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Sensitivity and Principal Component Analysis-Driven Bayesian Optimization of Process Parameters for Enhancement of Mechanical Strengths in 3D-Printed Biocomposites

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Abstract

This paper presents an in-depth investigation into the effects of process parameters affecting various mechanical properties of the 3D-printed biocomposite produced through the material extrusion (MEX) process. The biocomposite material under investigation is specially prepared polylactic acid reinforced with biochar. The process parameters such as biochar content (BC), raster angle (RA), infill pattern (IP), layer thickness (LT), and infill density (ID) are systematically varied. Test samples were prepared using MEX for tensile, flexural, and impact properties. The dataset gathered from the experimentation was used for analysis and optimization. Sensitivity analysis using SCILib revealed that the most tensile and flexural strength are highly sensitive to the ID and impact strength is sensitive to % of biochar added in the biocomposite. Principal component analysis was employed to reduce the complexity of the output features. A Bayesian approach was used for the optimization of the resultant principal strength component and further, the optimal MEX process parameters were extracted. The optimization results show that 2% BC, 0.25 mm LT, 0° RA, 99% ID, and octet IP are the optimum process parameters for obtaining the best possible mechanical strength of MEX printed biocomposite.

Categories: Advanced Manufacturing Technologies, Advanced Materials, Data Science and Analytics for Engineering
Keywords: 3d-printing, sensitivity analysis, principal component analysis, bayesian optimization, material extrusion

Introduction

3D printing has revolutionized the way of designing and manufacturing products. Among all the techniques of 3D printing, material extrusion (MEX), also known as fused deposition modeling (FDM), is a commonly used method due to its operational simplicity, versatility, and cost effectiveness [1]. Initially, the use of MEX was restricted to prototyping, but in recent years, technology is being used to produce functional parts in automotive, aerospace, biomedical, and consumer products [2]. Traditionally, acrylonitrile butadiene styrene (ABS) and polylactic acid (PLA) materials are popularly used for MEX [3]. However, the requirement in the case of mechanical properties, MEX, has some limitations. Researchers are exploring the use of various materials as well as optimization of the control parameters to enhance the mechanical performance [4].

Buican et al., fabricated the composite structure reinforced by carbon fiber and glass fiber using FDM and showed considerable improvement in the flexural rigidity of the material [5]. However, the use of synthetic fiber has adverse effects on the environment, so there is a need to explore the use of natural fibers. Shahar et al., examined the effect of adding kenaf fiber to PLA on the impact properties of a 3D-printed composite. The study shows the resistance to impact decreased with an increase in the amount of kenaf particles [6]. The tensile strength (TS) of the composite manufactured through the MEX for composite reinforced by *Hedysarum coronarium* increased from 18 MPa to 33 MPa [7]. Natarajan et al. developed a PLA-based biocomposite reinforced with *Acacia concinna* fiber and tested 3D-printed specimen for various mechanical properties. The maximum tensile, flexural, and impact strengths observed were 33 MPa, 46 MPa, and 16 kJ/m^2, respectively [8]. Osman and Atia developed a novel ABS/rice-straw filament for MEX process, and mechanical testing showed decrease in the TS of 3D-printed composite specimens [9]. Mechanical performance not only depends on the material characteristics but also on the process parameters of the 3D printing methods.

Kam et al. employed Taguchi techniques to understand the influence of the 3D printing process parameters on TS, and the result shows that layer thickness (LT) was the most critical parameter [10]. Kumar et al. found using Analysis of Variance that the effect of raster angle (RA) was dominating the flexural strength (FS) of ABS/Carbon fiber composites [11]. Murali et al. observed that increasing infill density (ID) led to a substantial increase in compressive strength (CS). While different infill patterns had a negligible effect on the CS [12]. The partial dependence plot technique was used by Kharate et al. to analyze the impact of critical printing parameters on various mechanical strengths [13]. Understanding the influences of process parameters and optimizing them to achieve desired mechanical characteristics is crucial.

Response surface methodology (RSM) was used for optimizing the printing parameters for ABS by Mushtaq et al., and the study identified optimal values of LT of 0.27 mm and printing speed of 51 mm/sec to achieve maximum ultimate tensile strength (UTS) and FS [14]. Gotkhindikar et al. proposed a deep neural network strategy for predicting suitable parameters of the 3D printing process to enhance CS and TS [15]. Murali et al. implemented a hybrid RSM and genetic algorithm to optimize FDM 3D printing parameters to minimize surface roughness [16]. Gray relational analysis was employed by Kumar and Singh for optimization of FDM process, and the result showed that a 45° deposition angle led to enhanced TS [17].

Although lots of work has been done to explore the effects of MEX process parameters on the mechanical properties of traditional materials, the systematic optimization of such parameters for biocomposites remains a research gap. This study uniquely utilizes sensitivity analysis to evaluate the influence of process parameters, including LT, ID, RA, IP, and biochar content (BC) on tensile (TS), flexural (FS), and impact (IS) strengths, providing a comprehensive understanding of their influence. As per the authors' knowledge, a principal component analysis (PCA)-driven Gaussian process-based Bayesian (GPB) optimization approach is used for the optimization of MEX process parameters. This methodology represents a novel and systematic approach, enabling comprehensive analysis and optimization of MEX process parameters for biocomposites.

Materials And Methods

Experimental data collection

Biochar-PLA filaments were developed by adding rice husk-based biochar to PLA in various percentages, namely (0%, 1%, 3%, and 5%) [4]. The printing parameters selected for investigation were LT, RA, ID, and IP. Refer Figure *1* for the variation in each of the process parameters. A Taguchi orthogonal array has been selected in order to design 16 experiments of these parameters and a certain concentration of biochar [4]. The additive manufacturing process selected for the printing test specimen was MEX, and the machine used was Smart Maker Dual Z200. Samples were fabricated for each experiment at three replication levels for reliability in achieving the exact mechanical behavior, and results were measured from their specimens considering the ASTM standards for mechanical analysis [4]. Process parameters along with results of UTS, FS, and IS of each sample were carefully recorded in Excel.

Process Parameter	FDM Settings
Infill Pattern (IP)	cubic, triangle, octet, and line
Infill Density (ID)	40%, 60%, 80% and 100%
Raster Angle (RA)	0°, 30°, 45° and 90°
Layer Thickness (LT)	0.1 mm, 0.2 mm, 0.3 mm and 0.4 mm

FIGURE 1: MEX process control variables and their operational ranges

MEX, material extrusion

Sensitivity analysis

The sensitivity analysis was performed to determine the impact of the input parameters on the output parameters. This analysis helped to identify the most influential parameter affecting the particular mechanical strength. The dataset in the Excel form was imported into Google Collaboratory, which is a cloud-based Python platform. A variance-based sensitivity analysis technique known as Sobol method from the "SALib" library was used in the study. Using Sobol, two key metrics, namely first-order (S1) and total-order sensitivity index (ST) were calculated. S1 quantifies the direct effect, and ST captures the direct as well as interaction effect of the input parameters on the strength. Higher values of S1 and ST indicate a more significant influence. Figure 2 presents the algorithm for sensitivity analysis using "SALib".

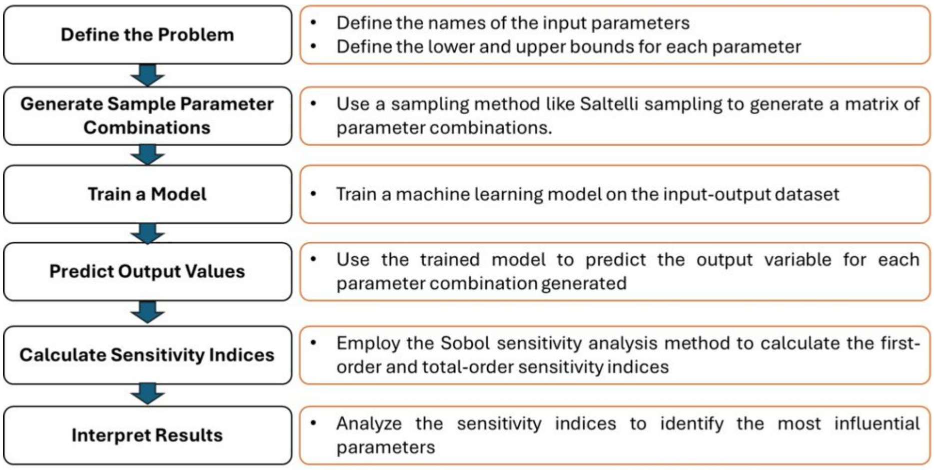

FIGURE 2: Sobol-based sensitivity analysis framework

Principal component analysis (PCA)

PCA is a dimensionality reduction approach used to transform data from its high-dimensional form to low-dimensional form retaining data's variability. PCA was utilized to reduce attributes to the single mechanical strength of the 3D-printed biocomposite from three different strengths namely UTS, FS and IS. Figure 3 shows the steps for PCA implemented in this research study. Initially, the UTS, FS, and IS values were extracted from the dataset. These values were standardized using the "StandardScaler" method in Python's "scikit-learn" library. A PCA model from "sklearn.decomposition" was then applied to the standardized data, configured to reduce the data dimensionality to one principal component. This step yielded the resultant principal strength (RPS), which captured the maximum variance across the three original mechanical strength parameters. The efficacy of RPS was validated by creating a separate PCA instance with three principal components for each mechanical strength.

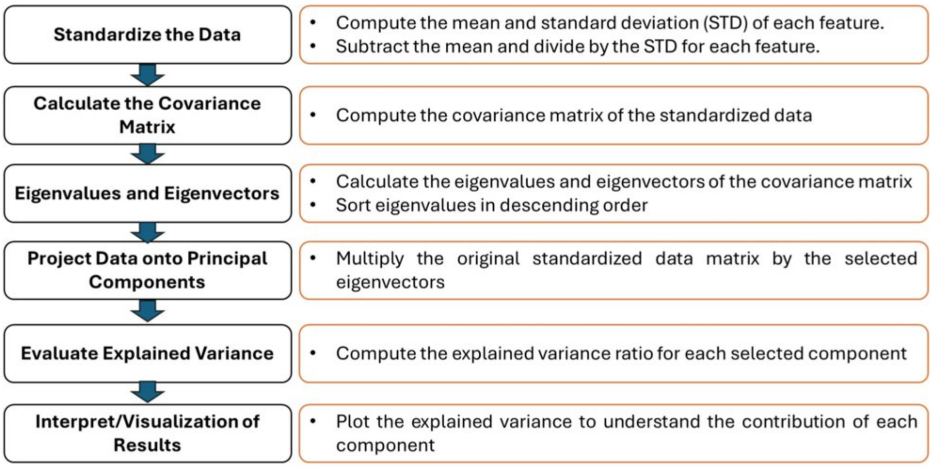

FIGURE 3: Step-by-step algorithm for principal component analysis (PCA)

Gaussian process-based Bayesian (GPB) optimization

The dataset contains number of input features and has highly non-linear interactions with output features. The GPB optimization approach was chosen because it is highly efficient for optimizing functions that are expensive, lack an explicit analytical form, and are complex in nature, such as the objective function of this research study. GPB optimization is an iterative optimizing algorithm that can look into a probabilistic model to efficiently explore the parameter space with proper exploitation and exploration to find the global optima of complex functions.

A systematic optimization methodology was applied to maximize mechanical strength by fine-tuning process parameters for a BC/PLA biocomposite material, and this methodology is presented in Figure *4*. The input parameters (BC, LT, RA, IP, and ID) along with corresponding values of RPS from PCA were taken for the optimization process. An eXtreme Gradient Boosting (XGBoost) regression model was then trained on the process parameters to predict this RPS. The objective function was defined to maximize RPS by minimizing its negative value in the GPB optimization approach. Optimization yielded a set of optimal parameters, which were further validated by transforming RPS back into its natural mechanical components: UTS, FS, and IS through inverse PCA and scaling. This allowed for the interpretation of each strength metric at the optimal conditions. This led to identifying optimal parameter settings that improve material performance with a clear, data-driven framework.

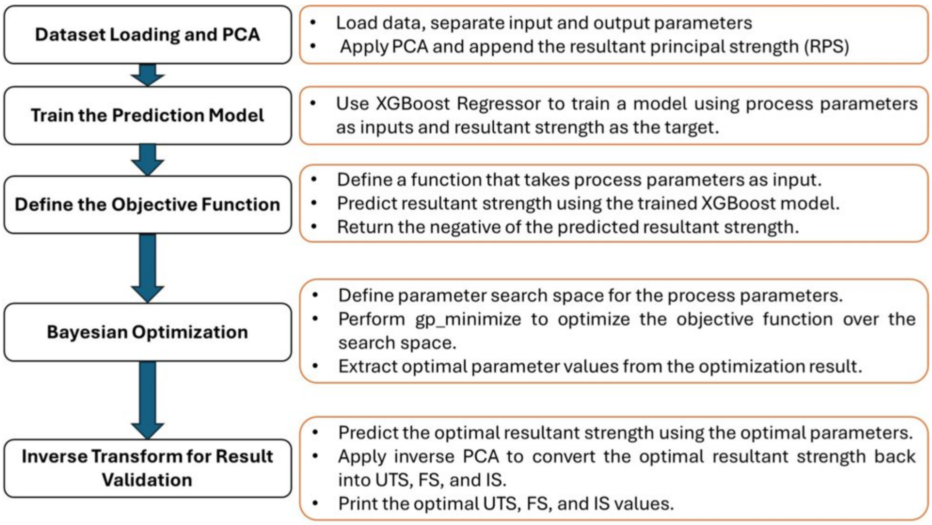

FIGURE 4: Algorithmic framework for optimizing mechanical strength via Gaussian process-based Bayesian optimization

PCA, principal component analysis; UTS, ultimate tensile strength; FS, flexural strength; IS, impact strength

Results

Experimental mechanical strength

Experimental test results were carried out for 16 different runs as per the design of experiments, with each run consisting of three tested samples, resulting in a total of 48 samples [4]. Figure *5* presents the test results of only the first 10 samples for illustrative purposes. The strengths in tension (UTS), bending (FS), and impact (IS) of MEX-produced biocomposite material are measured experimentally [4]. The results indicate that the maximum UTS obtained is 36.95 MPa for 5% biochar composition [4].

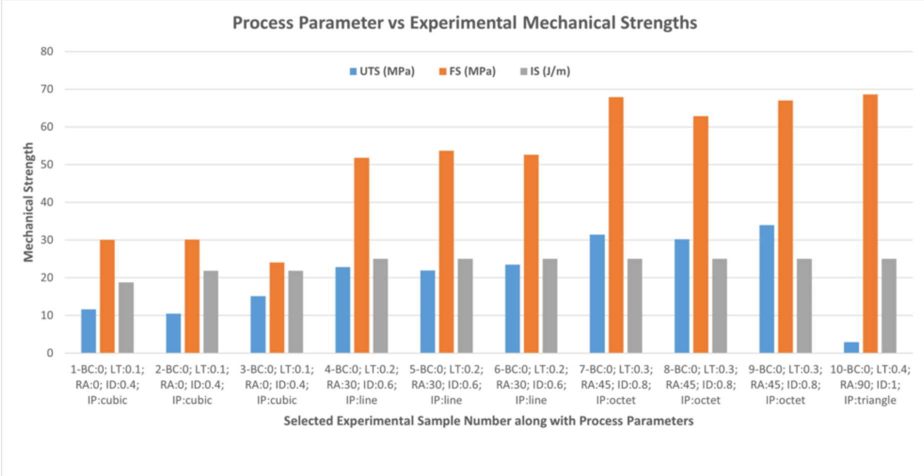

FIGURE 5: Measured mechanical properties of biocomposite materials produced via MEX for representative test specimens

MEX, material extrusion; UTS, ultimate tensile strength; FS, flexural strength; IS, impact strength; BC, biochar content; LT, layer thickness; RA, raster angle; ID, infill density; IP, infill pattern

Sensitivity analysis

The results of sensitivity analysis using Sobol show a similar trend for S1 and ST values. Figure 6 presents the ST values obtained for each input parameter from the analysis corresponding to the mechanical strengths, i.e., UTS, FS, and IS.

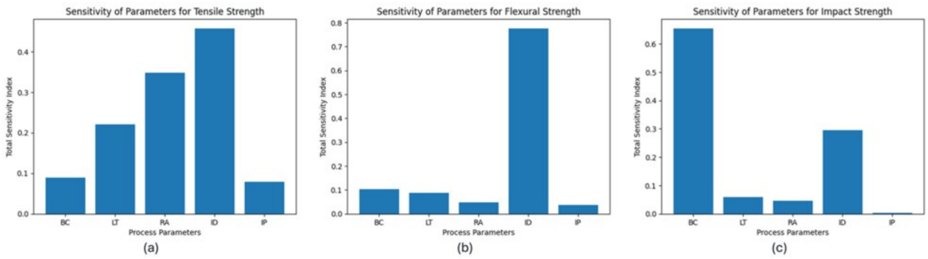

FIGURE 6: Process parameter's total sensitivity indices for (a) UTS, (b) FS, and (c) IS.

UTS, ultimate tensile strength; FS, flexural strength; IS, impact strength

Gaussian process-based Bayesian optimization driven by PCA

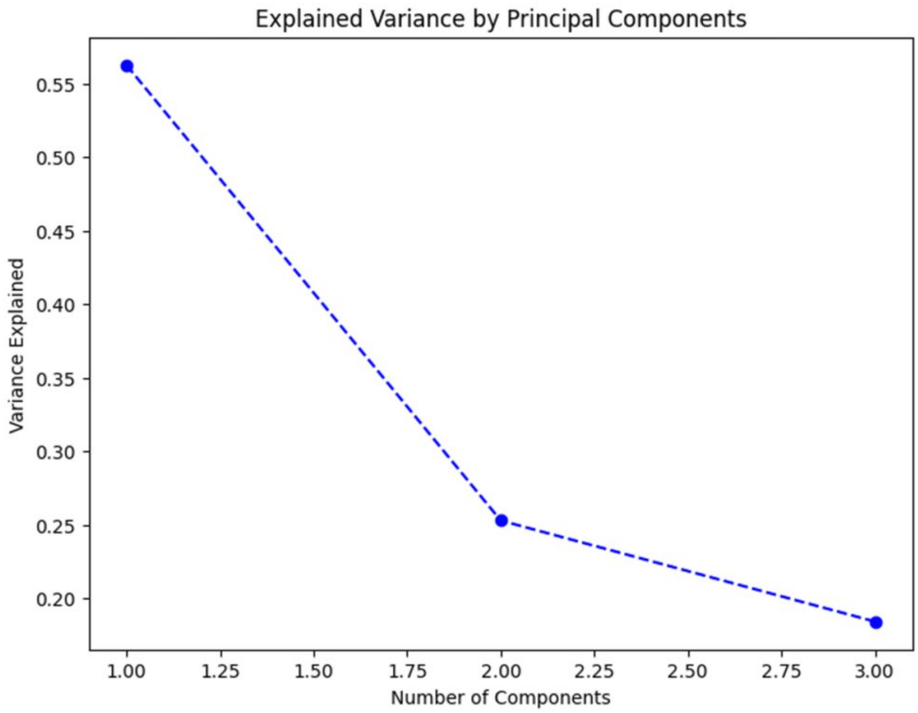

FIGURE 7: Explained variance by principal components

The PCA conducted on the mechanical strength data, i.e., UTS, F,S and IS, resulted in the formation of single composite indexes termed RPS. RPS consolidates the variation in these three mechanical strengths. Figure 7 provides an explanation of the variance captured by the RPS component. It reveals that UTS has the strongest impact on the RPS with a variance of 56.3%, followed by FS (25.3%) and IS (18.4%). The GPB optimization driven by the PCA successfully identified the optimal process parameters well suited for enhancing the total mechanical strength of biochar/PLA biocomposite. Table 1 presents a summary of the results of GPB optimization, including optimum values of the process parameters and maximum RPS.

Optimization Results	Value
Optimal Parameters	
Biochar Content (BC)	2%
Layer Thickness (LT)	0.256 mm
Raster Angle (RA)	0°
Infill Density (ID)	99.17%
Infill Pattern (IP)	octet
Optimization Outcome	
Maximum Resultant Strength	1.7205
Predicted Optimum Mechanical Strengths	
Ultimate Tensile Strength (UTS)	30.96 MPa
Flexural Strength (FS)	64.28 MPa
Impact Strength (IS)	30.20 J/m
Optimization Details	
Total Iterations	50
Time Taken for Final Iteration	1.8042 sec

TABLE 1: Summary of results of GPB optimization driven by PCA

GPB, Gaussian process-based Bayesian; PCA, principal component analysis

Discussion

The addition of BC negatively affected FS and enhanced IS. It is foremost essential to understand the influence of process parameters on the three mechanical strengths. From sensitivity analysis, it is observed that for UTS, ID is the most influential parameter, as it has the highest ST value of 0.4573 (refer Figure *6a*). In the case of FS, again, the ID is the most dominant parameter, as it has the maximum ST value, and it has also been observed that the remaining parameters have negligible effect (refer Figure *6b*). Higher values of ID result in a larger material volume, enhancing the structural integrity and, consequently, improving both TS and FS. Unlike UTS and FS, BC has the highest effect on the impact properties, i.e., IS (refer Figure *6c*). The addition of biochar to the PLA material provided better reinforcement, which may have resulted in better cushioning during impact. This result indicates that to increase the impact properties of the 3D-printed materials, one can consider adding reinforcing fillers or fibers to the virgin materials. The results from sensitivity analysis reveal that there is a negligible effect of IP on all types of mechanical strengths.

The results of PCA indicate that for representing the whole mechanical strength, the most important property is UTS. By using PCA, complex and multi-dimensional mechanical data is reduced to simple yet comprehensive and single-dimensional data. These RPS values enabled more streamlined optimization by providing a single objective measure of the mechanical strength for tuning the process parameters. Bayesian optimization enabled systematic examination of parameter space: the sequences of every step fine-tuned the increase in values of the parameters to converge on a global optimum. After 50 iterations, optimization indicated a maximum Resultant Strength value of 1.7205. Using inverse PCA transformation, the result of the maximum RPS value was translated back to the UTS, FS and IS and these values are also presented in the same table (refer Table *1*). The optimum predicted values for UTS, FS, and IS are 30.96 MPa, 64.28 MPa, and 30.20 J/m, respectively. These values are considerably higher, suggesting that the optimal process parameters found the equilibrium condition along with the enhancement of individual mechanical strengths. This approach illustrates the capability of employing PCA-guided Bayesian optimization for the tuning of process parameters aimed at achieving multi-objective improvements in material strength.

Conclusions

This study demonstrated a systematic approach to enhance the overall mechanical strength of MEX-produced biocomposites by integrating PCA with GPB optimization. Sensitivity analysis revealed that the most influential parameter is ID for UTS and FS, while BC significantly influenced IS. PCA identified UTS as the primary contributor to overall mechanical strength. PCA produced a composite index termed RPS, simplifying multi-dimensional mechanical data into a single objective function. GPB optimization predicted mechanical strengths of 30.96 MPa for UTS, 64.28 MPa for FS, and 30.20 J/m for IS, each indicating considerable improvements. The optimization results indicate that the optimal process parameters for maximizing the mechanical strength of MEX-printed biocomposites are 2% BC, an LT of 0.25 mm, RA of 0°, ID of 99%, and an octet IP. Many improvements are reported, but this study is not without its limitations. Although the experimental dataset was comprehensive, the process conditions were constrained to a certain range that can limit generalizability. The study was confined to only biochar-PLA composites. Different composite materials or additives may have different results.

Additional Information

Author Contributions

All authors have reviewed the final version to be published and agreed to be accountable for all aspects of the work.

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Critical review of the manuscript for important intellectual content: Prashant Anerao, Atul Kulkarni, Yashwant Munde, Namrata N. Wasatkar

Supervision: Atul Kulkarni

Disclosures

Human subjects: All authors have confirmed that this study did not involve human participants or tissue. **Animal subjects:** All authors have confirmed that this study did not involve animal subjects or tissue. **Conflicts of interest:** In compliance with the ICMJE uniform disclosure form, all authors declare the following: **Payment/services info:** All authors have declared that no financial support was received from any organization for the submitted work. **Financial relationships:** All authors have declared that they have no financial relationships at present or within the previous three years with any organizations that might have an interest in the submitted work. **Other relationships:** All authors have declared that there are no other relationships or activities that could appear to have influenced the submitted work.

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