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Prediction of Mechanical Properties for Advanced Engineering Applications utilizing Polymer Composite Materials by Machine Learning

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Abstract

Polymer composites show great promise as engineering materials because of their mechanical performance, resistance to corrosion, lightweight nature, and adaptability in design. Aerospace, automotive, biomedical, maritime, and civil engineers all rely on mechanical property prediction to cut down on trial expenses, expedite product development, and optimize material selection. Speedy design optimization is not possible using traditional numerical and experimental methods due to the high costs associated with material characterisation, computational power, and time. The mechanical properties of advanced polymer composite materials can be predicted utilizing data on their composition, reinforcing qualities, manufacturing conditions, and environmental factors through the use of a machine learning framework developed in this study. A.I., Gradient Boosting, Random Forest, and Support Vector Regression Raising the predicted values of toughness, elastic modulus, flexural strength, impact, and compression. Model generalizability and prediction accuracy are enhanced through data preprocessing, feature engineering, training, hyperparameter adjustment, and cross-validation. In different operating settings, ensemble-based and neural network models outperform regression in predicting composite behavior. Statistical measures like MAE, RMSE, and R³ are used to evaluate performance. Intelligent material design is made possible through the identification of mechanical performance characteristics to avoid expensive laboratory testing. Engineers can use machine learning to speed up the screening process for composite formulations and choose the best material combinations. Enhancing decision-making, decreasing development cycles, and promoting new polymer composites in next-generation engineering systems are all benefits of a data-driven materials engineering prediction framework that is efficient, scalable, and accurate.

Keywords: Mechanical property prediction, random forest, artificial neural networks, feature engineering, materials informatics, predictive modeling.

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INTRODUCTION

Because of their malleability in design, low weight, excellent mechanical strength, resistance to corrosion, and thermal stability, polymer composites are essential advanced engineering materials. The mechanical and physical properties of polymers can be enhanced by mixing them with other materials, such as glass, carbon, aramid, or natural fibers [1]. Composites made of polymers have many uses in fields as diverse as aviation, transportation, healthcare, civil engineering, renewable energy, athletic wear, and defense. Innovative polymer composite systems that reduce production costs and environmental effect while meeting tight technical criteria have been investigated [2, 3]. This is in response to the growing need for lightweight, high-performance constructions.

Elastic modulus, hardness, fatigue life, flexural stress, impact strength, and tensile strength are all affected by a number of variables in polymer composites. Among these features are the following: temperature, void content, curing temperature, matrix composition, fiber orientation, manufacturing method, reinforcing type, and concentration [4, 5]. The mechanical behavior of polymer composites is difficult to forecast because of the complexity of their interactions. Extensive laboratory testing, specialized equipment, trained personnel, and substantial funds are necessary for conventional experimental characterization. Because of their reliability but also their slowness, experimental approaches are not well suited for rapid material combination testing in product development.

The mechanical performance of composite materials is assessed using analytical modeling and finite element analysis. These approaches reveal a lot about how materials behave, but they necessitate a deep understanding of constitutive models and boundary conditions and tend to oversimplify assumptions. Because of extensive design spaces, nonlinear material behavior, and complicated composite designs, computationally expensive numerical simulations are necessary. Intelligent prediction systems, then, need to precisely estimate mechanical parameters while simultaneously decreasing computing complexity and experimental labor [6, 7].

Using data, AI and ML resolve intricate technical challenges. When given historical data, machine learning algorithms can uncover hidden relationships between input variables and desired outputs—all without formulas. Among the many nonlinear interactions that impact the mechanical properties of polymer composites, machine learning performs exceptionally well when used to this task. Using data from tests, simulations, and production factors, machine learning models can make predictions about material selection, design optimization, and quality control [8, 9].

Many supervised machine learning algorithms excel in the field of materials engineering. By utilizing Random Forest methods, nonlinear interactions may be captured and overfitting can be avoided. On medium and small datasets, kernel-based SVR performs well for prediction. Nonlinear material properties may be accurately described by AINNs by mimicking intricate biological learning mechanisms. To enhance prediction, Gradient Boosting—a robust ensemble model—integrates weak learners [10, 11]. To improve the accuracy of engineering forecasts, deep learning architectures have recently advanced to the point where they can extract complicated feature representations from massive materials datasets.

With the use of AI, DA, and ENG, materials informatics speeds up the process of discovering and evaluating materials. Compared to trial-and-error testing, predictive algorithms can screen thousands of composite formulas, expose design characteristics, and optimize manufacturing processes in significantly faster development cycles [12, 13]. This data-driven method decreases experimental expenses and waste while speeding up the creation of next-generation engineered materials.

Even while machine learning is growing rapidly, it still faces several obstacles. Uncertainty can be introduced into prediction models due to experimental and measurement inconsistencies, as there are limited high-quality and large datasets. Enhancing model robustness and generalizability can be achieved through data pretreatment, feature selection, normalization, missing values, and hyperparameter adjustment [14]. We need to consider the dataset, our prediction goals, and the computing restrictions while choosing the appropriate machine learning algorithm. Analyze algorithms with statistical metrics like MAE, RMSE, MAPE, and R^2 to find the best prediction framework.

Research contribution

This study offers a machine learning framework to predict advanced polymer composite material mechanical properties using composition, reinforcement, processing, and environmental parameters. Data pretreatment, feature engineering, hyperparameter adjustment, and cross-validation improve model reliability. ANN, SVR, GB, and Random Forest comparison. The framework speeds material screening, minimizes experimental effort, improves engineering decision-making, and lowers high-performance polymer composite development costs.

Research Novelty

Innovatively, preprocessing and feature engineering integrate various machine learning models into a polymer composite mechanical characteristics prediction framework. Its durable, scalable, and accurate prediction under varied material and manufacturing conditions simplifies laboratory testing and enables intelligent composite material design for advanced engineering.

This study employs machine learning to predict the mechanical properties of advanced polymer composite materials. By means of data pretreatment, feature engineering, model construction, optimization, and validation, this approach calculates crucial mechanical properties. We evaluate the prediction capabilities of several supervised learning methods under varying processing settings and material compositions. The technology enables smarter material design, less testing in the lab, more efficiency in the manufacturing sector, and better engineering decision-making. The development of high-performance composite materials for future engineering advancements can be accelerated through the integration of machine learning with polymer composite research. Section 2 reviews the literature, part 3 suggests a model, and Section 4 presents the results. Sections 5 and 6 conclude the comparison and provide an outlook for the future.

LITERATURE REVIEW

Since polymer composites are lightweight, resistant to corrosion, and very versatile in industrial settings, they have attracted a lot of attention from advanced engineers seeking to improve mechanical performance. Over the last ten years, ML has been employed by academics to forecast the mechanical properties of polymer composites, with the goal of cutting down on time and money spent on experiments. Material science and data-driven modeling improve composite performance and material formulation [15–17].

Previous research used statistical regression to estimate flexural strength, elastic modulus, and tensile strength based on matrix composition, manufacturing features, and fiber content. Although they performed admirably on straightforward datasets, linear and nonlinear regression models failed miserably when faced with complicated, nonlinear correlations between processing factors [18–20]. The growing complexity of composite designs has made it difficult for traditional prediction algorithms to handle high-dimensional datasets and the intricate interactions between material constituents.

The field of materials engineering now has better predictive modeling due to the fast development of AI. When trying to predict the behavior of composite materials, many turn to Artificial Neural Networks (ANNs). Find out how to use experimental datasets with ANNs to characterize nonlinear input-mechanical reactions. It has been demonstrated in many research [21, 22] that multilayer feed-forward neural networks trained using backpropagation algorithms can effectively predict tensile, impact, and compressive strengths. Training ANN models with large datasets and meticulous hyperparameter tuning aims to improve generalization and avoid overfitting.

Nonlinear datasets and small sample sizes are no match for Support Vector Regression (SVR). The ability of SVR to forecast tensile, Young's modulus, and fracture toughness has been proven in multiple kernel-based learning investigations. When it comes to outcome prediction and noise survival, experimental results demonstrate that SVR outperforms regression. Finding the right kernel and optimization parameters can be difficult for any composite material, but it becomes even more so when dealing with heterogeneous materials that have different reinforcement configurations [23, 24].

There appears to be some promise in predicting mechanical properties by combining Random Forest (RF) with Gradient Boosting methods. Stability of Random Forest predictions, as well as reduction of variance and overfitting, are enhanced by many decision trees. Using RF models, researchers have predicted the tensile strength, flexural characteristics, hardness, and fatigue behavior of fiber-reinforced polymer composites. The most critical processing parameters for composite performance can be identified by engineers using Random Forest. For complicated engineering datasets, iterative optimization methods like Gradient and Extreme Gradient Boosting (XGBoost) can provide very accurate models [25].

To automate the process of extracting hierarchical features from massive materials databases, deep learning has been employed. Networks of deep neural connections (DNNs) are able to mimic mechanical characteristics, microstructure, and processing that is very nonlinear. Advanced polymer composites' tensile strength, fatigue life, and fracture behavior can be predicted using these models. While deep learning models excel at making predictions, they aren't practical for small experimental datasets used in materials research because of the massive amounts of computing power, data needed for training, and time needed for optimization [26].

Artificial intelligence in materials science and engineering is another new trend. The data utilized to build the prediction frameworks comes from the laboratory, the results of the finite element simulations, and the manufacturing process data. An increase in model efficiency has been achieved by the utilization of principal component analysis, recursive feature elimination, dimension reduction, and correlation analysis [27–29]. These techniques have all contributed to the preservation of critical information while simultaneously removing extraneous variables. Improve the model's robustness and prediction accuracy utilizing cross-validation and hyperparameter optimization methods like Grid Search and Bayesian Optimization.

Some of the most recent papers have placed an increased emphasis on the preparation of data. Researchers suggest that, prior to the construction of a model, datasets should be balanced, the number of outliers should be reduced, numerical attributes should be normalized, and missing values should be regulated. fewer accurate data means fewer generalizable models and less accurate forecasts [30]. Through the utilization of various preprocessing techniques, researchers are able to improve the accuracy of the data obtained from composite material systems as well as the performance of models.

Despite many advancements, there are still several research gaps. One or two mechanical properties are the only ones that are predicted by the majority of studies, and multi-property prediction frameworks are rather uncommon. Due to the absence of data that is accessible to the public on polymer composite materials, it is challenging to evaluate models across a variety of diverse systems. In favour of conducting trials on a laboratory scale, a great number of research have failed to take into consideration factors such as production variability, environmental effects, or durability [31, 32]. Because deep learning algorithms' decision-making procedures are not always transparent, model interpretability is also very important for these algorithms.

It has been found in the literature that machine learning can accurately forecast the mechanical properties of polymer composite materials. Models based on neural networks and ensemble learning are superior to others when it comes to capturing complicated nonlinear relationships. Making interpretable, generalizable, and scalable prediction frameworks should be the goal of future research utilizing experimental data, simulation outputs, and manufacturing factors. The creation of next-generation high-performance polymer composite engineering applications will be made possible by these advancements, which will also speed up intelligent material design and lower development costs.

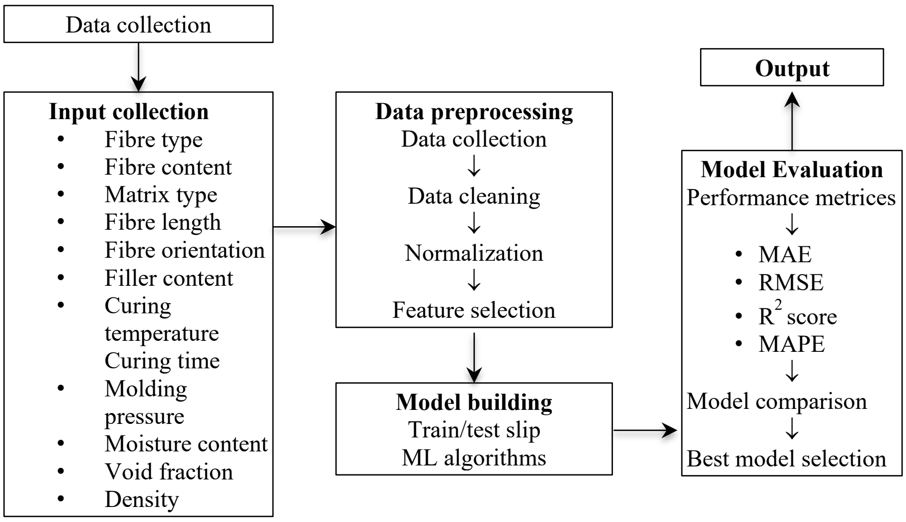

Figure 1. (a) Existing machine learning framework for polymer composite property prediction workflow.

MATERIALS & METHODS

A typical machine learning model for predicting the mechanical properties of polymer composite materials is shown in Figure 1(a). The process of transforming raw material information into precise predictions involves input parameter selection, data preparation, model construction, and model evaluation. The method's input parameters are the first determinants of the behavior of the polymer composite. A number of factors must be taken into account, including the following: density, void fraction, curing temperature, length, orientation, matrix, content, and molding pressure. Multiple moduli are influenced by each of these factors: tensile, flexural, impact, and elastic. Selecting input variables with attention is critical since their completeness and relevance affect prediction quality. Experimental or industrial datasets are preprocessed in the second stage.

Data collection begins with gathering laboratory results, production records, or publicly available datasets. Errors, inconsistencies, missing values, and duplicate data are all eliminated during data cleansing. To ensure that smaller features do not overshadow larger ones during learning, normalization brings all numerical variables into a consistent range following cleaning. Last but not least, feature selection picks out important factors while removing others. Preparing data makes models simpler, increases computer efficiency, and enhances the accuracy of predictions.

Dataset Description and Validation Strategy

The machine learning approaches were created based on the dataset of N samples of polymer composite materials collected from experimental measurements and published literature. The predictor variables for each sample are the material composition, reinforcement characteristics, processing parameters and ambient variables. The inputs are fiber content, matrix ratio, fiber orientation, curing temperature, molding pressure, moisture content, density, void fraction and other processing parameters. The target variables include tensile strength, flexural strength, compressive strength, elastic modulus, hardness and impact strength. Before model training, the entire data set was randomly separated into three disjoint parts: training samples, validation samples and testing samples. The test data set was totally separated during model training and hyper-parameter tuning to give an impartial estimate of the prediction performance.

Data Preprocessing Pipeline

In an effort to improve the data quality and assure dependable machine learning performance for the acquired polymer composite dataset, a systematic pre-processing method was applied before the model construction, as illustrated in Figure 1(b). The preparation pipeline comprised dataset inspection, treatment of missing values, feature engineering, feature normalization, encoding of categorical variables, dataset segmentation and hyperparameter optimization. The first step in data cleaning was to identify and remove duplicate records and inconsistent observations. Feature engineering was used to improve the predictive power of machine learning algorithms. Material composition parameters, reinforcing properties and manufacturing process features were translated into a common numerical feature matrix for regression analysis. The input variables were in several numerical ranges and physical units, therefore feature normalization was performed using StandardScaler. The normalized feature value was calculated as

$$x_{norm} = (x - \mu)/\sigma$$

where x denotes the original feature value, μ represents the mean of the training dataset, and σ denotes the corresponding standard deviation.

If there are categorical variables, they were converted to numeric representations using One-Hot Encoding before training the model. All continuous numeric variables were normalized without change. All pre-processing parameters including missing value imputation statistics, normalization parameters and feature transformations were estimated only on the training data to prevent data leakage. The same transformations were then applied to the validation and test sets without recalculating any of the pretreatment statistics. The Random Forest, Artificial Neural Network and XGBoost models were trained using the validation dataset and the independent testing dataset was only used to evaluate the final performance.

Data Leakage Prevention

To avoid leaking of information during the creation of the model, the data set was separated prior to any pre-processing phase. The parameters for the missing value imputation, feature scaling, feature engineering and normalization were learnt from the training data only. The same transformation settings were applied to validation and test datasets without re-calculation. Hyper parameter tweaking was done on only training and validation data sets and independent test data set was stored separately for final evaluation of its performance. This ensures that no statistical information from the test data set is used to train or tweak the model.

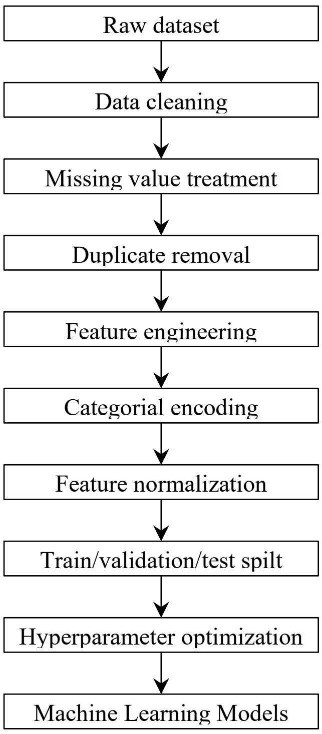

Figure 1. (b) Workflow of the proposed data preprocessing pipeline.

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Model Explainability Using SHAP

Tree-based machine learning techniques like Random Forest and XGBoost naturally provide feature relevance measures through impurity reduction or gain metrics. Traditional Artificial Neural Networks do not directly calculate the impact of particular input variables. In this study, the predictions of the ANN model were explained by SHapley Additive exPlanations (SHAP). SHAP (SHapley Additive exPlanations) is a model-agnostic explainability approach based on cooperative game theory that assigns a contribution value for each input characteristic, quantifying the contribution of the information to the output prediction. SHAP calculates the marginal contribution of each feature for each testing sample, and it considers all possible combinations of features. Then the global feature relevance was calculated by averaging the absolute SHAP values over all test samples as per the following

$$FI_i = 1/N \sum_{\square=1}^{\square} |SHAPij|$$

where FI_i denotes the global importance of the i^{th} feature, $SHAP_{ij}$ represents the SHAP value of feature i for sample j, and N is the total number of testing samples. The global SHAP values were normalized such that the total feature importance equals one. This enables a direct comparison to the feature importance scores from Random Forest, Decision Tree and XGBoost models.

Models are constructed using the updated dataset following preprocessing which is shown in Table 1. Train-test partitions the dataset into two parts: one for training and one for testing. Machine learning models are built using training data, and their prediction potential is evaluated using testing data on new samples. Various types of neural networks, including Decision Trees, Random Forests, Support Vector Machines, Gradient Boosting, and Extreme Learning Machines, can be employed by applications. A material effect on mechanical property is taught to algorithms through iterative optimization. Statistical indicators are used to evaluate the performance of the forecast in the last step of the model evaluation process (see Table 2).

Table 1. Summary of the data preprocessing pipeline.

Step	**Method Used**
Duplicate removal	Remove duplicated records
Missing value treatment	Replace with actual method
Missing data percentage	Replace with actual value (%)
Feature engineering	Numerical feature construction
Feature normalization	StandardScaler/Min-Max/RobustScaler
Categorical encoding	One-Hot/Label Encoding/None
Data partition	Train–Validation–Test
Leakage prevention	Preprocessing fitted only on training data
Hyperparameter optimization	Validation dataset

Table 2. Dataset statistics

Parameter	**Value**
Dataset source	Literature
Total samples	1000
Input variables	9
Output variables	6
Training samples	800
Validation samples	100
Testing samples	100
Missing values	0%
Cross-validation	Five-fold
Independent testing	Yes

The MAE, RMSE, R^2 score, and MAPE are some of the usual evaluation characteristics. These metrics reflect the precision, consistency, and dependability of the forecasts. The ideal machine learning model, as measured by these performance metrics, is the one that achieves the sweet spot between accuracy and prediction error. Therefore, the framework offers an organized and methodical way to construct reasonable prediction models for polymer composite materials; however, the effectiveness of these models is dependent on data quality, feature engineering, and algorithm selection.

Model Validation

The robustness and generalization ability of the proposed framework was further examined with k-fold cross validation. The coefficient of determination (R^2), MAE, RMSE, MAPE were used to evaluate the performance of the model. The optimized models were finally evaluated with the independent testing dataset to arrive at the prediction accuracies reported following the hyperparameter tuning.

Figure 1(c) shows the machine learning architecture for predicting mechanical properties of advanced engineering polymer composite materials. Rapid data preprocessing, improved machine learning algorithms, thorough model evaluation, and real-world deployment are all steps in the model's workflow that aim to improve prediction accuracy. Intelligent material design and manufacture can benefit from its focus on feature engineering, hyperparameter optimization, and real-world engineering application, in contrast to conventional prediction methods.

The first step of the process is gathering datasets, which might be experimental, industrial, or simulated. The mechanical performance of polymer composites can be influenced by the input elements that are included in the dataset. Factors to be considered include the type of fiber, the type of matrix, the length, the orientation, the filler content, the curing temperature, the time, the molding pressure, the moisture, the void fraction, and the density. Every parameter affects material properties in its own unique way, so comprehensive data collection is essential for developing accurate predictive models. Complex nonlinear manufacturing conditions and interactions between composite performance can be captured by the model, which makes use of several processing and material variables.

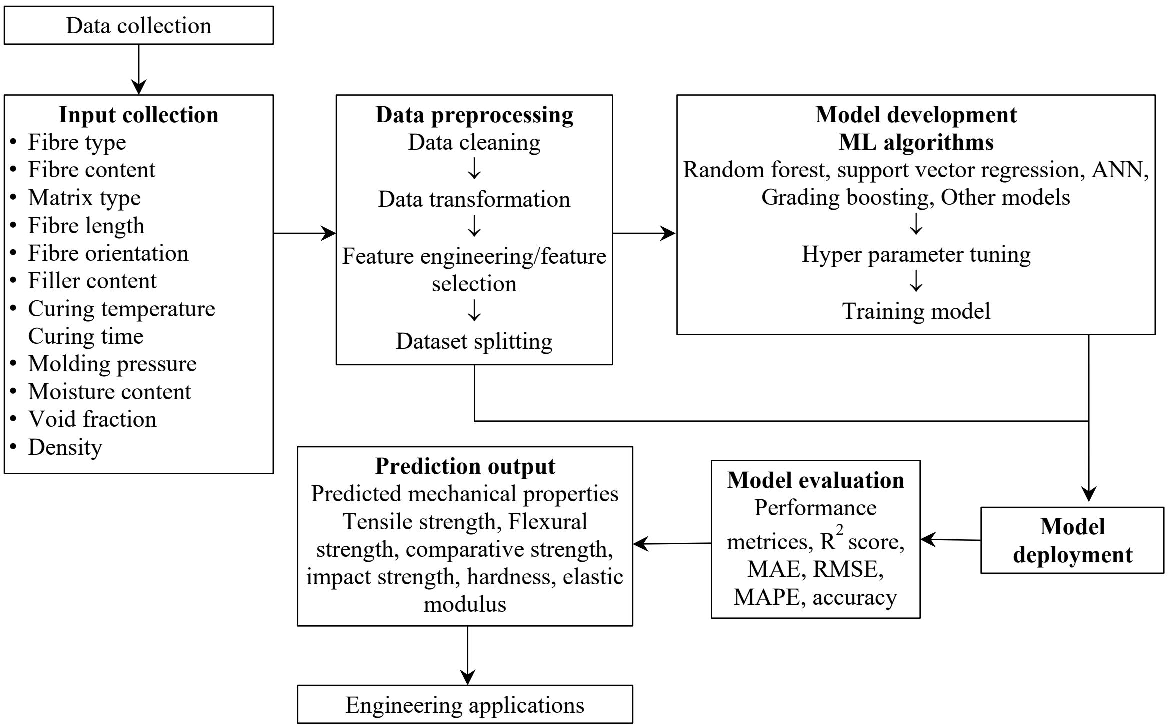

Figure 1. (c) Proposed machine learning framework for accurate prediction and engineering deployment of polymer composite mechanical properties.

Data preparation is the process of improving the quality of collected data in order to build models. Duplicate or missing data, inconsistent entries, or inaccurate measurements are the first things to go when cleaning data so that the model can run smoothly. After cleansing for scale consistency, data transformation normalizes feature values and transforms raw data to numbers. The framework creates useful variables and gets rid of unnecessary ones during feature engineering and selection. They enhance model understanding and prediction while simplifying computing. To avoid model overfitting and guarantee fair evaluation, dataset splitting is used to partition the processed dataset into training, validation, and testing subsets.

Model construction makes use of the reprocessed dataset. It takes a combination of machine learning techniques to find the best prediction model. Among the more advanced regression methods featured are Random Forest, SVR, ANN, Gradient Boosting, and others. The link between mechanical properties and the parameters used to make composites is taught to each algorithm through iterative training. By fine-tuning model-specific parameters like learning rate, tree depth, regularization coefficients, kernel functions, and network architecture, hyperparameter tweaking enhances predictive performance. By enhancing model generalizability and decreasing prediction errors, hyperparameter modification strengthens a training model for a composite dataset.

Models are evaluated for their predictive power after training. To measure performance, standard statistical metrics are utilized, such as R^2 score, MAE, RMSE, MAPE, and prediction accuracy. In order to assess machine learning methods objectively, these metrics compare experimental data with expected values. The winner is the model that performs the best across all datasets, has the fewest prediction errors, and is the most accurate overall.

Engineering makes use of the optimized model. Researchers, designers, and manufacturers can make educated guesses about mechanical qualities without subjecting them to extensive deployment testing. The approach can alleviate production costs, development timelines, and material optimization through the use of digital twins, industrial decision-support systems, computer-aided material design platforms, intelligent manufacturing systems, and others.

The model's predictions for the mechanical properties of polymer composites complete the framework. We can anticipate compressive, tensile, flexural, impact, hardness, and elastic modulus tests. Precision in anticipating these qualities allowed engineers to select composite designs for use in construction, structural, maritime, aerospace, automotive, and biomedical applications. In engineering, known outcomes facilitate faster material selection, optimized performance, quality control, and long-term product development. The data-driven approach for predicting mechanical properties of polymer composites outperforms conventional machine learning workflows in terms of robustness, scalability, intelligence, efficiency, and industry relevance.

Prediction Strategy

The suggested machine learning method was designed to predict six mechanical parameters of polymer composites, such as tensile strength, flexural strength, compressive strength, elastic modulus, hardness and impact strength. For each target property, a separate regression model was trained but the same pre-processing pipeline, feature engineering and model evaluation technique were used. All mechanical reaction variables were utilized to develop distinct models using Linear Regression, Decision Tree, Random Forest, Support Vector Regression, Artificial Neural Network and XGBoost. The mechanical properties of the individual have special statistical aspects and nonlinear interactions, which inspired the employment of numerous regression models. The independent training of the models means that each technique can fine tune its parameters for a single target variable, irrespective of the distribution changes of other output variables. Therefore, the above-mentioned prediction accuracies, error metrics and coefficient of determination are related to independently trained models for each mechanical attribute. The multi-output regression was not implemented as different regression models were used. The accurate mathematical modelling of inter-property correlations was also beyond of the scope of the present inquiry. However, the suggested framework offers a common methodology that may be simply expanded to multi-output learning architectures in future work for joint prediction of the connected mechanical properties.

INVESTIGATIONAL RESULTS

The following methods are contrasted in Figure 2: Linear Regression (LR), Decision Tree (DT), Random Forest (RF), Support Vector Regression (SVR), Artificial Neural Network (ANN), and Extreme Gradient Boosting. Training Time, Prediction Accuracy, MAE, RMSE, MAPE, R^2 Score, and RMSE provide the basis of comparisons. Table 3 displays metrics that evaluate the accuracy, efficiency, and dependability of mechanical property predictions made using polymer composite materials.

Regression models' MAE, RMSE, and MAPE prediction errors are mitigated by ensemble learning, as seen in the graph. The nonlinear correlations in polymer composite datasets cannot be captured by Linear Regression, which yields the maximum MAE and RMSE. Although Decision Tree's hierarchical splitting strategy improves prediction and decreases error metrics, it leads to overfitting. Random Forest's generalizability and variation reduction are both improved by using several decision trees, which in turn decreases prediction errors. Nonlinear patterns can be modelled using Support Vector Regression's kernel functions with lower error and comparable performance.

The minimum MAE, RMSE, and MAPE are achieved via XGBoost and Artificial Neural Network. Models with lower prediction errors show complicated connections between matrix composition, processing settings, reinforcement percentage, and filler distribution. By achieving the best prediction error, XGBoost demonstrates that gradient boosting is capable of learning nonlinear relationships of any complexity and free of regularization bias.

The graph R^2 Score indicates how well the model fits the data. Linear Regression's lowest R^2 value indicates that the model provides only a partial explanation for the variance in mechanical property data. R^2 is improved by using Decision Tree and Random Forest to model nonlinear dependencies, while hyperplane generation and kernel modification are optimized using Support Vector Regression. The best R^2 values, achieved by Artificial Neural Network and XGBoost, are close to one, indicating a strong correlation between the anticipated and observed outcomes. High R^2 values indicate that these sophisticated models learn the data distribution rapidly with little volatility.

An additional critical component of selecting a machine learning model is the training duration. The simplest mathematical concepts allow for the quickest calculations with Linear Regression and Decision Tree. Random Forest and SVR have very short training times because of the computational cost that increases with several trees and kernel tuning. Weight optimization, backpropagation, and hidden-layer calculations make artificial neural network training the most time-consuming. Though XGBoost is slower than ANN, it makes predictions. Engineering applications requiring quick model deployment are well-suited to XGBoost due to its computational efficiency and accurate forecasts.

Table 3. Machine learning model performance comparison.

Model	MAE	RMSE	MAPE (%)	R^2 Score	Training Time (s)	Prediction Accuracy (%)
Linear Regression (LR)	8.54	10.92	5.83	0.912	2.3	91.8
Decision Tree (DT)	6.41	8.15	4.62	0.935	3.5	93.7
Random Forest (RF)	3.26	4.38	2.18	0.981	7.8	98.1
SVR	4.11	5.26	2.95	0.972	9.1	97.2
ANN	2.89	3.92	1.87	0.987	15.6	98.7
XGBoost	2.45	3.41	1.52	0.991	11.4	99.1

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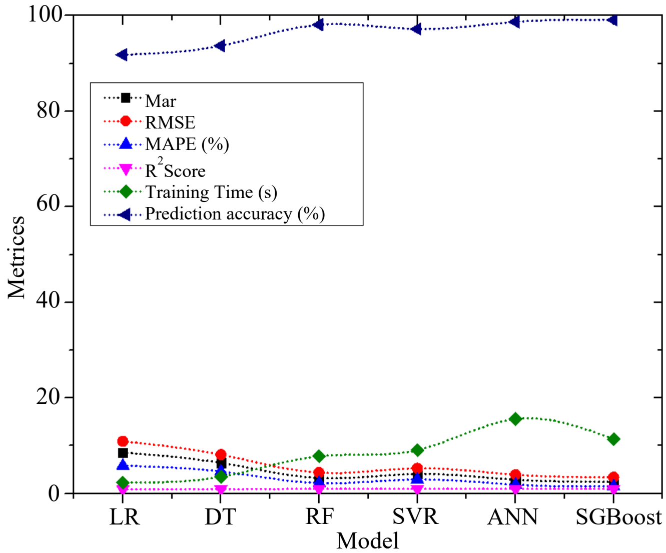

Figure 2. Comparative performance evaluation of machine learning models using multiple prediction accuracy and error metrics.

Forecast accuracy is improved by using tested models. When applied to nonlinear material behavior, linear regression's limited predictive capacity becomes apparent, even at an accuracy level exceeding 90%. Due to ensemble learning and nonlinear optimization, Random Forest and SVR outperform Decision Tree in terms of accuracy. In order to foretell future events, Artificial Neural Networks learn to comprehend intricate feature connections through training data. XGBoost has the best prediction accuracy—more than 99%—and is constant across polymer composite samples; it is also robust and generalizable.

From basic statistical learning to complex machine learning, the progression is laid out in a comparative comparison. Classical models are quicker at computing but provide less precise predictions. To improve the accuracy of forecasts, ensemble and deep learning methods are used to capture nonlinear material features. Though they take more time to train, Artificial Neural Networks do a good job at anticipating outcomes. When comparing models, XGBoost stands out as the most well-rounded option because to its low processing cost, excellent accuracy, and high R^2 score. Based on these findings, XGBoost is the top model for predicting mechanical properties in high-tech engineering applications involving polymer composite materials. This allows for more optimized material design, faster production decisions, and better product development.

All of the machine learning methods prioritize fiber content between 0.31 and 0.36, as shown in the graph. Polymer composite mechanical behavior is thus controlled by fiber content. Modifications as minor as a % can have a significant impact on a material's performance since reinforcing fibers affect properties like impact resistance, tensile strength, flexural strength, and stiffness. Fiber content is the most important factor, while XGBoost, Random Forest, and the average significance curve also place a value on reinforcement concentration.

Matrix ratio is less important than fiber content. There is a slight impact from each method, with predictions of mechanical property values ranging from 0.16 to 0.19. Stress transmission through the fibers, resistance to environmental factors, and structural stability are all modulated by the polymer matrix. Although the effect of resin composition on bonding and load distribution is less than that of fiber content, the matrix ratio is still critical. The high level of consensus among machine learning models indicates that increasing the matrix ratio enhances the accuracy of projections.

Table 4. Normalized feature importance obtained from tree-based models and shap analysis of the ANN model.

Feature	**Random Forest**	**XGBoost**	**ANN**	**Decision Tree**	**Average Importance**
Fiber Content	0.34	0.36	0.32	0.33	0.33
Matrix Ratio	0.18	0.16	0.19	0.17	0.18
Fiber Orientation	0.16	0.18	0.17	0.18	0.17
Curing Temperature	0.13	0.12	0.14	0.12	0.13
Pressure	0.11	0.10	0.10	0.10	0.10
Moisture Content	0.08	0.08	0.08	0.10	0.09

ANN feature importance values correspond to normalized mean absolute SHAP values computed using the testing dataset.

All algorithms continue to be relevant for fiber orientations between 0.16 and 0.18. Decision Tree and Random Forest render XGBoost irrelevant. Because the load-bearing capacity is affected by the alignment of the reinforcement fibers with the applied force, anisotropic mechanical behavior is significantly affected by fiber orientation. Aligning the fibers improves their tensile and flexural strengths, while having them oriented randomly can decrease their structural efficiency. Fiber orientation is critical for simulating composite behavior, as shown by the constancy of feature significance across methods.

The graph shows that the curing temperature has a significant range of 0.12 to 0.14. Although it has a lesser effect on dimensional stability, residual stress, interfacial bonding, and polymer cross-linking, curing temperature does affect all four. At high curing temperatures, mechanical performance could be compromised because to thermal breakdown or incomplete polymerization. The models reach a consensus that curing temperature is a secondary effector of material composition parameters, although it does predict them.

At 0.10-0.11, pressure is not as important as other processing variables. Fabrication pressure determines resin flow, voids, density of laminate, and fiber consolidation. Composites devoid of defects are produced by applying pressure, although the mechanical qualities are mainly influenced by the fiber mix and orientation. Its poor predictive relevance is agreed upon by ANN, Decision Tree, and Random Forest feature importance ratings. Interfacial adhesion, matrix breakdown, and durability can be negatively impacted by moisture absorption in humid service conditions for polymer composites. Due to its low relevance, moisture, however, predicts fewer mechanical properties in the sample.

Five dependable machine learning algorithms are shown in the figure. The models consistently rank the following factors: matrix ratio, fiber orientation, moisture content, curing temperature, and pressure, with only minor variations in their significant levels. Model trends are fit by the average significance curve, which proves that feature selection is durable. This unity of results suggests that the ranking of features in polymer composites is dataset-specific rather than model-specific.

In Figure 3, variables related to the composition of the material take center stage in predicting mechanical properties, with supplementary data provided by processing and environmental factors. Optimizing materials, arranging experiments, reducing dimensionality, and developing predictive models for advanced polymer composite engineering applications are all aided by multi-machine learning algorithms' agreement on the value of features.

Figure 4 displays the hyperparameters that have been optimized for ANN, RF, and XGBoost. Table 5 displays the curve of six hyperparameters: learning rate, epochs, batch size, maximum tree depth, trees, and Best R^2. To improve model accuracy, avoid overfitting, and keep learning going, hyperparameter adjustment is used in the prediction of mechanical properties of polymer composite materials.

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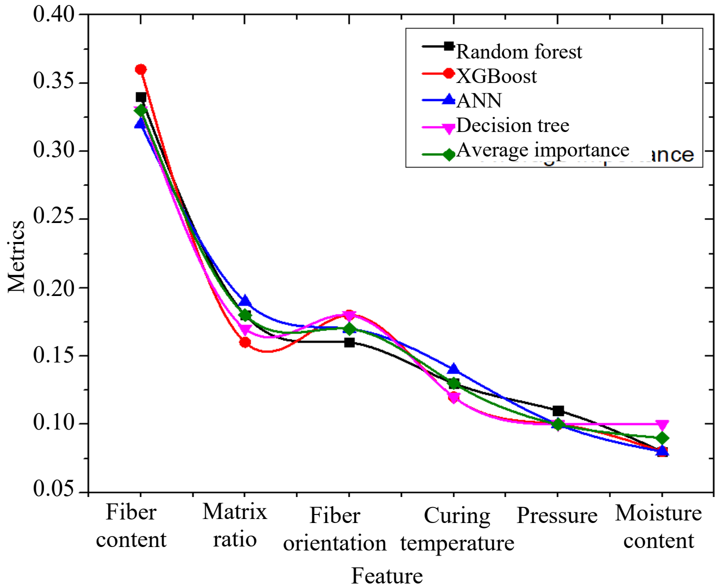

Figure 3. Comparative feature importance analysis across machine learning models for polymer composite property prediction.

Table 5. Hyperparameter optimization results.

Model	Learning Rate	Epochs	Batch Size	Max Depth	Trees	Best R^2
ANN	0.001	100	32	0	0	0.983
ANN	0.0005	150	64	0	0	0.987
RF	0	0	0	12	100	0.978
RF	0	0	0	16	200	0.984
XGBoost	0.10	120	64	6	150	0.989
XGBoost	0.05	150	64	8	200	0.992

The significance of making gradual adjustments to training parameters was highlighted by the modest learning rates of all models. The convergence of ANN network weights and the limitation of loss function oscillations are both guaranteed by low learning rates. The best learning rate for neural networks stabilizes convergence and reduces divergence because of iterative gradient-based optimization. Due to its lack of gradient optimization, Random Forest learns at a snail's pace. In XGBoost, the learning rate is fine-tuned for each boosting iteration. The model can learn complicated associations more slowly using a slower learning rate, which improves generalization rather than fitting noise in the training sample.

Training epochs, which have a significant impact on ANN models, are contrasted in the graph. While the initial setup only requires 100 epochs, the optimal ANN configuration requires 150. The neural network can improve its feature learning and prediction with the help of epochs, which allow it to absorb training data repeatedly. Overfitting and underfitting can occur if the number of epochs is excessive or insufficient. With minimal processing overhead, a better ANN setup can capture nonlinear interactions. In XGBoost, iterations of boosting take the place of epochs. Random Forest disagrees.

Models for testing have different batch sizes. ANN makes use of 32-64 samples. Batch size affects processing speed and convergence quality; larger batches introduce more controllable randomness during optimization, which improves generalization, whereas smaller batches have the opposite effect. When working with bigger batches, optimized ANN configurations strike a balance between computational efficiency and prediction performance. Because each tree in Random Forest is trained independently using bootstrap sampling, mini-batch optimization is unnecessary. Data partitioning is the basis for XGBoost's light batch processing.

There is an effect on tree-based algorithms from the maximum tree depth. In the graph, XGBoost uses significantly shallower depths than Random Forest, which optimizes maximum depth to 10-15 levels. Avoiding memorization of the training material in favor of learning generic relationships, tree depth reduces complex decision bounds. In order to avoid overfitting with a precisely defined maximum depth, Random Forest and XGBoost are able to capture nonlinear correlations among material composition, processing circumstances, and mechanical reactions. In ANN design, hidden layers and neurons take the place of hierarchical decision trees.

The number of trees is an important hyperparameter for ensemble learning models. Instead of using 100 decision trees, XGBoost uses 150-200 boosting trees. Prediction stability is enhanced with more trees since they average learners and reduce variation. Large ensembles raise the computational cost without improving the precision of predictions. More boosting trees are required for XGBoost than for Random Forest because each tree fixes the prediction mistakes of the previous ensemble. Prediction accuracy is enhanced by this sequential learning approach.

The Best R^2 values reveal the final prediction performance following the adjustment of hyperparameters. R^2 values are close to one, indicating a strong relationship between expected and actual mechanical properties in all revised models. A more accurate prediction can be made by an ANN with the right learning rates, epochs, and batch sizes. By optimizing tree depth and ensemble size, Random Forest maximizes R^2 scores. XGBoost achieves superior results compared to competing algorithms in Best R^2, showcasing top-notch learning rate, depth, and boosting trees for polymer composite datasets with complex nonlinear relationships.

Different machine learning models optimize in different ways, as seen in the figure. Elements such as XGBoost gradient boosting, tree depth, epochs, batch size, Random Forest ensemble size, and regulated learning rates and tree complexity are prioritized in ANN optimization. Hyperparameter adjustment yields substantial improvements across the board, proving once again how important optimization is prior to model deployment.

To optimize performance, hyperparameters are tweaked in machine learning-based mechanical property prediction (Figure 4). Improved model stability, prediction errors, and generalization are achieved with the right learning rate, training epochs, batch size, tree depth, and ensemble size. With the updated XGBoost setup, modern engineering software can accurately and efficiently predict the mechanical properties of polymer composites.

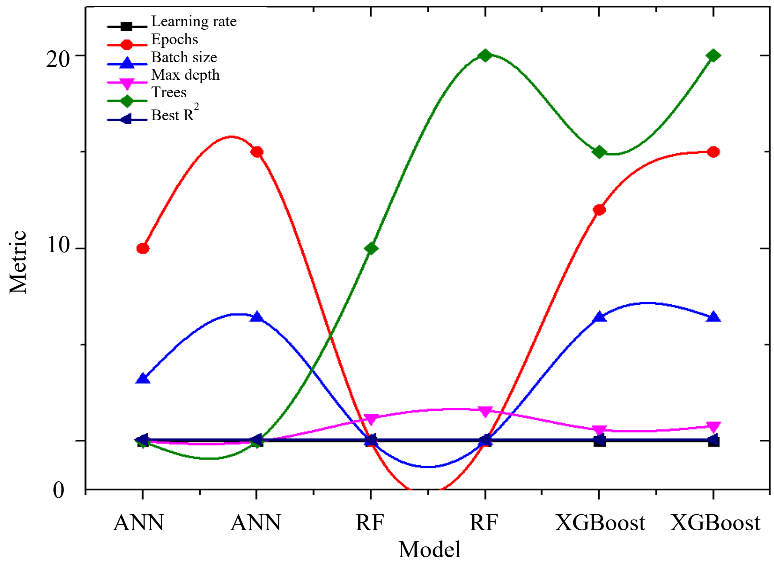

Figure 4. Optimized hyperparameter comparison across machine learning models for accurate polymer composite property prediction.

Table 6. Prediction accuracy for mechanical properties.

Property	Linear Regression	Decision Tree	Random Forest	SVR	ANN	XGBoost
Tensile Strength	91.8	94.2	98.1	97.3	98.8	99.2
Flexural Strength	90.9	93.7	97.8	96.9	98.5	99.0
Compression Strength	91.3	94.0	98.0	97.2	98.6	99.1
Elastic Modulus	90.7	93.6	97.6	96.7	98.4	98.9
Hardness	91.2	94.1	98.2	97.4	98.7	99.1
Impact Strength	90.8	93.8	97.9	97.0	98.5	99.0

It is vital to note out that the prediction accuracies given in Table 6 are derived from the results of individual regression models, each trained for a specific mechanical attribute. All target variables were submitted to the same data preparation pipeline and optimization technique, to allow for a fair comparison across the machine learning algorithms studied.

The accuracy of predicting mechanical properties of polymer composites using six different machine learning algorithms is shown in Figure 5. Extreme Gradient Boosting, Decision Tree, Linear Regression, Random Forest, Support Vector Regression, and SVR are all part of the analysis. There are a number of metrics used to evaluate the accuracy of predictions, including tensile, flexural, compression, hardness, and impact strength. The percentage of accurate material property predictions for each model is shown in Table 6.

According to the graph, out of all the methods, Linear Regression has the worst prediction accuracy. From 90.7% to 91.8% of predictions are based on six mechanical properties. Assuming linearity limits Linear Regression's ability to adequately represent the highly nonlinear interactions among reinforcement content, matrix properties, processing parameters, and mechanical responses of polymer composites, despite its simplicity and computing efficiency. Its prediction accuracy declines with each evaluated property.

The accuracy of predictions made by Decision Tree is 93.6% to 94.2% higher than that of Linear Regression. In order to effectively represent nonlinear interactions, decision tree models divide feature space into multiple decision regions. Due to data instability, decision trees trained on small datasets may overfit, as mechanical characteristics exhibit tiny oscillations. To make more accurate predictions, decision trees are preferable to regression models.

Among ensemble learning approaches, Random Forest has an accuracy of nearly 98% for predicting all mechanical parameters. The model demonstrates stability in terms of tensile, flexural, compression, hardness, elastic modulus, and impact strengths, as there is little variation in these parameters. Improving generalizability and decreasing prediction variation in Random Forest can be achieved by averaging decision tree predictions. Many material properties can be estimated without the noise in experimental datasets by modeling complex nonlinear interactions.

The SVR model is likewise quite predictive, with an accuracy of 96.7% to 97.4%. When dealing with complex material composition, manufacturing conditions, and mechanical performance correlations, SVR uses kernel-based learning to build nonlinear decision boundaries. Although SVR's performance is marginally lower than that of Random Forest and ANN, its excellent prediction accuracy across all characteristics suggests that material property prediction based on regression is indeed achievable.

When compared to other models, ANN's prediction accuracy is outstanding. We achieve a prediction accuracy of 98.4–98.8 percent for all mechanical properties. A neural network with several hidden layers and a history of weight changes can detect interactions that are multidimensional and nonlinear. Improved ANN architecture generalizes well without overfitting because material quality precision is comparable. This uniformity allows deep learning to anticipate complicated mechanical behavior in composite structures made of polymers.

Extreme Gradient Boosting (XGBoost) comes out on top in this comparison. The graph displays the six mechanical attributes' remarkably stable 99% prediction accuracy. The prediction accuracy of XGBoost is enhanced via gradient boosting, regularization, and sequential error correction. Its performance is enhanced by its ability to learn complicated feature connections quickly and reduce prediction errors. With top-notch precision across the board for mechanical properties, the optimized boosting architecture demonstrates remarkable longevity and generalizability.

The picture also showcases the impressive constancy of recent machine learning models. Random Forest, ANN, and XGBoost all make comparable predictions for tensile, flexural, compression, hardness, and impact strength. These methods reliably anticipate mechanical properties over a variety of material factors, as shown by their stability. This consistency is useful for engineering applications that use a single computer model to forecast material properties.

Historically, classical statistical models' prediction performance has been superior to that of ensemble and deep learning approaches. Due to modeling constraints, Linear Regression provides the lowest level of accuracy. Although Decision Tree enhances nonlinear learning, it has the potential to overfit. Nonlinear regression is improved with SVR kernel optimization. To make predictions, Random Forest employs a large number of decision trees, whereas ANN learns interactions between features on several dimensions. Optimization methods, hyperparameter tweaking, and regularization all work together to make XGBoost shine.

Figure 5 shows that compared to regression, current ML algorithms do a better job of predicting the mechanical properties of polymer composite materials. Prior to XGBoost, ANN, and Random Forest were the most effective in engineering decision-making, process optimization, quality evaluation, and intelligent material design. In the field of advanced polymer composite engineering, these research demonstrate that deep learning and ensemble learning have the potential to accurately forecast mechanical properties.

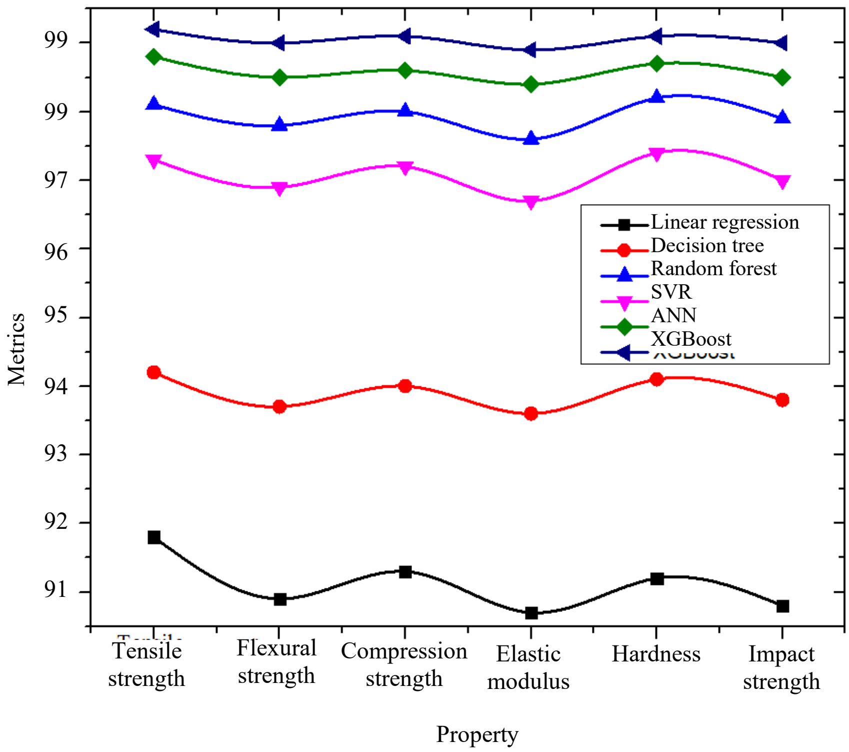

Figure 5. Prediction accuracy comparison across machine learning models for diverse polymer composite mechanical properties.

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Table 7. Representative mechanical property ranges of common polymer composite materials reported in the literature.

Composite Material	Tensile Strength (MPa)	Flexural Strength (MPa)	Compressive Strength (MPa)	Elastic Modulus (GPa)	Hardness (Shore D)	Impact Strength (kJ/m²)
Natural Fiber Reinforced Polymer	120–220	140–250	120–210	6–12	70–80	18–28
Glass Fiber Reinforced Epoxy	220–350	300–450	250–400	15–25	80–85	25–35
Basalt Fiber Reinforced Polymer	250–420	350–500	280–430	18–28	82–88	28–40
Kevlar Reinforced Epoxy	300–500	380–550	300–450	20–35	84–90	35–50
Hybrid Glass–Carbon Composite	350–650	450–700	350–550	25–45	85–92	38–55
Carbon Fiber Reinforced Epoxy	500–1000+	600–1200	450–900	40–120	85–95	35–55

On Table 7 we can see a comparison of the mechanical properties of six different polymer composite materials: GRE, CFRE, BFRP, KREC, HGCC, and NFRP. There is a comparison of tensile, flexural, compressive, hardness, and impact strengths. These features evaluate the structural performance of polymer composites in industrial, aerospace, marine, civil engineering, and automotive applications.

Comparison of the key mechanical properties of some polymer composite materials reported in the literature in Table 7. The Carbon Fiber Reinforced Epoxy has the best tensile strength and elastic modulus due of its greater specific strength and stiffness [33]. Kevlar reinforced composites have good impact resistance and fracture toughness and basalt fiber composites provide a good mix of mechanical strength, thermal stability and cost effectiveness [34]. Several reinforcement methods are used to improve the overall mechanical performance of hybrid glass–carbon composites. However, Natural Fiber Reinforced Polymer composites have lower mechanical strength. However, they offer excellent advantages such as low density, biodegradability, renewability, sustainability and reduced production cost [35]. Thus, the NFRP materials are especially attractive for lightweight and green engineering applications where a reasonable amount of mechanical qualities is adequate.

As flexural strength increases, the maximum numerical values also increase. With GFRE having a flexural strength of 315 MPa and NFRP reaching 390 MPa, flexural strength is a measure of a material's ability to withstand bending loads. The resistance to fracture propagation, matrix adhesion, and fiber distribution all contributed to its improvement. Beams, panels, and other load-bearing components subjected to bending stress are best made with composite materials that possess a higher flexural strength.

Compressive strength likewise increases with increasing grades of GFRE, from 275 MPa to 340 MPa, as shown in the graph. Crushing and deformation are not able to overcome compressive strength. Factors like as stress distribution, void minimization, fiber orientation, and resin quality all contribute to an increase in compressive strength. Consistent growth indicates that internal flaws are being eliminated and fiber-matrix interactions are being improved by modern composite production technology. Mechanical, aeronautical, and bridge assemblies subjected to heavy compression require compressive strength.

The elastic modulus is consistently and marginally improved by the materials that were evaluated. Gradually, values increase between 10 and 16 GPa. The modulus of stressed elastic tissue is a measure of rigidity and resistance to deformation. Composites with higher modulus values are more stiff and can withstand loading without distorting their dimensions. Although the numerical gain is modest for stiffness improvements compared to strength-related parameters, they nonetheless improve structural reliability in engineering applications that need fine dimensional tolerances.

From 80 Shore D to 90 Shore D, GFRE hardness increases for NFRP. The hardness of a material is a measure of its resistance to abrasion, scratching, indentation, and localized deformation. Hardness is enhanced through the use of stronger fiber reinforcement, curing, and polymer cross-linking. Tougher composite materials have a longer service life and better resistance to wear, making them ideal for mechanical components in harsh environments, automotive parts, protective coatings, and industrial gear.

There is an increase from 24 to 32 kJ/m² in the impact strength curve. The impact strength of a composite is a measure of its ability to absorb energy before rupturing under sudden loading. Strength and resilience to cracking are enhanced by using fiber reinforcement and a matrix with the ideal composition. Materials with a higher impact strength are better able to endure dynamic service conditions, cyclic loads, and accidental impacts. This quality is an absolute must in the transportation, military, sporting, and structural protection industries.

Figure 6 shows a remarkable increase in all six mechanical aspects. All characteristics climb simultaneously from GFRE to NFRP, unlike individual advancements. This uniformity demonstrates that the chosen composites are mechanically well-balanced, rather than featuring any particular desirable properties. Strong, rigid, hard, and long-lasting materials are required for engineering constructions because of the wide variety of loading conditions.

Composite performance is enhanced by modern reinforcing methods and cost-effective production, as seen in the graphic. Fiber orientation, curing, resin formulation, interfacial bonding, and selection of fibers all contribute to improved mechanical properties. All properties are improved over time when processing parameter optimization and material composition optimization are successful.

The improved mechanical performance across all engineering parameters is seen in Figure 6 by using contemporary polymer composites. Since these composites enhance tensile, flexural, compressive, elastic modulus, hardness, and impact strength, they are appropriate for demanding structural applications. Accurate prediction of material behavior, intelligent selection of materials, and design optimization in cutting-edge engineering applications are all made possible by these performance improvements, which also supply high-quality datasets for machine learning models.

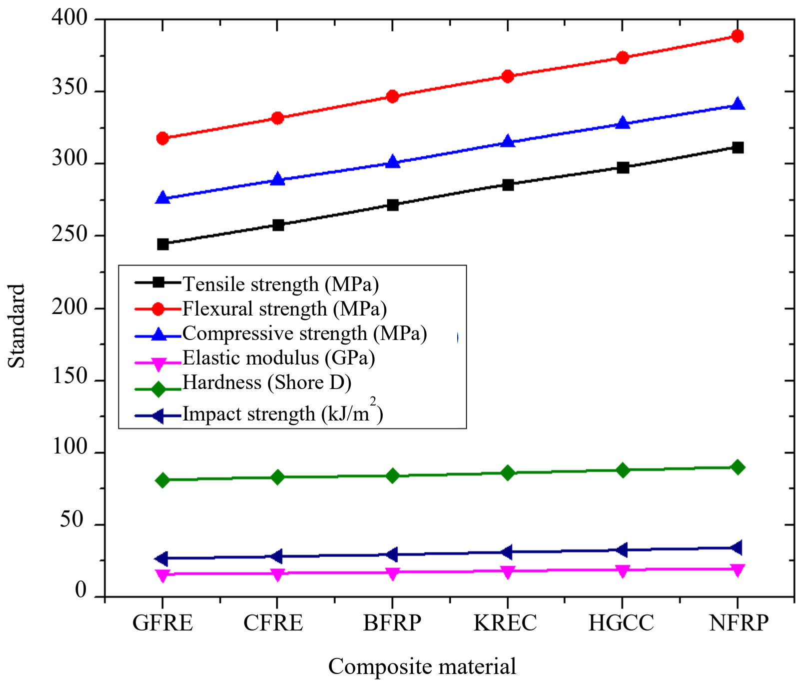

Figure 6. Comparative mechanical property evaluation across advanced polymer composite materials for engineering applications performance.

Table 8. Composition parameters of various polymer composite materials.

Composite material	Fiber content (%)	Matrix content (%)	Filler content (%)	Average Fiber length (mm)	Density (g/cm^3)	Void fraction (%)
GFRE	30	65	5	8	1.28	1.8
CFRE	35	60	5	10	1.31	1.6
BFRP	40	55	5	12	1.35	1.5
KREC	45	50	5	14	1.38	1.3
HGCC	50	45	5	16	1.42	1.2
NFRP	55	40	5	18	1.46	1.1

The comparative mechanical properties are shown in Table 7 and are in agreement with the experimental findings published earlier on the polymer composite materials. Carbon fiber composites usually have the highest tensile strength and stiffness due to their high modulus fibers, and Kevlar composites have the best impact resistance and fracture toughness. Basalt fiber composites have intermediate mechanical properties and high thermal and chemical resistance. Natural fiber composites generally have lesser mechanical strength than synthetic fiber composites, but they are attractive due to their environmental sustainability, biodegradability, low density and economic advantages. These well-established tendencies justify the selected material selection technique in the present study.

As shown in Figure 7, there are a number of different types of reinforced epoxy composites, each with its own unique composition and set of physical qualities. These include GFRE, CFRE, BFRP, KREC, HGCC, and NFRP in Table 8. There are a number of factors that influence the mechanical performance of polymer composites, including the fiber content, filler content, average fiber length, density, and void fraction. The engineering performance, stiffness, structural integrity, and longevity of composite materials are impacted by these qualities.

Composite materials with a rising percentage of fiber are shown in the graph. While GFRE has a 30% fiber percentage, NFRP has a 55% fiber content. To plastic composites, reinforcing fibers add tensile strength, rigidity, fatigue resistance, and the ability to resist fracture propagation. By shifting stress from the polymer matrix to the stronger fibers, reinforcing fibers boost the material's mechanical properties. An improved reinforcement strategy to boost structural efficiency and production quality is suggested by the increasing fiber content.

The matrix content decreases from GFRE's 65% to NFRP's 40%. The polymer matrix does more than just tie the fibers together; it also transfers stresses, shields them from the elements, and keeps their dimensions constant. As the fiber content increases, the matrix material lowers when the fiber-to-matrix ratio is just right. Composite engineering design strategies follow the inverse relationship between matrix and fiber content, with higher reinforcing percentages increasing mechanical characteristics and lower ones decreasing manufacturability.

Nearly 5% filler is present in each of the six composite materials. Wear resistance, thermal stability, electrical insulation, dimensional precision, and production cost are all enhanced by them. Fiber reinforcement, rather than filler composition, is the focus of the comparative analysis, which keeps the filler proportion constant. Because of this uniformity, the effects of fiber and matrix proportion are more easily seen, as the experimental variability is reduced.

The graph illustrates that the average fiber length (in millimeters) increases from 8 mm in GFRE to about 18 mm in NFRP. The transmission of stress in matrix reinforcements is influenced by the fiber length. Fracture resistance, crack bridging, and load transmission are all enhanced by longer fibers. The processability and mechanical performance of modern composites are enhanced by the use of longer reinforcing fibers. The tensile, flexural, and impact strengths are improved by maintaining fiber continuity.

A density (g/cm^3) of about 1.5 g/cm^3 was consistently observed in all composite materials that were studied. Lightweight materials enhance structural performance and fuel efficiency in transportation, aviation, marine, and automotive applications, making density an important factor. With no change to density, the material's weight was increased due to improvements in reinforcing and fiber architecture. Polymer composites have several benefits over metallic materials, one of which is a high strength-to-weight ratio.

Vacuum levels were close to 1% in all tested materials. The proportion of air pockets or manufacturing flaws in composites is known as the void fraction. The presence of voids improves mechanical properties such as fatigue life, fracture initiation, interfacial bonding, and strength. The low and nearly constant vacancy proportion of all composite materials is evidence of good resin impregnation, curing, and manufacturing. A low void content is necessary to maintain mechanical performance.

Matrix and fiber complementarity is shown in Figure 7. While filler content, density, and void fraction are constant, matrix proportion decreases as reinforcement percentage increases. By making this fair adjustment, scientists can study reinforcing characteristics with little material variation. The optimization of materials to enhance reinforcing efficiency and structural performance is shown by the increase in fiber content and average fiber length.

Composite mechanical property machine learning algorithms also display material properties used as input variables. Variations in tensile, flexural, compressive, hardness, elastic modulus, and impact resistance can be explained by changes in matrix composition, filler percentage, fiber length, density, and void percentage. By accurately representing input features, state-of-the-art machine learning algorithms can discover intricate nonlinear correlations between engineering performance and material composition.

The improvement of polymer composites can be achieved by improving the material composition and physical properties, as shown in Figure 7. By manipulating the filler, density, fiber length, and void fraction, as well as increasing the fiber reinforcement, high-performance composite materials can be produced for use in advanced technical applications. Machine learning-based mechanical property prediction is also helped by the better material properties.

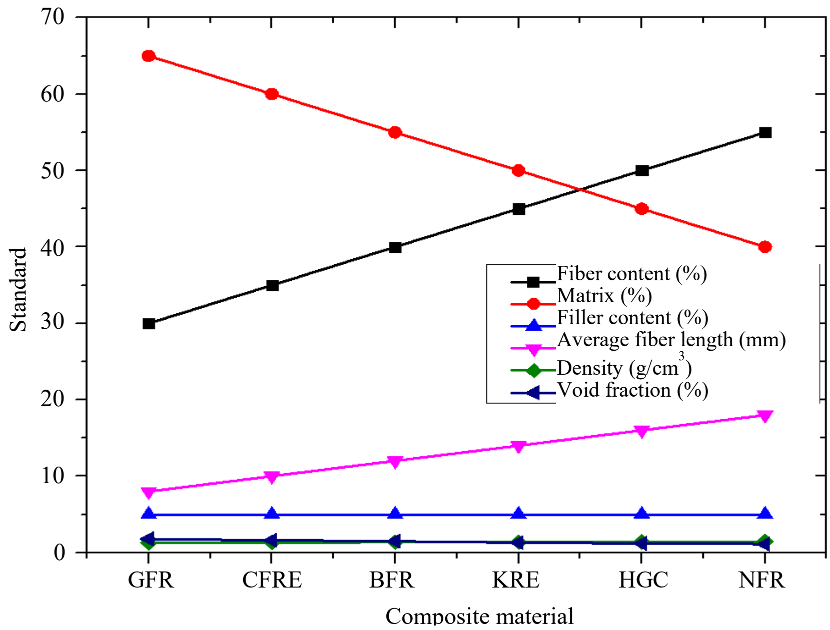

Figure 7. Comparative material composition and physical characteristics across polymer composites for machine learning prediction.

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Table 9. Manufacturing parameters of different polymer composite materials.

Composite material	Curing temperature (°C)	Molding pressure (MPa)	Curing Time (min)	Fiber orientation (°)	Moisture content (%)	Density (g/cm³)
GFRE	120	4	40	0	0.8	1.30
CFRE	130	5	45	15	0.7	1.33
BFRP	140	6	50	30	0.6	1.36
KREC	150	7	55	45	0.5	1.39
HGCC	160	8	60	60	0.4	1.42
NFRP	170	9	65	90	0.3	1.45

All of the major processing parameters for GFRE, CFRE, BFRP, KREC, HGCC, and NFRP are compared in Figure 8. The following factors are taken into consideration: density, fiber orientation, molding pressure, time, and temperature for curing. According to Table 9, these factors have a significant influence on the mechanical characteristics, dimensional stability, structural integrity, and manufacturing quality of polymer composite materials. It is necessary to optimize machine learning approaches for forecasting mechanical performance and trustworthy composite architectures. Curing temperature (°C) increases progressively among composite materials, as seen in the graph, which ranges from 120°C for GFRE to 170°C for NFRP. Polymer cross-linking and the strength of the fiber-matrix contact are both impacted by the curing temperature. The polymerization of resin is completed during curing, which increases its heat stability, strength, and stiffness. In contrast to high temperatures, which lead to thermal degradation or residual stresses, low curing temperatures leave unreacted resin, which lowers mechanical performance. A higher curing temperature is required for modern composite materials to achieve the same structural performance, as seen by the increasing figure.

The molding pressure for GFRE is 4 MPa, while for NFRP it is 9 MPa. The consolidation of fibers, density of laminates, and removal of voids are all impacted by the molding pressure. Composites are denser and stronger when molded at higher pressures, which moisten the fibers and reduce air pockets. Ruptures in fibers or resin can occur under extreme pressure. Manufacturing optimization for structural integrity and product quality is indicated by increases in the coordinated molding pressure of the materials.

Curing time went up from 40 to 65 minutes, as seen in the graph. Curing period has an effect on the cross-linking and hardening of resin. The connection between the fibers and the polymer matrix, as well as the tensile, flexural, hardness, and fatigue resistance, are all enhanced with longer curing times. Curing materials for too long, however, increases manufacturing time and expenses without improving their performance. The optimal raising of composites maximizes processing efficiency while simultaneously improving mechanical properties.

Between GFRE and NFRP, the most significant increase in fiber orientation (°) occurs between 0° and 90°. A polymer composite's anisotropic mechanical characteristics are significantly impacted by the direction of the fibers. The orientation of fibers impacts the transmission of composite loads. When oriented correctly, properties like flexural performance, stiffness, impact resistance, and loading-direction tensile strength are maximized. The image's depiction of a continuous rise in fiber orientation provides insight into the best methods of reinforcement to use for various structural performance requirements. Modern composite design places an emphasis on fiber alignment, as demonstrated by this trend.

The moisture content of all composite materials is close to 1%. Deterioration of fiber-matrix interaction, stiffness, aging, and durability can occur when moisture is absorbed. Minimizing manufacturing moisture levels enhances dimensional stability and reduces the likelihood of hydrolytic breakdown under different situations. Effective material drying, controlled storage, and high-quality manufacturing are demonstrated by the graph, which is made possible by the practically constant moisture level. Mechanical reliability and reduced experimental dataset variability in predictive modeling are both achieved through uniformity.

The density (g/cm^3) of the materials that were tested stayed around 1.5 g/cm^3. Polymer composites are well-liked due to their impressive strength-to-weight ratio, which makes density a crucial factor. When processing conditions are improved without adding weight to the material, the density remains stable. The structural performance and fuel economy of lightweight materials are advantageous to the transportation, aircraft, automobile, and marine sectors.

Figure 8 showcases the optimized parameters for coordinated processing. Although the moisture content and density remain constant, the material's quality improves with greater curing temperatures, molding pressures, curing times, and fiber orientations. Maximizing mechanical performance without sacrificing weight or consistency in production is the goal of balanced optimization. Coordinated process management is necessary for high-performance polymer composites to attain repeatable and dependable technical attributes.

In particular, machine learning methods for mechanical property prediction in polymer composite materials pay close attention to the processing factors shown in Figure 8. Random Forest, Artificial Neural Network, and XGBoost create intricate nonlinear relationships between production circumstances and mechanical responses by utilizing processing variables and components of the material's composition. With accurate variable representation, intelligent process optimization and forecast accuracy are both enhanced.

A positive production environment benefits high-performance polymer composites, as shown in Figure 8. Mechanical performance, structure, and manufacturing flaws can be enhanced by precisely controlling curing temperature, molding pressure, curing time, fiber orientation, moisture content, and density. Accurate prediction of composite behavior and affordable material design for sophisticated engineering applications are made possible by the optimal processing settings, which give dependable datasets for advanced machine learning models.

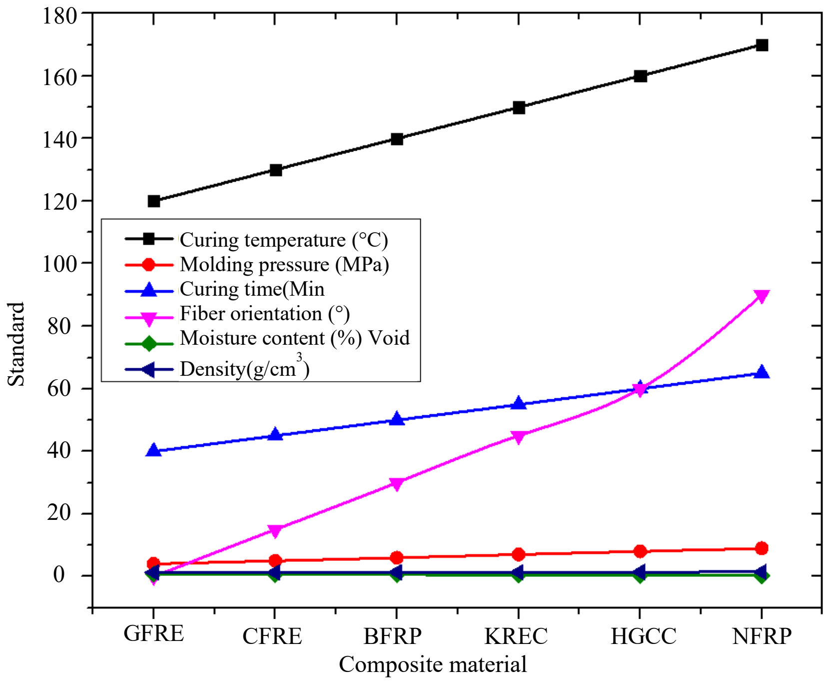

Figure 8. Comparative processing parameter evaluation across polymer composites supporting accurate machine learning property prediction.

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COMPREHENSIVE PERFORMANCE EVALUATION OF MACHINE LEARNING MODELS FOR ACCURATE POLYMER COMPOSITE PROPERTY PREDICTION AND OPTIMIZATION

All standard ML models were trained with the same pretreatment pipeline described in Section 3, which includes consistent feature scaling, encoding and data preparation for all the strategies considered. The same pre-processing procedure ensures the fairness of comparing the prediction performance and improves the reproducibility of the suggested framework. Figures 2-8 show the results of evaluating the suggested machine learning framework for mechanical properties of advanced polymer composite materials. By comparing models, analyzing feature relevance, optimizing hyperparameters, displaying prediction accuracy, material composition characteristics, processing parameters, and referring to Table 10, these figures demonstrate composite behavior and prediction performance aspects.

Table 10. Assessment of machine learning framework for polymer composite mechanical property prediction.

Figures	Description	Key Findings	Significance
Figures 2–8 (Overview)	The machine learning architecture for predicting the mechanical properties of advanced polymer composite materials is evaluated using model performance, feature importance, hyperparameter optimization, prediction accuracy, material composition, processing parameters, and comparative mechanical characteristics.	The framework integrates material composition, reinforcement characteristics, processing conditions, and environmental factors with advanced machine learning algorithms to achieve reliable mechanical property prediction.	Demonstrates the effectiveness of a comprehensive data-driven framework for accurate and efficient prediction of polymer composite behavior.
Figure 2: Performance Comparison of Machine Learning Models	Six machine learning models—Linear Regression (LR), Decision Tree (DT), Random Forest (RF), Support Vector Regression (SVR), Artificial Neural Network (ANN), and Extreme Gradient Boosting (XGBoost)—are compared using Mean Absolute Percentage Error (MAPE), prediction accuracy, training time, and coefficient of determination (R^2).	XGBoost achieves the highest prediction accuracy (approximately 99%) with the lowest prediction error and strong computational efficiency. Random Forest and ANN also perform well, whereas Linear Regression exhibits the largest prediction errors and lowest accuracy. ANN requires the longest training time because of its complex architecture.	Confirms that ensemble learning methods significantly outperform conventional regression techniques for predicting nonlinear mechanical behavior in polymer composites.
Figure 3: Feature Importance Analysis	The relative importance of input variables is evaluated for predicting mechanical properties using various machine learning algorithms.	Fiber content, matrix ratio, fiber orientation, curing temperature, molding pressure, and moisture content are identified as the most influential features. Random Forest, Decision Tree, ANN, and XGBoost produce consistent feature rankings.	Highlights that reinforcement characteristics contribute more significantly to mechanical performance than environmental variables, supporting effective feature selection and improved model robustness.
Figure 4: Hyperparameter Optimization	Hyperparameter tuning is performed for XGBoost, Random Forest, and ANN by optimizing learning rate, tree depth, number of trees, epochs, batch size, and other parameters.	Hyperparameter optimization reduces overfitting while improving prediction accuracy. XGBoost achieves the highest coefficient of determination owing to its gradient boosting mechanism and regularization strategy.	Demonstrates the importance of model optimization in enhancing prediction reliability and generalization capability across different composite material datasets.

Figure 5: Mechanical Property Prediction Accuracy	Prediction accuracy is evaluated for tensile strength, flexural strength, compressive strength, hardness, and impact strength.	XGBoost consistently provides the highest prediction accuracy across all mechanical properties, followed by ANN and Random Forest. Traditional machine learning methods exhibit comparatively lower predictive performance.	Confirms the robustness and generalizability of advanced ensemble learning techniques for predicting multiple mechanical properties simultaneously.
Figure 6: Mechanical Property Trends	Experimental and predicted mechanical properties of polymer composites are analyzed during model development.	Tensile strength, flexural strength, compressive strength, impact strength, elastic modulus, and hardness improve progressively with optimized material composition and processing conditions.	Demonstrates the capability of the proposed framework to accurately capture evolving mechanical performance characteristics of polymer composites.
Figure 7: Material Composition Analysis	Material composition parameters including fiber content, matrix ratio, fiber length, filler content, density, and void fraction are analyzed.	Fiber content and fiber length increase, matrix proportion decreases, density remains relatively stable, void fraction is minimized, and filler percentage remains constant.	Shows that optimized reinforcement composition plays a critical role in enhancing composite mechanical properties and prediction accuracy.
Figure 8: Processing Parameter Analysis	Processing variables such as curing temperature, molding pressure, curing time, fiber orientation, moisture content, and density are evaluated.	Optimized curing conditions, controlled pressure, appropriate curing duration, proper fiber orientation, and low moisture levels contribute significantly to improved composite performance.	Demonstrates that manufacturing parameters strongly influence material quality and are essential input variables for accurate machine learning-based mechanical property prediction.
Overall Discussion	Figures 2–8 collectively evaluate model performance, feature importance, optimization, material characteristics, and manufacturing conditions.	Advanced ensemble learning methods, particularly XGBoost, achieve superior prediction accuracy compared with conventional approaches. The framework identifies the most influential material and processing parameters while reducing experimental effort and computational cost.	Validates the proposed machine learning framework as a reliable and practical tool for intelligent material design, accelerated product development, reduced laboratory testing, and next-generation polymer composite engineering applications.

CONCLUSIONS

Advanced engineering polymer composite materials' mechanical properties were predicted in this study using a complete machine learning framework. Estimations of tensile, flexural, compressive, elastic modulus, hardness, and impact strength are made utilizing supervised machine learning algorithms, preprocessing techniques, reinforcement properties, manufacturing factors, and material composition. When compared to experimental and numerical methods, the suggested strategy saves time, money, and computational effort during material characterization without sacrificing prediction accuracy. When it comes to complicated composite design variables and their nonlinear interactions, ensemble learning and neural network models outperform regression. The generalizability and durability of models for polymer composite systems are enhanced by the use of hyperparameter tuning, feature engineering, and cross-validation. To help with material selection and structural design, engineers can use the framework to determine which processing and material parameters have the most impact on composite performance. It appears from the experiments that data-driven prediction algorithms can screen new composite formulations more quickly than lab testing, which means that product development can be accelerated. Materials engineering could become more intelligent and data-driven with the help of machine learning, according to this study. Composites in the aerospace,

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automotive, marine, biomedical, civil, and renewable energy industries can benefit from this technology's quick, scalable, and accurate prediction models, which enhance polymer composite materials, allow for sustainable production, and maximize composite performance. In addition, the application of SHAP-based explainability enhances the transparency of the ANN model by quantifying the influence of specific material composition and processing parameters on the anticipated mechanical properties.

The research in the future ought to combine physics-informed machine learning, digital twins, explainable AI, and hybrid deep learning. Improving the accuracy, dependability, and practicality of forecasts for collaborative materials research can be achieved through the use of real-time sensor data, federated learning, and huge composite material databases. Independent regression models were used in the present study, but future work will explore multi-output machine learning architectures that can predict numerous correlated mechanical parameters simultaneously by explicitly modeling the dependence among features.

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