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Characterization and Modeling of Mechanical Properties of Additively Manufactured Coconut Fiber-Reinforced Polypropylene Composites

George Mosi*, Bernard W. Ikua, Samuel K. Kabini, James W. Mwangi

Department of Mechatronic Engineering, Jomo Kenyatta University of Agriculture and Technology, Juja, Kenya
Email: *mosigmosi@gmail.com

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Abstract

In the face of the increased global campaign to minimize the emission of greenhouse gases and the need for sustainability in manufacturing, there is a great deal of research focusing on environmentally benign and renewable materials as a substitute for synthetic and petroleum-based products. Natural fiber-reinforced polymeric composites have recently been proposed as a viable alternative to synthetic materials. The current work investigates the suitability of coconut fiber-reinforced polypropylene as a structural material. The coconut fiber-reinforced polypropylene composites were developed. Samples of coconut fiber/polypropylene (PP) composites were prepared using Fused Filament Fabrication (FFF). Tests were then conducted on the mechanical properties of the composites for different proportions of coconut fibers. The results obtained indicate that the composites loaded with 2 wt% exhibited the highest tensile and flexural strength, while the ones loaded with 3 wt% had the highest compression strength. The ultimate tensile and flexural strength at 2 wt% were determined to be 34.13 MPa and 70.47 MPa respectively. The compression strength at 3 wt% was found to be 37.88 MPa. Compared to pure polypropylene, the addition of coconut fibers increased the tensile, flexural, and compression strength of the composite. In the study, an artificial neural network model was proposed to predict the mechanical properties of polymeric composites based on the proportion of fibers. The model was found to predict data with high accuracy.

Keywords

Additive Manufacturing, Artificial Neural Network, Mechanical Properties, Natural Fibers, Polypropylene

1. Introduction

Polymeric composites have been used in various areas, such as the aerospace, automotive, and construction industries. They are also commonly used in medical areas, including dental, orthopedics, and biomedical and tissue engineering [1]. Polypropylene (PP), polyethylene (PE), polyvinyl chloride (PVC), and polystyrene (PS) are some of the common thermoplastics that have been used as matrices in polymeric composites. In contrast, polyester and epoxy are the commonly used thermosetting plastics in developing polymer-based composites. Polymers are reinforced with fibers mainly to improve their mechanical properties, such as high strength-to-weight ratio [2].

Synthetic fibers such as those of carbon and glass have been traditionally used to reinforce these polymers due to their high mechanical strength. However, due to increased environmental awareness and the need for sustainability in manufacturing, many research works have explored various natural fibers as alternatives to conventional synthetic fibers. Natural fibers offer benefits such as relatively lower cost, renewability, good mechanical properties, biodegradability, and flexibility [3]. Different natural fibers such as those of hemp, jute, cotton, kenaf, sisal, banana, and palm have been used to reinforce different thermoplastic and thermosetting polymers [4]-[7]. Various research works have reported improvements in mechanical properties such as tensile strength, flexural stiffness, impact resistance, and compression properties for polymeric composites reinforced with natural fibers [8].

Natural fibers mainly comprise hemicellulose, cellulose, lignin, pectin, and moisture content [9]. The hydroxyl group in natural fibers contributes to their hydrophilic nature, which is the main drawback of the fibers. Since polymer matrices are hydrophobic, the difference in properties makes the polymeric composites less resistant to moisture adsorption and, therefore, vulnerable to environmental attacks. As a result, there is normally swelling of fibers along matrix-fiber interfaces, which leads to deterioration in mechanical properties content [9]. Another limitation of natural fibers is their poor dispersion in the matrix. Currently, studies are being conducted to improve inter-facial adhesion between the fibers and matrix. Various chemical treatments, such as alkali treatment, are usually employed to modify the fiber surfaces to enhance the mechanical characteristics of the polymer composites. Chemical treatments increase the fiber surface roughness and decrease the hydroxyl groups, reducing the fibers' water adsorption [10] [11].

The effects of chemical treatment on plant-based natural fibers' physical and mechanical properties have been explored. Venkatesh *et al.* [12] studied the impacts of alkali treatment on tensile, flexural, impact, and water absorption properties of natural fiber-reinforced polyester composites. They used sisal and bamboo fibers as reinforcing agents. The incorporation of fibers was found to increase mechanical properties and water absorption. They then exposed the fibers to 10 wt% NaOH solution for one day. The properties of untreated and treated fibers were then studied again. The composites reinforced with the treated fibers exhibited an increase in impact, flexural, and tensile strength by 36.9%, 27.4%, and 30%, respectively. A sharp decrease in moisture absorption by composites with treated fibers was also noticed.

Bachchan *et al.* [13] reviewed the influence of chemical treatment of fibers on their water absorption and mechanical properties. They noted a direct correlation between chemical treatment, water absorption, and mechanical properties. The researchers concluded that subjecting natural fibers to chemical treatment reduces their water absorption rates and improves their mechanical properties.

The most commonly used processing techniques for polymeric composites include hand lay-up, injection molding, bag molding, filament winding, and spray-up process [14]. However, these techniques are characterized by high energy consumption, material wastage and high level of rework, poor part consolidation, and limited design freedom. To address some of these challenges, embracing new fabrication techniques, such as additive manufacturing, is necessary. The present work investigated the mechanical characteristics of fused filament fabricated coconut fiber (Coir fiber) reinforced polypropylene for application in automotive vehicle parts such as dashboards, door handles, and bumper fascia. Fused filament fabrication is one of the fastest-growing additive manufacturing (AM) technologies, and it is the most commonly used in preparing natural fiber-reinforced polymeric composites. FFF offers various benefits such as the capability to produce small parts, reduced material wastage, and high energy efficiency. Additionally, the technique is relatively cheaper compared to other AM techniques [15].

One of the critical performance characteristics of a vehicle's part is its ability to remain intact when under impact. High flexural, tensile, and compression strength are desirable features of material properties used for developing car body parts. Material's flexural properties are its resistance to bending loads. The measurable flexural properties include flexural yield stress, flexural modulus, and ultimate flexural strength. Compression strength is the ability of a material to withstand loads tending to reduce its size. On the other hand, the tensile properties of a material are the characteristics that enable it to resist loads tending to elongate its size. Tensile characteristics include' tensile yield strength, Young's modulus, tensile yield strength, and ultimate tensile strength [16].

Comparatively, coconut fibers are among the most accessible natural fibers [17]. For instance, the fibers are abundantly available in most of the coastal areas and are underutilized. They can spur manufacturing growth in a country. Coconut husks are mainly used to make sawdust, briquettes, and biochar. The remaining volume of the husks is disposed into the environment, sometimes causing environmental pollution [18]. The coconut fiber extracted from the coconut husks can be processed to produce value-added engineering products such as reinforcement in polymer-based composites.

Automobile parts such as bumper fascia and dashboards are mainly manufactured from polypropylene (PP) reinforced with synthetic fibers such as carbon and glass [19]. Polypropylene is a suitable choice for the matrix in developing composites due to its advantages, such as high resistance to temperature, high resistance to chemicals, and good mechanical properties. In addition, it is semi-crystalline in nature with good resin characteristics, hence possessing high compatibility with most of the natural fibers [20].

The current research work aims to analyze and model the mechanical properties of coconut fiber-reinforced polymeric composites. The influence of the proportions of coconut fibers on the composite's tensile, compression, and flexural properties has been analyzed and modeled using an artificial neural network. The composites have been processed via fused filament fabrication.

2. Materials and Methods

2.1. Materials Preparation

The main materials used in this research work were coconut fibers, polypropylene, and sodium hydroxide (NaOH) pellets. Coconut fibers were obtained from Kwale County in Kenya. Sodium Hydroxide with a molarity of 40.00 g/mol was used to treat the coconut fibers. The coir fibers were sun-dried for 24 hours to reduce the moisture content. The dry fibers were then shredded into small pieces, which were then soaked in 5% w/v NaOH for 14 hours to improve their surface properties [11] [21]. The interfacial bonding between the fiber and matrix becomes more stable and stronger when the fiber is subjected to chemical treatment, thus enhancing the mechanical strength of the final composite [22].

The treated coir fibers were thoroughly washed with distilled water to remove the particles of NaOH on their surfaces and were then dried at 105˚C in an oven for 6 hours [23]. The moisture content of dry fibers was measured using a moisture content analyzer. The mechanical properties of biofiber-reinforced polymeric composite decrease with an increase in the fiber's moisture content [24] [25]. In this study, the fibers' moisture content was reduced to below 10% since achieving zero moisture content was impossible. The oven-dried coir fibers were crushed into powder using a ball milling machine. Coconut fiber particles of at most 150 μm in size were obtained via sieving. The summary of coir fiber processing steps is presented in **Figure 1**.

The coir fiber/polypropylene filaments were developed through extrusion. The processed coir powder and polypropylene pellets were dried in an oven at 105˚C for two hours before extrusion to minimize the moisture content. Different fractions of coir fiber and polypropylene pellets were measured and mixed using a mechanical mixer at a temperature of 85˚C for 4 minutes for homogeneity. The PP/coir fiber mixture was then fed into a screw extruder with two heating zones. Composite filaments with 0 wt%, 2 wt%, 3 wt%, 5 wt%, and 10 wt% of fiber were prepared. The levels of proportions of coconut fiber in the composites were determined through preliminary experiments. The composite filaments with more than 10 wt% of the fibers were discontinuous and could not be used for 3D printing. The extruder parameters used were similar to those of Sotohou *et al.* [26] and are shown in **Table 1**.

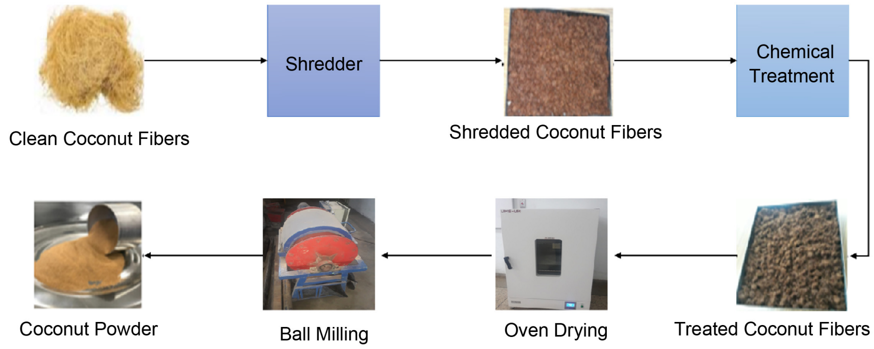


Figure 1. Coir fiber processing steps.

Table 1. Extrusion parameters.

Parameter	Level
Nozzle temperature	165˚C - 170˚C
Nozzle diameter	1.75 mm
Barrel temperature	170˚C - 180˚C

The filaments were passed through a water bath at room temperature for cooling. The filament preparation process is illustrated in **Figure 2**.

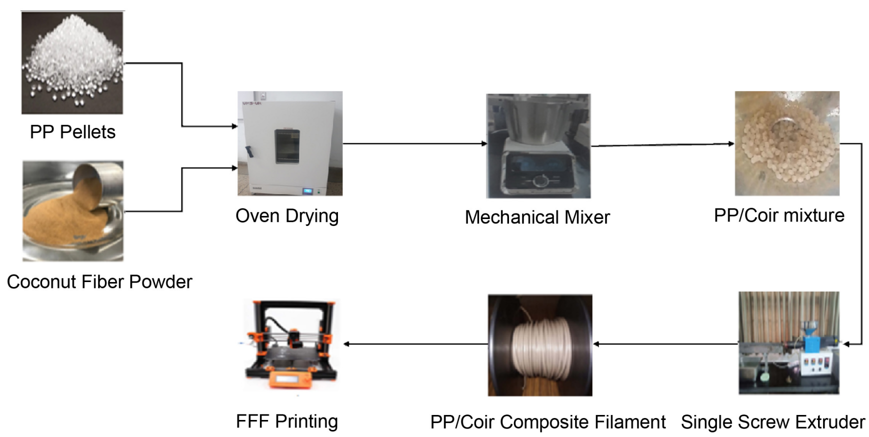


Figure 2. Composite filament preparation process.

2.2. Preparation of Test Specimens

The test specimens were fabricated from the composite filaments using a fused filament fabrication 3D printer. Autodesk Inventor, Education Version (version 2020) software was utilized to generate 3D models of the test samples. The specimens were prepared according to the American Society for Testing and Materials (ASTM). The test specimens for the tensile test were prepared according to ASTM D6382-Type IV [27] [28], while those for the compression and flexural tests were prepared according to ASTM D695 and ASTM D790 [29], respectively. The 3D CAD virtual geometries of the test samples were exported as stereolithographic (STL) files and printed using an FFF Prusa Printer (Prusa i3 MK3). The FFF printing parameters used were similar to those of Sotohou *et al.* [26] and Anerao *et al.* [30]. These parameters are shown in **Table 2**, while the printer's nominal print speed moves are presented in **Table 3**. The test specimen preparation process is shown in **Figure 3**.

Table 2. Parameters used in fabrication.

Parameter	Level
Nozzle temperature	210˚C - 220˚C
Infill density	100%
Layer thickness	0.15 mm
Infill pattern	Diamond
Nozzle diameter	0.4 mm
Bed temperature	60˚C - 65˚C
Raster angle	45˚
Airgap	0 mm
First layer height	0.2 mm
Printing speed	100%

Table 3. FFF printer's nominal print speed moves.

FFF print moves	Nominal speed (mm/s)
Perimeter	45
Infill	80
Bridge	25
Gap-fill	40
Ironing	15
First layer	20

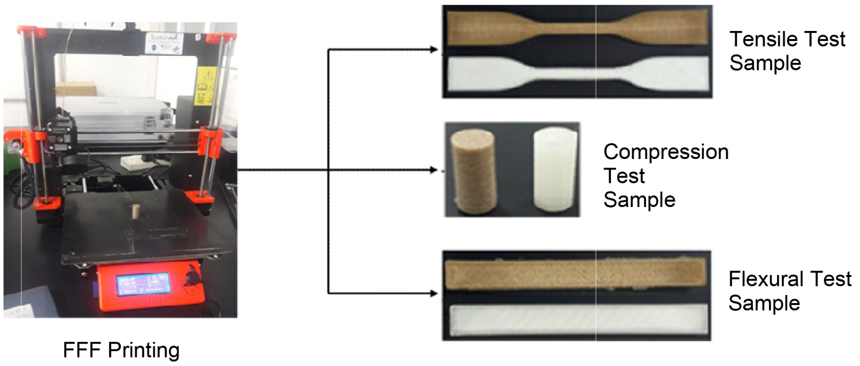


Figure 3. Test specimen preparation process.

2.3. Determination of Mechanical Properties

All the mechanical tests were conducted using a Universal Testing Machine (UTM)-Shimadzu. Under the tensile tests, properties such as tensile yield strength, Young's modulus, tensile yield stress, and elongation at the breakpoint were determined. The compression strength of the composites was computed under the compression test. The composite's flexural yield stress, flexural modulus, and ultimate flexural strength were determined under the flexural tests. The setups for mechanical tests are illustrated in **Figure 4**. The mechanical properties were determined as per the standard equations.

(a) Tensile Test Setup (b) Flexural Test Setup (c) Compression Test Setup

Figure 4. Mechanical test setups.

2.4. Modelling of the Composite's FFF Process

Traditionally, mechanical tests have been conducted to determine the mechanical properties of materials. However, these methods have drawbacks, such as being destructive, costly, and sometimes time-consuming. The mechanical tests are also associated with errors arising from testing inaccuracies and machine issues [31]. In an attempt to address these challenges, data prediction models based on simulation techniques have been introduced to predict the mechanical properties of materials. Compared to experimental methods, simulations offer many benefits, such as minimal or no material consumption and minimized equipment requirements [32]. In the current work, an artificial neural network data prediction model has been proposed to predict mechanical properties as a function of the proportion of coir fiber. Tensile yield stress, Young's modulus, ultimate tensile strength, elongation at break point, compression strength, flexural yield stress, flexural modulus, and ultimate flexural strength have been considered dependent variables and the process outputs. The proportion of coconut fiber has been taken as the input to the system and an independent variable.

Artificial neural networks are among the most commonly used machine learning techniques due to their ability to process nonlinear and complex data. Many research works have explored the possibility of using artificial neural network models to predict the mechanical properties of materials based on the inputs [33]-[35]. The proposed artificial neural network model consists of input, hidden, and output layers. The nodes (neurons) of the input layers take the inputs, the hidden layers process the input data, and the outputs predict the results based on the training data [33]. An artificial neural network with one neuron in the input layer, ten neurons in the hidden layer, and eight neurons in the output layer has been developed in this research work. The model is designed to take the proportion of coconut fiber as an input and predict the corresponding tensile yield stress, ultimate tensile strength, elongation at break point, Young's modulus, compression strength, flexural yield stress, flexural strength, and flexural modulus as illustrated in Figure 5.

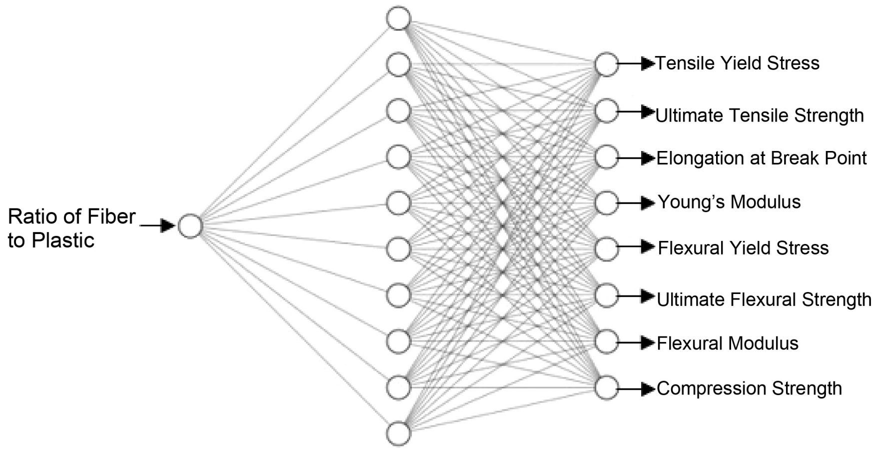


Figure 5. Artificial neural network model.

The network was designed and trained with the experimental data using the Neural Network Toolbox (nntool) available in MATLAB software (version R2021A). The tool supports unsupervised and supervised machine learning and automatically partitions the data in the ratio of 60%:20%:20% for training, validation, and testing data, respectively. The nntool supports unsupervised and supervised machine learning. Back-propagation learning with Tangent Sigmoid (TANSIG) and PURELIN activation functions in the input and output layers, respectively, was adopted for the model as shown in Figure 6. The percentages of coconut fiber in the composite were taken as inputs to the model and the corresponding mechanical properties were taken as outputs.

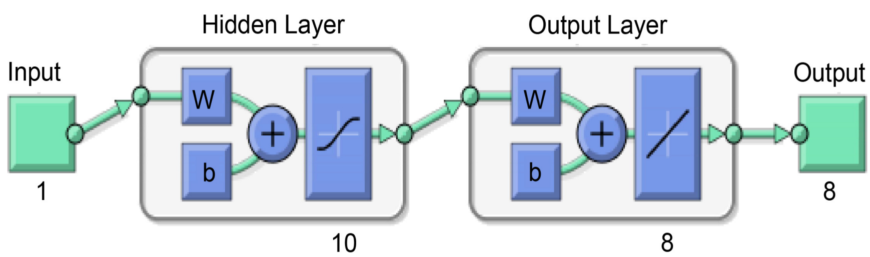


Figure 6. Data prediction neural network.

Regression squared (R^2) was used to evaluate the performance of the designed neural network model. R^2 is a statistical indicator that shows the relationship between the predicted and actual (experimental) values. It measures how well a regression model approximates data. The value of R^2 ranges between 0 and 1.

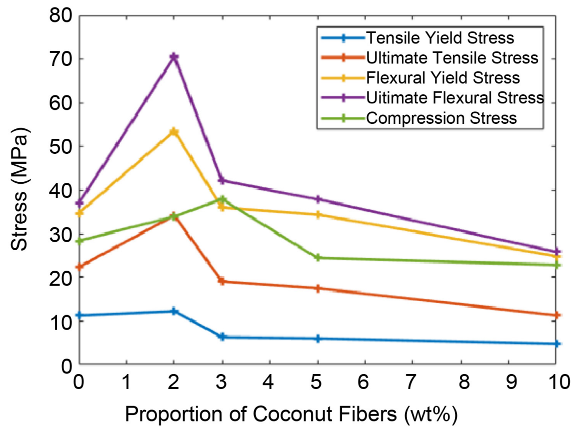
i.e., R ∈ [0, 1], with 0 showing a random correlation between the actual and predicted values and 1 indicating a close fit between the actual and predicted data. The experimental data sets were used to train the model in the present work. The number of neurons in the hidden layer was varied through trial and error, and the network's general performance was checked. A neural network with ten neurons in the hidden layer produced the highest value of R^2.

The number of hidden layers and their neurons is critical in designing a neural network model. Artificial neural network models with a single hidden layer have been determined to be more accurate in a research study by Khanam *et al.* [36]. The study further established that increasing the number of neurons in the hidden layer increases the network's power but leads to over-fitting.

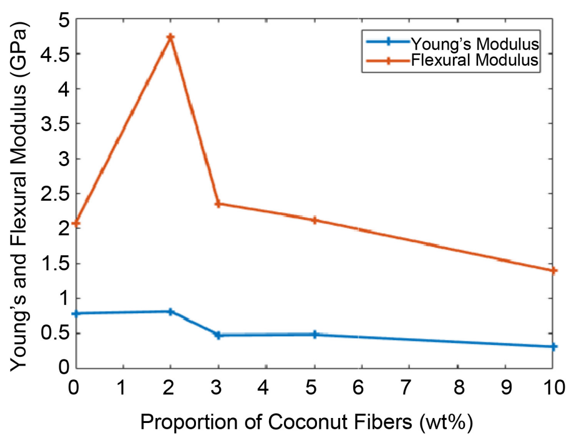
3. Results and Discussion

3.1. Mechanical Properties

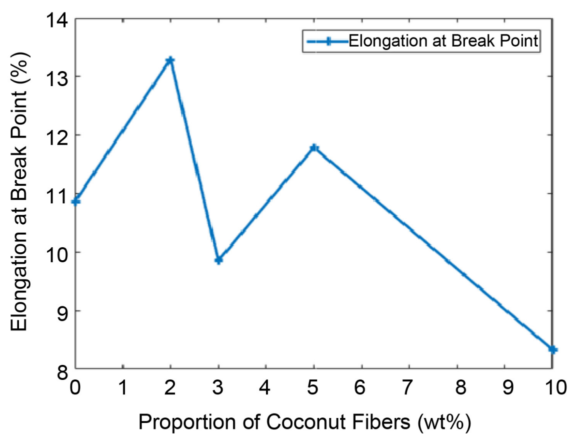
The effects of fiber loading on tensile, flexural, and compression properties are presented in shown in **Figure 7**. Tensile yield stress (TYS), ultimate tensile



(a) Stress versus proportion of fiber



(b) Young's and flexural modulus versus proportion of fiber



(c) Percentage elongation versus proportion of fiber

Figure 7. Effects of fiber content on various mechanical properties.

strength (UTS), elongation at break point (EBP), Young's modulus (YM), compression strength, flexural yield stress, ultimate flexural strength, and flexural modulus are seen to increase with the increase in the proportion of fiber coir in the composite to certain optimum fiber proportions. Further increase in fiber loading beyond the optimum was noted to decrease the mechanical properties of the composite.

The composite samples loaded with 2 wt% of the coir fibers exhibited the highest tensile and flexural properties, while those loaded with 3 wt% exhibited the highest compression strength. It is seen in **Figure 7** that increasing the coir fiber content beyond 2 wt% leads to a decrease in the mechanical strength, with the composite reinforced with 10 wt% of coir yielding the lowest tensile and flexural properties. 5 wt% fiber loading produced the lowest compression.

Coconut fibers contain a high lignin content of up to 45% [37]. Lignin gives the natural fiber its structural strength. However, it leads to poor interfacial adhesion between the fibers and polymer and limits the incorporation of more fibers into a polymer composite. Compared to pure polypropylene, the percentage increases in mechanical properties at optimum coconut fiber contents are summarized in **Table 4**.

Table 4. Comparison of the composites' mechanical properties at optimum fiber to neat polypropylene.

S/N	Mechanical Properties	Pure Polypropylene	Composite Mechanical Strength at Optimum Fiber Loading	Percentage increase in Mechanical Properties
1	Tensile Yield Stress (MPa)	11.27	12.28	8.89%
2	Ultimate Tensile Strength (MPa)	22.34	34.13	52.77%
3	Percentage Elongation at Break Point (%)	10.86	13.29	22.37%
4	Young's Modulus (GPa)	0.79	0.82	3.57%
5	Flexural Yield Stress (MPa)	34.70	53.47	54.09%
6	Ultimate Flexural Strength (MPa)	36.95	70.47	90.70%
7	Flexural Modulus (GPa)	2.07	4.73	128.09%
8	Compression Strength (MPa)	28.37	37.88	33.54%

The increase in the composite's tensile strength with the increase in fiber loading can be attributed to the reinforcement offered by the fibers, allowing the transfer of load from the matrix to the fibers. At low fiber content, the impact of crack initiation is dominant, hence poor tensile properties [38]. The role of a matrix in a polymeric composite is to wet the fiber surfaces, increasing the fiber-matrix interfacial adhesion. Increasing fiber loading results in an increased matrix-fiber ratio, hence insufficient wetting of the fiber surfaces, and leading to poor bonding between the fibers and the matrix. As reported by Das *et al.* [39]. increasing the proportion of fibers leads to agglomeration, hence blocking load transfer between the matrix and fibers.

The increase in flexural strength of the composite with an increase in the percentage of fibers may be due to the binding effects of the polymeric matrix. The polymeric matrix acts as a binding agent and also transmits and distributes stress to the fibers, resulting in increased flexural characteristics. Increasing the fractions of fibers resulted in proper weight distribution within the composite. The decline in flexural characteristics of the composite with an increase in fiber proportions above 2 wt% can be attributed to poor interfacial adhesion between fibers and matrix occasioned by the increased fiber-to-matrix ratios. Plant-based fibers are hydrophobic and absorb resin [40]. Since the matrix also acts as a resin, increasing the percentage of fibers in the composite beyond 2 wt% may have led to insufficient resin, causing brittleness and reduced flexural properties.

The composite's compression strength was also observed to increase with an increase in the proportions of coir fibers. The highest compression strength was obtained for a composite containing 3 wt% of coconut fiber. Adding 3 wt% of coconut fiber was found to enhance the compression strength by 33.54%. Increasing the fiber contents beyond 3 wt% was found to decrease the compression strength. A composite reinforced with 5 wt% was expected to produce higher compression strength than that reinforced with 10 wt%. However, this was not the case. The composite reinforced with 5 wt% produced lower compression properties than that reinforced with 10 wt%. They may be due to poor processing of the fibers. Fiber proportions above 5 wt% yielded compression strength lower than that obtained for pure polypropylene. Fibers act to minimize the initiation and propagation of vertical cracks in a composite part under compression, thus increasing its compression strength [41].

Increasing the fiber contents in the composite results in poor flowability and increased microstructural defects in the composite. Thus reducing its compression strength [42]. The force-extension curves for mechanical properties are shown in **Figure 8**. As seen in the figures, the samples undergoing compression required the highest magnitude of force, followed by the ones under tension. The samples under bending required the least force. It can also be seen that the composites loaded with 2 wt% required the highest force for tension and bending, while the composites loaded with 3 wt% required the highest force for compression.

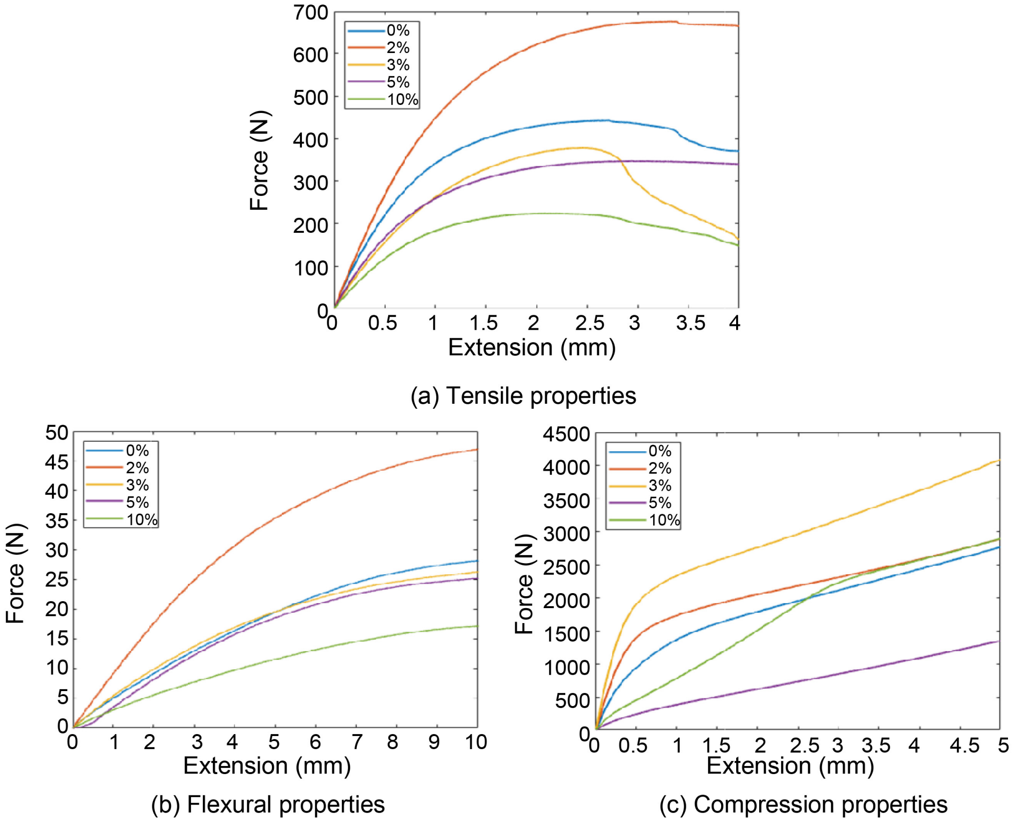


Figure 8. Force-extension curve for composite's mechanical properties at various fiber contents.

Figure 9 shows a comparison of the mechanical properties of carbon fiber-reinforced polypropylene and carbon fiber-reinforced polypropylene composites. The mechanical properties of carbon fiber-reinforced polypropylene were reported by Arun *et al.* [16] and Yoko *et al.* [43]. It is seen that the mechanical properties of coconut fiber-reinforced polypropylene composite are comparable to and better than those of carbon fiber-reinforced polypropylene composites. It can be concluded that coconut fibers are a viable replacement for carbon fibers.

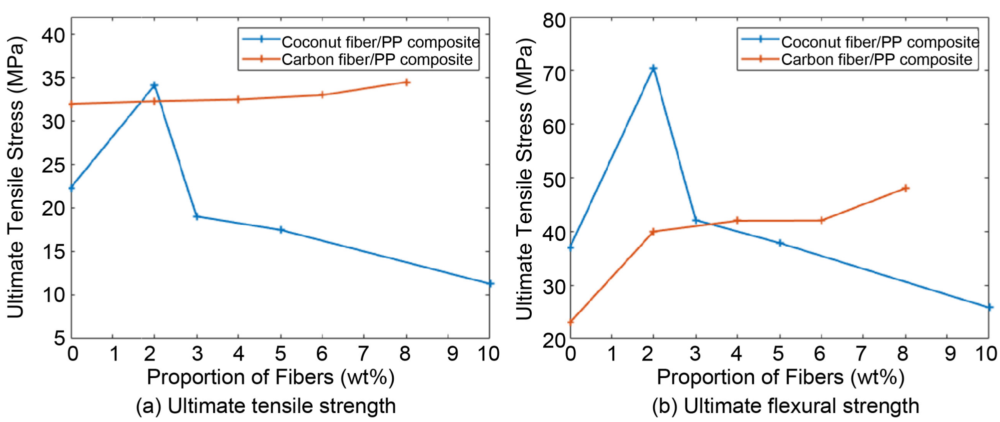


Figure 9. Comparison of mechanical properties of coconut fiber/PP and carbon fiber/PP composites.

3.2. Modelling Results

The regression plots for the artificial neural network model are presented in Figure 10. The maximum values of the coefficient of determination (R^2) obtained for the training, validation, and test data are 0.9984, 0.9996, and 0.9884, respectively. The value of R^2 for all the responses was determined to be 0.9785, which shows a good fit between the artificial neural network predicted values (Y_j) and target values ($\hat{Y}_j$).

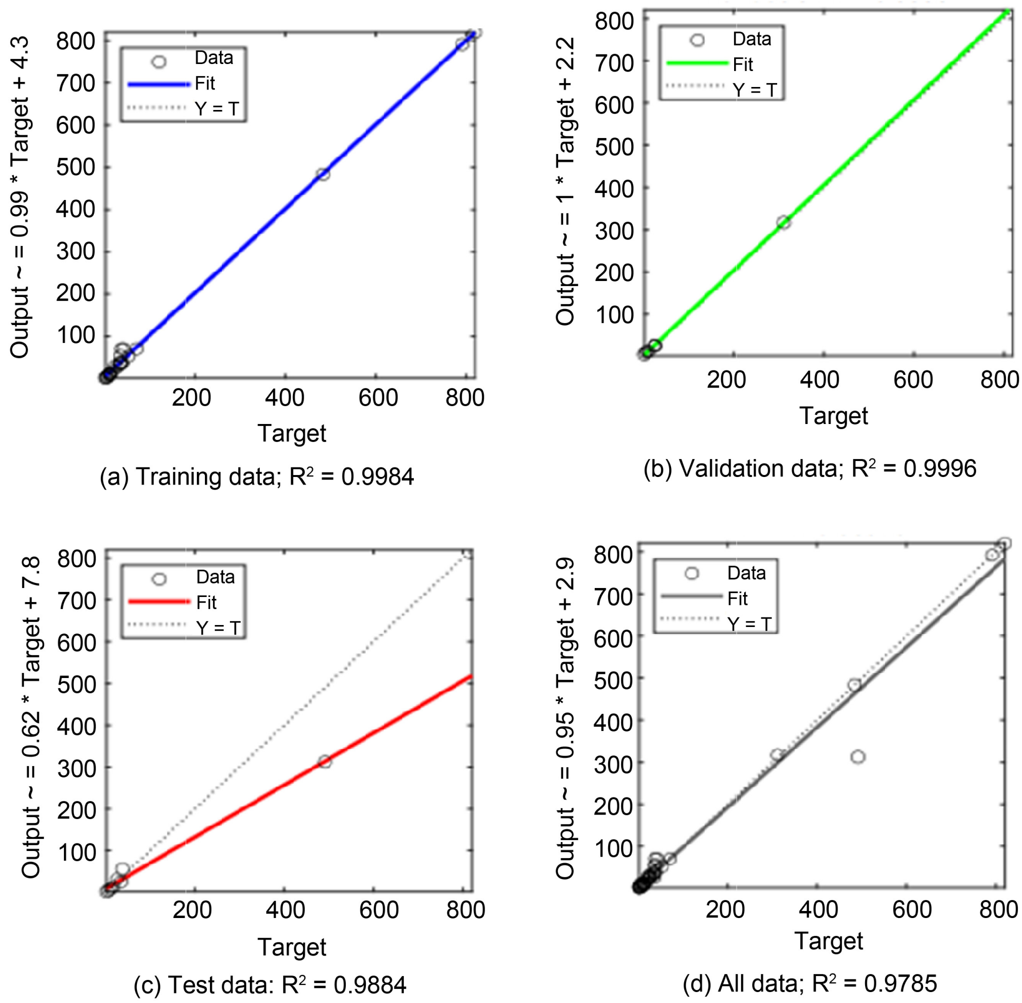


Figure 10. Artificial neural network regression plots.

Comparisons of the actual and predicted tensile properties are presented in Figure 11. It can be seen in the figure that there is a close correlation between the predicted and experimental (experimental values). Figure 12 shows a comparison of comparison of actual and ANN-predicted flexural properties. A fairly close fit between the two data sets is revealed in the figure. The model developed, however, did not produce accurate results in some instances. This may be due to overfitting since the data set used for training was small. The model can, therefore, be said to be indicative and not generalized.

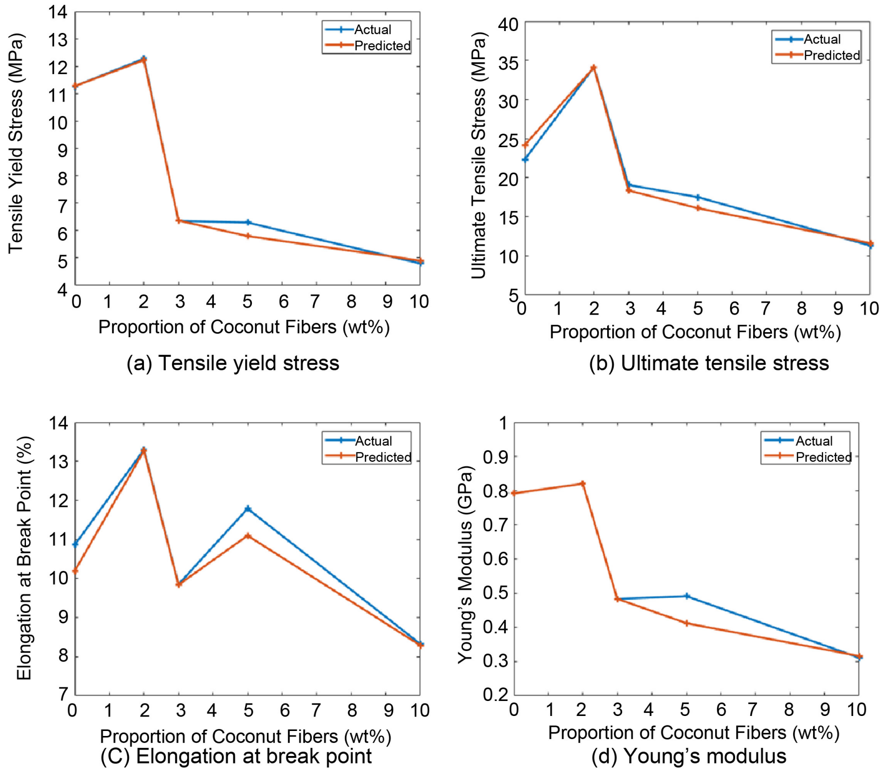


Figure 11. A comparison of actual and ANN-predicted tensile properties.

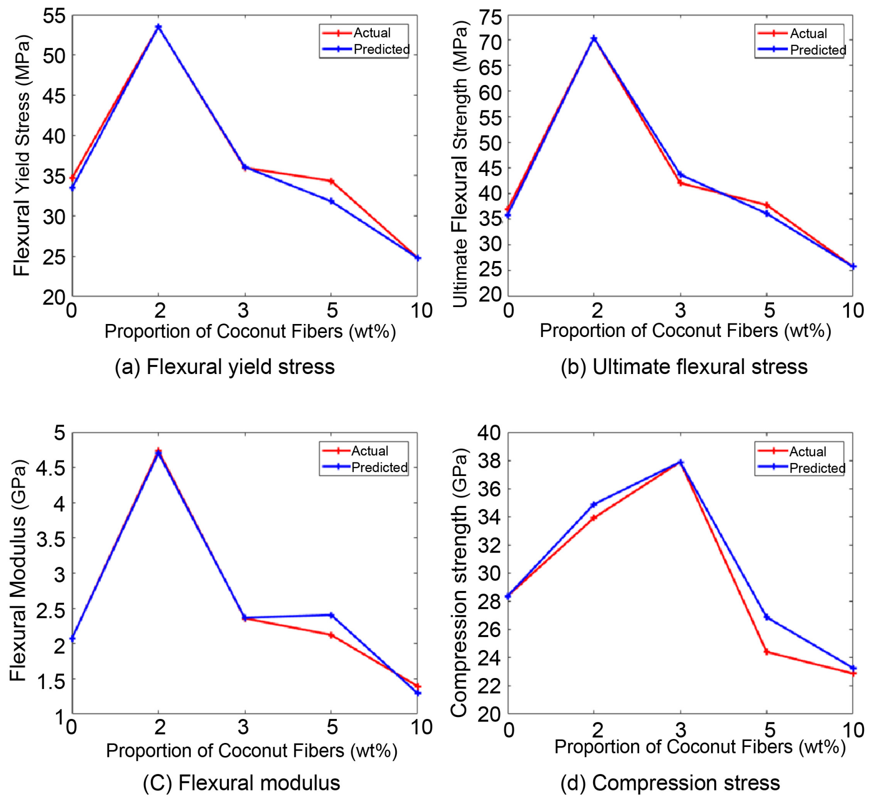


Figure 12. A comparison of actual and ANN-predicted flexural and compression properties.

4. Conclusion

This research work has demonstrated the feasibility of using coconut fibers as a reinforcement agent in polymer-based composites. The composite samples were additively manufactured using the fused filament fabrication method. The effects of the fractions of coconut fibers on the composites' tensile, compression, and flexural properties have been explored. It was observed that these properties are greatly affected by the quantity of coconut fibers in the composite. The mechanical strengths of the composite were found to increase with the increase in the percentage of coconut fibers in the composite and then decrease after some optimum points. The maximum tensile and flexural strengths were obtained for the composites reinforced with 2 wt% of coconut fiber, whereas a composite loaded with 3 wt% of coconut fibers yielded the highest compression strength. The tensile and flexural strengths of the reinforced polypropylene were found to be better than those of carbon fiber-reinforced polypropylene, which is currently used to fabricate automobile parts such as bumper fascia and dashboards [16]. The developed composites can be an alternative to carbon fiber-reinforced polypropylene composite. The artificial neural network model developed generally showed a close correlation between the actual and predicted values. However, in some instances, the model produced inaccurate data. This may have been due to overfitting, which was occasioned by the small amount of training data. Future research should focus on using a large data size to produce a generalized model.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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