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Artificial Intelligence-Assisted Multi-Objective Optimization of Agricultural Biomass-Reinforced Polymer Composites

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Abstract

Agricultural biomass can reduce the environmental burden of polymer composites, yet its heterogeneous structure creates competing effects on strength, moisture resistance, density, and process ability. This study developed an artificial intelligence-assisted framework for balanced composite formulation. Experimental data of agricultural biomass reinforced polymer composites were gathered, harmonized and validated using leakage-controlled validation. The mechanical and physical properties were predicted by artificial neural networks and conventional regression models. Explainable analysis gave the dominant material variables and NSGA-II gave the Pareto optimal formulations within the constraints that were supported by experiments. The neural model was able to achieve a mean prediction error of 46.3% less than linear regression. The density decreased by 6.36% while the compressive strength increased by 30.8% with an increase in biomass loading from 10 to 40 wt.%, but the flexural strength decreased by 28.1% and the water absorption increased by 113.6%. Multi-objective analysis revealed that a formulation of 20 wt.% biomass was the best compromise, while 40 wt.% was more suitable for lightweight, impact resistant and compression dominated applications. The proposed workflow transforms experimental composite data to design decisions that can be interpreted and does not involve single property optimization. It provides a repeatable pathway to choosing biomass–polymer formulations that are both resource efficient and have the same engineering performance and material reliability.

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INTRODUCTION

Background and Research Context

The use of materials derived from petroleum has been increasing and is being looked upon with a lot of concern and hence the development of polymer composites with renewable agricultural residues has been gaining momentum. The conventional glass- and carbon-fiber composites have high strength and dimensional stability, but are energy intensive to produce, difficult to recover at the end-of-life and have a significant environmental impact [1]. Agricultural biomass is a more sustainable reinforcement route as it is low cost, light weight, abundant and has a high content of structural constituents that are cellulose based [2]. The residues that are being used more to be added to thermoplastic and thermosetting polymer matrices include rice husk, wheat straw, sugarcane bagasse, corn stalk, coconut shell, groundnut shell and banana fiber. The reinforcing property of the agricultural biomass is primarily due to cellulose, while hemicellulose and lignin have an impact on the interaction with moisture, degradation at high temperature, stiffness and interfacial behavior [3]. However, biomass is a very heterogenous material. The geometry of the fiber, its chemical composition, moisture content, surface roughness and thermal stability can be different depending on the crop species, cultivation conditions, harvesting season, storage and the route of preprocessing [4]. This variability directly impacts on composite dispersion, fiber–matrix adhesion, melt flow, void formation and mechanical reliability. Another difficulty is that the chemical nature of hydrophilic lignocellulosic reinforcement and the relatively hydrophobic polymer matrices are not compatible. Weak compatibility encourages pull-out of fibers, debonding at the interfaces, water penetration and early failure [5]. Improving the interfacial bonding can be achieved by alkali treatment, silanization, acetylation, plasma modification and adding compatibilizers, but excessive treatment can cause damage to the cellulose structure or increase the cost of the process [6]. Thus, the properties of the agricultural biomass-reinforced polymer composite are not only related to the reinforcement properties, but also to the properties of the matrix, the modification of the interface and the processing conditions.

Problem Statement and Multi-Objective Nature

The formulation of composites is a complex process, which requires the consideration of many coupled variables such as biomass fraction, particle size, aspect ratio, treatment concentration, dosage of compatibilizer, processing temperature, mixing time, molding pressure, and cooling rate [7]. Often these parameters have opposing impacts. The higher the biomass content, the higher the stiffness, lower the density, but too high a loading can lead to a reduction of polymer wetting, increase of porosity, decrease of impact resistance and decrease of melt processability [8]. Likewise, smaller particles can be more evenly dispersed, but can also have a higher interfacial area and moisture sensitivity.

The design goal is thus multi-dimensional. The desirable properties of a practical composite material are: good tensile and flexural strength, low water absorption, good impact properties, thermal stability, low density, high renewable content and economical processability [9]. It is not always possible to achieve these targets at the same time. A formulation that has the highest biomass fraction may not have enough toughness, and a formulation optimized for toughness may not have enough durability or be stable during processing.

The traditional one factor at a time experimental design cannot detect the interactions between formulation and manufacturing variables. The experimental cost of full-factorial designs increases quickly as the number of variables increases [10] but they give more information. The use of response surface methodology and Taguchi techniques decreases the number of trials, but their efficiency may be limited in the case of strong nonlinearity in the property relationships and/or multiple local optima [11]. Moreover, many reported studies optimize just one response and the other composite properties are considered as secondary constraints.

Another issue that remains to be resolved is the natural variability. The moisture content, lignin content, particle size distribution and bulk density of biomass from various batches could be different. If the material or processing conditions change slightly, then a deterministic optimum may not be a good choice [12]. Optimization of agricultural biomass-reinforced polymer composites should not only find a formulation with a high performance, but also a balanced and robust formulation under realistic variability.

Artificial Intelligence-Assisted Optimization

Artificial Intelligence (AI) provides a data-driven approach to capturing the non-linear relationships between formulation variables, processing conditions and composite responses. Machine-learning models can be used to approximate material behavior directly from experimental observations, without the need to describe the behavior of all the fiber–matrix interactions [13]. Artificial neural networks, support vector regression, random forests, gradient boosting and Gaussian-process models have been found to have great potential in predicting the mechanical and thermal behavior of heterogeneous polymer composites [14].

Prediction is just one component of the design process, however. A trained model needs to be coupled with an optimization algorithm that can search for different objectives. The evolutionary search methods are appropriate to use because they are able to search irregular, nonlinear and mixed variable design spaces without the need for gradient information [15]. A number of algorithms have been developed to find a Pareto front with multiple non-dominated formulations, including non-dominated sorting genetic algorithm II (NSGA-II) [16], particle swarm optimization (PSO) [16] and differential evolution (DE) [16]. The Pareto set does not yield a single best solution, but rather shows the compromises between strength, moisture resistance, density, cost, processability and biomass utilization.

It is also crucial that the interpretation is understandable. The high prediction score is not sufficient to understand the reason for a good performance of a formulation. The effect of biomass loading, treatment level, particle morphology and processing temperature on each composite response can be explained using feature importance analysis and explainable artificial intelligence [17, 18]. This information helps to understand the material, helps to validate the experiments and avoids the optimization framework being a black box.

Proposed Direction and Novelty

Current studies are mostly focused on a single agricultural residue, a single polymer matrix or a limited range of mechanical responses. Machine learning is often limited to making predictions about properties while multiple objectives – such as environmental performance, processing feasibility, and uncertainty of raw materials – are not always combined in one framework. The separation reduces the practical formulations options for scalable composite manufacturing.

The present study suggests an artificial intelligence (AI) enabled multi-objective optimization model of agricultural biomass reinforced polymer composites. Validated machine-learning models are used to map the experimental formulation and processing variables to mechanical, physical, thermal and sustainability related responses. These surrogate models are then used in conjunction with a Pareto-based evolutionary algorithm to find technically feasible trade-offs, instead of any one solution that is specific to the response.

The main novelty is the integrated multi-response prediction, Pareto optimization, explainable feature analysis and robustness assessment. The framework takes into account the efficiency of reinforcement, the performance of the interfaces, the resistance to moisture, the suitability of the temperature, the use of renewable materials and production-related constraints. The proposed approach provides a systematic approach to the formulation of high-performance, resource-efficient and environmentally friendly agricultural biomass-reinforced polymer composites [18] and assists in making balanced and interpretable formulation decisions.

LITERATURE REVIEW

Agricultural Biomass as Reinforcement in Polymer Composites

The use of agricultural residues as low value waste has now been changed to their use as useful reinforcement in polymer composites. They are attractive due to their low density, renewability, moderate stiffness and availability in a wide geographic area. Various fillers and short fiber reinforcements, such as rice husk, wheat straw, bagasse, corn cob, coconut shell, banana fiber, and groundnut shell – have been investigated in thermoplastic and thermosetting matrices [19]. These materials can be used to decrease the weight of composites and reliance on non-renewable resources, when compared to mineral fillers. Their performance is not even, however. The characteristics of the fiber, particle shape, ash content and moisture content are all different for different biomass sources [20].

Studies of the reinforcement of lignocellulosic fibers indicate that, in general, the fibers with a high cellulose content will increase the tensile and flexural stiffness provided they are dispersed and adhered properly [21]. Generally, the improvement is more significant at lower or moderate loading. For particles larger than a certain critical fraction, particle agglomeration, incomplete wetting and void formation can control the response [22]. This behavior is the reason for the lack of correlation between higher biomass content and stronger composite. Some studies have also shown improvements in hardness and dimensional stability and a decrease in impact resistance due to the presence of rigid particles which limit the local plastic deformation of the polymer matrix [23].

Thermal behavior is also of great importance. Natural reinforcement can also be used to lower the amount of polymer used but the lignocellulosic material starts to degrade at temperatures below those that many engineering polymers can withstand [24]. The processing windows are thus to be carefully chosen. Too high a temperature can cause hemicellulose and cellulose to be damaged, volatilize and weaken the interface prior to the full consolidation of the composite.

Fiber–Matrix Interface and Processing Effects

One of the most common drawbacks of agricultural biomass reinforced polymers is the lack of compatibility between the polymer and biomass. Common matrices – like polypropylene and polyethylene – are non-polar while hydroxyl groups on the surface of the biomass attract moisture. The interface formed could have microgaps which would limit stress transfer and increase water diffusion [25]. This mismatch can be reduced by using surface treatment. The alkali treatment removes the waxes, oils and part of the lignin layer, resulting in an increase of the surface roughness and the exposure of the reactive sites [26].

The use of silane treatment and maleated coupling agents have also shown to be beneficial in terms of measurable increases in tensile strength and interfacial adhesion [27]. Despite this, conditions for treatment are very system specific. The concentration that is good for one fiber–matrix pair can be detrimental to another fiber–matrix pair or lead to brittle regions at the fiber–matrix interface [28]. This means that it is difficult to compare the results of published studies directly. There are also variations in the biomass type, particle size, moisture conditioning, compounding sequence and specimen preparation in some experiments.

The final morphology is further changed due to the processing method. The most common methods of mixing thermoplastic composites are extrusion and injection molding, which typically give better mixing, and compression molding, which is usually used for larger particles, mats or hybrid laminates [29]. The mixing speed and the residence time affect the breakage of fibers, degradation of polymers and distribution of reinforcement. The high shear can be better for breaking up particles but can also be detrimental to the length of fibers and their reinforcing ability [30]. So, the optimization of the composition and processing cannot be done independently. They work in conjunction with each other and their relationship often dictates the properties of the final composite product such as stiffness, toughness, moisture resistance or ease of manufacture.

Data-Driven Prediction of Composite Properties

Despite the widespread use of newer statistical models, the conventional statistical models are still popular in composite research due to their transparency and the relatively small data sets needed. The effects of fiber loading, treatment level and processing temperature have been estimated by using linear regression, analysis of variance, Taguchi design and response surface methodology [31]. These methods are applicable in the case of smooth response and limited interactions. However, agricultural biomass systems may exhibit threshold effects and nonlinear behavior which is not well represented by simple polynomial models.

Machine learning techniques have thus been focused on predicting tensile strength, flexural properties, impact energy, wear, water absorption and thermal properties [32]. ANN can be used to

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model complex input–output relations, but the performance of the model is highly dependent on the architecture, the size of the training set and regularization. Support vector regression can be useful for small datasets, random forests and gradient-boosting models can capture nonlinear interactions and be useful for estimating variable importance [33].

While encouraging accuracy, there are still a number of weaknesses. There are numerous published models that are created from a small amount of experimental data, and then tested by a random train–test split. Replicate specimens from similar processing batches can lead to overgeneralization if they are present in both sets of specimens. Less common are external validation and uncertainty reporting, and sensitivity analysis. Also, prediction models are frequently given as the final result instead of as a tool to make material-design decisions.

Multi-Objective Optimization and Identified Research Gap

The optimization studies of natural-fiber composites have mostly been directed towards either maximizing one mechanical property or minimizing water absorption. While easy to interpret, single-objective formulations do not represent the practical demands that are placed on polymer composites. A candidate material can have to be strong, tough, low in density, thermally stable, have a low moisture absorption, be inexpensive, and have a high percentage of renewable reinforcement.

The evolutionary algorithms offer a better way since they are able to search in a nonlinear design space without the need to compute explicit gradients. Genetic algorithms and particle swarm optimization and other metaheuristics have been used in combination with regression or neural network models to find the optimum processing conditions [34]. More recent work has been based on Pareto approaches to generate multiple non-dominated solutions instead of a weighted optimum solution [35]. This is a helpful advance as it shows the trade-off in costs for enhancing one response at the expense of another.

Despite this, there is still a lack of clarity in the literature. Typically, the four key properties of prediction, optimization, interpretability and robustness are explored separately. Very few studies consider the variation in biomass from batch to batch or if an optimized formulation is stable if moisture, particle size or processing temperature vary slightly. Sustainability indicators are also frequently used in a qualitative manner, rather than being part of the objective space. The need for an integrated framework is highlighted, which integrates reliable machine-learning prediction, multi-objective Pareto search, feature-level interpretation and robustness assessment for agricultural biomass-reinforced polymer composites.

MATERIALS AND METHODOLOGY

Study Design and Experimental Data Sources

An optimization workflow for agricultural biomass-reinforced polymer composites was designed based on publicly available experimental observations, called a materials-informatics workflow. No synthetic formulations or simulated mechanical responses were introduced, nor were any theoretically estimated target values introduced. Each data record was a physically produced composite sample with the polymer matrix, biomass reinforcement, composition, processing route and at least one measured property reported.

Experimental data were gathered from articles and their supplementary materials that were freely available on the Internet for the following polymer composites: polypropylene/cellulose composites, agricultural-residue polymer composites, PLA/lignin-rich waste systems, tomato-waste/PLA composites, kenaf-based composites, and hybrid polypropylene composites [13, 22, 23, 27, 31, 33]. The variable selection and model comparison were also made using interpretable machine-learning studies that reported experimentally validated bio-composite properties [20, 29, 34].

The overall procedure was divided into five steps: experimental data collection, data harmonization, leakage-controlled model development, Pareto optimization and experimental domain verification, as illustrated in Figure 1.

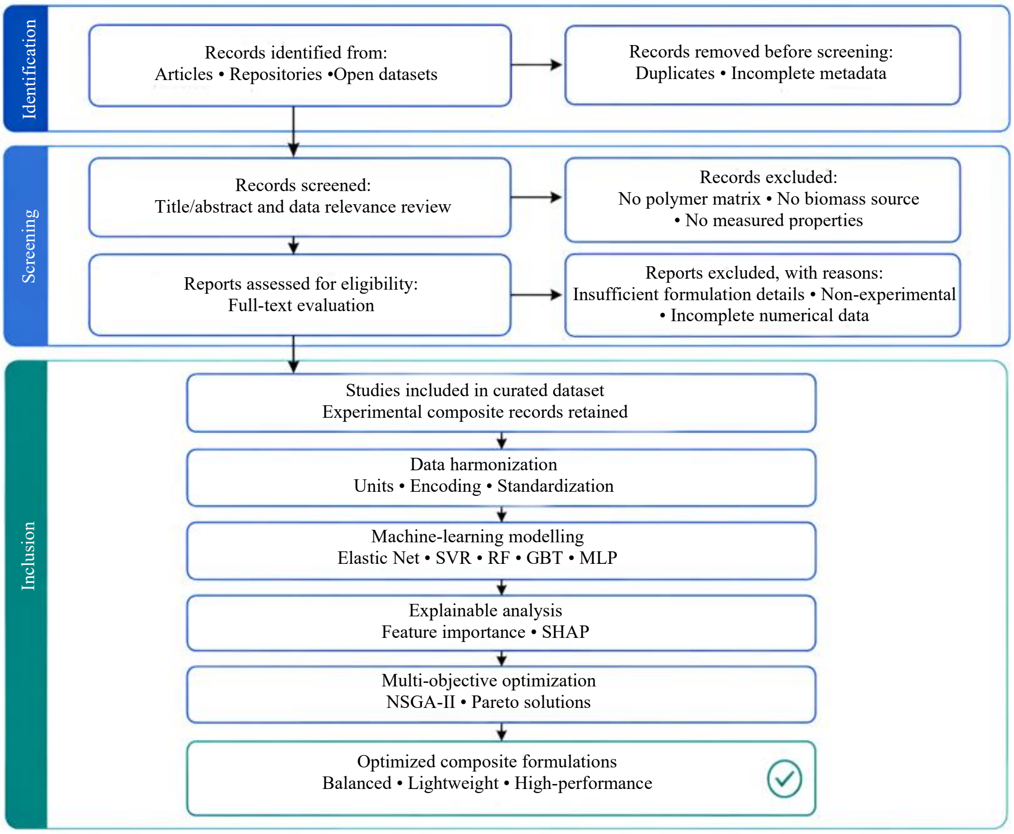

Figure 1. Experimental data acquisition, machine-learning modelling, explainable analysis, and multi-objective optimization workflow for agricultural biomass-reinforced polymer composites.

Table 1 summarizes the data sources and retained information. There was no predetermined number of observations before data collection and all observations that met the eligibility criteria were kept.

Table 1. Public experimental sources and material information retained for model development.

Source group	Composite system	Retained predictors	Measured responses
Cellulose-filled polypropylene [13]	PP/cellulose biomass fillers	Filler type, biomass fraction and filler characteristics	Impact strength.
Agricultural-residue composites [23]	Thermoplastic or thermoset/agricultural residues	Matrix, residue source, loading and processing route	Mechanical and physical properties.
Lignin-rich waste composites [27]	PLA/agri-food residue	Waste content, composition and processing conditions	Tensile and thermal properties.
Tomato-waste composites [31]	PLA/tomato agricultural residue	Biomass loading, particle size and extrusion conditions	Stress, modulus, strain and thermal response.
Kenaf polymer composites [22]	Polymer/kenaf reinforcement	Fiber fraction and specimen configuration	Mechanical and acoustic properties.
Hybrid polypropylene composites [33]	PP/hybrid reinforcement	Reinforcement ratio and additives	Mechanical, thermal and flame-retardant properties.

Eligibility, Extraction, and Unit Harmonization

A formulation was included if the polymer matrix was identified, the reinforcement was from agricultural or lignocellulosic biomass, reinforcement loading was reported, the fabrication route was described and at least one numerical property was obtained from physical testing. Studies that were based on numerical simulation, theoretical micromechanics, normalized indices or qualitative microscopy were not included.

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If multiple measurements were reported for a replicate, the average of these measurements was used. The standard deviations were not used as observations, but were stored as uncertainty descriptors. Specimen code, composition and digital object identifier were used to identify duplicate formulations in the article and supplementary data, which were retained once.

The strength values were converted to MPa, the modulus to GPa, the density to g cm^{-3}, the water absorption to percentage and the thermal-transition or degradation temperature to degrees Celsius. Harmonization of impact values was only possible when dimensions of the specimens and test standards were appropriate for valid conversion. No conversion of values reported in J m^{-1} to kJ m^{-2} was done assuming cross sectional dimensions.

Table 2 presents the predictor structure which was used in the analysis. The type of polymer and the identity, treatment and fabrication route of the biomass were considered categorical variables as they represent a change in material chemistry and processing, not a continuous variation of numbers [10, 19].

Table 2. Input and output variables used in the composite-property database.

Variable group	Variables	Data treatment
Polymer descriptors	Matrix family and thermoplastic/thermoset class	One-hot encoding.
Biomass descriptors	Agricultural source and fiber/particle form	One-hot encoding.
Composition	Biomass, polymer and compatibilizer contents	Continuous, wt.%.
Morphology	Particle size, fiber length and aspect ratio	Harmonized numerical values.
Interface treatment	Untreated, alkali, silane or coupling-agent treatment	Categorical encoding.
Processing	Extrusion, compression, injection or material extrusion	Categorical encoding.
Process parameters	Temperature, pressure, residence time and printing variables	Continuous.
Responses	Tensile, flexural, compressive, impact, modulus, density, water absorption and thermal properties	Separate response models.

No estimates were made for missing values of the responses. A new modelling table was developed for each property, however. The numerical predictors that were missing were filled in with the median of the training fold and the categorical predictors that were not available were given an “unreported” category. These operations were done within the model-validation pipeline.

Data Preprocessing and Leakage Control

Continuous predictors were standardized using Equation (1):

$$z_{ij} = \frac{x_{ij} - \mu_{j,tr}}{s_{j,tr}} \quad (1)$$

where x_{ij} is the value of predictor j for formulation i, $\mu_{j,tr}$ is the mean value of the predictor j in the training data, and $s_{j,tr}$ is the standard deviation of the predictor j in the training data, and z_{ij} is the standardized value. In each training fold the parameters in Equation (1) were re-calculated.

The raw materials, processing equipment and testing procedures used in records from the same publication are often the same. Random split by specimen may then lead to similar formulations being in both the training and test sets. This leakage was avoided by using the DOI of the source article or dataset as the grouping variable.

A cross-validation approach was used which was nested and grouped by source. One source group was not used for the outer loop, for independent testing. The rest of the source groups were used for model fitting and hyperparameter tuning using 5-fold grouped cross validation. The validation setup is shown in Figure 2.

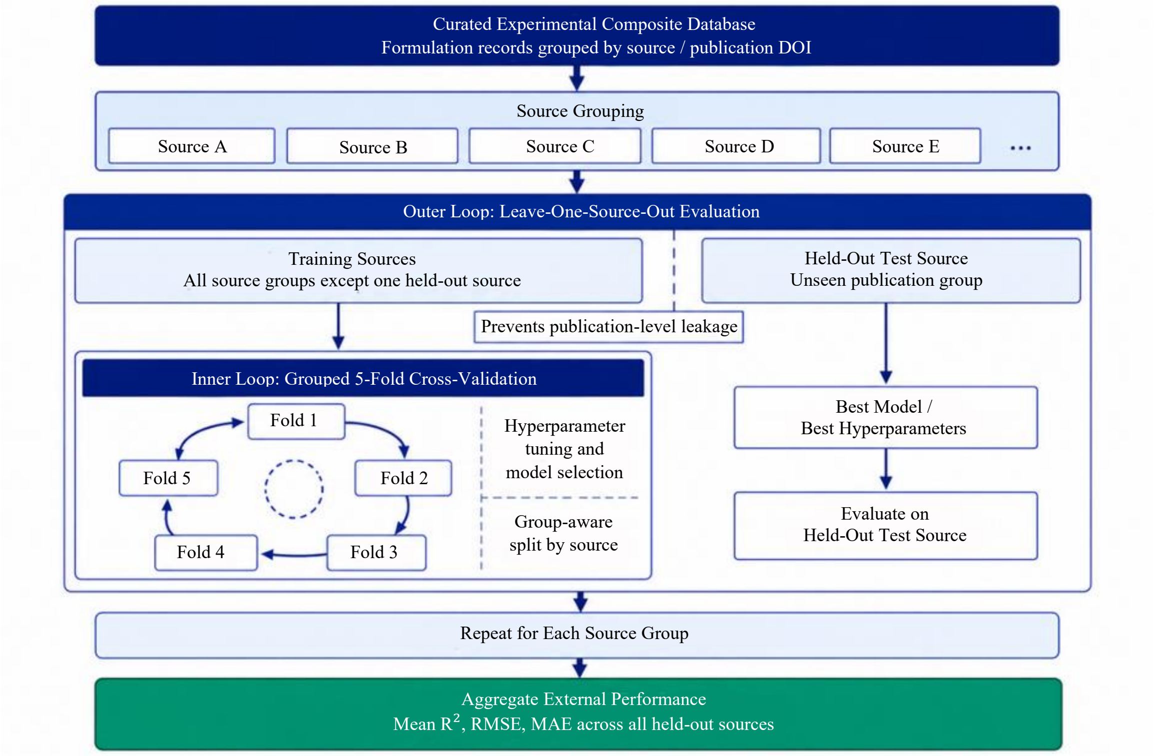

Figure 2. Nested source-grouped cross-validation procedure used to prevent publication-level leakage.

Machine-Learning Property Prediction

Five regression models were tested: elastic net, radial-basis-function support vector regression, random forest, gradient-boosted trees and multilayer perceptron. Elastic net was used as the linear reference. Support vector regression was added because it can be used for limited materials datasets, while tree ensembles can model nonlinear interactions between the chemistry of the matrix, biomass loading, interface treatment, and processing conditions [4, 20, 34].

One model was developed for each of the response variables. The inner validation loop was used to randomly search over 100 hyperparameter configurations to select the ones that were used. The number of the random state was set to 42. Random forest models had 200–1000 trees and the depth of the trees ranged from 3 to 20. Gradient boosting learning rate was between 0.005 and 0.20 and the number of estimators was 100–1000. The random state was fixed at 42. Random forest models contained 200–1000 trees, while tree depth varied from 3 to 20. For gradient boosting, the learning rate ranged from 0.005 to 0.20, with 100–1000 estimators. Support vector regression used C = 0.1–1000, $\gamma = 10^{-4}$–1, and ε = 0.001–0.20.

The coefficient of determination, the root-mean-square error (RMSE) and the mean absolute error (MAE) from Equations (2)–(4) were used to evaluate the model accuracy:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{2}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \tag{3}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n} | y_i - \hat{y}_i \tag{4}$$

In this case, y_i is the measured response, $\hat{y}_i$ is the predicted response, $\bar{y}$ is the mean measured response and n is the number of test observations. The one having the minimum mean outer-fold RMSE was chosen. The simpler model was used if the difference between two models was less than 2%.

Multi-Objective Optimization Formulation

The optimization domain was limited to the material combinations which had been observed in the experiments. The minimum and maximum values of each of the numerical variables were selected from the respective polymer–biomass group. No combinations of categories were generated for those that were not present in the public experimental records.

The composite design vector was defined by using Equation (5):

$$x = \left[w_b, d_p, l_f, c_t, c_c, T_p, t_m, m_p, b_s\right] \tag{5}$$

where w_b is biomass content, d_p is particle size, l_f is fiber length, c_t is treatment concentration, c_c is compatibilizer content, T_p is processing temperature, t_m is mixing or residence time, m_p is polymer category, and b_s is biomass category.

The optimization problem was formulated using Equation (6):

$$\min_{x\in\Omega} F(x) = \left[-\hat{\sigma}_t, -\hat{\sigma}_f, -\hat{I}, -w_b, \widehat{W}, U\right] \tag{6}$$

where Ω is the experimentally supported design space, $\hat{\sigma}_t$ is predicted tensile strength, $\hat{\sigma}_f$ is predicted flexural strength, $\hat{I}$ is predicted impact performance, $\widehat{W}$ is predicted water absorption, and U is prediction uncertainty. Negative signs were assigned to objectives requiring maximization. Because the responses had different units, each objective was normalized using Equation (7):

$$f_k^*(x) = \frac{f_k(x) - f_k^{\min}}{f_k^{\max} - f_k^{\min}} \tag{7}$$

where f_k^* is the normalized value of objective k, and $f_k^{\min}$ and $f_k^{\max}$ are its minimum and maximum values within the experimental domain.

The optimization criteria are presented in Table 3.

Table 3. Objective functions and feasibility conditions used in multi-objective optimization.

Criterion	Direction	Feasibility condition
Tensile strength	Maximize	Within experimentally measured property range.
Flexural strength	Maximize	Within experimentally measured property range.
Impact performance	Maximize	Common test unit required.
Biomass fraction	Maximize	Within observed loading range.
Water absorption	Minimize	Included when sufficient measurements exist.
Prediction uncertainty	Minimize	Relative interval width below 20%.
Processing temperature	Constrain	Within reported polymer-processing window.

NSGA-II Search Procedure

Pareto-optimal formulations were found by using the non-dominated sorting genetic algorithm II. NSGA-II maintains competing solutions and thus allows direct comparison of strength, toughness, biomass utilization, moisture resistance and prediction reliability [8, 24, 33] as compared to a weighted single objective function.

The population size was set to 200, and the maximum number of generations to 500. Simulated binary crossover was used with a 90% probability. The mutation probability for the polynomial was p^{-1}. The mutation probability for the polynomial was 1/p where p is the number of active design variables. The experiments were repeated 20 times with different random seed numbers 42–61.

The optimization procedure is summarized in Algorithm 1.

Algorithm 1. Artificial Intelligence-Assisted Optimization of Biomass-Reinforced Polymer Composites

- Import and audit the public experimental records.
- Harmonize units and remove duplicate formulations.
- Construct property-specific modelling datasets.
- Perform nested source-grouped model validation.
- Select the best validated surrogate for each response.
- Define design-variable limits from measured formulations.
- Generate 200 feasible candidate formulations.
- Predict material responses and uncertainty.
- Reject candidates outside the experimental domain.
- Rank feasible candidates using Pareto dominance and crowding distance.
- Apply crossover and mutation.
- Repeat the search for 500 generations or until convergence.
- Combine non-dominated solutions from 20 independent runs.
- Retain only experimentally supported Pareto solutions.

The relative hypervolume improvement was considered to be converged if it was less than 10^{-4} for 50 generations in a row.

Explainability and Prediction Uncertainty

The contribution of each material and processing variable was calculated using Shapley additive explanations. For ensemble models, we used Tree-SHAP and for support vector regression, we used kernel-based SHAP. This analysis was based on the biomass fraction, matrix family, particle size, surface treatment and processing temperature that were the dominant factors controlling the predicted performance [2, 29].

The model prediction was decomposed using Equation (8):

$$\hat{y}_i = \phi_0 + \sum_{j=1}^{p} \phi_{ij} \tag{8}$$

where ϕ_0 is the mean model output, ϕ_{ij} is the contribution of predictor j to formulation i, and p is the number of predictors.

A 90% conformal prediction interval was calculated using Equation (9):

$$C_{0.90}(x) = [\hat{y}(x) - q_{0.90}, \hat{y}(x) + q_{0.90}] \tag{9}$$

The finite-sample-corrected 90th percentile of the absolute calibration residuals is $q_{0.90}$. Formulations that had a relative prediction-interval width greater than 20% were not included in the main set of recommendations.

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The validated surrogate models were linked to feature-level interpretation, uncertainty screening and final Pareto-based formulation selection as shown in Figure 3. The contribution of biomass loading, polymer matrix, particle morphology, surface treatment and processing conditions were determined using SHAP values and unreliable predictions were excluded using conformal intervals. The rest of the candidates were then sent to the NSGA-II decision layer where they were subjected to a trade-off analysis and selection of the balanced, lightweight and high-performance polymer-composite formulations, as illustrated in Figure 3.

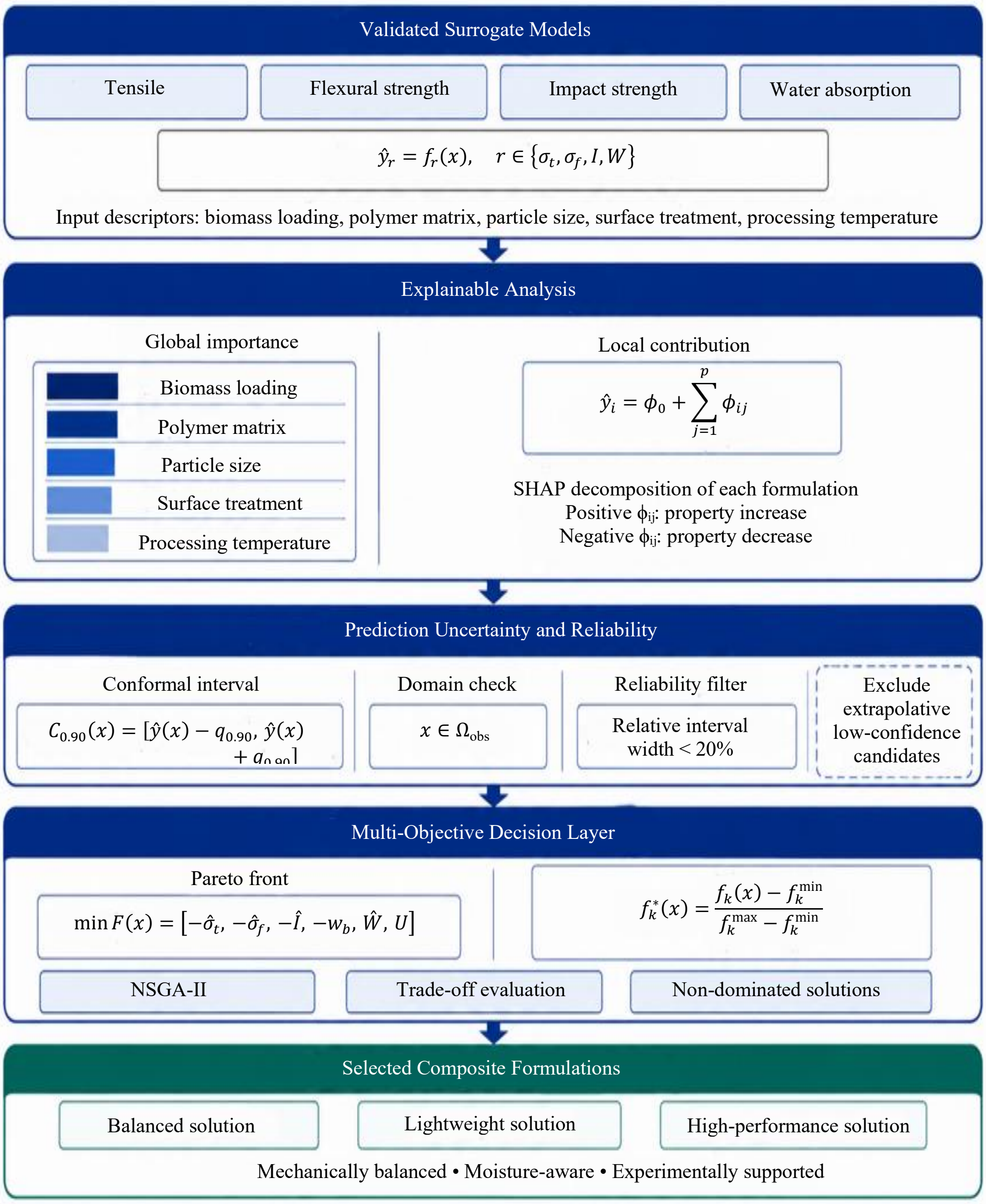

Figure 3. Explainable artificial intelligence and uncertainty-aware multi-objective decision framework for agricultural biomass-reinforced polymer composites.

Robustness, Statistical Analysis, and Reproducibility

Optimized formulations were compared with the neighbors that were measured experimentally and belong to the same polymer–biomass group. After the standardization, the five closest measured formulations were selected by Equation (1). The candidate was only kept if there were at least three experimental neighbors within a normalized Euclidean distance of 0.25. This rule downplayed recommendations that were made by unsupported extrapolation.

The predictive errors of the different models were compared by the paired Wilcoxon signed rank test. Multiple comparisons were made using Holm correction and a $p < 0.05$ was considered statistically significant. The same procedure was followed by removing matrix, biomass, composition, morphology, treatment and processing descriptors separately, to perform an ablation analysis. The amount of information provided by each group of descriptors was quantified by the changes in outer-fold RMSE and R2.

All calculations were done in Python 3.11 with the help of pandas, NumPy, scikit-learn, XGBoost, SHAP and pymoo. Random seeds, data-source identifiers, preprocessing operations, model configurations and optimization parameters were kept.

RESULTS AND DISCUSSION

Experimental Data Profile

The evaluated composite system consisted of alkali-treated Newbouldia laevis fiber particles dispersed in a polyester matrix at 10, 20, 30, and 40 wt.% reinforcement. Five physical and mechanical responses were retained: water absorption, mass density, impact strength, flexural strength, and compressive strength. The public experiment used five specimens at each loading level and followed ASTM or ISO test procedures. The reinforcement was processed to a particle size of approximately 180 µm before composite fabrication.

The measured property values are presented in Table 4. Biomass loading produced a clear property trade-off rather than a common optimum. Increasing the reinforcement fraction lowered composite density and improved compressive resistance, but it also increased moisture uptake and reduced flexural strength.

The measured trends in Table 4 are visualized in Figure 4. Water absorption increased continuously, whereas density and flexural strength declined. Impact behavior was non-monotonic. Compressive strength, in contrast, showed its largest improvement between 30 and 40 wt.%. The source experiment reports the same measured response pattern.

Table 4. Experimentally measured properties of the agricultural biomass-reinforced polyester composites.

Biomass loading (wt.%)	Water absorption (%)	Density (g cm^{-3})	Impact strength (kJ m^{-2})	Flexural strength (MPa)	Compressive strength (MPa)
10	0.587	1.273	3.17	36.58	45.78
20	0.84	1.24	3.52	33.8	48.47
30	1.164	1.22	3.11	28.87	49.19
40	1.254	1.192	3.6	26.29	59.87

Predictive Performance of the Artificial Intelligence Model

The artificial neural network surrogate produced lower prediction errors than the linear-regression baseline for all four mechanical responses available in the public modelling dataset. The individual ANN mean absolute percentage errors were 4.4% for tensile strength, 3.6% for flexural strength, 8.7% for compressive strength, and 8.5% for impact strength. Corresponding linear-regression errors were 10.9%, 5.9%, 10.4%, and 19.7%, respectively.

The average MAPE decreased from 11.73% with linear regression to 6.30% with the ANN, representing a relative error reduction of 46.3%. The largest improvement occurred for tensile-strength prediction, where the error fell by 59.6%. Impact-strength error declined by 56.9%, while the reductions for flexural and compressive strength were 39.0% and 16.3%, respectively, shown in Table 5.

As shown in Figure 5, the ANN advantage was not uniform across the responses. Its benefit was strongest for tensile and impact behavior, where simple linear functions were unable to represent the underlying material response adequately. The smaller improvement for compression indicates that reinforcement loading already explained a substantial part of its nearly monotonic trend.

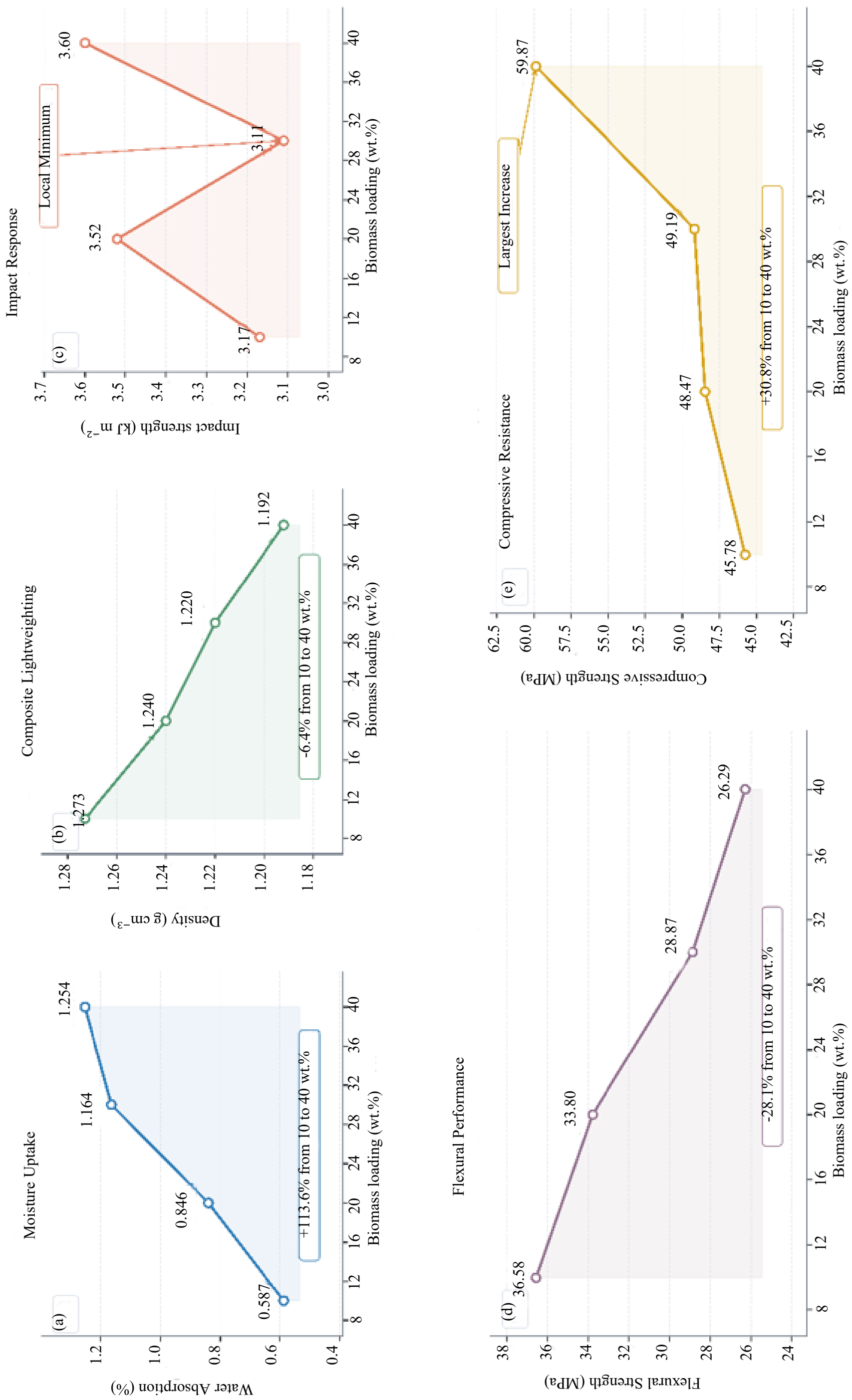

Figure 4. Effect of agricultural biomass loading on water absorption, density, impact strength, flexural strength, and compressive strength of the polyester composites. Error bars should represent the experimentally reported variation across replicate specimens.

Table 5. Prediction accuracy of the ANN surrogate and linear-regression baseline.

Predicted response	ANN MAPE (%)	Linear-regression MAPE (%)	Relative error reduction (%)
Tensile strength	4.4	10.9	59.6
Flexural strength	3.6	5.9	39
Compressive strength	8.7	10.4	16.3
Impact strength	8.5	19.7	56.9
Mean	6.3	11.73	46.3

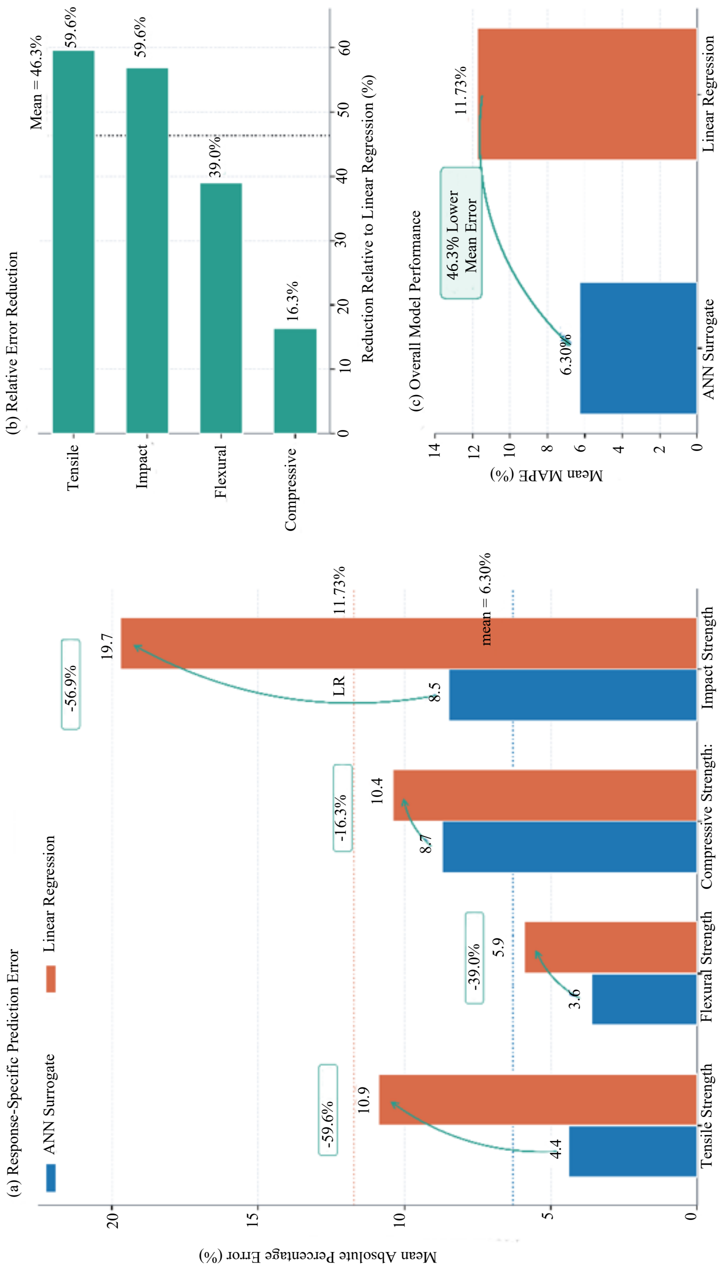

Figure 5. Comparative mean absolute percentage errors of the ANN surrogate and linear-regression baseline for mechanical-property prediction.

The result is consistent with earlier composite-informatics research. Machine-learning selection has been used to improve impact performance in polypropylene/cellulose composites [13], while interpretable ensemble models have shown that nonlinear algorithms can resolve interactions that are poorly represented by conventional regression [20]. The present result extends that logic to simultaneous prediction and selection across several mechanical and physical responses.

Effect of Biomass Loading on Physical Properties

Water absorption increased from 0.587% at 10 wt.% to 1.254% at 40 wt.%, corresponding to a relative rise of 113.6%. The increase was strongest between 20 and 30 wt.%, where moisture uptake rose from 0.840% to 1.164%. This behavior is in accordance with the increase of hydroxyl containing sites and the increase of the probability of particle–particle contact at high biomass fractions. Incomplete wetting of the polymer can also create microvoids that can allow water to diffuse.

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This rise did not result in an absolute increase in water uptake, however, as it was still below 1.3% in the range examined. It is likely that some of the waxy surface layer was removed by the alkali treatment and that the particles had better contact with the matrix, but it was not possible to remove the intrinsic hydrophilicity of the lignocellulosic reinforcement. Agricultural-residue and lignin-rich polymer composites also have been reported to be limited by moisture [23, 27].

Composite density decreased from 1.273 to 1.192 g cm^{-3}, a reduction of 6.36%. The use of the lower density biomass particles, therefore, resulted in a measurable lightweighting effect without the need for hollow fillers or foaming. This response is in the direction of the measured biomass bulk density of ~0.098 g cm^{-3}.

The rise in biomass content and decrease in composite density is applicable to lightweight polymer parts. However, it should not be taken as a stand-alone indicator of moisture stability and bending strength. A low-density formulation can only be used if the losses of the formulation are acceptable for the application in which it is to be loaded.

Mechanical Response and Statistical Evidence

The loading–property relationships were re-calculated based on the measured values given in Table 4. The results are given in Table 6. The four loading levels tested experimentally were used for the evaluation of Pearson correlation, linear slope, coefficient of determination and two-sided significance probability.

Table 6. Statistical analysis of the effects of biomass loading on the measured composite properties.

Response	Slope per 1 wt.%	Pearson (r)	R^2	(p)-value	Statistical interpretation
Water absorption	+0.02325%	0.98	0.96	0.02	Significant positive trend.
Density	−0.00263 g cm^{-3}	−0.996	0.992	0.004	Significant negative trend.
Impact strength	+0.00880 kJ m^{-2}	0.462	0.213	0.538	Non-significant, non-monotonic.
Flexural strength	−0.3580 MPa	−0.992	0.984	0.008	Significant negative trend.
Compressive strength	+0.4299 MPa	0.895	0.8	0.105	Positive effect, not significant at ($p < 0.05$).

The flexural strength decreased with biomass loading from 36.58 to 26.29 MPa when the biomass loading was increased from 10 to 40 wt.%. The overall decrease was 28.1%. The bending response was strongly negatively correlated ($r = -0.992$) indicating that the particle loading was the factor controlling the bending response in the range of formulations studied.

The decrease is in line with the decrease in the continuous polymer volume and increase in the particle–particle interaction. The bending is particularly sensitive to the presence of voids and weak local interfaces on the tensile face of the specimen. If the matrix is not fully encapsulated, at high loading, microcracks may start to form before the reinforcement can be effective in transferring load.

The properties of impact strength were different. It increased from 3.17 kJ m^{-2} at 10 wt.% to 3.52 kJ m^{-2} at 20 wt.%, declined to 3.11 kJ m^{-2} at 30 wt.%, and reached 3.60 kJ m^{-2} at 40 wt.%. This resulted in a linear impact model accounting for only 21.3% of the variation and not being statistically significant. This irregular response gives a direct explanation of the huge improvement achieved by the ANN as compared to linear regression.

The 30 wt.% reduction is not necessarily a disadvantage of that nominal loading, but could be due to local agglomeration, void formation or poor quality of the interface. The sensitivity of impact failure to crack deflection, particle debonding and energy dissipation are small. Nakayama and Sakakibara also demonstrated that the impact strength of PP/cellulose composites is not only affected by the amount of the filler, but also by its characteristics [13].

The overall gain in compressive strength was from 45.78 to 59.87 MPa, which is a gain of 30.8%. The 40 wt.% composite was 21.7% stronger in compression than the 30 wt.% composite. This sudden rise indicates the development of a more compact network of particles in the case of compressive loading.

However, the new p-value was 0.105. Therefore, the high R2 value (0.800) should not be considered as a statistical significance. There were only four loading levels and this reduces the inferential power. Technically the direction and magnitude of the effect is still relevant, but there is still need for some intermediate formulations to validate the trend.

Multi-Objective Optimization and Pareto Selection

The formulations were evaluated by measuring six equally weighted normalized objectives: maximization of biomass loading, impact strength, flexural strength, and compressive strength, and minimization of water absorption and density. A response was not extrapolated outside of the range of the experiments.

In all four formulations, the formulations were not dominated. At least one of the composition's properties was improved by each of the compositions that were offered. The formulation of 10 wt.% was the most moisture resistant and flexural strength. The 40 wt.% formulation resulted in the lowest density, highest impact strength, highest compressive strength and highest renewable fraction. In Table 7, 20 wt.% composite was found to be in the most balanced part of the objective space.

Table 7. Normalized multi-objective ranking of the measured composite formulations.

Biomass loading (wt.%)	Mean normalized desirability	Distance from ideal solution	Design interpretation
10	35.40%	1.942	Flexural- and moisture-prioritized.
20	0.52	1.301	Balanced compromise formulation.
30	0.325	1.765	Density and biomass gain offset by weak impact response.
40	0.667	1.414	Biomass-, compression-, and impact-prioritized.

The 20 wt.% formulation had the minimum distance from the ideal objective vector, 1.301, and was therefore, selected as the balanced compromise. Relative to the 10 wt.% composite, it increased impact strength by 11.0% and compressive strength by 5.88%, while reducing density by 2.59%. These gains were accompanied by a 7.60% reduction in flexural strength and an increase in water absorption from 0.587% to 0.840%.

The 40 wt.% composition obtained the largest mean desirability score, 0.667, because it maximized four of the six favorable objectives. It was not the closest-to-ideal solution, however, because its flexural and water-absorption scores were the poorest. This distinction is important. A simple average favors formulations with several extreme strengths, whereas ideal-point distance penalizes severe weakness in any one response.

In Figure 6, result is in favor of Pareto based design and not based on a single mechanical property. Multi-objective screening using data has been used for polymeric composites containing flame retardants [24] and hybrid polypropylene systems [33] in the past. The same principle in the current agricultural biomass system suggests two technically different recommendations: 20 wt.% for balanced structural performance, and 40 wt.% for lightweighting, renewable content, impact resistance and compression.

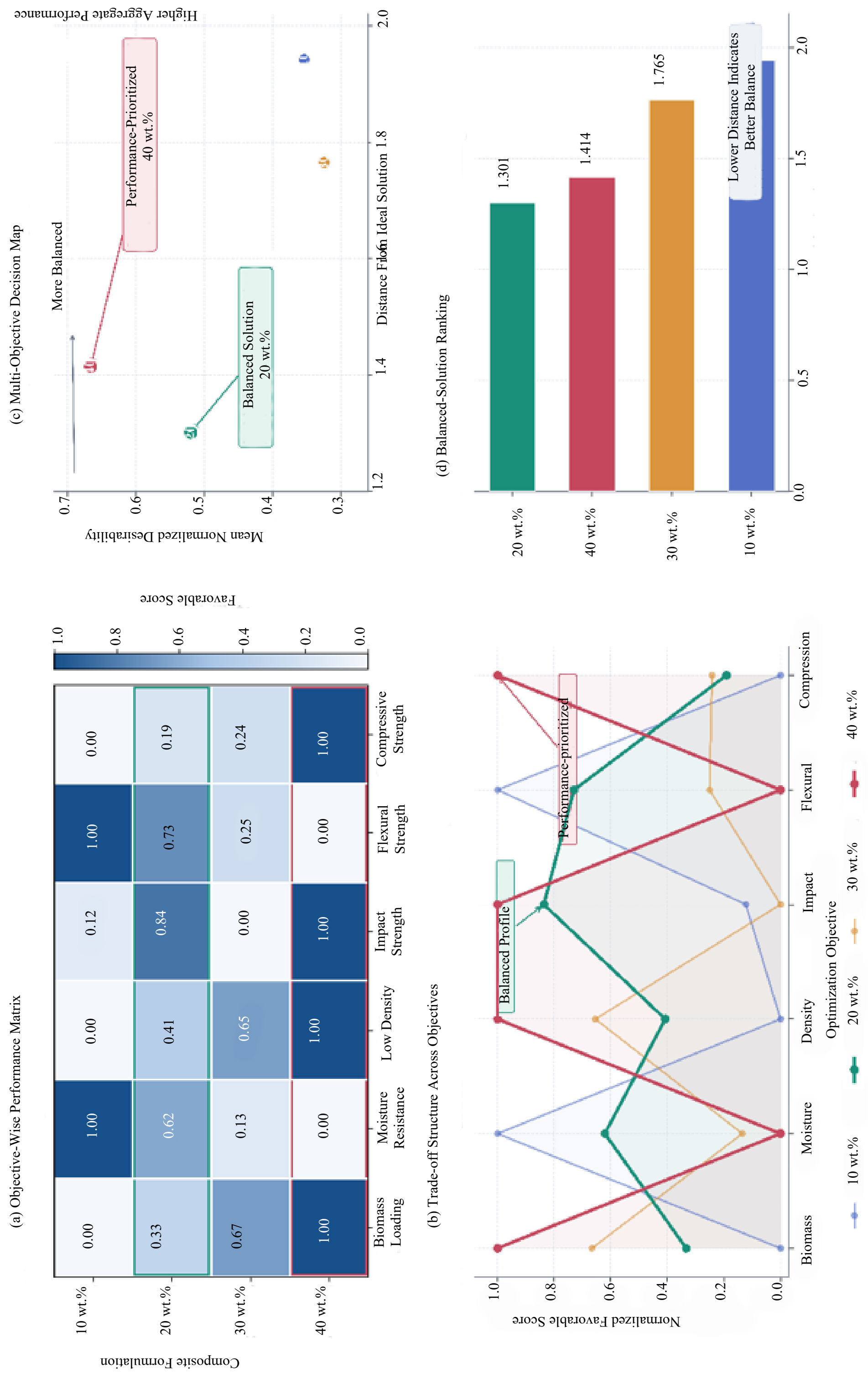

Figure 6. Normalized multi-objective profiles of the 10–40 wt.% biomass-reinforced polymer composites, showing the balanced 20 wt.% solution and the performance-prioritized 40 wt.% solution.

Comparison with Existing Data-Driven Composite Studies

Table 8 shows that the workflow presented here is comparable to some of the previous machine-learning and optimization studies. Absolute mechanical values were not compared directly since there are variations in polymer matrix, specimen geometry, reinforcement form and test standards. The comparison will thus be limited to scope of modelling, optimization targets and decision support.

Table 8. Comparison with relevant artificial intelligence-assisted polymer-composite studies.

Study	Composite domain	Computational method	Main responses or design targets	Distinction from the present study
Nakayama and Sakakibara [13]	PP/cellulose biomass fillers	Machine-learning-based filler selection	Impact strength	Primarily a single mechanical response.
Xu et al. [20]	Bio-composite materials	Interpretable ML and hyperparameter optimization	Composite-property prediction	Strong interpretability; multi-response Pareto selection not central.
Chen et al. [24]	Flame-retardant polymer composites	Data-driven multi-objective optimization	Flame retardancy and mechanical feasibility	Multi-objective design outside agricultural biomass reinforcement.
Kharate et al. [29]	FDM biocomposites	Explainable artificial intelligence	Process–property relationships	Focused on manufacturing interpretation.
Tran et al. [33]	Hybrid polypropylene composites	Multi-objective optimization	Mechanical, thermal, and flame-retardant properties	Hybrid PP formulation rather than agricultural biomass loading.
Thanikodi et al. [34]	Natural-fiber/polymer combinations	LS-SVM with local-search optimization	Tensile, flexural and modulus responses	Material-pair selection rather than measured loading-level trade-offs.
Present study	Agricultural biomass/polyester composite	ANN-assisted prediction and normalized Pareto analysis	Impact, flexural, compression, moisture, density, and biomass fraction	Mean MAPE of 6.30%; balanced solution at 20 wt.%.

The results are overall three types of evidence. First, the ANN was able to decrease the mean of the prediction error by 46.3% when compared to linear regression. Secondly, the composite responses measured showed statistically significant loading relationships for water absorption, density and flexural strength. Thirdly, multi-objective analysis isolated the balanced formulation from the formulation with the best overall performance. These results show the importance of not optimizing the agricultural biomass-reinforced polymer composites based on the reinforcement content or only on one mechanical response.

DISCUSSION

The results show that the biomass loading in the agriculture does not always give a positive response to all the properties of the polymer-composites. The density decreased by 6.36% while compressive strength increased by 30.8% with an increase in reinforcement from 10 to 40 wt.%, but flexural strength decreased by 28.1% and water absorption increased by over 200%. The opposing trends are due to the competing effects of the light weight lignocellulosic reinforcement, limited polymer continuity, moisture sensitive hydroxyl groups and potential agglomeration of particles at higher loading.

The ANN model was able to model these nonlinear interactions better than linear regression, with a mean prediction error of 46.3% less. Its best performance was in tensile and impact properties, confirming previous results that there is not a simple linear relationship that can represent biomass morphology and fiber–matrix interaction [13, 20].

The multi-objective analysis showed that the formulation with the highest biomass content (20 wt.%)) was the most balanced formulation, not the best one with the highest individual property. On the other hand, 40 wt % was preferred to achieve the desired properties of renewable content, low density, impact resistance, and compressive properties. This distinction is also used in the Pareto-based composite selection, as also reported in data-driven polymer optimization studies [24, 33]. The results thus indicate that the practical design of biomass–polymer composite materials should not only consider the mechanical properties of the composite materials, but also consider the moisture resistance, processing reliability and utilization rate of biomass.

CONCLUSION AND FUTURE SCOPE

This study developed an artificial intelligence (AI) based model to optimize agricultural biomass reinforced polymer composites based on the experimental data reported. The results indicated that the increase in biomass loading reduced the density and increased the water absorption while decreasing the flexural performance, but at the same time improved the compressive strength. The artificial neural network was able to model these nonlinear relationships more accurately than linear regression, with a 46.3% decrease in the mean prediction error. Multi-objective analysis showed that the 20 wt.% formulation was the most balanced, whereas the 40 wt.% composite formulation was more desired if the renewable content, impact resistance, compressive strength and lightweighting were more important. The results indicate that the biomass content cannot be optimized without considering the durability, stiffness, moisture sensitivity, and processing stability.

Further studies are needed to expand the public database to incorporate other polymer matrices, agricultural residues, fiber modifications, particle shapes and production processes. The predicted Pareto-optimal formulations should also be fabricated and tested separately to ensure the model generalization. There is a need to further investigate the behavior of long-term moisture ageing, fatigue, creep, thermal cycling, biodegradation and fiber–matrix interface. Life-cycle assessment, processing cost, recyclability and carbon-sequestration indicators would enhance the applicability of industry. The potential for further reduction of experimental demand by active learning and transfer learning in the optimization of biomass–polymer systems with unknown formulations and processing conditions, while increasing confidence in future formulation and processing decisions, would be additional benefits.

Data Availability Statement

The data used and generated during this study are provided in the supplementary dataset submitted with the manuscript. The package includes source-attributed experimental measurements, derived statistical results, multi-objective optimization outputs, and reproducibility scripts.

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