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Predictive Model for Compressive Strength of Geopolymer Concrete Produced from Metakaolin and Fly Ash with Bagasse Ash

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Abstract: This study aimed to investigate the effects of various parameters on the compressive strength of geopolymer concrete produced using met kaolin and Costus lacerus (CL) bagasse ash. A mix model was developed as a function of curing age and temperature, sodium hydroxide concentration, activator ratio, and bagasse ash using data from experiments. The model was then used to predict the compressive strength of concrete and compared to the measured compressive strength. The model was found to be effective in predicting compressive strength with an R^2 value of 0.9667 and a root mean squared error (RMSE) of 2.353, indicating that 96.67% of the measured compressive strength was estimated by the model with 0.0235% error. Therefore, the predicted compressive can be used to predict the compressive strength of geopolymer concrete for the given mix proportions and curing conditions, and the efficient prediction of the compressive strength would save cost and energy required in performing the compressive strength test experimentally.

Keywords: Compressive Strength, Metakaolin, Mix Variables, Geopolymer Concrete

1. Introduction

Geopolymer concrete is a type of concrete made from industrial waste materials, such as fly ash, slag, metakaolin and silica fume. It has been the subject of many research studies in recent years due to its potential to reduce the environmental impact of traditional cement-based concrete. The compressive strength of concrete is an important indicator of concrete performance and durability. In recent years, there have been several studies on the use of predictive models to estimate the compressive strength of geopolymer concrete.

Predictive models for the compressive strength of geopolymer concrete have been developed using a variety of techniques, including artificial neural networks, multiple linear regression, and genetic algorithms. These models have been used to predict the compressive strength of geopolymer concrete based on various input variables, such as the amount of the raw materials used, the curing conditions, and the chemical composition of the geopolymer.

A study by Li et al. (2018) used artificial neural networks (ANNs) to predict the compressive strength of fly ash-based geopolymer concrete. They found that the ANN model was able to accurately predict the compressive strength with a high coefficient of determination (R^2) value of 0.958.Sun et al. (2018) also used a neural network model to predict the compressive strength of geopolymer concrete, and found that the model was accurately predicted the compressive strength of the concrete, with a mean absolute error of less than 2%.

Multiple linear regression method is another method used in developing model involving several independent variables from experimental studies. Al-Jabri et al. (2019)used the multiple linear regression (MLR) to predict the compressive strength of geopolymer concrete made with different types of industrial waste materials, such as fly ash, slag, and silica fume, it was reported that the MLR model was able to accurately predict the compressive strength with an R^2 value of 0.902.Gupta et al. (2020) also used the multiple linear regression model to predict the compressive strength of geopolymer concrete, with results showing that the model was effective and the predicted compressive strength was comparable to the measured values with minimal error.

Another model called "random forest model" was applied by El-Gendy et al. (2021) to predict the compressive strength of geopolymer concrete. The study found that the model predicted the compressive strength of the concrete, with a coefficient of determination of 0.94. Also, Wang et al. (2020) used a support vector machine (SVM) model to predict the compressive strength of fly ash-based geopolymer concrete. They found that the SVM model was able to accurately predict the compressive strength with a high coefficient of determination (R2) value of 0.974. In another study, Ahmed and Ali (2022) developed a model for prediction compressive strength of geopolymer concrete using the combination of Artificial Neural Network and Genetic Algorithm, and a predictive accuracy reported with a coefficient of determination of 0.95.

In conclusion, many studies have been conducted to predict the compressive strength of geopolymer concrete using various predictive models, such as artificial neural networks, multiple linear regression, support vector machine, and hybrid models combining artificial neural networks and genetic algorithms or particle swarm optimization. These studies have reported high coefficient of determination (R^2) values, indicating that the models are able to accurately predict the compressive strength of geopolymer concrete.

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determination (R^2) values, indicating that the models are able to accurately predict the compressive strength of geopolymer concrete. Therefore, this study developed the a mix model for the prediction of compressive strength as a function of curing age and temperature, sodium hydroxide concentration, activator ratio, and bagasse ash.

2. Materials and Methods

2.1 Materials

The materials used include fly ash, Costusafer, sodium hydroxide (NaOH), sodium silicate (Na_2SiO_3), water, fine and coarse aggregates.

2.2 Preparation of Samples

All samples used in the study were according to standards as discussed in the following section.

2.2.1 Bagasse ash preparation

The Costusafer (CA) plants was collected from the bush and cut into pieces before transported to the laboratory. The pieces of CA were carbonized in the furnace at 300 – 400 °C temperature. The carbonized products were pulverized using ball millto obtain fine ashes, which were sieved to through a 90μm particle size sieve.

2.2.2. Metakaolin preparation

Metakaolin was prepared from natural clay. Clay samples were collected from Bori Community in swampy area at about 1 - 2m depth. The clay samples were packaged in polythene bags and transported to the laboratory for processing into metakaolin. The method described by Srilai et al. (2018) for synthesis of natural clay to metakaolin was adopted. Firstly, the raw natural clay in a container was dissolved and dispersed in distilled water, and allowed to settle for about 2 hours. Suspended solid particles were separated via decantation. More water was poured into the container and stirred to remove more particulate maters. Thereafter, the washed raw clay sample was transferred into Teflon lined autoclave and mixed with deionised water at 200 °C for 12 hours to obtain kaolin clay. The kaolin was dried, crushed in ball mill crusher to powdered form and sieved to 90μmparticle size. After crushing, the kaolin clay was calcined via heating in electric furnace to obtained metakaolin. Several samples of the washed clay, weighing about 2kg each, were separately placed in the oven and heated gradually to 700°C temperature at constant rate of 10°C/min for 4 hours to obtain the metakaolin. The heated samples were quenched at ambient conditions to avoid crystallization of amorphous metakaolin (Sánchez et al., 2020).

2.2.3 Alkaline Activators

Sodium hydroxide and sodium silicate were used as alkaline activator. Both activators were obtained from a science and laboratory store in Port Harcourt, Rivers State. The sodium hydroxide is a technical grade sodium hydroxide in flakes form (3mm), with a specific gravity of 2.130 and 98% purity. The sodium hydroxide (NaOH) solution was prepared by dissolving the pellets in water at predetermined weight to obtain the desired molar concentration. The molar concentration of NaOH was varied from 8, 10, 12, 14 and 16M. To calculate weight required to obtain the desired molar concentration, the molecular weight of NaOH (40g/mol) is multiplied by the desired molar concentration per volume of the solution. For instance, the weght required to make 12M, was obtained by multiplying 12 x 40 = 480g. Each of the NaOH concentration was mixed with a measured weight of sodium silicate to obtain the ratio of sodium silicate to sodium hydroxide of 0.5:1, 1:1, 2:1 and 2.5:1.

2.2.4 Aggregates

Aggregates were obtained from a retailer. Both the coarse and fine aggregates were crushed and sieved to a uniform sizes according to standard method.

2.3 Experimental procedure

Different weights of the metakoalin were mixed with5%, 10%, 15% and 20% bagasse ash to obtain a combined-constant geopolymer composite weight of 417.7kg/m^3 in concrete mixer. Each of the prepared activator solution was added into the concrete mixer at a mix ratio of geopolymer to activator solution of 2.5:1, to produce the geopolymer paste. Fine and coarse aggregates were then added to the geopolymer composite in the mixer at the ratio of 1:2:4, and mixed properly in the concrete mixer. After the mixing, the concrete paste was poured into moulds and compacted. After setting, the samples were cured in the oven for 24 hours at different temperatures (27, 60, 70, 80, 90 and 100°C). The temperature cured concrete specimens were wrapped in thin waterproof and air cured for 7, 14, 21, 28, 56 and 90 days. Table 1 shows the concrete mix design.

Table 1: Geopolymer concrete mixdesign

	Quantity (kg/m^3)				
CL (%)	Coarse aggregate	fine aggregate	MK	AS	CL
0	1176.1	578.5	417.7	208.85	0
5	1176.1	578.5	396.81	208.85	20.89
10	1176.1	578.5	375.93	208.85	41.77
15	1176.1	578.5	355.04	208.85	62.66
20	1176.1	578.5	334.16	208.85	83.54

AS = Activator solution, CL = Costuslacerus, MK = Metakaolin

2.4 Compressive strength test

The compressive strength test on the geopolymer concrete was performed on the casted cubes in accordance with BS 1881-116 (BSI, 1983) in the laboratory. The dimensions of the casted geopolymer concrete cubes were 100 x100 x 100 mm. On the test day, representative concrete specimens from the different mixes were randomly selected from the fog room and tested for compressive strength.

2. 5 Development of Model for Compressive Strength Prediction

The compressive strength of the geopolymer concrete was studied using a developed model. Thus, the compressive strength model is expressed as a function of bagasse ash (Costusafer and Costus lacerus) percentage in the concrete mix, curing age, curing temperature, NaOH concentration and activator ratio. The multiple regression technique was used in formulating the models. The model is expressed as:

$$f_c = \psi \gamma_B^{a_1} t^{a_2} T^{a_3} C_a^{a_4} \lambda_{AR}^{a_5} \tag{1}$$

Where: f_c = Compressive strength (MPa)

γ_B =Weight fraction of bagasse ash (kg/kg)

t =Curing age (Days)

T =Curing temperature (°C)

C_a =NaOH concentration (M)

λ_{AR} =Activator ratio, AR(ml/ml)

ψ = Model coefficient

a_1, a_2, a_3, a_4 and a_5 =Power index relating the independent variables

Equation (1) was solved using Microsoft Excel Analysis Tool Pak. The evaluated constants were substituted into equation (1), and used to predict the compressive strength at any given mix proportion and curing condition. The experimental plan data used for the development of the model is given in Table 2.

Table 2: Mix data for development of compressive strength model

γ_B	t (days)	T (°C)	C_a (M)	λ_{AR}
0.05	28	80	10	2
0.1	28	80	10	2
0.15	28	80	10	2
0.2	28	80	10	2
0.1	7	80	10	2
0.1	14	80	10	2
0.1	21	80	10	2
0.1	56	80	10	2

0.1	90	80	10	2
0.1	28	27	10	2
0.1	28	60	10	2
0.1	28	70	10	2
0.1	28	90	10	2
0.1	28	100	10	2
0.1	28	80	8	2
0.1	28	80	12	2
0.1	28	80	14	2
0.1	28	80	16	2
0.1	28	80	10	0.5
0.1	28	80	10	1
0.1	28	80	10	1.5
0.1	28	80	10	2.5

Further, the results predicted by the model were compared with the measured values using the root mean-square error (RMSE). This is stated as:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}\left(X_{predicted} - X_{measured}\right)^2}{N}} \quad (2)$$

Where: $X_{predicted}$ = Predicted strength at any time or referent point

$X_{measured}$ = Measured strength at any time or referent point

N = Number of data points

The resulted RMSE value was also multiplied by 100% to estimate the percentage of error or deviation between the predicted and measured compressive strength.

3. Results and Discussion

The experimental measurement and predicted compressive strength of geopolymer concrete produced from metakoal in (MK) with Costus lacerus (CL) bagasse ash have been obtained as presented in Tables 3 and 4.

Table 3: Measured and predicted compressive strength at 28 days

Ash (%)	**Compressive strength, f_c (MPa)**	
	Measured	Predicted
5	52.18	56.80
10	56.44	53.51
15	49.39	51.67
20	47.55	50.41

Table 4: Measured and predicted compressive strength at 10% bagasse ash

Age (Days)	Compressive strength, f_c(MPa)	
	Measured	**Predicted**
7	48.4	46.18
14	50.57	49.71
21	52.77	51.9
28	56.44	53.51
56	61.37	57.59
90	62.55	60.57

3.1 Model for compressive Strength Prediction

The compressive strength of geopolymer concrete is affected by several factors, particularly the parameters used in making the concrete. These factors, in extension, are influenced by the geopolymer type and the amount present, the synthesis conditions, and the curing conditions. Therefore, the mix model was developed as a function of curing age and temperature, sodium hydroxide concentration, activator ratio and bagasse ash. The formulated model equation (Equation 1) was implemented in Microsoft Excel Tool PaK, utilizing the experimental data. The resulting model was used to predict the compressive strength of concrete at any experimental design condition and compared with the measured compressive strength to estimate the degree of prediction and efficacy of the model.

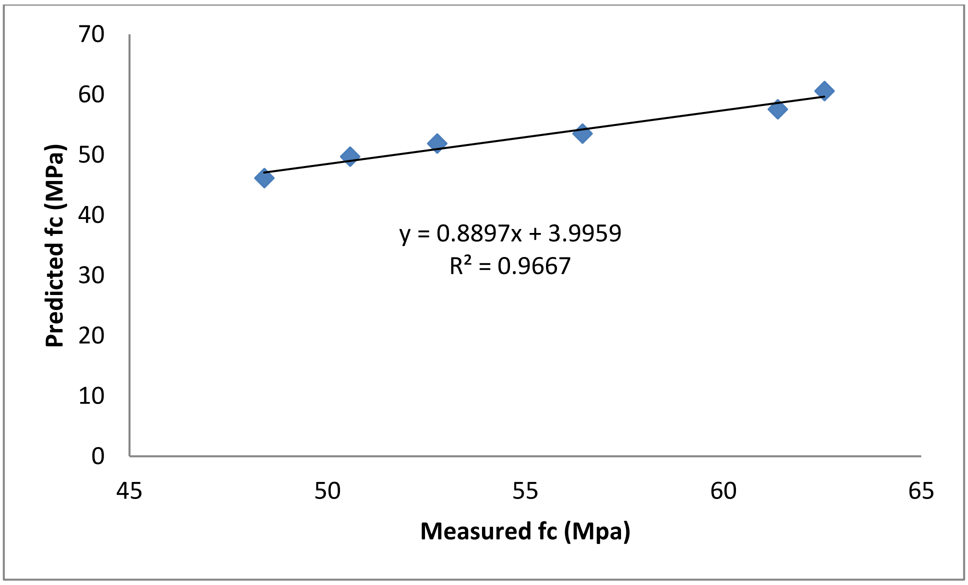

Figure 1: Measured and predicted compressive strength of concrete

Figure 1 shows the plot of the predicted compressive strength against the measured values obtainedas a function of Costuslacerus (CL) bagasse ash, curing age, curing temperature, sodium hydroxide concentration, and activator ratio. The obtained constant coefficients were substituted into equation (1) to obtain the predictive model for estimation of compressive strength of geopolymer concrete produced from MK and CL. The obtained model is expressed as $f_c = 0.5078\gamma_B^{-0.086}t^{0.106}T^{0.926}C_a^{-0.062}\lambda_{AR}^{0.279}$. The indicted R^2 value of0.9667 implied that 96.67% of the measured compressive strength was predicted by the model. In addition, the RMSE was evaluated as 2.353, which showed that the predictive model only resulted in an error of 0.0235% compared to the measured compressive strength. Thus, the model is effective in predicting the compressive strength of the concrete for the given mix design.

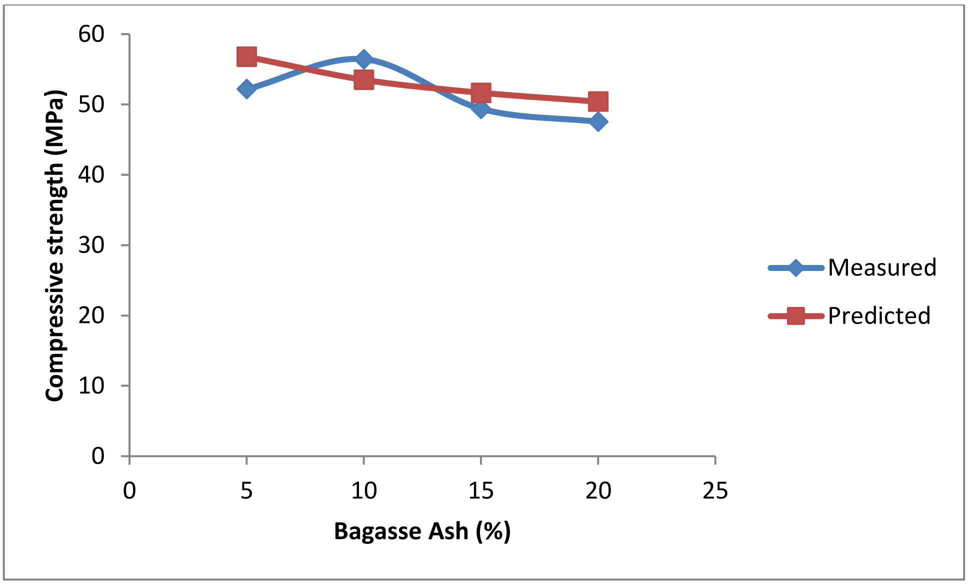

Figure 2: Measured and predicted compressive strength against CL percentage

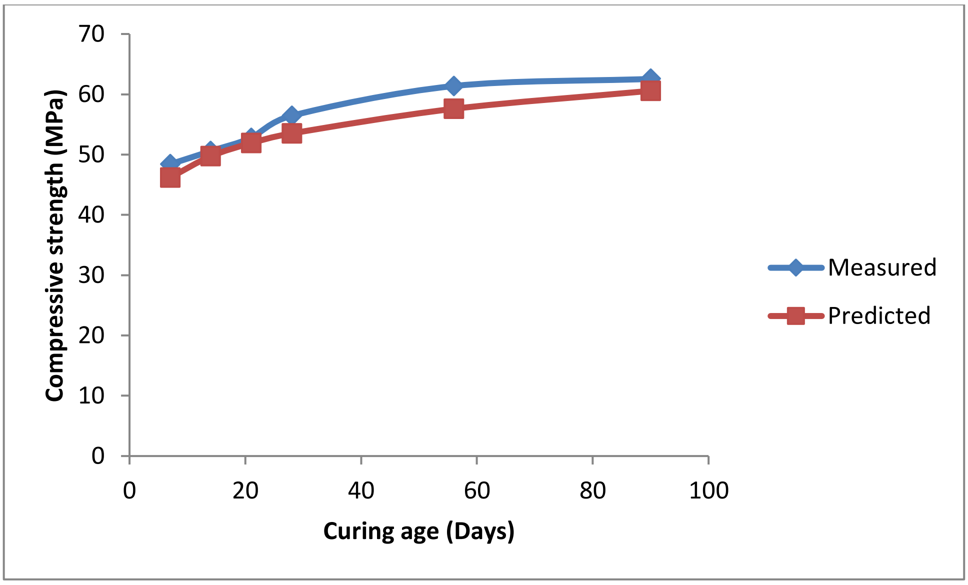

Figure 3: Predicted Compressive strength for a given curing age

Figure 2is the comparison of predicted and measured compressive strength at 28 days curing age, 80°C curing temperature, 10M sodium hydroxide concentration, 2:1 activator ratio and at varying CL bagasse ash from 5 – 20%. The predicted compressive strength decreased with increasing bagasse ash from 5 – 20%, but from the experimental measurement, the compressive strength initially increased from 5 – 10% CLbagasse before decreasing thereafter as the bagasse ash was increased to 15% and 20%. Thus, from the results presented in Table 3, the predicted compressive strength ranged from 50.41 – 56.80MP, while from the experiment, it ranged from 47.55 – 56.44MPa. The maximum strength was recorded at 5% CL from the predictive model and 10% from the experimental measurement.

However, by varying the curing age while keeping the bagasse ash constant alongside with curing temperature, sodium hydroxide concentration and activator ratio, the predicted and measured compressive strength increased with increasing curing age with similar trend as shown in Figure 3. At the given mix proportions and curing ages of 7 to 90 days, the predicted compressive strengths increased from 46.18 – 60.57MPa, while the measured strength ranged from 48.40 – 61.37MPa(Table 4). The values of compressive strength predicted by the model were slightly lower than the compressive strength obtained from the experimental measurement. The observation from the model is that compressive strength behaves uniquely with changes in the different independent model variables. Notwithstanding the variability, the model can be used to predict the compressive strength geopolymer concrete at any change in mix variables or curing conditions.

It is worthy of note that several authors have developed mathematical models for prediction of geopolymer concrete compressive strength as variable that depends on concrete mix parameters, but most of the developed models considered compressive strength as a function of few variables in the mix parameters. Thus, compressive strength was considered as a function of oxides composition in coal gangue-based geopolymer concrete (Zhang et al., 2021), while in another study, it was modeled to depend only on alkaline activators (Beskopylny et al., 2021). In the workby Zhang et al. (2022),the compressive strength was modeled in terms of temperature only. However, other studies have developed models for compressive strength prediction by considering quite a number of parameters that influenced the mechanical properties of geopolymer concrete. The developed modelby Kishore et al. (2021) expressed the compressive strength of fly ash-based geopolymer concrete as a function of sodium hydroxide concentration, activator-to-binder ratio, curing temperature and coarse aggregate content, with the RMSE obtained as 5.37 MPa. Also, Ahmed et al. (2022) expressed the compressive strength as variable which depends on the alkaline liquid to binder ratio, fly ash content, sodium hydroxide concentration and sodium silicate content. Generally, it is important to consider all influential variables on the properties of geopolymer concrete when developing a model for prediction of compressive strength.

4. Conclusion

This study developed a mix model to predict the compressive strength of geopolymer concrete as a dependent variable on curing age, curing temperature, sodium hydroxide concentration, activator ratio and bagasse ash. The predicted results compared well with the measured compressive strength with an R^2 value of 0.9667 and RMSE of 2.353. However, the predicted compressive strength decreased with increasing percentage of bagasse ash, while in the experiment, it first increase from 5 -10% CL before decreasing as the CL percentage was increased further. Overall, the model proved effective for the prediction of compressive strength of concrete for any given mix design using metakaolin and Costus lacerus bagasse ash.

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