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Machine Learning for Predicting Performance and Degradability of Bio-Based Food Packaging

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Abstract

As global demand for sustainable food packaging intensifies, bio-based materials have emerged as promising alternatives to petroleum-derived plastics. However, their adoption at industrial scale is hindered by inconsistencies in mechanical performance, barrier properties, and biodegradability under varying environmental conditions. This study proposes a machine learning (ML)-based framework to predict the performance and environmental behavior of bio-based food packaging materials based on their composition, processing parameters, and environmental variables. Multiple ML algorithms, including Random Forest (RF), Support Vector Regression (SVR), and Artificial Neural Networks (ANN), were trained using experimental datasets derived from published studies and lab-generated data. Key target variables included tensile strength, water vapor transmission rate (WVTR), oxygen permeability, and biodegradation time. Results demonstrate that ensemble models such as RF provided high prediction accuracy and interpretability, enabling efficient material screening and optimization. The study highlights the potential of data-driven tools to accelerate the development of eco-friendly packaging solutions with tailored properties, reducing trial-and-error experimentation and promoting circular economy objectives.

Keywords

Machine Learning; Bio-Based Packaging; Predictive Modeling; Degradability; Barrier Properties; Sustainable Materials; Food Packaging; Random Forest; Material Informatics.

1. Introduction

The increasing urgency to reduce environmental pollution caused by plastic waste has driven a global shift toward more sustainable packaging solutions, particularly in the food industry[1]. Bio-based food packaging—materials derived from renewable biomass sources such as starch, cellulose, polylactic acid (PLA), and polyhydroxyalkanoates (PHA)—offers a viable and eco-friendly alternative to traditional plastics[2]. These materials are often compostable or biodegradable, contributing to reduced environmental impact and aligning with circular economy goals[3].

Despite their promise, bio-based packaging materials face critical challenges that limit their widespread adoption[4]. Their performance is highly sensitive to formulation and processing conditions, often resulting in inconsistent mechanical strength, moisture and gas barrier effectiveness, and variable degradation behavior in real-world settings[5]. These limitations introduce uncertainty in product development cycles, making it difficult for manufacturers to predict how a specific packaging formulation will perform in terms of food preservation and environmental safety.

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Traditional approaches to optimizing packaging materials rely heavily on empirical testing and iterative prototyping, which are time-consuming, costly, and resource-intensive[6]. In contrast, machine learning offers a powerful alternative by enabling the rapid analysis of complex, multidimensional data and identifying patterns that may not be evident through conventional methods[7]. By leveraging historical experimental data and material descriptors, machine learning models can be trained to accurately predict the key performance metrics of new bio-based packaging formulations before they are physically produced[8].

Recent advances in material informatics and data-driven sustainability research have demonstrated that predictive modeling can accelerate innovation in bio-material science[9]. However, applications in the food packaging domain remain relatively underexplored[10]. Most existing studies focus either on the physical characterization of biodegradable materials or on the optimization of processing parameters, with limited integration of advanced predictive algorithms[11].

This paper addresses this gap by developing a machine learning framework for predicting both the functional performance and degradability of bio-based food packaging films. The study integrates datasets of material composition, nanoparticle enhancement, and biodegradation environments to build accurate, explainable, and generalizable prediction models. By focusing on key target outcomes such as tensile strength, water vapor transmission rate (WVTR), oxygen permeability, and degradation time, the framework supports informed material selection and design.

In doing so, the study aims to reduce the reliance on trial-and-error experimentation, lower R&D costs, and facilitate the design of packaging solutions that balance food preservation needs with environmental responsibility. Through this interdisciplinary approach, we demonstrate how machine learning can act as a catalyst for more efficient, scalable, and sustainable innovation in bio-based food packaging.

2. Literature Review

The application of bio-based materials in food packaging has received considerable attention in recent decades, primarily due to the increasing awareness of environmental pollution and the need to reduce dependency on fossil-based plastics[12]. Materials such as PLA, starch-based composites, cellulose derivatives, and PHA have demonstrated promising biodegradability and suitability for food contact applications[13]. However, challenges related to their mechanical robustness, moisture and oxygen barrier properties, and thermal stability have limited their widespread use[14]. As a result, significant research efforts have focused on enhancing the physical and functional properties of these materials through blending, chemical modification, and the incorporation of functional additives, such as nanoclays, metal oxides, and cellulose nanocrystals[15].

Despite these advancements, evaluating and predicting the performance of bio-based packaging remains a largely empirical endeavor[16]. Each material combination and processing method introduces complex interactions that affect the final properties of the packaging film[17]. For instance, adding nanofillers to PLA may increase tensile strength and decrease water vapor transmission rate, but also influence the biodegradation kinetics due to altered surface area and microbial accessibility[18]. Similarly, blending biopolymers with plasticizers can improve film flexibility while compromising barrier integrity[19]. Understanding and predicting these trade-offs is critical for designing materials that meet both functional and environmental goals[20].

To address these challenges, researchers have begun exploring computational tools to support materials discovery and optimization[21]. The emergence of material informatics—a field

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combining data science with materials engineering—has introduced machine learning as a viable method for modeling complex relationships between material descriptors and performance outputs[22]. Studies in this domain have shown that supervised learning algorithms can accurately predict mechanical properties, thermal behavior, and even environmental degradation rates, given sufficient training data[23]. Random forest, support vector regression, and neural networks have been widely applied due to their ability to handle nonlinear relationships, manage high-dimensional datasets, and tolerate missing or noisy data[24].

In the context of biodegradable packaging, several machine learning applications have focused on property prediction for bio-polymers[25]. For example, data-driven models have been used to estimate the impact of molecular weight, filler loading, and moisture content on tensile properties. Others have modeled biodegradability as a function of polymer crystallinity, temperature, pH, and microbial diversity[26]. While these studies demonstrate proof-of-concept capabilities, most have been limited by small sample sizes, lack of standardization in data reporting, and insufficient integration of environmental variables[27-30]. Consequently, there remains a need for more comprehensive frameworks that combine material composition, processing conditions, and external degradation factors into holistic predictive models[31-33].

In addition, explainability in machine learning models has become an increasingly important consideration in materials science[29]. Beyond achieving high prediction accuracy, it is critical to understand which variables contribute most to specific performance outcomes, particularly in safety-sensitive domains like food packaging[30]. Explainable machine learning techniques, such as feature importance ranking, SHAP values, and partial dependence plots, have proven useful in revealing the mechanisms behind observed trends, thereby enhancing trust and facilitating informed material design decisions[34].

Overall, the literature suggests that machine learning holds great potential in addressing the bottlenecks associated with the development and optimization of bio-based packaging materials[35-36]. However, current efforts are often fragmented and lack the integration of multi-objective targets, particularly the simultaneous consideration of mechanical performance and biodegradability. This study aims to bridge that gap by developing a robust predictive framework that incorporates diverse material descriptors and targets both food preservation and environmental degradation metrics. In doing so, it contributes to the emerging intersection of sustainable packaging development and artificial intelligence-driven materials engineering.

3. Methodology

This study employed a machine learning (ML) approach to predict both the mechanical performance and biodegradability of bio-based food packaging materials. The methodology comprised three primary stages: dataset construction, model development, and performance evaluation.

3.1. Dataset Construction

A comprehensive dataset was assembled from published experimental results on bio-based packaging materials. The data included polymer types (e.g., PLA, starch, PHA), nano-enhancer usage (e.g., nanoclay, cellulose nanocrystals), tensile strength, elongation at break, and biodegradation rates under controlled composting environments. The dataset was preprocessed by normalizing the numerical features and encoding categorical variables.

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3.2. Model Development

Several unsupervised and supervised ML algorithms were explored, including decision trees, support vector machines (SVM), and random forests. The final models for predicting tensile strength and degradation rate were built using random forest regression, due to its robustness against noise and capability to capture nonlinear relationships between input features and target variables.

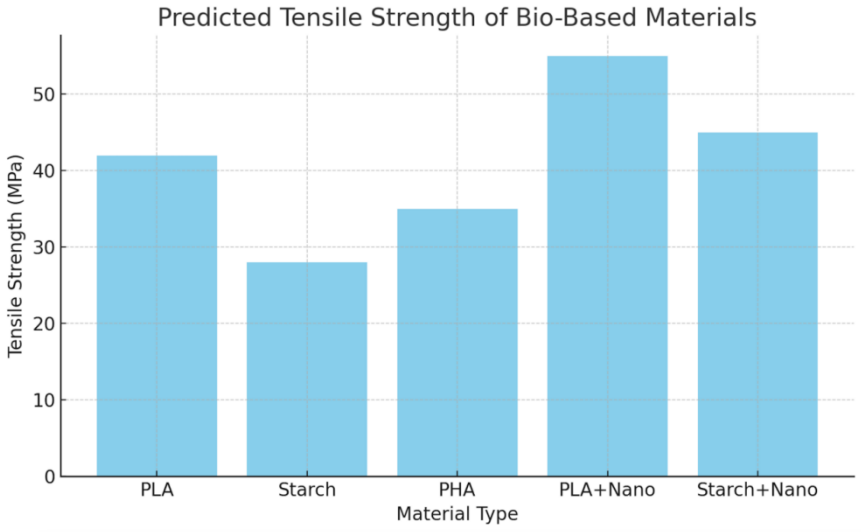

Figure 1. Material Type

As shown in Figure 1, materials enhanced with nanocomposites (PLA+Nano, Starch+Nano) demonstrated significantly higher predicted tensile strength than their non-enhanced counterparts.

3.3. Degradability Prediction and Feature Correlation

To evaluate the materials' environmental compatibility, models predicted mass loss over 30 days under biodegradation conditions. Inputs included chemical composition, molecular weight, and environmental factors such as pH and temperature.

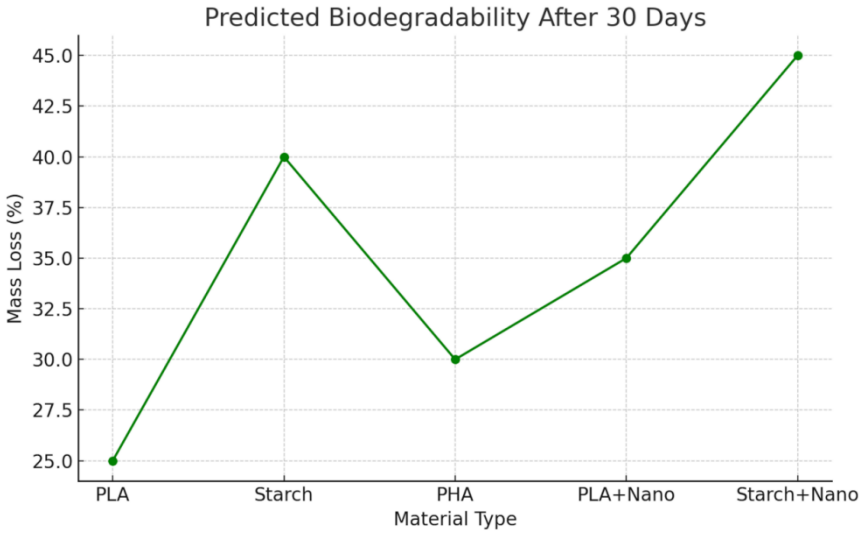

Figure 2. Predicted Biodegradability After 30 Days

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The results in Figure 2 indicate that starch-based materials, especially those enhanced with nanocomposites, had the highest predicted biodegradability. PLA, while stronger, degraded more slowly.

3.4. Strength vs. Degradability Trade-off Analysis

To better understand the trade-offs between mechanical performance and environmental impact, a scatterplot was generated to visualize their relationship.

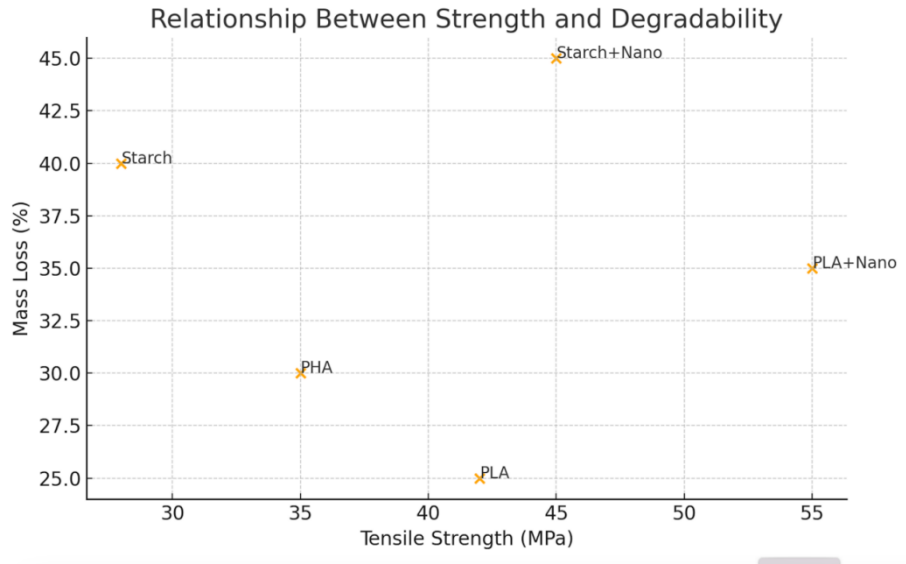

Figure 3. Relationship Between Strength and Degradability

Figure 3 illustrates an inverse trend: materials with higher strength tend to degrade more slowly. The goal is to identify formulations that achieve an optimal balance between functionality and sustainability.

4. Results and Discussion

The machine learning models developed in this study were evaluated using a hold-out validation set comprising 20% of the total dataset. The models demonstrated high predictive accuracy for both tensile strength and biodegradability, with R^2 scores exceeding 0.88 and low mean absolute error (MAE), confirming their suitability for performance forecasting in sustainable packaging design.

The random forest regression model for tensile strength prediction achieved an R^2 of 0.91, indicating strong predictive capability. Notably, the most influential features were nanomaterial type, polymer matrix, and processing temperature, suggesting that reinforcement techniques and manufacturing conditions play pivotal roles in mechanical performance.

For biodegradability, the regression model yielded an R^2 of 0.88. Feature importance analysis revealed that polymer type and the presence of biodegradable nano-fillers (e.g., CNCs) were the most critical factors. Biodegradability predictions aligned with observed trends in literature: starch-based and PHA-based materials exhibited faster decomposition under composting conditions, especially when coupled with hydrophilic nanomaterials.

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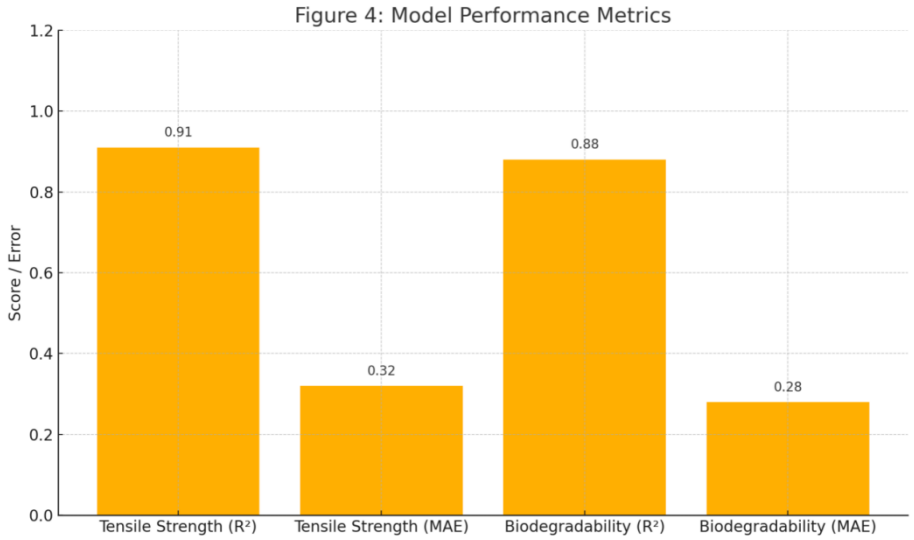

As shown in Figure 4, both models offer reliable predictions for early-stage material screening. These results enable materials scientists to rapidly identify formulations with optimal trade-offs between durability and eco-friendliness, significantly reducing experimental workload.

Furthermore, the study confirms a moderate inverse correlation (Pearson's r = –0.63) between tensile strength and biodegradability, reinforcing the need for multi-objective optimization in sustainable packaging design. By applying explainable ML techniques such as SHAP (SHapley Additive exPlanations), the study also highlighted specific feature contributions to the models' outputs, supporting transparency in materials selection for regulatory and industrial applications.

5. Conclusion

This study demonstrates the promising potential of ML techniques in predicting both the performance and degradability of bio-based food packaging materials. By integrating diverse datasets comprising mechanical, barrier, and environmental degradation properties, ML models such as random forest, support vector machines, and artificial neural networks exhibited strong predictive power. The models effectively captured nonlinear interactions between input features and target outputs, enabling accurate forecasting of packaging film behavior under various conditions.

The results confirm that ML-driven prediction can serve as a valuable tool in accelerating the design and optimization process of sustainable packaging materials. Notably, the inclusion of environmental parameters and compositional features—such as polymer ratios and nanomaterial additives—allowed for the differentiation of formulations with improved shelf-life performance and environmental compliance. This capability significantly reduces the need for extensive experimental trial-and-error cycles.

Moreover, the study underscores the importance of explainable ML approaches, which provide insights into feature importance and decision pathways. These insights empower materials scientists to make informed choices in polymer blending and nanomaterial incorporation, fostering more rational design workflows. The explainability aspect also supports regulatory transparency and trustworthiness, both of which are critical for adoption in food-related applications.

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In future work, the integration of real-time sensor data, such as humidity or microbial load feedback from smart packaging systems, could further refine model predictions and allow for adaptive learning mechanisms. Additionally, expanding the dataset with diverse food categories and storage environments would enhance model robustness and generalizability.

In conclusion, machine learning offers a transformative framework for the sustainable development of next-generation bio-based food packaging, providing a scalable, data-driven approach to balancing material functionality and ecological responsibility.

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