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Review Article

A REVIEW OF MACHINE LEARNING TECHNIQUES FOR SUSTAINABILITY PREDICTION IN COMPOSITE MATERIALS

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ABSTRACT

Composite materials are renowned for their exceptional mechanical properties and customizable functionalities, rendering them essential across a wide array of industries. Nevertheless, their inherent complexity presents challenges in forecasting sustainability indicators, including environmental impact, circularity potential, and economic viability throughout their entire lifecycle. Machine learning (ML) techniques have emerged as potent tools for addressing these multifaceted prediction tasks by employing data-driven modeling approaches. This review offers a comprehensive examination of the current state of ML applications in the sustainability prediction of composite materials. It scrutinizes critical components such as dataset curation, feature engineering, ML algorithm selection, and model validation. Furthermore, this work delves into ML applications for predicting environmental footprints, recyclability, and lifecycle costs. The review also underscores existing challenges, potential research directions, and the prospects for integrating ML with other computational techniques to unveil new sustainability insights. By bridging the domains of composite materials and ML, this work aspires to expedite the transition toward a circular economy while advancing the development of high-performance, eco-friendly composites.

1 Introduction

Composite materials have revolutionized various sectors due to their exceptional strength-to-weight ratio, tailorable properties, and multifunctionality. From aerospace and automotive to construction and renewable energy, these engineered materials have become indispensable [1]. However, their inherent complexity, involving intricate compositions and manufacturing processes, poses significant challenges in predicting

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sustainability indicators across their entire lifecycle [2]. These indicators encompass environmental impacts, circularity potential, and economic viability, which are crucial for transitioning toward a circular economy and achieving sustainable development goals.

Traditionally, sustainability assessments of composite materials have relied on physics-based modelling, analytical techniques, and experimental characterization [3]. While these approaches provide valuable insights, they often suffer from limitations such as high computational costs, simplified assumptions, and resource-intensive experimentation. Additionally, capturing the intricate interplay between material composition, processing conditions, and sustainability outcomes remains a formidable task [4].

In recent years, machine learning (ML) techniques have emerged as powerful data-driven tools for sustainability prediction, offering a complementary approach to conventional methods [5]. By leveraging large datasets and sophisticated algorithms, ML models can uncover intricate patterns and relationships, enabling accurate predictions of sustainability indicators without relying on explicit physics-based equations or extensive experimentation [6].

This review provides a comprehensive overview of the state of the art in applying ML for the sustainability prediction of composite materials. It examines critical aspects such as dataset curation, feature engineering, ML algorithm selection, and model validation. Additionally, this study delves into specific ML applications for predicting the environmental footprints, recyclability, and lifecycle costs of composites. This review also highlights existing challenges, prospective research directions, and the potential for integrating ML with other computational techniques to unlock new sustainability insights. By bridging composite materials and ML, this work aims to accelerate the transition toward a circular economy while bolstering the development of high-performance, eco-friendly composites.

2 Composite Materials and Sustainability Challenges

2.1 OVERVIEW OF COMPOSITE MATERIALS

Composite materials are engineered by combining two or more constituents with distinct properties, resulting in a material with enhanced characteristics tailored for specific applications [7]. These materials typically consist of a reinforcing phase, such as fibers or particles, embedded in a matrix phase, such as polymers, ceramics, or metals. The synergistic combination of these phases endows composites with superior mechanical properties, thermal resistance, and durability compared to their individual constituents [8]. Common examples of composite materials include the following:

Fiber-reinforced polymers (FRPs): FRPs are glass, carbon, or aramid fibers embedded in a polymer matrix and are widely used in aerospace, automotive, and wind turbine blades [9].

Particle-reinforced composites: Ceramic or metallic particles dispersed in a metal or polymer matrix enhance strength and wear resistance [10]. Laminated composites: Layers of different materials bonded together, such as carbon-fiber reinforced polymer (CFRP) laminates or metal-ceramic laminates [11]. Structural composites: Concrete reinforced with steel rebar or fiber-reinforced concrete for construction applications [12].

2.2 SUSTAINABILITY CHALLENGES IN COMPOSITE MATERIALS

Despite their remarkable properties, composite materials pose significant sustainability challenges throughout their lifecycle, from raw material extraction and manufacturing to use and end-of-life management [13]. These challenges can be categorized into three main aspects

- **Environmental Impact:** The production of composite materials often involves energy-intensive processes and the use of non-renewable resources, which contribute to greenhouse gas emissions and resource depletion [14]. Additionally, the disposal of composites can be problematic due to their complex nature, leading to potential environmental contamination [15].
- **Circularity Potential:** Composite materials are inherently difficult to recycle or reuse due to their heterogeneous composition and strong interfacial bonding between constituents [16]. This hinders the transition toward a circular economy, where materials are continuously cycled back into the supply chain, minimizing waste and maximizing resource efficiency[17].
- **Economic Viability:** The manufacturing of composites can be costly, especially for high-performance applications, which can impact their economic viability [18]. Moreover, the lack of

efficient recycling and reuse strategies can further increase lifecycle costs and hamper the adoption of composites in cost-sensitive sectors [19]. Addressing these sustainability challenges is crucial for realizing the full potential of composite materials while minimizing their environmental footprint and promoting a circular economy. Accurate prediction and quantification of sustainability indicators throughout the lifecycle are essential for informed decision-8making, optimizing material designs, and implementing effective mitigation strategies [20].

3 Machine Learning for Sustainability Prediction

3.1 OVERVIEW OF MACHINE LEARNING TECHNIQUES

Machine learning (ML) is a subset of artificial intelligence that enables computers to learn from data and make predictions or decisions without being explicitly programmed [21]. ML algorithms can discover patterns and relationships within complex datasets, allowing them to perform tasks such as classification, regression, clustering, and anomaly detection [22].
The two main categories of ML techniques are as follows:

- **Supervised Learning:** In this approach, the algorithm learns from labelled training data, where the input features (e.g., material composition, processing conditions) are mapped to known output values (e.g., mechanical properties, environmental impact) [23]. Common supervised learning algorithms include linear regression, decision trees, support vector machines, and neural networks.
- **Unsupervised Learning:** Here, the algorithm learns from unlabelled data without any predetermined output values [24]. It aims to discover inherent patterns, structures, or relationships within the data. Examples of unsupervised learning techniques include clustering algorithms (k-means, hierarchical clustering) and dimensionality reduction methods (principal component analysis, t-SNE). In the context of sustainability prediction for composite materials, both supervised and unsupervised learning techniques can be employed, depending on the specific task and available data.

3.2 ADVANTAGES OF MACHINE LEARNING FOR SUSTAINABILITY PREDICTION

ML offers several advantages over traditional physics-based modeling and experimental approaches for the sustainability prediction of composite materials:

- **Data-driven Modelling:** ML algorithms can leverage large datasets encompassing material compositions, processing conditions, and sustainability indicators, enabling data-driven modelling without relying on explicit physical equations or assumptions [25].
- **Handling Complexity:** Composite materials exhibit complex relationships between their constituents, manufacturing processes, and sustainability outcomes. ML techniques can effectively capture these intricate patterns and nonlinearities, providing accurate predictions [26]
- **Rapid Evaluation:** Once trained ,ML models can quickly evaluate new material compositions or processing conditions, enabling rapid screening and optimization of sustainable composite designs [27]. Transfer Learning: Pretrained ML models can be fine-tuned on specific composite datasets, leveraging knowledge from related domains and reducing the need for extensive training data [28]. Uncertainty Quantification: Advanced ML techniques, such as Bayesian methods and ensemble models, can provide uncertainty estimates along with predictions, enabling more informed decision-making [29].
- **Integration with Other Techniques:** ML can be combined with physics-based models, experimental data, and other computational techniques (e.g., density functional theory and molecular dynamics) to enhance predictive capabilities and gain deeper insights [30]. By harnessing the power of ML, researchers and industries can accelerate the development of sustainable composite materials while minimizing environmental impacts, promoting circularity, and ensuring economic viability throughout the lifecycle.

4 Data Acquisition and Pre-processing

4.1 DATA SOURCES AND CURATION

The performance of ML models relies heavily on the quality and quantity of the training data. In the context of composite materials, relevant data sources can include the following: Experimental Databases: Published literature, technical reports, and proprietary datasets containing measurements of composite properties, environmental impacts, and lifecycle assessments [31].

- Simulation Datasets: Data generated from computational modelling techniques, These methods include finite element analysis, molecular dynamics simulations, and process simulations [32].
- Industrial Data: Manufacturing process data, quality control records, and lifecycle inventory data from composite material producers and end-users [33].
- Open Data Repositories: Publicly available databases and online repositories hosting composite material data, such as the NIST Material Data Repository [34]. and Materials Project [35].
- Consolidating data from these diverse sources is crucial for creating comprehensive and representative datasets for ML model training. However, this process often involves addressing the following challenges:
- Data Heterogeneity: Disparate data formats, units, and nomenclatures across different sources require standardization and harmonization [36].
- Data Quality: Missing values, outliers, and measurement errors are eliminated through data cleaning and pre-processing techniques [37].
- Data Privacy and Security: Ensuring proper anonymization and protection of sensitive industrial data while maintaining data utility [38].
- Effective data curation strategies, involving domain expertise, automated tools, and collaborative efforts, are essential for assembling high-quality datasets suitable for ML modelling.

4.2 FEATURE ENGINEERING

Feature engineering is the process of selecting, transforming, and creating relevant input features (predictors) from the raw data to improve the performance of ML models. In the context of composite materials, feature engineering involves careful consideration of factors that influence sustainability indicators, such as:

- Material Composition: Weight fractions, volume fractions, or ratios of constituent materials (fibres, matrices, fillers, additives) [39].
- Processing conditions: temperature, pressure, curing time, cooling rate, and other manufacturing parameters [40].
- Structural Properties: Fiber orientation, void content, layer thickness, and other microstructural characteristics [41].
- Environmental Factors: Operating conditions (temperature, humidity, and UV exposure) and service life data[42].
- The feature engineering techniques may include the following:
- Domain Knowledge: Leveraging expert knowledge and establishing relationships from materials science and engineering to identify relevant features [43].
- Dimensionality reduction: Techniques such as principal component analysis (PCA) or t-distributed stochastic neighbour embedding (t-SNE) are used to reduce the feature space while preserving relevant information [44].
- Feature Transformation: Applying mathematical transformations (e.g., logarithmic, polynomial) or encoding categorical features to improve model performance [45].
- Feature Selection: Identifying the most informative features and eliminating redundant or irrelevant ones using methods such as recursive feature elimination or regularization techniques [46].

Effective feature engineering can significantly improve the predictive power of ML models, reduce overfitting, and enhance interpretability by capturing the most relevant information from the raw data.

5 MACHINE LEARNING ALGORITHMS FOR SUSTAINABILITY PREDICTION

5.1 SUPERVISED LEARNING ALGORITHMS

Supervised learning algorithms are widely employed for predicting quantitative sustainability indicators, such as environmental impacts (e.g., carbon footprint and energy consumption), recycling potential, and lifecycle costs. Common algorithms used in this context include the following:

Regression algorithms

- Linear Regression: Linear relationships between the input features and the target variable are modelled
- (Csányi Gáborand Willatt, 2020)
- .
- Decision Tree Regression: A tree-like model is built by recursively partitioning the feature space based on decision rules[48].
- Support Vector Regression (SVR): Mapping input features to a high-dimensional space and finding the optimal hyperplane for regression [49].
- Gaussian Processes: Probabilistic models that can capture complex, nonlinear relationships and provide uncertainty estimates [50].

Neural Networks

- Feedforward Neural Networks: Multilayer networks with interconnected nodes that can model intricate, nonlinear relationships [51].
- Convolutional Neural Networks (CNNs): CNNs specialize in processing structured data such as images or spatial representations of composite microstructures [52].

Ensemble Methods

- Random Forests: Multiple decision tree models are combined to improve the predictive accuracy and robustness [53].
- Gradient boosting: This method iteratively combines weak models (e.g., decision trees) to build a strong predictive model [54].
- Stacking/Blending: Combining predictions from multiple algorithms using meta-learners or weighted averaging [55].

The choice of algorithm depends on factors such as the complexity of the problem, the nature of the data (linear or nonlinear relationships), interpretability requirements, and the trade-off between model accuracy and computational efficiency.

5.2 UNSUPERVISED LEARNING ALGORITHMS

Unsupervised learning techniques can be valuable for exploratory data analysis, identifying patterns and clusters within composite material data, and potentially uncovering new insights related to sustainability. Common unsupervised algorithms include the following:

Clustering Algorithms

- K-Means Clustering: Partitioning data into k clusters based on similarity measures, which is useful for grouping materials with similar sustainability characteristics [56].
- Hierarchical Clustering: Creating a hierarchy of clusters by iteratively merging or splitting clusters, enabling multilevel exploration of material groups [57].

Dimensionality Reduction Techniques:

- Principal component analysis (PCA): Transforming high-dimensional data into a lower-dimensional space while preserving the most relevant information facilitates visualization and feature extraction [58].
- t-Distributed stochastic neighbour embedding (t-SNE): This is a nonlinear dimensionality reduction technique for visualizing high-dimensional data in a low-dimensional space, revealing underlying structures and patterns [59].

Anomaly detection:

- One-class support vector machines (OC-SVMs): These methods identify outliers or anomalies in composite material data that deviate significantly from normal patterns and are useful for quality control and identifying sustainability risks [60].
- Isolation Forests: Ensemble-based anomaly detection method that isolates anomalies by constructing random decision trees [61].

Unsupervised learning can provide valuable insights into the inherent structures and relationships within composite material data, potentially leading to the discovery of new sustainable material designs or the identification of critical factors influencing sustainability indicators.

6 Model Evaluation and Validation

6.1 PERFORMANCE METRICS

Evaluating the performance of ML models is crucial for assessing their predictive accuracy and ensuring reliable sustainability predictions. Common performance metrics used for regression tasks (e.g., predicting environmental impacts or lifecycle costs) include the following:

- Mean squared error (MSE) and root mean squared error (RMSE): The average squared difference between the predicted and actual values is measured, with the RMSE providing an interpretable scale[61].
- Mean absolute error (MAE): The MAE measures the average absolute difference between the predicted and actual values and is less sensitive to outliers than the MSE.
- Coefficient of determination (R^2): Quantifying the proportion of variance in the target variable explained by the model, ranging from 0 to 1 [62].
- For classification tasks (e.g., predicting recyclability or material selection), common metrics include the following:
- Accuracy: The proportion of correctly classified instances [63].
- Precision, Recall, and F1-Score: Measuring the trade-off between precision (fraction of true positives among predicted positives) and recall (fraction of true positives identified) [64].

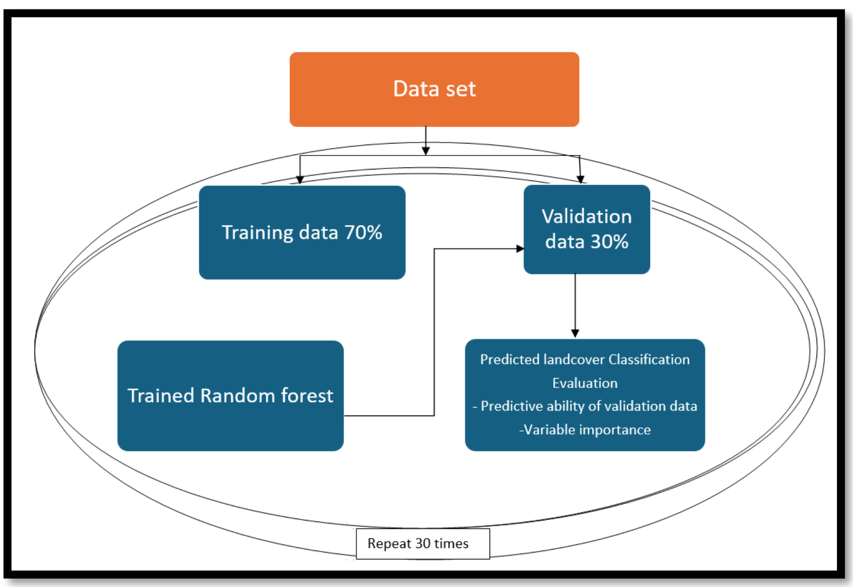

Figure 1: Data selection process, model validation and evaluation.

From figure 1 can state that, the classifier was developed using 70% of the dataset as training data and 30% as validation data. The dataset split and classifier was run 30 times. Classifier performance mean and variance as well as variable importance values were calculated from the outputs. The figure illustrates a structured approach to building a reliable landcover classification model using Random Forest, a popular machine learning algorithm. Let us have a full dataset of satellite images or geographical data, and need to train a model to classify different land types (like forest, water, urban, etc.).
Step by step illustration
Split the Dataset

First, we divide the dataset into two parts: 70% for training the model and 30% for validation. This split is done carefully using a stratified random method, ensuring that each landcover class is well-represented in both sets.

Train the Random Forest

A Random Forest model is then trained using the 70% training data. In this case, the model is made up of 500 decision trees to ensure robustness and accuracy.

Evaluate the Model

Once trained, the model is tested using the 30% validation data. The goal is to see how well the model predicts landcover types that it hasn't seen before. During this step, two things are evaluated:

First, how accurately the model predicts landcover and second which variables (features) were most important in making those predictions.

Repeat for Reliability

To make sure the model's performance isn't just a fluke due to random splits, the entire process—from splitting the data to evaluating predictions—is repeated 30 times. This repetition improves confidence in the results.

By this way Data selection process, model validation and evaluation can be done. Figure 2 explains Precision vs. Accuracy (Based on the Target Diagram), helps to understand two key concepts in data science and measurement systems: precision and accuracy. Let's assume as throwing darts at a target (like in archery or darts). The centre of the target — marked "X" — represents the true or ideal value.

High Precision, Low Accuracy It looks like: All darts land close together — but far from the bullseye.

It means: Results are consistent (can repeat the same result), but they are consistently wrong.

Real-life example: A faulty thermometer that gives you the same wrong temperature every time.

High Precision, High Accuracy It looks like: All darts are tightly grouped and close to the bullseye.

It means: Measurements are consistent and correct — the ideal situation!

Real-life example: A well-calibrated sensor or a machine learning model that performs consistently well.

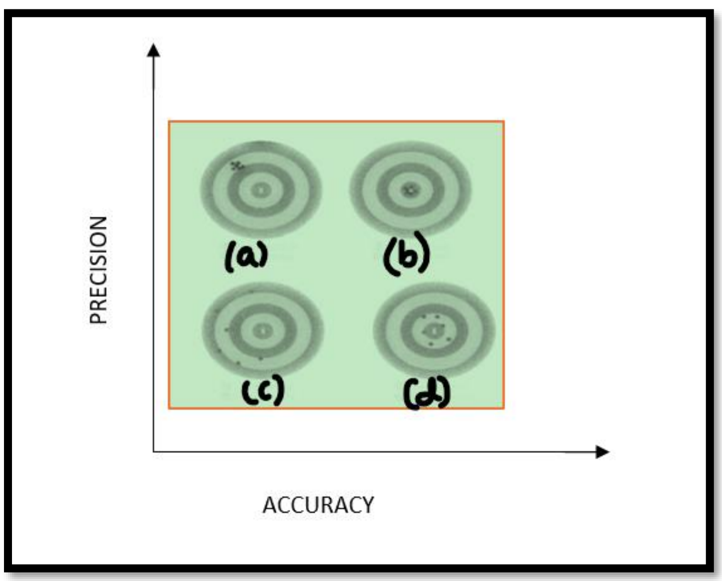

Figure 2: Illustrates the difference between precision and accuracy in machine learning [65].

Low Precision, Low Accuracy It looks like: Darts are scattered all over the place, and none are near the bullseye. It means: The results are inconsistent and wrong — the worst case. Real-life example: A broken or misaligned measuring tool giving random values each time. Low Precision, High Accuracy It looks like: The darts are spread out, but their average position is near the bullseye. It means: Generally getting the right answer on average, but the results are inconsistent. Real-life example: A scale that fluctuates slightly each time you weigh the same object, but the average is correct. Summary can be illustrated based on ideal data, which can be the Accuracy as how close they dart are to the true value. Precision as how consistent the measurements are.

To build reliable systems, whether in science, engineering, or machine learning, usually aim for both high accuracy and high precision. Area under the receiver operating characteristic curve (AUC-ROC): The area under the receiver operating characteristic curve (AUC-ROC) is used to evaluate the model's ability to distinguish between classes at various classification thresholds [66]. Additionally, domain-specific metrics tailored to composite material sustainability, such as lifecycle impact scores or circularity indices, can be employed for more contextualized model evaluation.

6.2 VALIDATION STRATEGIES

To ensure the reliability and generalizability of ML models, proper validation strategies are essential. Common validation approaches include the following:

- Hold-out Validation: The dataset is split into training and test sets, where the model is trained on the training set and evaluated on the unseen test set [67].
- Cross-validation: The data were partitioned into multiple folds, the model was trained on a combination of folds, and the remaining folds were evaluated; this process was repeated for all fold combinations [68].
- Nested cross-validation: Cross-validation is performed within an outer cross-validation loop, enabling unbiased model selection and hyperparameter tuning[69].

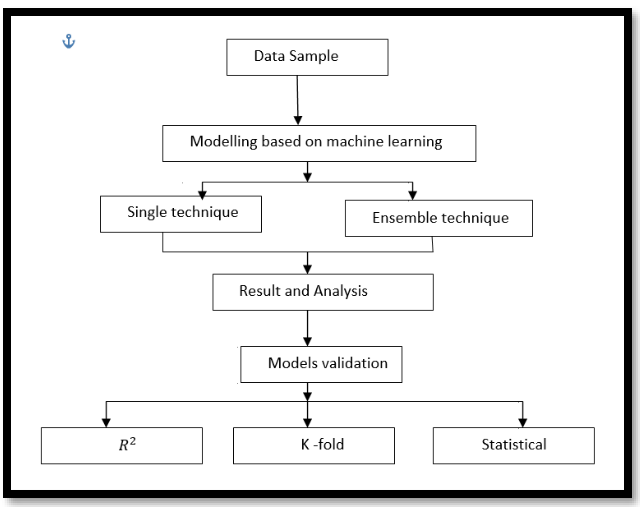

Figure 3:Sequence of ML and validation strategies adopted [67].

Figure 3 shows the sequence of ML and validation strategies which are stated. Validation strategies help assess the model's ability to generalize to unseen data, mitigate overfitting, and provide realistic estimates of predictive performance.

- A data sample is first generated through an experimental strategy. (This refers to collecting data, often in a lab or simulation, based on planned experiments.)
- The collected data is then modeled using machine learning techniques. (This means algorithms are applied to understand patterns or predict outcomes.)
- Two modeling approaches are considered:
- In one path, a single technique is used.
- In the other, an ensemble technique is applied, where multiple models are combined to improve performance. From both paths, results are obtained and analyzed. (The outputs of the models are compared, visualized, or summarized.)

- Model validation is carried out to assess the trustworthiness and generalizability of the model's predictions.
  (This ensures the model works not just on training data, but also unseen data.)
- Finally, model performance is evaluated using validation metrics, such as:
- R^2 (Coefficient of Determination) – to measure how well predictions match actual values.
- K-fold cross-validation – to check model performance across multiple subsets.
- Statistical tests – to verify the reliability and significance of results.

6.3 INTERPRETATION AND EXPLAIN-ABILITY

While ML models can achieve high predictive accuracy, understanding the underlying reasons and factors driving their predictions is crucial, especially in the context of sustainability and decision-making. Several techniques can be employed to enhance the interpretability and interpretability of ML models:
Feature Importance Analysis: This analysis quantifies the relative importance of input features in the model's predictions, providing insights into the most influential factors for sustainability [70].

- Partial Dependence Plots (PDPs) and Individual Conditional Expectation (ICE) Plots:
- Visualizing the marginal and individual effects of input features on the model's predictions [71].
- Local Interpretable Model-Agnostic Explanations (LIME): Approximating complex models with locally interpretable surrogate models to explain individual predictions [72].
- Shapley Additive explanations (Shapley Additive explanations (SHAP): A game-theoretic approach that attributes the model's prediction to the input features, providing local and global explanations [75].

Explainable AI techniques can help domain experts understand the rationale behind ML predictions, validate models against established domain knowledge, and gain insights into the critical factors influencing composite material sustainability.

7 APPLICATIONS OF MACHINE LEARNING FOR SUSTAINABILITY PREDICTION

7.1 ENVIRONMENTAL IMPACT PREDICTION

Predicting the environmental impact of composite materials throughout their lifecycle is crucial for mitigating adverse effects and developing eco-friendly materials. ML techniques have been successfully applied to predict various environmental indicators, such as:
Carbon footprint and greenhouse gas emissions:
ML models have been developed to estimate the carbon footprint and greenhouse gas emissions associated with composite manufacturing processes, considering factors such as material composition, energy consumption, and transportation [73]. These models can aid in identifying low-emission material alternatives and optimizing process parameters for reduced environmental impact.
Energy consumption and resource depletion:
ML algorithms have been employed to predict the energy consumption and resource depletion associated with composite production, use, and end-of-life management [74] . This information can guide the design of energy-efficient manufacturing processes and material selection for minimizing resource exploitation.
Life cycle assessment (LCA):
An LCA is a comprehensive methodology for assessing the environmental impacts of products or processes across their entire lifecycle. ML techniques have been integrated into LCA frameworks to streamline impact assessments, reduce computational costs, and enable rapid evaluation of composite material alternatives [75]. ML models can be trained on existing LCA data or coupled with physics-based LCA models for improved accuracy and efficiency.

7.2 CIRCULARITY POTENTIAL PREDICTION

Enhancing the circularity of composite materials is crucial for transitioning toward a circular economy. ML models can assist in predicting the circularity potential of composites, including the following:
Recyclability and reusability:

ML algorithms can be trained to predict the recyclability and reusability potential of composite materials based on their composition, manufacturing processes, and end-of-life characteristics [76]. These models can guide the design of easily recyclable composites and identify suitable recycling strategies.

Degradation and Durability:

The durability and degradation behaviour of composites over time can impact their circularity potential. ML techniques have been employed to predict material degradation rates, remaining useful life, and the possibility of reuse or refurbishment [77]. This information can inform maintenance strategies and extend the service life of composite products.

Disassembly and Separation:

The effective disassembly and separation of composite constituents are crucial for recycling and reuse. ML models can be developed to predict disassembly complexity and separation efficiency based on factors such as material composition, bonding characteristics, and geometries [78]. These models can assist in designing composites with improved disassembly and separation potential.

7.3 ECONOMIC VIABILITY PREDICTION

Ensuring the economic viability of composite materials is essential for their widespread adoption and sustainable development. ML techniques can contribute to predicting economic indicators, such as the following: Manufacturing Costs ML models can be trained to predict the manufacturing costs of composite materials based on factors such as raw material costs, energy consumption, labour, and equipment [79]. These models can aid in optimizing manufacturing processes, identifying cost-effective material alternatives, and conducting economic feasibility assessments. Lifecycle costs: ML algorithms can be employed to predict the total lifecycle costs of composite materials, considering factors such as manufacturing, transportation, maintenance, and end-of-life management [80]. This information can support informed decision-making and enable cost–benefit analyses for composite material selection and design optimization. Market Demand and Pricing: ML techniques can be used to forecast market demand and pricing trends for composite materials based on historical data, economic indicators, and industry trends [81]. This can assist in strategic planning, investment decisions, and the identification of potential market opportunities for sustainable composite materials.

8 CHALLENGES AND FUTURE DIRECTIONS

8.1 DATA AVAILABILITY AND QUALITY

One of the significant challenges in applying ML for the sustainability prediction of composite materials is the limited availability of high-quality, comprehensive datasets. Many existing datasets are fragmented, proprietary, or lack critical information, such as detailed material compositions, processing conditions, and lifecycle impact assessments. Addressing this challenge requires the following:

- Collaborative Data Sharing Initiatives: Fostering collaborations between academia, industry, and research organizations to share and consolidate composite material data while addressing privacy and intellectual property concerns.
- Standardized Data Formats and Ontologies: Developing standardized data formats, nomenclatures, and ontologies to facilitate data integration and interoperability across different sources.
- Automated Data Curation and Quality Assurance: Leveraging advanced data mining, cleaning, and curation techniques to ensure data quality, consistency, and completeness.

8.2 INTEGRATING PHYSICS-BASED MODELLING AND EXPERIMENTAL DATA

While ML techniques can effectively capture complex patterns in data, they may struggle to extrapolate beyond the training data distribution or incorporate physical constraints and domain knowledge. Integrating ML with physics-based modeling and experimental data can address these limitations and enhance the predictive capabilities of sustainability models. Potential approaches include:

- Hybrid Models: These models combine ML models with physics-based equations or simulations to leverage the strengths of both approaches, such as using ML to capture complex nonlinearities and physics-based models to enforce physical constraints.

- Multifidelity Modeling: Integrating high-fidelity experimental data or high-resolution simulations with lower-fidelity data sources using multifidelity ML techniques, enabling efficient and accurate sustainability predictions.
- Active Learning: Employing active learning strategies to iteratively refine ML models by identifying critical data points for targeted experimental characterization or high-fidelity simulations, reducing the need for extensive data.

8.3 UNCERTAINTY QUANTIFICATION AND SENSITIVITY ANALYSIS

Quantifying the uncertainties associated with ML predictions and understanding the sensitivity of the models to input features is crucial for reliable decision-making and risk assessment in sustainable composite material development. Advanced techniques such as Bayesian neural networks, ensemble methods, and sensitivity analysis techniques (e.g., SHAP, permutation importance) can be explored to provide uncertainty estimates and identify the most influential factors impacting sustainability predictions.

8.4 EXPLAINABLE AND TRUSTWORTHY AI

As ML models become more complex and accurate, ensuring their transparency, interpretability, and alignment with domain knowledge is paramount. Explainable AI techniques, as discussed in Section 6.3, play a crucial role in fostering trust and adoption of ML-assisted sustainability predictions among domain experts, decision-makers, and stakeholders. Ongoing research in this area aims to develop more interpretable ML architectures, post hoc explanation methods, and human-AI interaction frameworks tailored to the domain of composite materials.

8.5 SUSTAINABILITY-DRIVEN MATERIALS DISCOVERY

Beyond predicting the sustainability of existing composite materials, ML techniques can be leveraged for sustainable material discovery and design. This involves combining ML with optimization algorithms, generative models, and Mult objective optimization frameworks to explore vast compositional and processing spaces and identifying novel composite material candidates with optimal sustainability characteristics. Integrating sustainability predictions into the early stages of material design can accelerate the development of ecofriendly, circular, and economically viable composite solutions.

8.6 DEPLOYMENT AND SCALABILITY

As ML models for sustainability prediction mature, their successful deployment and scalability in industrial settings become crucial. This may involve developing user-friendly interfaces, integrating models into existing computational frameworks or decision support systems, and addressing computational resource requirements for large-scale predictions. Cloud computing, distributed computing, and model compression techniques can facilitate the scalable deployment of ML models for sustainability predictions across different sectors and applications.

9 CONCLUSION

Machine learning techniques have emerged as powerful tools for addressing the complex challenge of sustainability prediction for composite materials. By leveraging data-driven modelling approaches, ML algorithms can accurately predict environmental impacts, circularity potential, and economic viability indicators throughout the lifecycle of composites. This review provides a comprehensive overview of the state of the art in applying ML for sustainability prediction, covering critical aspects such as data acquisition, feature engineering, algorithm selection, model evaluation, and validation. Furthermore, this review highlights specific applications of ML in predicting the carbon footprint, energy consumption, recyclability, durability, manufacturing costs, and lifecycle costs of composite materials. These predictions can inform sustainable material design, process optimization, and decision-making, contributing to the transition toward a circular economy while promoting the development of high-performance, eco-friendly composites. Although significant progress has been made, several challenges remain, including limited data availability, the need to integrate physics-based modelling and experimental data, uncertainty quantification, explainable AI, and scalable deployment. Addressing these challenges through collaborative efforts, interdisciplinary research, and innovative computational approaches will be crucial for realizing the full potential of ML-assisted sustainability prediction. As composite materials continue to play a pivotal role across various industries, the integration of ML techniques with sustainability assessments will be instrumental in achieving sustainable development goals, mitigating environmental impacts, and fostering a circular, resource-efficient future. This review paves the way for further advancements in this emerging field, catalysing the development of sustainable and high-performance composite materials through the synergy of machine learning and materials science.

10 Future Outlook

The integration of machine learning and sustainability prediction for composite materials presents numerous exciting opportunities for future research and innovation. Key areas of focus include the following:

10.1 AUTONOMOUS MATERIALS DISCOVERY AND OPTIMIZATION

Combining machine learning with optimization algorithms, generative models, and multi-objective optimization frameworks can enable autonomous material discovery and optimization. This approach can explore vast compositional and processing spaces, identifying novel composite material candidates with optimal sustainability characteristics while meeting performance requirements. Integrating sustainability predictions into the early stages of material design can accelerate the development of eco-friendly, circular, and economically viable composite solutions.

10.2 DIGITAL TWINS AND REAL-TIME MONITORING

The advent of Industry 4.0 and the Internet of Things (IoT) has paved the way for real-time monitoring and digital twin technologies. By integrating machine learning models with sensor data and digital representations of composite materials and processes, it becomes possible to continuously monitor and predict sustainability indicators in real-time. This can enable proactive interventions, process adjustments, and predictive maintenance strategies to optimize sustainability throughout the entire lifecycle of composite materials.

10.3 BLOCKCHAIN-ENABLED TRANSPARENCY AND TRACEABILITY

Incorporating blockchain technology into a composite material supply chain can enhance transparency, traceability, and data integrity. By creating immutable and decentralized records of material compositions, processing conditions, and sustainability assessments, blockchain can facilitate collaborative data sharing, enable secure data provenance, and promote trust among stakeholders. This transparency can drive more informed decision-making and support the development of sustainable and circular composite materials.

10.4 HYBRID INTELLIGENCE AND HUMAN-AI COLLABORATION

While machine learning offers powerful data-driven modelling capabilities, domain expertise and human intuition remain invaluable. Hybrid intelligence approaches that combine machine learning with human domain knowledge and interactive interfaces can unlock new synergies. Human-AI collaboration can facilitate the intuitive exploration of sustainability predictions, enable interactive what-if scenarios, and foster a deeper understanding of the underlying factors influencing composite material sustainability.

10.5 SUSTAINABILITY-DRIVEN ADDITIVE MANUFACTURING

AM techniques, such as 3D printing, offer unique opportunities for sustainable composite material production. By integrating machine learning with AM process simulations and predictive models, it becomes possible to optimize print parameters, material compositions, and geometries to minimize waste, reduce energy consumption, and enhance circularity. This synergy can drive the development of sustainable and tailored composite materials through additive manufacturing processes.

10.6 REGULATORY COMPLIANCE AND POLICY SUPPORT

As sustainability regulations and policies evolve, machine learning can play a crucial role in supporting compliance and informing policymaking. By leveraging predictive models and data-driven insights, regulatory bodies and policymakers can assess the environmental impacts, circularity potential, and economic viability of composite materials across various sectors. This can enable evidence-based decision-making, support the development of sustainable material standards, and promote the adoption of eco-friendly composite solutions. The future of machine learning-assisted sustainability prediction for composite materials is promising and multifaceted. Collaboration among researchers, industries, and policymakers will be essential for navigating this exciting journey, fostering innovation, promoting sustainability, and unlocking the full potential of composite materials in a circular economy.

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