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Yaghoubi, Vahid; Kumru, Baris

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Retrosynthetic Life Cycle Assessment: A Short Perspective on the Sustainability of Integrating Thermoplastics and Artificial Intelligence Into Composite Systems

Vahid Yaghoubi and Baris Kumru**

Over the past 30 years, the polymer composite industry has flourished, producing advanced structural materials for the aviation, energy, and transportation sectors. However, the use of crosslinked thermoset matrices has been linked to significant end-of-life challenges, presenting a critical issue for the industry. Moreover, the industry is characterized by numerous labor-intensive processes. In alignment with Industry 4.0 principles, two major routes have been identified to enhance sustainability: the utilization of high-performance thermoplastic matrices and the integration of artificial intelligence in manufacturing. Nevertheless, there are substantial concerns regarding the life cycle assessment of these technologies, which are not accounted for in the initial calculations, including the environmental footprint of polymer synthesis and energy requirements for training AI. This perspective aims to address potential and significant CO_2 emissions from chemical feedstocks and the high computing requirements of these new technologies.

1. Introduction

Polymers are important class of materials being utilized in various objects and engineering materials across diverse scales. Performance of bare polymers can be boosted when composite systems are designed, which offers attractive thermomechanical properties to be employed for transportation and energy industry.[1] Fibre reinforced polymer composites (FRPC) serve this purpose, which is generated by merging polymer matrix with continuous fibre systems (i.e., carbon, glass).[2] Carbon, glass and aramid fibres offer high thermal stability, low density and high mechanical performance ideal for structural applications, whereas biobased fibres such as flax and bamboo are suited for secondary structures.[3] Polymer matrices are classified based on the nature of crosslinking, and crosslinked thermoset matrices are dominant choices in structural parts (i.e., aircraft wings and fuselage, wind turbine blades) in industry.[4] Thermosetting resins such as epoxy and cyanate esters are employed for this aim.[5] For thermoset composite formation, monomers are impregnated into fibres and cured to afford thermosetting composites since thermosets are not processable after curing.[6] It is important to mention that there are serious developments on vitrimer matrices (resins with dynamic reversible crosslinking behavior, some commercial vitrimeric hardeners such as Recyclamine and Vitrimax), however it currently takes no part in industrial systems.[7]

It is inevitable that for such a big market with high production volumes, sustainability metrics play a vital role for circular development of composite industry.[8] Thermoset composites face serious circularity problems despite great performances, mainly due to crosslinked resin which prevents reformability and recyclability.[9] Hence, fibre-matrix separation is not possible therefore composite waste is a serious concern in society today despite advancements on pyrolysis, solvolysis and mechanical recycling.[10] The production process of fibers and matrix constituents in the industry is a matter of concern when evaluating sustainability standards. These processes often demand the consumption of substantial amounts of energy and involve the use of toxic chemicals. Additionally, curing prepregs requires the maintenance of high temperatures. These aspects collectively represent a significant challenge, as they do not align with the principles of sustainability. In addition to landfill, losing such valuable materials at the end of life possesses a serious loss. Although the industry is highly skilled in thermoset composite manufacturing and joining over few decades, non-repairability and non-recyclability resulted in a search for alternative matrices. Thermoplastic polymers (TP) are non-crosslinked plastics which can bear amorphous or semicrystalline structure.[11] TPs are vastly abundant in daily life in non-composite form and address diverse range of applications.[12] Introducing TP as matrix to composite structures offer advantages of remoldability, repairability and recyclability which can not be achieved by thermosetting resins.[13] Additionally, joining techniques of thermoplastic composites (i.e., welding) enable lightweight solution compared to riveting.[14] TP composites are being used

V. Yaghoubi, B. Kumru
Aerospace Structures & Materials Department
Faculty of Aerospace Engineering
Delft University of Technology
Delft 2629 HS, The Netherlands
E-mail: v.yaghoubi@tudelft.nl; b.kumru@tudelft.nl

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in many sectors employing TPs such as polyamides, poly(lactic acid), polyacrylates and polypropylene using various manufacturing methods.[15] On a molecular scale, thermomechanical performance of a resin can be translated into chemical structure of starting products, so that highly aromatic systems are affiliated to improved thermomechanical properties compared to aliphatic systems.[16] Therefore, when higher thermomechanical properties are strived, high-performance thermoplastics are chosen.[17] Polymers such as poly(phenylene sulfide) (PPS), polyether sulfone (PES), poly(ethylene imide) (PEI), polyether ether ketone (PEEK) and polyaryl ether ketone (PAEK) are promising candidates for structural applications and notable amount of research, funding and products based on such composites are being developed.

The integration of artificial intelligence (AI) into composite manufacturing is anticipated to revolutionize this field in the coming years. AI offers unparalleled capabilities in the design and optimization of manufacturing processes and structural configurations. These advanced technologies have the potential to significantly reduce waste, thereby enhancing efficiency and sustainability. The application of AI in this domain ranges from predictive maintenance of manufacturing equipment to the optimization of material usage and minimization of defects during production. Such improvements not only contribute to cost savings but also reduce the environmental footprint of manufacturing operations.

On the other hand, a prevailing trend in AI development poses a big challenge to these sustainability gains. The current trajectory in AI research and application is towards the creation of increasingly large and complex models.[18] These models, while offering higher accuracy and improved predictions, come with a steep environmental cost. The computational power required to train, test, and run these large-scale AI models leads to substantial energy consumption. Consequently, this results in a significant carbon footprint, potentially offsetting the sustainability benefits that these technologies aim to achieve.

In this insightful perspective article, we delve into an alternative examination of the use of high-performance thermoplastics and artificial intelligence (AI) in manufacturing, with a specific focus on sustainability. These two technological frontiers are redefining the landscape of the composite industry by presenting unprecedented opportunities for sustainable operations. However, it is imperative to highlight several crucial aspects that warrant attention. Firstly, while high-performance thermoplastics offer a promising pathway towards more sustainable materials, their production processes and life cycle impacts need thorough evaluation. The intricate balance between their advanced properties and the environmental footprint of their synthesis is a critical consideration for true sustainability.

Secondly, the integration of AI in manufacturing processes represents a groundbreaking advancement. AI has the potential to optimize production efficiency, reduce waste, and enhance the lifecycle performance of composite materials. However, the environmental impact of developing and running these sophisticated AI systems, including their energy consumption and the resources required for their operation, must be critically assessed. This perspective aims to provide a comprehensive understanding of these technologies not just as isolated advancements but as part of a larger ecosystem where their sustainability implications are deeply intertwined with their operational benefits. By doing so, it underscores the importance of a holistic approach in evaluating technological innovations in the composite industry, ensuring that the pursuit of sustainability remains at the forefront of these developments.

1.1. High Performance Thermoplastics and Sustainability

High-performance TP are increasingly recognized for their myriad advantages over traditional thermoset matrices, particularly in terms of their impact on the life cycle assessment (LCA). These advanced materials offer a suite of benefits crucial for sustainable and efficient manufacturing. Notably, their potential for welding to join layers represents a significant advancement, potentially eliminating the need for riveting and thereby achieving considerable weight reduction.[19] This is complemented by their reformability, repairability, and exceptional chemical and aqueous stability, culminating in enhanced recyclability.[20] In contrast to thermoset prepregs, which are characterized by high reactivity and necessitate cold-temperature transportation to inhibit curing, thermoplastic prepregs exhibit remarkable stability with an almost infinite shelf life.[21] This stability significantly simplifies logistics and storage, presenting a more practical solution for manufacturing processes.

Furthermore, the adaptability of high-performance thermoplastics to additive manufacturing methods opens avenues for fabricating complex and precise geometries.[22] Such technological adaptability is critical in advancing manufacturing capabilities across various sectors, including aerospace, automotive, and energy. However, it is crucial to acknowledge the inherent challenges posed by the physical properties of high-performance thermoplastics. Their high melting points and viscosities can introduce complications in impregnation processes, presenting a technical hurdle that requires addressing.[23] This underscores the necessity for ongoing research and innovation in processing techniques to fully harness the potential of these cutting-edge materials.

The field of composite materials is witnessing a pivotal shift, with the LCA of thermoplastic composites gaining increasing prominence in recent years. This burgeoning interest is a testament to the potential of high-performance TP in structural composite systems, challenging the long-standing dominance of thermoset systems. A thorough review of the literature reveals a common trend: the LCA of thermoplastic composites typically commences from the manufacturing phase of the composite. This approach predominantly focuses on quantifying and comparing the energy requirements and CO_2 emissions associated with the manufacturing processes of thermoset versus thermoplastic composites.[24]

Furthermore, extensive investigations delve into the potential recycling pathways, the energy demands of these processes, the value of the output products, and their cumulative effect on the environment.[25] Such studies are integral in painting a comprehensive picture of the sustainability of these materials. However, we contend that there exists a critical oversight in the current methodology for performing the LCA of high-performance thermoplastic composites. The significant impact of the chemical feedstocks and the processes involved in synthesizing these

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polymers are often underrepresented in LCA evaluations.[26] This gap in analysis represents a substantial limitation, as it overlooks a crucial element in the lifecycle of these materials. The chemical synthesis stage, with its inherent energy consumption and potential environmental impacts, is a pivotal factor that warrants serious consideration.

Recent article by Beckham and colleagues elucidated the impact of chemical feedstock and supply chain energy requirements of commodity polymers on total calculated energy demands.[27] Shockingly, but expected from chemistry point of view, generation of starting products from petrorefinery and synthetic procedures to manufacture polymers (i.e., catalyst, heat) have impressive effect on LCA, which is normally hidden in general calculations. As an example, calculations on energy requirement increase 3 times when chemical feedstock input is considered, which is brutal.

In the realm of sustainable composites, high-performance thermoplastics (TP) such as Polyether Ether Ketone (PEEK) and Polyphenylene Sulfide (PPS) stand out as particularly noteworthy matrices. The fabrication of these polymers presents a fascinating area of study, especially considering their potential impact on the Life Cycle Assessment (LCA) of thermoplastic composites when the chemistry involved is accounted for in LCA calculations. Adopting a bottom-up approach to assess the potential impacts of polymer synthesis conditions and monomers is essential to gain a more comprehensive understanding of thermoplastic matrices.

Given the complexities involved in obtaining accurate LCA data for such polymer production, we advocate the use of a *"retrosynthetic LCA"* methodology. This approach involves a reverse engineering process of a polymer. To effectively implement this method, one must first identify the monomers composing the polymer, followed by an exploration of their synthesis starting from petrorefinery products, if feasible. Acknowledging that each step in this process requires energy (and potentially catalysts) for chemical conversion, as well as various separation and purification steps, and energy for processing polymers into forms such as films or pellets, the focus should be on the impact of the base molecules themselves. It's also crucial to note that current commercial synthetic routes, which may employ different solvents and conditions, could vary slightly. This variability necessitates consideration of conversion rates and mole reactivities in the retrosynthetic LCA. Additionally, chemical hazard symbols offer valuable insights into the toxicity of the molecules used in these processes.

To illustrate this concept, we present two potential examples focusing on PEEK and PPS. These examples are designed to provide a clearer understanding of the retrosynthetic LCA approach and its implications for evaluating the sustainability of high-performance thermoplastics. This approach underscores the importance of a thorough and nuanced analysis of polymer production processes in assessing the environmental impact of thermoplastic composites (**Scheme 1**).

Example approach on PEEK

PEEK is manufactured from a polycondensation reaction of monomers 4,4′-Difluorobenzophenone and disodium salt of hydroquinone at high temperatures (above 250 °C) using diphenyl sulfone solvent (**Scheme 2**). This reaction is known with high conversion affording polymer and sodium fluoride byproduct. In the second step, we identify how monomers are manufactured. 4,4′-Difluorobenzophenone is made from the reaction of fluorobenzene and p-fluorobenzoyl chloride in presence of aluminium chloride catalyst affording hydrochloric acid byproduct. Disodium salt of hydroquinone is prepared by treating hydroquinone in sodium hydroxide solution. One can delve further into the synthesis of fluorobenzene, p-fluorobenzoyl chloride and hydroquinone for further analysis to access LCA of smaller organic molecules. However, it has been already challenging to obtain a commercial synthetic route for p-fluorobenzoyl chloride.

Example approach on PPS

PPS is manufactured from a polycondensation reaction of monomers 1,4-dichlorobenzene and sodium sulfide at high temperatures using N-methyl-2-pyrrolidone solvent (**Scheme 3**). This reaction is known with high conversion affording polymer and sodium chloride byproduct. In the second step, we identify how monomers are manufactured. 1,4-dichlorobenzene is obtained from the reaction of benzene and chlorine in presence of ferric chloride catalyst affording hydrogen chloride byproduct. In this case, one can easily conclude from literature that components benzene, chlorine and 1,4-dichlorobenzene are notoriously toxic. Sodium sulfide is generated from the reduction reaction of sodium sulfate in presence of carbon affording two moles of CO_2 as byproduct. This stage can already generate enough input on potential LCA of sodium sulfide monomer component in PPS polymerization. If not, one can delve further on the production stages of sodium sulfate.

Our analysis reveals critical deficiencies in the LCA of high-performance TP. These deficiencies stem from four key areas: the nature and toxicity of chemical inputs, the intricacies of a global supply chain, the substantial energy demands, and the complexity inherent in the production process. These factors significantly influence the LCA outcomes for high-performance TPs and their monomers, yet they remain largely underrepresented in current assessments.

To rectify this, we propose a refined best practice for LCA calculations of high-performance TP composites. This approach involves incorporating the impacts of material composition at their most fundamental level, focusing on the simplest monomer forms. For example, in the case of PPS, this would mean accounting for the environmental impacts of basic constituents such as benzene, chlorine, sodium sulfate, and carbon. By adopting this methodology, LCA calculations can provide a more accurate and holistic representation of the environmental footprint of high-performance TPs, thereby facilitating more informed and sustainable material choices in various industries.

1.2. Sustainability and Artificial Intelligence

Sustainability and AI can be seen as sustainability with AI, and sustainability in AI. The former is more appreciated and can be interpreted as using AI to optimize, automate or predict different processes in order to achieve sustainability.[28] However, the latter is not that clear and thus is the main focus of this section.

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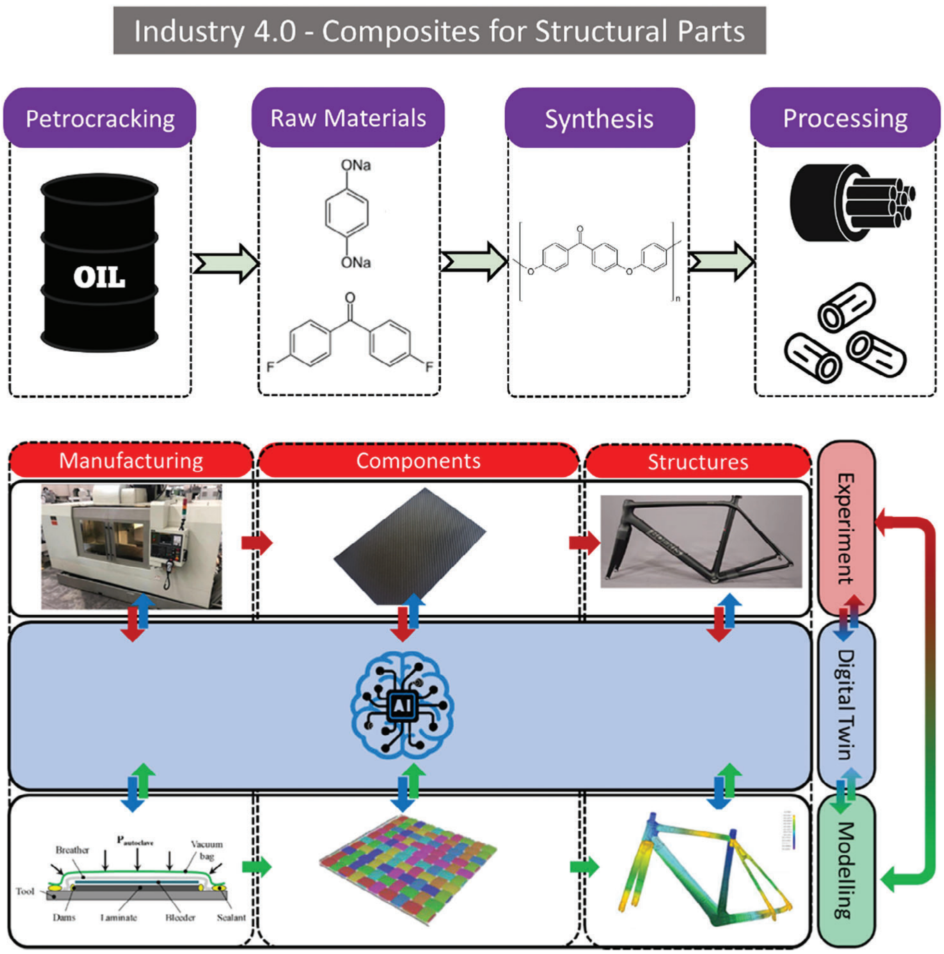

Scheme 1. Retrosynthetic LCA flowchart on high-performance thermoplastic pellet production (PEEK is exemplified) starting from petrocracking, and integration of AI in composite manufacturing.

It should be mentioned that, in this paper, we will focus on the environmental sustainability, although it will have indirect effect on the other two pillars of sustainability, i.e., social and economic.

An in-depth analysis of environmental sustainability in artificial intelligence necessitates a comprehensive evaluation of the entire life cycle of an AI model, which encapsulates three critical stages: data collection and storage, model development, and deployment. A prevailing trend in the field is the development of increasingly complex models, trained on expansive datasets to achieve optimal accuracy. This approach is vividly depicted in **Figure 1**, which chronicles the evolution of model training costs over the past decade. The comparison ranges from AlexNet in 2012, with a training cost of 5.4e-3 petaflop-seconds per day (pfs-day)[1], to the much more advanced GPT-4 in 2023, requiring a staggering 2.4e5 pfs-day. This trajectory highlights the escalating computational demands in AI model training, underscoring the need for substantial resources and raising critical questions about the environmental implications of these technologies (**Figure 2**).

Table 1 indicates that this rise in training cost resulted from the increase in model complexity, from 62.3 M parameters in AlexNet[29] to 170 trillion parameters in GPT-4[30] and will lead to generating large carbon footprint at the model training stage, primarily due to electricity usage for powering computing equipment and cooling systems. For instance, a transformer with 213 million parameters generate about 283.5 tons of CO_2 during training with Neural Architecture search (NAS). This is nearly five times the lifetime emissions of the average American car (including the manufacturing of the car itself).[31] This CO_2 emission increased to 552 tons for training GPT-3.

The advent of Industry 4.0, which is characterized by integrating AI and digital technologies in industrial processes, can potentially exacerbate the environmental impact of AI.[34] For instance, a study shows that the number of IoT devices is expected to reach 75 billion by 2025[35] and they will generate about 217.3 petabytes (PB) of data per day meaning 79.4 ZB in year 2025.[36] This not only indicates the carbon footprint in the data generation and processing stage but also shows the increasing demand for AI models and consequently their environmental footprint.

This highlights the urgent need for responsible and optimized use of AI. It is imperative to develop energy-efficient algorithms and promote the use of renewable energy in data centers.[37] Additionally, research into low-power hardware and quantum

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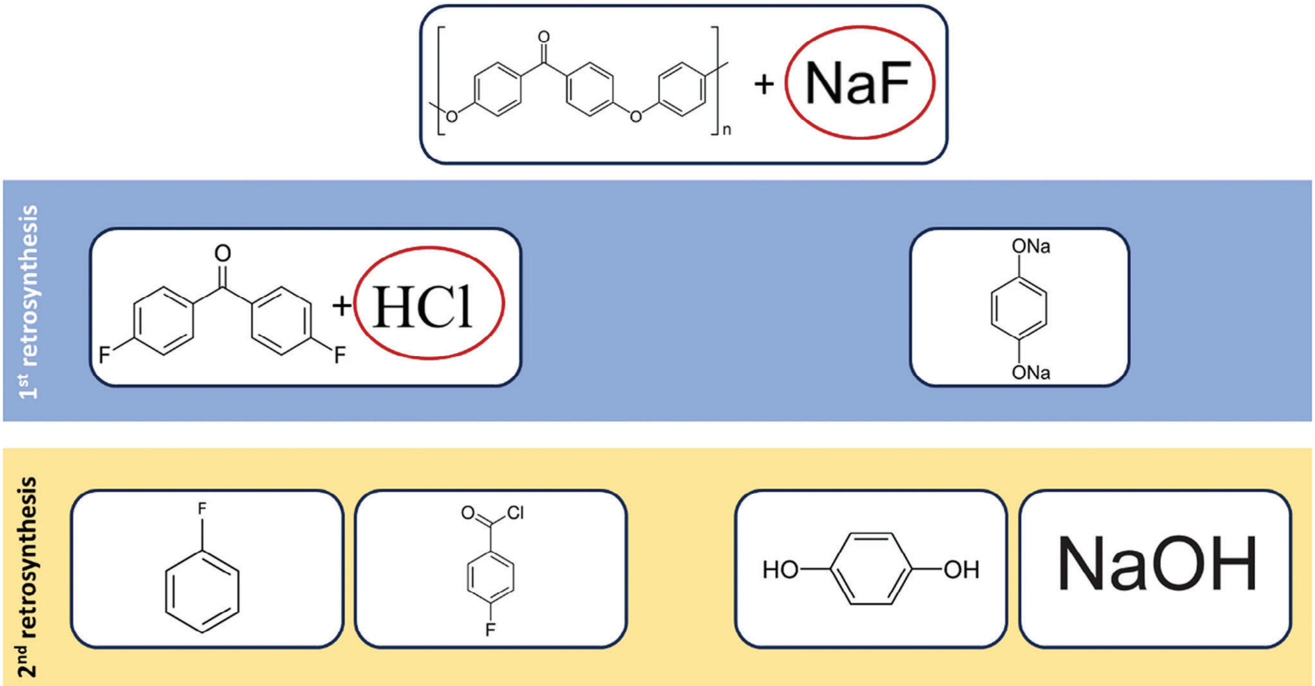
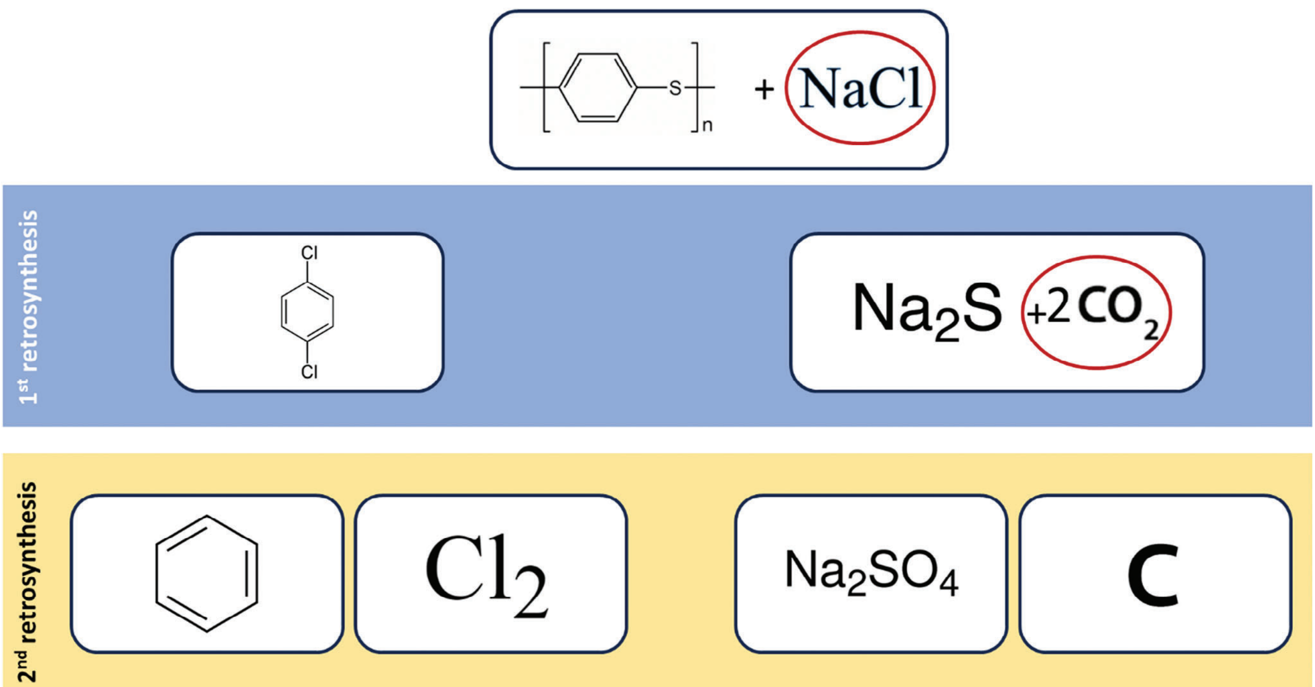


Scheme 2. Retrosynthetic approach for PEEK (chemicals in red circle are byproducts from reaction to synthesize a molecule/polymer next to it).

computing could also play a pivotal role in reducing the carbon footprint of AI. The goal should be to strike a balance between technological advancement and environmental sustainability.[29]

In the rapidly evolving landscape of artificial intelligence, a paradigm shift is being observed in the deployment of AI models, emphasizing the importance of positioning these systems near the end-user, at the very edge of the network. This strategic placement, in close proximity to where the data originates, is known as Edge AI[38] and increasingly recognized for its critical role in promoting environmental sustainability. The implementation of



Scheme 3. Retrosynthetic approach for PPS (chemicals in red circle are byproducts from reaction to synthesize a molecule/polymer next to it).

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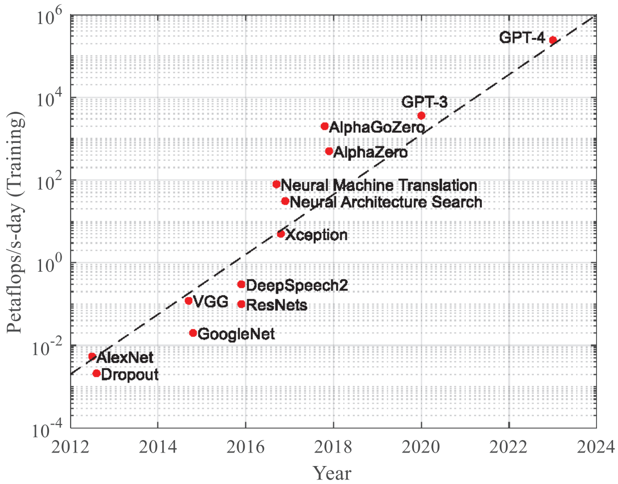

Figure 1. Training time of the common deep learning models, inspired from.[32]

Table 1. Comparison between complexity and training cost of AI models.

Model	Year of Development	Number of Parameters	Training Cost (Peatflops/s-day)	Training (tons CO_2)
AlexNet[29]	2012	6.23E+07	5.4E-03	–
Transformer w. NAS[31]	2019	2.13E+08	–	283.5
GPT-3[33]	2020	1.75E+11	3.6E+03	552
GPT-4[30]	2023	1.70E+14	2.4E+05	–

Edge AI brings a plethora of additional advantages that are pivotal in today's interconnected world. One of the primary benefits is enhanced reliability. By decentralizing the processing of data, Edge AI reduces the dependency on central servers, thereby mitigating the risks associated with server downtimes and network disruptions. This local processing ensures that critical AI applications remain operational even in the face of connectivity issues, which is especially crucial in sectors like healthcare and autonomous vehicles where uninterrupted service is imperative. Another significant advantage of Edge AI is its ability to drastically reduce latency. In traditional cloud-based AI systems, data must travel to distant servers for processing, resulting in notable delays. Edge AI, by contrast, processes data on local devices, enabling real-time or near-real-time responses. This immediacy is essential for applications requiring swift decision-making, such as in manufacturing automation and real-time analytics.

Moreover, Edge AI substantially enhances privacy and data security. By processing data locally, sensitive information does not need to traverse the internet to reach a central server, thereby reducing the exposure to potential data breaches. This aspect is increasingly relevant in the era of stringent data privacy regulations and growing cybersecurity threats. Efficient bandwidth usage is another hallmark of Edge AI. Traditional cloud-based models often involve transferring large volumes of data over the network, consuming significant bandwidth and incurring costs. Edge AI, by processing data locally, minimizes the need for data transmission, thereby alleviating network congestion and reducing operational costs.

Given that edge devices are resource-constrained and energy-sensitive, designing effective neural network architecture for specific edge devices is an urgent yet complex task. In this regard, Neural Architecture Search (NAS) can play a crucial role. NAS is an automated framework to optimize the architecture of artificial neural networks for, computational cost, energy efficiency, and performance.[38] NAS has already outpaced the best human-designed architectures on many tasks. However, NAS also faces some issues in terms of energy and time consumption, which limit its scalability and applicability. Therefore, the recent NAS methods have been mainly focused on developing strategies to reduce the energy and time consumption of NAS, by Early stopping, Weight sharing, One-shot and zero-shot methods, etc.[38]

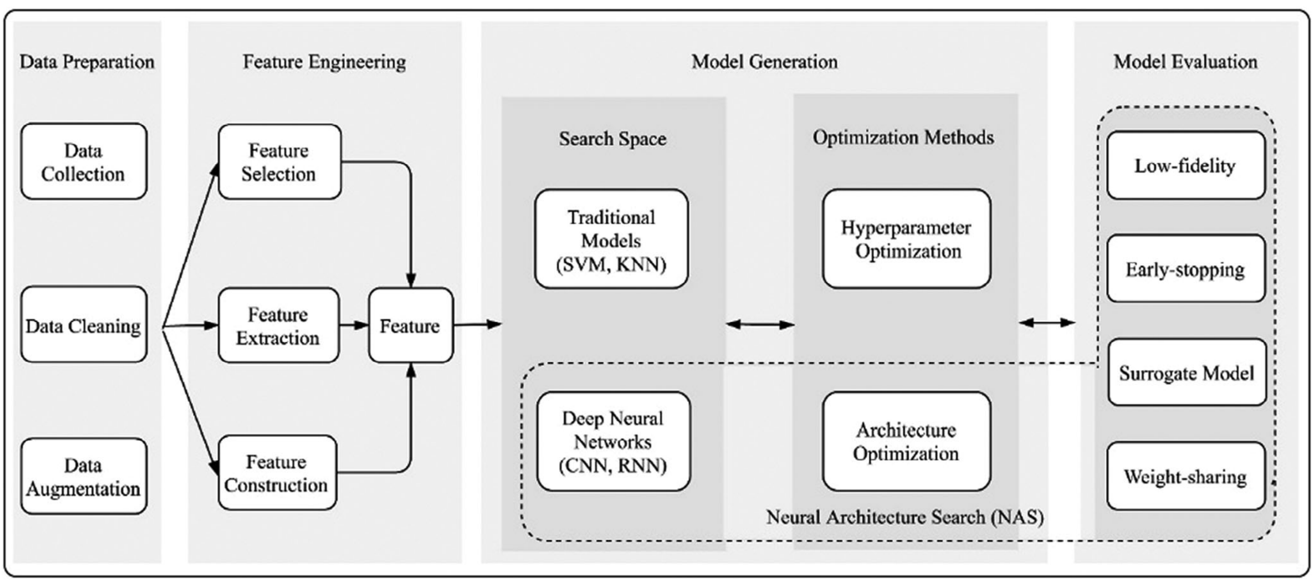

Figure 2. Overview of the current AutoML and NAS pipeline.[41]

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These strategies can make NAS more efficient and sustainable for AI systems. Besides that, to take into account the other constraints for developing and deploying optimized AI models, such as latency, memory requirement, energy consumption, robustness, fairness, etc.[39] NAS methods are being integrated with multi-objective optimization approaches. These methods aim to find a set of Pareto-optimal architectures, which are the ones that cannot be improved in one objective without degrading another. By doing so, they can offer a range of trade-offs between different aspects of performance and sustainability for AI systems.[40]

With the advancement of quantum computers and their associated algorithms, on the other hand, one can see its high potential to revolutionize the fight against climate change. It could help develop climate technologies able to abate carbon on the order of 7 gigatons a year of additional CO_2 impact by 2035. Quantum computing is also an environmentally friendly technology itself. A study jointly published by NASA, Google, and Oak Ridge National Laboratory showed that a quantum computer required only 0.002% of the energy consumed by a classical computer to perform the same task.

Quantum Machine Learning (QML) is a promising paradigm that harnesses the power of quantum computing to address complex problems in various domains, including new material discovery, climate change, and sustainability. It was shown that using QML can lead to exponential speed up provided that the data is available in the quantum format.[42] For instance, IBM Research has proposed a new approach to accelerate the discovery of new materials. This approach uses AI, hybrid cloud, automation, and eventually quantum computing. The goal is to speed up the discovery of new materials by 10 to 100 times.[43]

While there have been significant advancements in Noisy Intermediate-Scale Quantum (NISQ) devices and QML algorithms, their application to industrial problems is not a trivial task due to the fundamental differences between quantum and classical computers. This can lead to quantum algorithms that are quite different from their counterparts in classical computers. As such, it's crucial to develop new methods and algorithms that can assist the modeling and analysis of applications along with the development of NISQ devices. Otherwise, powerful quantum computers with very limited means to use will be formed.[44]

2. Conclusion

The composite industry is undergoing a significant transformation, guided by an unwavering commitment to sustainability. This evolution is particularly evident in the context of recycling challenges associated with crosslinked thermoset matrices. A promising solution has emerged in the form of high-performance thermoplastics for structural applications. These materials boast numerous benefits, including recyclability, repairability, and weldability. However, a more refined understanding of their LCA values is crucial.[45] A critical issue lies in the synthesis of polymers, which are not directly derived from petrorefineries. Instead, they undergo complex synthetic steps to form monomers, often involving highly toxic chemicals and harsh chemical processes. This raises significant sustainability concerns. A realistic assessment of the LCA for high-performance thermoplastic polymer synthesis is essential for a transparent understanding of the sustainability of these systems.

Moreover, the manufacturing processes for composite materials, whether using thermoplastic or thermoset resin matrices, differ markedly. These processes range from curing in epoxy resin composites to high-temperature impregnation in thermoplastic composites, each with distinct energy implications that must be factored into sustainability calculations. Our current vision suggests a retrosynthetic approach to the LCA of high-performance thermoplastics. This involves investigating the monomers of these thermoplastics and their synthetic steps, starting from petrocracking. A critical examination of chemical structures and their toxicity, especially the use of halogenated compounds, strongly indicates that the production of high-performance thermoplastics is currently far from sustainable. Achieving true circularity, where both fiber and matrix properties are preserved, thus eliminating the need for new production, may be the key to sustainability. Collaboration across academia, the composite and chemical industries, and government support is vital for fostering sustainable composite design in the near future.

From an AI perspective, this paper delves into two significant areas: Neural Architecture Search (NAS) and Quantum Machine Learning (QML). We explore how these technologies can contribute to sustainable AI development. NAS optimizes neural network architectures for specific performances, such as accuracy and complexity, while considering constraints like latency, memory usage, energy consumption, robustness, CO_2 emissions, and fairness. Quantum Computing, on the other hand, offers promising avenues towards meeting environmental sustainability goals. This cutting-edge technology has the potential to balance AI innovation with environmental conservation, heralding a new era of technological advancement in harmony with ecological preservation.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Data is available by corresponding authors on demand.

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artificial intelligence, neural architecture search, retrosynthetic LCA, sustainable AI, thermoplastic composites

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