a sustainable solution for the digitalisation of value chains, especially for SMEs, and supports the collaborative effort enabled through participation of multiple stakeholders. The Catena-X foundations are based on open source solutions that are transparently available to all. Other industries and ecosystems can be integrated at any time.

24 "Catena-X Automotive Network." Catena-X, accessed February 2023.

"There is a large reluctance to share data across the value chain in the chemical sector. There is a need to create standardised open data ecosystems connecting companies, similar to Catena-X for the automotive industry of the future."

Nicole Graf, Global Co-Lead Digital & Sustainability Innovation, BASF

Another good source of inspiration is the battery industry, which by 2026 will be one of the first sectors to implement the Digital Product Passport concept established by the EU's action plan for the circular economy. Key stakeholders in this industry and its supply chain, such as producers, suppliers, and civil society members, have together formed the Global Battery Alliance (GBA).[25]

This organisation is in the process of defining a framework to increase transparency across the battery production value chain, foster a responsible and sustainable circular battery economy, and fulfil high-level requirements for data exchange. To achieve this, it needs to address complex issues around data standardisation and data ontology, data control and governance, protection of trade secrets, and cover the costs of technical implementation across a wide and dynamic ecosystem. Interestingly, the GBA is fully impartial as to the digital technologies selected for implementation of the solution.

Among the high-level requirements that may apply for specific data sharing use cases, the most important considerations include the following abilities:

- **Trust** — offering guarantees that shared data will not be tampered with in any way.
- **Data control** — limiting what other participants can do with shared data.
- **Data quality** — ensuring that data entering the system is valid and accurate.
- **Performance** — exchanging large data volumes with low latency.
- **Scalability** — easily incorporating new players and attributes in the data sharing model.
- **Inclusivity** — avoiding high operational costs and technical hurdles that exclude small economic actors.
- **Efficiency** — keeping total operational costs and energy consumption at reasonable levels.

On the one hand, external data sharing can be conducted through a more centralised approach, relying on a central player in charge of designing and managing a data sharing platform built with traditional technologies, such as cloud-based software and application programming interface (API) gateways. Even though such a centralised approach may not fully solve the trust issue, its implementation is relatively simple and straightforward. It is also more inclusive and tends to offer comparatively better scalability and performance. This type of data sharing platforms is becoming increasingly accessible and suggests robust and future-proof solutions. For instance, common cloud service providers, which have become key players in many companies' digital journeys, have developed specific data sharing lines of services. Also, specialised data governance and data integration software providers have extended their internal data sharing features to the outside world. In addition, large commercial software companies have established partnerships to facilitate the emergence of common standards and methods for data sharing.

On the other hand, in a decentralised approach, blockchain technologies offer an open and neutral solution for external data sharing.[26]

"There is an opportunity for an interoperable ecosystem where suppliers and customers are able to seamlessly collaborate and share transactional data."

Colja Boennemann,
Sustainability Product Manager, ExxonMobil

25 "Global Battery Alliance." GBA, accessed February 2023.
26 "Blockchain Now and Tomorrow: Assessing Multidimensional Impacts of Distributed Ledger Technologies." European Commission Joint Research Centre, 2019.

"If we do not facilitate a data sharing solution as a whole industry that enables smaller players to be able to participate, we will never be able to drive circularity."

Daniel Pereira, Director,
Digital Corporate Technology & Sustainability, Eastman

Thanks to blockchain technologies, trust among stakeholders is created algorithmically on the operational level by removing the idea that data can be controlled by a few central nodes. In addition, blockchain ensures a high level of fault-tolerance and robustness, which can make it a technology of choice for collaboration on external data sharing. However, even though blockchain technologies have made significant progress over the past few years, scalability potential, energy consumption, and latency remain issues for most implementations, and addressing use cases that involve large data volumes and time-sensitive data may still prove to be challenging. Likewise, for data sharing initiatives to be successful, many participants with different levels of data, technological maturity, and diverse IT landscapes need to be involved. To this point, experience with blockchain technologies is still rather limited among SMEs.

Presently, the chemical sector is exploring blockchain technology as a possible option for cross-industry data sharing. There is a range of blockchain solutions, allowing companies to find the right compromise between decentralisation, scalability, and energy consumption (see "The blockchain potential").

Building trust for today & tomorrow with blockchain

Generally speaking, blockchain is considered a tool that promises to facilitate transactions between multiple suppliers, customers, partners, regulatory bodies, consumers, and even competitors. Blockchain technology promises to reduce transaction times from days to minutes, since time-consuming business reconciliations among the network members are eliminated. It also builds trust as end-to-end transactions and confidential

The blockchain potential

It is important to distinguish between different types of blockchain applications. First, public blockchains offer a decentralised, distributed, and shared database (ledger) used to record transactions between various stakeholders at different stages of a product's lifecycle across a network of partners (nodes) in a secure way, so that records cannot be altered retroactively. It is open to the public and does not require any form of authentication to join the network. It can be useful in use cases where different stakeholders need a shared ledger of publicly available transactions in order to avoid dealing with multiple bilateral data exchanges, have conflicting interests regarding the data they share, and are not willing to trust a third-party to maintain this shared database and must ensure immutability of the data.

Private blockchains, on the other hand, differ from public ones in the fact that a single entity or consortium is responsible for granting permissions to participants to join the network, based on identity management tools and processes. It also defines access rights to the data for different participants and the consensus mechanism for registering each block of transactions in the blockchain. From this point of view, private blockchains cannot be considered as fully decentralised and may not always guarantee immutability of the data. Implementations of private blockchains typically favour lighter consensus mechanisms compared to public ones, making private blockchains more efficient in terms of energy consumption and ability to handle larger volumes of data. Considered as a distributed ledger, private blockchains offer interesting non-functional features like security, since data is fully encrypted and split into pieces stored on different nodes, and resilience, as there is no single point of failure for this database. They may be useful for controlled exchange of immutable or sensitive data.

records are shared only with specific network participants to whom access is granted, while greater security features protect data against tampering, fraud, and cybercrime. Moreover, blockchain technology allows monitoring of operations across the supply chain, tracking authenticity and origin of products, exchanging trusted data about product properties and quality certifications, understanding how customers use products, and retrieving products at the end of their lifecycle.

In the chemical industry, blockchain is increasingly experimented with as an enabler of the transition to the circular economy and sustainable innovation. Today, chemical companies experience a growing need to prove the circularity of their products, and blockchain technology seems particularly suited for this purpose. While existing tracing systems are complex to operate, may contain information gaps, and cannot always guarantee protection of sensitive and confidential information, blockchain platforms can provide a trusted and globally accepted open-source infrastructure to store, exchange, build, and track chemical-related information along the value chain. Every time materials and chemicals change owners, related information can be documented, creating a permanent history and understanding.

Blockchain promises to address other lingering chemical industry challenges as well: with blockchain and integrated smart contracts, many standard business operations can be streamlined, such as product sales, payment flows, shipments, regulatory compliance, and customs activities. In addition, since blockchain technology is capable of tracing transactions across multiple steps along the value chain, it can provide valuable insights to the chemical companies, allowing prediction of market variations, identification of demand and consumption patterns, tailoring of offerings to customer needs, and boosting of innovation and growth.

Blockchain technology in the chemical sector is still evolving into a practical business solution and its use is currently limited to several trials and pilots illustrating its benefits (e.g., Solvay, Mitsubishi Chemical Europe, Eastman). Other chemical companies — such as BASF, Covestro, and Evonik, as well as a number of start-ups — are also exploring blockchain applications, and this ecosystem will only continue to grow. Indeed, with the introduction of Digital Product Passports as a key element enhancing the traceability of products and their components to promote circularity in the EU, almost three times as many chemical companies indicate in the survey their firm intention to explore the potential of blockchain technology within a short time frame.

Although blockchain technology will certainly have its place to solve specific problems requiring the distinctive features of blockchain, there are equally valid arguments to take a broader view. As promising as it may be as a secure and decentralised means to store and distribute data, blockchain as a technology does not solve all the challenges associated with data sharing. For instance, data sharing governance requires participants to agree on a common language and data model, common standards for cataloguing, discovering, and contracting access to shared data, as well as a way to express, negotiate, and document

Eastman traces certified recycled content across the value chain with blockchain technology

Blockchain technology, being an important enabler of the circular economy, allows traceability of sustainable products across the entire value chain, from raw materials to final consumers. Understanding where materials and products come from is a vital part of any brand's sustainability story. Eastman leverages a blockchain-based platform to give visibility to the specialty plastics produced with the company's certified molecular recycling technologies. Through data transparency enabled by blockchain, the platform is designed to provide brands and consumers with traceable information on the sustainability attributes of products, including their percentage of certified recycled content. This circular solution is fast becoming a key prerequisite for sustainable offerings made with renewable bio-based and molecularly recycled waste, and is a step forward to allow customers and end users to opt for more sustainable products.

the rules under which data is shared and with whom. Such governance needs to rely on some form of cooperation and include all ecosystem participants, regardless of their size, technical maturity, and expertise. The chemical sector is encouraged to think beyond the existing use cases and continue exploring other technological solutions and approaches for data sharing in the future ecosystems.

ENABLING INFRASTRUCTURE

Let cloud solutions assist you

In the process of digital transformation, business organisations already gain efficiency from storing all pieces of information, documentation, and datasets in one central data storage, allowing workers to easily and securely access, share, and synchronise files from anywhere and at any time. Handling large volumes and a wide variety of data from disparate sources, however, is best suited to a cloud platform.

Cloud solutions eliminate the need to manage data and services using traditional onsite storage and IT systems. Based on a pay-for-use model, there is no need to acquire and maintain costly infrastructure (such as servers, software licenses, data space, electricity, and extra IT workforce). In addition to location-agnostic collaboration opportunities promoting real-time workflows and updates, companies (e.g., Clariant, DuPont, and Repsol, among many others) can benefit from cloud-based data analytics (i.e., a range of advanced analytical tools and algorithms to extract and present valuable insights from massive amounts of unstructured data). Cloud platforms greatly accelerate digital transformation as they can support hundreds of digital initiatives carried out in different business units, such as various solutions for data ingestion, data governance tools, development labs and machine learning models, as well as a wide variety of self-service tools. In the future, these features will make it possible for any employee, regardless of their knowledge of analytics, to make data-driven decisions.

The survey shows that over 35% of the companies in the chemical sector have at least partially migrated to cloud computing and 15% plan to do so in the coming years, as they see an obvious financial advantage in adopting software that will be externally maintained and automatically upgraded as global business processes evolve. The inherent flexibility and scalability of cloud solutions can help chemical companies to become faster and more responsive as well as increase their ability to exploit a standard set of applications or processes enterprise-wide. Cloud services also allow chemical companies to collaborate effectively with suppliers, customers, and business partners, and overcome common barriers to such collaboration, such as data readiness, accessibility, data sharing, trustworthiness, compliance, and security.

Vital elements of Industry 4.0 for chemicals

In the chemical industry, advanced sensors are used to monitor different industrial processes, measure a wide range of specific parameters (e.g., temperature, humidity, vibration, flow, pressure), eliminate noise from results, and pass cleansed data to a centralised cloud computing platform or other edge device via a network connection, where all information is collected and analysed for patterns. The key advantages of advanced sensors include improved sensitivity during data capture, transmission with next to no loss, real-time data analytics, and continuous monitoring of processes, which increase efficiency of operations and overall productivity. Battery-less sensors are especially promising as they require very low power and can be deployed at large scale. Among other

"To support successfully the digital transformation and sustainability of chemical companies, it is important to create an architecture and application landscape based on cloud-native principles. This is true even if not all systems migrate to a cloud."

Heiko Ofer, Product Family Manager, Cloud-Native Computing, BASF

Evonik increases efficiency of production processes with IIoT platform

Following a comprehensive digital agenda to transform production and supply chain processes, Evonik introduced an IIoT platform for rapid development of applications that can be securely scaled from edge to cloud and rolled out across the enterprise, so that numerous sites can benefit from the same applications and easily adapt them to meet specific site needs. This platform does not influence the existing processes. It is connected to the existing IT and operational technology (OT) systems, and extracts data necessary to develop new applications and complement other programmes that increase efficiency of production-related processes. This IIoT platform is crucial for the automation of processes in the production environment and its data structure forms the basis for the digital twin. Among the first applications the company implemented is a digital checklist for plant inspections combined with process information systems and current plant data, allowing quicker identification of trends and deviations. Through various dashboards it is possible to perform condition-based monitoring, predictive maintenance, and root cause analysis, as well as to implement other optimisation measures at the plants to ensure more efficient production processes.

characteristics to be considered when selecting sensors for a chemical production site are their low cost, low maintenance, ability to operate in harsh environments, reliability, accuracy, and, of course, their security.

A variety of connected sensors embedded into existing production assets and facilities, together with wireless Internet connectivity and cloud computing platforms for data processing, represent the main components of the Industrial Internet of Things (IIoT) and are an indispensable part of Industry 4.0 ecosystems. IIoT sensors communicate with the cloud by transmitting critical production data through the Internet to a remote server, where data analytics services extract valuable insights. Real-time feedback and instructions are then returned to IIoT devices for performing an action without human intervention. There are millions of connected IIoT sensors already deployed at multiple production plants, and the survey results confirm that many more will be added in the chemical sector, especially in light of 5G wireless technology (i.e., the fifth generation of wireless networks providing higher speed and lower latency), which continues to roll out across the world.

Together, these digital technologies form an enabling infrastructure that allows chemical companies to gain strategic awareness, automate daily operations, and gather data in a single IIoT platform that can be accessed by authorised users from any location and at any time for further computations and decision-making purposes. Additionally, visibility on large amounts of crucial real-time data unlocks further opportunities in conjunction with deployment of AI and digital twins in industrial settings, such as predictive maintenance, efficient use of energy and resources, increased productivity, and reduced costs, as illustrated by an example from Evonik (see “Evonik increases efficiency of production processes with IIoT platform”).

IoT has a vast range of other applications in supply chain management and optimisation. For instance, it facilitates tracking and monitoring of raw materials and products, brings more transparency to the communication process, and increases the precision of planning.

AUTOMATION/LIMITED HUMAN INVOLVEMENT

Bridge the gap in automation & robotics

Next-generation progressive robotics and automation are turning the chemical industry into a safer and more productive space, thereby contributing to sustainability objectives. Industrial automation involves access to real-time data with the aim of further optimising production processes, increasing energy and resource efficiency, and making more informed decisions. Industrial automation is interconnected with the deployment of AI and digital twins in production. In addition, robotics and automation are highly advantageous for the chemical sector as they allow the elimination of many tedious and dangerous activities traditionally performed by humans.

Today, chemical production plants often rely on drones for aerial inspections, sparing employees from working at height. Continual safety inspections of sensitive ground areas are increasingly conducted by autonomous robots with thermal imaging cameras and adjustable sensors, which can alert workers of any impending danger. Chemical tank cleaning used to be one of the most dangerous tasks performed by humans, due to confined spaces and the presence of toxic gases and hazardous chemicals. Now, tank-cleaning robots do this job with excellent efficiency and keep workers away from a multitude of health and safety risks. Additionally, robotics and automation systems can be used to improve the consistency of lab experiments, especially for precise tasks like measurements, chemical dispensing, and testing.

Our survey revealed that around 35% of companies in the chemical industry (including Solvay, Evonik, and Merck) have already been automating certain workflows and supporting their workers with robotic systems. This number will continue to grow as benefits of the changing face of robotics and automation develop further. To showcase examples of innovation excellence in this domain, Wacker Chemie (see "Wacker relies on mobile robots for autonomous inspection of industrial plants") and Lanxess (see "Lanxess employs analytics platform supporting automation of its global production plants," see page 37) share their best practices in robotics and automation in production.

"Autonomous robots exceedingly improve routine inspections at production facilities and make work safer for humans."

Hartmut Manske, Director,
Head of Automation & Robotics, Merck

Wacker relies on mobile robots for autonomous inspection of industrial plants

Wacker puts into service autonomous robots to avoid human contact with dangerous or health-threatening work environments at production facilities, while increasing the quality and frequency of inspections of industrial plants. With the help of integrated sensors and cameras, these mobile robots can easily follow pre-determined inspection routes, while recording and transmitting information about onsite operations. They can read analogue devices, use thermal imaging to detect defects in pipes, monitor temperature levels, and collect data from local sensors and measuring points, including those that are difficult for people to reach. This data is transmitted to a cloud-based system and can be used to detect anomalies such as excessive temperature, leaks or contaminations at an early stage, and monitor flow rates and pressure values. Wacker intends to further expand the adoption of autonomous robots for inspection missions at production facilities to relieve employees from repetitive work in hazardous environments and ensure the company's high safety standards.

Lanxess employs analytics platform supporting automation of its global production plants

Lanxess continues to break new grounds in the chemical industry with its high-quality, sustainable products and innovative solutions, while increasing capacity utilisation, optimising resource efficiency, and reducing maintenance costs at its major production sites. At the core of these improvements is a novel self-service analytics platform for sensor-generated time-series data produced by its numerous global plants, which ensures an end-to-end capability to drive digital automation in production. Equipped with this advanced analytical system, production employees can autonomously analyse measurements data and manufacturing processes, reveal patterns and trends, and detect production anomalies. After a successful digital upgrade of its production sites as part of the overall digitalisation initiative, Lanxess particularly benefits in terms of more efficient raw material and energy use, improved product quality, higher production capacity, and timely asset maintenance.

Welcome to the immersive journey

AR and VR are the two principal immersive technologies commonly used in various industrial settings. Whereas AR blends interactive digital elements into a real-world environment through a smartphone, tablet, or headset, VR provides a full sense of immersion into a simulated environment, where realistic interactions with people and objects become possible. Up to now, AR and VR applications have mainly spanned commercial industries such as healthcare, education, architecture, tourism, and entertainment.

Specific to the chemical industry, these technologies help to address safety-related issues and workforce shortages by providing an alternative to bringing experts physically into a production plant. To keep running numerous facilities smoothly, improve efficiency, and reduce downtime, daily operations must be precisely coordinated, including periodic onsite security assessments looking for vulnerabilities, missing configurations, and other security risks.

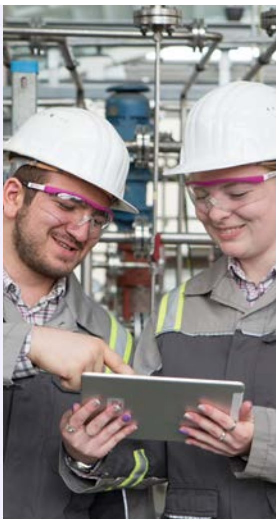
The latter process, however, can be significantly streamlined through remote assistance in real-time, enabled by immersive technologies and a network providing higher speed, lower latency, and greater capacity.

These technologies also ensure tacit knowledge transfer among workers and their effective training, and facilitate digital documentation.

AR and VR technologies are no longer considered novel. During the global pandemic, they proved their value to stay connected and have now become more pervasive in the chemical sector. They have evolved to be an integral part of modernised production facilities and their utilisation is expected to continue growing at the same rate for the foreseeable future. The example of Evonik (see "Evonik supports its employees with AR on the road to the digital future") demonstrates how one company emphasises immersive capabilities to enhance occupational safety, reinforce digital collaboration, and streamline inspection and maintenance activities.

Evonik supports its employees with AR reality on the road to the digital future

Following a comprehensive digital agenda, Evonik strives to design improved workflows and make daily work easier, while improving the company's sustainability performance. For instance, AR is among the modern technologies used to simplify work and boost production efficiency at Evonik's chemical plants. Thanks to the ability to combine virtual information with the real environment, operators maintaining highly complex production facilities can receive detailed information about a detected failing component, storage location of replacement parts, safety equipment checks, and designated routes to the specific site where the work needs to be performed, using a tablet. This approach not only streamlines work processes and reduces production downtime, but also makes the necessary formalities easier as logs now can be filled out directly on the site using a tablet, and digital documentation becomes available everywhere in real-time.



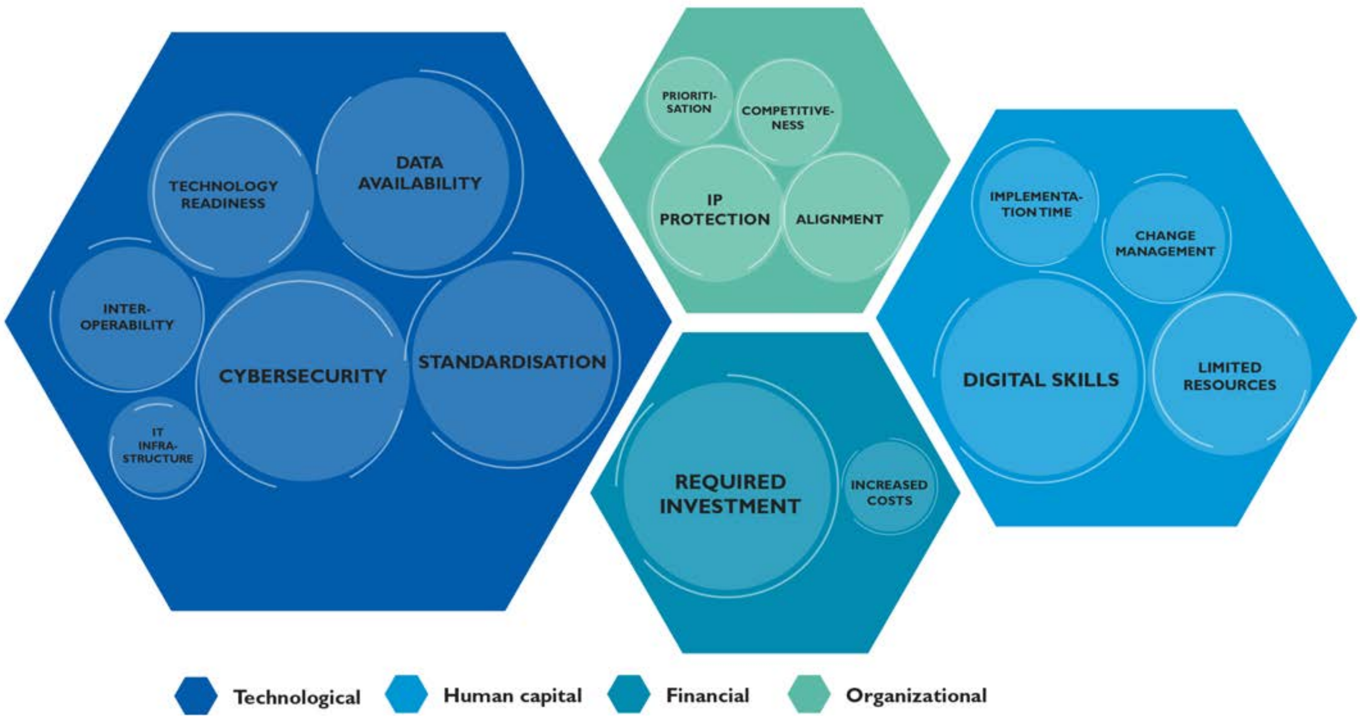
3. DRIVING CHANGE — DIGITAL TRANSFORMATION CHALLENGES THE CHEMICAL INDUSTRY MUST OVERCOME

In this section we consider the range of technological, financial, human capital, and organisational challenges that need to be overcome to further drive and accelerate implementation of digital technologies in the chemical sector (see Figure 6). As we have seen, overcoming these barriers will deliver both sustainability and other business benefits, such as efficiency, effectiveness, innovativeness, and competitiveness.

TECHNOLOGICAL CHALLENGES

- **Data availability.** Successful digital transformation and data-driven processes require access to the relevant data of interest. However, until recently, chemical companies did not value data as a strategic asset and data remained fragmented. Bringing data together in a data lake, building an internal data integration platform to enable authorised users to access required data in the right format, and deploying advanced analytics and data visualisation tools still represent major challenges for 35% of the companies we surveyed. These challenges impede them from making the best use of the available data for the benefit of the business over time. Given the complexity and competitiveness of the chemical sector, it is even more difficult to gather data from across the value chain, despite the actionable insights on sustainability it may provide. In this case, not only data availability but also trust in data quality and its provenance is vital.

Figure 6. Challenges in implementing digital technologies in the chemical sector



Source: CEFIC

- **Interoperability.** It is clear that upcoming regulations will mean that chemical companies will need to share data externally with other players to enable circularity and true end-to-end traceability of products across the value chain. Understanding what information is required by respective stakeholders and ensuring the right data is available in usable formats are problems the industry currently faces. Traceability requires specific mechanisms and data structures to validate data accuracy and provenance and to enable participation of all upstream and downstream stakeholders in the ecosystem, including smaller players that may not be technically advanced. The biggest challenge in achieving interoperable data exchange and transparency is gaining an agreement on industry-wide standards and ways of tracking sustainability, which must be integrated into existing processes and platforms.

- **Standardisation.** According to 45% of the chemical companies we surveyed, data sharing at the ecosystem level needs to address two main sets of issues: first, the means of technical implementation, and second, the need to protect IP and preserve competitive advantage. Creating a set of common standards and methodologies to incentivise and facilitate data sharing across the value chain will allow chemical companies to automate data flows and collaborate more effectively. To meet different levels of transparency without impacting business competitiveness, limited subsets of data may be shared with different stakeholders, based on access rights and rules determined for specific groups of products. Defining cybersecurity standards will also ensure a higher degree of data security and privacy.

- **Cybersecurity** is recognised by 45% of the survey respondents as one of the most prominent concerns, showing that this topic may still be rather underestimated. Bidirectional data flow, transmitting information for analysis, and sending actionable feedback directly to machines makes them extremely vulnerable to cyberattacks. For this reason, cybersecurity is particularly important for the chemical industry as disruption can have a serious impact both in terms of financial losses and brand image. Major data breaches and industrial espionage have become a severe threat in recent years, forcing chemical companies to take a more proactive approach to securing their sensitive data and intellectual property. Legacy cybersecurity tools are not capable of dealing with the rapidly growing complexity of enterprise attack surfaces. Consequently, chemical companies frequently lack full visibility of their cybersecurity posture and remain susceptible to cyber threats and breaches. To adequately protect sensitive information from access by unauthorised third parties, enterprises across the industry need a robust security platform safeguarding data across all endpoints, networks, and storages as well as in the cloud. High-level encryption standards should be applied to data storage, and there should be mechanisms to share this valuable data with authorised individuals. Reliable and resilient digital transformation can only be achieved when it is built on a foundation of robust cybersecurity practices.[27]

- **Technology readiness.** Some concerns have been raised around technology readiness at the industry level. While several digital technologies have been in use for many years, other digital solutions are still emerging and gaining traction at an incredibly fast rate (e.g., private 5G networks to strengthen cybersecurity and expand automation). It is important to understand the evolution of digital technologies and the highly interdependent relationships between them in order to start transitioning. At early stages, a pilot environment is typically exploited to demonstrate the maturity and performance of new digital solutions, and once the most advanced level is achieved, actual implementation in industrial settings begins.

- **IT infrastructure.** Chemical companies acknowledge the need to modernise their existing IT infrastructure in a business-oriented fashion to deliver the agility and efficiency required for implementing novel digital solutions while supporting current operations. Traditionally, IT infrastructures have been deployed within company-owned facilities. Management of a large enterprise IT environment requires a lot of space, power, personnel, and maintenance costs. Today, part of this infrastructure can be virtualised and rented from a cloud service provider.

27 "The EU's Cybersecurity Strategy for the Digital Decade." European Commission Joint Communication to the European Parliament and the Council, JOIN 18, 16 December 2020.

Following the cloud-native principle, data becomes more accessible, and processes are unified within an enterprise through a coherent set of interconnected applications. There are certainly some positive trends observed across the chemical sector regarding the transformation of legacy composite hardware, software, and network services. However, a lot still remains to be done.

FINANCIAL UNDERTAKINGS

- **Required investment.** Although the benefits of implementing digital technologies in chemical companies of all sizes are becoming more and more transparent, securing the required investment still represents the most predominant bottleneck. At least 50% of the surveyed companies hesitate to invest in digital transformation that may not deliver the desired outcome immediately, especially in the light of the challenging economic situation affecting every business. Also, pursuing the chemical industry transformation to a net-zero and circular future will require a colossal financial commitment. However, there is a strong consensus that investment in digital technologies must be one of the pillars of the intended recovery and will ultimately transform the chemical industry into a green, innovative, resilient, and competitive ecosystem.
- **Increased costs.** Several additional, recurring costs arise in the effort to meet digital transformation goals. These include the costs associated with upgrading legacy systems, platforms, and applications, maintenance, restructuring, new partnerships with technology providers, and deficient digital expertise.

HUMAN CAPITAL

- **Digital skills.** The digitalisation rate in the chemical sector strongly depends on the successful attraction and retention of highly skilled individuals with advanced digital competencies. Currently, around 45% of the surveyed chemical companies find it particularly challenging to attract digital professionals. Advanced digital skills are in high demand; thus, to be successful in the global race for digital talent, the chemical industry must be seen to be attractive as other sectors and large high-tech companies. Additionally, it is increasingly important to complement digital expertise with general green skills to support value creation in the context of the double twin transition.
- **Limited resources.** Driving the adoption and scaling of digital initiatives requires additional skill sets, and it may not be possible to run all of them with the limited resources available to a company. Existing competencies need to be complemented via continuous training measures that are appropriate to requirements. Developing new skills among existing personnel allows for a more flexible resource allocation across different projects. In addition, targeted recruitment can be used to overcome the current barriers and fully exploit growth opportunities.
- **Implementation time.** Digital transformation does not happen quickly. It may take several years, and even then, the task is never over, as digital technologies will continue to evolve rapidly and require constant upskilling. However, there is no reason for standing still. Even though digital maturity will be different for each chemical company, there is always a starting point.
- **Change management.** To embrace new digital technologies and deploy them in daily operations, chemical companies need first to create environments that are receptive to change by communicating the advantages of digitalisation, gaining employee trust, and providing a clear vision to jump-start the transition process. Placing emphasis on a change-oriented mindset, bolstered risk taking, agility and collaboration, rapid experimentation, investment in talent, and development of digital skills will foster effective management of the people side of the digital transformation. It is important to stay focused and maintain the pressure to achieve the desired outcome.

"The toughest challenge is to attract talent with the right skills to drive digital transformation and shift the mindset of existing employees."

Zoltán Szabó,
Head of Downstream Digital Development, MOL Group

ORGANISATIONAL CHALLENGES

- **IP protection.** Just like in many other industries, IP is at the center of a chemical company's value. Among the biggest challenges for chemical companies is implementing systems that enable a free flow of information inside the company as well as throughout the supply chain, while simultaneously protecting their valuable data, confidential business information, and IP from unauthorised access. It is crucial to gain better visibility and control over security in the entire supply chain by thoroughly vetting security practices of all participants and examining areas of risks with deeper scrutiny. Individual players will have to work together to find and implement new practical solutions for data sharing across the supply chain.
- **Competitiveness.** Most chemical companies agree that innovation requires new ways of collaborating and data sharing with ecosystem partners and other third-party organisations. However, collaboration is often associated not only with security risks but also concerns about losing competitive edge. Today's technologies will need to convince businesses that competition and collaboration can indeed go hand in hand. Competitive businesses that also cooperate when it is to their advantage are said to be in 'co-opetition.'
- **Prioritisation.** The chemical industry itself is changing very quickly, and given the current business uncertainties and constantly changing market conditions, companies must regularly reassess innovation projects to prioritise them correctly. The impact of specific digital technologies is often hard to estimate, thus digital initiatives are not always accurately compared and prioritised with respect to other projects running in parallel and, as a result, lack the required attention and investment. Instead, chemical companies must drive digital initiatives with the highest potential to deliver value and help organisations become more competitive, profitable, efficient, and sustainable.
- **Organisational alignment** is one of the most important drivers of digital success. Digitally savvy chemical companies are already aligning their people, structure, activities, processes, and culture to facilitate achieving organisational goals with the help of digital technologies. However, preparing for the digital future is no easy task. Companies can move forward with the digital transformation successfully and confidently if they ensure that all operational and strategical aspects fire in sync.

MIND THE DIGITAL CARBON FOOTPRINT

There are strong theoretical arguments and model-based reasons asserting that digital technologies can indeed help achieve sustainable development objectives in various industrial sectors.[28] However, due to the lack of empirical evidence, the role of digital technologies in achieving green growth has been a topic of opposing opinions and misleading conclusions. Widespread industrial digitalisation has raised reasonable concerns about energy consumption and environmental footprints. The digital industry currently estimates its share of consumption of the world's total electricity to be in the range 5%-9% and it accounts for around 2%-3% of the global CO_2 emissions (comparable to air traffic).[29] To ensure that these impacts are properly addressed, an agreed EU-level framework is needed for measuring the environmental impact of digitalisation in terms of GHG emissions, resource use, and energy consumption, including possible rebound effects; that is, occasions when energy savings achieved in one area get dissipated and absorbed by reuse of energy in another area.

Whereas the widespread adoption and use of digital technologies will inevitably continue to increase its energy and environmental footprint, further efforts can be made to significantly improve digital technology energy efficiency and to ensure green electricity supply. Moreover, the increase in energy consumption caused by digitalisation is more acceptable if it can be clearly shown to deliver energy-efficiency gains in other sectors of the economy. It is therefore most appropriate to stimulate digital transformation in energy-intensive sectors where the potential gain is expected to be the highest.[30] In this regard, digitalisation has raised great hopes that it can contribute to the reduction of emissions and energy demand, particularly in the energy-intensive chemical industry, both in terms of processes and products.[31]

28 "Digital with Purpose: Delivering a SMARTer 2030." GeSI and Deloitte, 2019.
29 "Shaping Europe's Digital Future." European Commission, COM 67, 2020.
30 "Digital Technologies and the Green Economy." EIT Digital, 2022.
31 "Molecule Managers: A Journey into the Future of Europe with the European Chemical Industry." Cefic, 2019.

CONCLUSIONS

The study forming the basis for this Report confirms that digital technologies will play an essential enabling role in the transformation of the European chemical industry required to address the climate, circular, health, safety, and environment objectives in the context of the European Green Deal. We have identified major priorities for the application of digital technologies in chemical companies as well as shared illustrative use cases. Several digital technologies are already well implemented in the chemical industry, while new ones will continue to emerge with high deployment potential in the chemical sector in the near future.

Considering the enormous potential of digital technologies and the challenges ahead, we have formulated a set of key recommendations for the chemical industry and the EU institutions that would ensure beneficial implementation of digital technologies in the chemical sector towards sustainable development.

For the chemical industry:

- **Explore what can be done collectively.** Investigate what is really needed to build scalable solutions for broader and more intensive implementation towards a sustainable future. Explore what can be done collectively within legal boundaries (e.g., future-ready data management, interoperability and cybersecurity, required IT infrastructure). Since the double twin transition does not only affect the chemical industry, broad collaboration with chemical value chain players and across ecosystems is key to further success.
- **Establish common data and technology standards.** Standardisation is a prerequisite, hence there is a need to establish common data and technology standards, including data sharing standards, that can ensure that the industry shares sustainability attributes across the entire value chain and with other industries.
- **Explore new business models.** As the double twin transition comes with major disruptions, the industry needs to explore new (digital) business models and anticipate possible challenges.
- **Drive targeted investment.** Invest in digital technologies with a view to achieving circularity and sustainability targets.
- **Train and attract digital talents.** Take actions to attract talents with advanced digital skills to the chemical sector. Additionally, collaboration with universities would facilitate the development of curricula and educational content that links digitalisation and sustainability aspects.
- **Demonstrate best practices.** Demonstrate and communicate the benefits of applying digital technologies for sustainability in the chemical sector through best practices and actively encourage broader adoption, explaining why improvements need to occur.
- **Engage more actively on policy and regulation.** Play a more active role in EU digital policies and regulations.

For EU institutions:

- **Align the regulatory framework.** Ensure that the EU regulatory framework allows for applying digital technologies and speeds up existing processes for the deployment of digital solutions that effectively contribute to sustainability objectives, including through new business models. The success of digital solutions that are in their development phase (e.g., AI applications) strongly depends on an innovation-friendly policy and regulatory framework.
- **Facilitate the creation of data standards.** Facilitate data standards creation to speed up the process and give more confidence to companies that develop digital tools and new business models based on those standards, contributing to sustainable development.
- **Facilitate data sharing mechanisms.** Facilitate mechanisms to share data with external stakeholders at the ecosystem level, taking into account, for example, cybersecurity concerns, confidential business information, and interoperability aspects and building on existing successful initiatives (e.g., Catena-X).
- **Consider risk-sharing measures.** Consider risk-sharing measures for the development of future-oriented solutions effectively addressing technology gaps and provide support especially to smaller companies in the context of sustainable development.

APPENDIX A — METHODOLOGY

The full study comprised three main phases. First, a number of interviews were conducted with innovation leaders in the chemical industry to lay the groundwork for the study. Based on the valuable inputs obtained from the experts during the interviews, the essential foundations and hypotheses were formulated, and the overall scope of the study was defined.

During the next phase, a chemical industry survey was launched to identify potential use cases where digital technologies can be an enabler for chemical companies to meet their sustainability targets. With input from more than 70 chemical industry respondents representing 50 different-sized enterprises and diverse chemical segments, it was possible to explore how companies prepare for and implement digital technologies within their value chains to address sustainability issues, and what others can learn from them. This was illustrated through distinguished examples with high-impact potential for broader application. The outcome of the survey not only identified a set of the most relevant digital technologies that are already in use or are planned to be deployed, but also assessed their expected impact and identified common bottlenecks for implementation. The second phase of the study was also complemented by desktop research, bringing additional information on the uptake of digital technologies and their concrete applications in specific areas of the chemical value chain.

Next, the results of the survey were exploited to map use cases, characterised in terms of: (1) chemical value chain position where the improvement is desirable, (2) sustainability goal being pursued, (3) corresponding problem specifics (e.g., efficiency, traceability, interoperability), and (4) type of digital technologies considered suitable to address the problems. These use case characterisations helped to define the current focus areas where digital technologies can play a significant role to help achieve sustainability objectives.

Finally, a technology expert consultation took place in the form of four thematic roundtable discussions with digital technology experts, including chemical industry representatives, to explore key digital technologies and their combinations, identifying which can offer the best available solutions with explicit benefits for each focus area, today and in the future.

APPENDIX B — GLOSSARY

Artificial intelligence (AI) is a machine simulation of human intelligence, which is able to carry out repetitive, rules-based, and judgment-related tasks after being trained on large amounts of data. AI makes traditional modelling processes more sophisticated through creation, training, and deployment of algorithms and models that emulate logical decision-making based on available data and support advanced intelligence methodologies such as real-time, predictive, and prescriptive analytics. AI is not just one thing; it represents a group of crucial methods and techniques that include machine learning, natural language processing, computer vision, mechanical automation, robotics, and many others. Each application of AI is designed to fulfil a relatively narrow purpose, but when combined, AI-driven tools have an immense transformational power and strongly influence the way we live and work on a global scale.

Big data is a term that describes large and complex datasets coming from a variety of sources and growing in volume at ever-increasing rates. It consists of both structured and unstructured data that is hard to store and process efficiently with traditional data management tools. Advanced analytical techniques are used to uncover hidden patterns, correlations, market trends, customer preferences, and other meaningful insights.

Blockchain is a decentralised, distributed, and shared digital database (ledger) that is used to store transactions and track assets across a network of computers in a secure way so that records cannot be altered retroactively. All participants have access to the shared ledger, where each immutable transaction is recorded only once as a block of data containing preselected information (who, what, when, where, how much, and other specific conditions), and none of the participants can tamper with the transaction once it is stored. Every time an asset moves from one location to another or changes ownership, a new block of data is added to the irreversible chain, strengthening the verification of the previous blocks and building the distributed database that members of the network can totally trust and refer to as a single point of truth.

Cloud computing refers to delivery of on-demand computing services over the Internet on a pay-as-you-go basis. Cloud infrastructure offers various configurable computing resources including networks, servers, data storage, software, analytical tools, and other IT capabilities. Instead of having to build and maintain massive IT infrastructure in-house, cloud computing allows companies to access large amounts of computing power virtually and consume computing resources as a utility.

Connectivity (5G) is the ability for the interconnection of various platforms, systems, and applications. The next generation of wireless networks is enabled by 5G connectivity, which is designed to weave virtually everyone and everything together, including machines, objects, and devices. 5G wireless technology delivers massive network capacity, significantly higher speed, ultra-low latency, and more reliability. Higher performance and improved connectivity will transform and disrupt industries like never before.

Cybersecurity is the practice of protecting computer systems and networks from digital attacks aimed to access, manipulate, or destroy sensitive information, steal electronic data for unauthorised use, maliciously disable or damage software and hardware, and interrupt normal business processes. Cyberattacks can be launched from anywhere by using various attack strategies. Thus, adopting a proactive approach to cybersecurity is crucial in the digital world.

Data lake is a centralised repository designed to store large amounts of structured and unstructured data in raw formats until it is used to run different types of analytics such as big data processing, machine learning, real-time analytics, and dynamic data visualisation to derive valuable insights and facilitate the decision-making process.

Digital twin is a virtual model that represents an exact digital counterpart of a physical object or process. Connected sensors collect data from functional areas of a physical asset in real-time and map it into the digital model, so that crucial information about the actual performance is easily accessible. With predictive analytics and machine learning algorithms, digital twins can also virtually simulate behaviour in real-world scenarios during design and testing phases, refine assumptions, study performance issues and generate possible improvements, predict future performance, and facilitate decision-making.

Information technology (IT) infrastructure is defined as composite hardware, software, and network components that represent the foundation of an enterprise IT environment. Hardware refers to physical components such as servers, computers, data storages, cooling systems, cables, routers, and other equipment. Software typically includes an operating system (OS), enterprise resource planning (ERP), customer relationship management (CRM), and various applications used for internal purposes as well as to provide services to customers. The network part consists of hardware and software elements necessary to ensure network enablement, Internet connectivity, firewall, and security.

Internet of Things (IoT) represents a network of physical objects that are embedded with sensors, software, and other technologies for the purpose of connecting and exchanging data with other systems and devices over the Internet or other communication networks. These devices range from ordinary household objects to sophisticated industrial tools. Among industrial IoT (IIoT) applications, the following are some common uses: smart cities, smart manufacturing, connected assets and predictive maintenance, connected logistics, and smart digital supply chains.

Quantum computing represents a new paradigm in computation that utilises the fundamental principles of quantum mechanics to perform calculations that are too complex for classical computing. Quantum computing is developing rapidly, and this powerful computing technology will be ideally suited to tackle issues relevant to materials discovery, drug development, traffic optimisation, cybersecurity, weather forecasting, and climate change.

Supercomputing relies on parallel processing, that is, executing multiple operations at once by a cluster of individual computers, instead of serial processing of an ordinary computer able to do one thing at a time. Supercomputing enables processing of large amounts of data and extremely complex computations in much shorter periods of time, including simulation tasks and testing mathematical models for complex physical phenomena (e.g., climate, weather), life sciences, manufacturing, and cryptology.

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- Adrinée Favé, Chief Information Officer, Solvay
- Pierrick Le Gallo, Vice President, DuPont Europe Middle-East & Africa
- Nicole Graf, Global Co-Lead Digital & Sustainability Innovation, BASF
- Stefan Haver, Head of Corporate Sustainability, Evonik

Chemical industry experts (roundtable discussions):

- Eric van den Berg, Group Chief Information Officer, Clariant
- Colja Boennemann, Sustainability Product Manager, ExxonMobil
- Stefan Dreher, Senior Vice President Digitalisation of R&D, BASF
- Japie van Heerden, Global IT sub-Domain Head Operations Solutions, Clariant
- Michael Nilles, Data & Knowledge Governance in R&D, BASF
- Heiko Ofer, Product Family Manager Compute Platform, BASF
- Daniel Pereira, Director, Digital Corporate Technology & Sustainability, Eastman
- Joerg Purwien, Head of Digital Labs, Evonik
- Dominik de la Rosa, BI Data Integration Manager, Clariant
- Helmut Winterling, Senior Vice President, Head of Digitalisation, Automation & Innovation Management, BASF

Digital technology experts (roundtable discussions):

- Claude Baudoin, Senior Consultant, Cutter Consortium
- Barry Devlin, Founder & Principal, 9sight Consulting
- Michael Eiden, Partner and Global Head of AI, Arthur D. Little
- Jon Geater, Chief Product & Technology Officer and Co-Founder, RKVST
- Cigdem Gurgur, Associate Professor of Decision and System Sciences, Purdue University
- Curt Hall, Senior Consultant, Cutter Consortium
- Vince Kellen, Chief Information Officer, University of California
- Phillip Laplante, Professor of Software and Systems Engineering, Penn State University
- Claudio Lima, Co-Founder, Blockchain Engineering Council
- Hod Lipson, Professor of Mechanical Engineering, Columbia University
- Sven Lohmann, Automation Solution Architect, Emerson Automation Solutions
- James Mitchell, Chief Strategy Officer, Strategic Blue
- San Murugesan, Senior Consultant, Cutter Consortium

MEET THE AUTHORS

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Innovation Manager, Cefic

Dr. Marina Samoylova is Innovation Manager at Cefic with exposure to the EU digital policies and digitalisation of the EU chemical industry. Prior to joining Cefic, she covered roles such as Innovation Lead at the EIT Digital Headquarters in Belgium, business analyst at Vodafone Italy, and research associate at the UK Quantum Technology Hub, working in close relation to new frontiers of digital technologies. Marina holds a PhD in applied physics from the University of Milan, Italy.

Dr. Sophie Wilmet,
Senior Innovation Manager, Cefic

Dr. Sophie Wilmet joined the Innovation Department of Cefic in 2007. She has covered various innovation priorities related to sustainable chemistry and is currently Senior Innovation Manager in charge of low CO_2 emissions technologies. She graduated as a chemical engineer and holds a PhD in chemistry from the University of Haute-Alsace, France.

Dr. Daniel Witthaut,
Executive Director Innovation, Cefic

Dr. Daniel Witthaut joined Cefic in 2021 as a secondee from Evonik and is assuming the role of Executive Director Innovation. He has 20 years of professional experience with Evonik, including several Leadership functions in the areas of innovation, new business development, controlling and strategy. He has worked in different areas of the chemical industry and lived in the USA, Singapore, and China. Daniel holds a PhD in organic chemistry from the University of Münster, Germany, and an MBA from the University of Chicago, USA.

Dr. Michael Kolk,
Managing Partner, Arthur D. Little

Michael Kolk is a Partner at Arthur D. Little (ADL), based in Amsterdam and Kuala Lumpur. He leads ADL's Technology & Innovation Management practice and coordinates the Chemicals practice. His consulting work focuses on growth and innovation performance enhancement. Prior to ADL, he worked for Shell Chemicals, providing technical support to internal customers in downstream oil and chemicals. Michael holds an MSc in biochemistry from the University of Amsterdam and a PhD in biophysical chemistry from Radboud University, the Netherlands. He has also attended the Executive Education program of INSEAD, France.

ABOUT CEFIC

Cefic, the European Chemical Industry Council, founded in 1972, is the voice of large, medium and small chemical companies across Europe, which provide 1.2 million jobs and account for 15% of world chemicals production. Based in Brussels, Cefic is a committed partner to the European Union, interacting on behalf of its members with European institutions, non-governmental organisations, the media and other stakeholders. Cefic is registered in the EU Transparency Register under n° 64879142323-90.

For further information, please visit www.cefic.org

ABOUT ARTHUR D. LITTLE

Arthur D. Little has been at the forefront of innovation since 1886. We are an acknowledged thought leader in linking strategy, innovation and transformation in technology-intensive and converging industries. We navigate our clients through changing business ecosystems to uncover new growth opportunities. We enable our clients to build innovation capabilities and transform their organizations.

Our consultants have strong practical industry experience combined with excellent knowledge of key trends and dynamics. ADL is present in the most important business centers around the world. We are proud to serve most of the Fortune 1000 companies, in addition to other leading firms and public sector organizations.

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