COMPARISON OF RESPONSE SURFACE METHODOLOGY (RSM) AND ARTIFICIAL NEURAL NETWORKS (ANN) IN OPTIMISATION OF INJECTION MOULDED POLYVINYLCHLORIDE--SAWDUST COMPOSITE

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ABSTRACT

This study focused comparison of the response surface methodology and the artificial neural networks in optimization of the injection moulded Polyvinylchloride-Sawdust (PVC-sawdust) composite. The PVC material and sawdust were mixed together to form a homogenous mixture with various percentage composition by volume as recommended by the central composite design (CCD). The two screw plunger injection moulding machine with maximum clamping force of 120 tons and shot capacity of 3.0oz was used to produce Polyvinylchloride-Sawdust (PVC-Sawdust) composite at various temperature. The produced composites were evaluated for their mechanical properties which included tensile strength, proof stress, percentage elongation and flexural strength. The response surface methodology (RSM) and artificial neural networks (ANN) were used to determine the effect of the interaction of temperature, material type and percentage by volume of material on the mechanical properties of the produced PVC-sawdust composite. The models were validated using coefficient of determination ($R^2$). The coefficient of determination ($R^2$) obtained ranged from 0.9627 (96.27%) to 0.9986 (99.86%) which indicates that a substantial good fit was achieved by the model developed. The ANN has performed better than RSM in the determination of $R^2$, adjusted $R^2$, RMSE and AAD

Keywords: Central composite design, Composite, Modeling, Polyvinylchloride, Sawdust.

1.0 INTRODUCTION

The demand for new materials with higher specifications has led to the concept of combining different materials to form a single material called composite. Such composite materials results in high performance, and high flexibility in design that cannot be attained by the individual constituents [1].

Moreover, it has been shown that technological development depends greatly on scientific research of materials, and this contributes to economic growth of any nation [2]. Furthermore, injection moulding is a cost-effective way to produce complex, three shapes at high volumes. In the plastic industry, injection moulding makes up approximately 32% weight of all plastic processing methods, second only to extrusion which is 36% weight. [3].

A qualitative analysis of the influence of these factors in this case barrel temperature on the mechanical properties of a moulded part will be helpful in gaining better insight into the presently used processing methods. Moreover, there are inadequate models to predict mechanical properties and determine the interaction of some process variables of PVC-sawdust composite.

Response surface methodology (RSM) explore the relationships between several explanatory variables and one or more response variables. The method was introduced by George E. P. Box and K. B. Wilson in 1951. The main idea of RSM is to use a sequence of designed experiments to obtain an optimal response. Box an Wilson suggest using a second-degree polynomial model to do this. [4], examined metal matrix composites (MMCs).
consisting of two or more physically/chemically distinct phases 
An Artificial Neural Network (ANN) is a mathematical 
model that tries to simulate the structure and functionalities 
of biological neural networks. Basic building block of every 
artificial neural network is artificial neuron, that is, a simple 
mathematical model (function). Such a model has three 
simple sets of rules: multiplication, summation and 
activation. At the entrance of artificial neuron the inputs are 
weighted what means that every input value is multiplied 
with individual weight. In the middle section of artificial 
neuron is sum function that sums all weighted inputs and 
bias. At the exit of artificial neuron the sum of previously 
weighted inputs and bias is passing through activation 
function that is also called transfer function [5] 
[6] modeling and production of injection moulded 
Polyvinylchloride-Sawdust composite using response 
surface methodology. This study however focuses on the 
comparison of response surface methodology and artificial 
neural networks in optimization of Polyvinylchloride-
Sawdust composite.

2.0 MATERIALS AND METHODS

2.1 Materials and Equipment

The following are the materials and equipment used for 
this study:

(i) Polyvinyl chloride (PVC) in powder form 
which were available at Adig plastics company Ltd.
(ii) Sawdust (from Mahogany tree) obtained from 
saw mill in Benin City, Edo State.
(iii) Two stage-screw plunger Injection machine 
Fox and offord, 120 tons two stage-screw 
plunger, A toggle clamp attached to the 
 injection end of injection moulding, An 
existing mould belonging to Adig Plastic Ltd,
(iv) Monsanto Tensometer, Type 'W' Serial No. 
8991, The mould was made of Silicon – killed 
forging quality steel AISI type H140 treated to 
252 –302 Brine 11. to use at high clamping 
pressures.

2.2 Design of Experiment

For this study, a two-variable central composite design 
(CCD) was used to plan the experiments, develop statistical 
models for predicting the chosen responses. The design 
points were made up of 2n factorial points as well as star 
points. The star points are particularly necessary for 
estimating the response for non-linear models [7].

2.3 Models Development

Design Expert software version 7.0.0, (Stat-ease, Inc. 
Minneapolis, USA) was used to design the experiment and 
to analyze the experimental data obtained. The factors 
considered were temperature and the level of polymer 
(PVC) in the matrix. The range and levels of these factors 
are shown in Tables 1 to 3 and they were calculated using 
Equation 1 [8]. In this case, the responses chosen for 
consideration were tensile strength, proof stress, percentage 
elongation, average deflection, flexural strength, and 
flexural modulus.

\[
x_i = \frac{X_i' - X_o}{\Delta X_i}
\]

(1)

Where \(X_i\) and \(X_i'\) are the coded and actual values of the 
factors respectively while \(X_o\) is the actual value of the 
factors at the centre point, and \(\Delta X_i\) is the step change in the 
value of the actual values of the factors.

In selecting the appropriate model for predicting the 
responses, different model types in the Design Expert 
software library were considered and these include linear, 
two-factor interaction (2FI), quadratic and cubic models.

The first type of model usually investigated is a linear 
model shown in Equation 2. It is usually proposed to 
predict the response of the dependent variables and to 
predict their optimum values when the relationship 
between the factors and the responses is thought to be linear.

\[
Y = b_0 + \sum_{i=1}^{N} b_i X_i + \sum_{i=1}^{N} e_i
\]

(2)

Where \(Y_i\) is the dependent variable or predicted response, 
\(X_i\) is the independent variables, \(b_i\) is offset term, \(b_i\) is the 
regression coefficient and \(e_i\) is the error term.

Equation (3) is a two-factor interaction regression model 
which was also proposed to predict the response of the 
dependent variables and to predict their optimum values.

\[
Y = b_0 + \sum_{i=1}^{N} b_i X_i + \sum_{i=1}^{N} b_{ij} X_i X_j + \sum_{i=1}^{N} e_i
\]

(3)

\(X_i\) is the independent variables or factors while \(b_{ij}\) is the 
coefficient of the interaction terms.

For situations where the relationship between the factors 
and the responses is thought to be nonlinear, a second 
order model as shown in Equation 4 can be used to predict 
the response.

\[
Y = b_0 + \sum_{i=1}^{N} b_i X_i + \sum_{i,j=1}^{N} b_{ij} X_i X_j + \sum_{i=1}^{N} b_i X_i^2 + \sum_{i=1}^{N} e_i
\]

(4)

The second order model is the most widely used model for 
response surface methodology, [9]. This is because it is 
flexible and parameters of the model are easy to estimate 
using the popular least squares method used by the Design 
Expert software. Beyond that, experience has shown that 
this model is most suitable in representing most real-life 
situations.
2.4 Statistical Analysis of Model Results

The statistical analysis of the results was carried out using the Design Expert software. The fit of the models representing the responses (tensile strength, proof stress, percentage elongation, average deflection, flexural strength, and flexural modulus) was determined using analysis of variance (ANOVA). The ANOVA results helped to also assess the statistical significance of the models representing the responses and this was done using parameters like p value, F value, sum of squares, mean square, lack of fit, standard deviation, coefficient of variation, coefficient of determination ($R^2$), adjusted $R^2$, adequate precision, predicted residual sum of squares (PRESS). These parameters are discussed in the following sections.

3.0 Determination of Optimal Training Algorithm

It is not usually possible to determine beforehand, the best algorithm to use for training a proposed neural network. Thus, it is usually necessary to iteratively test several training algorithms to determine the one most suitable for a particular network [10]. The same thing applies to the network architecture. Hence, in this work, two networks architectures were considered and trained using different training algorithms to determine the one that will be most suitable to model the responses. The network architectures evaluated were the multilayer normal feed forward (MNFF) and multilayer full feed forward (MFFF) while the training algorithms evaluated were incremental back propagation (IBP), batch back propagation (BBP), quick propagation (QP), generic algorithm (GA), and Levenberg-Marquardt (LM) algorithm. The results of the training exercise are shown in Table 1 for the PVCsawdust composite. The results showed that the best network was a multilayer normal feed forward neural network trained with the incremental back propagation algorithm. This was found to be suitable for predicting all the responses. The decision to select this network architecture and training algorithm was because it resulted in the highest $R^2$ value and lowest RMSE value for the responses under consideration.

Table 1: $R^2$ and RMSE values of MNFF and MFFF using different training algorithms for average deflection (PVC composite)

<table>
<thead>
<tr>
<th>Network architecture</th>
<th>Training algorithm</th>
<th>$R$ squared</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>*MNFF</td>
<td>IBP</td>
<td>0.9627</td>
<td>0.1390</td>
</tr>
<tr>
<td></td>
<td>BBP</td>
<td>0.9486</td>
<td>0.1633</td>
</tr>
<tr>
<td></td>
<td>QP</td>
<td>0.9602</td>
<td>0.1437</td>
</tr>
<tr>
<td></td>
<td>GA</td>
<td>0.9580</td>
<td>0.1475</td>
</tr>
<tr>
<td></td>
<td>LM</td>
<td>0.9451</td>
<td>0.1688</td>
</tr>
<tr>
<td>MFFF</td>
<td>IBP</td>
<td>0.9627</td>
<td>0.1391</td>
</tr>
<tr>
<td></td>
<td>BBP</td>
<td>0.9203</td>
<td>0.2033</td>
</tr>
<tr>
<td></td>
<td>QP</td>
<td>0.9091</td>
<td>0.2171</td>
</tr>
<tr>
<td></td>
<td>GA</td>
<td>0.9591</td>
<td>0.1451</td>
</tr>
<tr>
<td></td>
<td>LM</td>
<td>0.8681</td>
<td>0.2615</td>
</tr>
</tbody>
</table>

*best learning algorithm and network

4.0 RESULTS AND DISCUSSION

The range and levels of these factors are shown in Table 2 and they were calculated using Equation.1 [8]. In this case, the responses chosen for consideration were tensile strength, proof stress, percentage elongation, average deflection, flexural strength, and flexural modulus.

Table 2: Coded and actual levels of the factors for PVC polymer composite

<table>
<thead>
<tr>
<th>Factors</th>
<th>Unit</th>
<th>Symbols</th>
<th>Coded and Actual Levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>°C</td>
<td>$X_1$</td>
<td>-1.414 -1 0 1 1.414</td>
</tr>
<tr>
<td>PVC level</td>
<td>%</td>
<td>$X_2$</td>
<td>210.00 224.64 260.00 295.36 310.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>60.00 61.46 65.00 68.54 70.00</td>
</tr>
</tbody>
</table>

4.1 Determination of Appropriate Model

Table 3 shows the summary of model fit results for PVC-Sawdust composite
Table 3: Summary of model fit results (PVC-Sawdust composite)

<table>
<thead>
<tr>
<th>Source</th>
<th>Standard deviation</th>
<th>$R^2$</th>
<th>Adjusted $R^2$</th>
<th>Predicted $R^2$</th>
<th>PRESS</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>1.82</td>
<td>0.8622</td>
<td>0.8347</td>
<td>0.7264</td>
<td>65.79</td>
<td></td>
</tr>
<tr>
<td>2FI</td>
<td>1.79</td>
<td>0.8797</td>
<td>0.8396</td>
<td>0.5772</td>
<td>101.66</td>
<td></td>
</tr>
<tr>
<td>Quadratic</td>
<td>1.50</td>
<td>0.9349</td>
<td>0.8885</td>
<td>0.5535</td>
<td>107.38</td>
<td>Suggested</td>
</tr>
<tr>
<td>Cubic</td>
<td>0.95</td>
<td>0.9814</td>
<td>0.9553</td>
<td>0.0110</td>
<td>243.09</td>
<td>Aliased</td>
</tr>
</tbody>
</table>

Table 4: Lack of fit test results (PVC-Sawdust composite)

<table>
<thead>
<tr>
<th>Source</th>
<th>Sum of square</th>
<th>degree of freedom</th>
<th>Mean square</th>
<th>F-value</th>
<th>p-value</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>32.43</td>
<td>6</td>
<td>5.40</td>
<td>30.88</td>
<td>0.0026</td>
<td></td>
</tr>
<tr>
<td>2FI</td>
<td>28.22</td>
<td>5</td>
<td>5.64</td>
<td>32.26</td>
<td>0.0025</td>
<td></td>
</tr>
<tr>
<td>Quadratic</td>
<td>14.95</td>
<td>3</td>
<td>4.98</td>
<td>28.47</td>
<td>0.0737</td>
<td>Suggested</td>
</tr>
<tr>
<td>Cubic</td>
<td>3.78</td>
<td>1</td>
<td>3.78</td>
<td>21.61</td>
<td>0.0097</td>
<td>Aliased</td>
</tr>
<tr>
<td>Pure Error</td>
<td>0.70</td>
<td>4</td>
<td>0.18</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Source: Aliyegbenoma et al 2019

Tables 3 and 4 shows the statistical results for PVC-Sawdust composite respectively. As seen from the results, the quadratic model was chosen as the most appropriate model to predict the responses. This decision was reached based on the statistical parameters backing up the quadratic model. Among a number of alternatives, the model chosen should be the one with the desirable statistical parameters such as high $R^2$ value, low standard deviation, and low PRESS. The quadratic model was found to have the highest $R^2$ values for all the responses as shown in Table 3 for PVC-Sawdust composite. The quadratic model was also found to have the lowest standard deviation and PRESS as shown in Table 4 for PVC-Sawdust composites. Thus, the quadratic model was adopted for predicting the responses under investigation in this study.

4.2 Comparison of RSM and ANN predictive performance

The accuracy RSM and ANN in predicting tensile strength, proof stress, percentage elongation, average deflection, flexural strength and flexural modulus is directly related to
their predictive capability. The model with the better predictive capability will be able to predict the responses with a higher accuracy. The predictive capability of RSM and ANN was assessed using $R^2$ value, adjusted $R^2$ value, root mean square error (RMSE) and absolute average deviation (AAD) as shown in Table 5 for PVC composites. A good and accurate model prediction is usually characterized by high values of the $R^2$ value and adjusted $R^2$ value as well as very low RMSE and AAD. A comparison of the predictive capability of RSM and ANN as observed from the $R^2$ value, adjusted $R^2$ value, root mean square error and absolute average deviation shows that ANN performed better than RSM. This is because ANN gave very high $R^2$ values and adjusted $R^2$ values as well as very low RMSE and AAD values compared with RSM as shown in Tables 5.

### Table 5: Comparison of RSM and ANN predictive performance (PVC composite)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>RSM</th>
<th>ANM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Tensile strength</td>
<td>Proof stress</td>
</tr>
<tr>
<td>$R^2$</td>
<td>0.9349</td>
<td>0.9247</td>
</tr>
<tr>
<td>Adj. $R^2$</td>
<td>0.8885</td>
<td>0.8709</td>
</tr>
<tr>
<td>RMSE</td>
<td>0.8845</td>
<td>0.9543</td>
</tr>
<tr>
<td>AAD</td>
<td>0.0148</td>
<td>0.0142</td>
</tr>
</tbody>
</table>

### 4.3 Polarity plot for RSM and ANN

![Polarity plot for RSM and ANN](image-url)
Figure 1: RSM parity plot for (a) tensile strength (b) proof stress (c) percentage elongation (d) average deflection (e) flexural strength (f) flexural modulus for PVC composite
Figure 2: ANN parity plot for (a) tensile strength (b) proof stress (c) percentage elongation (d) average deflection (e) flexural strength (f) flexural modulus for PVC composite
Figures 2 show the ANN parity plot of the responses for PVC sawdust composites. It is a plot of the predicted response values versus the experimental response values. The purpose is to detect a value, or group of values, that are not easily predicted by the model. Comparison of the experimental values of the response and those predicted by the ANN model showed that there was an acceptable level of fit between the experimental and model predicted results. This is evident from the fact that the data points all clustered around the 45° diagonal line showing that there was minimal deviation between experimental and predicted values thus indicating optimal fit of the model. Comparing these results with those presented in Figures 1 for the RSM prediction, it can be seen that the data points in Figures 2 clustered around the 45° diagonal line closer than for the RSM results. This is an indication that the ANN model has better predictive capability compared to the RSM model.

### 4.4 Response Surface and Contour Plot

Figure 3 shows the response surface and contour plot showing the effect of temperature and polymer level on (a) tensile strength (b) proof stress of PVC sawdust composite. Increasing the level of PVC in the composite material resulted in a decrease in the tensile stress of the material as shown in Figure 3 (a). Increasing the temperature resulted in only a slight increase in the tensile stress of the material and this observation was recorded at high levels of PVC. For proof stress, Figure 3 (b) shows a similar trend to that shown in Figure 3(a). In the same way, increasing the level of PVC in the composite material resulted in a decrease in the proof stress of the material. Increasing the temperature resulted in only a slight increase in the proof stress of the material and this observation was recorded at high levels of PVC.
Figure 3: Response surface and contour plot showing effect of temperature and polymer level on (a) tensile strength (b) proof stress for PVC composite.
5.0 CONCLUSION

Models were developed for predicting the mechanical properties (tensile strength, proof stress, percentage elongation and flexural strength) for the produced composites. The models were validated using coefficient of determination ($R^2$). The coefficient of determination ($R^2$) obtained ranged from 0.9627 (96.27%) to 0.9986 (99.86%) which indicates that a substantial good fit was achieved by the model developed. The ANN has performed better than RSM in the determination of $R^2$, adjusted $R^2$, RMSE and AAD.

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