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Empirical Modelling of Developed Polyvinyl Chloride –Grass Composite

Olodu D.D[1*] and Osarenmwinda J.O[2]
[1*]Department of Mechanical Engineering, Faculty of Engineering, Benson Idahosa University, PMB 1100, Benin City, Edo State, Nigeria
[2]Department of Production Engineering, Faculty of Engineering, University of Benin, PMB 1154, Benin City, Edo State, Nigeria
E-mail: *dolodu@biu.edu.ng (Tel: +234-8065325363),
E-mail: joosarenmwinda@uniben.edu (Tel: +234-8023718684)

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ABSTRACT

Inadequate empirical models to predict the mechanical properties of composites pose great challenges in polymeric industries. This study was carried out to develop empirical models for predicting the mechanical properties of injection moulded Polyvinyl Chloride-Grass composite. The experimental results obtained from the mechanical properties of the developed Polyvinyl Chloride-Grass composite was used to develop the empirical models for tensile strength, proof stress, percentage elongation and flexural strength respectively. The purpose of this study is to produce new fangled empirical models for predicting the mechanical properties of composite. Furthermore, the experimental values and the developed models adequacy were determined using coefficient of determination (R^2) and mean absolute percentage error (MAPE). The coefficient of determination obtained for tensile strength, proof stress, percentage elongation and flexural strength were 0.9828 (98.28%), 0.9385 (93.85%), 0.9787 (97.87%) and 0.9847 (98.47%) respectively. This indicates that a substantial good fit was achieved by the models developed. The mean absolute percentage error (MAPE) of the developed models for tensile strength, proof stress, percentage elongation and flexural strength were also 4.21%, 5.10%, 6.53%, and 0.20% respectively which was below 10% recommended. The values obtained from the validation of these models were therefore found to be satisfactory, and shows good predictability of the model and its adequacy.

1. Introduction

Inadequate investigation of process parameter and their interaction in the production of composites is a great challenge. Moreover, there are inadequate empirical models to predict mechanical properties of some process variables of plastic-grass composites. Chunping et al. [1] carried out a study aimed to model fundamental bonding characteristics and performance of wood composite. In their study, mathematical models were developed to predict the variation of inter-element (strand) contact during mat consolidation. The mathematical predictions agree well with each other based on the results obtained. Their results showed that the relationship between the inter-element contact and the mat density was highly nonlinear and was significantly affected by the wood density and the element thickness. Harless et al. [2] examined mechanical properties of composite panels, from their study it was observed that the density variations have relation with the pan thickness. They then proposed an analytical tool to predict density profile as a function of the manufacturing processes. Osarenmwinda and Nwachukwu [3] focused *on* the development of empirical models to estimate properties of produced composite material from agro waste (sawdust and palm kernel shell). The empirical model was used to predict the properties of composite material (hardness, yield strength, ultimate tensile strength, modulus of elasticity, modulus of rupture, internal bond strength, density, thickness of swelling and water absorption) taking the inputs as percentage composition of sawdust and palm shell respectively. The empirical model was developed using "Mathematical Product" software program expressing the outputs in the quadratic form. The model performances were found to be satisfactory and show good predictability.

Adeyemi and Adeyemi [4] developed empirical formulas based on the diffusion model, they determined the moisture ratios with its drying times for composite obtained from sawdust. The results were computed and presented for various curing temperature and at different percentages of hardener resin addition. The physical parameters of four kinds of composite boards were determined by them in their study. The unsteady-state diffusion coefficients and surface emission coefficients of moisture in boards were separated in one experimental period by using the method of linear regression. Then the moisture transfer processes in board were analyzed by using finite element method (FEM), and the moisture absorption processes of four kinds of boards were observed experimentally. By comparing the computed results with the experimental results, it showed that the error was within 10%. Therefore, they came to the conclusion that the processes of moisture transfer in composite can be described by using FEM. Olayinka Oderinde [5] examined Bio-inspired and lanthanide-induced hierarchical sodium alginate/graphene oxide composite paper with enhanced physicochemical properties. His reports was based on an artificial nacre-like composite paper based on sodium alginate (SA) and graphene oxide (GO) by lanthanide ions cross-linking. SA-coated GO were used as building “bricks and mortar” and self-assembled into aligned GO/SA composite hydrogel by the coordination of lanthanide ions. Subsequently, the hierarchical GO/SA composite paper was formed under evaporation. According to Olayinka [5], the lanthanides enhanced the mechanical properties of the GO/SA composite papers (strength of 255.8 ± 8.52 MPa and toughness of 4.83 ± 0.28 MJ m^{-3}), this endowed the papers with high stability. These features greatly expand the application of the composite papers, which were believed to show competitive advantages in aerospace, electronic devices, and thermal interface materials [5].

This study therefore focused on empirical modeling of developed Polyvinyl Chloride-Grass for predicting the mechanical properties of injection moulded Polyvinyl Chloride-Grass composite.

2. Materials and Method

2.1 Equipment and Tools

i. Two stage-screw plunger injection machine (Fox and Offord, 70 tons two stage-screw plunger)
ii. A toggle clamp attached to the injection end of injection moulding machine was used.
iii. The mould was made of Silicon – killed forging quality steel AISI type H140 treated to 252–302, Brine 11. Such steel was used for moulds that require high quality parts, long production runs and is s safe to use at high clamping pressures.
iv. MonsantoTensometer, Type ‘W’ Serial No. 8991was used for tensile testing experiment.

2.2 Materials used for Processing

(a) The grass used for this research work is giunea grass (*Panicum maximum*), it was obtained from Benin City, Edo State, Nigeria**;**
(b) The plastic material used for this study was polyvinyl chloride (PVC), it exist in powder form and was obtained from Adig Plastic Company Limited in Lagos State, Nigeria

2.3 Preparation and Processing of Grass

The harvested grass was washed and soaked with dilute sodium hydroxide (NaOH) of concentration 0.10mol/dm^3 for 6 hours to ensure effective bonding between the grass and the plastic (Polyvinyl Chloride) materials. The grass was grinded to granules using crushing machine. The grasses were first air dried in the sun and later transferred to an oven and dried at 105^{o}C. It was continuously monitored until moisture content of about 4$\underline{+}$0.2% was obtained [6]. The ground grass was screened to a particle size of 300μm diameters using vibrating sieve machine.

2.4 Mixing, Compounding and production of Composite

Polyvinyl Chloride (PVC) was mixed with grinded grass in the proportion shown in Table 1.The prepared polyvinyl chloride-grass composite was blended in a cylindrical container until a homogenous mixture was obtained in the composite. The homogenous mixture of the composite was feed into the hopper of injection moulding machine and was produced at barrel temperature ranging from 210^{o}C to 310^{o}C respectively.

Table 1: Composition of the Produced PVC-Grass Composite [3, 7, 8]

Serial Number	Percentage by Volume of Plastic (PVC)	Percentage By Volume of Grass
1	80	20
2	70	30
3	60	40
4	50	50
5	40	60
6	30	70
7	20	80

The produced composite was evaluated for mechanical strength (tensile strength, proof stress, percentage elongation and flexural strength). In this study, all empirical models were developed using experimental values (E) obtained from the mechanical properties test results (tensile strength, proof stress, percentage elongation and flexural strength respectively). The empirical models were used to predict the mechanical properties of the developed composite by taking the inputs as percentage by volume of PVC (M), percentage by volume of grass (K) and barrel temperature (T).

The output was obtained through the interaction between M, K and T. A quadratic model of second order regression was obtained for the PVC-Grass composite for mechanical properties (Tensile Strength, Proof Stress, Percentage Elongation, and Flexural Strength). A code was written in a MATLAB program (MATLAB software, version 7.5.0; R2007b) to investigate the interactions of the various parameters of the developed empirical model. The empirical model was expressed in the form shown in Equation 1.

$$Z=\text{Constant}+\alpha_1T+\alpha_2M+\alpha_3K+\alpha_4TM+\alpha_5TK+\alpha_6MK+\alpha_7T^2+\alpha_8M^2+\alpha_9K^2 \quad (1)$$

2.5 Tests for the Adequacy of Models Developed

The mean absolute percentage error, and coefficient of determination were used to test for the adequacy of models developed. They were determined using Equation 2-3.

$$\text{Absolute percentage error} = \left|\frac{\text{Experimental value}-\text{Predicted Value X100\%}}{\text{Experimental Value}}\right| \quad (2)$$

$$\text{Coefficient of Determination, } R^2 = \left[1 - \frac{\sum(Yi - \hat{Y})^2}{\sum(Yi - \bar{y})^2}\right] \tag{3}$$

The Conditions for the Models Development are as follows:

i. The composite was produced from polyvinyl chloride and guinea grass.

ii. The injection pressure remained constant i.e160kg/mm^2.

iii. Guinea grass with particle size of 300µm was used.

iv. All the composite production parameters were kept constant except percentage by volume of material and barrel temperature of the injection moulding machine.

3. Results and Discussion

3.1 Empirical Model Development

Table A1-A4 in the appendix shows the results obtained for tensile strength, proof stress, percentage elongation and flexural strength respectively for PVC-Grass composite; experimental (E), predicted (P) and absolute percentage error .

The empirical models developed for PVC-Grass composite for tensile strength, proof stress, percentage elongation and flexural strength are shown in Equation 4-7 respectively.

$$\langle \text{Tensile Strength for PVC} - \text{Grass Composite } (6_T) = -93.4725 - 0.0629T + 0.5717M + 0.8493K + 0.0069TM + 0.0105TK - 0.0376MK - 0.0014T^2 + 0.0204M^2 - 0.0356T^2 \rangle \tag{4}$$

$$\text{Proof Stres for PVC} - \text{Grass Composite } (6_P) = -61.6083 - 0.0264T + 0.4261M + 0.2420K + 0.0044TM + 0.0070TK - 0.0213MK - 0.0010T^2 + 0.0124M^2 - 0.0192T^2 \tag{5}$$

$$\text{Percentage Elongation for PVC} - \text{Grass Composite } (P_E) = -24.3775 - 0.0130T + 0.1316M + 0.1362K + 0.0018TM + 0.0028TK - 0.0083MK - 0.0004T^2 + 0.0050M^2 - 0.0085T^2 \tag{6}$$

$$\text{Flexural Strength for PVC-Grass Composite (EI)} = -26.8877 - 0.0596T + 0.5647M + 0.4228K + 0.0033TM + 0.0055TK - 0.0212MK - 0.0007T^2 + 0.0071M^2 - 0.0116T^2 \tag{7}$$

Figure 1-4 shows the effects of barrel temperature on the tensile strength, proof stress, percentage elongation and flexural strength for PVC-Grass Composite, both for Experimental (E) and Predicted (P) Values.

3.2. Adequacy of Models for PVC-Grass Composite

The models adequacies were verified by comparing the predicted values from empirical models with its experimental data. In this study, a prediction error of 10% was noted according to the study of Osarenmwinda and Nwachukwu [3]. The results of the predicted values in this study were found to compare favourably with the measured values. The models adequacies were verified using coefficient of determination (R^2) and mean absolute percentage error (MAPE). The coefficient of determination (R^2) were determined to be 0.9828 (98.28%) for Tensile Strength, 0.9385 (93.85%) for Proof Stress, 0.9787 (97.87%) for Percentage Elongation, and 0.9847 (98.47%) for Flexural Strength respectively which indicates that a substantial good fit was achieved by the regression models developed. These values compared favourably with the values obtained by Olodu and

Osarenmwinda [9] with coefficient of determination of 0.92 for tensile strength and 0.88 for flexural strength for HDPE-Sawdust composite respectively.

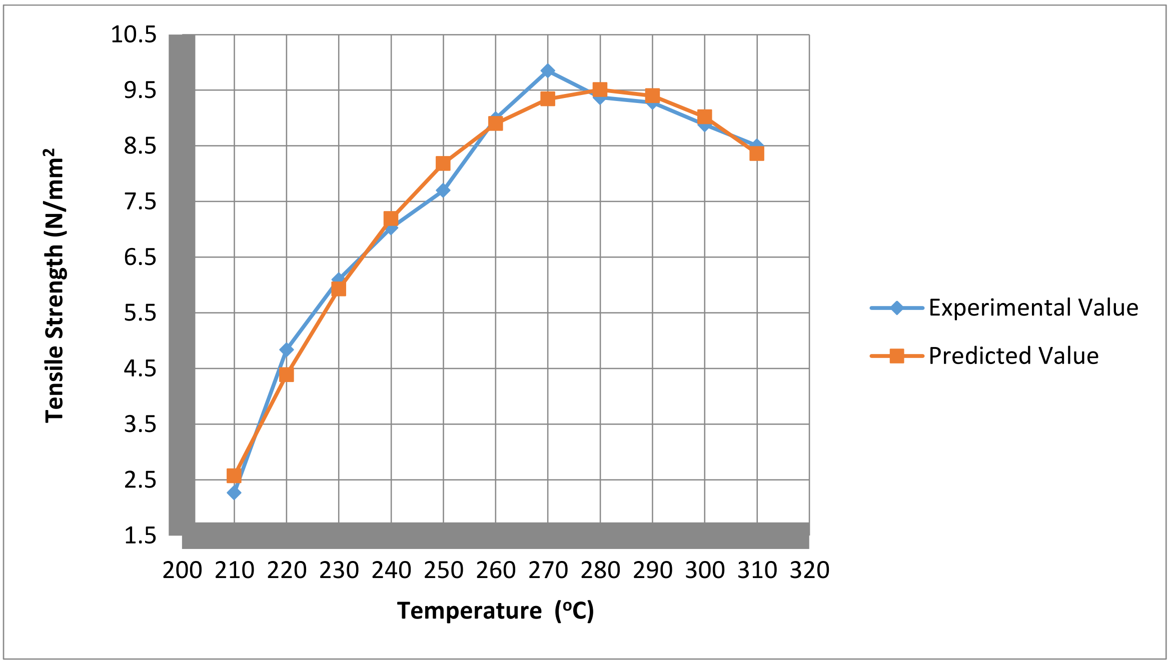

Figure 1: Effects of Barrel Temperature on the Tensile Strength for PVC-Grass Composite; Experimental (E) and Predicted (P) Values

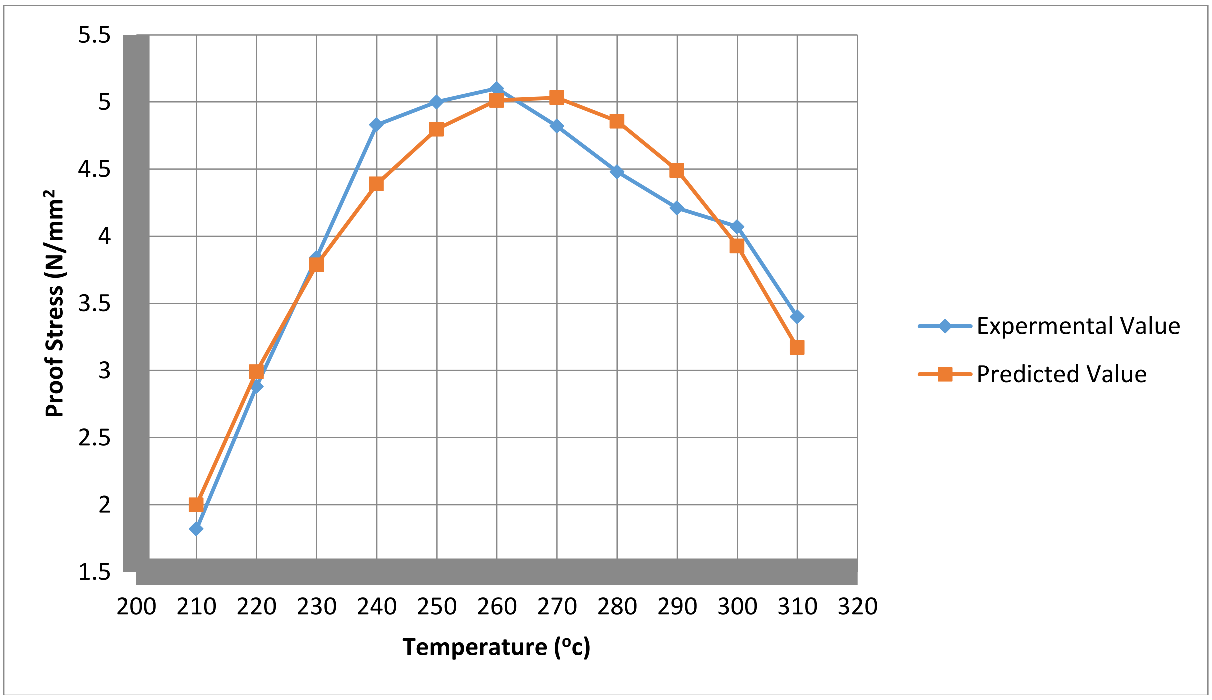

Figure 2: Effects of Barrel Temperature on Proof Stress for PVC-Grass Composite; Experimental (E) and Predicted (P) Values.

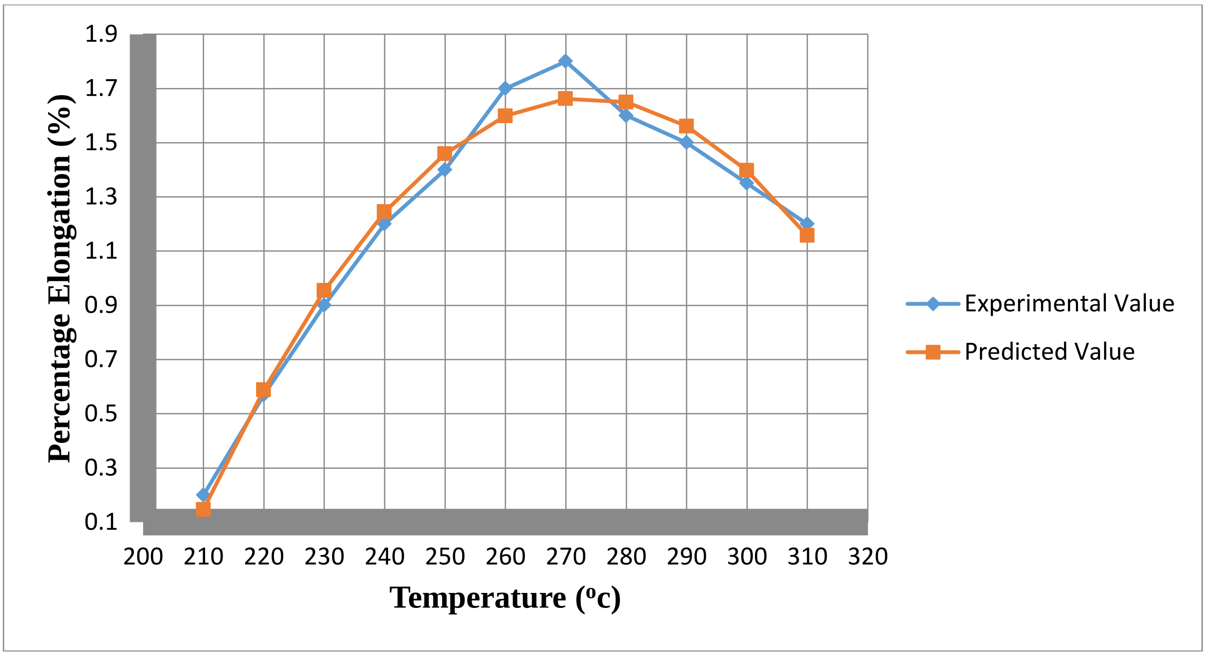

Figure 3: Effects of Barrel Temperature on Percentage Elongation for PVC-Grass Composite; Experimental (E) and Predicted (P) Values

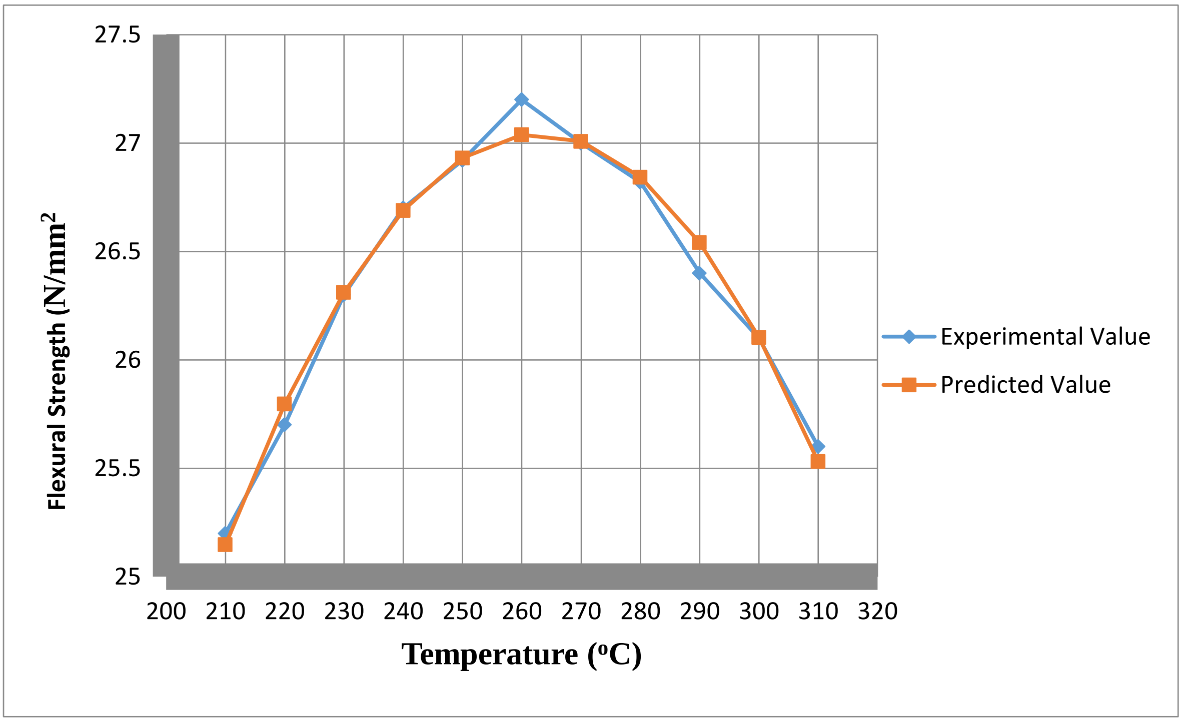

Figure 4: Effects of Barrel Temperature on Flexural Strength for PVC-Grass Composite; Experimental (E) and Predicted (P) Values

Moreover, the mean absolute percentage error of predicted values from model when compare with the experimental values were determined to be 4.21% for Tensile Strength, 5.10% for Proof Stress, 6.53% for Percentage Elongation and 0.20% for Flexural Strength respectively. These values are significantly small and below the maximum error of 10% proposed by Osarenmwinda and Nwachukwu, Liping and Deku [3, 8]. These values were therefore found to be satisfactory and show good predictability of the model and its adequacy.

4. Conclusion

The study of the empirical modelling of developed polyvinyl chloride-grass composite has been achieved. The results from the tests of models adequacy shows that the coefficient of determination obtained for tensile strength, proof stress, percentage elongation and flexural strength were 0.9828 (98.28%), 0.9385 (93.85%), 0.9787 (97.87%) and 0.9847 (98.47%) respectively. The mean absolute percentage error (MAPE) of the developed models for tensile strength, proof stress, percentage elongation and flexural strength were also 4.21%, 5.10%, 6.53%, and 0.20% respectively which was below 10% recommended. These values obtained were therefore found to be satisfactory, and shows good predictability of the model and its adequacy.
It is hopeful that the developed models will also be useful to researcher, industrialist and small scale manufacturers to ease the production of Polyvinyl Chloride-Grass composite.

Nomenclature

The empirical models were expressed in the form
$Z=\text{Constant}+\alpha_1T+\alpha_2M+\alpha_3K+\alpha_4TM+\alpha_5TK+\alpha_6MK+\alpha_7T^2+\alpha_8M^2+\alpha_9K^2$
M= Percentage by volume of plastic (%)
K= percentage by volume of grass (%)
T= Temperature (^oC)
Z= Output (Mechanical properties)
Where $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, \alpha_7, \alpha_8,$ and α_9 are the coefficient of T, M, K, TM, TK, MK, T^2, M^2, and K^2 respectively.
R^2 =Coefficient of determination
Y_i= Experimental value
$\hat{Y}$ = Mean of predicted values
$\bar{y}$= Mean of experimental values

5. Acknowledgement

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6. Conflict of Interest

There is no conflict of interest associated with this work.

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Appendix

Table A1: Value for Tensile Strength for PVC-Grass Composite, Experimental, Predicted and Absolute Percentage Error

Temperature (^{O}C)	**Tensile Strength (N/mm^2). Experimental**	**Tensile Strength (N/mm^2) Predicted**	**Absolute Percentage Error (%)**
210	2.27	2.5749	13.43
220	4.84	4.3890	9.32
230	6.10	5.9287	2.81
240	7.03	7.1939	2.33
250	7.70	8.1845	6.29
260	8.99	8.9007	0.99
270	9.85	9.3423	5.15
280	9.37	9.5095	1.49
290	9.28	9.4022	1.32
300	8.88	9.0203	1.58
310	8.50	8.3640	1.60
Mean Absolute Percentage Error (%)			4.21
Coefficient of determination = 0.9828			

Table A2: Value for Proof Stress for PVC-Grass Composite, Experimental, Predicted and Absolute Percentage Error

Temperature (^{O}C)	Proof Stress (N/mm^2), **Experimental**	Proof Stress (N/mm^2), **Predicted**	Absolute Percentage Error (%)
210	1.82	1.9989	9.83
220	2.88	2.9897	3.81
230	3.84	3.7864	1.40
240	4.83	4.389	9.13
250	5.00	4.7974	4.05
260	5.10	5.0117	1.73
270	4.82	5.0318	0.78
280	4.48	4.8577	8.43
290	4.21	4.4895	6.64
300	4.07	3.9272	3.51
310	3.40	3.1707	6.74
Mean Absolute Percentage Error (%)			5.10
Coefficient of determination =0.9385			

Table A3**:** Value for Percentage Elongation for PVC-Grass Composite, Experimental, Predicted and Absolute Percentage Error

Temperature (^{O}C)	**Percentage Elongation (%), Experimental**	**Percentage Elongation (%), Predicted**	**Absolute Percentage Error (%)**
210	0.2	0.1467	26.65
220	0.57	0.5885	3.26
230	0.9	0.9546	6.07
240	1.2	1.245	3.75
250	1.4	1.4596	4.26
260	1.7	1.5986	5.96
270	1.8	1.6618	7.68
280	1.6	1.6493	3.08
290	1.5	1.5611	4.07
300	1.35	1.3972	3.50
310	1.2	1.1576	3.53
Mean Absolute Percentage Error (%)			6.53
Coefficient of determination = 0.9787			

Table A4**:** Value for Flexural Strength for PVC-Grass Composite, Experimental, Predicted and Absolute Percentage Error

Temperature (^{O}C)	Flexural Strength (N/mm^{2}) **Experimental**	Flexural Strength (N/mm^{2}) **Predicted**	Absolute Percentage error (%)
210	25.2	25.1471	0.21
220	25.7	25.797	0.38
230	26.3	26.311	0.04
240	26.7	26.6891	0.04
250	26.92	26.9314	0.04
260	27.2	27.0377	0.60
270	27	27.0081	0.03
280	26.82	26.8426	0.08
290	26.40	26.5412	0.53
300	26.10	26.1039	0.02
310	25.6	25.5308	0.27
Mean Absolute Percentage Error (%)			0.20
Coefficient of determination = 0.9847			