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The Role of AI in Driving the Sustainability of the Chemical Industry

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Abstract: Sustainability is here to stay. As businesses migrate away from fossil fuels and toward renewable sources, chemistry will play a crucial role in bringing the economy to a point of net-zero emissions. In fact, chemistry has always been at the forefront of developing new or enhanced materials to fulfill societal demands, resulting in goods with appropriate physical or chemical qualities. Today, the main focus is on developing goods and materials that have a less negative impact on the environment, which may include (but is not limited to) leaving behind smaller carbon footprints. Integrating data and AI can speed up the discovery of new eco-friendly materials, predict environmental impact factors for early assessment of new technological integration, enhance plant design and management, and optimize processes to reduce costs and improve efficiency, all of which contribute to a more rapid transition to a sustainable system. In this perspective, we hint at how AI technologies have been employed so far first, at estimating sustainability metrics and second, at designing more sustainable chemical processes.

Keywords: Artificial intelligence · Chemical industry · LCA · Sustainability

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1.Introduction

1.1 *A Broader View*

Specific definitions of sustainability are difficult to agree on. In 1987, the United Nations released their final report, *Our Common Future*,[1] that famously defines sustainable development as "development that meets the needs of the present without compromising the ability of future generations to meet their own needs". Practically, they realized that economic development at the cost of social equity and ecological health was not building a prosperous long-lasting future. 'Harmonization' was, and is, the watchword. Sustainability is based on three major pillars: the environment, the economy, and the society.[2,3] Environmental sustainability aims at building a society where all earth's ecological systems are kept in balance, natural resources are replenished, even if consumed. The economic pillar on the other hand, focuses on the independence of the communities and on the ability they have to access the resources that they need. This is strictly linked to societal sustainability where the ultimate goal is to dismantle any form of discrimination and make fundamental human rights and basic necessities accessible to everyone. Even though there are a lot of people who think that the environmental pillar ought to be the most essential one,[4,5] it is impossible for it to be successful without the development of the other two. For this reason, the adoption of environmentally sustainable practices should always take into account the societal and economic consequences, making sure that the other pillars are not penalized in the process.

1.2 *Chemical Industry, a Main Player in Sustainability*

First and foremost, sustainability presents the chemical sector with a window of opportunity for new product development and expansion. Because it is one of the industries that is significantly involved in the use of energy as well as the substantial use of fossil fuels as raw materials, the chemical industry accounts for 10% of the global energy demand and is therefore one of the largest

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emitters on the planet.[6] Most importantly, the chemical sector is currently unable to meet the targets established by downstream industries. In the future, a crucial difference will be a company's leadership in cutting-edge innovations, such as those related to recycling or biomaterials. Instead of pushing innovation in the absence of obvious market demands, the use of technologies that enable businesses to anticipate and meet their consumers' evolving demands will provide a competitive advantage. In this journey, the chemical sector needs strong allies in order to keep up with the constantly shifting standards for environmental sustainability. What was considered to be sustainable development fifty years ago is not considered to be sustainable development today, and the rate at which new solutions are required has reached an all-time high. Effectively promoting research and innovation has emerged as one of societal major priorities.[7,8] The timeframe for a game-changing material/catalyst discovery process, from concept to market, can take up to a few decades,[9] which cannot be afforded in a sustainability-focused world. In the field of research, the scientific method is the golden standard to drive innovation.[10] However, it often follows a straight and segregated process, which means that the lab chemist, the theoretical and computational researcher, the industrial engineer, and lastly the government authorities, seldom communicate during the process. Closing the loop only at the end leads inevitably to bottlenecks and delays. The successful development of new chemicals, though, is only half the battle. There is a need for well-defined metrics, real-time monitoring of chemical production and finally dynamic analysis and responses to lessen the severity of unforeseen events. As well as methods for constant improvement and adaptation of the processes in response to changes in demand and legislation.

1.3 *AI as a Driver for Sustainability*

The leveraging of the unprecedented volume of data that chemical industries produced over the course of the last few decades poses a considerable challenge. AI is a key enabling technology in the journey toward sustainability. Nonetheless, AI has seen only a modest uptake in the chemical sector. Limitations to widespread AI adoption stem primarily from a scarcity of quantitative tools for gauging the true benefit in terms of sustainability metrics. The task is complicated by the blurriness of these metrics, with no comprehensive set of quantitative sustainability indicators available at the time of this publication.

As a consequence, research on AI has focused more on technical advancements[11] with only few studies clearly reporting the impact of the technology in terms of sustainability indicators (from economical, to environmental and societal). If a chemical company wants to successfully transition from the traditional process industry to the AI-based one, it will need a clear road-map outlining how various factors of sustainability will be affected by various types of AI technology. Liao *et al.*[11] reviewed 63 articles at the interface of the chemical industry and artificial intelligence in an effort to identify methods that facilitate the assessment of how the adoption of a particular AI technology affects various aspects/indicators of sustainability.

In light of their findings, we will begin by discussing how AI has recently been applied to quantify and measure the sustainability of chemical processes. And secondly, we will present recent advances in AI technologies for the design of chemical processes with the primary objective of being environmentally friendly.

We conclude with few considerations on the *sustainability of AI*, a topic that is vastly undervalued in comparison to *AI for sustainability*.[12]

2. AI to Measure Sustainability of Chemical Processes

Sustainability metrics were built on top of the 12 Green Chemistry (GC) principles[13] and today are gaining increased attention,[14] with the broader community constantly improving the processes' evaluation criteria.[15–17] However, these metrics tended to concentrate solely on the used materials or on their chemical processing while ignoring the wider context of their entire life cycle. In addition, in GC economic considerations are rarely addressed and societal issues often neglected.[17] Derbenev *et al.*[18] provide an overview of these case-specific metrics and of the tools available for their calculations.[19–21] Some of the approaches presented are AI-based like structure-to-yield predictors or greener solvents selection. However, sustainability metrics arise as more comprehensive and holistic metrics to measure concurrently economical, environmental and societal impacts going beyond the calculation of quantities like, for example, process mass efficiency (PME).[15,17] Liao *et al.*[11] complied an extensive list of methods that can be used to quantify indicators for sustainability goals, divided by impact category. We will elaborate on key approaches, where we believe recent developments in AI could be the most impactful: indicators estimations such as Life Cycle Assessment (LCA), Material Flow Analysis (MFA), Techno-Economic Analysis (TEA) and energy & exergy analysis.

2.1 *LCA*

An integral part of designing a chemical process is the evaluation of its impact on the health and environment. The evaluation of a product's inputs and outputs of energy and materials as well as the environmental impact caused by its production throughout its entire life cycle is referred to as a life cycle assessment (LCA). It is a crucial framework that provides insights into upstream and downstream trade-offs associated with environmental pressures and consumption of natural resources and energy, allowing us to evaluate and reduce the overall environmental burden of a chemical process. Comprehensive studies of how LCAs can be beneficial can be found in literature.[22–25] Often one of the limitations of LCA is the availability of information on all the chemicals (Life Cycle Inventory - LCI). To this end, AI can facilitate LCAs even with limited data from LCIs. In fact, AI models can be utilized to extrapolate unknown impact factors of chemicals such as, but not limited to, global warming *IPCC 2007*,[26] acidification *TRACI*,[27] human health *Impact 2000+*,[28] ecosystem quality *Impact 2000+*,[28] *Ecoindicator99* (*I and total*).[29] Through the use of LCA, Zhu *et al.*[30] were able to determine that the feedstock used in the production of sitagliptin is responsible for up to 80 percent of the life cycle impact. They used a dataset of 224 chemicals to train a neural network to learn to predict LCA impact categories *Ecoindicator99* and *ReCiP*. They investigated a variety of alternative feedstock choices and discovered a new environmentally friendly route. A similar approach was used by Song *et al.*,[31] where they trained a neural network to predict the life-cycle impacts of 166 chemicals according to six impact categories. Their studies concluded that these models are useful to estimate the impact of chemicals in absence of more reliable data sources. Calvo-Serrano *et al.*[32] focused on predicting the cradle-to-gate life cycle production impact of 88 organic chemicals by means of mixed-integer programming methods successfully. They used a combination of molecular descriptors and thermodynamic properties to represent the organic molecule and predicted nine impact categories. In a second publication, Calvo-Serrano *et al.*[33] built mathematical models to represent the LCA impact of chemicals based on a network representation of the petrochemical industry which allows them not to rely on fixed mass and energy flows. Finally, Liao *et al.*[34] developed LCA for activated carbon from diverse biomasses, combining process simulations with ANN (artificial neural networks).

All these above-mentioned approaches and many more[11,35,36] mainly rely on simple machine learning architectures and do not take advantage of newer deep-learning models, since for the training of more complex neural networks often larger data sets are required.[37,38] No literature to date was found where deep-learning models were employed. In view of the recent advancement on ChatGPT[39] and the relevance of language models in capturing chemical knowledge[40–42] we foresee that new datasets can be extracted from existing literature, with the main goal of improving sustainability metrics thanks to state-of-the-art AI models. These new AI models would be able to quickly evaluate LCA impact categories over a broad spectrum of chemicals and processes and could be a key tool to convince the earlier adoption of LCA at the stage of designing a new chemical process.

2.2 *MFA*

Achieving a circular economy in production is one of the most important steps that must be taken in order to successfully make the chemical industry more sustainable. For instance, a byproduct of one process can be used as feedstock in another process. Material flow analysis has become increasingly popular as a means of tracking the flow of materials throughout a process and of locating and quantifying the points at which material flows are produced, reused, consumed, and lost.[43] The MFA spans from the individual chemical process, to broader economic impacts[44] or even planetary considerations.[45–47] We foresee great potential in the combination of MFA and AI. One example is teaching an AI system to predict the combined effects of two different chemical pathways into a final product within the boundaries of the system. If, for example, the first alternative produces fewer byproducts than the second, but the second alternative's byproducts can be used as feedstock in another process, then AI could learn to recommend the second option.[48]

2.3 *TEA*

The term techno-economic analysis, or TEA, refers to a method that combines the operational costs, capital costs, and economic costs of, for instance, equipment sizing. This method is used to quantify the economic sustainability of processes. There is already some application of artificial intelligence in this area, such as assisting with the sizing of distillation columns[49] and the cost of the energy[50] they use.

By optimizing complex chemical processes like the production of ethylene, AI has also assisted in lowering operational costs and the carbon footprint.[51] In some cases, the greatest challenge is finding a single set of operating parameters for a chemical process that simultaneously maximizes profit and minimizes environmental impact. Schweidtmann *et al.*[52] presented a multi objective optimization strategy to balance these two factors (space time yield vs E-factor or % impurity) which allowed to find improved operating conditions for the nucleophilic aromatic substitution reaction.

2.4 *Energy and Exergy Analysis*

If a system is brought to its reversible equilibrium with its environment the maximum amount of useful work that can be extracted from this system is called exergy. Exergy destruction corresponds to a degradation of both energy and material in a system.[53] Lowering the energy, respectively exergy, consumption of a chemical process also improves its environmental and economical sustainability. Therefore, it is a vital indicator of sustainability and an opportunity for AI contributions. Because calculations of exergy are dependent on thermodynamic information for the molecules involved in the chemical process of interest, artificial intelligence already demonstrated its value directly predicting exergy values for a series of applications.[54–56]

3. How AI Has Been Used to Improve Sustainability of Chemical Processes

While on one hand AI can be used to conduct a purely analytical evaluation of the viability of a chemical process, on the other, it can be utilized to directly optimize that process. Even if literature is scarce, we attempt to present few works where any of the sustainability indicators have been estimated before and after the adoption of AI. We split the review into two different categories: (1) research and development (2) production.

3.1 *R&D*

Research and Development (R&D) is thriving in the chemical industry, focusing on the discovery and development of new chemical reactions or new catalytic species in a variety of applications. However, the long-term effects of integrating AI into R&D procedures are largely unexplored at this time.

In a general discovery pipeline, a few investigated chemicals are chosen as candidates for the solution of a specific challenge in a target application (*e.g.* catalyzing a chemical process with enzymes). These compounds are then tested and analyzed. The process is iterated until suitable species are identified which satisfy a figure of merit (*e.g.* reaction yield), often limited to the research scenario.

While several R&D teams apply ML and AI to improve the discovery process,[57–61] none perform their analysis to directly optimize sustainability metrics, and few compare their value to the AI-free approach. Few works focus their optimization based on sustainability indicators. AI is known to reduce time for the design, experiment, and computation, which can indirectly reduce environmental impact and costs. However, time reduction is rarely quantified in detail. In the field of heterogeneous catalysis funded by the NCCR catalysis Suvarna *et al.*[62] focused on the development of an ML model which predicts the space–time yield of 1425 catalysts (an indicator of process and material efficiency), extracted from literature, involved in the methanol synthesis from CO_2 hydrogenation. However, they do not recommend an alternative catalyst with a promising space-time yield increase. Ten *et al.*[63] implement a computer-aided molecular design framework where the selected molecules are optimized for desirable properties and at the same time meet the safety and health criteria. They conducted a case study in order to determine the most effective molecule to use as a solvent in the process of removing hydrogen sulfides, carbon dioxide, and mercaptans from natural gas in order to make it suitable for transport and sale. However, in order to evaluate the molecular performance, they make use of standard predictive models (the Group Contribution Method), and they only integrate safety and health considerations during the performance analysis stage and not during the design stage. Angello *et al.*[64] report a simple closed-loop workflow to discover general reaction conditions for the heteroaryl Suzuki-Miyaura cross-coupling. They identified conditions that double the average yield with respect to the reference approach. Polykovskiy *et al.*[65] developed a framework based on conditional adversarial autoencoders to generate a novel inhibitor of Janus kinase 3, implicated in rheumatoid arthritis, psoriasis, and vitiligo. Their method optimizes for numerous properties, including synthetic accessibility (SA). Even if their AI approach is not directly related to a sustainability indicator, it can be used as a starting point to improve upon more conventional techniques.

3.2 *Production*

If we take a step up from the laboratory (R&D) to the chemical factory (production), we can see that the long-term viability of AI adoption has been more thoroughly evaluated, despite the fact that data-driven technology adoption is still in its infancy. Diverse studies and articles highlight the positive impact of AI at the manufacturing level.[66,67] Maintenance is a key operation for every manufacturing business. It enables the reduction of downtimes and extends the life of the equipment. It ensures higher financial safety for the manufacturing company and has a positive impact on resource management. Predictive maintenance (PdM) has been widely analyzed with AI[68–70] and many deep learning models have been proposed. The central concept is to track operational data and analyze it for signs of equipment failure or degradation based on past experiences and current understanding.[71] Strictly related to PdM is the reliability and safety of the chemical plant. Hanif and Gunawan[72] use random forests to predict catalyst deactivation, a crucial indicator for a maintenance schedule, based on actual data from relevant multitube-reactor sensors. Their approach leads to increased quality assurance, again with a positive impact on downtimes and costs. Another example is provided by Bao *et al*.,[73] which proposes a classification model based on RNNs to identify abnormal conditions, for the Tennessee Eastmann process (TE).

AI can also bring benefits to process optimization, which we refer to as the set of techniques to increase production, improve quality and, reduce energy/costs.[74] Golkarnarenji *et al*.[75] used heuristic algorithms to optimize the energy consumption of a carbon fiber production line, reaching an optimized scenario where energy was reduced by 40%. Most recent advances in process optimization and control have been done through the use of reinforcement learning (RL).[76,77] Examples are distillation columns, pumps, and polymerization processes.[71] A challenge is surely the necessity of many experiments to achieve good performance, which in the industrial chemical setting can be limited or even prohibited for quality and safety reasons. Model-based RL with the use of hybrid approaches combining AI and first-principles models, together with the use of historical data, can be the way forward. Another important point in plant management is the planning and scheduling of production, known as the supply chain. Here AI can be employed in predicting future trends and consequently optimize supplies. Here as well RL has demonstrated success for solving planning and scheduling problems. A deep RL-based agent has been applied to automatically make scheduling decisions for a continuous chemical reactor.[78]

4. A Note on Sustainable AI

While fascinating and powerful, AI itself is a technology for which we cannot afford to ignore environmental costs. Alongside reporting the improved values in the sustainability metrics after AI adoption, the environmental impact of the use of the AI IT infrastructure needs to be evaluated. van Wynsberghe[12] highlights in his perspective article how the use of AI embodies the tension between two complementary worlds: the first of AI for sustainability, where the focus is on innovation to reach sustainable development goals,[3] and the second, the sustainability of AI, more focused on the use of sustainable data sources, power supplies, and infrastructures. The author underlines how addressing the sustainability of AI is the third step in the ethical analysis of AI, which has gone from science fiction concerns about robots uprising, to practical issues of algorithms (*e.g.* the problems of explainability,[79,80] biases[81] and privacy[82]). Sustainable AI ought to address the entire life cycle of AI from design, training, development, validation, deployment, use and update. A famous study analyzes the carbon dioxide emissions in training a deep-learning model.[83] In the future, scientists need to account for the environmental impact of the development and use of AI. TURINTECH[84] developed evoML, an optimization platform where metrics related to the development and use of AI models, such as carbon emission and electricity consumption, can be optimized alongside performance metrics such as accuracy and precision. They also provide a way for code optimization which can increase the efficiency by over 50% without compromising accuracy. Far from being exhaustive on this discussion, we leave the AI practitioners with two other tools available for calculating emissions[85,86] as well as recent literature on this important and overlooked topic.[87–91]

5. Conclusions

AI is a promising sustainability driver to mutate the chemical industry. However, its wide adoption is somehow delayed by the lack of data and, therefore, examples that help understand and quantify its impact. In this brief perspective we tried to hint at the examples on how AI as been employed so far to either measure sustainability or improve sustainability of chemical processes. We foresee that more recent advances in the field of AI (deep learning) will facilitate, with renewed vigor, the transition to more sustainable practices. And the more examples will be generated, the more trust will be created in the adoption of these technologies, enabling the chemical industry to match the ambitious goals of the long-term EU strategy for the year 2050.

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