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Numerical Optimization of the Input Factors and Responses of an Experimental Design Reinforce PVC Composite

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Abstract: In this study, the input factors (PVC, rattan, plantain peduncle, and temperature) and the responses (flexural strength and modulus of elasticity) of an experimental design to reinforce PVC composite were investigated. The assessment of suitability and ultimately the choice of the models were done based on the values of statistical parameters like coefficient of determination (R^2 value), p value, F value, etc. The experimental data was carried out by fitting a second-order model in the Design Expert model library to the data to estimate the unknown model parameters. This process was accomplished by applying multiple regression analyses to the data. The optimum values of the responses were obtained by numerical optimization based on the criterion of desirability. The results obtained showed that the design was adequate, and the models developed from it were useful because the off-diagonal values were close to zero. Also, increasing the proportion of PVC resulted in a steep and significant increase in the flexural strength of the composite. More so, this trend was similar to the flexural strength for the response surface and the corresponding contour plots representing the relationship between PVC, rattan, and modulus of elasticity. Besides, at higher temperatures, the PVC material could act as a binder, which results in a strong interaction between the components of the composite material.

Keywords: Numerical optimization, flexural strength, reinforce PVC, composite, modulus of elasticity

1. Introduction

Polyvinyl chloride (PVC) has essentially replaced metals in a broad variety of applications because of its many advantages over conventional materials [1-3]. Their extensive usage is a result of their effectiveness, affordability, and flexibility. However, mechanical properties such as flexural strength and modulus of elasticity are inadequate for some applications. Several techniques have been developed to improve such qualities. The flexural strength and high modulus requirements of PVC are often satisfied by the addition of fillers and fibers [4,5]. This has enhanced the mechanical properties of PVC, such as flexural strength, modulus of elasticity, hardness, and tensile strength [6-8], which have broadened the application of the material. The limitations of PVC need quick improvement. Reinforced PVC is a composite material composed of a PVC matrix with reinforcing components, which are often chopped, or continuous fibers used in weaving or nonwoven applications [9]. In addition to textiles, reinforcements occur in several forms, including powder, beads, and flakes. Reinforcements improve the mechanical properties of composites, particularly flexural strength, modulus of elasticity, and stiffness [10, 12]. Their influence on other metrics, such as the coefficient of thermal expansion, conductivity, etc., is also noteworthy. The most challenging aspect of PVC reinforcement is achieving the optimal balance between young modulus and impact resistance. Maintaining tight control over the dispersion of the

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filler and the adhesion of the polymer matrix may provide the best outcomes [13, 14]. After a certain concentration of filler, the impact resistance and modulus of elasticity would be significantly altered [15-18].

Furthermore, the construction of composites comprises different manufacturing processes, which include extrusion and injection molding [32]. Besides, these techniques are used in the direct integration of short fibers into polymers [33, 34]. Also, knowing the behavior of reinforced plastic composites via a predictive model is vital because such knowledge can help improve the mechanical properties of the composites by using the appropriate mix ratios [35, 36]. Response surface methodology (RSM), introduced by Box and Wilson [32, 37], has been used in previous research work to optimize the conditions for the manufacturing of composites [38-40]. Also, the Box-Behnken design and the central composite design are the two most dominant designs utilized in RSM [37, 41]. Nevertheless, among RSM, the Box-Behnken design is far better since it does not only have axial points, but all design points fall within the safe [36, 42-44]. The elastic constants of a coir fiber powder-reinforced plasticized polyvinyl chloride composite were investigated by means of impulsive excitation vibration by [32]. In their study, the optimization of the elastic constants was carried out using Box–Behnken experimental design, and this was based on response surface methodology, which has three factors: fiber content (wt.%), fiber size (μm) and chemical treatments. The outcome of their study using analysis of variance and regression analysis showed that a Young's modulus of 18.2 MPa and a shear modulus of 6.6 MPa were obtained for a blend of fiber content (2 wt%), fiber size (225 μm), and triethoxy (ethyl) silane treatment.

Today, most PVC composites are reinforced composites. In these structural materials, PVC is employed as the matrix, completely encasing the reinforcements. Without the reinforcements, the PVC's mechanical properties would be severely diminished. Several studies [19, 20] have investigated how various kinds of reinforcing materials impact the features of the finished composite, as well as other pertinent issues such as pretreatment. Extensive research has been conducted on PVC natural fiber composites, and their properties have been widely published. As filler/reinforcing components, at least nine distinct kinds of natural fibers have been used to date. Examples include bamboo, pine, rice straw, sisal, oil palm, sugarcane bagasse, banana, and coconut [2,18-23]. A mix of PVC and natural fibers is fascinating due to the "environmental tolerance" of natural fibers. In addition, the use of PVC composites has expanded faster than that of other polymer composites, and they offer a vast array of possible applications. PVC is an excellent material due to its improved chemical resistance to a wide range of corrosive fluids, as well as its higher strength and stiffness compared to other thermoplastics. It is easy to make, has a long lifetime, and is well-suited for usage in specialized technical applications as a consequence of its capacity to generate both rigid and flexible items [24]. Although plantain peduncles and rattan may be found in abundance as municipal solid waste in Nigerian towns, cities, and especially local markets, no research on their possible applications has been recorded to our knowledge. Consequently, a reinforced PVC composite will be the focus of this study, and the inputs and outputs will be numerically optimized. Besides, sufficient study has not been carried out on the flexural strength and modulus of elasticity of an experimental design to reinforce PVC composites.

2. Materials and Methods

The experimental design was employed in Design Expert® software version 7.0.0, (Stat-ease, Inc. Minneapolis, USA). In this study, the design entails five variables, three of which are the composite constituents, which include the amount of PVC, raffia palm, and plantain peduncle, and the remaining two production variables, modulus of elasticity and flexural strength. The Design Expert® software utilizes the concept of randomization to generate the experimental design. This is usually done by scheduling the experiments in a random manner to minimize the effects of unexplained variability in the response. The quadratic model is easily the most commonly used model for random surface methodology (RSM), and this is because it is very flexible and the unknown model parameters can easily be estimated using the least squares method algorithm in the Design Expert software. The models in the Design Expert library were assessed for their suitability in adequately representing the relationship between the factors under investigation (PVC, rattan, plantain peduncle, and temperature) and the responses selected (flexural strength and modulus of elasticity). The assessment of suitability and ultimately the choice of the models were done based on the values of certain key statistical parameters like coefficient of determination (R^2 value), p value, F value, etc. The second-order model in the Design Expert model library, as shown in Equation (1) [25], was selected, and it is a two-factor interaction (2FI) model. The condition of optimality of the second-order model is that the Hessian matrix obtained from the model (after incorporating the Lagrange multipliers) with respect to the independent variables must be positive definite for a minimization problem and negative definite for a maximization problem.

$$Y = b_o + \sum_{i=1}^{N} b_i X_i + \sum_{i,j=1}^{N} b_{ij} X_i X_j + \sum_{i=1}^{N} e_i \tag{1}$$

where X_j is the independent variable or factor and b_{ij} is the coefficient of the interaction terms. The experimental data was obtained by fitting Equation (1) to the data to estimate the unknown model parameters. This process was accomplished by applying multiple regression analyses to the data. At the end of the process, the estimated model parameters were incorporated into the equations representing the models for flexural strength, and modulus of elasticity, in terms of the independent variables (PVC (X_1), rattan (X_2), plantain peduncle (X_3), temperature (X_4), and pressure (X_5)) as presented in Equations (2) and (3).

$$\text{Flexural strength} = 4.37 - 0.093X_1 - 0.29X_2 + 0.20X_3 + 0.0041X_4 + 0.012X_5 + 0.0056X_1X_2 - 0.0039X_1X_3 + 0.0024X_1X_4 - 0.0029X_1X_5 + 0.012X_2X_3 - 0.0039X_2X_4 + 0.0019X_2X_5 - 0.0015X_3X_4 - 0.0025X_3X_5 - 0.00014X_4X_5 + 0.00055X_1^2 - 0.0072X_2^2 - 0.017X_3^2 - 0.000025X_4^2 + 0.00011X_5^2 \tag{2}$$

$$\text{Modulus of elasticity} = 8.17 - 0.30X_1 - 0.10X_2 + 0.45X_3 + 0.0046X_4 + 0.015X_5 - 0.0010X_1X_2 - 0.0060X_1X_3 - 0.000050X_1X_4 - 0.00025X_1X_5 - 0.00032X_2X_4 + 0.00073X_2X_5 + 0.00029X_3X_4 - 0.0012X_3X_5 - 0.000010X_4X_5 + 0.0038X_1^2 + 0.00063X_2^2 - 0.00057X_3^2 - 0.0000021X_4^2 - 0.000018X_5^2 \tag{3}$$

The optimum values of the responses were obtained by numerical optimization based on the criterion of desirability. The optimization process searches for a combination of factor levels that simultaneously satisfy the criteria placed on each of the responses and factors. To include a response in the optimization criteria, it must have a model fit through analysis or be supplied via an equation-only simulation. For this work, the optimization was done by choosing the desired goal for each factor and response. The independent variables were kept at their natural levels, while a minimum and a maximum level were set for the responses. A weight was assigned to each goal to adjust the shape of its particular desirability function. The default setting was used for the goal, which was that all goals be equally important at a setting of 3 pluses (+++). The goals were combined into an overall desirability function, which was maximized by the software. Contour, 3D surfaces, and perturbation plots of the desirability function at each optimum were then used to explore the function in the factor space. The model was validated by comparing the results predicted by the models with those of the actual experiments.

3. Results and Discussion

Tables 1 and 2 show the correlation matrix of regression coefficients and the correlation matrix of factors, respectively. These two matrices are used to compare the capability of a design. They give an indication of how much the regression coefficients and the factors of a design model are correlated with each other. The desirable situation is that the off-diagonal values should be close to zero. If that is the case, then it means that there is no correlation between the model terms. That was indeed the case, with the results presented in Tables 2 and 3 showing that the design was adequate, and the models developed from it were useful.

Table 1 - Correlation matrix of regression coefficients

	Intercept	**X_1**	**X_2**	**X_3**	**X_4**	**X_5**	**X_1X_2**
Intercept	1	-	-	-	-	-	-
X_1	0	1	-	-	-	-	-
X_2	0	0	1	-	-	-	-
X_3	0	0	0	1	-	-	-
X_4	0	0	0	0	1	-	-
X_5	0	0	0	0	0	1	-
X_1X_2	0	0	0	0	0	0	1
X_1X_3	0	0	0	0	0	0	0
X_1X_4	0	0	0	0	0	0	0
X_1X_5	0	0	0	0	0	0	0
X_2X_3	0	0	0	0	0	0	0
X_2X_4	0	0	0	0	0	0	0
X_2X_5	0	0	0	0	0	0	0
X_3X_4	0	0	0	0	0	0	0
X_3X_5	0	0	0	0	0	0	0
X_4X_5	0	0	0	0	0	0	0
X_1^2	-0.60	0	0	0	0	0	0
X_2^2	-0.60	0	0	0	0	0	0
X_3^2	-0.60	0	0	0	0	0	0
X_4^2	-0.60	0	0	0	0	0	0
X_5^2	-0.60	0	0	0	0	0	0

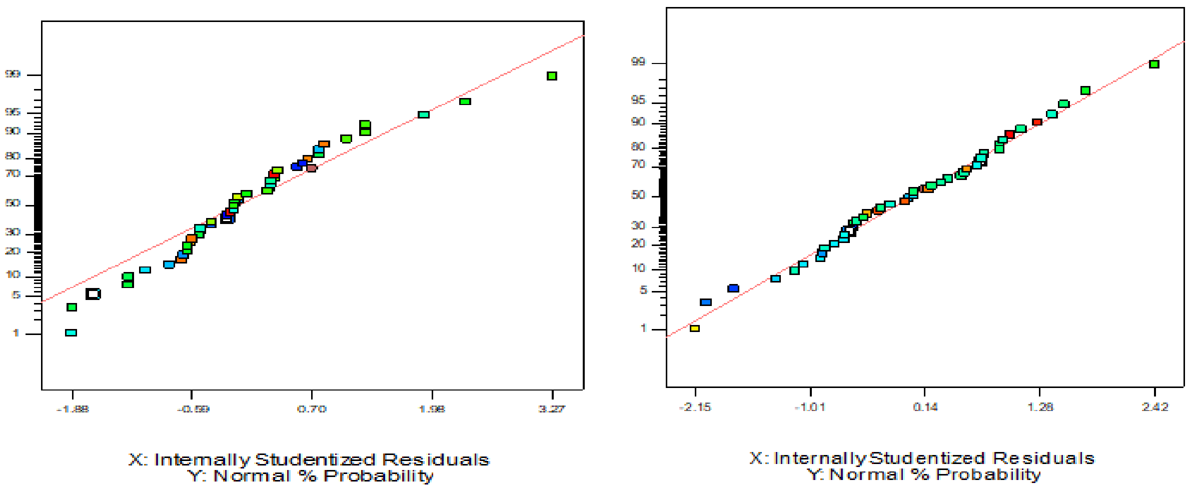
	X_1X_3	X_1X_4	X_1X_5	X_2X_3	X_2X_4	X_2X_5	X_3X_4
X_1X_3	1	-	-	-	-	-	-
X_1X_4	0	1	-	-	-	-	-
X_1X_5	0	0	1	-	-	-	-
X_2X_3	0	0	0	1	-	-	-
X_2X_4	0	0	0	0	1	-	-
X_2X_5	0	0	0	0	0	1	-
X_3X_4	0	0	0	0	0	0	1
X_3X_5	0	0	0	0	0	0	0
X_4X_5	0	0	0	0	0	0	0
X_1^2	0	0	0	0	0	0	0
X_2^2	0	0	0	0	0	0	0
X_3^2	0	0	0	0	0	0	0
X_4^2	0	0	0	0	0	0	0
X_5^2	0	0	0	0	0	0	0
	X_3X_5	X_4X_5	X_1^2	X_2^2	X_3^2	X_4^2	X_5^2
X_3X_5	1	-	-	-	-	-	-
X_4X_5	0	1	-	-	-	-	-
X_1^2	0	0	1	-	-	-	-
X_2^2	0	0	0.27	1	-	-	-
X_3^2	0	0	0.27	0.27	1	-	-
X_4^2	0	0	0.27	0.27	0.27	1	-
X_5^2	0	0	0.27	0.27	0.27	0.27	1

Table 2 - Correlation matrix of factors

	X_1	X_2	X_3	X_4	X_5	X_1X_2	X_1X_3
X_1	1	-	-	-	-	-	-
X_2	0	1	-	-	-	-	-
X_3	0	0	1	-	-	-	-
X_4	0	0	0	1	-	-	-
X_5	0	0	0	0	1	-	-
X_1X_2	0	0	0	0	0	1	-
X_1X_3	0	0	0	0	0	0	1
X_1X_4	0	0	0	0	0	0	0
X_1X_5	0	0	0	0	0	0	0
X_2X_3	0	0	0	0	0	0	0
X_2X_4	0	0	0	0	0	0	0
X_2X_5	0	0	0	0	0	0	0
X_3X_4	0	0	0	0	0	0	0
X_3X_5	0	0	0	0	0	0	0
X_4X_5	0	0	0	0	0	0	0
X_1^2	0	0	0	0	0	0	0
X_2^2	0	0	0	0	0	0	0
X_3^2	0	0	0	0	0	0	0
X_4^2	0	0	0	0	0	0	0
X_5^2	0	0	0	0	0	0	0
	X_1X_4	X_1X_5	X_2X_3	X_2X_4	X_2X_5	X_3X_4	X_3X_5
X_1X_4	1	-	-	-	-	-	-
X_1X_5	0	1	-	-	-	-	-
X_2X_3	0	0	1	-	-	-	-
X_2X_4	0	0	0	1	-	-	-
X_2X_5	0	0	0	0	1	-	-

X_3X_4	0	0	0	0	0	1	-
X_3X_5	0	0	0	0	0	0	1
X_4X_5	0	0	0	0	0	0	0
X_1^2	0	0	0	0	0	0	0
X_2^2	0	0	0	0	0	0	0
X_3^2	0	0	0	0	0	0	0
X_4^2	0	0	0	0	0	0	0
X_5^2	0	0	0	0	0	0	0
--	X_4X_5	X_1^2	X_2^2	X_3^2	X_4^2	X_5^2	-
X_4X_5	1	-	-	-	-	-	-
X_1^2	0	1	-	-	-	-	-
X_2^2	0	-0.15	1	-	-	-	-
X_3^2	0	-0.15	-0.15	1	-	-	-
X_4^2	0	-0.15	-0.15	-0.15	1	-	-
X_5^2	0	-0.15	-0.15	-0.15	-0.15	1	-

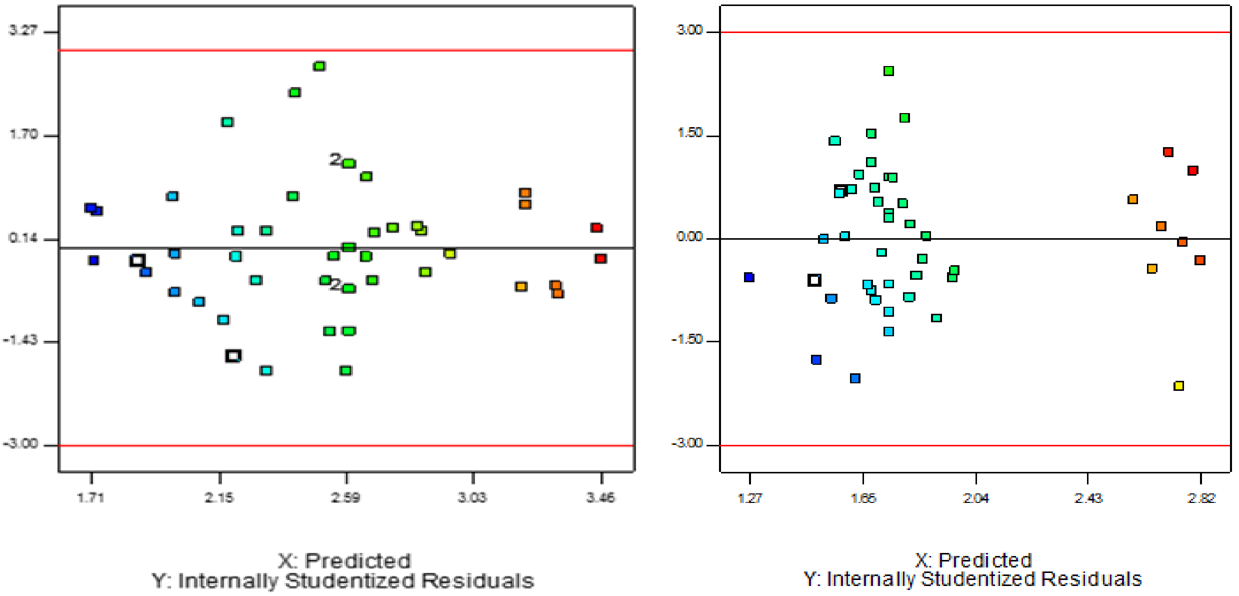
Statistical diagnostics of the models developed were carried out to further assess the adequacy and accuracy of the models. This was done by utilizing normal probability plots, residual plots, leverage plots, difference in fit plots, difference in beta plots, and Cook's distance plots. The normal probability plots for the model representing flexural strength and modulus of elasticity are shown in Figure 1. This plot is used for determining the normal distribution of the residuals. In an ideal situation, it is desired that the residuals follow a normal distribution, and this is usually indicated by the points in the normal probability plot clustering around the straight line. This is a desirable situation for a model to be considered acceptable, and that was indeed the case for the results presented in Figure 1.



i. Flexural strength ii. Modulus of elasticity

Fig. 1 - Normal probability plot

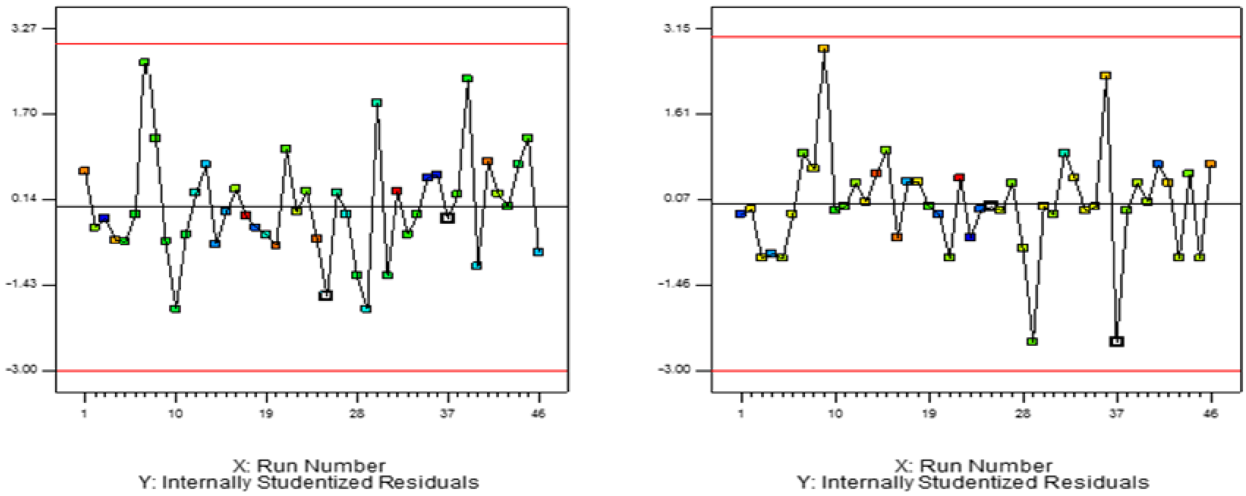
The plots of the internally standardized residuals against the predicted values for the model representing flexural strength and modulus of elasticity are shown in Figure 2. The plot is used to determine if the responses exhibit constant variance. Normally, a response that exhibits constant variance will have the plot of residuals display a random scatter. If this is not the case, then it means that the response does not show a constant variance, and this might necessitate a transformation [26]. The plots presented in Figure 2 clearly show a random scatter, indicating that the responses display constant variance.



i. Flexural strength ii. Modulus of elasticity

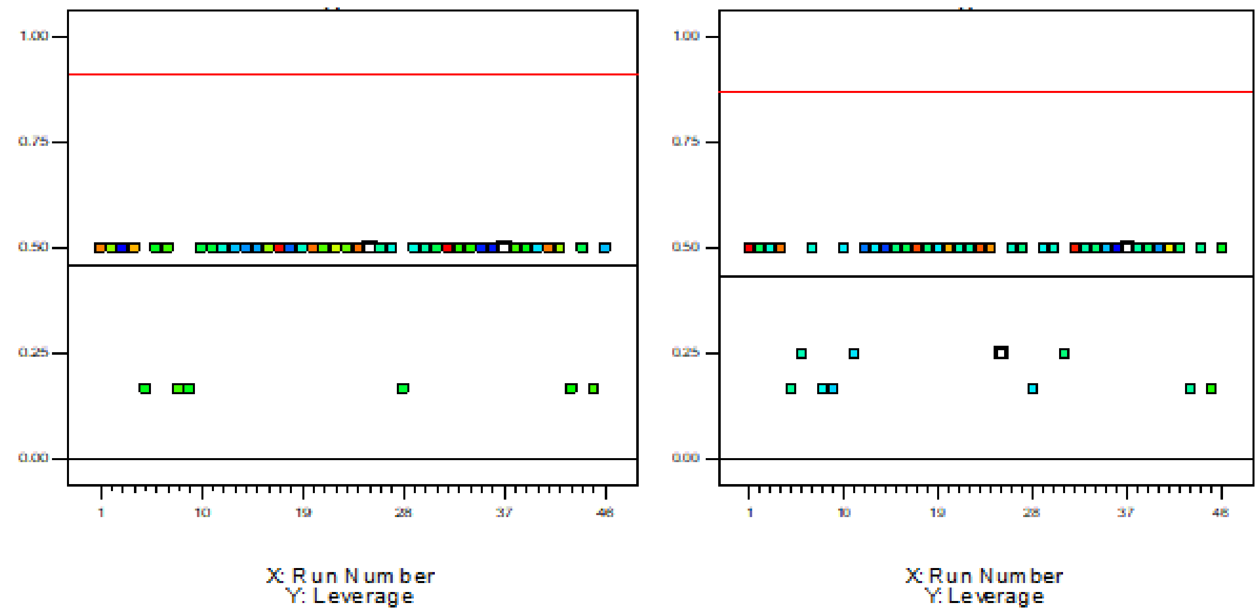
Fig. 2 - Plot of residuals versus predicted response

The plots of the internally standardized residuals versus the experimental run order for the model representing flexural strength and modulus of elasticity are shown in Figure 3. The plot is used to determine the presence of any unexplained variables that might affect the results of the experiment. A desirable situation only occurs if the plots show a random scatter. If that is indeed the case, then it means that there are no unexplained variables lurking in the background, and this was the case for the results presented in Figure 3. The plots of leverage versus the experimental run order for the model representing flexural strength, and modulus of elasticity are shown in Figure 4. The plot is used to determine the presence of any extreme experimental observation or statistical outlier that might impact the integrity of the results of the experiment. A desirable situation is that the leverage value for each experimental run should not exceed the maximum value of one. If that is indeed the case, then it means that there are no outliers in the experimental design, and this was the case for the results presented in Figure 4. However, if any run has a leverage value greater than one, then it is an indication of a possible outlier, and that run would have to be repeated.



i. Flexural strength ii. Modulus of elasticity

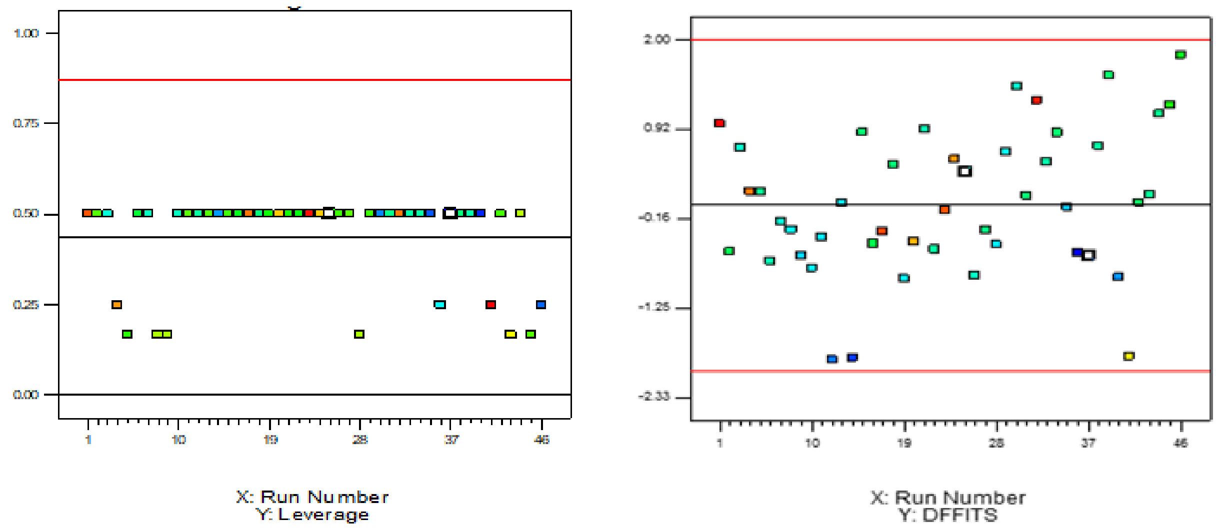
Fig. 3 - Plot of residuals versus experimental run order



i. Flexural strength ii. Modulus of elasticity

Fig. 4 - Plot of leverage versus experimental run order

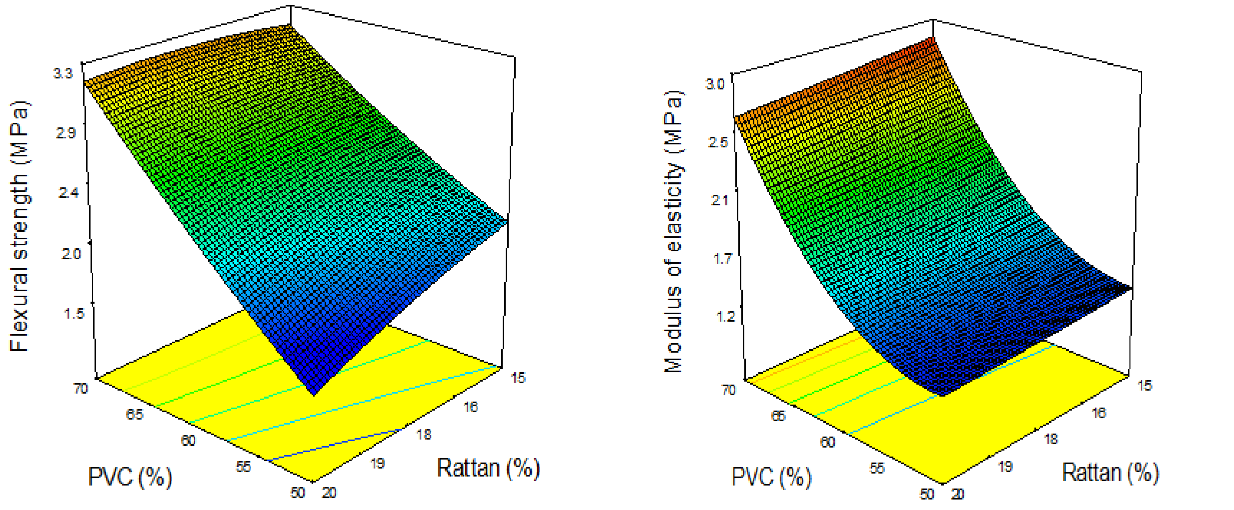
Figure 5 depicts the plots of difference in fits (DFFITS) versus experimental run order for the model expressing flexural strength and modulus of elasticity. Using two fits to the data, one with and one without the ith response, the DFFITS is used to determine the change in the expected value of the ith response. It is the difference between the expected value with observation I and the predicted value without observation I that has been standardized. According to the DFFITS statistic, the criteria for determining whether an observation is important depend on both the sample size and the number of predictor variables in the model. The greater its absolute value, the greater its influence on the fitted model. A run is deemed influential when the DFFITS value is outside the boundaries. Since the DFFITS is used to determine the influence of suspected outliers, it can be deduced from Figure 5 that there were no suspected outliers because the DFFITS values were within the acceptable range.



i. Model representing flexural strength ii. Model representing modulus of elasticity

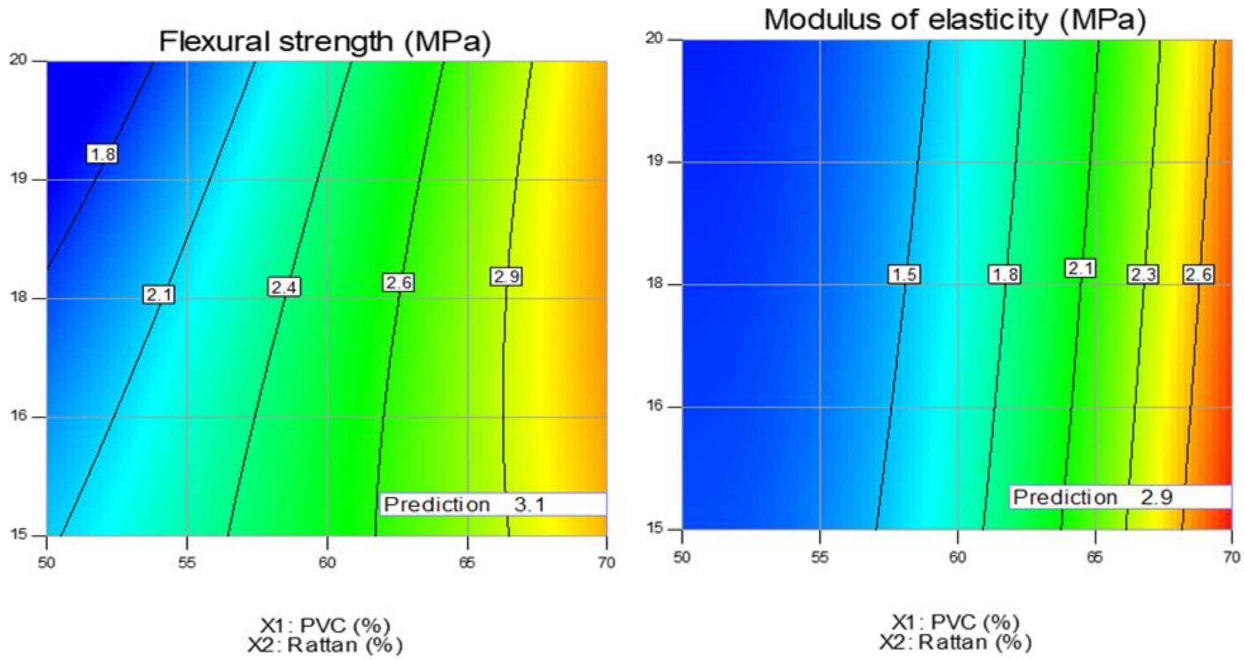
Fig.5 - Plot of DFFITS versus experimental run order

Figures 6a and 6b show the 3D response surface and corresponding contour plots illustrating the simultaneous effect of the amount of PVC and rattan on the flexural strength and modulus of elasticity of the composite. The trend observed in the figure shows that increasing the proportion of PVC resulted in a steep and significant increase in the flexural strength of the composite. This observation was recorded both at low and high levels of rattan. Again, this observation could be a result of the strength of the PVC material, which was consequently imparted to the composite. Also, it was observed that the trend is similar to the flexural strength for the response surface and the corresponding contour plots representing the relationship between PVC, rattan, and modulus of elasticity. Similar observations have also been reported by previous researchers. For instance, [25] investigated the effects of the number of kenaf layers, heating time, and kenaf weight fraction on the modulus of elasticity of the composite specimen using lightweight laminate composites made from kenaf and polypropylene (PP) fibers by press forming. Their observations showed that the modulus of elasticity increased with an increasing number of kenaf layers.



i. Effect PVC and rattan composition on flexural strength ii. Effect PVC and rattan composition on modulus of elasticity

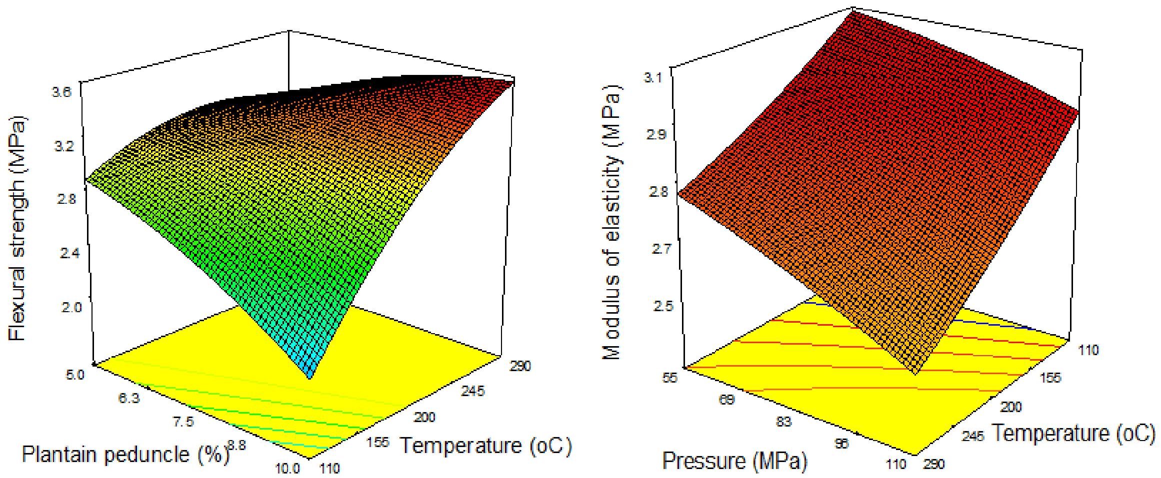
Fig. 6a - Response surface plot



i. Effect PVC and rattan composition on flexural strength ii. Effect of PVC and rattan composition on modulus of elasticity

Fig.6b - Contour plot

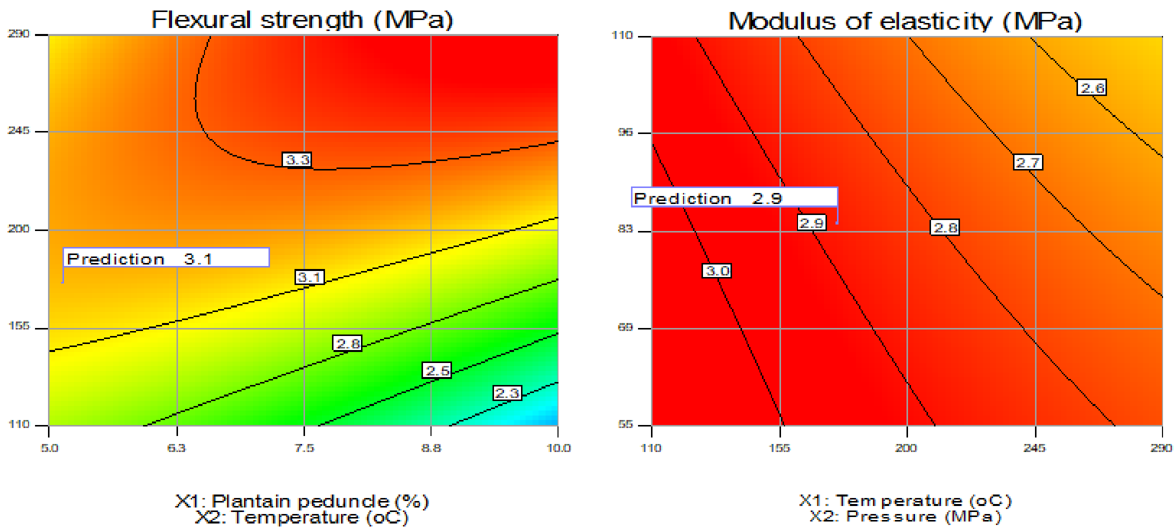
Furthermore, at higher temperatures, the PVC material could act as a binder, which results in a strong interaction between the components of the composite material. Similar observations have been reported by other researchers who produced composites from similar materials. [27] used palm ash to produce brake pads by varying the composition of polychlorinated biphenyl waste (PCB) and palm ash. Thermoset resin was employed as a binder. The observations showed that as the palm ash content increased in the composition, the compressive strength also increased. The results showed that a high content of PA composition gave better mechanical properties. Figures 7 and 8 show the effect of temperature and pressure on the flexural strength of the composite. The temperature positively affected the flexural strength of the composite. Similar observations were reported by other researchers [28-30]. Temperature had antagonistic effects on the modulus of elasticity of the composite pipes (Figures 7 and 8), and as stated previously, this could be attributed to variations of the viscosity of the polymer material at higher temperatures and therefore variations of the fiber wetting and/or different binder-network structures formed under different temperature/pressure conditions [31].



i. Effect of temperature and plantain peduncle composition on flexural strength

ii. Effect of temperature and plantain peduncle composition on modulus of elasticity

Fig.7 - Response surface plot



i. Effect of temperature and plantain peduncle composition on flexural strength

ii. Effect of temperature and plantain peduncle composition on modulus of elasticity

Fig.8 - Contour plot

4. Conclusion

The numerical optimization of the input factors and responses of an experimental design to reinforce PVC composite was successfully carried out. It was observed that the normal distribution of the residuals was in an ideal situation, and this was a desirable situation for a model to be considered acceptable, and that was indeed the case in this scenario. Also, the plots of the internally standardized residuals against the predicted values for the model representing flexural strength and modulus of elasticity exhibit constant variance, thus, plot of residuals displaying a random scatter. The plots of the internally standardized residuals versus the experimental run order for the model representing flexural strength and modulus of elasticity revealed that the presence of any unexplained variable would not affect the results of the experiment. The results of the 3D response surface and corresponding contour plots illustrating the simultaneous effect of the amount of PVC and rattan on the flexural strength and modulus of elasticity of the composite showed that increasing the proportion of PVC resulted in a steep and significant increase in the flexural strength and modulus of elasticity of the composite. This trend was similar to the flexural strength for the response surface and the corresponding contour plots representing the relationship between PVC, rattan, and modulus of elasticity. Above and beyond that, at higher temperatures, the PVC material could act as a binder, which results in a strong interaction between the components of the composite material. This observation was recorded both at low and high levels of rattan. However, this observation could be a result of the strength of the PVC material, which was consequently imparted on the composite. Also, increasing the proportion of PVC resulted in a steep and significant increase in the flexural strength of the composite.

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