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Perspective

Transition to sustainable chemistry through digitalization

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SUMMARY

Modern chemistry is the backbone of our society, but it is also a major contributor to global environmental pollution and the ongoing climate crisis. The transition toward a sustainable future requires a radical transformation of how chemistry is designed, developed, and used. This represents a "break it or make it" challenge for the chemical industry with significant technology lock-in and high entry barriers to radical innovations. We propose that urgently required systemic changes in chemical industry, research and development (R&D), chemicals assessment and management, and education to advance sustainable chemistry are attainable through increased and more rapid adoption of digitalization and new digital tools. This will enable flexible data exchange, increased transparency of information flows along cross-country chemical, material, and product life cycles, and chemistries that are safe and sustainable by design, addressing the complexity of chemicals-environment-health interactions and lowering the costs of entry into chemical R&D and manufacture, and new, more sustainable and collaborative business models.

INTRODUCTION

Advances in chemistry over the past century are widely praised for the technological and developmental achievements of human civilization, but are also associated with environmental degradation, loss of biodiversity, threats to human health, and the ongoing climate crisis. Yet, in the modern technological society, chemistry is ubiquitous, and innovations in chemistry and materials are responsible for the majority of new products in most areas of human endeavor.[1] The innovation potential of chemistry is at the core of current efforts to solve complex challenges, including the development of energy storage materials to support the wider adoption of renewable energy, the production of hydrogen as a clean energy vector, the direct utilization of carbon dioxide to introduce technogenic circulation of carbon, and the development of infinitely recyclable synthetic polymers.[2–8] Nevertheless, the transition of chemistry toward a sustainable development model requires a paradigm shift in (1) chemical research and development (R&D); (2) how businesses protect intellectual property and profit from chemicals; and (3) chemicals, materials, and products design and manufacturing being safe and sustainable-by-design (SSbD).

It is no surprise that the definition of "sustainable development" (see https://sdgs.un.org/goals) includes "organizational" change. A systemic change to how the chemical industry is structured is urgently needed that would encompass the entire life cycle of molecules toward full circularity. This includes what feedstocks are being

The bigger picture

Achieving the various goals of the global sustainable development agenda poses complex challenges for the chemical industry and society as a whole. Systemic innovation in chemical research and development, assessment, management, and education is required to facilitate a transition toward a sustainable future. Such an innovation can benefit, to a large extent, from the increased uptake and systematic adoption of digitalization and digital tools to optimize the management of entire chemical life cycles, from chemical supply chains and chemical manufacturing to use and end-of-life. Digitalization in chemistry will enable development of more flexible data exchange models, more transparent international and cross-sector chemical information transfer, and chemistries that are both safe and sustainable by design. With that, digitalization is key to a radical transformation to more sustainable and collaborative business models in the growing chemical industry sector.

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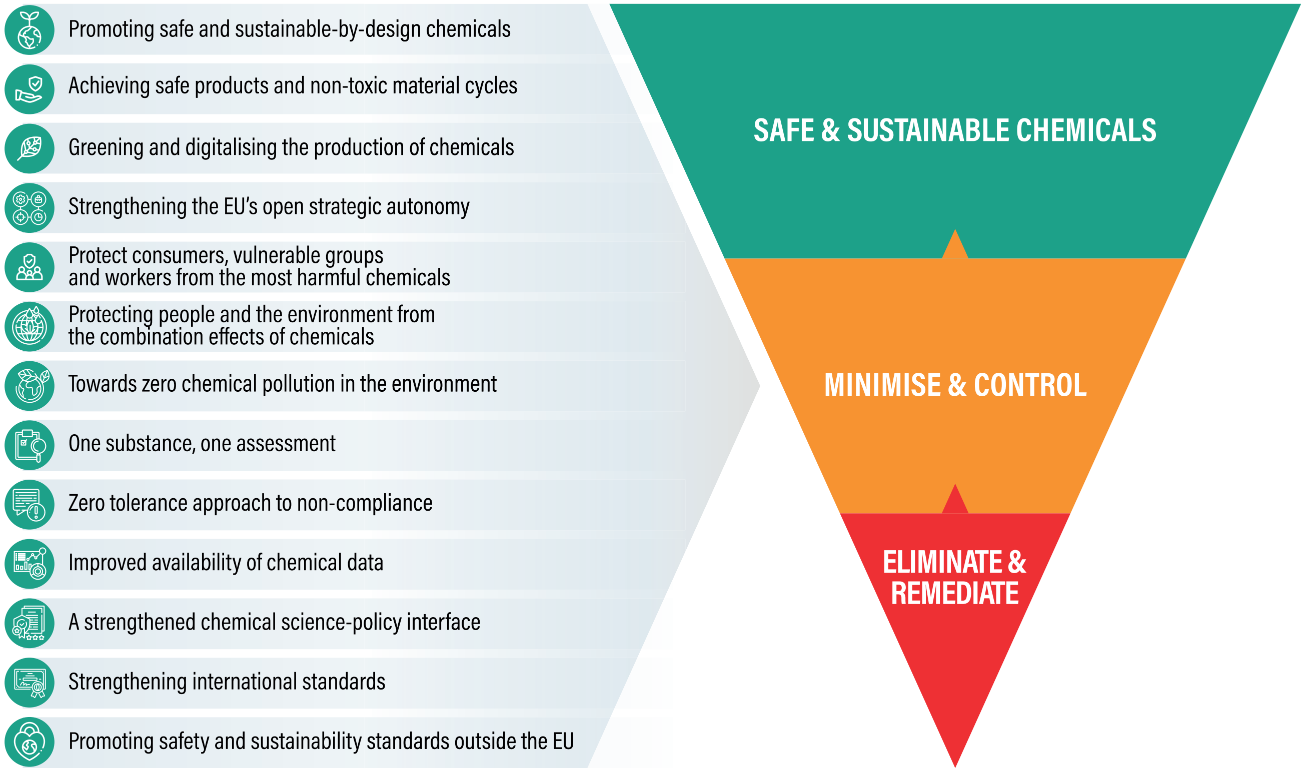

Figure 1. Overarching EU strategy and objectives for moving toward sustainable chemicals

used, what molecules are incorporated into materials and products to achieve the desired functional performance, how manufacturing of new molecules is developed, and how molecules are treated for remanufacturing, reusing or at end-of-life.[9,10]

Chemistry has long been described as a complex system.[11,12] When all its aspects are considered together—its highly complex supply chains, business models, wide range of stakeholders, interactions of molecules with products, humans, and the environment—chemistry becomes an example of a complex dynamic interacting system, a class of problems that are not amenable to classical reductionist solutions.[13,14] Finding chemical solutions with positive impacts toward sustainability depends on making chemical data more transparent and available for decision-support tools that are suitable for addressing complex problems, including emerging tools from the field of artificial intelligence (AI) and digitalization. There is an ongoing development in the discourse on potential positive and negative implications of digitalization approaches.[15] We outline the rationale for an urgently needed, rapid, and radical transformation of the chemical industry with the aid of digitalization, in support of achieving the ambitious objectives of intergovernmental strategies, such as the EU Chemicals Strategy for Sustainability[16] (Figure 1).

Structural transformation of chemical industry

Scientific institutions,[17,18] industry associations,[19,20] and financial market actors[21,22] point to major shifts in global environmental, social, and economic conditions over the next decades, risking societal fractures with deep global consequences.[23] The chemical industry, along with all other sectors of human activity, must radically change toward sustainable models. We argue that digitalization will facilitate this transition and create knowledge on how best to adapt and

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perform. The "low-carbon" and "pollution-free" paths to mitigate the current climate crisis and ongoing environmental degradation must be based on the transition toward a circular economy model, as well as significantly emphasizing the importance of stronger protection of human and environmental health. Such pathways indicate great opportunities ahead for the chemical innovation ecosystem of academia, private and public sectors, but they also pose many uncertainties as existing structures will be tested.

Manufacturers are progressively acknowledging consumer and government calls for providing product sustainability information based on principles of reliability, relevance, clarity, transparency, and accessibility.[24] Climate-driven initiatives, such as "carbon-neutrality" roadmaps, are a first step toward a more sustainable chemical industry but are currently limited to greenhouse gas (GHG) emissions and not directly addressing the wider realm of impacts from chemicals on human and environmental health, including biodiversity impacts. Furthermore, "sustainable," "circular," or "green" public procurement has the potential to leverage sustainability information via policymaking[25] in a sector with great purchase power—public procurement accounts for an average of 12% of gross domestic product (GDP) in countries of the Organization for Economic Co-Operation and Development (OECD) and up to 30% of GDP in many developing countries. Assessing the complete life cycle of chemicals, materials, and products, based on transparent, standardized, and accessible scientific methodologies, will become the major foundation for gaining the trust of the public and enabling evidence-based policies.[26] To understand how far we currently are from this target, it is enough to consider that life cycle assessment (LCA) studies published today almost never contain full verifiable datasets and are not supported by detailed annotated models.[27]

Although many calls for action agree on the ultimate goals, viable decision pathways toward these goals need to be developed, tested, and adjusted in iterative cycles, based on the reality of evolving elements of a complex system. Current innovation activities are slowed down by the lack of robust frameworks that align the interests of citizens, communities, shareholders, private enterprises, and the environment. Regulatory intricacy at all levels,[28] short-term financial incentives, and incipient business models for a circular and low-carbon chemical industry all compound the technological challenges. This translates into uncertainty over future strategies in the private sector and stalls implementation of even those scientific and technical solutions that are ready for scale-up today. Furthermore, companies often lack an insight into the environmental, social, and economic impacts of their products beyond the immediate scope of their own operations. Thus, direct actionable cause-effect relationships and the resulting responsibilities still need to be established on a systemic level.[29] Regulating agencies and government entities also lack such insights, preventing the development of policies and regulations that cover the full extent of the chemical value chain.

Would acceleration of the transformations in the whole innovation ecosystem help to respond to these challenges faster? How can we build frameworks that mitigate planning uncertainty on the systems level? How can we make environmental, social, and economic-sustainability ambitions actionable based on rigorous scientific standards and tools that capture relevant complexities and interactions?

Assuming that uncertainty over future regulations and multiple conflicting business drivers are only slowly resolved, the private sector and the wider innovation ecosystem, including academia, governmental agencies, and nonprofit R&D agencies, can already work toward the more rapid alignment of visions—circular economy for plastics,[30] mass balance,[31] value chain carbon transparency,[18] and sustainability impact accounting[29] represent the emerging industry frameworks that have the potential to align the interests of communities, companies, shareholders, and the environment. These frameworks follow the principles of scientific rigor and shared responsibility for products' eventual impact, considering how products are designed, created, manufactured, brought to market, reused, and recycled.

The recent surge of research and investments in data-driven innovation and chemical manufacturing operations is creating the comprehensive data foundation required for industry-wide data sharing and deployment of state-of-the-art machine-learning, AI and big-data applications.[32–34] Pilot projects on distributed trust technologies have started to tackle the challenge of proprietary data and intellectual property protection.[35] Considering recent progress, initiatives for cross-sector, precompetitive technology roadmaps and standards[36] could be implemented at a much faster pace than what is observed today. However, the sustainability challenge in such efforts transcends a single organization of any type in the chemistry value chain. To address this challenge, new solutions in the field of sustainable technologies are urgently needed, which combine conventional chemistry and sustainability assessment expertise with innovations in digitalization technologies. Since it is nearly impossible for a single entity to capture all the required technology components, a wider structural change is required, which should also include much broader cross-organizational cooperation.

Needs for increased digitalization

At the level of individual entities, "Industry 4.0" has become reality in many companies since 2011,[37] and automation has led to measurable increases in productivity and efficiency. Many attributes of Industry 4.0 are rapidly being adopted across different industry sectors. For example, measurements of extensive process parameters in real-time are in place and used for visualization, as well as for economic optimization, although the latter is still fairly rare.[38] Predictive maintenance and augmented reality for maintenance have arrived in some chemical companies.[39] Within the chemical industry, there are also significant structural changes already taking place, such as interlinking of processes with upstream and downstream, as well as raw materials and residue management within the network of plants and entire production facilities.

However, for several applications, more data are collected than are being used because data are not integrated into a single, consistent (centralized or distributed) platform nor standardized, whereas for many running "legacy" processes, the relevant data are not collected or otherwise available. The challenge of data is especially complex in the estimation of environmental aspects of sustainability, such as toxicity and degradability,[40,41] or mapping detailed chemical flows for complex multi-material products. For these two very different challenges, there is a common set of problems—access to data, transparency, and traceability of data—which require the same solution through digitalization of the complete system of chemical processes. To address these problems, digitalization should aid in the transformation of chemical business models, as well as breaking organizational obstacles to the exchange of know-how and data.[42]

We ask the questions "What opportunities would emerge, if chemical value chain stakeholders standardize data and establish data sharing in an economically viable

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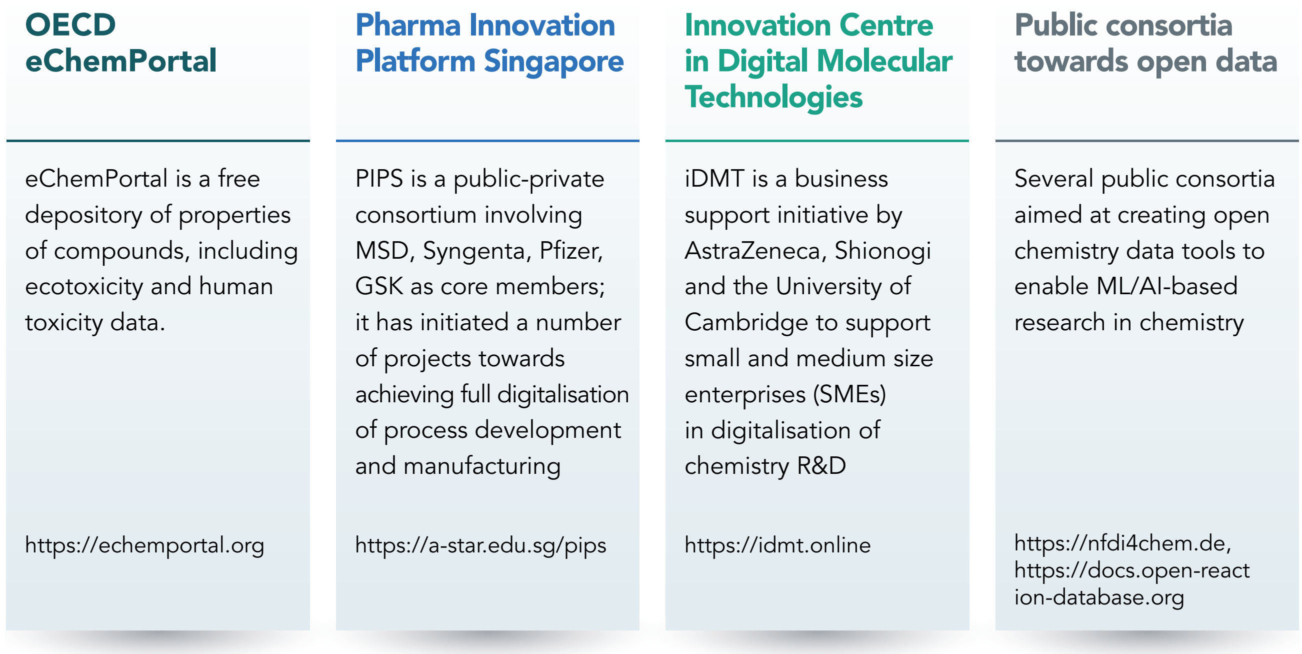

Figure 2. Examples of international collaborative efforts in digitalization of chemical industry

and secure manner that respects intellectual property rights, confidentiality of enterprise data, and privacy of citizens?'' and ''Would the environmental, social, and economic benefits of data sharing and data availability significantly outweigh concerns that are levied from the position of maintaining the status quo?''

The creation of digital twins of production processes and digital representations of products is a prerequisite to the virtualization of value chains. Virtualized value chains are required for cost optimization and comprehensive tracking and evaluation of environmental impacts. This would represent a radical departure from the currently used one-off estimates that depend on laborious field and literature studies and come with significant uncertainties. In the fully digital chemical design and manufacturing paradigm, factories and production sites learn from each other, designers systematically adopt SSbD principles, and manufacturers learn how to produce with fewer emissions and health hazards, ultimately staying within planetary and other boundaries for chemicals.[43]

The digitized value chain with transparent data flows will enable to rapidly translate customer-defined product functions into the most sustainable function delivery, whereas emerging digital rights identification methods protect intellectual property. It is feasible with current digital technologies to enable data transparency, business-to-business cooperation, and intellectual property protection at the same time. There are emerging examples of collaborations that are spearheading the development of data transparency and full digitalization of value chains in the chemical industry (see Figure 2).

There are also examples of new business models, which require extensive data-driven services being trialed out, such as chemical leasing and industrial symbiosis.[44] Although the manufacturing industry is experimenting with these data spaces and business models, the chemical process industry is lacking behind. A similar situation exists with the commercial

Box 1. Challenges and enabling factors of introducing digitalization into chemistry R&D and manufacturing

Increasing transparency: It is expected that digitalization of chemistry will facilitate wider access to (raw) data, providing the ingredients for disruptive-innovation alternatives and unveiling bottlenecks, similar to the introduction of open standards in computing and the development of digital collaboration tools for coding. Increasing transparency of the value chain will advance the knowledge of manufacturing processes of compounds that are currently restricted. A wider and more systemic adoption of digitalization may be required to trace those procuring materials for synthesis of restricted materials.[46] Blockchain can tackle the security and privacy issues of such data being exchanged.

Reskilling/upskilling of professionals: The digitalization of chemical R&D and manufacturing requires a new set of skills. This can be obtained by reskilling/upskilling the current workforce or bringing new professionals to work within the chemical industry. Chemists and material scientists would benefit from being able to work with large datasets, assisted by AI and machine learning. Engineers working with robotic instruments would support complex multi-instrument infrastructure of robotic labs and manufacturing facilities within the chemical industry. As the amount of routine and repetitive tasks will decrease, technicians and engineers who currently perform such types of activity would have to be reskilled/upskilled to remain active in the industry.[47] Although digital transformation brings along operational benefits, large companies have enough resources to bring or develop new skills within its workforce. Nevertheless, the impact of change tends to be harder for small and medium enterprises, especially when competing for highly skilled workforce.[48]

Providing additional high-performance infrastructure and new devices: Digitalization of chemistry entails increasing the use of smart devices and sensors to collect more data and pushing computational performance to interpret increasingly larger amounts of data. The manufacturing of new electronic devices, especially on a large scale, will increase the over-exploitation of natural resources, such as (scarce) metals required for processors and batteries. Toxic wastes generated from production, recycling, and end-of-life of electronics are a serious environmental concern. The path toward sustainable and non-polluting digitalization should consider these aspects and push for longer product lifetimes through circularity processes, such as repair, reuse, and remanufacture, and especially designing devices within a circular and life cycle-based approach. E-wastes should be appropriately included in related chemical and product life cycle performance assessments.[49] Furthermore, efficiency of computing power should be paired with clean energy consumption (as it is the case currently with internet giants). It is key that environmental benefits brought by digitalization are not cancelled by the infrastructural environmental costs.

adoption or scale-up of promising new clean technologies. Currently, scaling of novel, potentially sustainable, and innovative chemical technologies to industrial production is mainly limited by uncertainty over the future shape of the chemical industry, which affects investments into capital projects. Investors are reluctant to pour capital into technologies that may not be able to offer an explicit demonstration of the benefits to sustainability. There have also been examples of early commercialization of new clean processes that resulted in ultimate commercial failure, such as the 2nd generation bio-ethanol plants in the UK, which are now shut. At present, investment decisions into developing sustainable technologies contribute around 5% of the ratio between economic versus sustainability criteria in corporate boardrooms. We attribute this, ultimately, to the lack of decision-support tools that are suitable for analysis of complex, dynamically interacting systems that could offer 5- to 10-year projections with regard to the impact of investment decisions on sustainability. Main reasons for this are the protection of companies' intellectual property and fear of losing competitive advantage, as well as the lack of transparent environmental information on large benchmark processes from established chemical companies.

The uptake of digitalization for developing and evaluating chemicals also introduces new requirements. These are related to changes in operational chemical R&D workflows and additional infrastructures for information and data management. Some of these requirements and related enabling factors are provided in Box 1. In parallel to industry, academia plays a key role in enabling digitalization, seeking transparency, decentralization and harmonization of data generation and curation, and reproducibility of new digitalization-based data for decision support. Centralized data cleaning and augmentation approaches create concerns around ownership, funding, and authorship. In response, blockchain-enhanced solutions have recently emerged as a possible, secure alternative to centralized data management. Academia provides an important forum for discussing and suggesting data standards, and for developing appropriate authorship and data identifiers using new digital technologies. Furthermore, a recent analysis of the potential applications of blockchain technology in the chemical industry[45] has identified opportunities through better sharing and logging of data and machine-to-machine "trading" paired with the internet of things (IoT). Nevertheless, that analysis also highlights the need for further development of blockchain technology to overcome some of its limitations for large-scale deployment without serious environmental impact, such as high resource consumption. This includes slow speed and computational costs that are currently being addressed by the 3rd generation crypto/blockchain start-ups and academic institutions, which elaborate on how to optimize a decentralized non-hierarchical network of (autonomous) agents and non-hierarchical data sharing protocols. However, given the early stage of this research area, there is limited knowledge about its performance and eventual impact.[18]

Despite the required adaptations, there are quantifiable benefits of moving toward increased digitalization in the chemical industry. For example, BASF has reported a 30% reduction in pilot-scale batch cycle times of emulsion polymerization by introducing real-time optimization based on better reaction sensors and improved predictive models.[50] This time reduction translates into lower operational costs, higher plant throughput, and, with the quality-oriented process control, a reduction in off-spec product waste. In automotive manufacturing, one of the key benefits of digitalization that translates into supply chain optimization is an 80% increase in forecasting accuracy.[51] A similar potential is expected when applied to optimizing chemical supply chains, where collaboration with digital market places allows to rationally forecast product demand. In these efforts, an improved access to data thereby enables new start-ups to challenge the traditional opaque chemicals market, and the use of machine learning algorithms enables deeper understanding of chemical supply chains with knowledge that can be used to reduce the number of harmful chemical products in the market. In chemical R&D, digitalization has already demonstrated a significant increase in performance gains of materials and molecules discovered with the aid of AI,[52,53] which will ultimately also be useful to identify and develop safer and more sustainable chemistries and materials to substitute harmful substances across applications. Although some benefits of digitalization can already be enumerated, the most significant benefit is expected from innovation in business models enabled by digitalization.

In the following, we will focus the discussion on the role of digitalization in relation to feedstocks, chemicals and materials design, and interactions in the chemicals-environment-health space.

The role of feedstocks

Global chemicals production still greatly relies on the oil and gas sectors as major feedstocks for chemicals, despite their significant contributions to global warming and environmental pollution. In parallel, the chemical industry is directly or indirectly implicated in the life cycle of most products globally, and its unaccounted release of hazardous chemicals and pollution is linked not only to environmental releases from resources extraction but also from chemical synthesis, chemical and product formulation and manufacturing, product use and recycling, remanufacture, and waste

Box 2. Data availability and digitalization needs associated with chemicals, oil and gas industries emissions, chemical pollution, and impacts on human and environmental health

Greenhouse gas emissions and related impacts on climate: Data show that fossil fuels, apart from coal, were responsible for 55% of the historic high of 33.1 Gt CO_2 global energy-related emissions in 2018.[54] The oil and gas industry is the second (after agriculture) largest emitter of CH_4 (82 Mt out of 342 Mt annual emissions from human activity[55]), a critical climate pollutant with a global warming potential over 80 times that of CO_2 on a 20-year timescale. In 2017, approximately 75 Mt of natural gas escaped into the atmosphere from global oil and gas operations, which represents roughly USD 34 billion of lost revenue at average 2017 delivered prices.[56] In relation to the chemical industry, its operations generate about 20% of all GHG industrial emissions and 7% of global GHG emissions, despite significant reductions in the past decade.[54]

Chemical pollution: When addressing chemical pollution, an appropriate assessment is not possible nor accurate due to the multitude of sources in selected countries, the lack of data—especially in low-to middle-income countries—and the lack of data from industrial accidents and disasters. Although simulation models have the potential to be used to estimate environmental releases and related impacts on human and environmental health, related data are only available in the lower percent range across the more than 100,000 marketed chemicals worldwide,[57] which emphasizes the strong need for innovative digitalization methods that help characterize and manage chemical releases and their potential impacts on humans and the environment.

Chemical impacts on natural ecosystems: Cumulatively, chemicals reaching the environment are reported to already threaten the integrity of ecosystems globally.[58] This trend is considered to worsen as the global chemical market is rapidly and continuously growing, with a 50-fold increase in global chemical production volume since 1950.[57] Chemical production is especially growing in emerging economies with mostly insufficient chemicals and waste management capacity, which affects entire product life cycles and cross-border value chains, urgently requiring innovative digitalization approaches along with additional and efficient technologies and chemicals management infrastructure.

Chemical impacts on human health: A recent WHO report estimated that two million human lives or an equivalent of 53 million disability-adjusted life years were lost globally in 2019 due to exposure to selected chemicals, including lead and some occupational carcinogens and asthmagens.[59] However, such figures are based on epidemiological data that are available only for a handful of chemicals, whereas humans are exposed to a wide range of chemicals in their daily life.[60] Hence, whereas these estimates are likely underestimating the true human health burden from chemical exposure, more straightforward digitalization methods are urgently needed to provide health burden estimates for the wider range of marketed chemicals, also accounting for the diversity of exposure settings, and inter-individual and spatiotemporal variability.

disposal. A dramatically increased availability of data, as well as the development and uptake of digitalization methods, is required to address these urgent challenges (see Box 2).

The ongoing global climate crisis, approaching or surpassing Earth's boundaries that include the finite assimilative capacity for chemical pollution,[43] is unquestionably a reason to accelerate the development of sustainable chemistry. Over the last decade, the search for alternative carbon sources for chemicals has significantly widened the R&D efforts in creating "new" feedstocks from municipal and industrial wastes, recycled/repurposed materials and bio-feedstocks,[61] such as lignocellulose and algae, as well as captured carbon dioxide.[3] These broadly align with the circular economy model[62] and move toward SSbD approaches. An increasing number of chemical companies realize the necessity to shift emphasis toward environmentally benign products and to prioritize investment toward sustainability and circular economy, in order to create low-carbon supply chains. However, the chemical supply chain and its networks are highly complex and usually non-transparent. The transition to "new" feedstocks with their widely acknowledged challenges of compositional complexity and variability, while retaining the opaque and complex nature of the chemical supply chain, is currently a major bottleneck.[63,64]

How could companies identify and capture long-term value from truly sustainable chemicals supply chains? Could we envisage decision-support tools, which would allow identification of optimal sustainable technology choices in different locations?

One key target for the utilization of digital technologies is the development of up-to-date databases on availability, scales, and geographies of specific feedstocks, combined with the demand for chemicals, as sustainable supply chains become localized. Some molecules can be produced or remanufactured from different feedstocks; identifying the most sustainable (and efficient) way of molecule production from a given choice of feedstocks becomes very important (for example, drop-in molecules from CO_2 obtained via carbon capture and utilization (CCU) technologies versus the same molecules produced from biomass).

An overall result of a sustainability assessment[65] depends on the combination of impacts of each life cycle stage, which, in turn, depends on the level of maturity of technology at each stage and hence is a dynamic variable. As businesses need to develop long-term strategies, prospective sustainability assessment that considers the likelihood of changes in energy systems and regulations could facilitate the currently stagnating investment decision making. For example, the utilization of second-generation biomass or the direct conversion of CO_2 to fuels and molecules is limited today due to environmentally costly energy requirements, which may soon be overcome if energy systems become renewable.[3] Machine-learning and AI-supported decision-making tools, capable of making viable predictions on optimized solutions, can bolster the chemical industry progress toward sustainable sourcing of feedstocks.

Design of chemicals and materials

Digitalization will help to transition toward more sustainable sourcing of feedstocks, as chemicals and materials design supported by new digitalization methods will increase transparency and sustainability along the entire chemical value chain. Many discoveries in chemical sciences are serendipitous and, despite significant progress in the field of molecular design,[66,67] the ability to rationally "design" a synthesizable molecule or a material that perfectly corresponds to the required "functional performance" remains an elusive target. This is related to the significant degree of complexity in most structure-property relations that are not only numerous (simultaneous competing objectives) but may also lack theoretical foundation for the link between molecular structure and the final product performance (quantitative structure-activity relationships, QSARs). This is why future innovations in chemistry will likely be based on integrated solutions, which are based on digital technologies.[57]

The use of AI and machine-learning tools for designing molecules and materials has transformed this field in recent years. Navigating complex multidimensional input-output relationships with machine learning has become possible through significant advances in computing, and many areas of material and molecular products are rich in data through access to high-throughput experimental and computational techniques. There are several early successes that serve as potent demonstrations of the future capabilities of digitalization in molecular/material sciences, such as predicting new protein folding with Alphafold 2 algorithm,[68] the creation of large-scale datasets for *in silico* design of catalysts,[69] designing new materials through a combination of datamining, training simplified predictive models, and searching a large chemical space for "functional" fit,[70] or designing formulations using machine learning models based on high-throughput data.[71] Published early advances already cover the widest range of chemistry, from energy materials, via consumer products, to catalysts and healthcare. The recent development of a hybrid physics/machine learning framework[72] is also promising rapid progress in the highly diverse areas of multiscale modeling, which can also be applied to a wider range of chemistry and chemical processes. However, these are individual achievements of early adopters, who have benefited until today from access to rare resources, such as expertise, computing power, datasets, or high-throughput experimental facilities.

The pace of developing digitalization tools for chemistry is already very high and will only increase. Increased participation is being facilitated through access to data and low-cost robotic equipment, welcoming a larger pool of talent into the field of chemistry. However, this field is massively hampered by the unresolved issues of lack of standards for data and knowledge models. To date, the majority of chemical reactions data are locked in few proprietary databases, which, in reality, offer only limited capability to digitalization research, since these datasets are highly biased (mostly positive data and not universal coverage), have a non-negligible error rate, and are accessible only via an expensive subscription. These databases also contain information that is insufficiently well labeled, and thus is difficult to use by algorithms. This increases the popularity of new databases generation efforts, such as a well-maintained and cleaned, but rather small Pistachio database.[73] In part, this is due to the fundamental difficulties in developing a universal canonical data standard for chemical information that could cover many areas of chemical sciences. Another aspect is the high dimensionality of chemical information. In order to describe the behavior of molecules in a specific situation, one requires at least a six-dimensional context descriptor.[74] This complexity further increases as we include supply chain and life cycle information. Although scientific output in chemical sciences continues to be largely on paper and the reported information is low-dimensional, it will remain almost entirely inaccessible and useless to algorithm-based research, unless innovations from the field of digitalization are more rapidly taken up.

CHEMICALS-ENVIRONMENT-HEALTH INTERACTIONS

Beyond the chemical design and feedstock sourcing, the increasing number and amount of marketed chemicals used in thousands of industrial and consumer product applications, creates additional challenges for achieving sustainability, which cannot be solved using conventional chemicals and environmental management approaches. Challenges range from (1) assessing and mitigating impacts on climate crisis and pollution from energy-intensive chemical production, via (2) environmental degradation from emissions and resources depletion along chemical, material, and product life cycles, to (3) human occupational exposures during manufacturing and waste treatment, and consumer exposure during product use. Although some challenges are directly connected to intrinsic properties of molecules, such as environmental persistence, bioaccumulation, or hazard potency, the problem is not related to chemicals alone. Instead, many challenges arise from insisting on designing molecules and materials in a linear rather than a circular model[75] with a focus on sales of volume rather than on performance (or on function), and the lack of transparency of the environmental "costs" (so-called externalities) of new products that would enable customers to make informed choices.

By following the "reduce-by-design,"[76] "sustainable-by-design,"[77] or "safe-by-design"[78] approaches, the design of molecules and materials would anticipate and plan for different alternatives to production, consumption, and end-of-life, avoiding mostly energy- and resource-intensive processing technologies, marketing that disregards the risk of using hazardous chemicals in non-essential applications, and prevailing end-of-life treatments that are mostly incinerating or landfilling products after use.[79] Consequences are that a wide range of chemicals used in consumer products and industrial processes is now found in virtually all environmental media

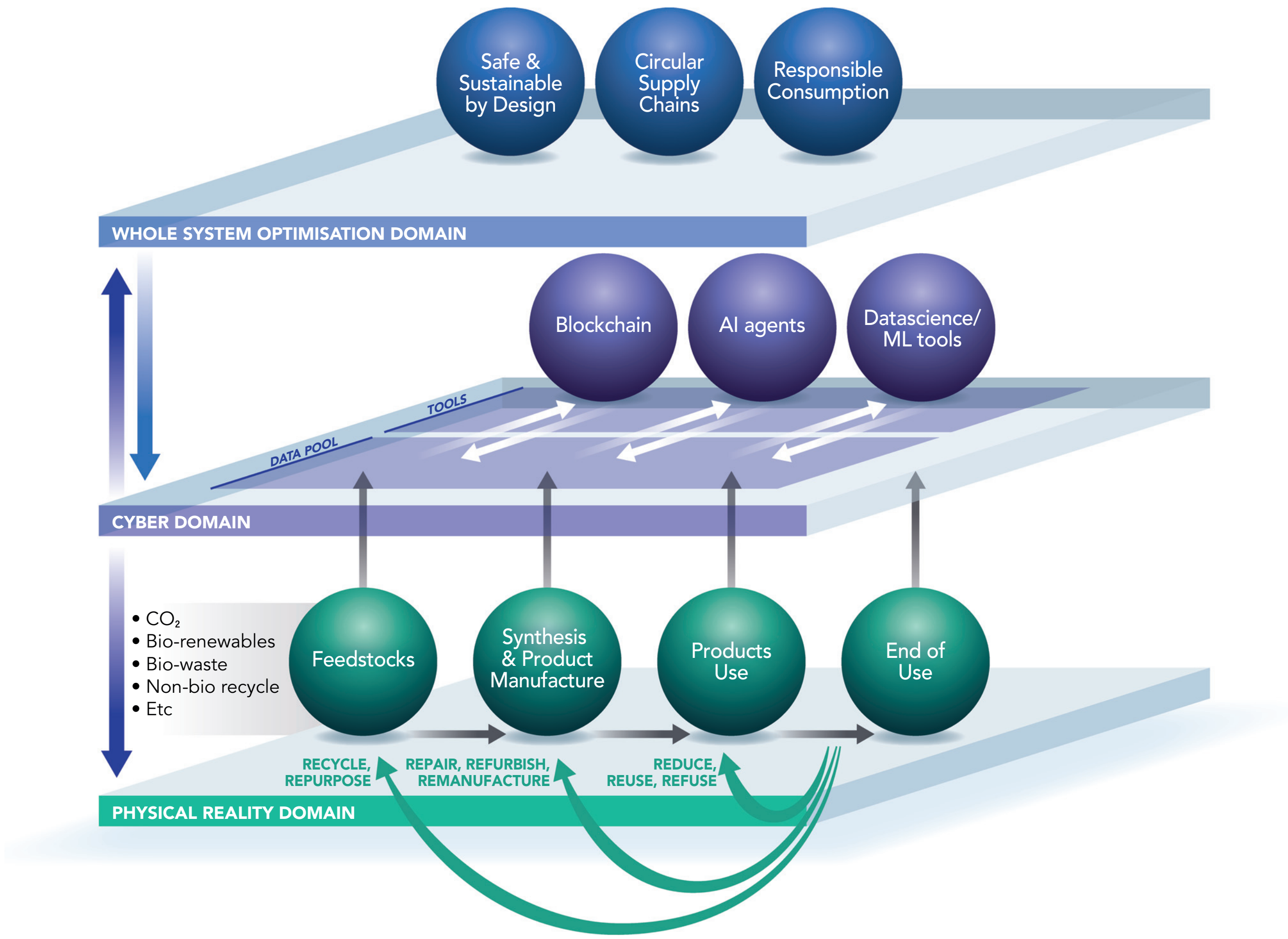

Figure 3. Data points on the value chain of the chemical industry from raw materials to finished products and interfaces for digitalization and big data approaches to boost safer and more sustainable chemistries

worldwide, in biota, and in human tissues, where they—individually or in combination—can cause health hazards and biodiversity loss.[80]

Which innovations are needed to successfully overcome these challenges, to successfully manage the ever-increasing demand for new chemistries and consumer goods? By what means can we ensure that the highly dynamic mixture of marketed chemicals is aligned with health and environmental sustainability targets and to manage increasingly complex, global chemical supply chains and waste streams? Answering these questions requires innovation in providing, collecting, curating, and structuring data, and developing prediction and assessment methods that are able to handle an ever-increasing complexity. It is clear that digitalization needs to become an important driver to overcome these challenges, adopting big data management approaches for structuring, curating, and preparing data, as well as AI- and machine learning-based approaches for processing data, filling-in data gaps, and producing input for relevant decision-support tools at the chemicals-environment-health nexus. Initial efforts focus on, for example, using such approaches for aiding the optimization of chemical synthesis and material manufacturing processes.[81–83] However, the need for radically increasing the use of digitalized chemicals management encompasses the entire value chain of the chemical industry (Figure 3), where different data and methods apply to each specific value chain segment

Table 1. Current challenges in sustainability assessments of chemicals across various fields of chemistry and possible application of digitalization approaches to overcome these challenges

Challenges in sustainability assessments of chemicals	Key limitations of existing data and approaches for sustainability assessments	Potential solutions to address the challenges
Process and supply chain levels: life cycle inventories		
Data gaps	Although the use of primary process data of a chemical production in environmental assessment is preferable, in reality, access to process data is very limited, owing to the fear of loss of commercial advantage or reputation.	Digital infrastructure for information and data management. The use of link-prediction estimation of incomplete data for new chemical processes.[84] The use of streamlined process simulation to estimate energy consumption of chemical manufacturing.[85] Changes in business models promoting data exchange.
Poor data quality	In the absence or high-quality process data, prediction methods based on molecular structures and thermodynamic properties are used[86,87]; these methods do not distinguish between different chemical production pathways and often suffer from poor extrapolation ability.	New, more accurate machine learning models for properties predictions.[88] Combining molecular and process descriptors in prediction models.[89]
Limited spatiotemporal resolution	Current data on feedstocks production are very patchy and difficult to obtain.	Creation of spatially resolved feedstock production databases.
Unconsidered chemical supply chain processes	Assessment of product and system life cycle performance usually does not consider the complexity and all relevant chemical synthesis and supply chain processes, such as emissions and related impacts from catalysts production.[90,91]	Transparency of supply chain through well-labeled process data, prices, and chemicals availability data. Efficient search of data using knowledge-graph technology.[92]
Chemical-related human and environmental health impacts		
Data gaps	Many existing methods, including life cycle impact assessment (LCIA), face data gaps yielding incomplete assessments (e.g., chemical content in products, dermal exposure, cancer effects, ecotoxicity effects for some species groups or environments, and general data from vulnerable locations, such as the Global South, where most end-of-life processes currently take place).	Imputation or other approaches (e.g., read across) for systematic data gap filling; regulatory framework for completeness of product data. Incentives for data collection in all locations impacted by chemical, material, and product life cycles, including vulnerable locations in the Global South.
Poor data quality	Many existing approaches use data of inconsistent, poor, or non-determined data quality (e.g., data on biodegradation, ecotoxicity, and human toxicity); several QSAR and extrapolation methods have a very limited data applicability domain (e.g., restricted to selected substance classes).	Systematic approaches for semi-automated data curation and quality assessment.[93]
Limited spatiotemporal resolution	Most current approaches do not consider a sufficiently high and flexible level of spatial and/or temporal resolution and/or inter-individual heterogeneity (e.g., for human exposure, consumer product applications, effect vulnerability, emission patterns).	Flexible digitalization approaches accounting for a sufficient level of spatiotemporal and inter-individual detail.[94,95]
Poor prediction models	Many prediction models use themselves input data that are (at least partly) predicted or otherwise estimated, and do not account for interactions across input parameters or strong non-linearities (e.g., predicting chemical function and concentration as function of product application, such as phthalates that are used as plasticizers in plastics but as solvents in cosmetics, non-linearities in phase partitioning in multilayer materials, saturation effects in bioaccumulation processes).	Prediction approaches that consider the right level of (input data) complexity, accounting for non-linearities and interdependencies.[96–101]
Oversimplified extrapolation models	Existing extrapolation approaches are often based on limited training data and various untested assumptions e.g., across effects or exposure routes, e.g., inhalation versus oral exposure or multi-species ecosystem exposure.	Collection of new and consistent integration with various existing and emerging data (e.g., from human and environmental biomonitoring), and training of machine learning models using more complex datasets.[102]

(*Continued on next page*)

Table 1. *Continued*

Challenges in sustainability assessments of chemicals	Key limitations of existing data and approaches for sustainability assessments	Potential solutions to address the challenges
Difficult-to-characterize chemicals	High complexity when addressing "difficult" chemicals, e.g., partitioning for per- and polyfluoroalkyl substances (PFAS) and siloxanes or transformation kinetics for inorganic substances.	Digitalization-based methods that consider the intrinsic complexity of reaction pathways in different environments[103] and chemical group-specific kinetics and environmental fate and degradation dynamics.[104]
Environmental systems level: Biome and biosphere; biotic regulation of the environment		
Lack of considering interdependency	Lack of ecosystem- and location-specific information to address chemical mixture-ecosystem interactions and interactions with chemical background levels, local species distributions, and high level of interdependencies in molecular properties, water chemistry, ecological species abundance for ecotoxicity.	Cross-disciplinary ontologies and data exchange frameworks to allow modeling interdependency across disciplines, as well as multi-stressor pressure prediction method that consider local environment and ecosystem conditions.[105]
Missing link between chemical pressure on ecosystems and ecological capacities for chemical pollution	Current attempts fail to account for spatiotemporal granularity of chemical fate, eco-exposure, and effects, to define local-to-regional ecosystem sensitivity for different chemical effects, and to translate species-level effects into damage on ecosystem integrity. The lack of data on dynamics of interaction of technogenic fluxes and natural fluxes that contribute to biotic regulation of the environment.	Absolute environmental sustainability approaches are needed that allow linking chemical pressure to ecosystem capacity for diluting chemical pollution, thereby considering spatiotemporal interactions between chemicals, ecosystems and environmental conditions.[106,107] Increased use of Earth satellite observation (sensors and images) and open data.[108]
Socio-economic-sustainability level		
Data gaps	True economic and social costs of loss of biodiversity and of climate change (i.e., including externalities). Only few, limited attempts have been made to quantify such impacts and costs of climate change and biodiversity loss.[109]	Advanced data science techniques for identifying emerging trends in "values," "ethics" and "wellbeing," which would inform cost formation and sustainability-driven evolution of economic concepts.
Methodological gaps	The current growth model is outdated, hinders the adoption of new, clean technologies, and is not compatible with the emerging and sustainability-conscious trends in the younger population. However, there is no accepted alternative model and no broadly accepted methods for incorporating social and economic trends into sustainability assessments.	New models based on considering complex systems dynamics, which would help to set and monitor global and regional priorities, and consistently and quantitatively integrating environmental, social, and economic-sustainability aspects.

to address distinct yet often systemic and complex aspects (Table 1). In the previous section, we have already provided examples of successful early implementation of digital technologies in different sectors across all fields of chemistry, from chemical synthesis and materials chemistry to pharmacology and environmental chemistry. Access to information enabled by digitalization will automatically enable breaking out of compromises within the complex chemicals-environment-health nexus that today, almost invariably, lead to negative consequences for the environment.

CONCLUSIONS AND PERSPECTIVE

The global goal to minimize adverse impacts of chemicals and waste was not achieved by 2020.[57] Going forward, digitalization is a key enabler of sustainable development within the chemical industry and chemistry R&D. The chemical industry must undergo a significant systemic-level transformation, and digitalization is an essential tool to support this evolution. Digitalization of chemistry and materials R&D will facilitate the access and interlinkage of data and knowledge, which are crucial for transforming chemistry from the subject of an elite, to the subject accessible to many more talented individuals and organizations. This requires rapid development of standards for chemical data and knowledge models, as well as the adoption of scalable infrastructure for data sharing and sustainability assessments.

Digitalization of chemical supply chains and chemical manufacturing is shown to lead to increased understanding and the potential for business innovation, which are necessary for transforming the current industry to a much more sustainable model. This also depends predominantly on the availability of data sharing and knowledge-management infrastructure. The emerging tools of digital identification of intellectual property rights and managed data privacy in the digital space are already being demonstrated in other sectors.

A significant change is required in the organization of chemistry R&D, facilitating the development of open collaboration between multiple science and technology areas, academia, private and public institutions, crossing geographical or geopolitical boundaries and including the Global South. Digitalization of research partnering, access to open data and digital experimental facilities globally, and an increased, sustainability- and circularity-driven assessment capacity promise a revolution in the speed of chemistry R&D and the possibility to pose research questions worthy of the challenge of developing a sustainable global society.

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