



Predicting and Improving the Mechanical Strength of a Modified Natural Fiber/TiO₂ Polymer Nanocomposite Using Artificial Intelligence

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ABSTRACT

Artificial Intelligence (AI) including methods such as artificial neural networks (ANN) and machine learning has been employed to address numerous technical challenges. This study employed titanium dioxide (TiO₂) and natural fibers derived from *Paederia foetida* (PF) to fabricate a high-performance hybrid nanocomposite reinforced for structural functions. A chemical mixture of KMnO₄ in acetone was utilized to modify the fibers, enhancing the internal properties and improving bonding with the PF/polymer matrix. To enhance the tensile strength (TS) and flexural strength (FS) of the synthesized PF/TiO₂ hybrid nanocomposite (PFMNC), an ANN model featuring hyper-parameter enhancement within a linear neural network of 3-5-1 was employed, incorporating 5 neurons in the internal layer, with the application of Box-Behnken Design (BBD). Scanning electron microscopic images indicate that KMnO₄ alteration influenced the mechanical strength of the composite. The mechanical assessment findings indicate that variables influenced the tensile strength (TS) and flexural strength (FS) of PFMNC, as demonstrated by the analysis of variance $R^2 = 0.9525$ and $R^2 = 0.9526$, respectively. The anticipated outcomes closely resembled the experimental results. The model forecasted an ideal TS of 47.5613 MPa and FS of 38.12 MPa. To validate the empirical experimental research, TS and FS analyses were conducted at the projected optimal settings. The TS data indicated an average strength of 40.67 MPa, while the FS exhibited an average value of 52.98 MPa. This work has shown that the ANN-BBD modeling technique effectively attains suitable mechanical property values rapidly, reduce production costs, and conserves resources.

Keywords: Artificial intelligence; Machine learning; Titanium dioxide; Natural fibers; Mechanical properties.

1. INTRODUCTION

The construction and industrial sectors have made natural fibre polymer composite (NFPCs) to meet a wide range of technical demands. *Desmostachya bipinnata* fibers in raw, 10% NaOH-treated, and 0.5% KMnO₄-treated forms were investigated for their reinforcement potential. Alkali treatment reduced fiber diameter, increased aspect ratio, and enhanced tensile strength while lowering density, while alkali-treated fibers also exhibited the highest crystallinity index and activation energy, confirming superior performance (Gnanaraj *et al.* 2024). *Abutilon indicum* fiber was extracted and chemically treated with varying concentrations of NaOH and KMnO₄ to evaluate its suitability for cement composites. The optimum treatment with 1% NaOH enhanced tensile properties, increased cellulose content (73.59%), reduced hemicellulose and wax, and improved crystallinity index

(74→77%) and thermal stability (335→347 °C) (Aarthipriya and Umarani, 2025). Epoxy composites reinforced with alkali-treated natural nanofibers and TiO₂. *Paederia foetida* fibres treated with NaOH and KOH showed reduced diameter and increased crystallinity (Gunasekar *et al.* 2024). Hybrid epoxy composites reinforced with *Paederia foetida* fibers (PFs) and carbon powder (CP) were fabricated in varying ratios by hot pressing to assess mechanical, thermal, and microstructural properties. The 20% PFs–10% CP composite (CDS20) showed the highest tensile strength (42.3 ± 2.7 MPa), modulus (2310.8 ± 91 MPa), and good thermal resistance (23.8% residue). (Sari *et al.* 2025). Jute–abaca hybrid laminates fabricated by hot-pressing showed that the 0/0/0/0/0 orientation delivered the best tensile, flexural, impact, and ILSS (3.35 MPa) performance. ANN predictions ($R^2 = 1.0, 0.98, 0.99$) and SEM confirmed strong fiber–matrix bonding (Ramesh *et al.* 2024). TiO₂-coated flax fibers in epoxy composites

enhanced tensile and flexural by strength 22% and 16%, respectively. Water diffusion dropped by 42% with 0.6 wt% TiO₂ due to silane-assisted nanoparticle grafting (Prasad *et al.* 2021). Fiber/ TiO₂-reinforced epoxy composites improved compressive (90 MPa) and hardness (45 HV) properties. Kulkual fiber-reinforced epoxy composites with TiB₂ particles were fabricated via open-mold casting to evaluate compression, hardness, and water absorption properties. The 5 vol% fiber composite achieved the best performance with 90 MPa strength, 87 MPa modulus, and 45 HV hardness, while higher fiber content mainly increased water uptake. (Shahapurkar *et al.* 2025). Coir pith nanocomposites with nano-silica and nanoclay (up to 4.5 wt%) enhanced tensile and thermal stability. A combination of 4.5 wt% NS and 3 wt% NC yielded the best mechanical and water resistance results. The SEM analysis confirmed improved interfacial bonding (Matheswaran *et al.* 2023).

Areca catechu L. peduncle fibers treated with alkali showed a 12.9% improvement in tensile strength and a 14.2% increase in crystallinity, with SEM/AFM revealing rougher surfaces that enhanced interfacial bonding for sustainable composite development. (Mansingh *et al.* 2024). Tamarind seed filler-sugarcane fiber composites demonstrated notable improvements in flexural and compressive strength, with the highest performance achieved at controlled filler-to-fiber ratios (Girimurugan *et al.* 2022a). Pineapple leaf fiber-based laminates showed enhanced tensile, flexural, ILSS, and fracture toughness, where an optimal stacking sequence reached 70.8 MPa tensile strength and 16.1 MPa ILSS (Gaddala *et al.* 2025). Bamboo-madar fiber composites optimized using machine learning and genetic algorithms exhibited strong predictive accuracy with high R² values, confirming their potential for lightweight automotive applications (Gupta *et al.* 2024). Luffa fiber/epoxy nanocomposites incorporated with TiO₂ nanoparticles achieved a 137% increase in dry tensile strength, only 2% water absorption, and 95% retention of wet tensile strength, with FESEM confirming structural improvements (Anbukarasi *et al.* 2025).

Paederia foetida/polyester biocomposites (2.5–25 vol.%) retained thermal stability (up to 800 °C) after 72–168 h of water immersion. Mechanical properties declined due to moisture uptake, but density and swelling increased. The composite remained viable for construction use, balancing strength and environmental durability (Sari *et al.* 2024a). Hybrid epoxy composites with PF and alumina powder (0–40%) were tested for strength, water absorption, and thermal stability. The best performance was from the SFD (30% PF + 10% Al₂O₃) with 49.1 MPa tensile strength and low swelling (<5%). Scanning electron microscopic studies showed fiber pull-outs and optimal bonding, indicating suitability for structural applications (Sari *et al.* 2024b). Pineapple leaf fiber (PALF)/High density polyethylene (HDPE)/polyethylene-grafted-maleic anhydride (MAPE) bio-

composites were optimized using Box-Behnken Design and ANOVA, targeting tensile, flexural, and impact strengths. Optimum performance was achieved at 13.67 mm fiber length, 16.84 wt.% PALF, and 2.95 wt.% MAPE, with TS of 32.35 MPa. Validation confirmed the accuracy of Response Surface Model (RSM) for predictive modeling and optimization (Mittal and Phutela, 2023). Banana fiber/vinyl ester composites were optimized by RSM-BBD using fiber content, length, and curing time as inputs. Maximum tensile strength and Young's modulus reached 85.64 MPa and 73.406 GPa, respectively. Response Surface Model coupled with desirability analysis effectively predicted improvements over base vinyl ester matrix (up to 276%) (Esonye *et al.* 2022). Sisal fiber-reinforced geopolymer composites were evaluated using BBD-RSM for compressive and split tensile strength. Best compressive (21.5 MPa) and tensile strength (4.6 MPa) occurred at fiber length of 20–35 mm, 5–15% of fiber content, and 8–12 M of alkali concentration. Results demonstrated that these composites are lightweight, eco-friendly cement alternatives (Debena *et al.* 2025).

Cellulose microfibrils from banana fibers were incorporated into epoxy composites and optimized by RSM-BBD. At 18.32% NaOH, 250 µm fiber diameter, and 4.05% volume fraction, TS and modulus reached 41.78 MPa and 10.38 GPa (Pragasam and Reddy, 2020). The ANN and fuzzy logic models predicted and optimized mechanical properties of 3D-printed PLA/wood composites. Raster angle and print speed had the highest influence, with ANN. Errors were below 2%, validating ML-driven parameter optimization in Fused Deposition Modeling (FDM) of natural fiber composites (Ulkir *et al.* 2025).

Banana fiber/nano-SiO₂ hybrid composites were optimized for mechanical properties using a combined Taguchi-ANN approach. Process parameters included nano-SiO₂ wt%, banana fiber wt%, compression pressure, and molding temperature, with an L16 orthogonal array guiding optimization. The composites achieved 47.36 MPa tensile, 64.48 MPa flexural, and 35.33 kJ impact strength under 5% SiO₂, 19 MPa, and 110 °C, while ANN predictions reached 95% accuracy, outperforming regression models (Natrayan *et al.* 2023). Jute/flax hybrid composites were reinforced with tungsten carbide (WC) and zinc oxide (ZnO) fillers to study mechanical and wear performance. WC enhanced tensile strength more effectively, with 1% WC and 1.5% ZnO improving strength by 41% and 24%, respectively, while impact resistance rose to 10.3 J/m² in WC-filled composites. Wear tests showed lower COF and reduced matrix damage, and ANN predictions closely matched experimental values, confirming reliable modeling (Demir, 2025). Mechanical performance of Poly (lactic acid)-wood composites fabricated by FDM was predicted using ANN and gene expression programming (GEP), which outperformed ANN with minimal

validation errors (0.04–0.82%). Raster angle was the most significant factor affecting strength, confirmed by ANOVA (Bhowmik *et al.* 2025). Jute/kenaf/glass fiber hybrid composites with Al_2O_3 nanoparticles were optimized for tensile and impact strength using RSM and ANN. Fiber orientation (90°), sequence (3 layers), and 5% Al_2O_3 yielded the best properties, with ANN predictions surpassing RSM in accuracy (Arunachalam *et al.* 2025). Polyethylene composites reinforced with pineapple fiber and potato waste filler were fabricated via compression molding for biomedical applications (Girimurugan, *et al.* 2022b). Taguchi–GRA, TOPSIS, and ANN optimization identified the best configuration as 3% NaOH treatment, 3 wt% filler, and 30 wt% fiber, achieving tensile strength of 22.3 MPa, flexural strength of 23.8 MPa, and impact strength of 18.3 kJ/m² (Ramakrishnan *et al.* 2024).

The tensile strength of a fiber-reinforced hybrid nanocomposite is influenced by various parameters, including fiber volume content and fiber-matrix bonding. Another further crucial factor for augmenting the maximum reactivity of composite is experimental design. In the present work, PF/TiO₂ hybrid nanocomposite treated with KMnO_4 were fabricated. The influence of KMnO_4 - TiO₂ volume concentration, treatment duration, and fiber weight content, together with their relationships to the tensile strength of the generated PFMNC, was evaluated using an analytical framework with precise parameter-based optimization by ANN-BBD. The measured data were connected within the collected outcomes to evaluate precision and determine potential differences.

2. MATERIALS AND METHODOLOGY

2.1 Materials and Preparation of PF/TiO₂ Hybrid Nanocomposite Samples

TiO₂, acetone, and KMnO_4 were procured from Matrics Enterprises, Nagercoil, India and used without additional treatment. Hardener and epoxy were procured from Kovai Seenu Enterprises, Coimbatore, Tamil Nadu, India. *Paederia foetida* fiber was harvested from the stems of *Paederia foetida* using a retting process. The collected PF fiber was maintained in 0.05% KMnO_4 in a $\text{C}_3\text{H}_6\text{O}$ solution. Subsequently, the mixture was filtered and thoroughly cleaned with acetone to eliminate any remaining solution. The treated PF fiber was maintained for durations of 1 min, 3 mins, and 5 mins. Then, the PF fiber was subjected to oven drying at $75 \pm 5^\circ\text{C}$ until a stable weight was achieved. After dispersing TiO₂ in 100% ethanol, the mixture was treated to 20 minutes of ultrasonic sonication at 40 kHz using an EINS SCI professional ultrasonic cleaner. The epoxy resin and hardener were mixed with TiO₂-ethanol dispersion. Afterwards, it underwent another 30 minutes of ultrasonic treatment. The solvent was gradually evaporated from the resin/TiO₂ mixture by heating it, and

then it was vacuum degassed for one hour. After evenly applying the resin/ TiO₂ mixture onto the PF in the mold, it was compressed and rolled to remove any air bubbles. The fabricated sample underwent compression molding to remove excess matrix material and thereafter allowed to cure for 1 day at ambient temperature. A TiO₂ volume content of 0%, 1%, and 2%, along with *Paederia foetida* concentration of 10%, 20%, and 30%, was utilized to fabricate a PF/TiO₂ hybrid nanocomposite

2.2 Characteristics of Fibers and the Composites

The surface morphology of PF and PF/TiO₂ hybrid nanocomposite samples was studied using a scanning electron microscope (ZEISS, GEMINI) in secondary electron imaging (SEI) and high vacuum mode. The accelerating voltages used were 20.0 KV for composite surfaces and 30 KV for fibers. During sample preparation, specimens were initially sized appropriately and affixed to a double-sided carbon tape on the specimen base, followed by sputter coating with carbon for two cycles prior to introduction into the scanning electron microscopy chamber for vacuum evaluation. Tensile strength measurements were conducted in accordance with ASTM Test Procedure D638 utilizing an Instron (Model 3369) testing machine at a crosshead speed of 2 mm/min, employing a dumbbell-shaped specimen at ambient temperature (28°C). Each sample was placed into the Instron universal testing machine and subjected to the load. The published data were based on the mean results of five effective analyses performed on each specimen after tensile testing. Flexural properties were assessed following ASTM D790-17 using the three-point bending setup of the universal testing machine (UTM) is shown in Fig. 1. The specimens used for this test measured $125 \times 12.7 \times 3.2$ mm. Each specimen was subjected to a load until fracture, at a constant crosshead speed of 2 mm/min. This evaluation provided insights into the bending strength and stiffness of the composite samples under flexural stress.

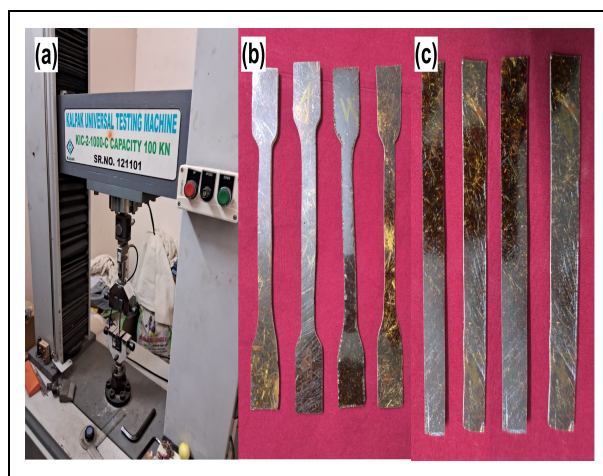


Fig. 1: (a) Universal testing machine (b) tensile test specimens and (c) flexural test specimens

2.3 Experimental BBD

The Box-Behnken Design in Design-Expert 13 edition was used in the work. A Central composite design (CCD) structure with three separate stages was chosen, comprising three factors within the three levels: low(1), middle(0), and high(+1) of the KMnO_4 treatment duration (minutes), TiO_2 volume concentration (%) and PF weight content (wt%). This research encompassed 20 experiments runs. An analytical study of the procedure was conducted to examine significant factors parts using multiple regression analysis (MRA) and analysis of variance as shown in Table 1.

2.4 Building Models for ANN

To represent the link between the predictors and the response variable, a perceptron was refined. As seen in Fig. 2, the model architecture utilized in this study was 3-5-1. This provided the model with three input variables, five neurons for the hidden layer, and two output for the output layer. Using a trial-and-error method, the ideal number of neurons was found. In order to ascertain which

number of neurons in the hidden layer best predicts the tensile strength, a variety of neuron counts were examined. Additionally, the multi-layer perceptron's efficacy was examined. In contrast, the single-layer perceptron model outperformed the multi-layer perceptron model in terms of computational time and mean square error during the model training phase. The gradient descent model that could be trained with an adjustable learning rate used a softmax transfer function as its activation function. This training approach is notable because it can retain a dynamic learning rate while potentially improving the steepest descent algorithm. The goal of the gradient descent with adjustable learning rate approach is to retain a large learning step size while achieving consistent learning. This study showed that ANN with multi-hidden layers best predicted composite performance compared to regression and single-layer models. Using the current learning rate, new weights and biases were produced at each iteration after identifying the initial network outcome and errors. Further calculations were made for errors and the revised network output.

Table 1. The code and actual variable chosen for BBD

Element	Name	Units	Low	High	Minimum	Maximum
A	KMnO_4 treatment time	Mins	- 1 - 1.50	+ 1 - 4.50	1.50	4.50
B	PF content	Wt. %	- 1 - 15.00	+ 1 - 25.00	15	25
C	TiO_2 volume concentration	%	- 1 - 0.00	+ 1 - 4.00	0	4

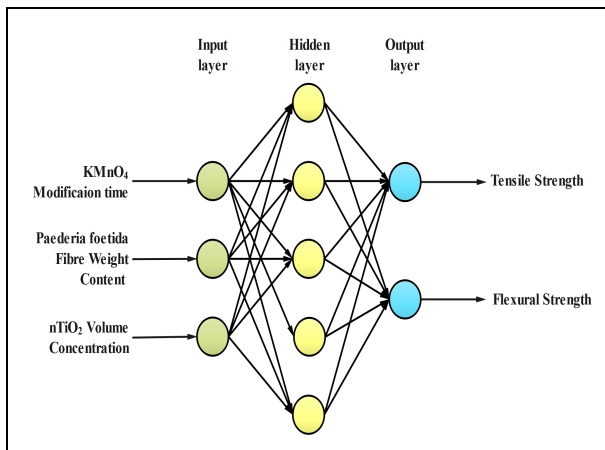


Fig. 2: The training architecture of the proprietary neural network

Eqn. (1) was used to update bias threshold and weights for every training set in the traditional steepest gradient descent algorithm. Artificial Neural Network models can accurately predict the mechanical response of composites based on input parameters such as geometry and surface treatment (Makri *et al.* 2024).

$$\theta_{t+1} \equiv \theta_t + \eta \cdot \nabla_{\theta} E(\theta_t; x^{(i)}; y^{(i)}) \quad \dots (1)$$

where $y(i)$ is the target label, $x(i)$ is the training sample input, θ represents the biases and weights, η represents the learning rate, while E denotes the loss function. Training and testing datasets were created using a 70%:30% split of the experimental dataset. This was done to ensure that the model gets trained using a significant amount of the dataset. An infinite training term was allowed to avoid the model converging at a local minimum due to training time limits. Additionally, a maximum of 1000 epochs were allowed.

2.5 Evaluation of the Model's Efficiency for PFMNC

In addition to the visual evaluation of prediction and projected outcomes, it is crucial to assess the efficiency of ML models to evaluate their efficacy in forecasting the result. A combination of efficiency analysis metrics is frequently advised to mitigate bias. Therefore, this study used well-established analytical performance metrics, such as Root Mean Square Error (RMSE), Mean Absolute Deviation (MAD), Mean

Percentage Error (MPE), Relative Coefficient of Variation (RCV), and relative mean bias error (rMBE). These metrics are computed utilizing equations (2)–(6) (Sheeba *et al.* 2023).

$$RMSE = \sqrt{\frac{\sum_{k=1}^N [y_k - \hat{y}_k]^2}{N}} \quad \dots (2)$$

$$MAD = \frac{1}{N} \sum_{k=1}^N |y_k - \bar{y}| \quad \dots (3)$$

$$MAPE = \frac{1}{N} \sum_{k=1}^N \left| \frac{y_k - \hat{y}_k}{y_k} \right| \times 100\% \quad \dots (4)$$

$$VAF = 1 - \frac{\text{var}(\hat{y}_k - y_k)}{\text{var}(y_k)} \times 100\% \quad \dots (5)$$

$$RCoV = \frac{\text{median} |\hat{y}_k - y_{k_median}|}{y_{k_median}} \quad \dots (6),$$

where y_k is the observed TS, $\hat{y}_k$ is the predicted TS, y_{k_max} and y_{k_min} , and y_{k_median} is the maximum, median, and minimum values of observed data, N denotes number of samples, and $\bar{y}$ is the average of recorded time series.

Table 2. ANN-BBD predicted and experimental TS and FS values

Std	A (mins)	B (wt.%)	C (%)	Actual TS Value	Predicted TS Value		Actual FS Value	Predicted FS Value	
					BBD	ANN		BBD	ANN
1	3	20	4	44.30	43.01	41.10	49.89	48.40	48.99
2	1.5	25	2	45.04	43.95	36.93	50.56	49.43	39.71
3	1.5	25	0	32.14	32.72	31.90	36.51	37.11	35.98
4	3	20	4	43.04	43.01	41.10	48.36	48.40	48.99
5	3	20	4	42.79	43.01	41.10	48.23	48.40	48.99
6	1.5	15	2	39.67	38.05	37.84	44.65	42.88	38.73
7	3	25	4	41.41	41.13	41.53	46.71	46.38	43.34
8	3	20	4	43.43	43.01	41.10	48.79	48.40	48.99
9	4.5	20	4	45.45	44.71	42.31	51.15	50.36	51.76
10	3	20	0	36.37	37.24	35.36	41.03	42.01	38.62
11	4.5	15	2	45.03	44.88	41.32	50.69	50.47	45.89
12	3	20	4	43.80	43.01	41.10	49.20	48.40	48.99
13	1.5	15	0	26.99	27.27	30.64	30.85	31.15	30.10
14	3	15	4	35.37	36.75	40.06	39.93	41.47	46.37
15	3	20	4	42.91	43.01	41.10	48.36	48.40	48.99
16	3	20	2	47.24	47.47	41.13	52.98	53.21	46.85
17	1.5	20	4	39.55	41.40	38.64	44.67	46.67	42.51
18	4.5	25	0	39.04	37.20	37.48	43.96	41.93	42.98
19	4.5	15	0	35.54	35.65	40.23	40.25	40.40	38.00
20	4.5	25	2	44.24	46.87	43.47	49.68	52.57	49.19

3. RESULTS AND DISCUSSION

3.1 Data Evaluation for the Tensile and Flexural Strength

After conducting tensile strength test and developing the Box-Behnken Design, this investigation made use of the Design Expert version 13 application.

$$\text{Tensile Strength} = + 47.47 + 2.435 A + 1.97 B + 2.88 C - 0.976 AB - 0.78 AC + 0.222 BC + 0.0391 A^2 - 4.071 B^2 - 7.343 C^2 \quad \dots (7)$$

$$\text{Flexural Strength} = + 53.205 + 2.68 A + 2.16 B + 3.19 C - 1.10 AB - 0.834 AC + 0.289 BC + 0.111 A^2 - 4.48 B^2 - 7.997 C^2 \quad \dots (8)$$

The variables for the duration of the KMnO_4 modification (A), the percentage of fiber weight (B), and the volumetric concentration of TiO_2 (C) were coded. Using the quadratic equation, the TS forecasts for all of the variables were determined. Table 3 shows the results of the TS ANOVA, while Table 4 shows the results of the FS ANOVA. The study shows the P-value and F-ratio by comparing the average square effect and mean square error. For TS, the pertinent parameters are shown in Table 3, whereas for FS, they are the sum of squares (SS) and mean square (MS), respectively. The Model F-values of 22.26 for tensile strength and 22.32 for flexural strength indicate that the model is significant. Noise could only cause such a large F-value 0.01% of the time. To be considered significant, model terms must have a P-value lower than 0.0500. The terms are not significant if the P-

The dataset, including the variables and the consequent estimated solutions is shown in Table 2. Important terms are A, B, C, AB, AC, BC, A^3 , B^3 , and C^3 , as shown by the second-order polynomial equation that represents the multiple regression analysis of the initial data. The net equation, as shown in equation (7), was generated using a multiple linear regression model, taking into consideration of the components for the coded variable.

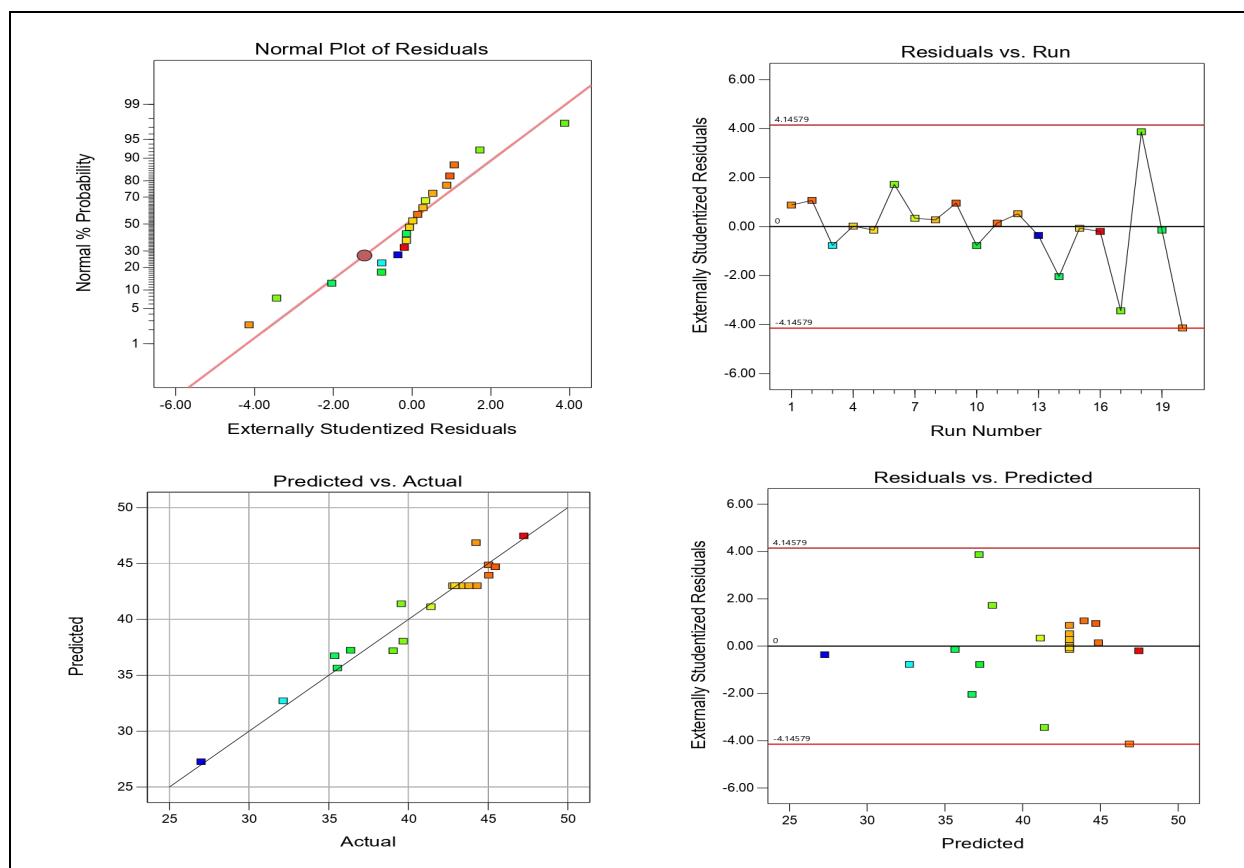
value is greater than 0.1000. Excessive unnecessary terms in model, except those necessary for hierarchy, may be reduced by model minimization. The tensile strength of R^2 at 0.9525 and the corrected R^2 at 0.9097 are significantly aligned, indicating a difference of <0.2 . The ratio over 4 is desirable, evidenced by Adeq Precision's assessment of SNR. The flexural strength of R^2 is 0.9526, and the adjusted R^2 is 0.9099, indicating a substantial agreement, with a discrepancy of <0.2 . A ratio over 4 is desirable, which is confirmed by Adeq Precision's assessment of the SNR. With just a 0.01% chance of noise playing a role, this magnitude of substantial lack-of-fit F-value is quite unlikely to occur. A proper signal is indicated by the TS ratio of 18.5147 and the FS ratio of 18.4530.

Table 3. ANOVA Results for the obtained TS quadratic model

Source	Sum of Squares	df	Average Square	F-value	p-value	
Model	477.04	9	53.00	22.26	< 0.0001	significant
A-KMnO ₄	55.34	1	55.34	23.24	0.0007	
B-Paederia Foetida Fiber	36.27	1	36.27	15.24	0.0029	
C-nTiO ₂	71.81	1	71.81	30.16	0.0003	
AB	7.62	1	7.62	3.20	0.1038	
AC	3.41	1	3.41	1.43	0.2592	
BC	0.2763	1	0.2763	0.1161	0.7404	
A ²	0.0042	1	0.0042	0.0018	0.9673	
B ²	45.57	1	45.57	19.14	0.0014	
C ²	170.68	1	170.68	71.69	< 0.0001	
Residual	23.81	10	2.38			
Lack of Fit	22.10	5	4.42	12.92	0.0069	significant
Pure Error	1.71	5	0.3420			
Cor Total	500.84	19				
Std. Dev.	1.54		R ²	0.9525		
Mean	40.67		Adjusted R ²	0.9097		
C.V. %	3.79		Predicted R ²	0.5449		
			Adeq Precision	18.5147		

Table 4. ANOVA Results for the obtained FS quadratic model

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	574.09	9	63.79	22.32	< 0.0001	significant
A-KMnO ₄	67.14	1	67.14	23.50	0.0007	
B-Paederia Foetida Fiber	43.66	1	43.66	15.28	0.0029	
C-nTiO ₂	88.05	1	88.05	30.81	0.0002	
AB	9.83	1	9.83	3.44	0.0933	
AC	3.90	1	3.90	1.36	0.2699	
BC	0.4686	1	0.4686	0.1640	0.6940	
A ²	0.0344	1	0.0344	0.0120	0.9148	
B ²	55.15	1	55.15	19.30	0.0013	
C ²	202.46	1	202.46	70.85	< 0.0001	
Residual	28.58	10	2.86			
Lack of Fit	26.52	5	5.30	12.87	0.0070	Significant
Pure Error	2.06	5	0.4120			
Cor Total	602.66	19				
Std. Dev.	1.69		R ²	0.9526		
Mean	45.82		Adjusted R ²	0.9099		
C.V. %	3.69		Predicted R ²	0.5463		
			Adeq Precision	18.4530		

**Fig. 3: (a) Normal probability plot against the residual, (b) residual against the run number following the TS response, (c) comparison of expected and actual values and (d) externally studentized versus projected residuals**

3.2 Evaluation of Residual Plots for PFMNC

The connection between the internal residual time series and the conventional probability distribution is shown in Fig. 3. Fig. 3 (a) shows that all of the residual points form curve that is more precisely aligned with the line that approximates the model data, with no abnormalities in the residual outcome. Fig. 3 (b) elucidates the correlation between the tensile strength behavior of the experimental and residual runs. Fig. 3 (c) illustrates actual and projected TS data. The discrepancy among the expected or modified values and the actual measured factors is quantified in points. The uniform dispersion of each scatter point along the axis indicates the strong correlation between the observed and estimated results, as illustrated in Fig. 3(d).

Fig. 4. illustrates the statistical and residual diagnostics related to the prediction of flexural strength utilizing the RF model. Fig. 4 (a) presents a normal probability plot of the residuals, demonstrating that the residual data points closely conform to the reference line, indicating adherence to a normal distribution. This

verifies the model's sufficiency and the lack of significant non-normality or skewness in the flexural strength forecasts. Fig. 4 (b) illustrates the residuals in relation to the experimental FS values. The near-zero centered residual values and their consistent distribution across the FS range signify homoscedasticity, indicating uniform variation in prediction errors. This indicates that the RF model preserves prediction accuracy throughout the entire range of measured flexural strengths. Fig. 4 (c) presents a scatter plot illustrating the correlation between actual experimental values and model-predicted FS values. The data points are clustered along the diagonal line ($y = x$), indicating a robust connection between the observed and anticipated values. The slight divergence from the diagonal validates the precision of the model's FS forecasts. Fig. 4(d) illustrates the graph of residuals versus expected FS values. The uniform distribution of residuals over the forecast range, devoid of any regular structure, confirms the model's impartiality. The uniform distribution corroborates the RF model's dependability in predicting flexural strength and reveals no signs of overfitting or underfitting.

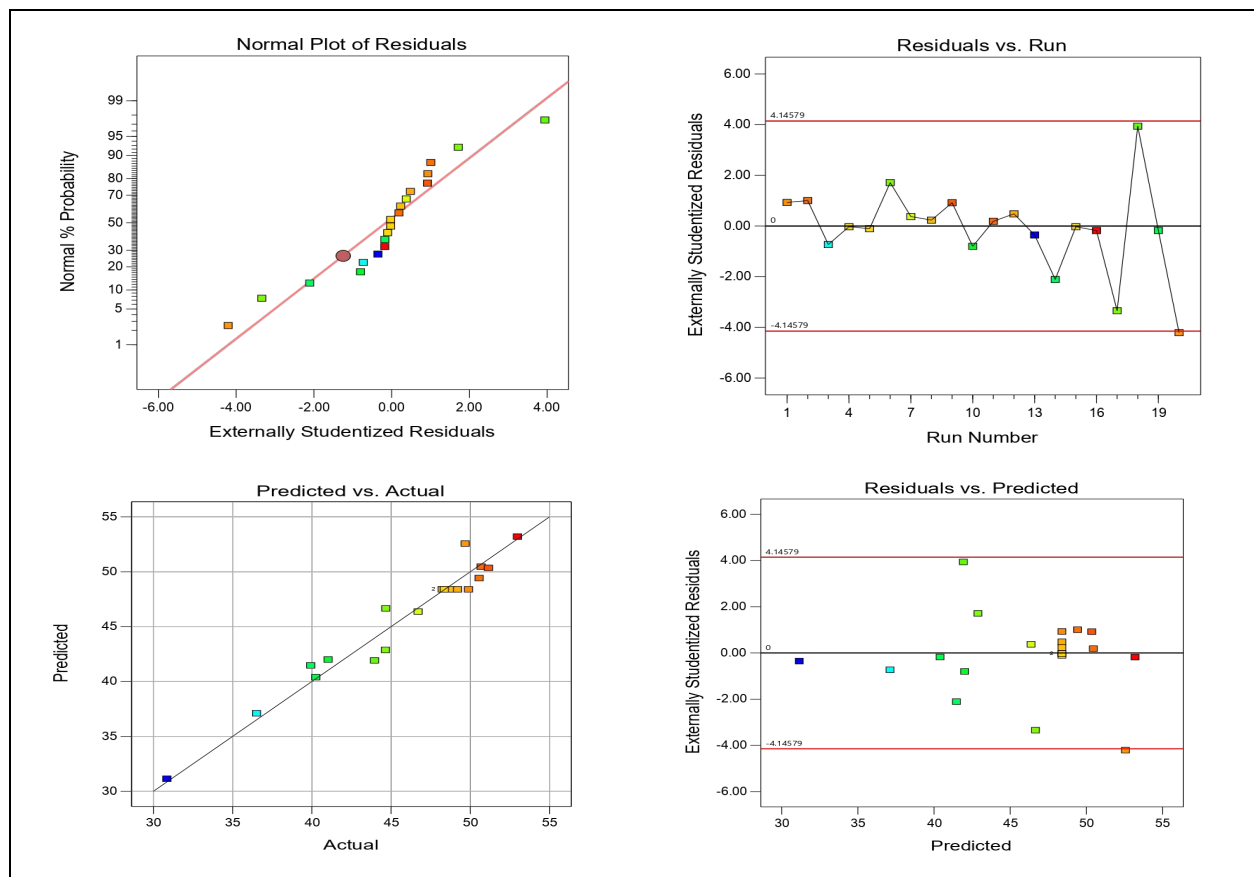


Fig. 4: Normal probability plot against the residual following the FS response, (b) run number versus residual, (c) comparison of expected and actual values and (d) externally studentized versus projected residuals

The variations in tensile and flexural strength are presented in Figures 3 and 4 (Table 2), respectively. The experimental results for both properties are very

close, which is reflected in the similar appearance of the figures. As the observed data approach, the baseline, the model's precision increases. The factor effect plot is

illustrated in Fig. 5, showing the association between each process variable and the TS response. The response of a single variable in relation to a fixed reference point, assuming all other variables remain constant is shown. Studies have reported that fibers treated with KMnO_4 exhibit the highest tensile strength among various treatments, demonstrating its effectiveness in enhancing interfacial bonding (Ezeamaku *et al.* 2023). This evaluation was based on the design area center point and the individual element's zero-coded level.

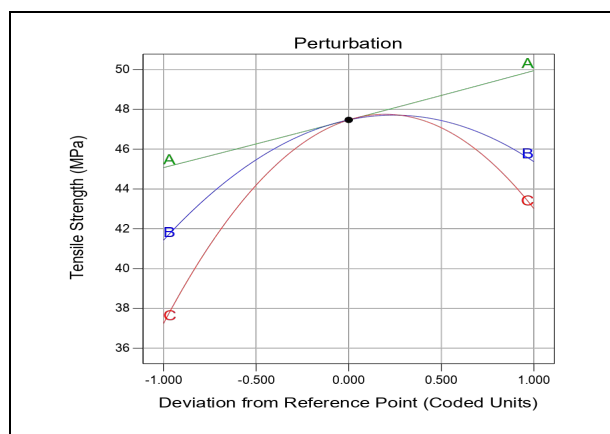


Fig. 5: Hybridized nanocomposite's perturbation plot after the TS test

The tensile strength increased with the rising volume concentration of TiO_2 , attributable to enhanced TiO_2 toughness and bonding with the epoxy matrix. The data indicate that the removal of cellulose and additional impurities like waxes from the *Paederia foetida* fiber surface result in an increase in TS as the modification duration (A) of KMnO_4 - acetone is extended. Nonetheless, as the fiber weight content (B) increased, the TS diminished, which is ascribed to reduced wetting of the fiber and less interaction between the fiber and the polymer matrix.

As the data points approach the reference line, the model's forecast accuracy for flexural strength improves. Fig. 6 presents a perturbation plot that demonstrates the sensitivity of FS to the chosen process parameters. It graphically illustrates the impact of various variables on the FS outcome in the RF model, with all other elements held constant. The response behavior is assessed in relation to a central reference point, which aligns with the center of the design space and the zero-coded level of each independent variable. Significant departures in the curve of any factor from the reference baseline imply greater sensitivity and a more pronounced effect on flexural strength, whereas gentler slopes suggest a relatively minor impact. Consequently, this figure functions as a diagnostic illustration to discern the predominant variables influencing FS and to assist in the subsequent optimization procedures for nanocomposite systems.

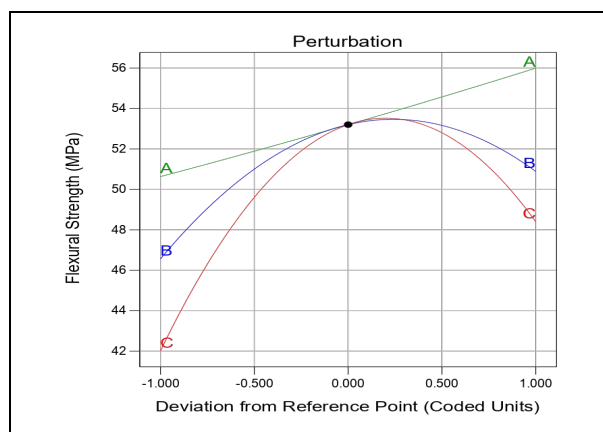


Fig. 6: Hybridized nanocomposite's perturbation plot after the FS test

An elevation in TiO_2 concentration (C) resulted in enhanced FS attributable to superior stiffness and interfacial bonding with the epoxy matrix. As the modification duration (A) of KMnO_4 -acetone increased, FS also improved, presumably due to the elimination of surface contaminants from PF, thereby improving bonding. Nonetheless, increased fiber content (B) led to diminished flexural strength, due to inadequate wetting and insufficient contact between the fiber and the matrix, which restricted efficient stress transmission during bending.

3.3 PFMNC TS Surface Response Contour Plots

Fig. 7 (a and b) presents a 3D and 2D contour map of the topography, demonstrating the influence of fiber weight and KMnO_4 modification duration on TS. The 3D surface graph analysis shows that increasing KMnO_4 alteration time from 1 to 3 minutes enhances tensile strength of the produced PFMNC, and a small decrease is seen at 5 minutes. This is due to PF deterioration caused by excessive oxidation with prolonged treatment duration. The optimal modification time for KMnO_4 was achieved after being treated for 3 minutes. The TS of the PFMNC declines from 15% to 25% PF by weight (Fig. 7 (a)). This problem might be caused by the insufficient wettability of the fibers in the matrix. The peak tensile strength value occurred at 15 wt %, while the minimum was at 25 wt%, as indicated by the 2D contour plot related to fiber content (Fig. 7 (b)).

Fig. 8 (a and b) presents a 3D surface plot and a 2D contour plot, demonstrating the influence of TiO_2 volume concentration and fiber weight content on the tensile strength. The study of 3D surface graph indicated that increasing volume content of TiO_2 to 2% enhances TS of the manufactured PF/ TiO_2 hybrid nanocomposite. However, as the TiO_2 concentration increases to 4%, the enhancement in dispersion becomes marginal. Inadequate TiO_2 dissipation, together with the effects of particle aggregation or residual within the PFMNC

matrix, all are contributing factors. Similarly, Sari *et al.* (2024c) documented that hybrid epoxy composites of *Paederia foetida* fibers achieve high tensile strength. Fig. 9 a and 9 b show the topography in three dimensions and two dimensions, respectively, demonstrating how the composite tensile strength is affected by the amount of TiO_2 and the length of time that KMnO_4 is applied. The evaluation of the 3D surface graph indicates that increasing the TiO_2 content to 2% enhances the tensile strength, which then experiences a slight decline as

concentrations rise to 4%. Multiple factors such as inadequate TiO_2 dispersion and nanoparticle aggregation inside the PFMNC matrix contribute to changes in tensile strength. The optimal KMnO_4 treatment significantly improved tensile strength (Supriya *et al.* 2024). The TS increased during the KMnO_4 modification period from 1.5 minutes to 4.5 minutes, attributable to the improved interconnection of the enhanced PF within the epoxy resin matrix.

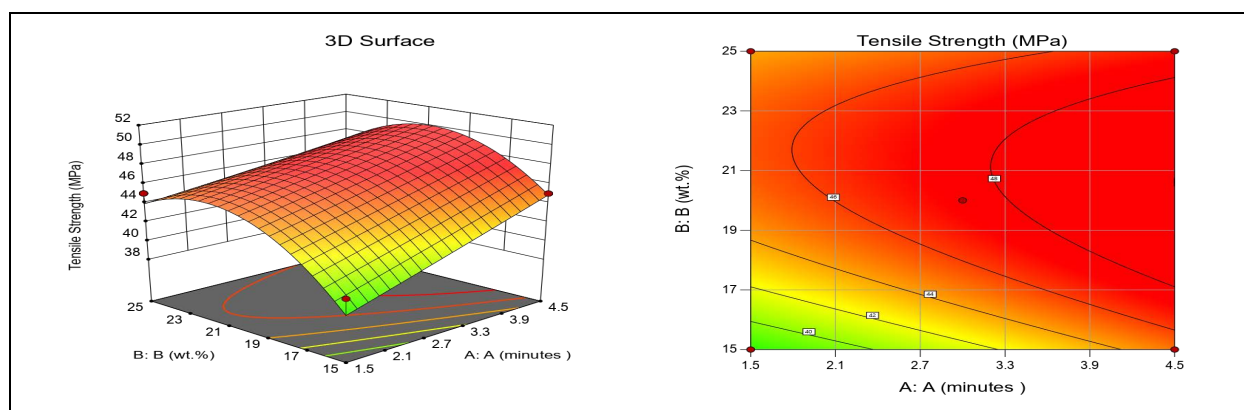


Fig. 7: Relationship between KMnO_4 change time and fiber mass fraction on the TS of PFMNC (a) 3D Surface Plot and (b) 2D contour

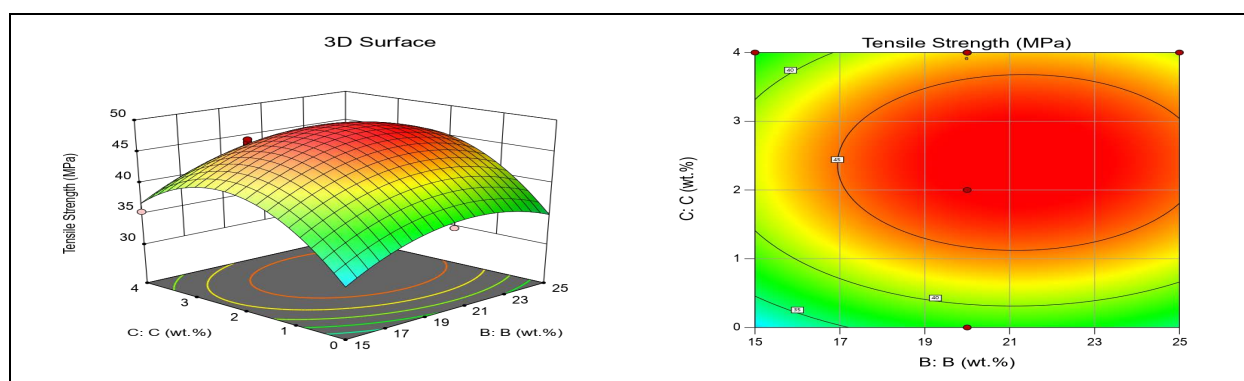


Fig. 8: TiO_2 volume content vs fiber mass content plots on PFMNC's TS (a) 3 D surface and (b) 2 D contour

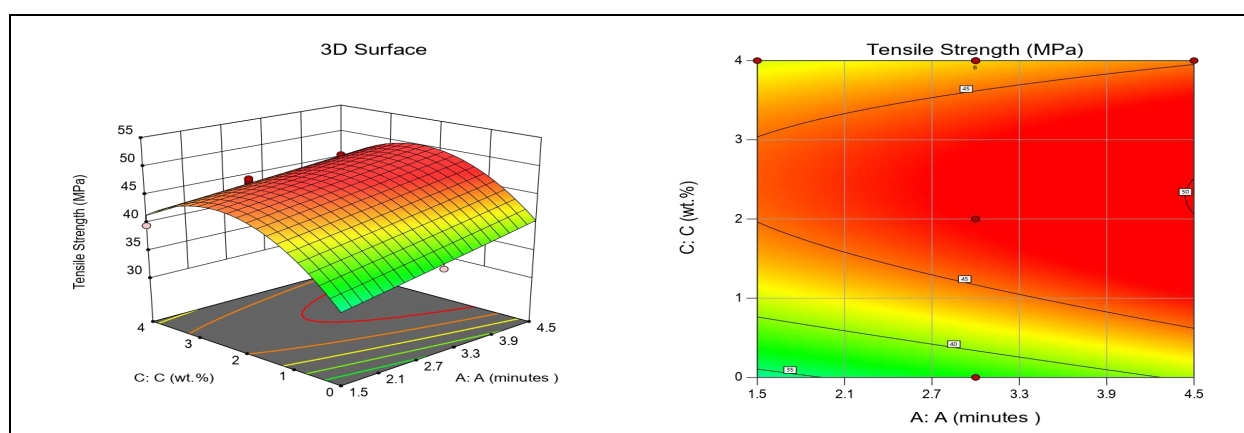


Fig. 9: Plots of PFMNC's TiO_2 volume concentration vs KMnO_4 modification time (a) 2D-contour and (b) 3D-surface plot

3.4 PFMNC FS Surface Response Contour Plots

Fig. 10 illustrates the impact of the data factors on the efficacy of the FS using 3D surface and 2D contour plots. The examination of the 3D surface plot indicates that extending KMnO_4 treatment period from 1 min to 3 mins enhances the FS of the fabricated PF/ TiO_2 hybrid nanocomposite, which subsequently experiences a minor decline when the modification time is prolonged to 5

minutes. This is caused by excessive oxidation with prolonged treatment duration. The optimal modification time for KMnO_4 was achieved after 3 minutes of processing. The FS of the PFMNC decreases when the PF weight content increases from 15% to 25%, as shown in the 3D surface plot in Fig. 10 (a). One possible cause of this problem is the matrix's insufficient fiber wettability. The peak FS value occurred at 15 wt %, while the minimum was at 25 Wt %, as indicated by the 2D contour plot presented in Fig 10 (b).

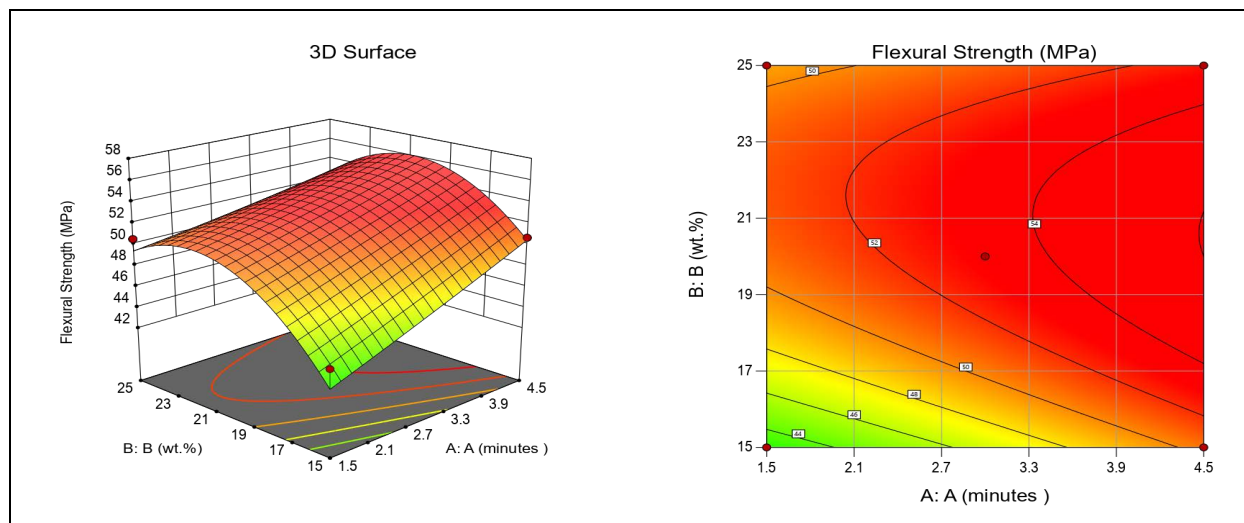


Fig. 10: Relationship between KMnO_4 modification time and fiber mass content for PFMNC's FS (a) 3 D surface and (b) 2 D contour plot

Fig. 11 (a and b) presents a 3D surface plot and a 2D contour plot, demonstrating the influence of TiO_2 volume content and fiber weight percentage on FS. The examination of the 3D surface graph indicated that increasing the TiO_2 volume content to 2% enhances the FS of the fabricated PF/ TiO_2 hybrid nanocomposite, which subsequently experiences a slight decline when TiO_2 concentrations increase to 4%. Inadequate TiO_2

dispersion, together with the effects of particle aggregation within the PFMNC matrix, all be contributing factors. Studies have reported that the addition of TiO_2 nanoparticles to natural fiber composites significantly improves their flexural strength due to better filler dispersion and matrix interaction (Mishra *et al.* 2025).

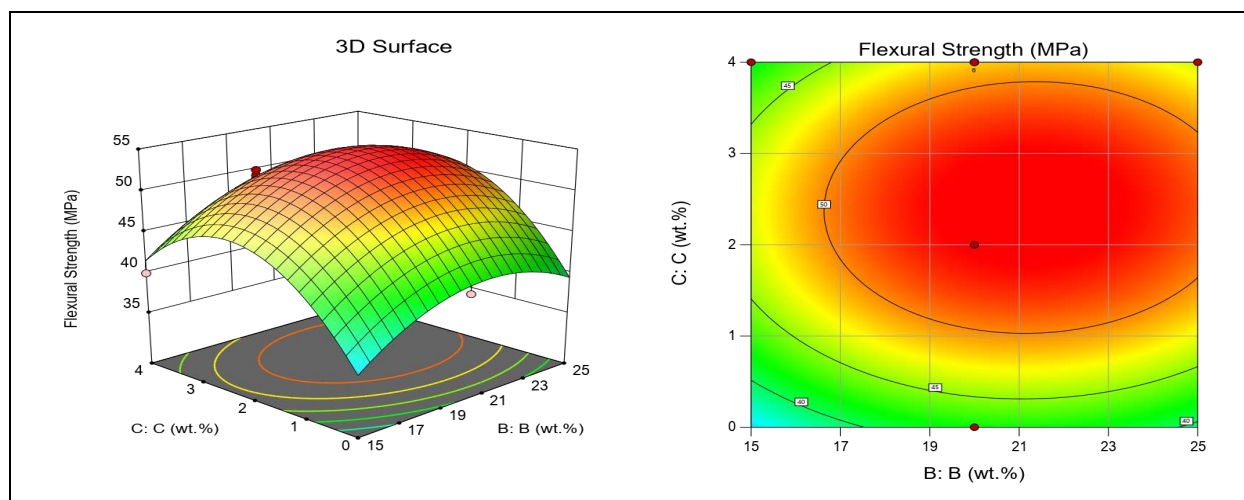


Fig. 11: Relationship between TiO_2 volume fraction and fiber mass content for PFMNC's FS (a) 3D surface and (b) 2D contour

Fig. 12 (a and b) illustrates the 3-Dimension surface and 2-Dimension contour plots of the topography, highlighting the influence of KMnO_4 treatment duration and TiO_2 volume content on the composite FS. The evaluation of the 3D surface graph indicates that increasing the TiO_2 content to 2% enhances the FS, after

which it experiences a slight decline as concentrations rise to 4%. Flexural strength of the composite was found to increase when KMnO_4 treatment duration was between 1.5 minutes and 4.5 minutes, attributable to the improved interconnection of the enhanced PF inside the epoxy resin matrix.

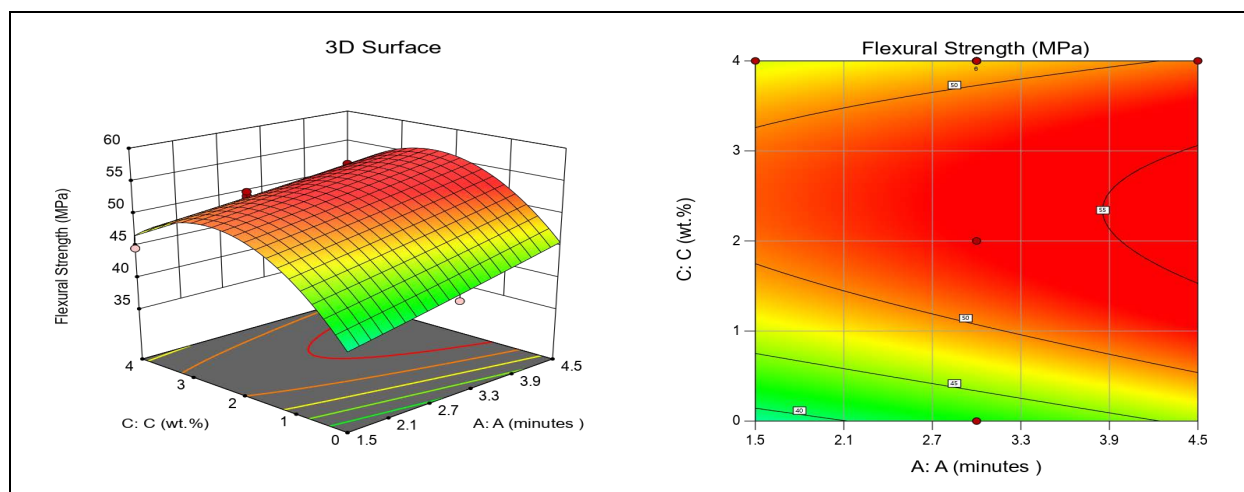


Fig. 12: Plots of PFMNC's TiO_2 volume concentration vs KMnO_4 modification time (a) 2D-contour and (b) 3D-surface plot

3.5 Results of the ANN Model Efficiency Metrics for The Fabricated PFMNC

The optimal model structure was evaluated using both the training and external validation data, and the subsequent regression graphs for both stages were generated. Fig. 13 (a) illustrates the post-regression plot of the training dataset. By comparing the expected output with the network's actual response, this performs a linear regression analysis. A correlation coefficient of $R = 0.9199$ was acquired. This factor approaches unity, indicating the efficacy of the training period. The dotted

line, which represents the best forecast was closer to the generated line of best fit. This proves the model's ability to accurately predict future data from unique datasets. The testing dataset was also subjected to the post-regression plot, as shown in Fig. 13 (b), produced a correlation coefficient of $R = 0.4208$. Weak correlations denote low interdependence, whereas strong correlations highlight a substantial and reliable relationship. The independent factors explain 94% of the variation in the dependent variable, according to a correlation coefficient of $R = 0.9440$. This also demonstrates the model can accurately forecast unique data in proximity to the anticipated tensile strength.

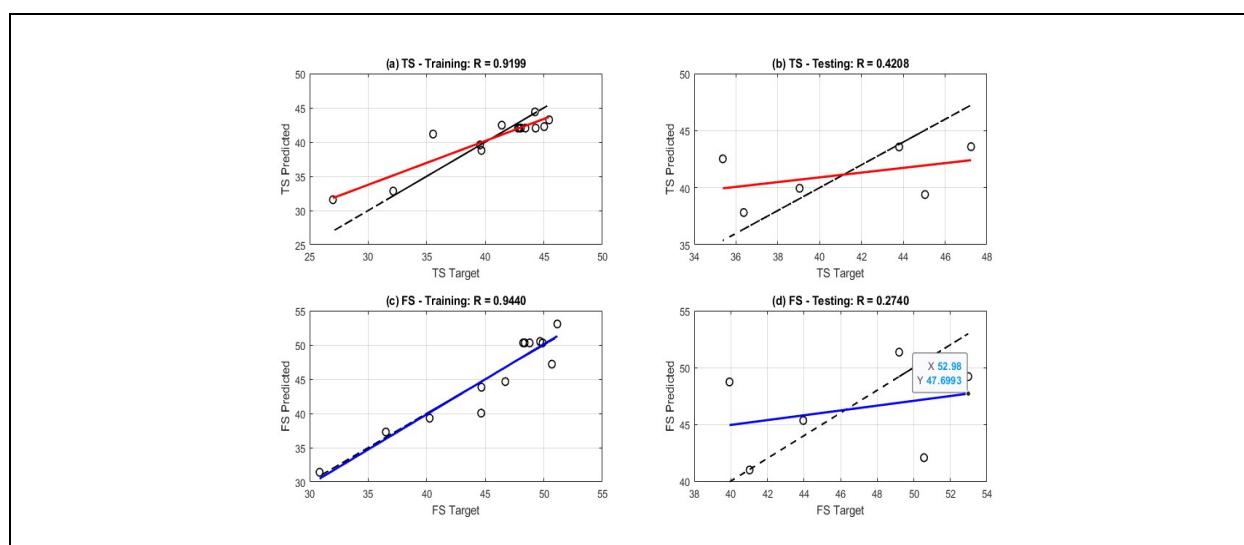


Fig. 13: PFMNC post-regression plots for the training and testing datasets

The model's accuracy was initially evaluated using its training data. A plot illustrating the difference between projected tensile strength and the experimentally acquired values was generated, as illustrated in Fig.14. The model demonstrated commendable accuracy in predicting the training datasets. Evaluating the model with novel datasets not employed during training is essential, as it serves as a method to assess the model's

predictive accuracy. A comparative graph illustrating the disparity between the predicted and experimentally obtained TS was created using 25% testing data, as depicted in Fig. 15. The anticipated tensile strength and the factors derived from testing demonstrated strong concordance. The tensile strength was found to be overestimated, potentially due to the model's insufficient training data.

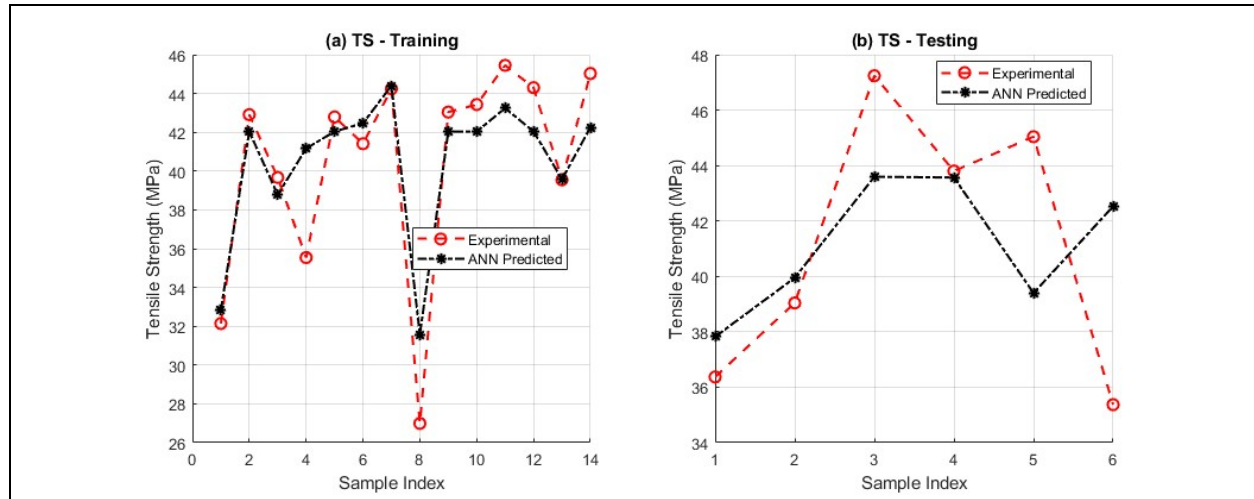


Fig. 14: PFMNC post-regression plots for the training and testing datasets

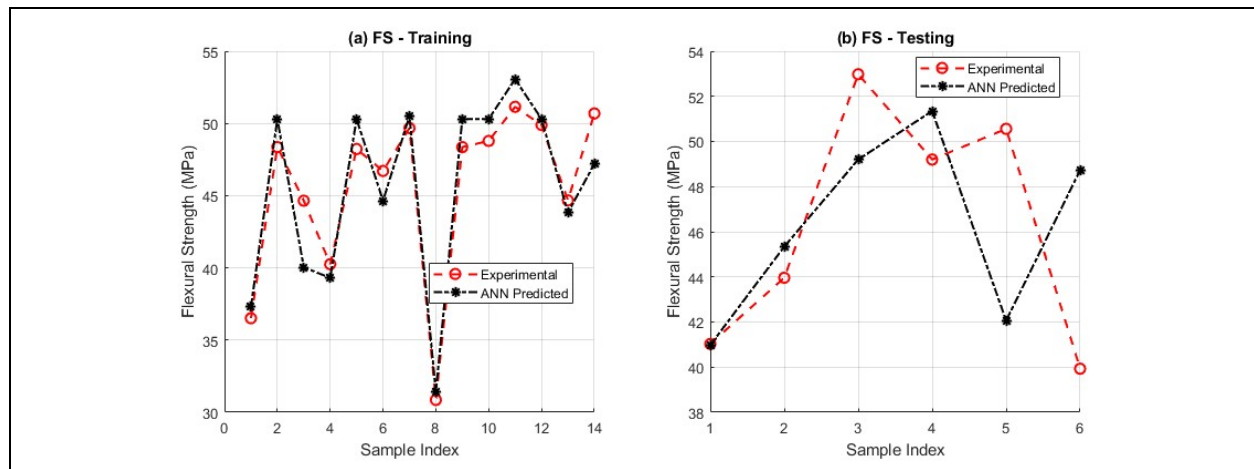


Fig. 15: PFMNC model testing using (a) training data and (b) FS testing dataset

3.6 The ANN Statistical Performance Metrics for PFMNC

The ANN model was further evaluated using the metrics presented in Tables 4 and 5 for known statistical performance indicators. A comparative analysis of the tensile strength model testing was conducted utilizing both training and testing datasets. Although the RMSE value for the training dataset was lower than that of the testing dataset ($\text{RMSE training} = 2.3467 < \text{RMSE testing} = 4.0694$), the MAD value was lower for the testing dataset ($\text{MAD testing} = 1.7364 < \text{MAD training} = 3.1733$). Subsequently, the flexural strength model was

evaluated using both the training and testing datasets. Although the RMSE value for the training dataset was lower than that of the testing dataset ($\text{RMSE training} = 2.0515 < \text{RMSE testing} = 5.3300$), the MAD value was lower for the testing dataset ($\text{MAD testing} = 1.7087 < \text{MAD training} = 4.1093$). The training data were estimated with minimal error; however, the error in the testing data between predicted and actual mechanical properties is only slightly greater than that of the training dataset. The average MAD metric distance between each observation and its mean in the testing dataset was less than that in the training dataset. This leads to reduced variability during testing relative to the training phase.

The training phase of TS exhibited a higher MAPE compared to the testing phase (MAPE Testing = 4.69% < MAPE training = 7.89%). However, the MAPE for the training phase of FS was less than that of the testing phase (MAPE Testing = 3.68% > MAPE training = 8.93%). From the perspective of utilizing unknown data during the model testing phase, the predicted accuracy of the model is approximately 97.65% for TS and 97.95% for FS. This endows the model with robust reliability for analogous time series and forecasting predictions. The assessment of model variability in predictive capability was also examined utilizing the RCoV metrics. There is very little variation between the training dataset's predictions and the actual values. Similarly, the model's ability to accurately predict TS from the new input dataset is supported by the small discrepancy (RCoV_testing = 0.73%) between the predicted and

experimentally measured TS in the testing data. Using the rMBE metric, the model's tendency to overestimate or underestimate was determined. The model's tendency to overestimate is shown by positive values, whereas the opposite is true for negative values. Table 5 indicates that the rMBE value for tensile strength during the training phase approaches a negative value (rMBE_(training) = 0.73%), but the testing period exhibits a rMBE value that leans towards the positive (rMBE_(testing) = 0.96%). This additionally explains the incorrect forecasts in the test data. Table 6 indicates that the rMBE value for flexural strength during the training phase approaches a negative value (rMBE_(training) = 0.02%), but the testing phase exhibits a tendency towards the positive (rMBE_(testing) = 0.91%). This additionally explains the incorrect forecasts in the test data.

Table 5. Metrics for ANN performance assessment for TS

	RMSE	MAD	MAPE	RCoV	rMBE
Training	2.3467	1.7364	4.69%	0.0429	0.73%
Testing	4.0694	3.1733	7.89%	0.0771	0.96%

Table 6. Metrics for ANN performance assessment in FS

	RMSE	MAD	MAPE	RCoV	rMBE
Training	2.0515	1.7087	3.68%	0.0374	0.02%
Testing	5.3300	4.1093	8.93%	0.0888	0.91%

3.7 Analysis of PFMNC's Validation and Optimization

A suitable parameter of the mechanical properties is identified by the investigation of various factors influencing the mechanical strength of the PF/TiO₂ hybrid nanocomposite. Table 2 indicates that the optimal range for enhancing mechanical strength is between 26.99 and 47.24 MPa for tensile strength and between 30.85 and 52.98 MPa for flexural strength. Fig. 16 (a and b) illustrates the optimization and cube ramp for tensile strength. The BBD optimization of tensile and flexural strength reveals the optimal analysis of the PFMNC's validation and anticipated operating conditions: (A) KMnO₄ treatment time: 3.72483 minutes, (B) fiber weight percentage: 18.6334%, (C) TiO₂ volume content: 2.89723%, (D) ultimate tensile strength: 47.5613 MPa. This is also consistent within the predictions from the artificial neural network. Fig. 16 (a) presents the BBD optimization results for flexural

strength, highlighting the optimal operating conditions of the hybrid nanocomposite: KMnO₄ treatment time (A) at 3.72483 minutes, fiber weight content (B) at 18.6334%, TiO₂ volume concentration (C) at 2.89723%, and FS at 53.3553 MPa.

Upon the completion of an experiment, data were gathered and the results were aligned with analytical predictions. If the outcomes align with anticipated range, the estimation is corroborated. If the results deviate from that range, it be essential to examine possible sources of error. Tensile strength was measured and duplicate samples were created using the expected ideal value to verify the statistical experimental analysis. The ideal location was identified, and there was significant concordance between the anticipated and observed results. This validated that the model is precise and effective in enhancement and estimation of natural fiber based composites.

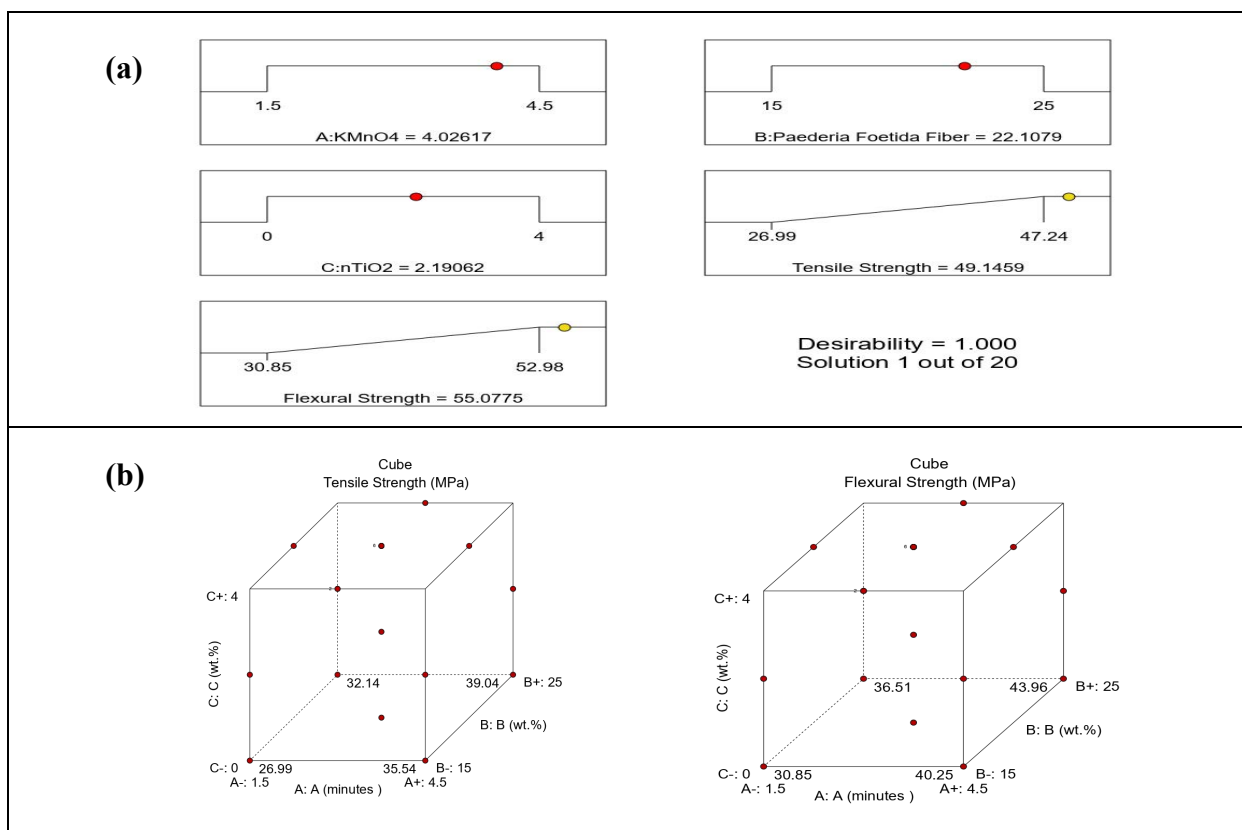


Fig. 16: Numerical optimization of the KMnO_4 change time, fiber mass content and TiO_2 volume content for tensile strength shown in (a) ramp and (b) cube plot

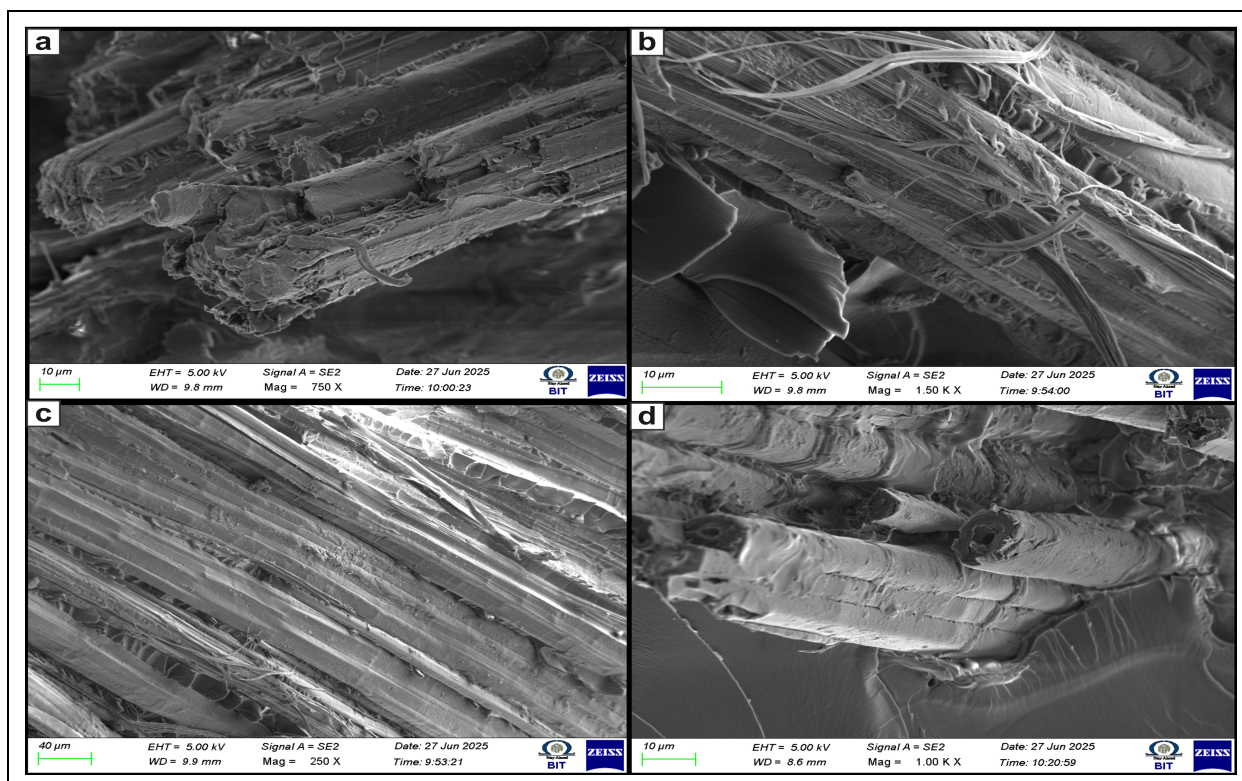


Fig. 17: PF fiber (a) SEM micrograph (b) maximum KMnO_4 modified fiber (c) fractured surface of improved PFMNC and (d) optimally treated KMnO_4 modified fiber

Fig. 17 (a–d) presents the scanning electron micrographs of *Paederia foetida* fibers, effectively processed KMnO₄-fiber, maximally treated KMnO₄-changed fiber (5 min), and the fractured surface of PF/TiO₂ hybrid nanocomposite. Fig. 17(a) illustrates the natural PF surface, coated with waxes and various surface contaminants. Natural fiber surfaces are typically coated with an amorphous layer composed of lignin and hemicellulose. The elimination of these compounds enhances the cellulose fraction at the fiber's surface, hence augmenting its strength. Fig. 17 (b) illustrates the microscopic image of optimally processed KMnO₄-treated fiber (2.29 min), demonstrating the removal of waxy substances, lignin, and other undesirable surface contaminants, resulting in a uniform roughness of the fiber surface. Cellulose manganate is formed when permanganate ions react with hydroxyl groups in cellulose. This reaction initiates graft copolymerization, hence enhancing the chemical interaction at the fiber interface. Fig. 17 (c) illustrates that fiber damage commenced following extended exposure to KMnO₄. Fig. 17(d) illustrates the failure surface of the optimal PF/TiO₂ hybrid nanocomposite, in which TiO₂ has been seamlessly integrated into the PF hybrid nanocomposite and demonstrates uniform diffusion within the epoxy matrix. The micrograph demonstrates enhanced interface cohesiveness among the epoxy matrix, PF, and TiO₂. The fabrication process employed in this work achieved a uniform dispersion of TiO₂ within the matrix, as no discernible aggregation of TiO₂ was evident in the SEM micrograph. Previous studies using FESEM have shown uniform dispersion of fillers and good matrix bonding (Sari *et al.* 2023).

4. CONCLUSION

This study investigated the efficacy and dependability of the ANN-BBD by modeling and optimizing the mechanical strength of PFMNCs, considering TiO₂ volume concentration, KMnO₄ modification duration, and fiber weight content. This research demonstrates that mastering hyperparameter tuning is essential for designing a high-performing neural network to predict the TS and FS of PFMNCs. Using the criterion of least error, the ideal ANN model (topology 3-5-1) was selected to establish the model's RMSE, MAD, MAPE, and R-values. An ANN model is expected to have an accuracy of approximately 97.65% to 97.95%. KMnO₄ modification time, fiber loading, and TiO₂ concentration affect the tensile and flexural strengths of PFMNC were analyzed through BBD.

The optimal factors for TS and FS were determined to be 3.72483 minutes for KMnO₄ alteration duration, 2.89723% for TiO₂ volume content, and 18.6334 wt%. The model projected TS to be 47.5613 MPa, which is close to the actual value of 44.24 MPa.

Similarly, for FS, it was 53.3553 MPa, which is close to the actual value of 52.98 MPa.

This work has demonstrated the efficacy of soft computing strategies in attaining optimal values for mechanical properties and facilitating cost-effective, energy-efficient production processes. The BBD is a practical choice for optimizing systems or processes of moderate complexity because it strikes a good balance between precision and the amount of experimental effort needed. The utilization of the ANN-BBD model for estimation and improvement must be considered in studies of the various mechanical properties of NFPCs for advanced applications.

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CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

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