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Mathematical Model for the Prediction of Compressive Strength of Metakaolin Blended Cement Concrete using Sheffe's Simplex Method

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ABSTRACT
Current policies on building materials require a new approach that would enable the development of novel ideas and reduce the overall cost of construction. Environmental regulations require that we must be more sensitive on energy utilization and waste management. Metakaolin as a bye product of high temperature controlled burning of Kaolin which occurs in large quantities in many parts of Nigeria has been proven to exhibit pozzollanic properties. Generally, mix proportions of the various components determine the compressive strength and other properties of concrete. In this study, a mathematical model was developed for optimizing the compressive strength of metakaolin blended cement concrete based on Scheffe's Simplex lattice theory. A total of ninety (90) cubes were cast, consisting of three cubes per mix ratio and for a total of thirty (30) mix ratios. The first fifteen (15) were used to obtain the coefficients of the model, while the other fifteen were used to validate the model. The five component second degree (5, 2) mathematical model compared favorably with the experimental data and the predictions from the model were tested with the statistical Fischer test ant t-test, hence, found to be adequate at 95% confidence level. The optimum 28-day compressive strength of the blended concrete was found to be 45.091 N/mm2 and the corresponding mix ratio was 0.929: 0.071:1.884: 3.568:0.565 for cement: metakaolin: sand: granites: water respectively. The model derived in this study can be used to predict mix ratios for any desired strength or mix ratio of metakaolin blended cement concrete within the factor space of the simplex design used in the study.

Key words: Blended Cement, Compressive Strength, Concrete, metakaolin, Mathematical model, Optimization

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1. INTRODUCTION

One of the basic needs of man is housing, but in many developing countries like Nigeria, lack of Novel ideas to facilitate the provision and availability of houses has been identified as a panacea to this endless problem. It was on this note that the world Engineering Conference held in Nigeria in 2014 recommended that Engineers should develop novel ideas to ensure efficient and quality delivery of infrastructure to the people of sub-saharan Africa. It is important to note that majority of infrastructural developments in Nigeria are constructed using concrete, which has Portland limestone cement as a basic constituent, hence needs for correct utilization. It has also been proved that blending of this cements with other pozzolans ensures better and efficient quality of the resulting concrete which exhibits better lasting and durable structures. The optimal use of some of these pozzolans has attracted interest from researchers which has prompted this research into the best Use of Metakaolin in concrete production as partial replacement of cement which has started in the 1960's and the interest in this material has considerably increased in recent years. Metakaolin has pozzolanic properties bringing positive effects on resulting properties of concrete. Pozzolanic properties cause chemical reaction of active components with calcium hydroxide (portlandite), which is formed as a product of cement hydration. Therefore ,the aim of this study is to develop mathematical model for the optimization of Compressive Strength of metakaolin blended cement concrete based on Scheffe's (5, 2) simplex theory.

Different percentages of metakaolin were used for partial replacement of cement in the designed mix ratios of grade 30 concrete and placing the resultant mix ratios as pure blend component at vertices of the pentahedron. This involves the interaction of the pure blends with binary pseudo values at intersections, ternary blends and complete blends at the controls using the relation S = AX, where S= actual component of mix, A=Matrix of all the component mixtures at vertices, while X are the pseudo values. Testing concrete from the different mix ratios where cement is partially replaced with metakaolin and to develop a mathematical model that can be used to predict the compressive strength of concrete given any mix ratio or predict mix ratios given a particular Compressive Strength of concrete. As the number of components increased, cost per m3 increased, making optimization of concrete mixtures necessary so as to obtain concrete with required a suitable properties at minimum cost.

2. MATERIALS

Some of the materials used for this study was tested to determine suitability for making concrete are as follows:

- Water that is good for drinking obtained from the mains of the Rivers State University, Port Harcourt, Nigeria. The water was clean, fresh and free from dirt, unwanted chemicals or rubbish that may affect the desired quality of concrete conforming to BS EN 1008:2002.
- Portland Limestone cement, grade 42.5N that conforms to BS 12(1978) with specific gravity of 3.14.
- River sharp sand as fine aggregate obtained from Ogbogoro River, Port Harcourt. The river sand was sharp and free from clay, debris and other deleterious materials. The grading of the sand was carried out to BS 812:103 (BS 812: Part 1, 1975). The sand belongs to grading zone 2.
- The coarse aggregate used for this research work were granite chippings quarried from crushed rock industries quarry, Ishiagu, along Enugu-Port Harcourt express way, Ebonyi state, Nigeria. The granite has a maximum size of 20mm. They were washed and sun-dried for seven days in the laboratory to ensure that they were free from excessive dust, and organic matter.
- The Metakaolin was bought from Ogbuwa Group of companies, 117 Azikiwe Road, Aba, Abia state, Nigeria, who in turn are one of the distributors in Nigeria. They imported the metakaolin from NEELKANTH MINECHEM Company, E-63, 1-pase, RIICO industrial Area, Boronada, India. The laboratory test shows that it has a specific gravity of 1.84.

The mix ratios used for the simplex design points were obtained using four-dimensional simplex lattice factor space for five–component two-degree mixture with reference concrete mix design of grade 30 concrete without admixture.

Table -1 Physical Properties of Aggregate Used in the Production of Metakaoilin Blended Cement Concrete

Characteristics	Fine Aggregates	Coarse Aggregates
Source	**Ogbogoro, Obio/Akpo LGA, Rivers State**	**Isiagu, Evo L.G.A, Ebonyi State**
Type of Aggregates	Coarse Sand	20 mm maximum size
Specific gravity	2.46	2.7
Bulk density(KG/m^3)	1788	-
Fineness Modulus	3.73	5.36
Class of sand	Fine	Nominal size
Zone	Two (2)	20 mm
Coefficient of Uniformity(C_U)	3.6	1.88
Coefficient of Curvature (C_C)	0.9	1.01

The values of the coefficient of curvature, coefficient uniformity and fineness modulus obtained for the aggregates shows that they are well graded and suitable for making satisfactory concrete according to BS 812.

2.1 Component Mix Ratios

The mix ratios for the five pure blends is given in equation 3 as obtained from design of grade 30 concrete which gives 1:0.55:1.56:3.32 for (cement, water, sand and granite) is shown in equation 3.

$$[A]=\left\{\begin{matrix} 0.57 & 0.95 & 0.05 & 2.0 & 4.0 \\ 0.50 & 0.90 & 0.1 & 1.2 & 2.4 \\ 0.55 & 0.85 & 0.15 & 1.5 & 2.0 \\ 0.60 & 0.80 & 0.20 & 2.1 & 4.2 \\ 0.60 & 0.75 & 0.25 & 1.2 & 4.0 \end{matrix}\right\} \quad (1)$$

A11=Water Cement Ratio, A12=Cement, A13= Metakaolin, A14=Sand, A15=Granite, with row1 to row 5 repeated like as the mix ratios at the vertices.

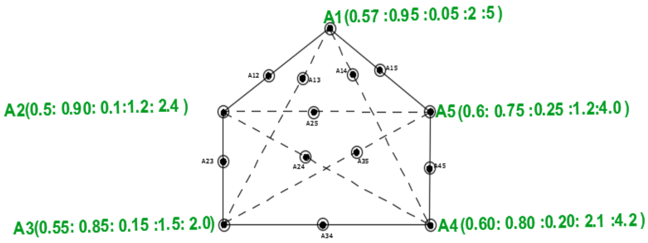

Fig. 1 Mix Ratios at the Vertices

2.2 Ratios at Vertices

As earlier mentioned, the actual component S and pseudo component, X, are related by a coefficient A. The relationship is expressed mathematically as

$$S=AX. \tag{2}$$

Which in a matrix form, gives Eqn.3

$$\begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{bmatrix} \begin{Bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \end{Bmatrix} \tag{3}$$

For the first 15 actual mix ratios, using pure and binary blends,

2.3 Computation of Actual Components of the First Fifteen (15) Mixes

At the design point P_{12}

Table -2 Pseudo values at intersections

Points	X_1	X_2	X_3	X_4	X_5
A_{12}	0.5	0.5	0	0	0
A_{13}	0.5	0	0.5	0	0
A_{14}	0.5	0	0	0.5	0
A_{15}	0.5	0	0	0	0.5
A_{23}	0	0.5	0.5	0	0
A_{24}	0	0.5	0	0.5	0
A_{25}	0	0.5	0	0	0.5
A_{34}	0	0	0.5	0	0.5
A_{35}	0	0	0.5	0	0.5
A_{45}	0	0	0	0.5	0.5

$$\begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \end{bmatrix} = \begin{bmatrix} 0.57 & 0.50 & 0.55 & 0.60 & 0.60 \\ 0.95 & 0.90 & 0.85 & 0.80 & 0.75 \\ 0.05 & 0.1 & 0.15 & 0.20 & 0.25 \\ 2.00 & 1.20 & 1.50 & 2.10 & 1.20 \\ 4.00 & 2.40 & 2.00 & 4.20 & 4.00 \end{bmatrix} \begin{Bmatrix} 0.5 \\ 0.5 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{4}$$

Solving for the actual components gives;

$S_1 = 0.535$, $S_2 = 0.925$, $S_3 = 0.075$, $S_4 =1.16$, $S_5 = 3.20$

The process of this solution was carried out for the rest of design points P_{13} to P_{45} to obtain S_1 to S_5 for P_{13} to P_{45}. The results of this process is presented in table 3

2.4 Computation of Actual Components 0f the Fifteen (15) Mixes for Controls

All the control points (C_1 C_2, C_3, C_4, C_5. C_6, C_7, C_8, $C_{9,}$ C_{10}, C_{11}, C_{12}, C_{13}, C_{14}, C_{15}) and are determined as follows by choosing ternary blends and complete blends whose addition must not be greater than one as pseudo values. When these pseudo values at selected points are multiplied by equation 3, all control points are obtained.

At the control point C_1

$$\begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \end{bmatrix} = \begin{bmatrix} 0.57 & 0.50 & 0.55 & 0.60 & 0.60 \\ 0.95 & 0.90 & 0.85 & 0.80 & 0.75 \\ 0.05 & 0.1 & 0.15 & 0.20 & 0.25 \\ 2.00 & 1.20 & 1.50 & 2.10 & 1.20 \\ 4.00 & 2.40 & 2.00 & 4.20 & 4.00 \end{bmatrix} \begin{Bmatrix} 0.333 \\ 0.333 \\ 0.333 \\ 0. \\ 0 \end{Bmatrix} \tag{5}$$

Solving for the actual components gives;

$S_1 = 0.539$, $S_2 = 0.899$, $S_3 = 0.100$, $S_4 = 1.565$, $S_5 =2.797$

This process of computation was carried out for the rest of design points C_3 to P_{15} to obtain control mixer's real components, $S_{1\text{-}5}$ for C_3 to C_{15}.

The proportions of the real mixes for laboratory compressive strength test are obtained by multiplying the actual mix ratios with concrete density of 2400kg/m^3.

Table -3 Experimental Material Composition Mixtures for Concrete from Metakaolin Blended Cement

Point	Water (Kg)	Cement (Kg)	Metakaolin (Kg)	Sand (Kg)	Chippings (Kg)
P1	2.013	3.354	0.177	7.062	14.124
P2	2.621	4.717	0.524	6.289	12.579
P3	2.911	4.499	0.794	7.940	10.586
P4	2.030	2.707	0.677	7.105	14.211
P5	2.359	2.948	0.983	4.717	15.724
P6	2.257	3.903	0.316	6.751	13.502
P7	2.372	3.813	0.424	7.413	12.708
P8	2.022	3.024	0.432	7.084	14.168
P9	2.176	3.162	0.558	5.952	14.881
P10	2.765	4.609	0.658	7.110	11.587
P11	2.262	3.495	0.617	6.785	13.571
P12	2.471	3.706	0.786	5.391	14.376
P13	2.374	3.406	0.722	7.431	12.797
P14	2.594	3.609	0.902	6.090	13.534
P15	2.182	2.818	0.818	6.001	14.911
Controls					
C1	2.444	4.073	0.453	7.090	12.671
C2	2.241	3.387	0.521	7.295	13.287
C3	2.124	3.001	0.600	6.361	14.643
C4	2.316	3.652	0.522	7.095	13.146
C5	2.270	3.278	0.636	6.653	13.893
C6	2.420	3.761	0.600	6.432	13.518
C7	2.315	3.858	0.370	7.081	13.106
C8	2.268	3.466	0.495	6.635	13.865
C9	2.247	3.584	0.443	7.087	13.369
C10	2.325	3.504	0.618	6.596	13.687
C11	2.268	3.395	0.576	6.672	13.820
C12	2.326	3.425	0.677	6.604	13.699
C13	2.356	3.636	0.555	6.518	13.665
C14	2.285	3.458	0.586	6.571	13.830
C15	2.135	3.148	0.523	6.387	14.537
	69.746	**106.395**	**17.563**	**200.200**	**407.995**

2.5 Compressive Strength Test

Batching of the ingredients was done by mass and shown in table 2. Cement/ metakaolin was thoroughly mixed together with a mixture of sand and granite. The entire component was cast in concrete mould of size 150 x 150x 150 mm using the procedures of BS1881. The concrete cubes were cured in a curing tank for 28 days and were crushed using universal testing machine. Compressive strength of the cubes was calculated using equation 6.

$$Compressive\ Strength(Y) = \frac{\text{Maximum Load at Failure}}{\text{Area of cube}}\ (\text{N/mm}^2) \qquad (6)$$

Compressive strengths of the concrete cubes from the laboratory as obtained from the thirty points of observations are shown in Table 4.

Table -4 Experimental and Schefe's Compressive Strength Result

S/No	Response Symbol	Experimental Compressive Strength (N/mm^2)	Scheffe's model Compressive Strength (N/mm^2)
1	P_1	42.52	42.52
2	P_2	48.15	48.15
3	P_3	37.33	37.33
4	P_4	45.78	45.78
5	P_5	24.59	24.59
6	P_{12}	47.85	47.85
7	P_{13}	45.48	45.48
8	P_{14}	38.37	38.37
9	P_{15}	33.04	33.04
10	P_{23}	34.81	34.81

11	P_{24}	38.07	38.07
12	P_{25}	37.33	37.33
13	P_{34}	32.00	32.00
14	P_{35}	30.37	30.37
15	P_{45}	20.56	20.56
16	C_1	43.41	42.73
17	C_2	37.19	37.53
18	C_3	27.11	28.33
19	C_4	38.22	37.43
20	C_5	29.19	31.18
21	C_6	37.19	38.15
22	C_7	45.33	44.69
23	C_8	38.37	39.11
24	C_9	41.93	39.77
25	C_{10}	33.19	33.46
26	C_{11}	33.93	34.00
27	C_{12}	29.63	30.77
28	C_{13}	38.67	38.68
29	C14	34.52	34.23
30	C_{15}	32.00	32.13

3. METHODS

5, 2 Scheffe's Simplex Design

Response equation of Scheffe's (5, 2) simplex design was given by (Obam, 2006) as:

$$Y= \beta_i X_1 + \beta_2X_2 + \beta_3X_3 + \beta_4X_4 + \beta_5X_5 + \beta_{12}X_1X_2 + \beta_{13}X_1X_3 + \beta_{14}X_1X_4 + \beta_{14}X_1X_5 + \beta_{23}X_2X_3 + \beta_{24}X_2X_4 + \beta_{25}X_2X_5 + \beta_{34}X_3X_4 + \beta_{35}X_3X_5 + \beta_{45}X_4X_5. \quad (7)$$

Where β_i and Xi are the coefficients of response equation and pseudo components of the mix respectively.

$$\{\beta_1= p_1, \beta_2= p_2, \beta_3= p_3, \beta_4= p_4, \beta_5= p_5, \beta_{12}=4p_{12}-2p_1-2p_2, \beta_{13}=4p_{13}-2p_1-2p_3, \beta_{14}=4p_{14}-2p_1-2p_4, \beta_{15}=4p_{15}-2p_1-2p_5, \beta_{23}=4p_{23}-2p_2-2p_3, \beta_{24}=4p_{24}-2p_2-2p_4, \beta_{25}=4p_{25}-2p_2-2p_5, \beta_{34}=4p_{34}-2p_3-2p_4, \beta_{35}=4p_{35}-2p_3-2p_5, \beta_{45}=4p_{45}-2p_4-2p_5\} \quad (8)$$

Where, y_1 to y_{15} are the compressive strengths from the laboratory testing of the mixtures in table 1 as shown in table 2.

3.1 Model for Predicting the Compressive Strength of Metakaolin Blended Cement Concrete

This model is obtained by substituting experimental compressive strength in table 5 of concrete compressive strength from the first fifteen points of observations (P_1, P_2, P_3, P_4, P_5, P_6, P_7, P_8, P_9, P_{10}, P_{11}, P_{12}, P_{13}, P_{14}, and P_{15}) into equation 2 and 3 to obtain:

$$Y=42.52X_1+48.15X_2+37.33X_3+45.78X_4+24.59X_5+10.07X_1X_2+22.22X_1X_3-23.11X_1X_4-2.07X_1X_5-31.70X_2X_3-35.56X_2X_4+3.85X_2X_5-38.22X_3X_4-2.37X_3X_5-58.49X_4X_5 \quad (9)$$

Equation (6) is the mathematical model for the optimization of compressive strength of Metakaolin Blended Cement concrete based on Scheffe's (5, 2) factor space.

3.2 Validation of Scheffe's Model

The model was validated by carrying out two tests. They are; Students T-Statistics test and Fisher F-Statistics Test at 95% confidence level on the compressive strengths at the control points (that is, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, and C15). In this test, two hypotheses were set as follows:

3.2.1 Null Hypothesis

There is no significant difference between the laboratory concrete cube strength and model predicted strength results.

3.2.2 Alternative Hypothesis

There is a significant difference between the laboratory concrete cube strength and model predicted strength results.

Fisher's F-Statistics Test

The summary of the F-test is given in Table 5.

From the table above, F critical (one Tail) of 2.4837 is greater than calculated F (1.3199), hence, Null hypothesis is accepted.

Students T-Statistics Test

The summary of the t-test is given in Table 6.

Table -6 t-Test: Paired Two Sample for Means

	Experimental Control Result	Scheffe's Model Result
Mean	35.99012346	36.14634157
Variance	28.14490822	21.32283628
Observations	15	15
Pearson Correlation	0.988808503	
Hypothesized Mean Difference	0	
df	14	
t Stat	-0.59877545	
P(T<=t) one-tail	0.279443624	
t Critical one-tail	1.761310136	
P(T<=t) two-tail	0.558887249	
t Critical two-tail	2.144786688	

From the table 4.5, both t-critical (one Tail) of 1.7613 and t-critical (two Tail) of 2.145 is greater than calculated t-statistics of -0.599, hence, this shows that Null hypothesis is accepted.

4. APPLICATION OF THE DEVELOPED MODEL FOR THE OPTIMIZATION OF METAKAOLIN BLENDED CEMENT

A computer program was written in Microsoft Visual Basic 6.0 which allows the user to input any compressive strength of choice while the software returns the mix ratios of the concrete materials that gives the strength.

Table -7 Microsoft Visual Basic 6.0 Optimum Predicted Compressive Strengths for grade 30, 32, 37, 40, 42 and 45 N/mm^2

Metakaolin-Cement Ratio (%)	Predicted Compressive Strength (N/mm^2)	Water-Cement Ratio	Cement Content	Metakaolin Content	Sand Content	Granite Content
22.55	30.079	0.57	0.816	0.184	1.475	2.84
20.05	32.083	0.568	0.833	0.167	1.505	3.12
10.98	37.97	0.579	0.902	0.099	1.939	4.038
9.65	40.096	0.574	0.912	0.088	1.98	3.88
8.33	42.075	0.569	0.924	0.077	1.936	3.772
7.64	45.091	0.565	0.929	0.071	1.884	3.568

5. CONCLUSION

In this study, Scheffe's modeling technique has been applied and used successfully to develop model for optimization of 28-day compressive strength of metakaolin blended cement concrete. On the basis of the analysis of experimental data of 30 concrete mixes results and the predicted results, the following conclusions can be made.

1. Optimization and prediction model of the compressive strength of metakaolin blended cement concrete was successfully developed in this study using Scheffe's Simplex lattice model.
2. The compressive strength tests carried out on the resultant 30 mixes from Scheffe's 5, 2 mix shows that strength of metakaolin blended cement concrete meets the requirement of reinforced concrete as stated in ACI 211.1.
3. The reliability of the model was validated with student's t-test and the fisher test which showed that the predicted results has no significant difference between the mean and variance of the laboratory result and predicted results. Hence the model developed is adequate within 95% confidence level and the Null Hypothesis (H_0) is chosen.

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