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A review of machine learning applications in polymer composites: advancements, challenges, and future prospects

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Machine learning (ML) is revolutionizing the development and optimization of polymer composites by enabling data-driven insights into material design, manufacturing processes, and property prediction. Polymer composites, widely used in aerospace, automotive, biomedical, and construction industries, require precise engineering to achieve desired mechanical, thermal, and physical properties. Traditional methods for predicting composite behavior and optimizing production are often time-consuming and resource-intensive. ML techniques such as supervised, unsupervised, and deep learning offer an efficient alternative by analyzing large datasets, identifying patterns, and making accurate predictions without the need for extensive physical testing. This review examines the integration of ML into polymer composite research, highlighting its role in material discovery, performance prediction, and manufacturing process optimization. Case studies illustrate how ML algorithms have successfully enhanced property estimation, reduced defects, and accelerated the identification of novel composite formulations. However, challenges such as limited standardized datasets, model interpretability, and the need for domain-specific knowledge hinder broader adoption. Addressing these issues is crucial for advancing AI-driven composite development. Despite its potential, the adoption of ML in polymer composite manufacturing remains limited. Many industries still rely on conventional trial-and-error methods, leading to inefficiencies in material selection, process control, and quality assurance. This review underscores the importance of integrating AI-driven solutions to improve cost-effectiveness, reduce human errors, and streamline production workflows. By overcoming current challenges, ML can facilitate the development of next-generation high-performance polymer composites with superior mechanical strength, durability, and environmental sustainability.

1. Introduction

The capacity of polymer composites to integrate the advantageous characteristics of several materials into a single system has made them a vital tool in contemporary engineering and industrial applications. Aircraft, automobiles, medicinal devices, and building materials are just a few of the many applications of composites, which include a polymer matrix reinforced with fibers, fillers, and other additives.[1,2] Because of their malleability, polymer composites have a wide range of potential uses; for example, they may be tailored to fulfill the needs of many industries, thanks to their high strength-to-weight ratios, excellent corrosion resistance, and improved thermal stability. Because of this adaptability in design, engineers may modify the composites' characteristics to meet the needs of a broad variety of harsh environments.[3]

Nevertheless, there are obstacles to overcome in the process of developing and optimizing polymer composites. There is a great deal of variation in the microstructures of these materials, and the processing techniques used to combine various matrices, fibers, and fillers all have an impact on the composite's ultimate characteristics.[4,5] Polymer composite behavior prediction is challenging due to the complex interplay between material composition, manufacturing processes, and the

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resultant characteristics. The examination and comprehension of these materials have traditionally relied on experimental methods and computational technologies such as finite element analysis (FEA). Although these approaches do a decent job to a certain degree, they aren't always suitable for capturing the whole complexity of composite behavior, and they may be expensive and time-consuming.[6,7]

The use of machine learning (ML) as a crucial technique for enhancing research and development in the area of polymer composites has lately caused a substantial shift.[8] Algorithms can learn from data, see patterns, and make predictions with little to no human intervention, thanks to machine learning (ML), a branch of AI. Polymer composites are highly sought after for their versatile mechanical qualities and extensive use in fields, including aerospace, automotive, construction, and biomedical engineering. This capacity opens up new possibilities for tackling the difficulties of these materials.[9,10] Research on polymer composites that makes use of ML may significantly impact many important domains, including material discovery, process optimization, and precise property prediction.

By sifting through mountains of data in search of optimal polymer and reinforcement combinations, ML may significantly quicken the process of discovering novel composite materials. To simplify and speed up the process of material creation, generative models may propose new formulae depending on the required mechanical and thermal characteristics.[11,12] When it comes to optimizing complicated manufacturing processes like injection molding, extrusion, and additive manufacturing, ML algorithms are just as successful as they are when it comes to material discovery. Algorithms like this assist in cutting down waste, boosting efficiency, and lowering manufacturing costs by studying the effects of various process factors on product quality. Furthermore, by using large datasets that include various material compositions and processing circumstances, ML enhances the precision of mechanical property predictions.[13] Improved forecasts of important qualities, including tensile strength, elasticity, toughness, and thermal stability, are made possible by ML's illumination of the complex interplay between material composition and performance. Composites with improved efficiency and performance are the result of engineers' ability to use this information to choose the most appropriate materials for each given application.[14,15]

By providing a more thorough understanding of the processes by which composite materials collapse, ML might completely transform the study of polymer composites. More resilient materials and constructions may be created with the help of ML algorithms that study failure data in the past to find patterns and early warning indicators of impending failure.[16] In sectors where structural failure may lead to disastrous outcomes, like aircraft and automotive, this predictive skill is very useful. By detecting and fixing problems before they worsen, predictive maintenance powered by ML may increase material life and safety in these industries. There are still a number of obstacles that must be overcome before ML can live up to its enormous promise.[17] The accessibility and accuracy of data are one of the main challenges. Standardized, high-quality datasets are generally in short supply when it comes to polymer composites due to their bespoke nature and the intricacy of the material combinations used in them. Inadequate data makes it hard to train ML models and provide accurate predictions. Making ML models interpretable is another major obstacle. Model accuracy is insufficient in materials science; engineers and researchers must also comprehend the fundamental mechanisms behind these predictions.[18] Integrating ML into research on polymer composites becomes much more complicated due to the demand for interpretability.

Notwithstanding these obstacles, ML is still a formidable instrument with enormous promise. An exhaustive examination of the present state of machine learning (ML) in polymer composites is the goal of this paper. Polymer composites and the ways in which their characteristics are influenced by various material combinations and processing procedures are introduced from the outset.[19,20] The overview continues by outlining major advances in the area of machine learning and then delves into several ML approaches, including supervised learning, unsupervised learning, and deep learning. This study does more than just summarising prior work; it also takes a look forward approach and discusses the major obstacles that still stand in the way of studying ML's complete integration into polymer composites. The development of sustainable and recyclable composite materials, autonomous experimentation, and the integration of ML with multi-scale modeling techniques are all promising areas for future research.[21] Development of next-generation polymer composites can become more innovative, faster, and cost-effective by overcoming current limitations and utilizing the full capabilities of ML. This will ultimately drive progress across a range of industries. On the whole, the polymer composite sector stands to benefit greatly from the use of AI in areas such as data analysis, process management, material selection, error reduction in human operators, and parameter selection during production. The sad truth is that manufacturers are still falling short in this area in the modern day. Research like this may help direct optimization efforts, which are particularly important for the polymer composite sector.

2. ML techniques in polymer composites

Machine learning has emerged as a powerful tool in the development and optimization of polymer composites, assisting researchers in addressing the complexity of these materials. Through the analysis of extensive datasets and the identification of patterns, machine learning models are capable of predicting properties, optimizing processes, and facilitating material discovery, thereby significantly accelerating research and decreasing costs. This section presents an overview of the primary machine learning techniques utilized in polymer composites and examines their particular applications.[22] Fig. 1 illustrates the primary machine learning techniques.

2.1 Supervised learning

Supervised learning is one of the most commonly used ML techniques in polymer composites. In supervised learning,

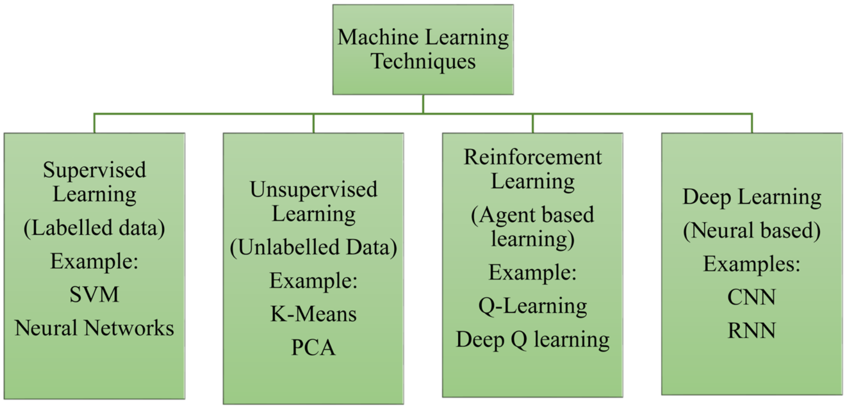

Fig. 1 Key ML techniques.

models are trained on labelled datasets where inputs (*e.g.* material composition and processing parameters) are mapped to known outputs (*e.g.* mechanical properties and failure data).[23] Supervised learning models play a pivotal role in the field of polymer composites, providing predictive capabilities and valuable insights in various applications. Fig. 2 shows the supervised learning process.

2.1.1 Property prediction. Supervised learning models such as decision trees, support vector machines (SVMs) and neural networks are trained on historical data to predict key mechanical, thermal and electrical properties of polymer composites.[24,25] This is particularly useful in materials science, where prediction of properties, such as tensile strength, Young's modulus, fracture toughness, thermal conductivity and dielectric properties, is essential. By learning from experimental data (*e.g.* fibre volume fraction, filler type, and resin properties), these models can predict the performance of new composite formulations, reducing the need for time-consuming and expensive physical testing.[26] For example, by inputting variables such as fibre type, resin and processing conditions into the model, researchers can predict the tensile or impact strength of hybrid composites before they are actually manufactured and tested.

2.1.2 Material classification. In material classification, supervised learning algorithms categorize polymer composites based on their composition, performance, or specific application areas. For instance, SVMs or random forests can classify materials into categories such as high-performance composites for aerospace, automotive, or marine applications based on their mechanical or thermal properties.[27,28] This is useful in industrial environments where rapid identification of suitable materials for a given application is critical. For example, a classification model could help engineers quickly determine whether a composite is suitable for structural load-bearing applications or whether it is more suitable for thermal insulation.[29,30]

2.1.3 Failure analysis. Supervised learning can significantly improve failure analysis by predicting the failure modes of composites (*e.g.* delamination, crack propagation, matrix cracking, or fibre pullout) using historical experimental failure data.[31] These models can help engineers identify weaknesses in composite structures and inform design adjustments to prevent premature failure in critical applications. For example, a neural network might predict that a particular fibre and resin combination is more susceptible to delamination under high-stress conditions, allowing researchers to modify the material

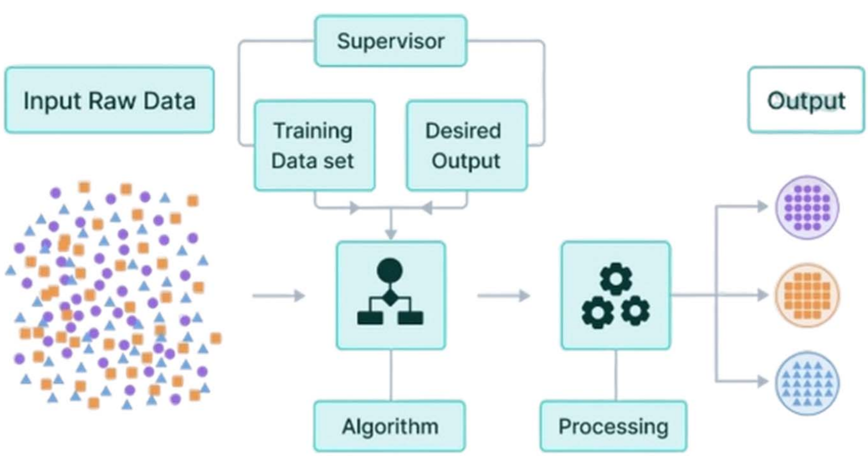

Fig. 2 Process of supervised learning.

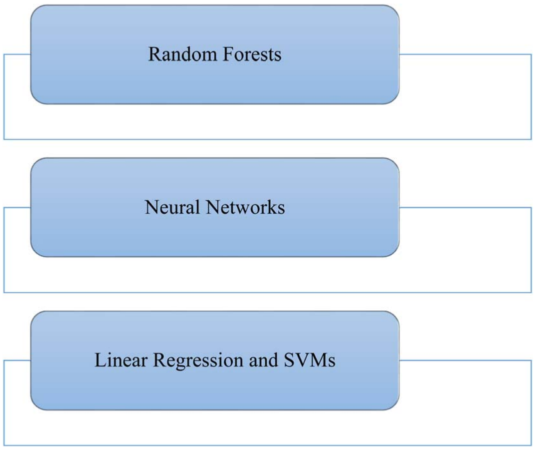

Fig. 3 Algorithms of supervised learning.

composition or lay-up design to improve the performance and longevity.[32] This approach is highly beneficial for industries such as aerospace, automotive, and marine, where material failure can lead to catastrophic consequences.[33] In all these cases, supervised learning reduces reliance on physical trials, allowing researchers to make faster, data-driven decisions when developing and optimizing polymer composites. This leads to cost and time efficiencies, along with more innovative material designs.[34]

2.1.4 Common algorithms in supervised learning. In supervised learning, various algorithms are applied based on the complexity and nature of the data involved. Here is a more detailed look at the common algorithms used in predicting properties and behaviors of polymer composites.[35] Fig. 3 shows the algorithms of supervised learning.

(1) Random forests: a collection of decision trees used to improve prediction accuracy by aggregating outputs from multiple models.

(2) Neural networks: models that capture complex, nonlinear relationships between inputs and outputs, useful for predicting multifaceted composite behaviors.

(3) Linear regression and SVMs: simpler models that are often used for predicting properties like stress and strain under specific conditions.

2.2 Unsupervised learning

Unsupervised learning techniques are used to analyze datasets without pre-defined labels, allowing models to uncover hidden patterns and relationships within the data. In polymer composites, unsupervised learning is useful for the following applications,[31,36] and the process of unsupervised learning is presented in Fig. 4.

2.2.1 Material discovery. Clustering algorithms are used to group materials based on shared properties or performance characteristics, especially when researchers don't have pre-defined labels or classifications.[37,38] This technique is invaluable for discovering new composite formulations by revealing patterns in the data. For example, clustering can identify groups of materials with high strength-to-weight ratios, making them ideal candidates for aerospace or automotive applications where lightweight yet strong materials are critical. By grouping composites with similar mechanical, thermal, or electrical properties, clustering helps researchers focus on promising material combinations, reducing the time and effort required for experimental testing.[39]

2.2.2 Anomaly detection. In manufacturing, unsupervised learning techniques such as clustering can be used to detect anomalies in processing data or material properties. These methods can identify unusual patterns or outliers in the data, signalling potential defects in the composite structure, such as delamination, voids or improper curing. For example, clustering methods such as *k*-means can highlight data points that deviate significantly from the norm, ensuring that these deviations are addressed before they lead to major problems.[40] This improves quality control, ensures production consistency and minimizes material waste, which are vital for industries that demand high reliability and safety.

2.3 Reinforcement learning

Reinforcement learning (RL) is a type of ML in which agents learn to make decisions by interacting with an environment and

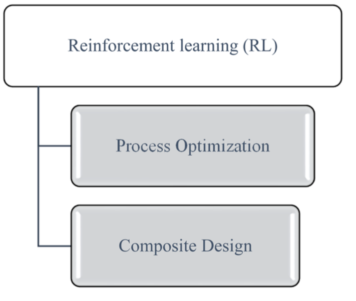

Fig. 5 Reinforcement learning (RL) uses.

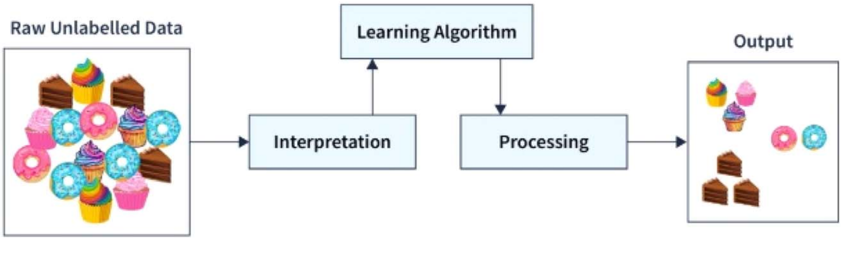

Fig. 4 Process of unsupervised leaning.

receiving feedback in the form of rewards or penalties.[41] Fig. 5 shows the application of RL.

Reinforcement Learning (RL) plays a crucial role in both process optimization and composite design. In process optimization, RL algorithms can dynamically adjust parameters such as temperature, pressure, and time in manufacturing processes such as curing, molding, or extrusion.[42] By learning through trial and error, RL identifies the optimal set of conditions that maximize performance and minimize defects, making it particularly effective in complex, ever-changing production environments.

In composite design, RL explores a wide range of design variables, including fibre orientation, matrix composition and filler content. Over time, RL models learn to balance competing performance criteria such as strength, durability and weight, leading to the development of optimized composites for specific applications, such as lightweight yet strong materials for aerospace or automotive use.[43]

2.4 Deep learning

Deep learning (DL), a subset of ML based on multi-layer artificial neural networks, excels at handling large, complex datasets and capturing intricate patterns.[44] In polymer composites, deep learning is particularly effective for the following and is shown in Fig. 6.

2.4.1 Complex pattern recognition. Deep learning models, such as Convolutional Neural Networks (CNNs), are highly effective in recognizing complex, non-linear relationships between composite microstructures and their properties.[45] For example, CNNs can analyse micrographs or 3D images of composite structures and identify critical features such as fibre orientation, voids or microcracks that affect the mechanical performance of the material. By automatically recognizing these patterns, CNNs help researchers better understand how microstructural arrangement affects properties such as tensile strength and fatigue resistance, leading to improved material design and more accurate predictions of material behavior.[46]

2.4.2 Prediction of nonlinear behaviors. Many properties of polymer composites, such as fatigue resistance, thermal expansion and creep, exhibit non-linear behaviour that is difficult to predict using traditional methods.[47] Recurrent Neural Networks (RNNs), which are designed to capture sequential dependencies, are well suited to modelling these complex time-dependent behaviours. RNNs can be used to predict the long-term performance of composites under varying conditions of stress, strain or temperature by learning from historical data. This allows engineers to predict the fatigue life or thermal stability of a material over extended periods of time, helping in the development of more durable and reliable composites.[48]

2.4.3 Defect detection. In composite manufacturing, deep learning models are transforming defect detection through their ability to analyse image data from non-destructive testing methods such as X-ray, ultrasound or thermography.[49] Trained deep learning algorithms can automatically detect defects such as delamination, voids or inclusions within the material, ensuring higher accuracy and consistency than manual inspection. This significantly improves quality assurance by identifying defects in real-time during production, reducing the likelihood of defective material entering the supply chain and improving the overall product reliability and performance.[50] Deep learning's ability to model high-dimensional data makes it a powerful tool for analyzing the complex behaviour of polymer composites. However, these models require large amounts of data and computational resources, which can be limiting in some cases.[51]

2.5 Hybrid models

Hybrid models combine ML techniques with traditional computational methods, such as FEA, to improve the accuracy and efficiency of predictions in polymer composites. These models leverage the strengths of both approaches: ML's data-driven pattern recognition and FEA's physics-based simulations.[52] Fig. 7 shows models in the ML.

2.5.1 ML-augmented FEA. ML can significantly enhance FEA by integrating predictive models to reduce computational costs and time. In this hybrid approach, ML algorithms can predict material properties or behaviors for specific configurations, which minimizes the need for extensive repeated simulations in FEA.[53] For instance, instead of running multiple simulations to determine how a composite material will respond under different loading conditions, ML can quickly provide estimates based on historical data, effectively streamlining the simulation process.[54] This is particularly beneficial in multi-scale modelling, where the behaviour of composites is

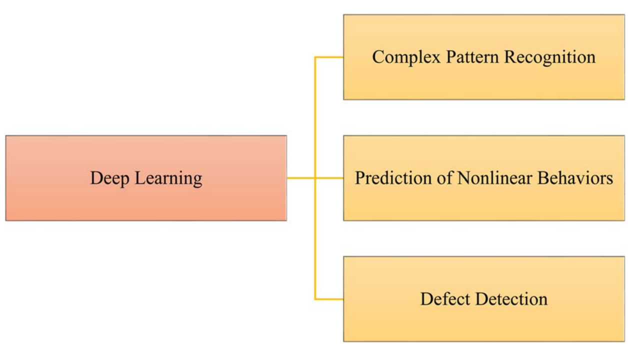

Fig. 6 Deep learning applications.

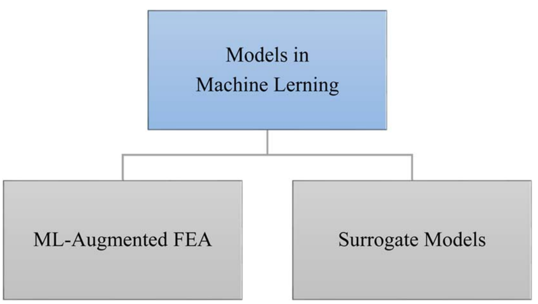

Fig. 7 Models in ML.

Table 1 The comparative analysis between different ML techniques and quantitative metrics

ML technique	Key applications in polymer composites	Advantages	Limitations	Accuracy	Computational efficiency
Supervised learning	Property prediction (*e.g.*, tensile strength and elasticity)	High predictive accuracy (85–95%)	Requires large labeled datasets	85–95%	Moderate
Artificial Neural Networks (ANNs)	Mechanical property estimation	Can model complex, nonlinear relationships	Prone to overfitting with small datasets	90–95%	Moderate
Support Vector Machines (SVM)	Classification of composite types	Effective with small datasets	Computationally expensive for large datasets	85–92%	Low (for large datasets)
Random Forest (RF)	Material selection and property prediction	Robust against overfitting	Requires careful parameter tuning	88–93%	Moderate
Unsupervised learning	Clustering materials based on properties	No need for labeled data	Limited for direct property prediction	N/A	High
Principal Component Analysis (PCA)	Feature reduction for composite datasets	Reduces dimensionality and improves efficiency	Can lose critical information	N/A	Very high
K-Means clustering	Grouping materials based on similarities	Fast and scalable	Requires predefined cluster number	N/A	High
Deep learning	Microstructural analysis and failure prediction	High accuracy with large datasets	Requires significant computational resources	92–98%	Low (for training) and high (for inference)
Convolutional Neural Networks (CNNs)	Microstructure and defect detection	Excellent at image-based analysis	Computationally expensive	95–98%	Low (for training) and high (for inference)
Recurrent Neural Networks (RNNs)	Time-series prediction for material degradation	Captures sequential dependencies	Difficult to train and prone to vanishing gradient	90–95%	Low
Reinforcement Learning (RL)	Process optimization (*e.g.*, injection molding and extrusion)	Learns optimal process parameters over time	Requires significant trial-and-error data	N/A	Low (training) and high (real-time use)

analysed at different length scales – from microstructural features to macroscopic properties. By combining the detailed analysis capabilities of FEA with the speed and efficiency of ML, researchers can achieve a more comprehensive understanding of composite behavior while significantly reducing the time and resources typically required for extensive simulations.[55]

2.5.2 Surrogate models. Hybrid models frequently utilize ML to create surrogate models that approximate complex FEA simulations. Surrogate models act as simplified representations of the intricate relationships and behaviors captured by FEA, allowing for rapid evaluation of different design parameters without the need for full-scale simulations.[56] This is particularly useful during the optimization of composite designs, where numerous configurations need to be assessed to identify the best-performing options. By using surrogate models, engineers can quickly explore the design space, testing different combinations of materials, geometries and loading conditions while significantly reducing the computational burden.[57] This approach not only accelerates the design process but also improves the predictive accuracy of polymer composite analysis, enabling faster innovation and more efficient development cycles. Overall, the integration of ML with traditional FEA and surrogate modelling represents a promising way to improve the efficiency and effectiveness of polymer composite analysis, ultimately leading to better designed materials with optimised properties.[58]

ML is revolutionizing the way polymer composites are developed and optimized. By harnessing a variety of ML techniques, researchers can more effectively navigate the complexities of these materials, enabling faster discovery, improved performance and reduced costs. In the next section, we will discuss specific case studies where ML has been successfully applied to polymer composites, showcasing its transformative potential.[59] Table 1 shows a comparative analysis between different ML techniques and quantitative metrics.[60]

This table provides a structured comparison of ML techniques in polymer composite research, helping researchers and industry professionals choose the most suitable approach based on accuracy, efficiency, and application needs.

3. Application of ML in polymer composites

Machine learning has advanced considerably in the domain of polymer composites, offering innovative solutions throughout multiple phases of material development, including design, discovery, manufacturing, and failure prediction. This section examines the practical applications of machine learning in polymer composites, emphasizing its role in accelerating material discovery, improving manufacturing processes, and predicting composite behavior.[61,62] Fig. 8 illustrates the applications of machine learning in polymer composites.

3.1 Material design and discovery

One of the most promising applications of ML in polymer composites is material design and discovery. Traditional methods for discovering new composites involve extensive experimentation and trial-and-error, which can be both time-consuming and expensive. ML models, trained on large datasets of existing materials, can predict the properties of new composites before they are even synthesized.[58]

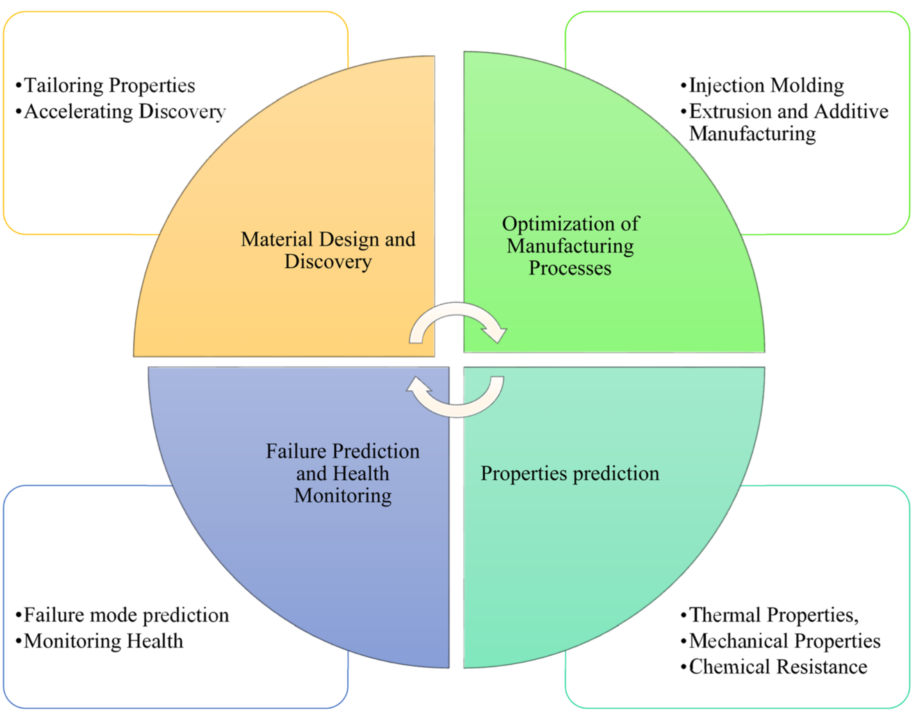

Fig. 8 Significant applications of ML in polymer composites.

3.1.1 Tailoring properties. By analyzing patterns in the relationships between composite compositions and their properties, ML algorithms can predict the outcomes of new combinations of polymers, fibres, and fillers. For instance, ML can help identify the optimal ratio of reinforcement to the matrix material that maximizes tensile strength, thermal conductivity, or other desired properties while minimizing weight.[59] This predictive capability is particularly useful in industries such as aerospace and automotive, where material performance is critical, and optimizing compositions can lead to significant advantages.[60] For example, in the automotive industry, ML-driven simulations have helped determine the best fiber–matrix ratio for high-impact-resistant composites, enhancing vehicle safety while maintaining lightweight characteristics. Similarly, in aerospace, ML models have been employed to design carbon fiber composites that optimize stiffness and strength while ensuring manufacturability.[63]

3.1.2 Accelerating discovery. ML enables the discovery of new materials that may not have been considered using traditional methods. Algorithms such as Bayesian optimization and genetic algorithms can explore vast design spaces more efficiently than manual approaches, identifying high-performance composites for specific applications.[62] This efficiency allows researchers to focus on the most promising material candidates, reducing the overall time and cost associated with material development.

Advanced ML algorithms, such as Bayesian optimization and genetic algorithms, efficiently explore large design spaces to identify high-performance polymer composites. Bayesian optimization, in particular, has proven effective in refining composite compositions to enhance mechanical properties such as tensile strength and flexural modulus.[64]

A recent study demonstrated how genetic algorithms were applied to develop hybrid bio-based composites with superior mechanical characteristics while maintaining environmental sustainability.[65] These models significantly reduce material discovery time, allowing researchers to focus on promising candidates rather than relying solely on experimental synthesis.

3.2 Optimization of manufacturing processes

Manufacturing processes for polymer composites, such as injection molding, extrusion, and additive manufacturing (3D printing), involve complex variables such as temperature, pressure, and processing time. ML has been successfully applied to optimize these processes, reducing waste, improving efficiency, and ensuring consistent material quality.[66]

For example, ML-based predictive models have enabled defect reduction in glass fiber-reinforced composites by optimizing cooling rates and mold flow dynamics, leading to improved component durability and reduced production costs.[59]

3.2.1 Injection molding. ML models can optimize critical injection moulding parameters such as mould temperature, cooling rate and pressure. By analysing historical production data, ML can predict settings that minimise defects such as warpage, voids or incomplete fills. This optimization ensures that the final product consistently meets stringent quality standards, ultimately enhancing production efficiency and reducing material waste.[67]

For example, ML-based predictive models have enabled defect reduction in glass fiber-reinforced composites by optimizing cooling rates and mold flow dynamics, leading to improved component durability and reduced production costs.[68]

3.2.2 Extrusion and additive manufacturing. In extrusion processes, ML can help control variables such as die shape and extrusion speed to achieve desired fibre alignment or material density. In additive manufacturing, ML models can predict the effects of layer thickness, print speed, and material feed rate on the mechanical properties of finished composites. By optimizing these parameters, manufacturers can produce parts with consistent quality and minimize the need for costly post-processing steps.[69]

In additive manufacturing (3D printing), ML plays a crucial role in predicting the effects of process parameters such as layer thickness, print speed, and material feed rate. These predictions help mitigate defects like porosity, layer delamination, and uneven fiber distribution.

For example, in thermoplastic-based composites, ML models have successfully identified ideal printing parameters to maximize interlayer adhesion and overall mechanical integrity, significantly improving the reliability of printed composite parts.[70]

3.3 Predicting mechanical, thermal, and chemical properties

Predicting the mechanical, thermal, and chemical properties of polymer composites is a critical step in ensuring their suitability for specific applications.[71] ML has been used to develop models that can accurately predict these properties based on material composition and processing parameters. Accurate prediction of polymer composite properties is essential for their application in structural, thermal, and chemically harsh environments.

3.3.1 Mechanical properties. ML models are widely used to predict key mechanical properties such as tensile strength, fracture toughness and fatigue resistance. By training the algorithms on experimental data, researchers can predict how a composite will behave under different loading conditions, eliminating the need for extensive physical testing.[72] This predictive capability not only speeds up the material evaluation process but also increases the reliability of performance predictions.

For example, in hybrid natural fiber-reinforced composites, ML models have been used to assess the impact of fiber orientation and fiber–matrix bonding on tensile and flexural strength. Researchers have utilized support vector regression (SVR) and deep learning models to estimate impact resistance under various loading conditions, streamlining material selection processes in structural applications.[73]

3.3.2 Thermal properties. In industries such as electronics or aerospace, predicting thermal properties such as thermal conductivity and expansion is essential.[74] ML algorithms trained on datasets of composite formulations can provide insight into how different reinforcement materials and matrix compositions affect thermal stability. This capability can assist designers in selecting appropriate materials for high-temperature environments, ensuring optimal performance and safety.[75]

In aerospace and electronics applications, predicting thermal conductivity and expansion behavior is crucial. ML models trained on composite formulations and thermal cycling data have been used to develop high-temperature-resistant composites for jet engine components.[76,77]

For instance, convolutional neural networks (CNNs) have been employed to analyze the effects of nanoparticle fillers on thermal stability in polymer composites, identifying optimal filler loadings that maximize heat dissipation while maintaining mechanical integrity.[78] Additionally, decision tree algorithms have assisted in selecting polymer matrices that provide superior thermal insulation for aerospace applications, preventing thermal degradation under extreme conditions.[79]

3.3.3 Chemical resistance. ML models can also predict the chemical resistance of polymer composites, which is crucial for applications in harsh environments. By analyzing the molecular structures of polymers and reinforcements, ML can predict how a composite will react to exposure to chemicals, moisture, or UV radiation. This predictive capability helps in the selection of materials that will maintain integrity and performance under adverse conditions.[79]

For example, an ML model trained on experimental data for bio-based epoxy composites successfully predicted long-term resistance to acidic and alkaline environments, assisting industries such as marine and chemical processing in selecting durable materials for extreme operating conditions.[80]

3.4 Failure prediction and health monitoring

Polymer composites are often used in critical applications where material failure can have severe consequences. ML has been used to predict failure modes such as delamination, cracking, or fibre–matrix debonding, allowing for preventive maintenance and improved safety.[80] ML-driven failure prediction and health monitoring techniques improve reliability and enable predictive maintenance.[81]

3.4.1 Failure mode prediction. ML models can analyze data from nondestructive testing (NDT) methods, such as ultrasound or X-ray, to predict when and how a composite will fail. By identifying early signs of damage or degradation, these models can estimate the remaining useful life of the composite, enabling proactive maintenance and reducing the risk of catastrophic failures. ML-based nondestructive testing (NDT) techniques, such as X-ray and ultrasound image analysis, detect early-stage defects in composites.

For instance, deep learning models trained on ultrasonic inspection datasets have successfully classified delamination patterns in fiber-reinforced composites with over 95% accuracy, allowing for early maintenance interventions. Additionally, reinforcement learning algorithms have been used to predict microcrack initiation and propagation in aerospace composites, preventing in-service failures and ensuring structural integrity.[82]

3.4.2 Health monitoring. Real-time health monitoring systems use sensors embedded in composite structures (such as wind turbine blades or aircraft wings) to collect continuous data on stresses, strains and environmental conditions.[83] ML algorithms process these data to detect anomalies, providing early warning of potential failures and facilitating timely intervention. This capability increases the overall safety and reliability of composites in critical applications.

Embedded sensor networks in composite structures collect real-time data on stress, strain, and environmental conditions. ML algorithms process these data to detect anomalies indicative of impending failure.[84]

For example, in wind turbine blades, recurrent neural networks (RNNs) have been used to analyze vibration and load data, predicting material degradation trends and enabling proactive maintenance. This approach has extended the operational lifespan of composite blades and reduced the maintenance costs significantly. Similarly, ML-driven anomaly detection in aircraft fuselage composites has improved safety by identifying stress concentration points that could lead to structural failures.[85]

4. Recent advancements in ML-IAPs for macromolecular/polymer systems

Machine learning has significantly enhanced the field of polymer composites by expediting material discovery, optimizing manufacturing processes, accurately predicting properties, and improving failure detection.[8,59,83] With ongoing advancements in ML algorithms and data availability, the integration of ML in composite research and manufacturing will continue to drive innovation and efficiency in various industries, including aerospace, automotive, and biomedical applications.

Recent advancements in machine learning-based interatomic potentials (ML-IAPs) have significantly enhanced the simulation and analysis of macromolecular and polymer systems. These developments bridge the gap between quantum mechanical accuracy and computational efficiency, enabling the exploration of complex molecular behaviors that were previously computationally prohibitive.[86]

4.1 Key developments

4.1.1 Integration of long-range interactions. Traditional ML-IAPs often focused on short-range interactions, neglecting long-range effects crucial for accurate simulations of polymers and macromolecules. Recent approaches, such as the Sum-of-Gaussian Neural Network (SOG-Net), integrate long-range interactions by employing a latent-variable learning network and efficient Fourier convolution layers. This method adaptively captures diverse long-range decay behaviors while maintaining computational efficiency, making it effective for large-scale simulations.[87]

4.1.2 Equivariant neural networks. To enhance the robustness and accuracy of ML-IAPs, researchers have developed equivariant graph neural networks that respect the symmetries of Euclidean space. These networks improve sample efficiency and model robustness, addressing challenges related to data scarcity and model generalization. Notable contributions include E(3)-equivariant models that have demonstrated data-efficient learning and high accuracy in predicting molecular properties.[88]

4.1.3 Deep learning for structure–property relationships. Deep learning models have been employed to connect molecular structural ordering to macroscopic properties. For instance, studies have demonstrated that deep-learning interatomic potentials can link the structural ordering of polyacrylonitrile at the molecular level to its macroscopic properties, providing insights into polymer design and performance.[89]

4.1.4 Incorporation of nonlocal interactions. Accurately modeling nonlocal interactions, such as dispersion and electrostatic effects, is essential for realistic simulations of polymer systems. Recent ML-IAPs incorporate these interactions by augmenting traditional models with dispersion corrections and electrostatic calculations derived from atomic environment descriptors. These enhancements improve the predictive power of ML-IAPs for complex molecular systems.[90]

Despite significant progress, challenges remain in developing ML-IAPs for polymer systems. Accurately modeling the hierarchical structures and diverse topologies of polymers requires sophisticated descriptors and comprehensive training datasets. Ensuring the physical interpretability of ML-IAPs is also crucial for their acceptance in the scientific community. Future research is directed towards refining these models, enhancing data diversity, and improving the integration of long-range interactions to fully harness the potential of ML-IAPs in polymer science.[91]

These advancements position ML-IAPs as powerful tools for simulating and understanding the complex behaviors of macromolecular and polymer systems, paving the way for accelerated discovery and design of novel polymer materials with tailored properties.

5. Machine learning for sustainable polymer composites

Sustainable polymer composites focus on utilizing bio-based, biodegradable, and recyclable materials to mitigate environmental impact. These materials play a crucial role in advancing green manufacturing and reducing the dependency on petroleum-based polymers. However, their development poses challenges such as optimizing mechanical properties, ensuring durability, and predicting degradation behavior.[92] Machine Learning (ML) offers powerful tools to accelerate research and development in sustainable polymer composites by analyzing large datasets, predicting material behavior, and optimizing formulations for better performance.[8,93]

5.1 Biodegradable and bio-based composites

Biodegradable and bio-based polymer composites are derived from renewable resources such as natural fibers (*e.g.*, jute, flax, hemp, kenaf, and banana), biopolymers (*e.g.*, polylactic acid (PLA) and polyhydroxyalkanoates (PHA)), and plant-derived resins.[94] ML algorithms are instrumental in selecting and optimizing these materials by predicting their mechanical, thermal, and degradation properties.

• ML-driven material selection: traditional trial-and-error methods for material selection are time-consuming and costly. ML models trained on extensive databases of natural fibers and bio-polymers help researchers predict the best fiber–matrix combinations for specific applications.[95]

• Example: a deep learning model trained on datasets of flax-reinforced bio-epoxy composites accurately predicted their tensile strength, impact resistance, and biodegradability, reducing the need for extensive experimental testing.

• Case study: a random forest algorithm successfully identified optimal processing conditions for kenaf fiber-reinforced PLA composites, improving their mechanical properties while maintaining biodegradability.

5.2 Waste polymer recycling and reusability

Recycling polymer waste into high-performance composites is a sustainable alternative to landfill disposal. However, maintaining mechanical properties while reusing polymer waste is challenging. ML helps optimize formulations of recycled polymer blends by predicting the best mixing ratios and identifying potential property enhancements.[96]

• Optimizing recycled polymer blends: ML models predict the impact of recycled polymer content on strength, elasticity, and durability by analyzing large datasets of experimental results.

• Example: researchers used a neural network to optimize the formulation of recycled PET-based composites, achieving a balance between mechanical performance and environmental sustainability.

• Hybrid ML approaches: combining genetic algorithms and artificial neural networks (ANNs) has enabled the design of recycled HDPE composites with enhanced toughness and reduced brittleness.

• Industrial application: companies leveraging ML have developed recycled polypropylene (PP) composites reinforced with cellulose fibers, successfully competing with virgin PP composites in mechanical performance.

5.3 Predicting the lifespan of sustainable composites

One of the major concerns with sustainable composites is their long-term stability and degradation behavior. ML-based predictive models assess the aging behavior and mechanical deterioration, reducing the need for extensive long-term testing.[97]

• Failure and degradation analysis: ML models analyze historical data on degradation pathways, enabling more accurate predictions of composite durability.

• Example: ML algorithms trained on biocomposites made from PLA and natural fibers predicted their aging behavior under different environmental conditions (humidity, temperature, and UV exposure).

• Predictive maintenance: in industries such as automotive and construction, ML-powered monitoring systems analyze composite wear and fatigue patterns, predicting failure points before they occur.

• Case study: a support vector machine (SVM) model was used to forecast the degradation of PHA-based marine biodegradable composites, ensuring their structural integrity in underwater applications.

By integrating ML-driven optimization, predictive analytics, and failure modeling, the development of sustainable polymer composites becomes more efficient, cost-effective, and environmentally friendly, paving the way for next-generation green materials.[98]

6. Machine learning in energy storage materials

Energy storage materials, such as batteries and supercapacitors, play a crucial role in advancing renewable energy technologies and electrification. Efficiency, longevity, and sustainability of these materials are essential for developing high-performance energy storage systems.[99] Machine learning (ML) accelerates the discovery, characterization, and optimization of these materials by enabling predictive modeling of their electrochemical behavior, stability, and environmental impact. By leveraging vast datasets and complex algorithms, ML-driven approaches reduce experimental trial-and-error efforts and enhance material selection and processing techniques. Some of the key ML applications in energy storage are provided in the following.[100].

6.1 Lithium-ion and next-generation batteries

• Electrode material discovery: ML models analyze extensive databases of electrode materials, identifying promising candidates with high energy density, fast charge/discharge rates, and long cycle life. Deep learning models trained on first-principles and experimental data provide insights into the electronic structure, phase stability, and diffusion properties of battery materials.[101]

• Example: a neural network trained on thousands of battery materials successfully predicted new lithium-rich cathode compositions with 20% higher energy density and improved thermal stability, reducing degradation over multiple charge cycles. Researchers also applied reinforcement learning techniques to optimize the composition of high-capacity silicon anodes, enhancing mechanical stability and charge retention.[102]

6.2 Sustainable supercapacitors and bio-based electrodes

• Bio-based carbon electrodes: ML aids in optimizing the synthesis of supercapacitor electrodes from biomass-derived carbon sources (*e.g.*, lignin, cellulose, coconut shell, and algae-based precursors).[103] By modeling the relationships between pyrolysis conditions, pore structures, and electrochemical performance, ML can predict the optimal processing parameters for high-performance bio-based electrodes.[104,105]

• Example: ML-driven optimization of lignin-derived activated carbon led to the development of high-surface-area electrodes with exceptional capacitance retention and low internal resistance. These sustainable electrodes improved the energy and power density of supercapacitors while reducing reliance on petroleum-derived carbon materials.[106]

6.3 Electrolyte and binder optimization

• Predicting green electrolytes: ML models facilitate the discovery of environmentally friendly electrolytes by screening potential solid-state or bio-derived electrolyte formulations. These models assess the ionic conductivity, thermal stability, and electrochemical window, enabling the replacement of hazardous organic solvents with safer alternatives.[107]

• Example: a random forest model identified novel ionic liquid-based electrolytes with high conductivity and low toxicity, making them ideal for next-generation batteries and supercapacitors. Additionally, ML-assisted molecular simulations helped design polymer-based electrolytes with improved ionic transport and mechanical flexibility, paving the way for flexible and wearable energy storage devices.[108]

By integrating ML into energy storage material research, scientists and engineers can accelerate the transition toward more efficient, sustainable, and eco-friendly energy storage solutions. ML-driven insights not only expedite material discovery but also improve the recyclability and environmental footprint of batteries and supercapacitors, contributing to a greener energy future.[109]

7. Machine learning for green manufacturing

Green manufacturing aims to improve efficiency while minimizing environmental impact by reducing energy consumption, material waste, and pollution in industrial production. ML has emerged as a transformative tool for optimizing manufacturing processes, enabling real-time monitoring, predictive analytics, and sustainability assessments.[110] By integrating ML into green manufacturing, industries can achieve higher efficiency, lower costs, and a reduced carbon footprint.

7.1 Process optimization in polymer production

Manufacturing polymer-based materials involves complex processes such as injection molding, extrusion, and additive manufacturing, requiring precise control over parameters like temperature, pressure, and cooling rates to ensure product quality and energy efficiency. Traditionally, process optimization relies on trial-and-error experimentation, which is time-consuming and resource-intensive.[111] ML provides a data-driven approach to dynamically optimize these processes, improving efficiency and reducing waste. Key applications of ML in polymer manufacturing include real-time process monitoring, where ML algorithms analyze sensor data to predict deviations and suggest immediate adjustments, adaptive process control, where reinforcement learning models continuously learn from production data to automatically adjust process parameters for improved quality and energy savings, and defect detection and correction, where computer vision and deep learning models identify defects in polymer production, minimizing the need for post-production inspections and rework.[112]

Example:

• An ML-powered predictive control system implemented in an industrial polymer extrusion plant optimized temperature and pressure parameters, reducing energy consumption by 15% while maintaining high product quality.[113]

• A convolutional neural network (CNN) was used to detect surface defects in polymer film production, minimizing material rejection rates and enhancing product consistency.[114]

7.2 Carbon footprint reduction and life cycle assessment (LCA)

Life Cycle Assessment (LCA) is a crucial method for evaluating the environmental impact of materials and processes from raw material extraction to end-of-life disposal. However, traditional LCA approaches are computationally expensive and time consuming due to the complexity of materials, energy flows, and emission data.[115] ML significantly enhances LCA by rapidly predicting environmental impacts based on material composition, processing methods, and energy consumption patterns, making sustainability assessments more efficient. Key ML applications in carbon footprint reduction include AI-powered sustainability assessments, where ML models analyze historical LCA datasets to estimate environmental impact without extensive manual calculations, eco-friendly material selection, where ML predicts the carbon footprint of different polymer formulations, enabling manufacturers to choose sustainable alternatives, and process emission optimization, where ML-based simulations refine production methods to minimize greenhouse gas emissions and improve overall environmental sustainability.[116]

Example:

• A deep learning model analyzed over 200 polymer manufacturing pathways, identifying process modifications that reduced carbon emissions by 30% without compromising material properties.[117]

• ML was used to predict the environmental impact of bio-based polymer composites, guiding industries toward low-carbon alternatives in automotive and packaging applications.[118]

7.3 Predictive maintenance for sustainable manufacturing

Equipment failures in polymer manufacturing result in unplanned downtime, material waste, and increased energy consumption. Predictive maintenance, powered by ML, mitigates these issues by identifying potential failures before they occur.[119] By analyzing historical performance data, real-time sensor readings, and machine operating conditions, ML models predict breakdowns and recommend preventive actions. Key ML applications in predictive maintenance include failure prediction, where time-series analysis detects early signs of machine wear, minimizing unexpected failures, intelligent scheduling, where AI-driven models optimize maintenance timing to reduce production disruptions, and defect minimization, where ML detects anomalies in production processes, enabling corrective actions before defective products are manufactured, ultimately improving the efficiency and sustainability.[120]

Example:

• A deep learning-based predictive maintenance system in a polymer injection molding plant detected early signs of machine failure, reducing unplanned downtime by 40% and material waste by 25%.[121]

• ML was used in 3D printing of polymer composites to predict and correct print defects in real-time, reducing the need for failed print iterations and minimizing material waste.[122]

8. Challenges and future directions

While machine learning (ML) has shown great potential in revolutionizing polymer composite research, several challenges need to be addressed for its widespread adoption and effective implementation. These challenges include data-related limitations, model interpretability, integration with traditional computational methods, and the necessity of physics informed ML models. Additionally, ensuring sustainability in polymer composite development remains a key concern.[123] This section discusses these obstacles and proposes future research directions to improve the reliability, accuracy, and applicability of ML models in this field. Fig. 9 illustrates the challenges in ML.

8.1 Data-related challenges

8.1.1 Scarcity of high-quality data. One of the most significant challenges in applying ML to polymer composites is the limited availability of high-quality datasets. Polymer composites encompass a wide range of materials with diverse compositions and properties, making data collection complex. Furthermore, many composite formulations are developed for niche applications, resulting in a lack of publicly available data. Insufficient datasets can lead to overfitting, where ML models perform well on training data but fail to generalize to new cases.[124]

8.1.2 Data standardization and quality. The lack of standardized data formats across industries and research domains further complicates ML applications. Inconsistencies in measurement units, experimental methods, and data recording practices hinder the development of robust ML models.[125] Moreover, experimental data may contain noise or inconsistencies, reducing the accuracy of ML predictions. Establishing comprehensive, high-quality, and standardized datasets is crucial for advancing ML applications in polymer composites.

8.2 Model interpretability and physical understanding

8.2.1 Trade-off between accuracy and interpretability. Many ML models, especially deep learning algorithms, function as "black boxes," offering high accuracy but limited interpretability. This lack of transparency poses a challenge in polymer science, where understanding the underlying material behavior

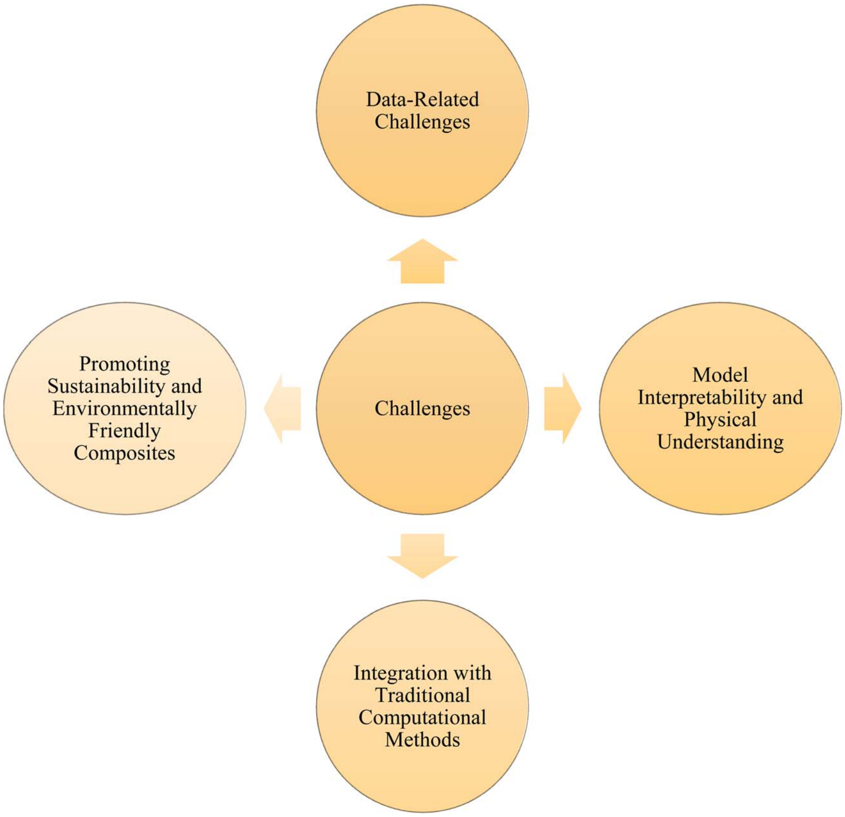

Fig. 9 Challenges in ML.

is crucial. Researchers must strike a balance between model accuracy and interpretability to ensure that ML predictions provide meaningful scientific insights.[126]

8.2.2 Physics-informed ML models. Integrating physics-based knowledge into ML models is essential for ensuring reliable and physically consistent predictions. Traditional ML approaches rely solely on data-driven learning, which may lead to physically implausible results.[127] By incorporating first-principles calculations, such as density functional theory (DFT) or molecular dynamics (MD) simulations, ML models can enhance their predictive capabilities while maintaining adherence to established physical laws.

8.3 Integration with traditional computational methods

8.3.1 Hybrid approaches for efficiency. Traditional computational techniques, such as finite element analysis (FEA) and computational fluid dynamics (CFD), provide high-fidelity simulations but are computationally expensive. ML models can accelerate these simulations by serving as surrogate models, significantly reducing computational costs.[128] For example, ML models trained on a subset of FEA simulations can predict stress distributions in composites without running full simulations, expediting the design and optimization process.

8.3.2 Enhancing ML with synthetic data. In scenarios where experimental data are scarce, physics-based simulations, including finite element analysis (FEA) and molecular dynamics (MD), can produce high-fidelity synthetic datasets that serve to enhance machine learning training.[129] This hybrid approach improves model generalization by integrating fundamental material behavior and physical laws, thereby minimizing dependence on extensive experimental datasets. Furthermore, physics-informed machine learning models have the capability to enhance predictions by applying constraints based on established scientific principles, thereby ensuring alignment with real-world phenomena.[130] Researchers can enhance the reliability and interpretability of machine learning models for polymer composites and related materials by integrating data-driven learning with first-principles calculations.

8.4 Promoting sustainability and environmentally friendly composites

8.4.1 Eco-friendly material discovery. ML can facilitate the discovery of biodegradable and recyclable polymer composites by predicting their environmental impact based on chemical composition and processing methods. By screening vast material libraries, ML can identify sustainable alternatives that balance performance with ecological benefits.[131]

8.4.2 Optimizing recycling and circular economy processes. ML algorithms can optimize polymer composite recycling by identifying the best conditions for material recovery and reuse. For instance, ML models can predict the mechanical properties of recycled polymers, allowing manufacturers to adjust processing conditions accordingly.[132] This approach reduces waste, promotes circular economy principles, and minimizes reliance on virgin raw materials.

8.5 Integration with traditional computational methods

The FEA computational fluid dynamics (CFD) and other traditional computational methods have long been used to simulate the behavior of polymer composites. However, these methods can be computationally expensive and time-consuming, especially for complex, large-scale problems. Integrating ML with traditional methods can offer a more efficient and comprehensive approach to composite analysis.[133]

8.5.1 Speed and efficiency. ML models can be trained to predict the outcomes of computational methods like FEA much more quickly, reducing the time required for simulations. For example, a trained ML model could predict stress distributions in composite materials without running a full FEA simulation, allowing for rapid optimization during the design process.[134]

8.5.2 Accuracy enhancement. Conversely, traditional computational methods can enhance ML models by providing high-fidelity synthetic data. These data can be used to train ML algorithms when experimental data are unavailable or insufficient.[135]

8.6 Promoting sustainability and environmentally friendly composites

Sustainability is an increasingly important consideration in materials science, and polymer composites are of no exception. The development of eco-friendly composites, efficient recycling methods, and sustainable manufacturing processes is essential to reduce the environmental impact of polymer composites. ML can play a critical role in achieving these goals.[136]

8.6.1 Eco-friendly material discovery. ML can accelerate the discovery of biodegradable or recyclable composites by identifying material formulations that combine high performance with environmental sustainability. Algorithms can predict the environmental impact of different composites based on their chemical compositions and manufacturing processes, guiding researchers toward greener alternatives.[137]

8.6.2 Optimizing recycling processes. ML models can also optimize the recycling of polymer composites by identifying the best processing conditions for recovering valuable materials such as fibres or polymers. This will enable more efficient reuse of composite materials, reducing waste and the need for virgin raw materials.[137]

9. Case studies on ML-guided experimental validation

9.1 ML-driven discovery of high-performance polymers

9.1.1 ML prediction and experimental validation. A research team aimed to develop a high-performance polymer blend for aerospace applications. They trained a machine learning model on large datasets of polymer properties, including molecular weight, chain structure, and cross-linking density. The model predicted polymer formulations with high strength and thermal stability.[138] Several polymer blends were synthesized and subjected to mechanical testing (*e.g.*, tensile strength and elongation at break) and thermal analysis (*e.g.*, thermogravimetric analysis and differential scanning calorimetry).

9.1.2 Experimental feedback and model refinement. Despite initial ML predictions, some synthesized blends exhibited inconsistent thermal stability in real-world tests. The ML model underestimated polymer chain rigidity and cross-linking behavior, leading to suboptimal performance. To improve accuracy, the model was retrained with additional features such as polymer chain stiffness and cross-linking density.[139] After refinement, the updated model successfully predicted a new polymer blend that met strength requirements and demonstrated superior thermal stability, resulting in an advanced composite material for aerospace applications.[79]

9.2 ML for high-energy lithium-ion batteries

9.2.1 ML prediction and experimental validation. A deep learning model was trained on a dataset of known cathode materials, focusing on chemical composition and electrochemical behavior. The goal was to predict materials with higher energy density and longer cycle life. Several ML-predicted cathode materials were synthesized and tested in coin cell batteries for charge/discharge capacity, cycle life, and rate capability.[140]

9.2.2 Experimental feedback and model refinement. Although some materials exhibited high energy densities, they degraded quickly after a few hundred charge cycles due to structural instability. This issue was not fully accounted for by the initial ML model.[141] The model was refined by incorporating additional descriptors related to structural stability, ionic conductivity, and crystallographic properties. With these refinements, the updated ML model successfully predicted a new cathode material that demonstrated both higher energy density and improved cycle life, outperforming traditional lithium cobalt oxide ($LiCoO_2$).

9.3 ML-driven discovery of sustainable biodegradable composites

9.3.1 ML prediction and experimental validation. Researchers used an ML model to predict optimal fiber–resin combinations for sustainable biodegradable composites. The model suggested several fiber (*e.g.*, flax and hemp) and resin (*e.g.*, PLA and PHA) combinations, which were synthesized and tested for mechanical strength (tensile and flexural) and biodegradability in soil and marine environments.[142]

9.3.2 Experimental feedback and model refinement. While some composites showed strong mechanical performance, their biodegradation rates were inconsistent due to fiber–resin interactions affecting water absorption. The ML model was refined by incorporating additional factors like fiber–resin bonding and environmental exposure conditions. After retraining, the updated model identified a fiber–resin combination with both high strength and rapid biodegradation, making it ideal for eco-friendly packaging materials.[143,144]

10. Future research directions

The application of ML in polymer composites is still in its early stages, and there are numerous opportunities for future research that can significantly enhance its impact in this field. The following areas highlight key research directions that can pave the way for more advanced applications of ML in polymer composites.[145]

10.1 Development of more robust ML models

Future research should focus on the development of more sophisticated ML models that can handle the complexity inherent in polymer composites. This includes the following.

10.1.1 Multi-scale modeling. Research should prioritize the development of ML models that can operate across different scales, from atomic and molecular levels to macroscopic properties. By integrating multi-scale modeling techniques, researchers can capture the hierarchical structure of composites, thereby improving the prediction of composite behaviors that depend on microstructural features.[146]

10.1.2 Nonlinear behavior handling. Many polymer composites exhibit nonlinear mechanical behaviors, particularly under varying loading conditions. Future models should incorporate algorithms capable of recognizing and accurately predicting these nonlinear responses, providing insights into how materials will perform under different stress and strain conditions.[147]

10.1.3 Adaptive learning. Incorporating adaptive learning techniques can enhance the ability of ML models to update themselves as new data become available. This can be particularly useful in dynamic applications where material performance may change over time or in response to different environmental conditions.[148]

10.2 Better data generation techniques

The creation of high quality, standardized datasets remains a priority for the advancement of ML applications in polymer composites. Key areas of focus include the following:

10.2.1 High-throughput experimentation. Advances in experimental techniques that allow for the simultaneous testing of multiple composite formulations will be crucial. High-throughput experimentation enables researchers to quickly collect large datasets covering a wide range of material compositions and processing parameters, providing a solid foundation for training accurate ML models.[149]

10.2.2 Synthetic data generation. In scenarios where experimental data are limited or difficult to obtain, the development of advanced simulation techniques to generate synthetic data can be beneficial. Researchers should focus on improving computational models that can simulate the behavior of composites under different conditions, creating a robust dataset that complements experimental findings.[8,150]

10.2.3 Data augmentation techniques. Exploring data augmentation strategies, such as using generative adversarial networks (GANs) or other statistical methods, can enhance the diversity and robustness of training datasets. This will help mitigate issues related to overfitting and improve the generalizability of ML models.[151]

10.3 Interdisciplinary collaboration

Collaboration between materials scientists, computer scientists, engineers and domain experts is essential to advance the application of ML in polymer composites. Interdisciplinary teams can achieve the following:

10.3.1 Bridging expertise gaps. By bringing together experts from different fields, teams can combine their knowledge of material behavior, computational methods, and ML techniques.[152] This collaboration will lead to the development of more effective ML models that consider both materials science principles and advanced computational methods.

10.3.2 Innovative solutions. Interdisciplinary collaboration can foster creativity and innovation, leading to the discovery of novel approaches to solve complex problems in polymer composites. The integration of different perspectives can lead to breakthrough solutions that address pressing challenges in materials design, manufacturing and application.[153]

10.3.3 Education and training. Promoting interdisciplinary education and training programs will help equip the next generation of researchers with necessary skills to work effectively in cross-functional teams. This will enhance the capacity for collaboration and innovation in the field.[154]

11. ML for new manufacturing techniques

As advanced manufacturing techniques such as 4D printing and smart materials develop, ML will be instrumental in optimizing these processes. Research opportunities in this area include the following:

11.1 Smart materials development

ML can help design composites that respond to environmental stimuli such as temperature, humidity or mechanical stress. This could lead to the creation of materials that can adapt their properties or configurations in real time, improving their functionality and performance.[155]

11.2 Self-healing composites

The design and development of self-healing polymer composites can benefit from ML by predicting the optimal formulations and processing conditions for enhancing healing capabilities. By analyzing the underlying mechanisms of self-healing, ML can guide the synthesis of materials that repair damage autonomously, thereby extending their service life.[156]

11.3 Process optimization for additive manufacturing

In additive manufacturing, ML can be used to optimize process parameters such as print speed, layer thickness, and material feed rates. By predicting the effects of these parameters on the mechanical properties of finished parts, ML can help manufacturers produce high-quality composites with reduced waste and improved efficiency.[24,157]

11.4 Real-time monitoring and control

The implementation of ML techniques for real-time monitoring and control of manufacturing processes can improve the quality assurance of polymer composites. ML algorithms can analyze sensor data during manufacturing to identify anomalies and adjust parameters on the fly to ensure consistent product quality.[158] In conclusion, the integration of ML into the field of polymer composites offers a wealth of opportunities for advancing material design, manufacturing, and performance prediction.[8,159] By addressing the challenges identified and pursuing the proposed research directions, the potential of ML can be fully realized, leading to innovative and sustainable solutions in polymer composite applications.[160]

12. Conclusions

The incorporation of machine learning into polymer composites presents a significant opportunity to enhance the design, manufacturing processes, and performance forecasting of these materials. As the field develops, several key conclusions can be drawn:

• Machine learning can significantly enhance the performance of polymer composites through discovery of novel material formulations and optimization of their properties. Neural networks, support vector machines, and random forests are techniques utilized for the analysis of complex datasets. These methods are capable of identifying patterns and correlations that may not be detectable through traditional analytical approaches. This facilitates the development of advanced composite solutions designed for particular applications, including lightweight structures in aerospace and biocompatible materials in medical devices.

• The effective implementation of machine learning in polymer composites depends on overcoming several challenges, such as data scarcity, standardization, and model interpretability. Joint initiatives aimed at producing thorough, high-quality datasets, coupled with the advancement of interpretable models *via* explainable AI (XAI) and physics-informed machine learning, will improve the dependability and usability of machine learning in this field.

• The intricate nature of polymer composites necessitates cooperation among various fields, such as materials science, computer science, and engineering. Interdisciplinary partnerships will facilitate the exchange of knowledge and expertise, resulting in enhanced ML models and novel strategies for material development and processing. Multi-fidelity modeling techniques can enhance collaboration by integrating high-fidelity simulations with machine learning predictions.

• ML-IAPs have revolutionized polymer simulations by enhancing the accuracy and efficiency. Advances in long-range interactions, equivariant networks, and deep learning have improved material design and property prediction. Challenges remain in data availability and model interpretability, but continued research will unlock ML-IAPs' full potential, accelerating polymer discovery and optimization.

• The increasing importance of sustainability in materials science highlights the potential of machine learning to advance eco-friendly composites and recycling methods. Techniques such as life cycle analysis (LCA) and optimization algorithms play a crucial role in identifying biodegradable materials and improving recycling strategies, thus contributing to the reduction of the environmental impact linked to polymer composites.

• Future research should focus on the advancement of robust machine learning models that can effectively capture the complexities inherent in polymer composites. Additionally, there is a need to enhance data generation techniques, including high-throughput experimentation and synthetic data generation. The investigation of advanced manufacturing methods, such as 4D printing and smart materials, presents significant opportunities for future research that may result in innovative applications across multiple industries.

The convergence of machine learning and polymer composites presents significant potential for advancing innovation and promoting sustainability within the field of materials science. Addressing current challenges, leveraging advanced techniques, and pursuing future research directions will enable the field to harness the full potential of machine learning. This approach aims to create high-performance, environmentally friendly composite materials that satisfy the requirements of contemporary applications.

Data availability

Data will be made available on request.

Author contributions

Manickaraj Karuppusamy: writing – review & editing, writing – original draft, conceptualization; Ramakrishnan Thirumalaisamy: writing – review & editing, writing – original draft, methodology; Sivasubramanian Palanisamy: writing – review & editing, writing – original draft, formal analysis, data curation; Sudha Nagamalai: writing – review & editing, writing – original draft, investigation, resources; Ehab El Sayed Massoud: writing – review & editing, writing – original draft, visualization; Nadir Ayrilmis: writing – review & editing, writing – original draft, funding acquisition.

Conflicts of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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