Simplex Lattice Method: A Predictive Tool for Concrete Materials

Claudius K. 1, Elinwa A. U. 2, Duna S. 3

1(Department of Civil Engineering, Abubakar Tafawa Balewa University, P.M.B. 0248 Bauchi, Nigeria)
2(Department of Civil Engineering, Abubakar Tafawa Balewa University, P.M.B. 0248 Bauchi, Nigeria)
3(Department of Civil Engineering, Abubakar Tafawa Balewa University, P.M.B. 0248 Bauchi, Nigeria)

ABSTRACT: This study was carried out to investigate the feasibility of using mixture experiment design and analysis method to optimize concrete mixture proportions. Estimation equations for concrete properties were developed based on the experimental data obtained from the compressive strength development of termite mound concrete specimen. The experimental data was obtained from the effect of termite mound on fresh concrete properties and the strength of the hardened concrete. The equations expresses the coefficient β, which indicates the effect of termite mound as a binder on slump and the compressive strength as a function of age and termite mound content. The termite mound was ground and sieved through 150 µm sieve size, the product was used to replace cement in the concrete mix in proportions of 0 %, 5 %, 10 %, 15 %, 20 % and 25 % by weight of cement. Polynomial models were generated for all response variables using multiple regression analysis (MRA) approach. The model incorporating 15 interactive terms was used to evaluate the response variables, these were expressed for model analysis by Scheffe’s quadratic model.

Keywords: Compressive Strength, Optimization, Scheffe’s Simplex Lattice, Termite Mound Material and T-Test.

I. INTRODUCTION

The problems encountered in the concrete industry are complex and dynamic for non-conventional concrete. This is due to the use of mineral and chemical admixtures either as replacements and/or additives in concrete production. The solution to these problems requires methods and tools for building adaptive intelligent systems that should be able to use available data to update their knowledge [1]. The use of cement replacement and additives has increased over the years due economical, technical, environmental considerations and in most cases the possibility of concrete with superior qualities to the reference mix [2].

Mix design is the process of choosing suitable ingredients of concrete and determining their relative quantities with the objective of producing concretes that are economical and durable. Mix design procedure/specifications provided in codes and standards and used for production of conventional concretes of various grades, but producing concrete with termite mound material as replacement for cement would require a different design procedure. Furthermore, to obtain the desired concrete workability in the laboratory, technical personnel must try several mix proportions [3].

One approach for determining appropriate mix proportion is the “Mixture Experiment”. In this approach two or more ingredients are mixed or blended together in varying proportions to form an end product. The quality characteristics of the end product of each blend is recorded to see how the quality varies from one another or from a reference blend. The measured characteristic (Response) is assumed to depend only on relative proportions of the constituents and not on the amount of mixture [4]. Therefore, in mixture experiment the response depends only on the proportions of the constituents present in the mixture and not on the amount of the mixture provided non-mixture variables are kept constant. Non-mixture variables are external conditions whose settings or levels, if changed can affect the values of the response or affect the blending properties of the mixture constituents [5].

In this research termite mound was used as a replacement material by weight of cement and in proportions of 0 %, 5 %, 10 %, 15 %, 20 % and 25 %, to produce concrete that would be tested to evaluate its effect. It will also apply the Scheffe’s simplex method to develop response models for optimization of the compressive strengths of termite mound concrete (TMC).
II. BACKGROUND OF OPTIMIZATION METHODS FOR CONCRETE MIXTURES

The optimization of constituents’ proportion of concrete to meet certain performance criteria which contain several constituents are often subject to performance constraints and are difficult and time consuming. Statistical design of experiments are developed for the purpose of optimizing mixtures such as concrete. The final mixture proportion depends on the relative proportion of the constituents rather than the individual volumes of the constituents [6][7]. Many methods have been employed for optimization of mixture experiments and are reviewed.

2.1 Fuzzy logic (FL)

Fuzzy logic is a popular artificial intelligence technique invented by Zadeh in the 1960s that has been used for forecasting, decision making and action control in environments characterized by uncertainty, vagueness, presumptions and subjectivity. It was found that between 1996 and 2005 fuzzy logic was used by many scholars in construction related research, either as single or hybrid techniques that are categorized into four types namely: decision making, performance, evaluation/assessment and modelling. Fuzzy logic consist of four major components namely: fuzzification, rule base, inference engine and defuzzification. Fuzzification is the process that uses membership functions to convert the value of input variables into corresponding linguistic variables. The result which is used by the inference engine stimulates the human decision making process based on fuzzy implications and available rules. In the final stage, the fuzzy set, as the output of the inference process is converted into crisp output and the process is known as defuzzification [8].

Despite the advantages of the fuzzy logic, the approach has a number of problems which includes, identifying appropriate membership functions and number of rules for application. This process is subjective in nature and reflects the context in which a problem is viewed. The more complex the problem, the more difficult membership functions construction and rules becomes [9].

For each implication \( R_i \), \( Y_i \) is calculated by the function \( f_i \) in the consequence:

\[
Y_i = f_i(x_1, x_2, ..., x_p) = b_i(0) + b_i(1)x_1 + ... + b_i(p)x_p
\]  

(1)

The weights are calculated from:

\[
r_i = (m_i^r \Delta m_i^r \Delta ... \Delta m_i^r)R^r
\]  

(2)

Where:

\[m_i^r, m_i^r, ..., m_i^r\] Denotes the \( \alpha \) cuts of membership functions according to input values for the \( r \)th rule.

The occurrences probability denoted by \( R^r \) and \( \Delta \) stands for minimum operations. The final output \( Y \) inferred from \( n \) implications is given as the average of all \( Y_i \) with the weights \( r_i \).

\[
Y = \frac{\sum_{i=1}^{n} r_i Y_i}{\sum_{i=1}^{n} r_i}
\]  

(3)

2.2 Support vector machines (SVM)

The theory that underlines support vector machines (SVM) represents a statistical technique that has drawn much attention in recent years. The learning theory is seen as an alternative training technique for polynomial, radial basis function and multilayer perceptron classifiers. SVM are based on the structural risk minimization induction principle, which aims to restrict the generalization error (rather than the mean square error) to certain defined bounds. SVM have proven to deliver higher performance than traditional learning techniques and have been introduced as a powerful tool to solve classification and regressional problems.

In most cases, identifying a suitable hyper plane in input space is an application that is overly restrictive in practical applications. The solution to this situation is to map the input space into higher dimension feature space, and then identify the optimal hyper plane within this feature space. Without any knowledge of the mapping, an SVM locates the optimal layer hyper plane using dot product functions in feature space known as “kernels”. The kernel trick based on the Mercer theorem is used in SVM to map input into high dimensional feature spaces, wherein simple functions defined on pairs of input patterns are used to compute dot products and design a linear decision surface [10].

It is expressed that SVM bandwidth and penalty parameter which determines the tradeoff between margin maximization and violation error minimization, represents an issue that requires attention and handling. Another point of concern is the setting of kernel parameters on the radial basis function, which must also be set properly to improve prediction accuracy [8]. The expression for support vector machines is given below:

\[
W(v^*, a) = -\varepsilon \sum_{i=1}^{n} (a_i + a_i^*) + \sum_{i=1}^{n} a_i \sum_{j=1}^{n} (a_i - a_j) - \frac{1}{2} \sum_{i=1}^{n} a_i^* (a_i - a_i^*)(a_j - a_j^*)k(V_i, V_j)...
\]  

(4)

Subject to the following constraints,

\[
\sum_{i=1}^{n} (a_i - a_i^*) = 0, \quad 0 \leq a_i, a_i^* \leq C
\]  

(5)
To obtain,

\[ f(v) = \sum_{i=1}^{n}(a_i - a_i^*)k(V, V_i') + b \]  

where \(a_i\) and \(a_i^*\) are language multipliers, \(k(V, V_i')\) is a kernel that measures non-linear dependence between two instances of input variables, and \(N\) is the number of selected input data points that explain the underlying snow/runoff relationship [11].

### 2.3 Time series analysis (TSA)

Time series analysis is a powerful data analysis technique with two specific goals. The first is to identify a suitable mathematical model for data, and secondly to forecast future values in a series based on established patterns [12].

Accurate and unbiased estimation of time series data produced by the linear techniques cannot always be achieved, as real word applications are generally not amenable to linear prediction techniques. Real world time series application are faced by highly non-linear, complex dynamic and uncertain conditions in the field. Thus, estimation requires development of a more advanced time series prediction algorithm, such as that achieved using an artificial intelligence approach [13].

Structural change as a time series data characteristic should always be taken into consideration on all methodological approaches to time series analysis. In light of these characteristics it is expressed that recent data provides more relevant information than distant data. Consequently, recent data should be assigned weights relatively greater than weights assigned earlier data [8].

The time series is created with the use of the Mackey-Glass (MG) time delay differential equation [14] defined as

\[ \frac{dx(t)}{dt} = \frac{0.2x(t-\tau)}{1 + x^2(t-\tau)} - 0.1x(t) \]  

With the assumption that time step is 0.1, \(x(0) = 1.2, \tau = 17\) and \(x(t) = 0\) for \(t < 0\)

Where \(t\) is the data points, \(t\) is a non-negative time delay in evaluating a signal and \(x\) is a variable.

### 2.4 Scheffe simplex lattice method of analysis

The Scheffe’s simplex lattice method is a single step multiple comparison procedure and employs the use of a single regression polynomial to compare all the constituents in a single step generating the value of the objective function. The method builds an appropriate model that relates the response to the mixture components, and is a classic mixture approach developed on the principle that all components of the mixture sum up to unity, thus, making the components not independent of one another. The Scheffe’s method gives a clear understanding of how proportioning the constituents of the concrete affects the engineering behaviors of the concrete [15].

In mixture problems, the blending surface for the experimental programme is modelled with some form of mathematical equations. This will predict empirically the response for any mixture of the ingredients.

The coordinate system for mixture proportions is a simplex coordinate system. Simplex lattice method is used if the number of components is not large. The response in a mixture experiment usually is described by a polynomial function and this represents how the components affect the response. An ordered arrangement consisting of a uniformly spaced distribution of points on a simplex is known as a lattice [16].

A \(\{q, m\}\) simplex lattice design for \(q\) components consist of points defined by the following coordinate settings: The proportion assumed by each component take the \(m+1\) equally spaced values from 0 to 1,

\[ X_i = 0, \frac{1}{m}, \frac{2}{m}, \ldots, 1 \quad i = 1, 2, 3, \ldots, q \]

And the design space consist of all the reasonable combinations of all the values for each factor, \(m\) is usually called the degree of the lattice.

An experimental region for a three component mixture \((X_1, X_2 \text{ and } X_3)\) defined by this constraint is the regular triangle (simplex) shown in figure 1.

![Fig. 1: Layout of experimental design for three component mixture](image-url)
The axis for each component \( X_i \) extends from the vertex it labels \( X_i = 1 \) to the midpoint of the opposite side of the triangle \( X_i = 0 \). The vertices represents points, 1, 3, 5 \( (X_1, X_2, X_3) \) are the pure components, while points 2, 4, 6 \( (X_1, X_2, X_3, X_4, X_5) \) are the interactions.

For three components, the linear polynomial for a response \( Y \) is

\[
Y = b_0 + b_1X_1 + b_2X_2 + b_3X_3 + e
\]

Where the \( b_i \) are constraints and \( e \), the random error terms. Equation 1 is reparametrized to,

\[
Y = b_1X_1 + b_2X_2 + b_3X_3 + e
\]

Using \( b_0 = \left( X_1 + X_2 + X_3 \right) \)

Equation 9 is called the Scheffe’s linear mixture polynomial, for a quadratic polynomial:

\[
Y = b_0 + b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{11}X_1^2 + b_{22}X_2^2 + b_{33}X_3^2 + e --- (11)
\]

Reparameterizing Equation 11:

\[
Y = b_1X_1^2 + b_2X_2^2 + b_3X_3^2 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + e --- (12)
\]

Using:

\[
X_1^2 = X_1(1 - X_2 - X_3) \\
X_2^2 = X_2(1 - X_1 - X_3) \\
X_3^2 = X_3(1 - X_1 - X_2)
\]

III. METHODOLOGY

In this study five constituents (water, cement, termite mound, fine aggregate and coarse aggregate) were used for concrete production. The concrete was designed for grade 25 using the absolute volume method in accordance with ACI 211. The mix ratio of the design is 1:2:3 with a water-cementitious ratio of 0.43. 24 blends were selected and the proportions of cement and termite mound were varied in each of the blends with termite mound material replacing cement by weight from 5 to 25%. The proportions of other constituents were also measured by weight. A second degree Scheffe’s polynomial \{5, 2\} was adopted for the study and its development is presented in Equations 14 to 23.

For a five component mixture \( (X_1, X_2, X_3, X_4, X_5) \) a quadratic Scheffe polynomial of the form

\[
Y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{11}X_1^2 + b_{22}X_2^2 + b_{33}X_3^2 + e --- (14)
\]

The coefficients in Equation 14 are 25, but because of symmetry these are reduced to 15 in Equation 15. That is \( \beta_{ij} = \beta_{ji} \)

\[
Y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{11}X_1^2 + b_{22}X_2^2 + b_{33}X_3^2 + e --- (15)
\]

If the 5-component mixture in a concrete mix is used and are given as:

\[
X_1 = \text{Water} \quad X_2 = \text{Cement} \quad X_3 = \text{Termite Mound} \quad X_4 = \text{Fine Aggregate} \quad X_5 = \text{Coarse Aggregate}
\]

Where:

\[
\begin{bmatrix}
1, 0, 0, 0, 0 \\
0, 1, 0, 0, 0 \\
0, 0, 1, 0, 0 \\
0, 0, 0, 1, 0 \\
0, 0, 0, 0, 1
\end{bmatrix}
\]

Pure Blends

And:
3.1 Calculations for the Polynomial Coefficients

These are calculated as functions of the responses at the lattices. From the Scheffe’s simplex lattice mode equation, the responses $y_{ij}$ for $X_i = 1$, $X_j = 0$ for $i, j = 1, 2, 3, 4, 5$. The effect at the vertices are:

$$y_i = \beta_i$$

The effect of the two corresponding vertices at the midpoint, substituting $y_{ij}$ at $X_i = \frac{1}{2}$, $X_j = \frac{1}{2}$ for $i, j = 1, 2, 3, 4, 5$ for $j < i$ are

$$y_{ij} = \frac{1}{2} \beta_i + \frac{1}{2} \beta_j + \frac{1}{4} \beta_{ij}$$

where:

$$\frac{1}{2} \beta_i$$ The effect of ion $i$

$$\frac{1}{2} \beta_j$$ The effect of ion $j$

and $$\frac{1}{4} \beta_{ij}$$ The non-linear blending between points $i$ and $j$.

Since: $y_i = \beta_i$

Equation (16) can be re-written as:

$$\beta_i = y_i$$

And Equation (17) can be re-written as:

$$\beta_{23} = 4y_{23} - 2y_2 - 2y_3$$

3.2 Estimation of the $(q, m)$ polynomials

To estimate the parameters, $\beta_i$ and $\beta_{ij}$, let $b_i$ and $b_{ij}$ denote the estimates of $\beta_i$ and $\beta_{ij}$ respectively then

$$b_{ij} = 4y_{ij} - 2y_i - 2y_j$$

for $i, j = 1, 2, 3, 4, 5$. for $i < j$, then

The quantity $b_{ij}/4$ represent the difference in interaction of the blends from the effect of the pure components. From the replicates of the observations collected, the averages $\bar{y}_i$, $\bar{y}_j$, and $\bar{y}_{ij}$ are calculated from the replicates, then the averages are substituted into equations (18) and (19), then the least-square calculating formulas for the parameter estimates becomes,

$$b_i = \bar{y}_i$$

and

$$b_{ij} = 4\bar{y}_{ij} - 2\bar{y}_i - 2\bar{y}_j$$

for $i, j = 1, 2, 3, 4, 5$. for $i < j$, then

Table 1 shows the tabular representation of the simplex lattice and the corresponding proportions of the constituents for pure and interaction blends.
reduction of strength forming compounds (C, S, and A) in the blended cement through partial replacement of cement with TMM.

IV. DISCUSSION OF RESULT

4.1 Slump

Figure 2 shows that the slump of the fresh termite mound concrete mix increases with increase in the replacement of cement with termite mound material (Table 2). At 5% replacement, the slump increases by 4.9% with respect to the control; at 15% replacement, the slump increases by 21.0%, while at 25% replacement, the slump increases by 31.5% with reference to 0% replacement of cement with termite mound material.

It is reported [17] that if the volume concentration of a solid is held constant, the addition of mineral admixtures reduces the workability of the concrete mix; however in the case of this study the addition of termite mound improves the workability of the concrete mix, this might be as a result of the spherical nature of the fine particles which easily roll over one another reducing inter-particle friction. The spherical shape also minimizes the particles surface to volume ratio, resulting into low fluid demands [18].

4.2 Compressive Strength

Figure 3 shows the compressive strength development for the termite mound concrete at different replacement levels of cement with termite mound material. A linear decrease in the compressive strength was recorded with increase in the replacement level of termite mound material (Table 2). For 5%, 10%, 15%, 20% and 25% replacements, 11.9%, 18.7%, 19.0%, 24.6% and 45.0% decrease in the values of the compressive strength was recorded respectively with respect to the control at 28 days compressive strength, the reduction in strength of the concrete specimens as the replacement levels of cement with TMM increases is attributed to the reduction of strength forming compounds (C, S, C2S and C3A) in the blended cement through partial replacement of cement with TMM.

### Table 1: Tabular Representation of the Simplex Lattice and Mix Proportions

<table>
<thead>
<tr>
<th>Points</th>
<th>Water</th>
<th>Cement</th>
<th>TMM</th>
<th>F/A</th>
<th>C/A</th>
<th>Water (kg/m³)</th>
<th>Cement (kg/m³)</th>
<th>TMM (kg/m³)</th>
<th>F/A</th>
<th>C/A</th>
</tr>
</thead>
<tbody>
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<td>0.00</td>
<td>0.00</td>
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<td>1260.0</td>
</tr>
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<td>0.50</td>
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<td>344.8</td>
<td>86.4</td>
<td>523.0</td>
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### Table 2: Test Result for Slump and Compressive Strength

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<tr>
<th>Mix No</th>
<th>Slump (mm)</th>
<th>3 Days  (N/mm²)</th>
<th>7 Days  (N/mm²)</th>
<th>28 Days  (N/mm²)</th>
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<td>10.64</td>
<td>15.35</td>
<td>16.74</td>
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</table>
Figure 2: Relationship between Slump and Replacement Levels

Fig. 3: Relationship between Compressive Strength and TMM Replacements

Fig. 4: Relationship between Compressive Strength and Curing Age

Figure 4 shows the relationship between curing age (days) with compressive strength development, it was observed that compressive strength increases with days. No significant increase was observed after 28 days of curing. This might be as a result of non-activation of the pozzolanic effect of the termite mound material.

V. MODEL DEVELOPMENT

Mixes N1 to N3 and N12 to N45 were used to set up experiments to generate the experimental data that was used to determine the regresional coefficients (β) for model development. Models for predicting the slump and compressive strength were developed by substituting the values of β into equation (13) with the experimental data. Equations 24 to 27 are the developed models.

**Slump (workability)**

\[
Y = 51.5X_1 + 57.5X_2 + 62.0X_3 + 68.0X_4 + 71.5X_5 - 4.0X_1X_2 + 3.0X_1X_3 + 7.0X_1X_4 + 8.0X_1X_5 - 27.0X_2X_3 - 7.0X_2X_4 + 4.0X_2X_5 - 2.0X_3X_4 + 9.0X_3X_5 + 3.0X_4X_5
\]  

(24)

**3 Days Compressive Strength**

\[
Y = 13.2X_1 + 12.6X_2 + 10.9X_3 + 10.7X_4 + 10.5X_5 - 0.4X_1X_2 + 2.6X_1X_3 - 2.8X_1X_4 - 0.2X_1X_5 - 1.5X_2X_3 - 4.3X_2X_4 - 2.9X_2X_5 - 2.1X_3X_4 - 0.5X_3X_5 + 0.2X_4X_5
\]  

(25)

**7 Days Compressive Strength**

\[
Y = 20.5X_1 + 21.0X_2 + 21.5X_3 + 19.1X_4 + 13.0X_5 + 5.0X_1X_2 - 5.3X_1X_3 + 6.7X_1X_4 + 18.3X_1X_5 + 6.7X_2X_3 - 0.9X_2X_4 + 5.9X_2X_5 - 2.9X_3X_4 + 10.9X_3X_5 - 2.7X_4X_5
\]  

(26)
28 Days Compressive Strength

\[ Y = 28.2X_1 + 26.0X_2 + 26.0X_3 + 24.2X_4 + 17.6X_5 - 3.1X_1X_2 - 2.1X_1X_3 - 0.6X_1X_4 + 10.4X_3X_5 - 0.3X_2X_3 - 4.1X_2X_4 - 2.1X_3X_4 - 16.5X_1X_4 + 10.6X_3X_5 - 15.6X_4X_5 \]

(27)

VI. VALIDATION OF DEVELOPED MODELS

It was observed that the differences in values of the experimental slump and the predicted slump is within acceptable limit. The highest percentage difference recorded in the values of the experimental slump and the predicted slump is 5.5 % as shown in Table 3. It was also observed that in all cases except one, the experimental values are greater than the predicted values and the implication being that in practice concrete mix with better workability is expected.

For the compressive strengths, the models predicted compressive strength values that are favourably comparable with the experimental values. The percentage difference between the observed and predicted values are below 10 %, except in two cases where the percentage difference is above 10 %.

Based on the difference between the predicted and observed values, it is therefore found that the two models developed are adequate for the prediction of the slump and compressive strength of concrete specimen.

VII. STATISTICAL VALIDATION OF THE MODELS

The T-test was conducted to compare the actual difference between the mean of the predicted values and that of the observed values in relation to the variation in the sets of data. All models are tested at 95 % significant level. From the T-test results, all models except for three days compressive strength are significant at 95 % significant level having P-values equal or less than 0.05. The results are shown in Tables 3 and 4.

### Table 3: Validation Result for Slump

<table>
<thead>
<tr>
<th>Mix No.</th>
<th>Experimental Slump Values (mm)</th>
<th>Predicted Slump Values (mm)</th>
<th>Difference (mm)</th>
<th>Difference (%)</th>
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<tbody>
<tr>
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<td>3.1</td>
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</table>

T-Value = 2.53, P-Value = 0.035, Remarks = Significant at 95 % significance level

### Table 4: Validation Result for Compressive Strength

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<th>Age (Days)</th>
<th>Experimental Value (N/mm²)</th>
<th>Predicted Value (N/mm²)</th>
<th>Difference (N/mm²)</th>
<th>Difference (%)</th>
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T-Value = 2.67, P-Value = 0.028, Remarks = Significant at 95 % significance level
VIII. CONCLUSION

From results obtained above, the following conclusions were drawn,

i. As the percentage replacement of cement with termite mound material increases, the slump of the fresh concrete mix improves. This implies that the termite mound can be used to improve workability of concrete at low-water-cement ratio.

ii. Increasing the percentage replacement of cement with termite mound material the compressive strength of the concrete decreases, this is attributed to reduction of strength forming compounds (C₃S, C₂S and C₃A) in the concrete blend.

iii. The percentage difference between the predicted and observed values were found to be within accepted limits of not more than 10 %.

iv. From the T-test conducted to determine the relationship between the predicted and observed, all the models except the model for three days compressive strength were found to be significant at 95 % significant level.

This shows that the model should not be for predicting compressive strength at stages later than 7 days.

REFERENCES


