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Machine Learning-Based Prediction and Optimization of 3D-Printed PLA Biocomposites Reinforced with Vegetal Fibers

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ABSTRACT: The behavior of 3D-printed biocomposites as substitutes for products made with plant fibers depends on the factors involved during the printing process. This study focuses on the use of a predictive model to evaluate the effect of printing parameters on the physical and mechanical properties of biocomposites printed with PLA filaments reinforced with vegetal pulverized fibers. During fabrication, the following factors were varied: reinforced filament type, build orientation, layer height, infill density, and infill pattern. The physical and mechanical properties of the printed specimens (density, absorption capacity, swelling percentage, rupture modulus, and flexural elasticity modulus) were determined following the procedures established in the ASTM D1037-20 and NTC 2261-03 standards. An analysis of variance based on response surface methodology was performed to verify the statistical significance of the printing parameters, as well as their interaction. To define the prediction model, two machine learning algorithms were implemented and compared: Extreme Gradient Boosting (XGBoost) and Gaussian Process Regression (GPR). XGBoost was selected, and SHAP analysis was performed to interpret the contribution of each parameter to the model predictions. A Non-dominated Sorting Genetic Algorithm II (NSGA-II) was implemented in order to optimize the printing parameters, enabling the identification of configurations that satisfy the minimum requirements for structural applications in humid environments. A total of sixteen optimal configurations met the standard criteria, including modulus of rupture (MOR) >16 MPa, modulus of elasticity (MOE) >2400 MPa, and swelling percentage (Sw) <10%. Two of the most representative configurations were experimentally validated to assess the optimization results. The results demonstrate that an increase of more than 75% in infill density does not result in significant changes in the mechanical behavior of the biocomposite.

KEYWORDS: Biocomposites; fused filament fabrication; 3D printing parameters; prediction; optimization

1 Introduction

The growing interest in sustainable materials has accelerated the development of bio-based alternatives that can reduce the environmental impact of conventional materials [1,2]. Among these materials, plant fiber-reinforced biocomposites have emerged as promising candidates, because they combine renewable resources with low density, competitive mechanical behavior, and a reduced carbon footprint [1–5]. Beyond these characteristics, they can represent a substitute for conventional wood-based composites, which often rely on the use of synthetic adhesives derived from fossil resources and can release formaldehyde during their useful life [6–8].

Advances in additive manufacturing have further expanded the potential applications of these sustainable materials. Among the available technologies, fused filament fabrication (FFF) has become one of the most adopted processes because of its low production cost and its compatibility with thermoplastic biopolymers such as polylactic acid (PLA) [9–13]. For this reason, increasing attention has been paid to its use for the manufacture of printed biocomposites from thermoplastic filaments reinforced with vegetable fibers for use in various branches of engineering [14–16]. However, the performance of FFF-printed materials depends strongly on the parameters selected during the design and manufacturing stages. The interaction between these parameters can affect the final physical and mechanical properties, often requiring extensive experimental campaigns to identify suitable manufacturing conditions, thus increasing production time and costs [17–21].

Several studies have shown that printing parameters can affect the behavior of printed materials [22–26]. For this reason, the need has arisen to optimize the parameters involved in the printing process in order to achieve a balance between material consumption, manufacturing time, and the properties of the resulting structure [27]. For example, Mihankhah et al. (2026) designed bio-inspired PLA scaffolds with sandwich geometries fabricated by FFF, incorporating different infill densities across the sample thickness. The authors evaluated the mechanical properties, weight, and printing time, demonstrating the versatility of FFF technology for lightweight structural engineering applications [28]. Likewise, Sumanth et al. (2026) evaluated the effect of infill density and fiber percentage on the properties of PLA-wood composites manufactured using fused deposition modeling (FDM). Their characterization included tensile, flexural, and impact tests. The results showed that the mechanical properties of the materials are strongly affected by both the infill density and the proportion of wood reinforcement [27]. Unlike models traditionally used to predict the physical and mechanical properties of materials, machine learning techniques allow the identification of non-linear patterns and the accurate capture of interactions between design parameters, which reduces the costs and time associated with experimental characterization, contributing to the optimization of the manufacturing process [29–33].

Recent studies have applied machine learning techniques for predicting the mechanical performance of materials manufactured using 3D printing. Harishbabu et al. (2025) employed models such as Extreme Gradient Boosting (XGBoost) and Gaussian Process Regression (GPR) to evaluate the effect of printing parameters (graphene nanoplatelet (GNP) content, printing speed, nozzle temperature, layer thickness, and build orientation) on the tensile behavior, deformation, and hardness of GNP-reinforced PLA specimens. They demonstrated that fiber composition and build orientation were the variables that most affected the material's performance under axial stress [29]. Similarly, Laurenti et al. (2025) implemented a system based on enhanced neural networks to predict the mechanical properties of FDM-printed biopolymers. The study evaluated properties such as stiffness, tensile strength, deformation, fracture, and material toughness. According to the authors, the methodology implemented proved effective for application in scenarios where collecting large volumes of data is not possible due to technical or economic limitations [30]. In another study, Abu-Shams et al. (2026) developed machine learning models to predict tensile strength and estimate energy consumption in FDM-printed parts. Layer height, printing speed, nozzle temperature, infill density, and infill pattern were used as input variables for the predictive model [31]. Meanwhile, Patil et al. (2025) applied the TOPSIS multi-criteria decision-making approach to establish a global performance index (MAPI) aimed at optimizing the mechanical response of PLA biocomposites reinforced with rice husk fiber [32]. Additionally, machine learning techniques have also been applied to the optimization of impact-related properties. Hasanzadeh (2025) investigated carbon fiber-reinforced PLA composites manufactured by FFF and proposed regression-based machine learning models to predict energy absorption from nozzle diameter, nozzle temperature, and cooling fan speed. Experimental impact testing combined with density

measurements demonstrated the ability of these predictive models to estimate and optimize the mechanical performance of 3D printed composites [33].

Currently, the optimization of 3D printing parameters has become a strategy for maximizing the mechanical and physical properties of parts manufactured using 3D printing while minimizing material consumption and manufacturing times [34–36]. Liu et al. (2025) evaluated the effect of printing speed, layer thickness, nozzle temperature, and print bed temperature in order to develop a methodology that allows optimizing the accuracy of printed parts by minimizing dimensional error in length, width, and height and reducing printing time [34]. Chowdhury et al. (2026) implemented a multi-objective optimization algorithm assisted by surrogate models to maximize interlayer strength and minimize processing time in specimens printed using fused deposition modeling (FDM) of PLA filaments. The study trained Random Forest (RF), Gradient Boosting Machine (GBM), Extreme Gradient Boosting (XGBoost), and Light Gradient Boosting Machine (LightGBM) machine learning models, which were then integrated as surrogate models into a hybrid algorithm that combines a Non-dominated Sorting Genetic Algorithm II and a technique for order of preference by similarity to ideal solution (NSGA-II–TOPSIS) framework to generate and rank Pareto-optimal solutions [35]. Dev and Srivastava (2020) presented results from an experimental and multi-objective optimization of FDM process parameters to produce strong and lightweight parts for smart structural applications, evaluating the effect of layer thickness, build orientation, and infill density on the material consumption and compressive strength of FDM-printed specimens. The study combined the Taguchi approach for experimental design with the development of empirical models using commercial statistical analysis software to obtain functions that were optimized using the Non-dominated Sorting Genetic Algorithm II (NSGA-II) [36].

The present study focused on implementing a model based on machine learning to predict the effect of 3D printing parameters on the physical and mechanical properties of biocomposites manufactured using fused filament fabrication (FFF). PLA filaments reinforced with 10% pulverized plant fibers were used for the 3D printing process. During the manufacturing process, the following parameters were varied: reinforced filament type (*Guadua angustifolia*, Amazonian Yare, and *Salix viminalis*), build orientation (0° and 90°), layer height (0.20 and 0.40 mm), infill density (25%, 50%, and 75%), and infill pattern (gyroid, concentric, and linear). Five replicates were manufactured for each combination of variables. The materials' properties, viz. density (D), absorption capacity (A), swelling percentage (Sw), modulus of rupture (MOR), and modulus of elasticity (MOE), were determined following the procedures established in ASTM D1037-20 [37] and NTC 2261-23 [38]. An analysis of variance based on response surface methodology was performed in order to verify the statistical significance of the 3D printing parameters, as well as their interaction. The Extreme Gradient Boosting (XGBoost) algorithm was implemented, and an analysis based on SHapley Additive exPlanations (SHAP) was performed to predict the material properties from the evaluated parameters. Finally, the Non-dominated Sorting Genetic Algorithm II (NSGA-II) was applied in order to optimize the printing parameters, determining the parameter combinations that satisfy the minimum performance criteria specified in NTC 5493 [39] for structural applications exposed to humid conditions, and two of the most representative configurations were printed and tested as part of the validation process.

2 Materials and Methods

2.1 Materials

Pulverized and dried fibers from three plant species, *Guadua angustifolia*, *Heteropsis flexuosa* (Amazonian Yare), and *Salix viminalis*, were mixed with polylactic acid (PLA) granules Ingeo™ 4043D (NatureWorks LLC) to obtain biofilaments by means of a single-screw extruder operating at 180°C and an extrusion

throughput of 18–25 kg/h. To ensure stable extrusion and minimize processing difficulties, 10 wt.% pulverized fibers were incorporated into the PLA matrix [40].

2.2 Characterization of Filaments

The properties of the filaments were determined using standard procedures. The density was determined according to ISO 1183-1:2019 [41]. Ten specimens were analyzed for each filament type. Tensile properties (strength, modulus for elasticity, maximum strain, and toughness) were determined following the guidelines of ASTM D3822-14 [42] in specimens 70 mm in length using a gauge length of 25 mm.

2.3 Experimental Design

To assess the effects of the manufacturing variables on the behavior of FFF-printed specimens, a factorial design of experiments was adopted. Three categorical and two numerical factors were considered in the study. These factors were the filament type (PLA filaments reinforced with Guadua fibers (GF), Yare fibers (YF), and *Salix viminalis* fibers (SF)), infill pattern (gyroid, concentric, and linear), printing orientation (0° and 90°), layer height (0.2 and 0.4 mm), and infill density (25%, 50%, and 75%). A total of 108 experimental combinations were obtained ($3 \times 3 \times 2 \times 3 \times 2$). Five replicas for each combination of variables were considered, resulting in a total of 540 specimens. The distribution of the factors and their levels is presented in Table 1.

Table 1: Factors used in the experimental design.

Factor	Type	Level 1	Level 2	Level 3
Fiber	Categorical	GF	YF	SF
Infill Pattern	Categorical	Gyroid	Linear	Concentric
Build Orientation (°)	Categorical	0	90	–
Infill Density (%)	Numerical	25	50	75
Layer Height (mm)	Numerical	0.2	0.4	–

2.4 3D Printing Process

To evaluate the physical properties, specimens measuring 50 mm × 50 mm × 15 mm were designed. For determining the mechanical properties, specimens with a width of 50 mm, a thickness of 6 mm, and a length of 195 mm were designed. The digital models were created using Ultimaker Cura (version 5.5.0). A commercial Creality Ender 5 S1 Pro was used for the manufacturing process. The printing conditions, which remained constant during the printing stage, are shown in Table 2.

Table 2: 3D printing parameters.

Parameter	Value
Nozzle diameter (mm)	0.6
Nozzle temperature (°C)	205
Build plate temperature (°C)	60
Printing speed (mm/s)	80
Cooling fan speed (%)	100
Wall line count	3

(Continued)

Table 2 (continued)

Parameter	Value
Top layers	4
Bottom layers	2
Retraction speed (mm/s)	30

2.5 Experimental Characterization

Density measurements were performed according to ISO 1183-1:2019 [41]. Water absorption (A) and swelling percentage (Sw) were assessed by measuring the variations in specimen mass and thickness following 24 h of water immersion at ambient temperature [38]. Flexural testing was conducted under three-point bending conditions following ASTM D1037-20 [37]. For the mechanical tests, a Landmark MTS 370.10 testing machine was used with a loading rate of 3 mm/min.

2.6 Statistical Analysis

An analysis of variance (ANOVA) combined with response surface methodology (RSM) was conducted to evaluate the effects of the 3D printing parameters on the properties of the biocomposites. Statistical significance was evaluated at a 95% confidence level ($\alpha = 0.05$). The contribution of each factor was identified, as well as their interaction effects. In addition, main effects plots were constructed to verify the influence of the processing variables on the measured responses.

2.7 Machine Learning Analysis

To predict the effect of 3D printing parameters on the properties of the biocomposite, two machine learning algorithms were implemented: Extreme Gradient Boosting (XGBoost) and Gaussian Process Regression (GPR). According to Nasiri et al. (2024), the XGBoost model is distinguished by its use of gradient-boosted decision trees, which gives it speed, efficiency, and the ability to accurately analyze large datasets [43]. On the other hand, GPR is a versatile regression algorithm, which is notable for managing data and its capability for the prediction of uncertainties [44]. Categorical variables were encoded using one-hot encoding, while numerical variables were directly incorporated into the model. To evaluate the performance and generalizability of the machine learning model, the K-fold cross-validation technique was implemented. The dataset was randomly divided into subsets of equal size. The model was trained on $k - 1$ subsets and tested on the remaining subsets. The final performance metric was the average of the performance metrics for each subset [45].

For the optimization process, a set of hyperparameters was used. The hyperparameters are shown in Table 3.

Table 3: Hyperparameters used for the machine learning models.

Model	Parameter	Symbol	Value
XGBoost	Number of trees	n-estimator	100
	Learning rate	η	0.1
	Maximum tree depth	max_depth	3
	Row subsample ratio	subsample	0.8
	Feature subsample ratio	colsubsample_bytree	0.8

(Continued)

Table 3 (continued)

Model	Parameter	Symbol	Value
GPR	L1 regularization	α	0.10
	L2 regularization	λ	1.0
	Kernel function	$k(x, x')$	Matern 5/2
	Length scale	l	0.87
	Noise level	α	17.91

The dataset ($n = 540$) was randomly partitioned into training and testing sets, representing 80% and 20% of the data, respectively. A five-fold cross-validation strategy was applied to the training subset. This procedure enabled the evaluation of model stability and generalization across different data partitions.

Statistical metrics were used to evaluate the model's ability to predict the physical and mechanical properties of the material based on the printing parameters. The coefficient of determination (R^2), root mean square error (RMSE), mean absolute error (MAE), mean absolute percentage error (MAPE), Pearson correlation coefficient (r), and mean cross-validation coefficient of determination (CV mean R^2) were determined. These metrics quantified the model's accuracy and its generalizability to data not used during the training phase. A Pearson correlation matrix was developed to represent the evaluation coefficients between the sets of variables. Accordingly, the information obtained from these coefficients (signs and values) can be contributed to improving the data analysis and therefore to improving the performance of machine learning models [31].

SHapley Additive exPlanations (SHAP) was employed to interpret the predictions generated by the machine learning models. According to Takefuji (2025), SHAP provides a comprehensive framework for explaining model behavior by quantifying the contribution of each predictor to the predicted outcome. In this study, SHAP dependence plots were generated to examine the relationships between the input variables and the model responses, thereby facilitating the identification of the most influential factors and their effects on the predicted properties [46].

2.8 Multi-Objective Optimization

The multi-objective genetic optimization algorithm, NSGA-II, was implemented to identify the combinations of 3D printing parameters that maximize the strength and stiffness of the biocomposite while minimizing its water absorption (A), swelling percentage (Sw), and density (D). The implemented algorithm explored the design space within the limits defined by the experimental values used to train the XGBoost model. For each solution, the machine learning model predicted the target properties, which were then used as functions in the optimization process. As a result, a composite Pareto front was obtained, from which the most balanced alternative was selected using a global performance function that simultaneously weighed all the evaluated properties.

3 Results and Discussion

3.1 Properties of Filaments

The density and mechanical properties of the filaments were determined following the procedures described in Section 2.2, and the results are presented in Table 4. Based on these results, there were variations of less than 5% in the values of the density. On evaluating the mechanical properties, reinforced GF filaments

exhibited greater tensile strength (69.36 MPa) and a higher Young's modulus (2766 MPa), while reinforced SF filaments exhibited lower tensile strength (63.32 MPa) and modulus (2511 MPa) but greater maximum strain (5.76%) and toughness (2.57 MJ/m³), suggesting that this filament exhibits greater ductile behavior and therefore a greater capacity to absorb energy before breaking. Additionally, reinforced YF filaments exhibited intermediate values for all the evaluated properties. According to Kreft et al. (2024), filament strength and stiffness can affect the quality of printed specimens by influencing the continuity and stability of material feeding. Filaments with low stiffness may be more susceptible to buckling within the feeding system, while brittle filaments may fracture before reaching the nozzle [47].

Table 4: Properties of reinforced filaments.

Properties	GF	YF	SF
Diameter, mm	1.75 ± 0.03	1.75 ± 0.03	1.75 ± 0.03
Density, kg/m ³	1220 ± 15	1200 ± 10	1230 ± 13
Tensile strength (R _t), MPa	69.36 ± 0.80	65.90 ± 2.60	63.32 ± 2.70
Young's modulus (E _t), MPa	2766 ± 38	2620 ± 41	2511 ± 29
Maximum strain, %	4.08 ± 0.15	4.82 ± 0.21	5.76 ± 0.18
Toughness, MJ/m ³	1.81 ± 0.076	2.16 ± 0.053	2.57 ± 0.085

3.2 Experimental Characterization

The properties of the printed specimens, to wit density (D), water absorption (A), thickness swelling (Sw), modulus of rupture (MOR), and modulus of elasticity (MOE), were evaluated following the procedures outlined in Section 2.3. The corresponding results are shown in Figs. 1–5 for specimens printed with GF-, YF-, and SF-reinforced filaments.

Based on the results shown in Fig. 1, the effect of the 3D printing parameters on the specimens' density can be verified. Specimens printed using GF-reinforced PLA filaments exhibited density values up to 36% higher than those produced with YF- and SF-reinforced filaments. The results indicate a relationship between infill density and specimen density, with an increase from 25% to 75% in the density values of the printed specimens. According to Akhondi et al. (2023), this behavior is attributable to the greater amount of material present per unit volume [48]. Furthermore, the density of samples printed with a gyroid-type infill pattern was up to 20% higher than those printed with a linear or concentric pattern. According to Sun et al. (2025), the internal geometry of 3D-printed elements is a parameter that affects the packing efficiency of the material and therefore its specific density [49]. A reduction of less than 10% in density values was observed when increasing the printing layer height and modifying the printing orientation from 0° to 90°. To evaluate the effect of the printing parameters on the water absorption capacity and dimensional stability of the material, it is important to understand the behavior of the material when exposed to a humid environment, which can affect its mechanical behavior and its durability [49]. The effect of the printing parameters on A and Sw values is shown in Figs. 2 and 3.

The results shown in Figs. 2 and 3 indicate that increasing the infill density reduced the A and Sw of the specimens by up to 30%. Samples printed with a gyroid pattern exhibited lower A (7.75 ± 0.47) and Sw (2.16 ± 0.15) values, while those printed with a concentric pattern exhibited the highest values (14.72 ± 1.12 and 7.75 ± 0.28, respectively). Additionally, increasing the layer height led to increases of 24.8% and 17.7% in A and Sw values, respectively. These results are consistent with those reported by Helouai et al. (2024) and can be related to the internal porosity of the material, which depends on both the density and the filling pattern as well as the adhesion between consecutive printed layers [50].

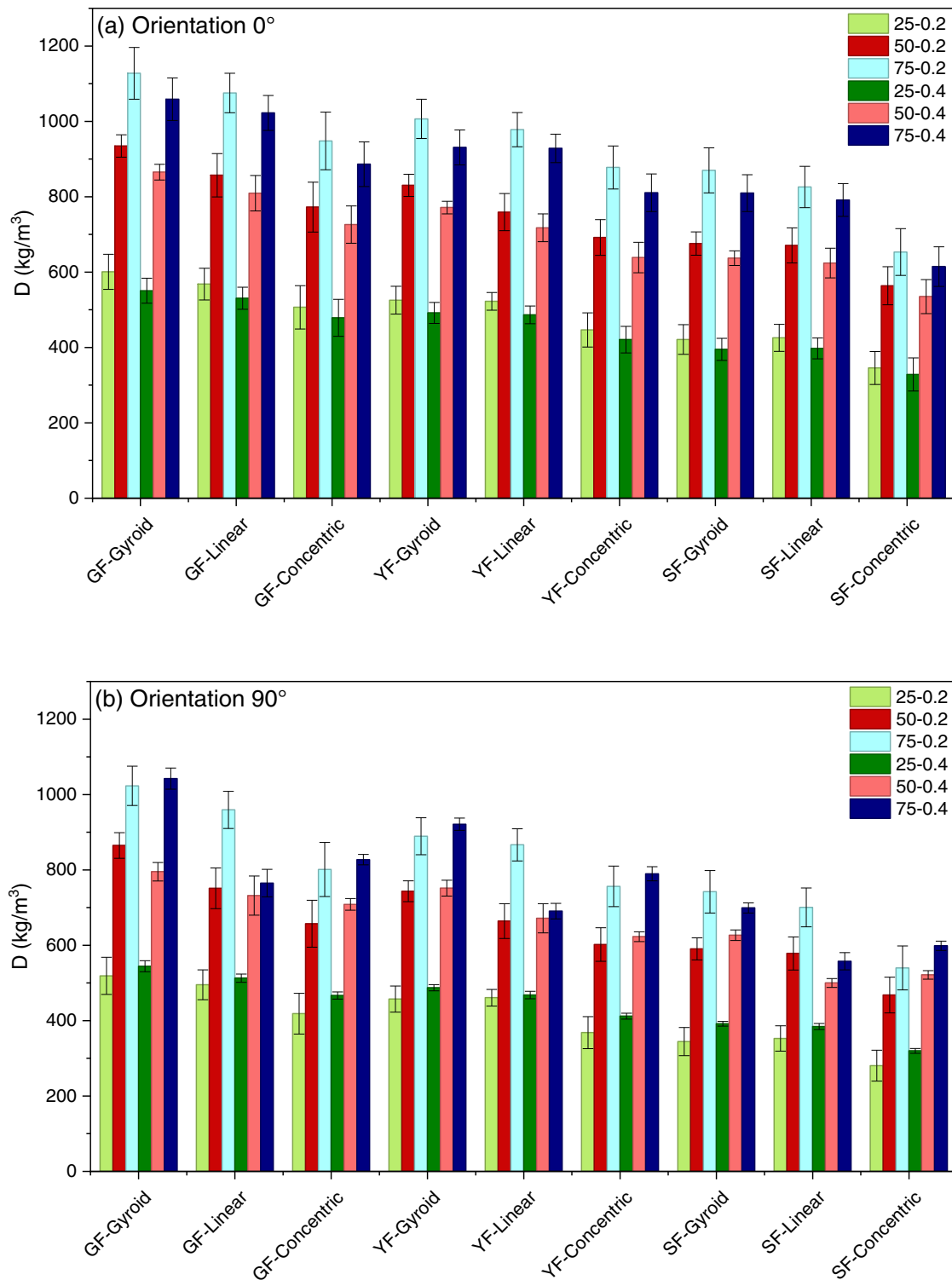


Figure 1: Experimental density (D) results for specimens printed at (a) 0° and (b) 90°.

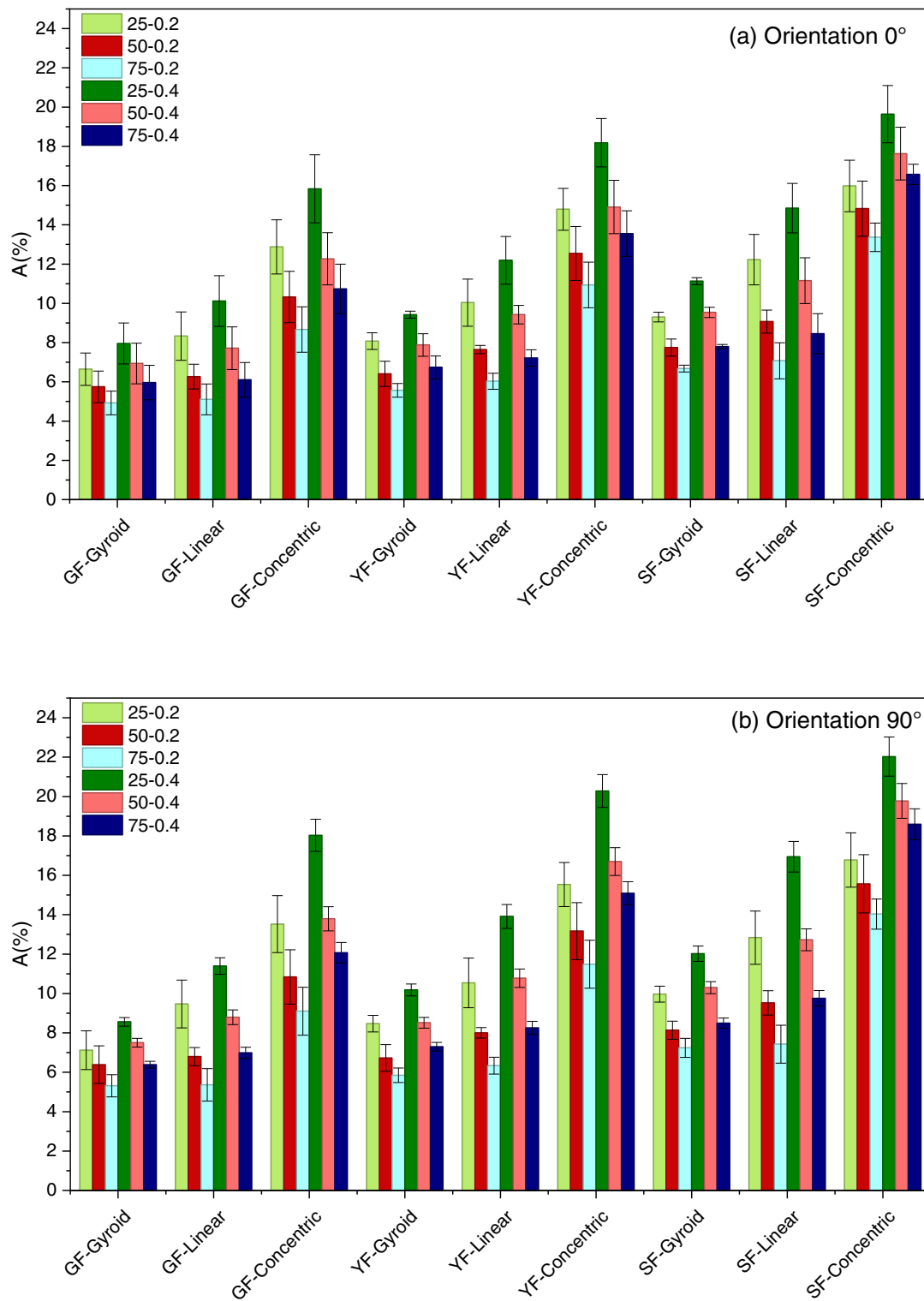


Figure 2: Experimental absorption (A) results for specimens printed at (a) 0° and (b) 90°.

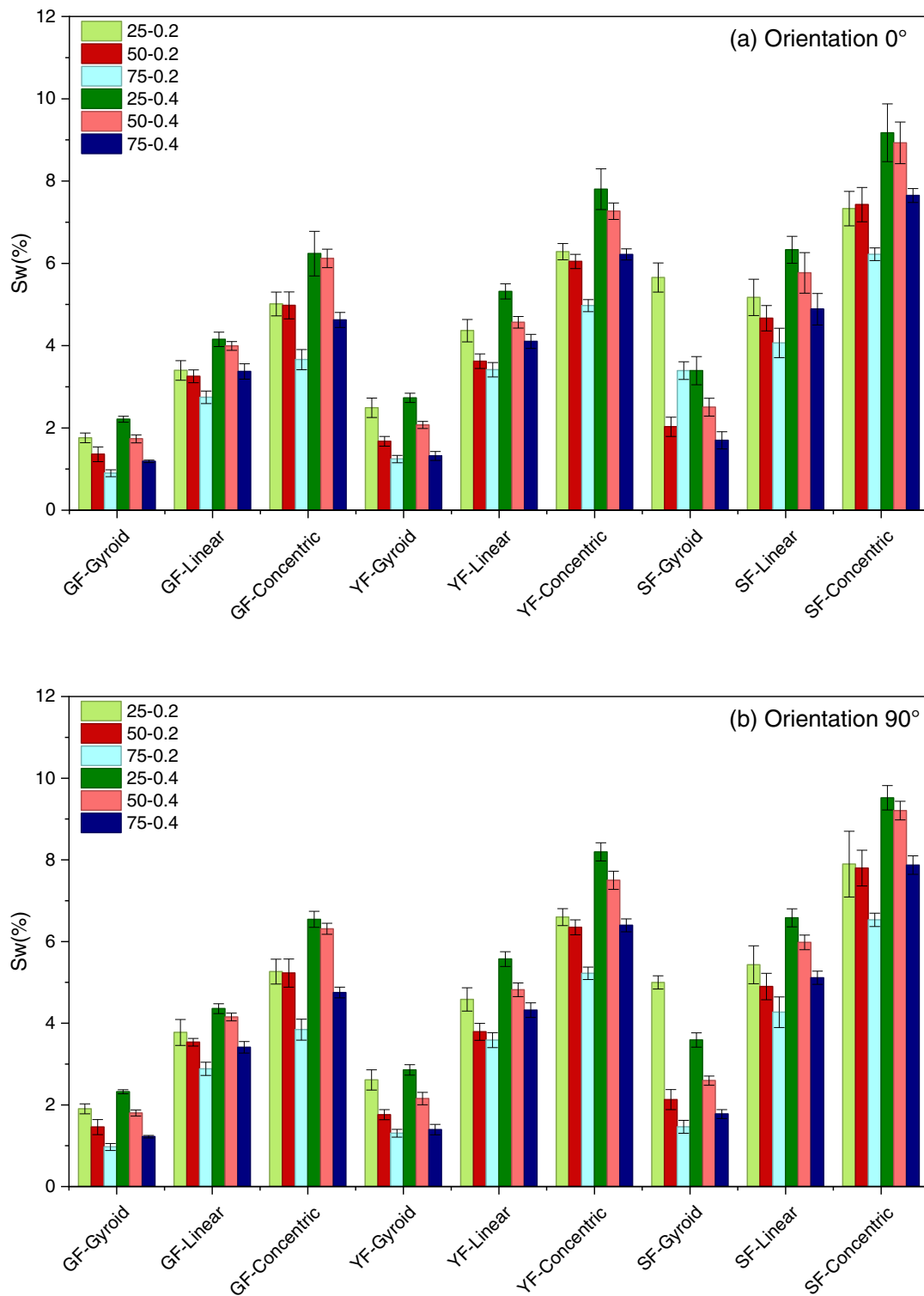


Figure 3: Experimental swelling percentage (Sw) results for specimens printed at (a) 0° and (b) 90°.

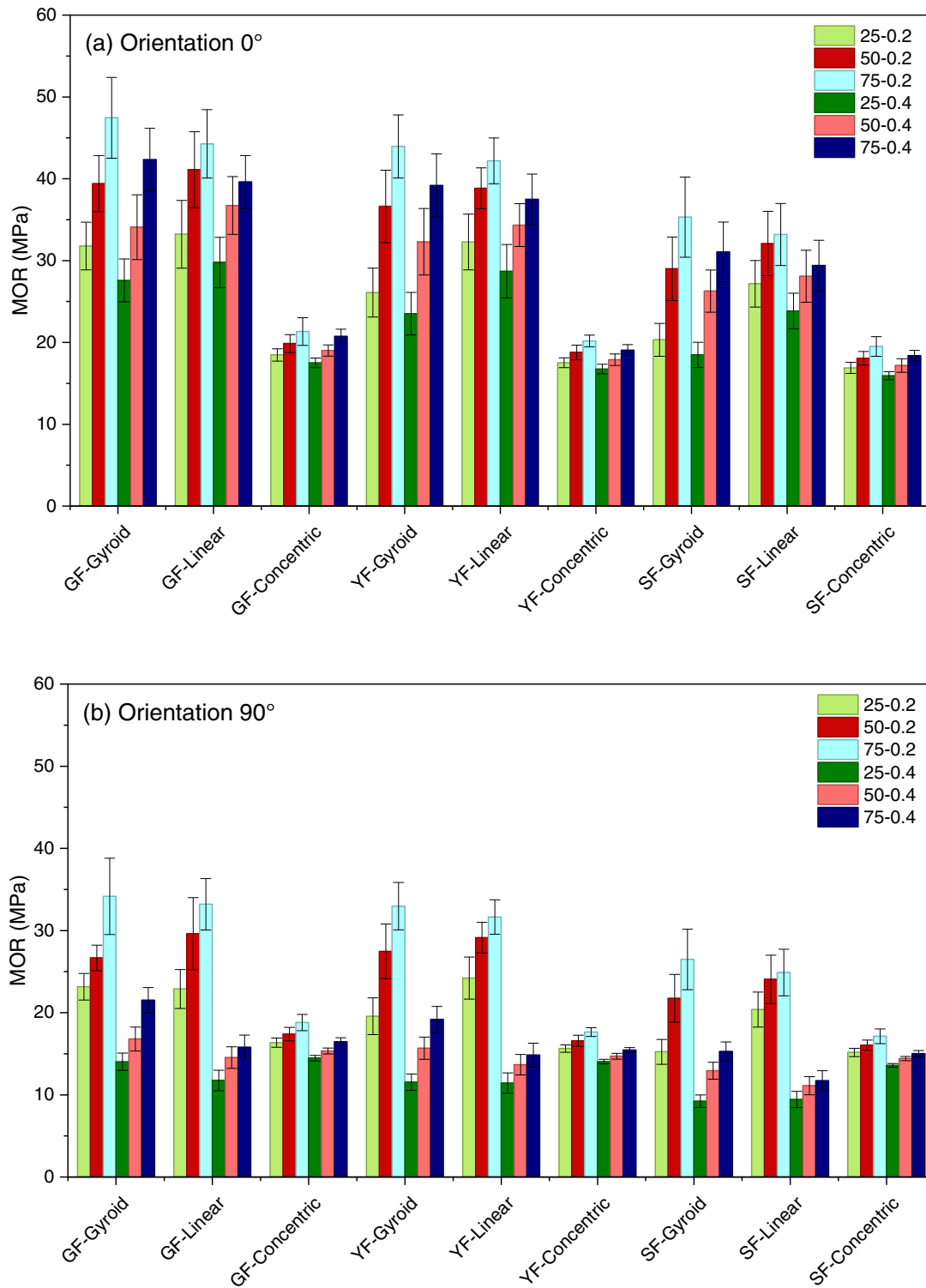


Figure 4: Experimental MOR results for specimens printed at (a) 0° and (b) 90°.

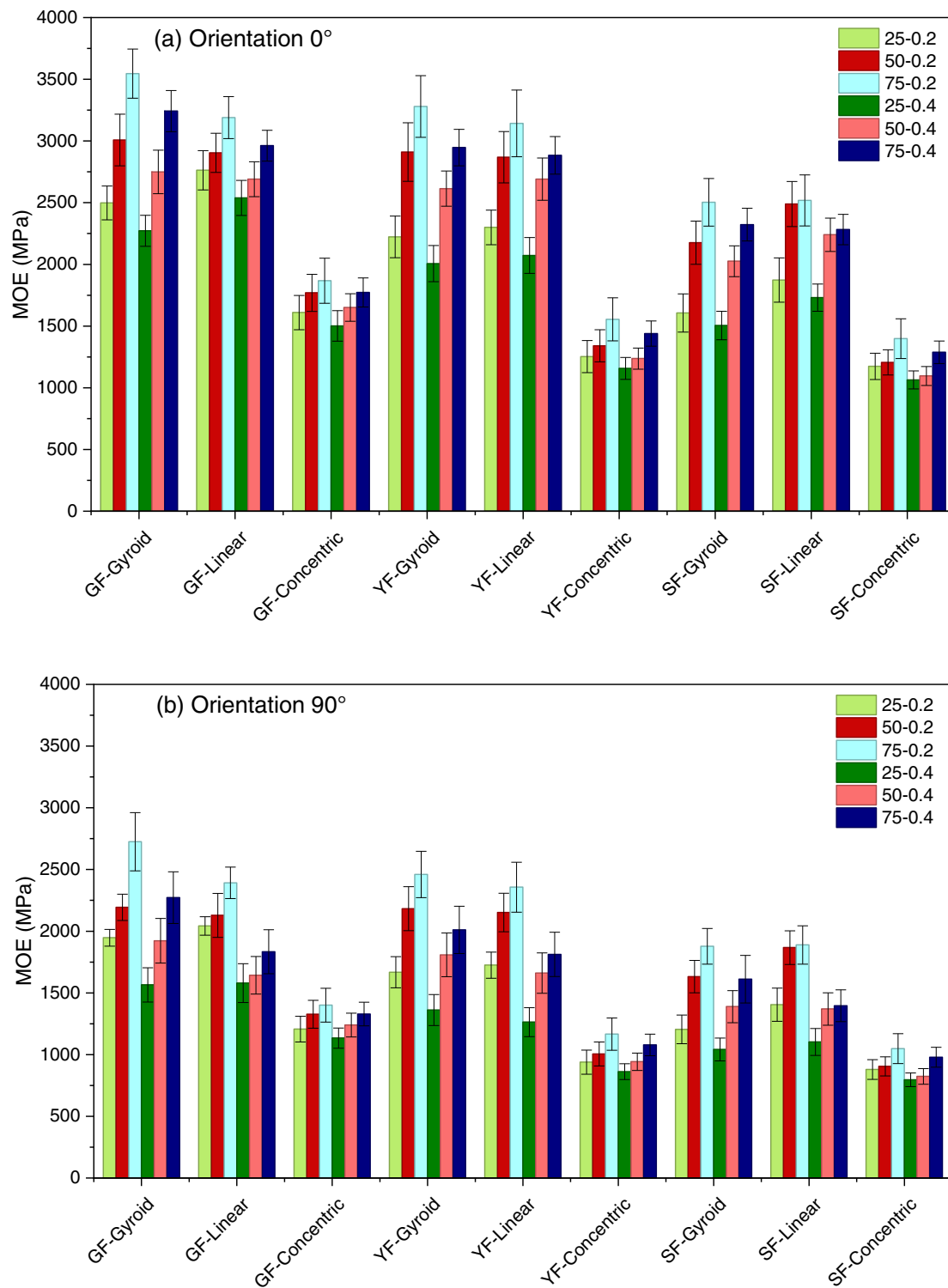


Figure 5: Experimental MOE results for specimens printed at (a) 0° and (b) 90°.

Figs. 4 and 5 show the effect of 3D printing parameters on the MOR and MOE values. According to these results, GF specimens printed at 0° with 75% infill, a gyroid-type pattern, and a layer height of 0.2 mm exhibited greater MOR and MOE values (47.45 ± 1.52 MPa and 3546 ± 199 MPa, respectively). According to Downing et al. (2021), the gyroid pattern consists of a continuous three-dimensional geometry that promotes uniform load distribution and stress transfer, thereby reducing local stress concentrations [51]. Furthermore, due to its strength and stiffness (see Table 4), the use of Guadua fiber-reinforced PLA filament contributed to enhancing the mechanical behavior of the biocomposites fabricated via FFF. Conversely, SF specimens printed with 25% infill, gyroid pattern, layer height of 0.4 mm, and printing at 90° exhibited the lowest MOR values (9.22 ± 0.76), while specimens printed with 25% infill, concentric pattern, and layer height equal to 0.4 mm and printing at 90° exhibited the lowest MOE values (796 ± 55 MPa). Experimental results suggest that the use of high percentages of filler and the selection of continuous three-dimensional geometries (as a filler pattern) can contribute to the uniform distribution of internal stresses in 3D printed specimens, improving their strength and stiffness when subjected to static bending [52].

3.3 Statistical Analysis

Analysis of variance (ANOVA) was performed to assess the statistical significance of the printing parameters and their interactions. The coefficient of determination (R^2), the adjusted R^2 (R^2_{adj}), the predicted R^2 (R^2_{pred}), and the root mean square error (RMSE) values are presented in Table 5. Despite the fact that statistical metrics show the stability of the model and its ability to predict the physical properties of the material, the results show a significant lack of fit for MOR, MOE, D, and Sw. These results suggest that the second-order polynomial equations obtained using the RSM model do not adequately describe the interaction between 3D printing parameters and their effect on the evaluated properties. According to Nikooharf et al. (2024), this behavior can be attributed to the fact that the physical and mechanical performance of biocomposites fabricated via FFF depends not only on the individual effects of the printing parameters but also on complex non-linear interactions between them [53]. In this context, machine learning approaches represent an alternative to response surface modeling [53,54]. For this reason, Extreme Gradient Boosting (XGBoost) and Gaussian Process Regression (GPR) were developed in order to represent these relationships more accurately and to improve the predictive capability regarding material properties.

Table 5: ANOVA metrics.

Properties	R^2	R^2 (Pred)	R^2 (Adj)	RMSE	Lack of Fit
D	95.33	94.75	95.08	43.89	<0.05
A	95.28	95.82	95.04	0.88	0.153
Sw	96.24	94.79	96.04	0.42	<0.05
MOR	92.91	92.12	92.54	2.51	<0.05
MOE	95.20	94.66	94.95	148.73	<0.05

The main effects of the 3D printing parameters on the properties are graphically represented in Figs. 6–8. The effects are represented by a line connecting the minimum and maximum levels of each factor. In the graphs, the slope of the line indicates the direction and magnitude of each factor on the response variable. From the results shown in Figs. 6 and 7, a significant effect of infill density on the physical properties of specimens can be seen (increasing the infill density enhances the density and dimensional stability of the printed specimens while reducing their water absorption capacity). These results suggest that increasing the amount of deposited material helps reduce internal voids and therefore the material's porosity.

Furthermore, the results indicate that the selection of the infill pattern and the type of fibers can affect the physical properties of the biocomposite, while layer height and print orientation had a smaller effect on the evaluated properties.

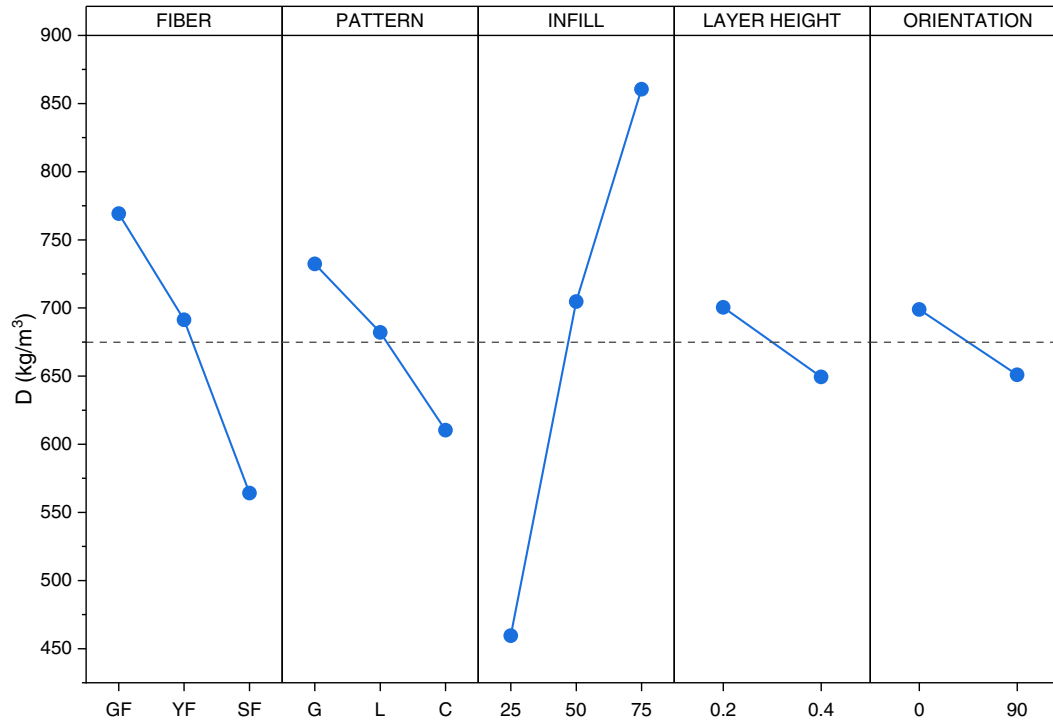


Figure 6: Main effects plot for density: G is gyroid, L is linear, and C is concentric pattern.

Fig. 8 shows the main effects plot for MOR and MOE. The results are consistent with those presented by Doshi et al. (2022) [55]. Due to the way the filament is deposited in a concentric pattern, the strength and stiffness values are lower than those obtained using three-dimensional patterns such as gyroid patterns, in which the load is distributed in several directions. Furthermore, it can be verified that the build orientation is one of the most important factors in the analysis of the flexural behavior of biocomposites, affecting their failure pattern. In specimens printed at 0° , the orientation along the specimen axis promotes the initiation of failure at the underside of the specimen, while in specimens printed at 90° , the bending strength can cause delamination of the material [55].

Fig. 9 shows the heat map of Pearson correlation coefficients (r) between 3D printing parameters and the physical and mechanical properties of the biocomposite. To incorporate categorical variables into the correlation analysis, the fiber type (FT) and infill pattern (P) variables were transformed using a one-hot encoding strategy, in which each category was represented as an independent binary variable. This procedure made it possible to calculate the r values without imposing an artificial order on the levels of the categorical variables, facilitating the interpretation of the effect of all the printing parameters on the properties of the material.

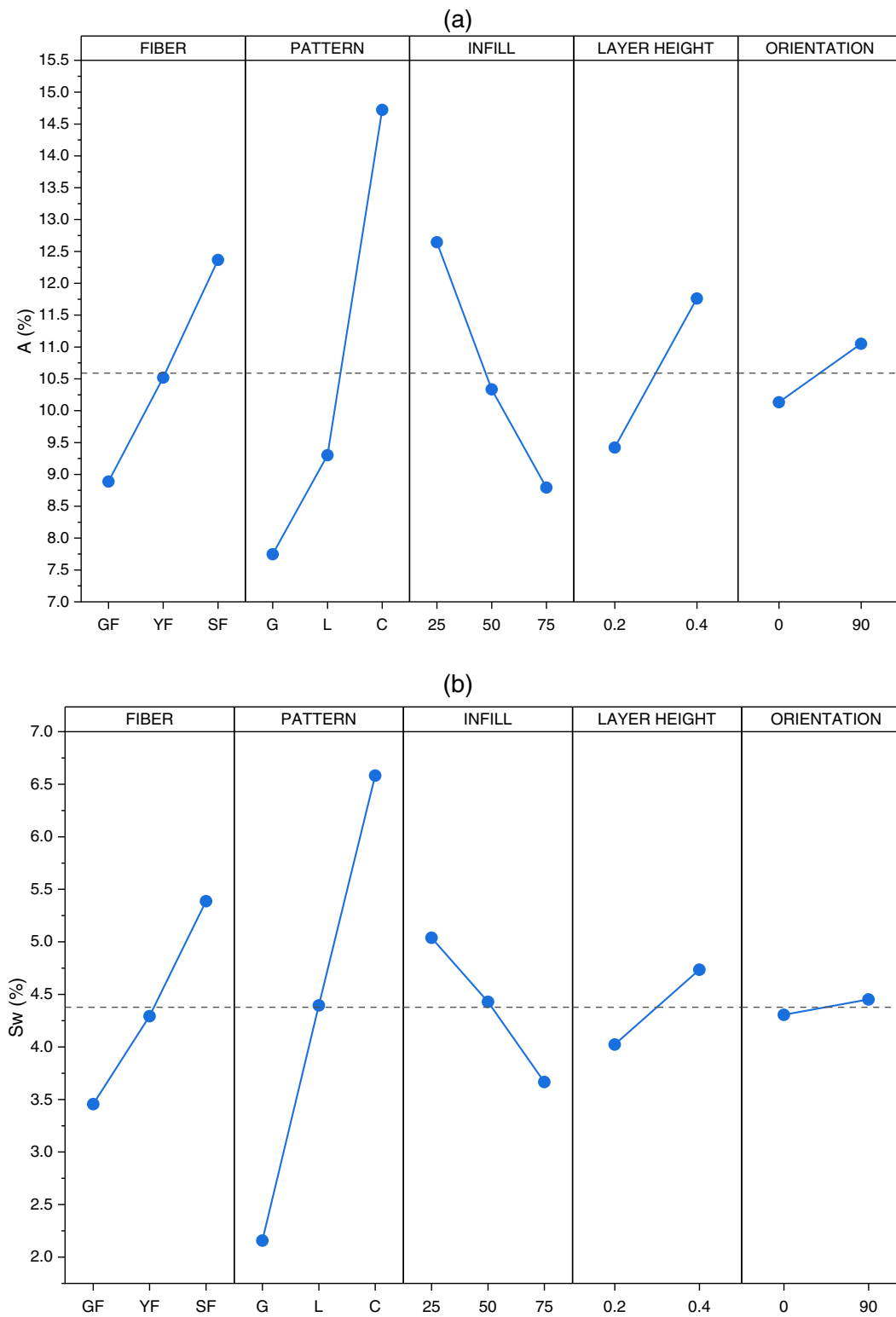


Figure 7: Main effects plots: (a) Main effects for A; (b) Main effects for Sw. G is gyroid, L is linear, and C is concentric pattern.

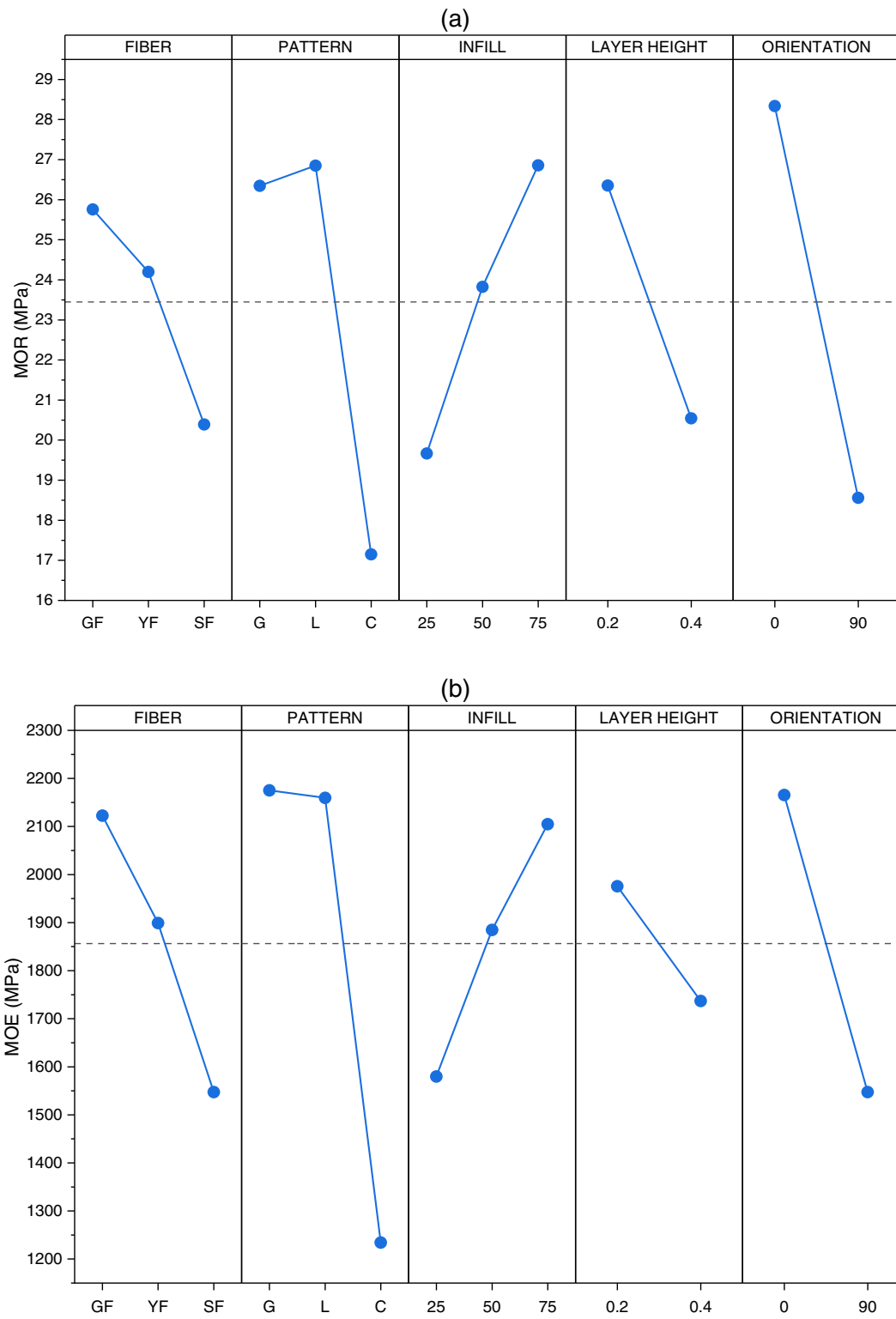


Figure 8: Main effects plots: (a) Main effects for MOR; (b) Main effects for MOE. G is gyroid, L is linear, and C is concentric pattern.

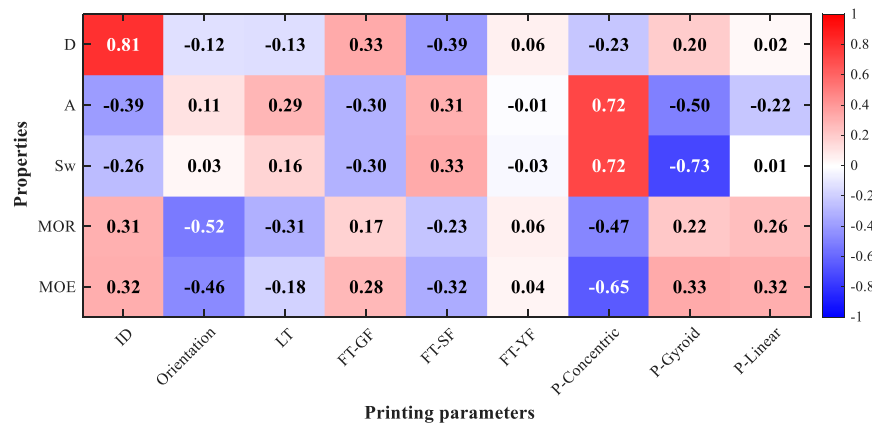


Figure 9: Correlation between printing variables and physical and mechanical properties.

The results shown in Fig. 9 confirm that the infill density (ID) is one of the parameters that most affects the material's physical properties, exhibiting a positive correlation coefficient of 0.81 for the biocomposite's density. Negative correlations ($r = -0.39$ and $r = -0.26$) were observed with water absorption (A) and swelling percentage (Sw), respectively. On the other hand, ID exhibits positive Pearson correlation coefficients with the evaluated mechanical properties ($r = 0.31$ for MOR and $r = 0.32$ for MOE). These results are consistent with those reported by Nikzad et al. (2025), who demonstrated that increased deposited material volume contributes to reducing the material's porosity and provides greater mass in order to resist strains and failure under load, promoting increased material strength and stiffness [56].

The effect of the build orientation can be seen in Fig. 9. A moderate negative r value for MOR and MOE allows verification that samples printed at 90° tend to have less strength and rigidity than those printed at 0° . Conversely, r values less than 0.12 suggest that this parameter does not significantly affect the physical properties of the material. On evaluating the effect of layer thickness (LT), negative correlations can be seen with the values of D, MOR, and MOE (r between -0.13 and -0.31), while positive correlation with absorption capacity ($r = 0.29$) and swelling percentage ($r = 0.16$) suggests that the use of thicker layers favors the formation of voids, increasing the porosity of the material and affecting its dimensional stability in the presence of moisture.

When evaluating the effect of the fiber type used to reinforce the filaments, it can be seen that GF fibers exhibited positive r values with D, MOR, and MOE ($r = 0.33$, $r = 0.17$, and $r = 0.28$, respectively), while exhibiting negative correlations with A and Sw. On the contrary, the use of SF fibers exhibited the opposite behavior, exhibiting negative coefficients of variation with the mechanical properties (MOR and MOE) and positive ones with A and Sw, indicating greater susceptibility to moisture absorption and lower structural efficiency. On the other hand, the use of YF fibers resulted in coefficients very close to zero ($r < 0.06$) for all the evaluated properties, suggesting that it did not significantly affect the evaluated properties. On the other hand, as to the effect of the infill pattern on the physical and mechanical properties of the biocomposite, it can be seen that the concentric pattern exhibits a positive correlation with A ($r = 0.72$) and Sw ($r = 0.72$) and negative r values with MOR and MOE. By contrast, the use of the gyroid pattern resulted in high positive correlations for MOR ($r = 0.22$) and MOE ($r = 0.33$), suggesting that the use of three-dimensional patterns can contribute to increasing flexural strength and stiffness.

3.4 Machine Learning Model

Fig. 10 presents the predictive performance of the RSM, XGBoost, and GPR models for all evaluated properties. As can be seen, the XGBoost and GPR models achieved coefficients of determination (R^2) greater than 0.94, along with RMSE, MSE, MAE, and MAPE values lower than those obtained via RSM. Furthermore, a comparison showed that the GPR and XGBoost models demonstrated equivalent predictive capabilities that surpassed those of the traditional statistical model. However, according to Liu et al. (2019), GPR models may face scalability limitations, because their computational cost increases with dataset size [57]. By contrast, XGBoost combines high predictive capability with greater computational efficiency, regularization mechanisms that reduce overfitting, and superior scalability for applications involving larger datasets. For this reason, XGBoost was selected as the final model for implementing the multi-objective genetic algorithm during the optimization stage.

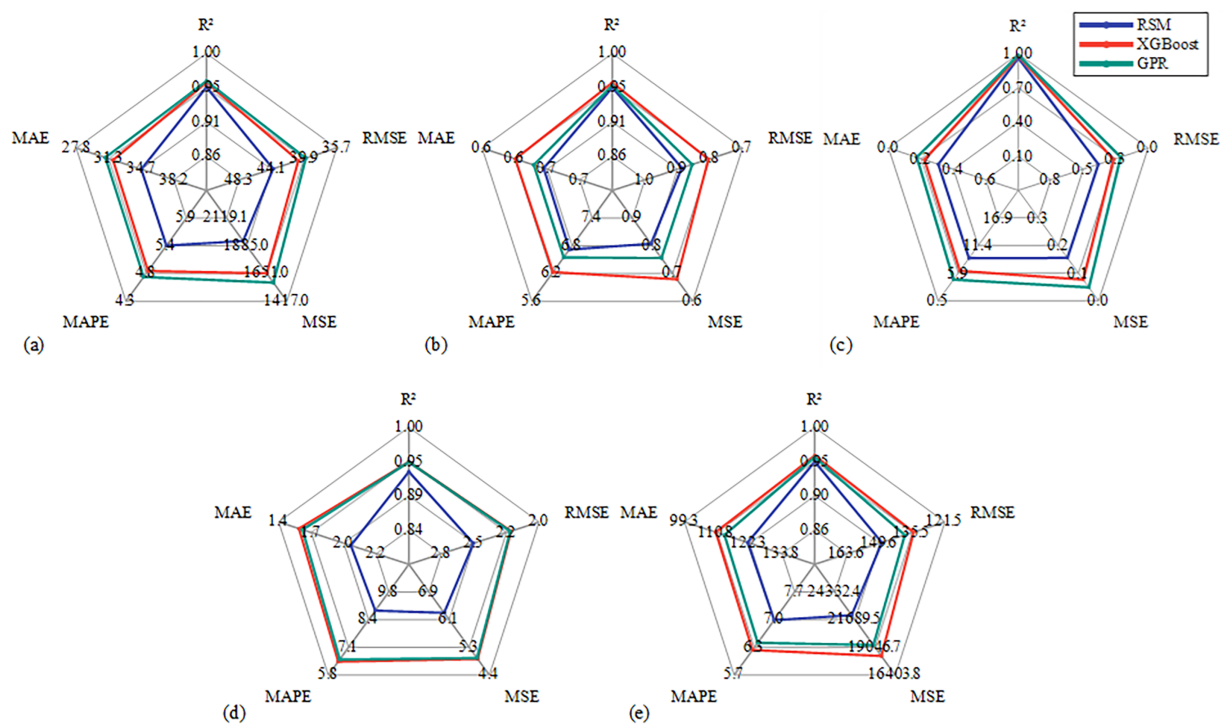


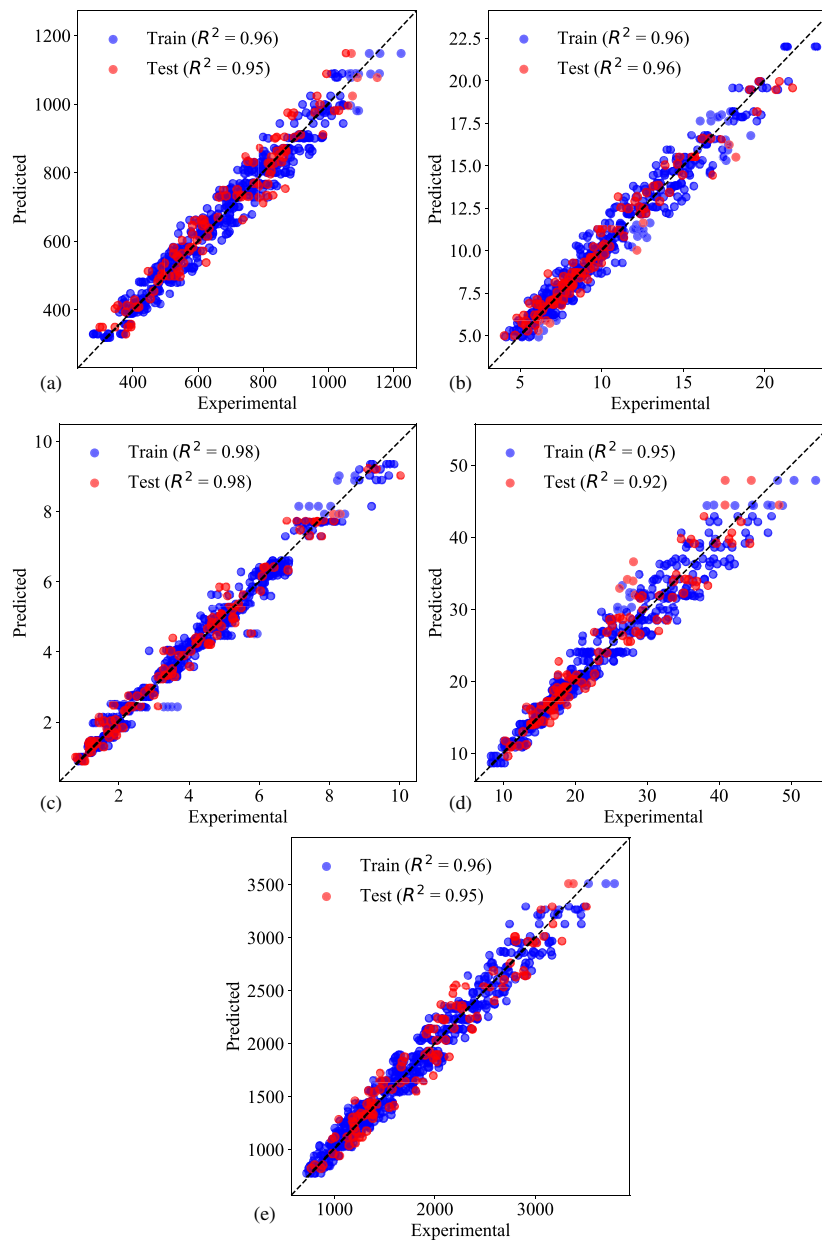
Figure 10: Comparison of models: (a) Density; (b) Absorption; (c) Swelling percentage; (d) MOR; (e) MOE.

The XGBoost performance metrics are presented in Table 6. The results show a coefficient of determination (R^2) > 0.90 for all evaluated properties. The MAPE values < 10% and the Pearson correlation coefficient ($r > 0.95$) validate the model's predictive capacity and the linear relationship between experimental and predicted values. Furthermore, the cross-validation values (CV mean R^2) suggest good model generalization and the absence of overfitting.

Fig. 11 shows scatter plots of the values predicted by XGBoost vs. experimental values for the target properties. The blue points correspond to the training and validation group used to calibrate the model, while the red points represent the test group. Additionally, the dashed line represents a reference line for a perfect fit. The high accuracy of the XGBoost model in predicting all the evaluated properties is verified based on these results, with $R^2 > 0.96$ for the training sets and $R^2 > 0.92$ for the test sets. This confirms the model's ability to generalize adequately and make accurate predictions for previously unobserved data.

Table 6: XGBoost performance metrics.

Properties	R^2	RMSE	MSE	MAPE	MAE	CV Mean R^2
D	95.99	40.65	1652.26	4.89	31.72	94.93
A	95.94	0.82	0.67	6.24	0.62	94.71
Sw	98.08	0.30	0.09	6.39	0.22	97.23
MOR	94.49	2.21	4.90	6.44	1.60	93.05
MOE	96.04	135.01	18,226.44	6.28	110.33	94.89

**Figure 11:** Scatter plots for predicted vs. experimental values: (a) D; (b) A; (c) Sw; (d) MOR; (e) MOE.

SHAP analysis was performed to quantify the contribution of each input variable to the XGBoost predictions for the evaluated physical and mechanical properties. Fig. 12a–c shows that the factors with the greatest impact on predicting density, absorption, and % swelling are fiber type, infill density, and infill pattern, respectively, which is consistent with the nature of these parameters. For the mechanical properties, MOR (Fig. 12d) and MOE (Fig. 12e), the graphs show that infill pattern and build orientation are the dominant variables, while layer thickness and fiber type have secondary effects. This indicates that the strength and stiffness depend primarily on the interaction between fiber direction and the applied load. Overall, the SHAP analysis confirms that the variables related to composition and internal geometry are the most decisive in the mechanical behavior of the biocomposite. These findings align with those reported by Yusoff et al. (2023), who demonstrated that fiber type and structural configuration are the primary drivers of mechanical and physical performance in PLA-based natural fiber composites [58].

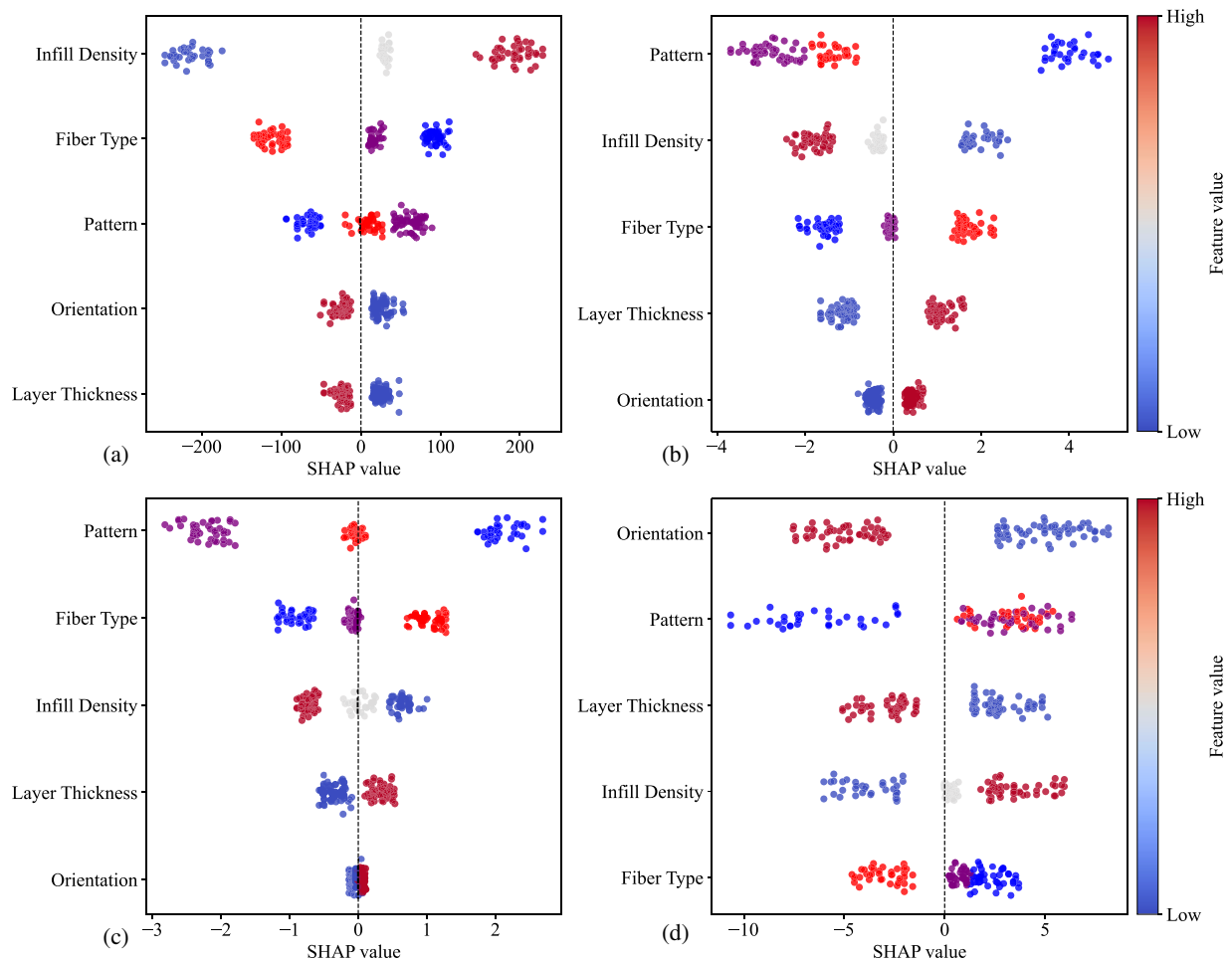


Figure 12: (Continued)

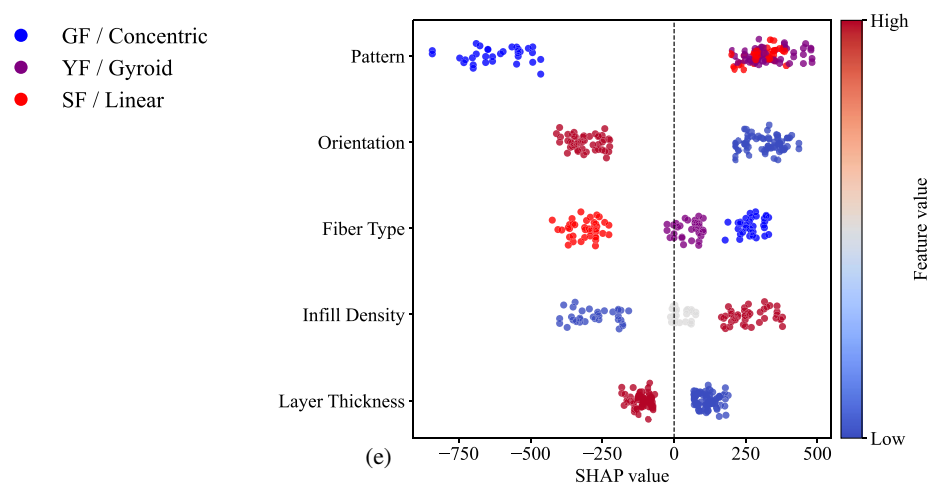


Figure 12: SHAP analysis: (a) D; (b) A; (c) Sw; (d) MOR; (e) MOE.

3.5 Optimization Algorithm

A Non-dominated Sorting Genetic Algorithm II (NSGA-II) was implemented to optimize the 3D printing parameters. The algorithm was designed to minimize the physical properties (density, absorption capacity, and swelling percentage) and maximize the mechanical properties of the material subjected to static bending. The decision variables were the parameters used in training the machine learning model. The solutions generated by the algorithm were evaluated using the XGBoost model, which predicted the properties of the biocomposite, thus avoiding the need for additional experimental tests. Fig. 13 shows the Pareto front obtained using the optimization algorithm. The minimum requirements established in NTC standard 5493 for wood particleboards designed for structural applications in humid environments ($MOR \geq 16$ MPa, $MOE \geq 2400$ MPa, and $Sw \leq 10\%$) were adopted as reference values [39]. Consequently, the optimal configurations were selected based not only on their mechanical behavior but also on their ability to meet engineering criteria regarding dimensional stability and mechanical behavior in humid environments. In Fig. 13, the limits corresponding to MOR and MOE were represented with horizontal lines, while Sw was not plotted, because all the solutions obtained have values lower than the maximum permitted limit.

Based on the optimization process results, 16 3D printing configurations (PC) were obtained that meet the mechanical requirements and dimensional stability of the material. Five of the most representative configurations are presented in Table 7.

Based on the results presented in Table 7, it can be seen that all the selected optimal configurations have a 0° printing orientation. Configurations with infill densities below 65% exhibited the highest A and Sw values and the lowest MOR and MOE values. This result confirms that reducing this 3D printing parameter reduces the material's load-bearing capacity and increases the probability of moisture penetration. On the other hand, increasing the infill percentage to approximately 76% increases the material's density to 980 kg/m^3 , resulting in an increase in the biocomposite's strength and stiffness. Furthermore, the results show that increasing the infill percentage above 76% does not produce significant differences in the evaluated properties. For this reason, the use of an infill density of 75%, gyroid pattern, and layer height of 0.22 mm can be considered to be the most efficient alternative within the configurations evaluated, since it provides practically the same mechanical performance as specimens printed with 95% infill while using a smaller amount of material and reducing printing time.

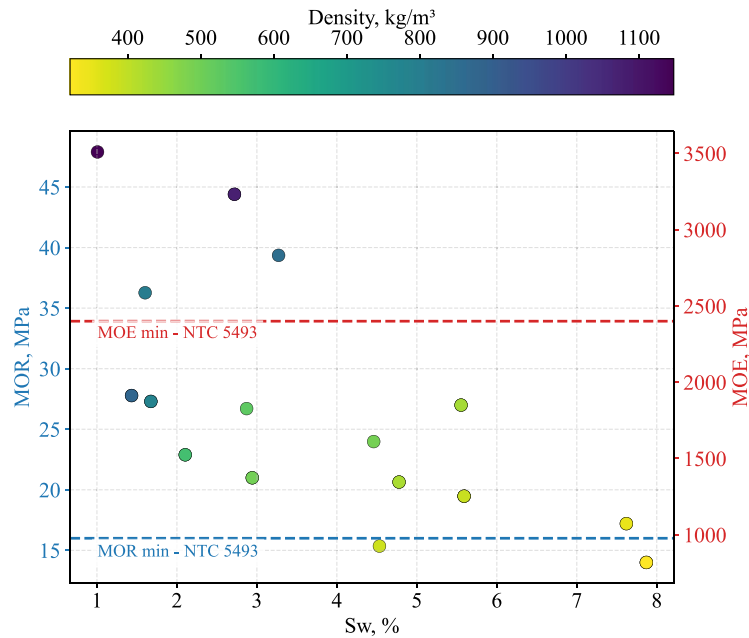


Figure 13: Pareto front for optimized designs.

Table 7: Optimal combinations obtained using the NSGA-II algorithm.

PC	FT	Pattern	ID	Orientation	LT, mm	D, kg/m ³	A, %	Sw, %	MOR, MPa	MOE, MPa
1	GF	Linear	51.60	0.00	0.21	852	6.22	3.27	39.36	2884
2	YF	Gyroid	65.51	0.00	0.20	803	6.35	1.60	36.27	2834
3	GF	Gyroid	75.75	0.00	0.22	1148	4.99	1.01	47.89	3509
4	GF	Linear	80.64	0.00	0.20	1077	4.92	2.72	44.40	3210
5	GF	Linear	95.00	0.00	0.20	1077	4.92	2.72	44.40	3210

For experimental validation, specimens were printed using two of the configurations shown in Table 7. Configurations 1 and 3 (PC 1, and PC 3), were selected because both correspond to specimens printed with filaments reinforced with guadua fibers (GF), which exhibited the best mechanical behavior during the optimization process. PC 1 represents a solution with low density (852 kg/m³) and MOR and MOE values that meet the minimum requirements established in NTC 5493 [39], while PC 3 corresponds to the solution that presented the highest strength and stiffness values (MOR = 47.89 MPa and MOE = 3509 MPa, respectively). Five specimens were evaluated for each of the selected configurations. The results are presented in Table 8.

The results presented in Table 8 demonstrate that the implemented multi-objective genetic algorithm adequately predicts the physical and mechanical properties evaluated. With the exception of the relative value found for the swelling percentage in specimens printed with the PC 3 configuration (12.22%), a difference of less than 5% was observed when comparing the experimental results with those obtained using NSGA-II. Furthermore, although the greatest relative error can be seen in the swelling percentage of the sample printed with the PC 3 configuration, the absolute difference between the optimized and experimental values was 0.11. According to Mukoroh et al. (2024), this difference can be attributed to the high sensitivity of swelling-related properties in biocomposite materials printed via FFF, as well as to the appearance of small internal defects

during the printing stage, and it does not affect the predictive capability of the implemented optimization model [59].

Table 8: Experimental validation of the optimized printing configurations.

PC	Property	Optimization Value	Experimental Value	Relative Error, %
1	D, kg/m ³	852	857 ± 57	0.58
	A, %	6.22	6.26 ± 0.63	0.64
	Sw, %	3.27	3.25 ± 0.16	0.62
	MOR, MPa	39.36	41.11 ± 4.63	4.26
	MOE, MPa	2884	2904 ± 158	0.69
3	D, kg/m ³	1148	1127 ± 69	1.86
	A, %	4.99	4.92 ± 0.60	1.42
	Sw, %	1.01	0.90 ± 0.08	12.22
	MOR, MPa	47.89	47.45 ± 4.94	0.93
	MOE, MPa	3509	3545 ± 199	1.02

4 Conclusions

The effects of printing parameters on the physical and mechanical properties of biocomposites manufactured using FFF were investigated. The results showed that the behavior of the material can be affected by the parameters selected during the printing stage: higher infill density increased the biocomposite's density and enhanced its strength, stiffness, and dimensional stability, whereas increased layer height and a 90° build orientation affected its mechanical behavior.

Specimens printed with PLA filaments reinforced with GF exhibited higher D, MOR, and MOE values. Additionally, the three-dimensional geometry typical of the gyroid infill pattern enhanced the material's performance under static bending.

The XGBoost model accurately predicted the properties of the biocomposites, achieving coefficients of determination greater than 0.94 for all evaluated responses and MAPE values below 10%. Compared to RSM, XGBoost provided greater predictive accuracy and lower prediction errors, demonstrating its ability to model the nonlinear relationships between printing parameters. In addition, SHAP analysis enabled interpretation of the relative contribution of each parameter to these responses.

Multi-objective optimization allowed the identification of printing configurations capable of simultaneously maximizing the mechanical properties and minimizing water absorption and swelling of biocomposites manufactured using FFF. The results demonstrated that increases above 75% infill density do not generate significant changes in the mechanical performance of the biocomposite.

Validating the configurations obtained during the optimization process allowed for a comparison between the values estimated by the optimization algorithm and the experimentally obtained results. For the majority of the properties analyzed (including density, water absorption, modulus of rupture, and modulus of elasticity), the differences between predicted and experimental values were less than 5%. Although the swelling percentage showed the highest relative deviation in one of the evaluated configurations (12.22%), the absolute difference was small, due to the low value of the experimental response.

The methodology proposed in this investigation combines experimental characterization, machine learning, SHAP explainability, and optimization using genetic algorithms, providing a starting point for the design and development of sustainable biocomposites printed using FFF. The use of machine learning methods reduces the experimental characterization stage and facilitates the identification of printing configurations necessary to ensure the material's good mechanical performance according to its application. However, experimentally validating a larger number of solutions belonging to the Pareto front is recommended, in order to evaluate the generalizability of the implemented model and verify its applicability to the development of biocomposites that can be used as substitutes for conventional wood-based panels for structural purposes in the construction sector.

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Abbreviations

The following abbreviations are used in this manuscript:

A	Absorption capacity
D	Density
Et	Modulus of elasticity in static bending
FFF	Fused filament fabrication
GF	Guadua reinforced filaments
MAE	Mean absolute error
MAPE	Mean absolute percentage error
MOE	Modulus of elasticity in in static bending
MOR	Modulus of rupture
MSE	Mean squared error
NSGA II	Non-dominated sorting genetic algorithm II
Rt	Tensile strength
RSM	Response surface methodology
RMSE	Root mean squared error
SHAP	SHApIey additive exPlanations
SF	<i>Salix viminalis</i> reinforced filaments

Sw	Swelling percentage
XGBoost	eXtreme gradient boosting
YF	Amazonian yare reinforced filaments

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