

Comparative Analysis of Artificial Intelligence Algorithms for Predicting the Elastic Modulus of Recycled Polypropylene-Tea Residue Composites

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Abstract

This study evaluates the effectiveness of different artificial intelligence (AI) algorithms in forecasting the elastic modulus of recycled polypropylene-tea residue composites. The research seeks to determine the most precise algorithm for this predictive task, thus aiding in the advancement of sustainable materials. Composite samples were formulated utilizing residues from Thai and green tea, with different proportions of polypropylene-graft-maleic anhydride (PP-g-MA) and thermoplastic elastomer (TPE). The elastic modulus of these samples was experimentally determined. Five artificial intelligence algorithms were assessed: Generalized Linear Model, Decision Tree, Random Forest, Support Vector Machine (SVM), and Artificial Neural Network (ANN). Performance metrics, such as Root Mean Square Error (RMSE), Relative Error, R², and P-value, were employed for comparison.

The results demonstrate that the ANN achieved the greatest prediction accuracy, evidenced by a $R²$ value of 0.883 and the minimal relative error of 3.11% \pm 0.47%. The Decision Tree and Random Forest algorithms exhibited commendable performance, whereas the SVM yielded the least accurate predictions. The research indicates that the correlation between composite formulation and elastic modulus is significantly non-linear, requiring advanced modeling methodologies. This study identifies the optimal AI algorithm for predicting the elastic modulus of these composites and elucidates the intricate interactions within the material system. The results have considerable implications for expediting the advancement and refinement of sustainable composite materials that incorporate recycled and natural elements.

Keywords: Artificial Intelligence Algorithms, Elastic Modulus Prediction, Recycled Polypropylene Composites, Tea Residue Composite.

1. Introduction

Wood-plastic composites (WPCs) derived from recycled polymers and natural fibers represent a significant advancement in sustainable materials research, offering a unique combination of environmental benefits and technical challenges. These innovative composites exemplify sustainability principles by incorporating recycled plastics and natural fibers, reducing waste and promoting resource conservation.

Incorporating natural fibers into wood-plastic composites enhances their mechanical qualities, particularly stiffness and strength. Employing compatibilizers enhances the interactions between the fibers and the matrix, making this particularly applicable. Moreover, the recyclability of WPCs, which permit numerous recycling cycles, highlights their potential in circular economy applications. However, the development and use of WPCs face significant challenges. Repeated recycling can significantly impair mechanical properties, with studies showing reductions in tensile strength of up to 17% and decreases in modulus of up to 28% across numerous recycling cycles. Furthermore, achieving suitable fiber-matrix compatibility during processing is a complex task that significantly affects the composite's overall performance and uniformity. While WPCs offer beneficial characteristics in terms of sustainability and initial mechanical performance, apprehensions about long-term durability and processing challenges necessitate comprehensive assessment and continuous research to maximize their potential across many applications. (Burgada et al., 2022; Spear et al., 2015; Vercher et al., 2018; X. Zhao et al., 2021)

Previous studies have employed Design and Analysis of Experiments (DoE) to investigate the effects of various factors on the mechanical properties, particularly the Elastic Modulus, of recycled polypropylene-tea residue composites. Prior research shows that specific basic components affect the mechanical properties of WPCs. However, the interaction analysis revealed that some covariate combinations had no statistically significant effects on these properties. Analysis of variance (ANOVA) showed that the three-way interaction among the studied components did not significantly affect the mechanical properties.

Previous research conducted regression analysis and developed linear prediction models for mechanical properties, yielding R² values between 46% and 66%. These moderate R² values indicate that the relationship between the factors and WPC mechanical properties may not be entirely linear. This finding highlights the limitations of conventional statistical methods in explaining and predicting WPC material behavior. Due to these non-linear relationships and the limited predictive capability of linear models, more sophisticated analytical methods are necessary to accurately characterize and predict the mechanical properties of recycled polypropylene-tea residue composites (Kongrit, Limsiri, & Meehom., 2024a; Kongrit, Limsiri, & Meehom., 2024b)

The examination of wood-plastic composites (WPCs) is hindered by significant variability in experimental data, resulting from the diverse characteristics of recycled materials and the intricate interactions among components. Conventional statistical techniques frequently fail to effectively model and forecast the mechanical properties of WPCs because of this significant volatility. The analysis of highdimensional data in Wood-Plastic Composite (WPC) research requires sophisticated statistical methodologies and specialized knowledge. The intricacy of the data and contemporary analytical methods poses difficulties in result interpretation and the suitable application of analytical procedures. Expertise in machine learning and advanced statistics is essential, as conventional methods may be inadequate for high-variance data. The issue is intensified by the persistent lack of adequate training among researchers in the advanced

statistical methods required for high-dimensional data processing. The lack of expertise hinders result interpretation and may lead to misunderstandings or misapplications of analytical techniques. An in-depth comprehension of machine learning and advanced statistical principles is crucial, as traditional methods often prove inadequate in high-variance scenarios. High-variance data in WPC research requires significant computational resources, often exceeding the limitations of traditional analytical techniques. Researchers are utilising error-pooling approaches and advanced modelling to address these challenges; nevertheless, these require a deep understanding of statistics. Although formidable, these challenges offer opportunities for innovation in WPC research analytics. The development of innovative statistical tools and targeted training programs can enhance the dependability of research results. Improving analytical capabilities in WPC research can yield more accurate results, hence enhancing decision-making in materials science and engineering. (Chiu et al., 2017; Garcia-Milian et al., 2018; Johnstone & Titterington, 2009; Park et al., 2007; Rahnenführer et al., 2023)

The utilization of artificial intelligence (AI) in materials science, especially in composite materials, has become a revolutionary method for improving predictive modeling and material characterization. Artificial neural networks (ANNs), a fundamental AI methodology, have exhibited significant effectiveness in assessing and forecasting the mechanical properties of diverse composite materials. Artificial neural networks have successfully predicted the shear stress-strain characteristics in epoxy composites reinforced with carbon and E-glass fibers, with a success rate of over 80% (Bezerra et al., 2007). It has been shown that neural network-based models are better than traditional mathematical models at showing the nonlinear stress-strain properties of graphite-epoxy laminates (Pidaparti & Palakal, 1993). These improvements highlight AI's ability to transform our understanding and enhancement of composite materials.

The implementation of AI in composite material research extends beyond the prediction of mechanical properties, offering substantial computational efficiency and diverse applications across several sectors. Research indicates that AI techniques significantly reduce the time required to calculate the properties of composite materials. This enables rapid estimation of materials' hydraulic, thermal, and mechanical properties based on environmental data and their characteristics (Brown et al., 2008). Furthermore, the integration of artificial neural networks with other artificial intelligence technologies has enhanced composite design, property prediction, and material selection in sectors like as aerospace and automotive. (Hasan et al., 2009).

Artificial intelligence exhibits considerable promise in the field of composite materials research for generating accurate forecasts. Nevertheless, obstacles remain in the standardization of procedures and the assurance of data accuracy. To significantly progress the domain of composite materials science, artificial intelligence must continue its research and development initiatives. Given the aforementioned characteristics, it is evident that use linear equations to predict the mechanical properties of composite materials is of restricted efficacy. This study seeks to utilize artificial intelligence algorithms to determine

the Elastic Modulusity in composite materials. The study will do a comparative examination of the efficacy of different algorithms utilized in this area. Moreover, subsequent studies of various composite materials may extrapolate research findings to anticipate additional evaluated mechanical qualities. This method is poised to substantially enhance and optimize high-performance composite materials, ultimately improving their design and development processes.

2. Objectives

To compare the effectiveness of various artificial intelligence Algorithms for Predicting the Elastic Modulus of Recycled Polypropylene-Tea Residue Composites

3. Research Question

Which artificial intelligence algorithm demonstrates the highest accuracy in predicting the elastic modulus of recycled polypropylene-tea residue composites?

4. Literature Reviews and Research Frameworks

The utilization of AI algorithms in wood-plastic composites (WPCs) is revolutionizing material characterization, optimization, and performance forecasting. These algorithms augment the comprehension of intricate relationships among diverse parameters, resulting in enhanced composite properties. Machine learning (ML) has become an influential instrument in forecasting the mechanical properties of wood-plastic composites (WPCs), providing considerable benefits in material science and engineering. Sharma and Kushvaha (2022) emphasize that the implementation of machine learning techniques has transformed material development, significantly accelerating the process and reducing costs by minimizing the necessity for extensive physical testing and facilitating rapid iterations in material design. The capability of machine learning in material characterization is illustrated by Fini et al. (2015), who effectively utilized artificial neural networks to assess the elastic behavior of wood-plastic composites under cold temperature conditions, showcasing the adaptability of machine learning methodologies in elucidating intricate material responses across diverse environmental factors. These studies collectively highlight the increasing significance and effectiveness of machine learning in enhancing our comprehension and predictive abilities regarding composite materials, especially in the realm of WPCs, thereby facilitating more efficient and innovative material development processes in the future.

This research's conceptual framework begins with the input variables, including tea residue type, PP-g-MA content, and TPE content, which determine the composite formulation. These formulations undergo material processing, followed by experimental measurements to obtain elastic modulus data. The core of the study involves applying five AI algorithms (Generalized Linear Model, Decision Tree, Random Forest, Support Vector Machine, and Artificial Neural Network) to this data, creating prediction models. These models are then evaluated using performance metrics such as RMSE, Relative Error, R², and P-value to

identify the best prediction model. The framework extends to the application phase, where the optimal model contributes to sustainable composites development through enhanced material design, property prediction, and optimization. This comprehensive approach integrates materials science with artificial intelligence, aiming to accelerate the development of sustainable composite materials by leveraging advanced predictive modeling techniques.

Figure 1: conceptual framework

5. Methodology

5.1 Composites Preparation and Mechanical Testing

The materials utilized in this study comprised recycled polypropylene (PP) derived from the thermoforming process of drinking cups, Thai tea residue, and green tea residue post-beverage preparation.

Local beverage establishments graciously provided the tea residues, and their preparation methods aligned with previous research protocols (Kongrit, Limsiri, & Meehom., 2024a; Kongrit, Limsiri, & Meehom., 2024b). Additional materials included polypropylene-graft-maleic anhydride (PP-g-MA) with an approximate maleic anhydride content of 1% (POLYB® AM-920), thermoplastic elastomer (TPE, ENGAGE™ 7447), and antioxidant (SUNOX® 168).

The composite formulation combines constant and variable elements. The defined parameters included 20% tea residue by weight and 0.1% antioxidant content by weight. The recycled polypropylene grade content varied from 79.9% to 64.9 wt%, depending on the residual composition. The composite properties were investigated by methodically changing a few experimental circumstances. The study examined two types of tea residue: Thai tea and green tea. The proportion of compatibilizer (PP-g-MA) was changed to 0%, 2.5%, and 5% by weight. The concentrations of thermoplastic elastomer (TPE) were set at 0%, 5%, and 10% by weight. Table 1 shows the formulations of composite materials made from tea residue for experimental design objectives. This experimental design allows for a thorough evaluation of the effects of tea residue type, compatibilizer content, and thermoplastic elastomer content on the elastic modulus of recycled polypropylene-tea residue composites. The systematic modification of these characteristics makes it easier to assess their individual and interaction effects on the resulting composite materials, particularly their elastic modulus.

A mechanical mixer was used to accomplish the initial dry mixing of recycled polypropylene, tea residue, and additives, followed by one hour of desiccation. The mixture was then melt compounded in a co-rotating twin-screw extruder (L/D=12) at temperatures varying from 200°C to 230°C between the feed and metering zones. Following air chilling and pelletizing, the material was hot-air dried. ASTM-compliant test specimens were manufactured for analysis using injection molding. Tensile testing was performed in accordance with ASTM D638 requirements on a LLOYD LR10K testing equipment equipped with a 10 kilonewton (10 kN) load cell. The test was carried out at a crosshead speed of 50 millimeters per minute. These tests found the Elastic Modulus, which is provided in MPa. Ten specimens were evaluated per experimental condition to assure statistical reliability. The elastic modulus test results are reported as mean values with standard deviations, as indicated in Table 1 and Figure 1 respectively.

5.2 Predictive Modeling of Elastic Modulus Using Machine Learning Algorithms

The study approach consists of several important phases. A computer-operated tensile testing machine first evaluated the mechanical qualities of the materials and entered the findings into CSV form. The total dataset consisted of 180 entries (18 formulations \times 10 specimens per experimental condition). The outliers were identified using the Interquartile Range (IQR) method, which effectively detects anomalies by measuring the spread of the middle 50% of data (Perez & Tah, 2020). The outlier detection and treatment system were written in Python and ran on Google Colab, a cloud-based Python development tool. From the total 180 entries, 6 data points were identified as outliers: two points each from rPP/T and rPP/G formulations, one point from rPP/T/MA5/TPE5, and one point from rPP/G/MA2.5/TPE10. The median

replacement method was chosen over mean replacement due to its superior robustness against extreme values. While mean values are significantly affected by outliers and can lead to skewed results (Insolia et al., 2021), median replacement helps maintain the central tendency of the data while minimizing the influence of extreme values on the dataset (Cursi & Yang, 2019). This approach ensures the integrity of the training data for machine learning models.

Table 1 Formulations of Tea Residue-Based Composite Materials for Experimental Design

Note: All mixing ratios throughout this study are expressed in weight percent (wt%).

The default parameters from Altair AI Studio 2024.1.0 were used for each algorithm as follows:

Generalized Linear Model: ridge regression with alpha = 0.0

Decision Tree: maximum depth = 10, minimum samples split = 4

Random Forest: number of trees = 100, maximum depth = 10

Support Vector Machine: dot kernel, C = 0.0, gamma = 'scale'

Artificial Neural Network: two hidden layers (3, 2 nodes), learning rate = 0.01, activation

function = sigmoid

These default parameters provided satisfactory prediction performance without the need for additional tuning.

For the analysis and prediction of the Elastic Modulus, multiple algorithms were employed, including General Regression, Decision Tree, Random Forest, Support Vector Machine, and Artificial Neural Network (ANN). These analyses were conducted using Altair AI Studio 2024.1.0 software, a specialized platform for machine learning and data analysis. The dataset was partitioned for training and testing using 10-fold cross-validation technique to ensure robust model performance. The predictive accuracy of the Elastic Modulusity was assessed using several statistical metrics: Root Mean Squared Error (RMSE), Relative Error, coefficient of determination (R^2) , and P-value at a significance level of 0.05. Following the predictive modeling, a comparative analysis was performed between the experimentally obtained Elastic Modulus values and those predicted by the models. Visualization of these comparisons was created using Python in Google Colab to provide a clear graphical representation of the results.

6. Results

6.1 Elastic Modulus of Recycled PP-Tea Residue Composites

Figure 2, the experimental findings demonstrate the influence of tea type, the percentage of PP-g-MA, and the percentage of TPE (Thermoplastic elastomer) on the elastic modulus of recycled polypropylene-tea residue composites. The elastic modulus of green tea-based composites varied between 442.13 MPa and 709.23 MPa, while Thai tea-based composites exhibited a range from 491.62 MPa to 758.24 MPa. The incorporation of PP-g-MA enhanced the elastic modulus in both varieties of tea. Green tea composites exhibited the highest average modulus of 685.5 MPa with 5% PP-g-MA and 0% TPE, whereas Thai tea composites demonstrated the highest average modulus of 740.4 MPa with the identical combination.

The incorporation of TPE (thermoplastic elastomer) into the composites resulted in a similar decrease in elastic modulus for both varieties of tea. This effect intensified with higher TPE percentages. When the amount of TPE in green tea composites with 5% PP-g-MA was raised from 0% to 10%, the average elastic modulus dropped from 685.5 MPa to 530.2 MPa. In Thai tea composites with 5% PP-g-MA, an increase in TPE content decreased the average elastic modulus from 740.4 MPa to 557.6 MPa. The findings indicate that PP-g-MA enhances the stiffness of the composites, whereas the incorporation of TPE renders the material more flexible, likely due to its influence on the interfacial adhesion between the polymer matrix and tea residues.

6.2 Comparative Performance Metrics of Artificial Intelligence Algorithms for Predicting Elastic Modulus

The main objective of this study is to compare the performance of different AI techniques in predicting the elastic modulus, rather than investigating the effects of material compositions. The features and their levels used in this study were based on preliminary experiments and material processing constraints, which were already described in the methodology section. The focus of the results and discussion is therefore on the predictive capabilities of various AI algorithms rather than the compositional analysis of the composites.The comparative analysis of various artificial intelligence algorithms for predicting the elastic modulus of recycled polypropylene-tea residue composites yielded diverse performance metrics, as summarized in Table 2. The evaluation criteria encompassed Root Mean Square Error (RMSE), Relative Error, coefficient of determination (R²), and P-value at a significance level of 0.05.

Differently performing five artificial intelligence algorithms for elastic modulus prediction of recycled polypropylene-tea residue composites was investigated. Under a significance level of 0.05, the algorithms were assessed using RMSE, Relative Error, coefficient of determination (R²), and P-value. With R² = 0.8828, the Artificial Neural Network (ANN) had the highest predictive accuracy; followed by the Decision Tree (R^2 = 0.88777) and Random Forest (R^2 = 0.8662). Whereas the Support Vector Machine (SVM) had the lowest accuracy (R^2 = 0.4970), the Generalized Linear model performed rather (R^2 = 0.7574). Closely followed by the Random Forest and ANN, the Decision Tree algorithm shown the lowest RMSE (21.965 \pm 5.132) and relative error (2.98% \pm 0.64%). With a P-value of 0.97425, the Random Forest algorithm showed the highest statistical significance; next in order was the Decision Tree with a P-value of 0.96803. Though the ANN showed the best R² value, its P-value (0.58638) shows less statistical relevance than those of the tree-based models. With P-values of >0.0000 and 0.20729 respectively, the Generalized Linear Model and SVM shown different degrees of statistical significance. The Support Vector Machine (SVM) showed the lowest prediction accuracy ($R² = 0.497$) due to its limitations in handling the complex non-linear relationships present in our composite material data. Unlike ANN and tree-based methods, SVM struggled with the high variability inherent in recycled materials and natural fibers. Additionally, the algorithm's performance may have been constrained by the challenges in capturing multiple interacting variables affecting the elastic modulus. The findings show that although the ANN produces the best fit to the data, the Decision Tree and Random Forest algorithms show a favorable mix of high accuracy and statistical dependability, so maybe more suitable for this given use.

Figure 3 illustrates the comparison of actual and predicted elastic modulus values for two distinct algorithms. Figure 3a illustrates the relationship between the actual elastic modulus and the predicted elastic modulus derived from the Generalized Linear algorithm. Conversely, Figure 3b illustrates the correlation between the actual elastic modulus and the predictive elastic modulus produced by the Artificial Neural Network algorithm. These plots visually represent the predictive accuracy of each model, facilitating a direct comparison of their performance in estimating the elastic modulus of the recycled PPtea residue composites.

Figure 3: Comparison of Actual vs. Predicted Elastic Modulus for Recycled PP-Tea Residue Composites: (a) Generalized Linear Algorithm and (b) Artificial Neural Network Algorithm

7. Discussion

The study on tea residue-based composite materials reveals intriguing relationships between material composition and mechanical properties, particularly elastic modulus. The addition of PP-g-MA generally increased the elastic modulus, with the effect more pronounced in Thai tea residue composites compared to green tea residue composites. This suggests that PP-g-MA may enhance interfacial adhesion between the tea residue and the polymer matrix, leading to improved mechanical properties. Conversely, the incorporation of TPE typically resulted in a decrease in elastic modulus, likely due to its elastomeric nature softening the overall composite. The complex interplay of these components presents challenges in predicting the elastic modulus, as evidenced by the comparative performance of various AI algorithms. Decision Tree, Random Forest, and Artificial Neural Network models demonstrated superior predictive capabilities, with relatively low RMSE and high R² values. This suggests that the relationship between composition and elastic modulus is non-linear and potentially involves complex interactions among variables. The high performance of tree-based models (Decision Tree and Random Forest) indicates that the data may contain distinct patterns or clusters based on composition, which these algorithms are adept at capturing. The strong performance of the ANN model further supports the presence of complex, non-linear relationships in the data. These findings not only provide insights into the material behavior of tea residuebased composites but also highlight the potential of machine learning techniques in materials science for predicting and optimizing material properties.

The investigation of tea residue-based composite materials uncovers significant correlations between material composition and mechanical properties, especially elastic modulus. The incorporation of PP-g-MA typically enhanced the elastic modulus, with a more significant impact observed in Thai tea residue composites than in green tea residue composites. This indicates that PP-g-MA may augment interfacial

adhesion between the tea residue and the polymer matrix, resulting in enhanced mechanical properties. In contrast, the addition of TPE generally led to a reduction in elastic modulus, probably because its elastomeric properties softened the composite. (Zulfia et al., 2015; K.; Ragunathan et al., 2016; Lin et al., 2020) The complex interaction of these elements complicates the prediction of the elastic modulus, as evidenced by the efficacy of various AI algorithms. The Decision Tree, Random Forest, and Artificial Neural Network models showed improved predictive performance, with low RMSE and high R² values. This indicates that the correlation between composition and elastic modulus is non-linear and may entail intricate interactions among variables. (Esmaeili & Rizvi, 2023; Upadhyay & Singh, 2014; Ho et al., 2021; Galimzyanov et al., 2023) The enhanced effectiveness of tree-based models (Decision Tree and Random Forest) suggests that the data may reveal unique patterns or clusters based on composition, which these algorithms can identify. (Rudar et al., 2023; Taskin et al., 2023) The ANN model's strong performance indicates the presence of complex, non-linear relationships within the data. These findings elucidate the material characteristics of tea residue-based composites, illustrating the potential of machine learning methodologies in materials science for forecasting and enhancing material properties. (May et al., 2008; Yoo et al., 2006; Hussain et al., 2023) Support Vector Machine (SVM) exhibited the least accurate predictions, characterized by a low R^2 value and high RMSE. This suboptimal performance may be attributed to SVM's limitations in handling highly complex relationships, particularly in scenarios involving high-dimensional data with significant non-linear interactions among variables. (Olorisade et al., 2022; Tang et al., 2020; Cipolla & Gondzio, 2022) The moderate efficacy of the Generalized Linear Model further substantiates that the connections among variables in this dataset are not wholly linear. (McCullagh & Nelder, 2005; Heit et al., 2024)These results emphasize the essential significance of choosing algorithms that correspond with the intrinsic attributes of the data to get high accuracy in forecasting composite material qualities.

8. Conclusions

This study evaluated the efficacy of different artificial intelligence systems in forecasting the elastic modulus of recycled polypropylene-tea residue composites. The findings indicate that the Artificial Neural Network (ANN) had the greatest accuracy in forecasting the elastic modulus, evidenced by a $R²$ value of 0.883 and a minimal relative error of $3.11\% \pm 0.47\%$. This exceptional performance is due to ANN's capacity to identify intricate, non-linear correlations between the composite constituents and their resultant mechanical properties. The Decision Tree and Random Forest algorithms demonstrated favorable outcomes, indicating that the data may exhibit discernible patterns based on composition.

The Support Vector Machine (SVM) produced the least accurate predictions, demonstrating its limitations in dealing with the complex interactions found in this material system. These findings not only address the research question by identifying the most effective algorithm, but also shed light on the nature of the relationship between composite formulation and elastic modulus. The study emphasizes the importance of using appropriate machine learning techniques to predict material properties in composite

systems, particularly those made from recycled materials and natural fibers like tea residues. Furthermore, these findings pave the way for more precise prediction models in materials science, potentially speeding up the development and optimization of sustainable composite materials.

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