

Modeling for Predicting the Mechanical Properties of Calcium Carbonate Filled Coir-silk Squash Hybrid Composites Using Response Surface Methodology and Artificial Neural Network

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Abstract

Presently, there is a need to switch for more sustainable and renewable materials because of its low weight, economic, eco-friendly, biodegradable and easily recyclable. The samples of coir, silk squash hybrid composites filled with calcium carbonate (CaCO_3) powder have been prepared using hand lay-up technique and the mechanical properties of the prepared hybrid composite material are determined. The aim of the present work is to evolve the knowledge-based system to estimate the mechanical properties (tensile strength, flexural modulus, and impact strength) of these hybrid composites. Mechanical properties like tensile strength, flexural modulus, and impact strength have been evaluated by varying the input parameters. The morphological properties of the polymer composites were studied in the present study. Feed forward neural networks were successfully trained and the model is validated by testing it with experimental data. Also, regression equations are developed for tensile, flexural and impact strengths in terms of the input variables using Response Surface Methodology (RSM). The prediction accuracy of both RSM and Artificial Neural Network (ANN) models is good and the three statistics namely R^2 , average absolute deviation error, and mean absolute error calculated for both the models suggest that ANN modelling has better predictability.

Keywords

Coir, Silk squash, Response surface methodology, Artificial neural network, Calcium carbonate

Introduction

The usage of artificial fibers (glass and carbon fibers) is widely used in various industrial application has quite common. However, these fibers are not up to the mark in work efficiency, non-degradable in nature and when they burn it generates large amount of pollution. Eventually the focus of the scientists shifted towards investigation on natural fiber reinforced hybrid composites [1, 2]. These days, remarkable attention has been perceived in natural fiber as an alternate for glass and ceramics owing to their environmental, renewable and degradable nature, economical, less weight, higher mechanical strength, etc. So far, natural fibers like bagasses, *Abutilon indicum*, jute, *Cardia dichotama*, ramie, loofah, oil palm, kenaf and hemp natural fibers have been examined as reinforcements to fabricate fiber reinforced polymer composites. Many investigations have been carried on different natural fibers from past few years, where good results are obtained from natural fibers in comparison with artificial fibers. These natural fibers are easy to obtain and also very cheap since they are deriving from natural and eco-friendly sources [3, 4].

Boukhoulda et al. [5], worked on alfa reinforced composites and observed micro structural and mechanical properties of alfa fibers through the various extraction processes; Accordingly, water retting, alkali treatment, and mechanical extraction are the accentuated areas of work. Henceforth, when the microscopic observations through scanning electron microscope were made, trachoma, uniformed layer formation, and porous surfaces were revealed. Significantly, the work highlights the importance of each process, especially as the best ecological approach and also the importance of alkali treatment-10% NaOH-leads to 976 MPa of strength at break and elastic modulus of 40 GPa. Mouhoubi et al. [6], investigated behavior of the alkali treated alfa fibers. In this regard, 5% NaOH solution is contrived for different immersed periods (2 - 72 h). Accordingly, the treatment contributed to a decrease of absorbance after 6 h cut off. Besides, alkali treatment increased the crystallinity and hence, their stiffness. Further, the treatment degrades the fiber surface, enabling better adhesion at the interface. Likewise, few researchers like Bessadok et al. [7], Bourahli and Osmani [8], Mohanthy et al. [9, 10] endeavoured on the effect of such alkali treatment to observe various aspects of fiber composites. Sumi et al. [11], investigated the hydrophobicity of coir fibers with special reference to surface modification. It is found that unmodified samples stayed in the oil-water mixed interface while surface modified samples moved towards the oil phase. Low polarity is reported in the work exhibiting hydrophobic nature. Jayaramudu et al. [12], have concentrated on establishing the relationship between alkali treatment, morphology and tensile properties of fiber-polycarbonate composites. The author reveals that the integrated approach enhanced the tensile properties of *C. dichotama* fabric. The hemi cellulose was found to be eliminated by the alkali treatment and voids were found to be filled by the polymer. Also, the treatment enhanced the interfacial adhesion among the matrix and fiber. In the Fourier transform infrared spectroscopy study, it was observed the peak at 3431 cm^{-1} identifies the hydrogen-bonded O-H peak in cellulose.

Jayaramudu et al. [13], studied on the structural and tensile strength of *C. dichotama* cellulose fabrics. The morphology was found to be mesh kind of structure for the raw, bleached and alkali-treated (5% NaOH) cellulose fabrics. The treated fibers reported maximum tensile strength of 36.2 MPa and elastic modulus of 3699.2 MPa in comparison to raw and bleached ones. This work provides detailed information on the aforementioned fiber, its availability and typical properties. Amin et al. [14], is also used as a filler element for the reinforcement and gave good results, due to its lowest thermal conductivity and bulk density. Coir fiber can be prominently a component in natural fiber hybrid composites. Prasad et al. [15], worked on the flexural properties of the different weight proportioned untreated coir reinforced composites and values are predicted using ANN tool and the values closure are to experimental flexural properties.

Sathiyamurthy et al. [16], carried out mechanical properties of different wt.% calcium carbonate filled coir-polyester composites and mechanical properties are predicted and optimized using ANN and RSM. They concluded that ANN predicted values are much closure to experimental results than RSM predicted. Nwobi-Okoye and Ochieze [17],

prepared aluminium/different wt.% cow horn particle filled metal matrix composites and evaluated hardness values. The authors are predicted and optimized the hardness values using RSM, ANN, and simulated annealing. ANN predicted values (99.21%) and RSM predicted values are 95.41% near to the experimental values. Experimental values are optimized using simulated annealing and these composites were used in brake drum applications. Saba et al. [18] studied the effect of oil palm nano fillers on kenaf fiber reinforced composites and observed that enhance the interfacial bonding between fiber-matrix and the mechanical properties were improved with the inclusion of nano fillers in the composites. Saba et al. [19] explored the importance of nano filler in natural fiber reinforced composites.

Jagadish et al. [20] developed sundi powder fiber reinforced composites; the experiment was carried on abrasive water jet machining and evaluated surface roughness and process time. The authors were also carried prediction and optimization using RSM. Nikzad et al. [21] reported modeling of the rice husk composites using RSM and ANN. In this, they considered pre-treatment time, solid concentration and NaOH concentration are the input parameters and glucose and xylose are the output parameters. For these input and output parameters RSM and ANN techniques were applied and they concluded ANN predicted values are better than RSM values and other researchers also carried by Parikh and Gohil [22].

Sen and Reddy [23], concluded that silk squash due to its less weight and more fiber content in (wt.%) is very useful as a natural fiber. The density of luffa fiber is around $0.82 - 0.92\text{ g/cm}^3$ which is lower when compared with other common natural fibers like hemp, cotton, sisal, etc., inclusion of inorganic filler in the composite processing increases the mechanical behavior of the hybrid composite. The particles filled coir-silk squash hybrid composites can be used as a source in many industrial sectors such as automotive, packing, aircrafts, etc. These hybrid composites are more advantageous due to its recycling capacity, eco-friendly, low weight, low cost, non-toxicity and no abrasion during processing.

Several studies have been carried out on different chemical treatments of natural fibers such as jute, flax, hemp, and kenaf to improve the mechanical characteristics of composite materials. Among these natural fiber hybrid composites calcium carbonate-coir-silk squash hybrid composite didn't gain much attention. Coir is an accessible, flexible, inexpensive, and biodegradable lignocellulose fiber that is used to make a wide range of products.

In this work, the mechanical properties of these natural fiber hybrid composites such as tensile, flexural, and impact strength are investigated. Study on these mechanical properties is very important in comparison to physical and chemical properties. The stiffness, flexibility and other aspects of the natural fibers can be determined by knowing the mechanical properties of the fiber composites. Mechanical Properties of the hybrid composites was precisely studied and compared the predicted results by ANN and RSM algorithm techniques. In using aforesaid techniques, optimization and prediction of the mechanical properties is possible, which is currently done in the work.

Experimentation

Materials

The main ingredients in the matrix are epoxy LY-5062 and hardener HY-5062 brought from Sri Lakshmi Industrial Composites, Hyderabad (Telangana, India). In the preparation of composite specimens, the epoxy and hardener were mixed in 10:1 ratio. The inorganic filler purchased from Hyderabad Composites, (Telangana, India) and mixed with equal properties before adding to the matrix 2% and 4% by weight.

Hand lay-up technique

For fabricating coir-silk squash hybrid composites, a hand lay-up process was generally preferred for the fabrication of the various hybrid composite laminates. Before fabrication of a release agent, Wax is applied to the mold's surface. The resin and fibers were impregnated in the mould and a load of 500 N applied for about 24 h to compress the composites, then the composite moulds were kept in a woven at 80 °C for 15 min. Followed by this, the specimen was released from the mold and further it was processed to cure at room temperature for 24 h. Different combinations of CaCO₃-coir-silk squash hybrid composites were prepared by the earlier process.

Evaluation of mechanical properties

For tensile test, ASTM D3039 standards were used; specimens were cut in definite dimensions of 150 x 15 x 3 mm³ from the fabricated composites and tested in universal testing machine (INSTRON). The INSTRON machine as per ASTM-07 standard was used to conduct three-point flexural tests of specimen with dimension 150 x 13 x 3 mm³. Izod impact testing machine as per ASTM 256-06 standard was used for impact strength testing. For impact test, the specimens were cut with dimension of 62.5 x 12.7 x 3 mm³ from the fabricated composites.

Statistical model of responses

Nonlinear regression is used for independent variables

(Coir, silk squash and filler weight) to estimate the mechanical properties like tensile strength (TS), flexural modulus (FS), and impact strength (IS) by using Minitab 17. Coefficient of determination (R²) values for tensile strength, flexural modulus and impact strength were determined to know the predictive capability of developed models.

ANN model

ANN module is used to predict the mechanical properties of CaCO₃ impregnated coir silk squash fiber hybrid composites. It produces analytical model to predict flexural, tensile, and impact strengths.

Each neuron has input which can produce an output and it can be observed as a reflection of local information. It has trained in Matlab software. Hidden neurons are identified if MSE (Mean square error) value was minimum by Betiku et al. [24]. ANN structure consists of three stages, input layer as input data to the network, hidden layer compute the mathematical operations on the known data, output layer considered as target to the given network. For the prediction, nonlinear sigmoidal or sigmoidal transfer computational functions used in the hidden layer and linear or other type of transfer computational function were used in output layer. From equation 1, P_i is input from unit i, W_{ji} is network weight, and bias b_j connected to jth unit.

$$\text{net}_j = \sum_{i=1}^n W_{ji}P_i + b_j \quad (1)$$

Because of sigmoidal or any other transfer computational function in jth unit, the algebraic sum of weighted input is altered to output O_j by using appropriate transfer computational function as given in equation 2 and transmitted as input (O_j) to the neuron in the following layer.

$$O_j = f(\text{net}_j) = \frac{1}{1 + e^{-(\text{net}_j)}} \quad (2)$$

After every neural network forward iteration, expected outputs (O_j) are compared with outputs (T_j) and MSE is cal-

Table 1. ANOVA table of outcomes.

Source	Impact strength (KJ/m ²)			Flexural modulus (MPa)			Tensile strength (MPa)		
	Adj SS	F-value	P-value	Adj SS	F-value	P-value	Adj SS	F-value	P-value
Model	143.454	23.23	0	1935662	31.01	0	92.58	8.43	0.002
Linear	269.876	43.7	0	4285153	68.66	0	14.48	1.32	0.328
C	694.3	112.4	0	1.1E+09	182.3	0	31.91	2.91	0.122
L	60.46	9.79	0.012	2459565	3.94	0.078	2.391	0.22	0.652
F	54.82	8.88	0.015	1229902	19.71	0.002	9.135	0.83	0.385
Square	9.122	1.48	0.279	5328995	8.54	0.008	241.6	22.01	0
c*c	3.868	0.63	0.449	4582617	7.34	0.024	460.1	41.9	0
f*f	14.37	2.33	0.161	6075373	9.73	0.012	23.25	2.12	0.18
2-way interaction	2.323	17.26	0	5213479	8.35	0.006	71.31	6.5	0.012
c*l	2.354	0.38	0.555	3824662	6.13	0.035	35.26	3.21	0.107
c*f	315.1	0.38	0.552	2395718	0.38	0.551	178.6	16.27	0.003
l*f	6.176	51.02	0	1157620	18.55	0.002	0.055	0	0.945
	R ² = 95.38%			R ² = 96.50%			R ² = 88.23%		

culated as follows:

$$MSE = \frac{1}{n} \sum_{i=1}^n (T_{ij} - O_{ij})^2 \quad (3)$$

Where, N is the number of input data points, O_{ij} is the predicted output, and T_{ij} is the experimental output.

Results and Discussion

Nonlinear regression models

Quadratic regression model was developed for every response based on the optimal fit of investigational data to study the effect of mechanical properties. The resulting model's statistical significance was assessed using Analysis of Variance (ANOVA). Maximum tensile strength is observed as 56.66 MPa at 20 g of coir and 6.2 g of silk squash, maximum flexural and impact strength were 58956.24 MPa and 68.42 kJ/m² at 30 g of coir and 5.7 g silk squash, respectively. The ANOVA and estimated regression coefficients on the mechanical properties are tabulated in the table 1. In RSM, if the p-value of the independent variable is <0.05, then it is considered as significant. In estimating the value of one variable from the given value of another, statistical tool and regression analysis are helpful. For co-relating the responses, tensile strength (T), flexural modulus (S) and impact strength (I), considered input variables such as coir fiber weight (C), silk squash weight (L) and filler content (F), a mathematical relationship is obtained from the coefficients. The mathematical equations for tensile strength, flexural modulus and impact strength were repre-

sented by equation 4, 5, and 6. For the prediction of future outcomes, the coefficient of determination (R^2) is used in context of statistical tool established on the other related information. The coefficient determination R^2 that fits the model is 88.23% for tensile strength, 96.5% for flexural modulus, and 95.38% for impact strength. If the R^2 value is nearer to 100%, then the model is treated as more significant to predict the responses as explained in the literature [17, 25, 26]. The proposed equations of the expected model in uncoded units are represented by the following equations.

$$\text{Tensile strength} = 72.8 + 0.52 \times c - 11.99 \times l + 3.6 \times f - 0.1072 \times c \times c + 0.603 \times f \times f + 0.686 \times c \times l - 0.2363 \times c \times f - 0.13 \times l \times f \quad (4)$$

$$\text{Flexural modulus} = 29065 + 6631 \times c - 28171 \times l - 34117 \times f - 33.8 \times c \times c - 974 \times f \times f - 714 \times c \times l - 27.4 \times c \times f + 6212 \times l \times f \quad (5)$$

$$\text{Impact strength} = 183.8 + 1.47 \times c - 24.31 \times l - 63.40 \times f + 0.0098 \times c \times c + 0.474 \times f \times f - 0.176 \times c \times l - 0.0271 \times c \times f + 10.25 \times l \times f \quad (6)$$

ANN models of outcomes

The feature coir fiber weight, silk squash fiber weight and filler weights were considered as inputs and tensile strength, flexural modulus, and impact strength are the outputs. For training the network, the input neurons and output neurons should be normalized between 0 and 1. 3-5-3-1 feed forward network is selected to predict tensile strength after training the ANN network. 3-7-4-1 and 3-5-4-1 networks are selected for flexural and impact strengths. For training of tensile strength

Table 2. Comparison of different model values.

S. No.	Factor1	Factor 2	Factor 3	Response 1			Response 2			Response 3		
				Tensile strength (MPa)			Flexural modulus (MPa)			Impact strength (KJ/m ²)		
				EXP	RSM	ANN	EXP	RSM	ANN	EXP	RSM	ANN
1	10	5.7	0	38.5	38.0	38.4	38278	35240	38232	50.2	50.8	50.2
2	10	5.7	2	42.5	41.4	42.6	29449	33378	29384	42.0	42.2	42.0
3	10	5.7	4	48.8	49.6	48.8	25173	23725	25028	36.4	37.4	34.8
4	20	5.7	0	50.7	50.1	50.6	50086	50712	50075	58.9	58.4	58.9
5	20	5.7	2	46.9	48.8	47.4	46391	48302	45860	53.0	49.3	53.0
6	20	5.7	4	51.3	52.3	49.9	39374	38101	39598	43.2	44.0	46.4
7	10	6.2	0	33.5	35.4	34.3	28350	30261	28519	36.7	37.4	36.8
8	10	6.2	2	35.4	38.7	34.3	35877	34612	35700	42.3	39.5	43.9
9	10	6.2	4	50.6	46.8	47.7	31188	31171	31258	44.7	44.9	44.7
10	20	6.2	0	56.6	51.0	54.3	42503	42163	42478	44.2	44.5	44.2
11	20	6.2	2	48.9	49.5	48.72	48990	45966	49397	42.7	45.6	42.7
12	20	6.2	4	49.5	52.9	49.2	39709	41977	39432	50.13	50.59	50.10
13	30	5.7	0	39.1	40.8	39.0	58956	59424	60124	68.4	68.0	61.2
14	30	5.7	2	36.8	34.8	36.3	58156	56466	58128	54.2	58.3	61.3
15	30	5.7	4	33.8	33.6	34.5	44928	45717	44205	54.3	52.4	54.2
16	30	6.2	0	42.2	45.1	42.4	46756	47305	46760	54.3	53.2	54.3
17	30	6.2	2	40.8	39	41.27	50232	50560	49792	54.2	53.8	58.5
18	30	6.2	4	37.1	37.6	40.8	46138	46023	45664	58.3	58.1	61.2

Table 3. Comparison of R² and AAD values for the three outcomes.

	Tensile strength		Flexural modulus		Impact strength	
	ANN	RSM	ANN	RSM	ANN	RSM
R²	0.96218	0.8823	0.9979	0.965	0.886	0.9538
AAD	0.02002	0.070749	0.006648	0.03978	0.02934	0.04400
Absolute mean error	0.015177	0.059697	0.005063	0.02609	0.02288	0.03220

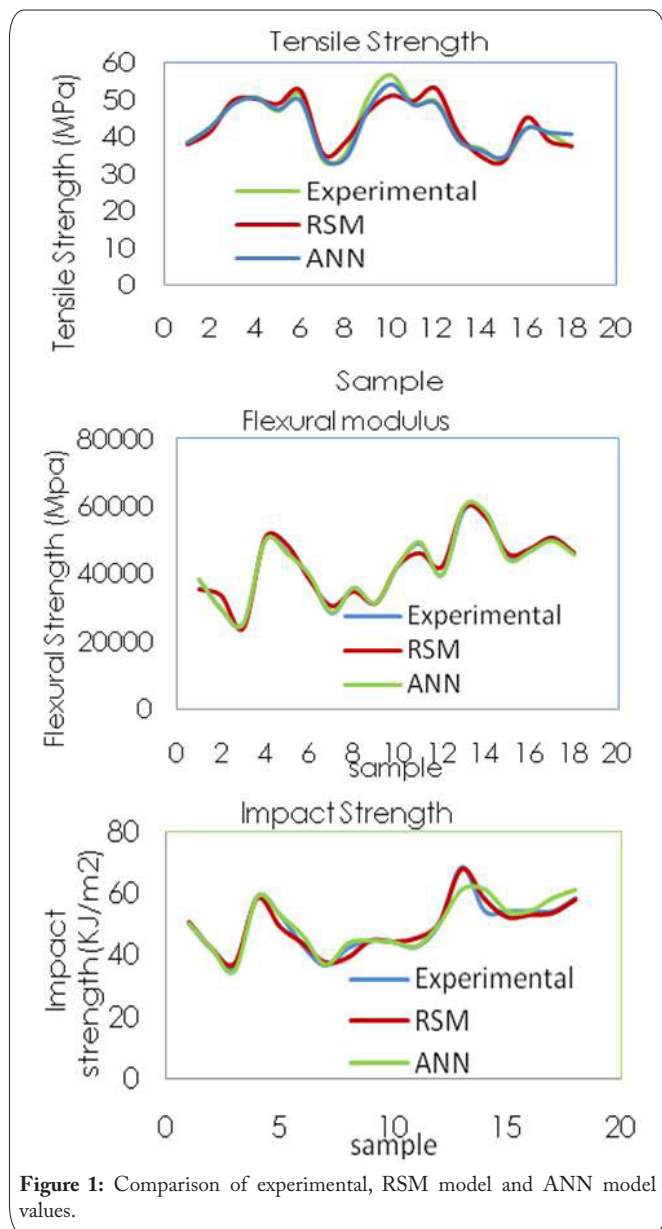


Figure 1: Comparison of experimental, RSM model and ANN model values.

values, training parameters of 1000 epochs and zero goal were used. By setting the same target values in learning processes, the performance curves for flexural and impact strength behaviours are also obtained.

The mathematical models were developed using RSM and ANN for predicting properties of the tensile, flexural, and impact strengths. The R² and AAD (Average absolute deviation) were evaluated, and their values were used to choose the best model. The R² and AAD were computed by equation 7 and 8, respectively.

$$R^2 = 1 - \frac{\sum_{i=1}^n (Y_{i,Cal} - Y_{i,Exp})^2}{\sum_{i=1}^n (Y_{avg,exp} - Y_{i,Exp})^2} \quad (7)$$

$$AAD = \left\{ \left[\sum_{i=1}^n \left(\frac{|Y_{i,exp} - Y_{i,cal}|}{Y_{i,exp}} \right) \right] \frac{1}{n} \right\} \times 100 \quad (8)$$

For forward neural network modelling, the experimental data was divided into three sets: training, validation, and testing sets. For training 12 samples are considered and for each validation and testing consist of 3 samples. For better overview of the model, experimental data was pre-processed in between 0 and 1, and after the training, post processed values are converted into the original form using appropriate Matlab codes. The performance of the trained model was judged on unseen data on the basis of R² and MAE.

For tensile strength, the best validation performance occurred at epoch 2 and the validation error is minimum. After the epoch 2, both the test set error and validation set error is displayed similar, till the validation was stopped at 31 epochs. The coefficient of determination value R² is 0.962 for tensile strength which indicates that the predicted values are very close to experimental output and the model provides accurate predictions. Similarly, for flexural and impact strength R² values are calculated. Further comparison of experimental values and predicted values are provided in table 2.

Figure 1 shows that ANN model values are close to experimental values, when compared to RSM values. The R², AAD, and absolute mean error values of ANN and RSM models for tensile, flexural and impact strengths of the composite are presented in table 3.

Conclusion

This work has investigated synthesis and the mechanical properties of CaCO₃ particles filled coir-silk squash hybrid composites which can be a significant source in automotive and packing industries. Further prediction of aforementioned mechanical properties was carried out using ANN and RSM algorithms. Furthermore, R² and AAD values are calculated for both the models. From these ANN is the best predictor when compared to RSM. The present study underlined the importance of prediction in the field of hybrid composites. The maximum tensile, flexural and impact strengths were retrieved at 20 g of coir, 6.2 g of silk squash and 30 g of coir, 5.7 g of silk squash, respectively.

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None.

Conflict of Interest

The authors declare that there is no conflict of interest.

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