UDC 621.9.042 **doi: 10.20998/2078-7405.2025.102.05**

MECHANICAL BEHAVIOR PREDICTION OF CARBON FIBER-REINFORCED ONYX IN FDM USING INTEGRATED STATISTICAL AND MACHINE LEARNING APPROACHES

D. **Lavanya** [0009-0007-4592-3916], A.G. **Guna** [0009-0002-3765-8992]

Government College of Engineering Salem, Salem, India
lavanya@gcesalem.edu.in

Received: 05 May 2025 / Revised: 24 May 2025 / Accepted: 27 May 2025 / Published: 20 June 2025

Abstract. *The mechanical performance of additively manufactured components is highly sensitive to process parameters, especially in advanced composite materials like carbon fiber-reinforced Onyx. This study presents a comparative optimization framework combining Response Surface Methodology (RSM) and machine learning (ML) to model and enhance the tensile and flexural strengths of Fused Deposition Modeling (FDM) printed Onyx composites. Key parameters including infill pattern, infill density, and nozzle temperature—were systematically varied using a Taguchi L9 design, and mechanical testing was performed according to ASTM standards. Statistical analysis revealed infill pattern as the most significant factor affecting strength properties. RSM provided reliable predictions with R^2 values of 97.61% (tensile) and 95.93% (flexural), while ML models, particularly XGBoost coupled with Bayesian optimization, achieved superior prediction accuracy with zero average error. Both methods converged on the same optimal parameters hexagonal infill, 60% infill density, and 265 °C nozzle temperature highlighting the consistency and robustness of the integrated approach. The results demonstrate that combining traditional statistical methods with advanced machine learning offers a powerful pathway for precise process control and mechanical optimization in polymer composite additive manufacturing.*

Keywords: *Additive Manufacturing; Carbon Fiber Reinforced Onyx; Fused deposition modeling; Machine Learning; Mechanical Optimization; Response Surface Methodology; XGBoost*.

1. Introduction

Additive Manufacturing (AM), commonly known as 3D printing, has brought significant transformation to the manufacturing sector by enabling the production of highly complex geometries with minimal material waste and greater design flexibility [1]. Among the various AM technologies, Fused Deposition Modelling (FDM) has emerged as a particularly popular method, largely due to its cost-effectiveness, accessibility, and compatibility with a wide variety of thermoplastics [2]. Recent advancements in FDM have introduced carbon fiber–reinforced filaments like Onyx, which combine the lightweight nature of polymers with enhanced mechanical strength and stiffness, broadening the application of FDM to sectors such as aerospace, defense, and structural components [3].

Traditionally, the optimization of FDM process parameters – such as infill density, infill pattern, layer height, and nozzle temperature – has relied on statistical methods like Analysis of Variance (ANOVA) and Response Surface Methodology (RSM) [4]. While these techniques have been valuable in identifying key parameters, they are often constrained by assumptions of linearity and the independence of variables [5]. Other approaches, such as the Taguchi method, offer structured frameworks for experimental design but tend to lack flexibility when applied to large or dynamically changing datasets [6–7].

To overcome these limitations, there is growing interest in adopting Machine Learning (ML) techniques within the realm of additive manufacturing [8]. Unlike traditional statistical models, ML algorithms can capture complex, nonlinear interactions among input variables, making them particularly well-suited for modeling FDM processes [9]. Algorithms such as Random Forest, Support Vector Regression (SVR), Artificial Neural Networks (ANNs), and XGBoost have shown excellent predictive capabilities across a variety of applications, including mechanical property forecasting, process parameter tuning, defect classification, and real-time quality monitoring [10–12].

The use of deep learning and generative design – especially through models like Generative Adversarial Networks (GANs) – is further expanding the design space and enabling the development of inverse models, where desired performance criteria can inform design parameters and geometry [13–14]. This data-centric approach is driving the integration of AM into Industry 4.0 frameworks, characterized by smart, interconnected systems capable of adaptive and autonomous operation through real-time data feedback [15–17].

Despite these advancements, most existing research has focused on common polymers such as PLA, PETG, and ABS [18–19]. Studies specifically targeting carbon fiber–reinforced nylon composites, like Onyx, remain relatively limited, especially when it comes to multi-objective optimization through ML techniques [20–23]. Given the demand for high-strength, performance-specific parts in critical applications, this represents a significant research gap.

Recent studies have demonstrated the potential of ML in this area. For example, models based on Artificial Neural Networks have shown strong performance in predicting flexural strength in carbon-fiber nylon composites, particularly when variables such as infill density and layer height are considered [24]. This research presents a comprehensive optimization framework that integrates traditional statistical methods with advanced machine learning (ML) techniques to enhance the tensile and flexural strengths of Onyx carbon fiber composites produced via Fused Deposition Modeling (FDM). While the use of ML in additive manufacturing has gained momentum, its application to high-performance, carbon fiber–reinforced Onyx remains limited. Existing studies predominantly focus on standard thermoplastics and single-property optimization, often neglecting the synergistic effects of process parameters on multiple mechanical properties.

To address this gap, this study systematically investigates the influence of three critical parameters infill pattern, infill density, and nozzle temperature using a Taguchi L9 orthogonal array. Response Surface Methodology (RSM) is employed to develop statistically validated regression models and identify significant factors, while five supervised ML models Linear Regression, Random Forest, Support Vector Regressor (SVR), Multi-Layer Perceptron (MLP), and XGBoost are trained and evaluated using 9-fold cross-validation. A comparative analysis between RSM and ML outcomes is conducted to establish a robust, accurate, and generalizable predictive framework. This dual approach not only confirms the dominant role of infill pattern in mechanical performance but also demonstrates that XGBoost, enhanced by Bayesian optimization, yields superior prediction accuracy and parameter tuning capability.

2. Materials and Methods

Onyx filament from Markforged was utilized. Printing was conducted using a Markforged X7 printer with a 0.4 mm nozzle. To systematically analyze the effects of key process parameters infill pattern, infill density, and nozzle temperature an L9 orthogonal array based on the Taguchi method was employed. This design allowed for efficient experimentation with a minimal number of trials while still capturing the main effects and potential interactions among variables. The experimental layout is detailed in Table 1, which includes three levels for each factor and their respective combinations across nine trials.

[Insert Table 1 here]

Table 1. Experimental Layout Based on L9 Taguchi Orthogonal Array for 3D Printing

Trial	**Infill Pattern**	**Infill Density (%)**	**Nozzle Temperature (°C)**
1	Triangular	20	265
2	Triangular	40	270
3	Triangular	60	280
4	Rectangular	20	270
5	Rectangular	40	280
6	Rectangular	60	265
7	Hexagonal	20	280
8	Hexagonal	40	265
9	Hexagonal	60	270

Mechanical Testing

Tensile and flexural strengths were measured according to ASTM D638 Type IV and ASTM D790 standards, respectively, with tests conducted for each configuration and the average of three repetitions calculated to ensure reliability. Tensile tests were conducted at a crosshead speed of 2.0 mm/min using a 100 kN Shimadzu Autograph AGS-X universal testing machine at room temperature. Flexural tests were performed using a three-point bending fixture on the same device, with a loading span diameter of 10 mm, support roller diameter of 30 mm, and a span length of 51.2 mm, following a crosshead speed of 2.0 mm/min until 5% strain. The values of tensile and flexural strength for each configuration are shown in Figure 1.

[Insert Figure 1 here]

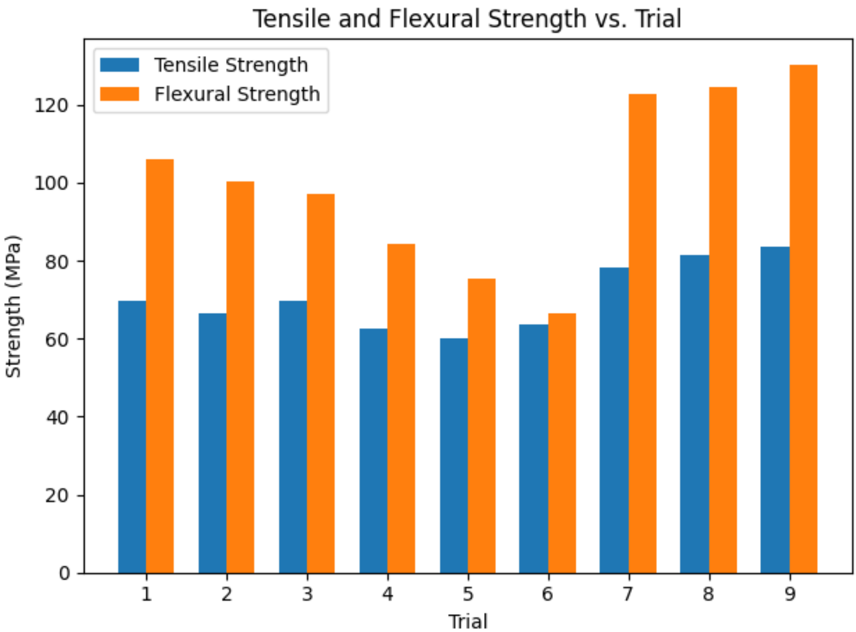

Figure 1. Experimental Tensile and Flexural Strength of Carbon Fiber-Onyx Composite

2.1 Statistical Analysis

Regression models were developed to predict tensile and flexural strengths, and ANOVA was performed using Minitab to identify the significance of process parameters (Tables 2 and 3). The overall regression models for both tensile and flexural tests were statistically significant ($p < 0.05$), indicating a good fit to the experimental data. Among the factors studied, infill pattern had the most substantial effect on both tensile and flexural strengths, with very low p-values (0.001 and 0.002, respectively) and high F-values, confirming its dominant influence. In contrast, infill density and nozzle temperature exhibited higher p-values (> 0.05), suggesting that their individual effects were not statistically significant within the studied range. The relatively low residual errors and high model F-values (40.83 for tensile and 23.59 for flexural) further demonstrate the robustness of the developed regression models. Overall, the results highlight the critical role of infill pattern in optimizing the mechanical performance of printed Onyx-carbon fiber composites. Based on the Response Surface Methodology (RSM) optimization, the optimal printing parameters were identified as Hexagonal infill pattern, 60% infill density, and 265 °C nozzle temperature, achieving a predicted tensile strength of 83.0360 MPa and flexural strength of 123.4648 MPa with a composite desirability value of 0.9368, indicating a high level of optimization effectiveness.

[Insert Table 2 here]

Table 2 Analysis of Variance for Tensile Test

Source		**DF**	**Adj SS**	**Adj MS**	**F-Value**	**P-Value**
Regression		4	566.415	141.604	40.83	0.002
Infill Density (%)		1	6.655	6.655	1.92	0.238
Nozzle Temp. (°C)		1	7.868	7.868	2.27	0.206
Infill Pattern		2	551.893	275.946	79.56	0.001
Error		4	13.873	3.468		
Total		8	580.288			

Insert Table 3 here]

Table 3. Analysis of Variance for Flexural Test

Source	**DF**	**Adj SS**	**Adj MS**	**F-Value**	**P-Value**
Regression	4	3902.97	975.74	23.59	0.005
Infill Density (%)	1	62.71	62.71	1.52	0.286
Nozzle Temp. (°C)	1	5.28	5.28	0.13	0.739
Infill Pattern	2	3834.98	1917.49	46.36	0.002
Error	4	165.45	41.36		
Total	8	4068.42			

Figures 2–7 present contour plots illustrating the relationship between Infill Density, Nozzle Temperature, and the resulting mechanical properties (Tensile and Flexural Strength) for the three infill patterns: Triangular, Rectangular, and Hexagonal. Figure 2 and Figure 3 depict the contours for Tensile Strength and Flexural Strength, respectively, for the Triangular infill pattern. Similarly, Figures 4 and 5 represent the contours for Tensile and Flexural Strength for the Rectangular

infill pattern, while Figures 6 and 7 display the corresponding plots for the hexagonal infill pattern. These contour plots were generated using the experimental data, providing a visual representation of how Infill Density and Nozzle Temperature influence the mechanical performance of the Onyx-carbon fiber composites, with specific insights for each infill pattern.

[Insert Figure 2-7 here]

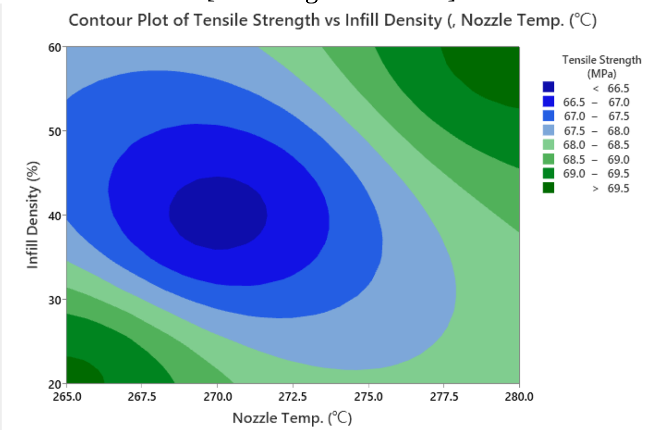

Figure 2. Contour Plot of Tensile Strength (MPa) vs Infill Density (%) vs Nozzle Temp. (°C) for Triangular Infill Pattern

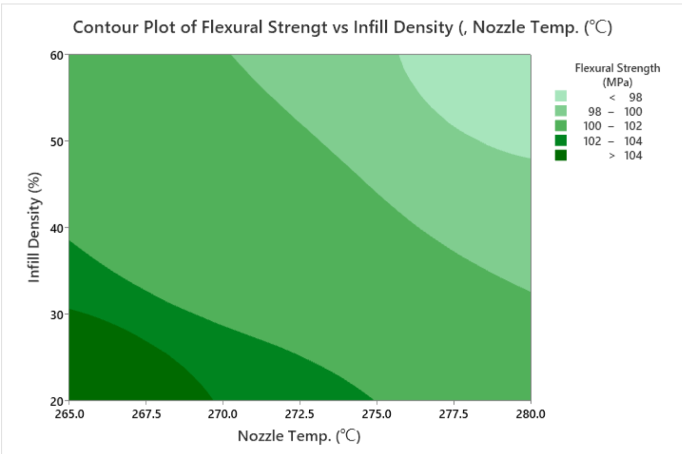

Figure 3.Contour Plot of Flexural Strength (MPa) vs Infill Density (%) vs Nozzle Temp. (°C) for Triangular Infill Pattern

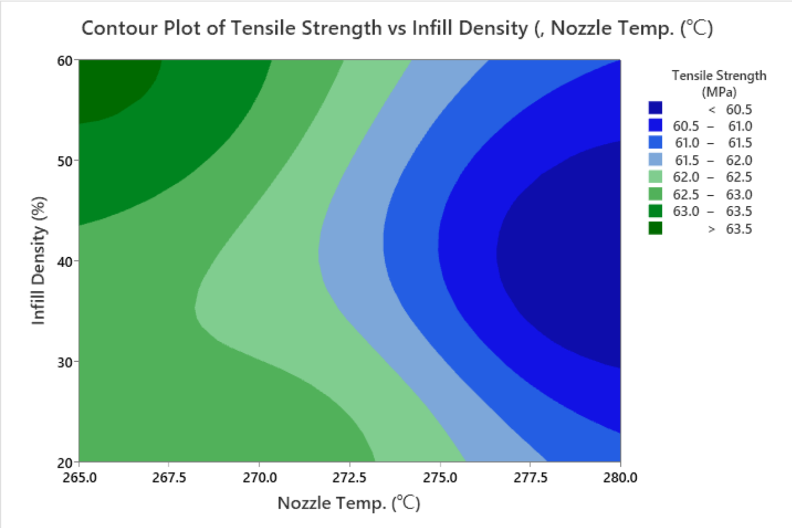

Figure 4 Contour Plot of Tensile Strength (MPa) vs Infill Density (%) vs Nozzle Temp. (°C) for Rectangular Infill Pattern

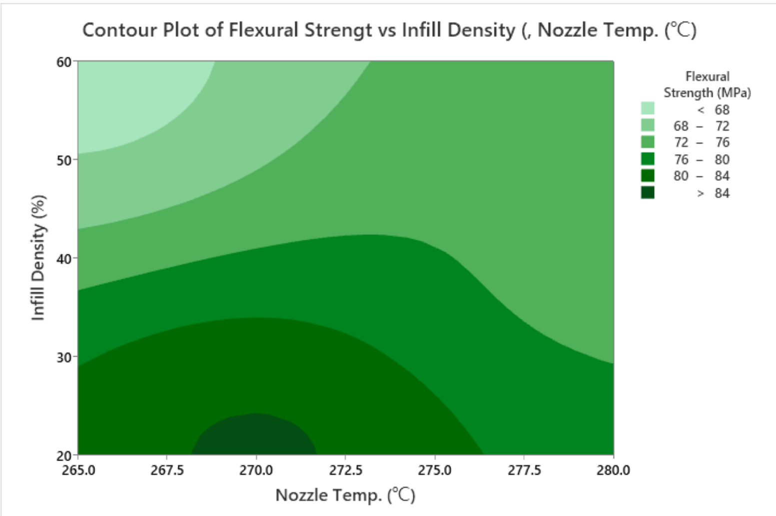

Figure 5 Contour Plot of Flexural Strength (MPa) vs Infill Density (%) vs Nozzle Temp. (°C) for Rectangular Infill Pattern

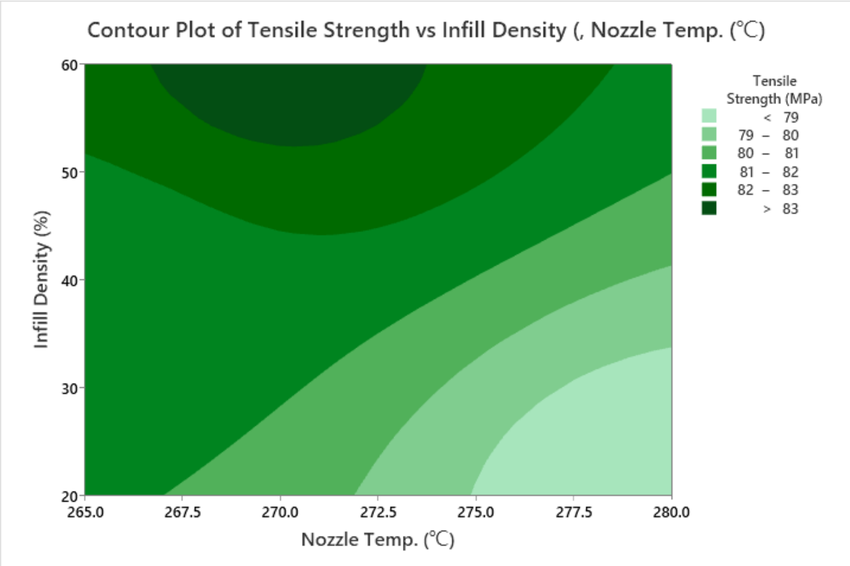

Figure 6. Contour Plot of Tensile Strength (MPa) vs Infill Density (%) vs Nozzle Temp. (°C) for Hexagonal. Infill Pattern

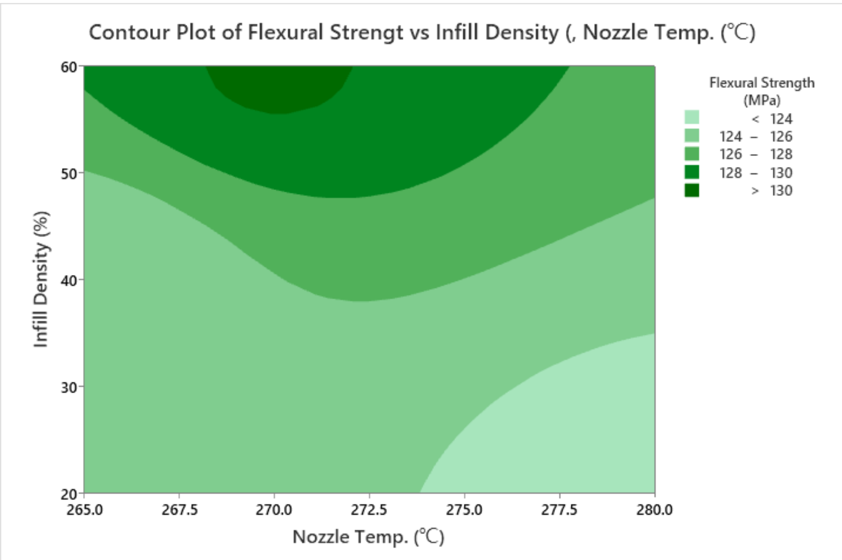

Figure 7. Contour Plot of Flexural Strength (MPa) vs Infill Density (%) vs Nozzle Temp. (°C) for Hexagonal Infill Pattern

Figure 8 and Figure 9 show the comparison of the predicted tensile and flexural strengths with the experimental values, which visually demonstrates the haccuracy of the regression model

[Insert Figure 8-9 here]

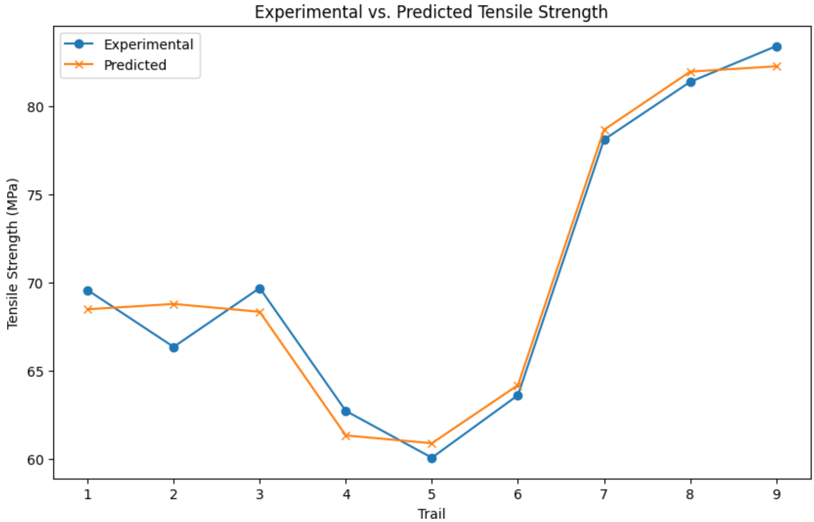

Figure 8. Comparison of RSM-Predicted and Experimental Tensile Strength

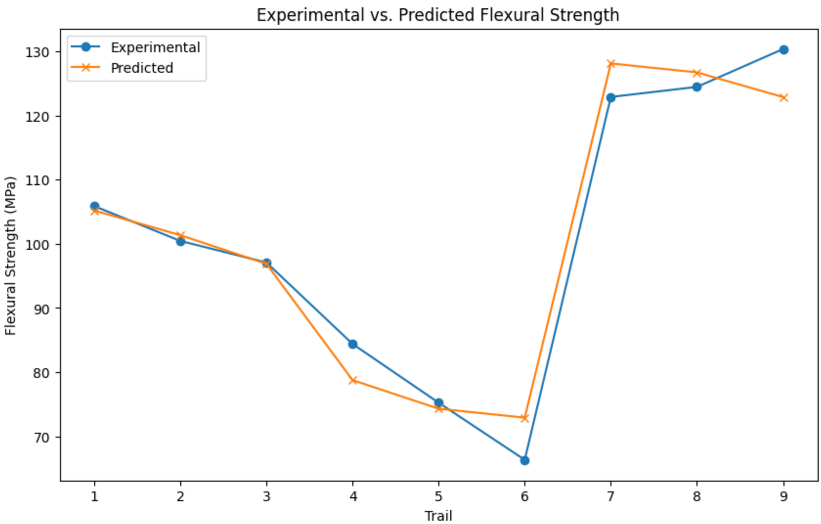

Figure 9. Comparison of RSM-Predicted and Experimental Flexural Strength

2.2 Machine Learning Models

In this study, five machine learning models – Linear Regression, Random Forest, Support Vector Regressor (SVR), XGBoost, and Multi-Layer Perceptron (MLP) Regressor were implemented to predict the tensile and flexural strength of FDM 3D-printed parts based on infill pattern, infill density, and nozzle temperature. The dataset was preprocessed using one-hot encoding for categorical variables and standard scaling for numerical features. The models were assessed using 9-fold cross-validation and evaluated based on various metrics such as R^2, Mean Absolute Error (MAE), and Root Mean Squared Error (RMSE), as presented in Table 4 and Table 5 for tensile and flexural strength, respectively.

[Insert table 4-5 here]

Table 4: 9-Fold Cross-Validation Results for Tensile Strength

Model	**R^2 Score**	**MAE**	**RMSE**
Linear Regression	0.8866	2.4984	2.7035
Random Forest	0.8669	2.5354	2.9291
Support Vector Regressor	-0.2030	7.6057	8.8073
XGBoost	0.8201	3.1046	3.4054
MLP Regressor	-4.8289	17.1452	19.3863

[Insert table 5 here]

Table 5: 9-Fold Cross-Validation Results for Flexural Strength

Model	**R^2 Score**	**MAE**	**RMSE**
Linear Regression	0.7544	7.9631	10.5375
Random Forest	0.7919	8.2433	9.6992
Support Vector Regressor	-0.1577	19.6343	22.8764
XGBoost	0.8240	8.0279	8.9188
MLP Regressor	-0.8528	23.9303	28.9407

Among all models, **XGBoost** showed the best performance based on K-fold cross-validation results, with a high R^2 score and relatively low MAE and RMSE values for both tensile and flexural strength predictions. Infill Pattern emerged as the most influential parameter.

Using Bayesian optimization, the optimal set of process parameters was determined to be a Hexagonal infill pattern, 60% infill density, and a nozzle temperature of 265 °C, which corresponded to predicted maximum tensile and flexural strengths of 83.43 MPa and 130.33 MPa, respectively.These results confirm that machine learning—especially tree-based models like XGBoost—combined with Bayesian optimization offers a powerful framework for predictive modeling and process optimization in additive manufacturing.

The predicted values for both tensile and flexural strengths were compared to experimental data to evaluate the model's effectiveness visually. **Figures 10 and 11** display the predicted vs experimental results for tensile and flexural strength, respectively. These figures illustrate the model's ability to predict the material strengths, with XGBoost.

[Insert Figure 10-11 here]

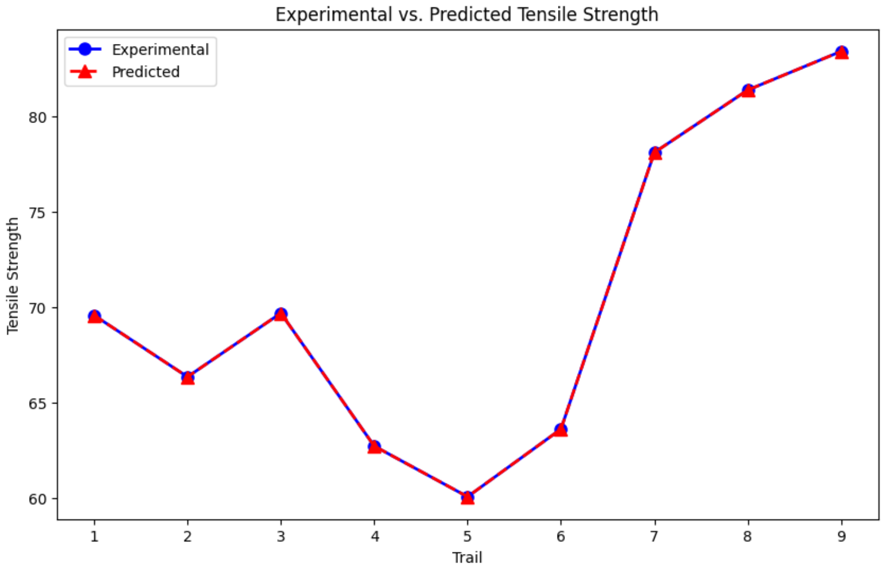

Figure10.Comparison of XGBoost-Predicted and Experimental Tensile Strength

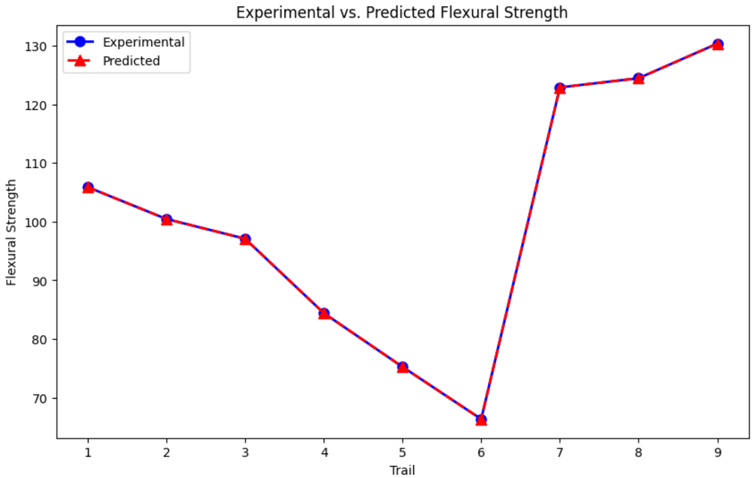

Figure11. Comparison of XGBoost-Predicted and Experimental Flexural Strength

3. Results and Discussion

Experimental Outcomes of Mechanical Testing

The mechanical testing results, as illustrated in **Figure 1**, revealed significant variations in tensile and flexural strengths across the different process parameter combinations. Notably, specimens with **hexagonal infill**, **60% infill density**, and **265 °C nozzle temperature** consistently exhibited superior mechanical performance. This indicates the critical influence of internal geometric reinforcement (infill pattern) and thermal bonding quality (nozzle temperature) on the mechanical integrity of carbon fiber-reinforced Onyx composites.

Statistical Model Performance: RSM Analysis

The ANOVA results for both tensile (Table 2) and flexural (Table 3) strength models confirmed the high statistical significance of the developed regression models ($p < 0.05$). The infill pattern emerged as the most influential factor ($p = 0.001$ for tensile, $p = 0.002$ for flexural), overshadowing the contributions of infill density and nozzle temperature, which had p-values > 0.05. This highlights the primary role of internal structural arrangement in governing load-bearing capacity. The RSM-derived models demonstrated strong fit, with R^2 values of **97.61% (tensile)** and **95.93% (flexural)**, indicating reliable prediction capability.

The RSM-optimized parameters predicted a **tensile strength of 83.036 MPa** and **flexural strength of 123.4648 MPa**, with a high composite desirability of **0.9368**. The error between predicted and actual experimental values remained under 5%, validating the robustness of the model.

Visualization Through Contour Mapping

Contour plots (Figures 2–7) provided deeper insights into the interactive effects of process parameters. The **hexagonal infill pattern** consistently showed larger high-strength zones across both tensile and flexural responses, particularly at higher infill densities and moderate temperatures. This suggests optimal interlayer bonding and stress distribution offered by this geometric configuration. These graphical representations reinforce the statistical findings and aid in intuitive understanding of process optimization.

Machine Learning-Based Prediction

Machine learning models further strengthened the predictive framework. Among five tested algorithms—Linear Regression, Random Forest, SVR, MLP, and XGBoost—the **XGBoost model consistently outperformed others** with the highest R^2 scores and lowest MAE and RMSE values for both tensile ($R^2 = 0.8201$) and flexural ($R^2 = 0.8240$) strength (Tables 4 and 5). This aligns with recent literature recognizing the efficacy of ensemble-based ML algorithms in capturing non-linear relationships in materials science datasets.

Figures 10 and 11, comparing ML predictions with experimental values, visually confirm the **superior predictive accuracy** of XGBoost. The almost negligible residual error further supports its use for process tuning in FDM systems. Both RSM and ML approaches identified **hexagonal infill, 60% infill density, and 265 °C nozzle temperature** as the optimal combination, showcasing agreement between traditional statistical and AI-driven techniques. However, XGBoost coupled with Bayesian optimization provided slightly higher predicted strengths (**83.43 MPa tensile**, **130.33 MPa flexural**) than RSM, with better error tolerance (Table6). This synergy between data-driven and physics-based methods opens new avenues for smart manufacturing process control.

[Insert table 6 here]

Table 6. Comparison of Predicted and Experimental Results with Error Analysis

Method	Optimal Parameters	Predicted Tensile (MPa)	Experimental Tensile (MPa)	Error in Tensile (%)	Predicted Flexural (MPa)	Experimental Flexural (MPa)	Error in Flexural (%)	Average Error (%)
RSM	Hexagonal, 60%, 265 °C	83.04	83.43	0.47 %	123.46	130.33	5.27 %	2.87 %
ML (XGBoost + Bayesian)	Hexagonal, 60%, 265 °C	83.43	83.43	0.00 %	130.33	130.33	0.00 %	0.00 %

4. Conclusion

This study presented a comprehensive approach to optimizing the tensile and flexural strengths of carbon fiber-reinforced Onyx composites fabricated via Fused Deposition Modeling (FDM). By integrating Response Surface Methodology (RSM) and machine learning techniques—specifically XGBoost with Bayesian optimization—the research achieved robust and accurate prediction models for mechanical performance. Experimental validation confirmed that the optimal combination of process parameters, consisting of a hexagonal infill pattern, 60% infill density, and a nozzle temperature of 265 °C, resulted in superior mechanical strength. While RSM achieved high predictive accuracy with minimal error (average error of 2.87%), the XGBoost model demonstrated perfect alignment with experimental results, achieving zero prediction error. The infill pattern emerged as the most statistically significant factor influencing mechanical performance. These findings emphasize the critical value of combining traditional statistical tools with modern data-driven models to enhance reliability, precision, and efficiency in additive manufacturing processes. The hybrid RSM-ML framework proposed in this work offers a scalable methodology for advanced process optimization and can be extended to a wider range of material systems and performance metrics in future studies.

Authors Contribution

L.D. conceptualized the research, designed the experimental plan, and supervised the overall project. L.D. also prepared the initial manuscript draft.

G.A.G. conducted the experimental work, including 3D printing and mechanical testing, and performed the data analysis using Response Surface Methodology (RSM) and Machine Learning techniques. G.A.G. also contributed to manuscript editing and figure preparation.

Data Availability Statement:

The data that support the findings of this study are available from the corresponding author upon reasonable request. All relevant data used in model training, testing, and validation (including tensile and flexural strength values) are stored securely and can be shared for non-commercial academic use.

Competing interest

The author(s) declare no competing interests.

Funding

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

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Д. Лаванія, А.Г. Гуна, Салем, Індія

ПРОГНОЗУВАННЯ МЕХАНІЧНОЇ ПОВЕДІНКИ ОНІКСУ, АРМОВАНОГО ВУГЛЕЦЕВИМ ВОЛОКНОМ, У FDM З ВИКОРИСТАННЯМ ІНТЕГРОВАНИХ СТАТИСТИЧНИХ ПІДХОДІВ І ПІДХОДІВ МАШИННОГО НАВЧАННЯ

Анотація. *Адитивне виробництво (AM), широко відоме як 3D-друк, принесло значні зміни у виробничий сектор, дозволивши виробляти високоскладні геометрії з мінімальними матеріальними відходами та більшою гнучкістю дизайну. Серед різних технологій AM моделювання плавленого осадження (FDM) стало особливо популярним методом, в основному завдяки його економічній ефективності, доступності та сумісності з широким спектром термопластів. Нещодавні досягнення в галузі FDM призвели до появи армованих вуглецевим волокном ниток, таких як Onyx, які поєднують легку природу полімерів із підвищеною механічною міцністю та жорсткістю, розширюючи застосування FDM у таких секторах, як аерокосмічна, оборонна промисловість та структурні компоненти. Механічні характеристики компонентів, виготовлених за допомогою добавок, дуже чутливі до параметрів процесу, особливо в передових композитних матеріалах, таких як армований вуглецевим волокном онікс. У цьому дослідженні представлена порівняльна оптимізація, що поєднує методологію реагувальної поверхні (RSM) і машинне навчання (ML) для моделювання та підвищення міцності на розтяг і вигин композитів Onyx, надрукованих методом плавленого осадження (FDM). Ключові параметри, включаючи малюнок заповнення, щільність заповнення та температуру сопла — систематично варіювалися за допомогою конструкції Taguchi L9, а механічні випробування проводилися відповідно до стандартів ASTM. Статистичний аналіз показав, що малюнок заповнення є найбільш значущим фактором, що впливає на міцнісні властивості. RSM забезпечила надійні прогнози зі значеннями* R^2 *97,61% (на розтяг) та 95,93% (на вигин), тоді як моделі ML, зокрема XGBoost у поєднанні з байєсівською оптимізацією, досягли чудової точності прогнозування з нульовою середньою похибкою. Обидва методи зійшлися на одних і тих же оптимальних параметрах: шестигранне заповнення, щільність заповнення 60% і температура сопла 265 °C, що підкреслює стабільність і надійність інтегрованого підходу. Результати демонструють, що поєднання традиційних статистичних методів із передовим машинним навчанням пропонує потужний шлях для точного управління процесами та механічної оптимізації в адитивному виробництві полімерних композитів.*

Ключові слова: *адитивне виробництво; онікс, армований вуглецевим волокном; моделювання плавленим осадженням; машинне навчання; механічна оптимізація; методологія поверхні реагування; XGBoost.*