Application of Machine Learning in Prediction of Strength Properties of GGBS based Geopolymer Concrete

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Abstract. The current study is one such initiative to analyze the effect of heat curing in geopolymer concrete made of Ground Granulated Blast Furnace Slag (GGBS) as base material. With higher sodium hydroxide concentrations (14M and 16M) and different alkaline activator ratios (1, 1.5, 2, and 2.5), the GGBS-based geopolymer concrete is examined to ascertain the strength, durability, flexural characteristics. The tests were conducted under exposed elevated temperature curing, which ranges from 100°C to 800°C. The proposed mixture planned for this study was 1:1.40:3.28:0.40. The combination contains of GGBS, river sand, coarse aggregate and the alkaline activator solution. To maintain the workability, 3% of water and 1% of superplasticizer were used in the mixture. After casting, all the geopolymer samples were heat cured at 60°C for 24 hours and kept in ambient temperature for 24 hours and exposed to 100ºC and 800ºC elevated temperature curing with an exposure of 1 to 6 hours using muffle furnace of 1000ºC capacity. The mechanical, durability and flexural properties of the specimens were studied and resulted the impact of elevated temperature and its exposure in the GGBS based geopolymer concrete. The theoretical relationships between mechanical properties have been developed with respect to elevated temperature and derived equations for split tensile strength (0.52 $\sqrt{fck}$ for both GP14M and GP16M) and flexural strength (1.03 $\sqrt{fck}$ for GP14M and 1.08 $\sqrt{fck}$ for GP16M). Machine Learning concept has been adopted to predict the mechanical properties based on different dependent variables such as alkaline ratio, molar concentration, temperature exposure and elevated temperature. The predicted results were highly compatible with experimental and theoretical investigations.

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1 Introduction

Geopolymer is formed by the fast chemical reaction between silica and aluminium minerals in an alkaline environment. This technique will result in a 3-D ring structure with Si-O-Al-O links. Also the said process considerably reduced the release of carbon dioxide emission by one-sixth time than the cement and considered as worthwhile alternative for cement. [1-2]To begin with natural minerals like metakaolin, clays etc. contains Si-Al were experimented as base material. Researchers acknowledged that the industrial by-products are most suitable base materials for geopolymer. In cement, calcium is the reactive material which acts as a binder but for geopolymer artificial binding need to be created using alkaline liquids. [3]

The researchers have used sodium/potassium hydroxides and silicates as alkaline liquids and found that the usage of sodium silicate and hydroxide solution has provided excellent chain structure with different base materials. The high compressive strength of geopolymer concrete can be achieved while using higher NaOH concentration and high ratio of Na2SiO3-NaOH liquid ratio.

Reference [4] investigated combination of fly ash and 4% slag and specified that the addition of slag enhanced the compressive strength considerably. This geopolymer concretes were cured under 30°C and 70°C for 14 days and given compressive strength of 50Mpa and 70MPa respectively. The results of XRD and FTIR showcased intense amorphous structure because of slag and which would be the reason for faster reaction and increment in strength. The decrease in binding energy was more favourable to zeolite formation.

Granulated Blast Furnace Slag (GGBS) geopolymer concrete was created and allowed to cure for 180 days, according to Reference [5]. The results derived that it has high alkali activator which led in to early strength achievement and later ultimate compressive strength was found as 50MPa after180 days. Reference [6] investigated the geopolymer against fire and derived the stress-strain behavior of geopolymer under elevated temperature. The results were shown remarkable contraction while increasing the temperature between 200°C to 290°C. Reference [7] also made an experiment with Australian fly ash to find the impact of increased temperature in geopolymer paste, mortar and concrete. The parameters considered were size and type of aggregates, super plasticizer and type of specimen. They determined that size of the specimen played a vital role in the thermal behavior than the aggregate size at 800°C. A 10mm size aggregate provided high strength characteristics in both ambient and higher temperatures.[8-12]

Numerous earlier studies concentrated on the residual qualities of geopolymer mortar and paste, and it was discovered that fly ash-based geopolymers preserved a fair degree of residual strength when subjected to high temperatures. This might be one of the many nanopores created by water escaping during the geopolymerization process.

The aforementioned literatures unequivocally declare that curing geopolymer concrete at a high temperature is essential.[13-16]

Subsequently, all the researchers were experimented with fly ash as base material or combination of fly ash with few percentages of GGBS or other industrial by-products as base materials. At an elevated temperature above 100°C, many researchers tried for the preparation of geopolymer paste or mortar with fly ash/fly ash combinations with other by-products. [17-20] With varying sodium hydroxide concentrations and alkaline ratios, this unique base material in geopolymer concrete and its effects on physical, residual strength, and durability capabilities at exposed high temperatures ranging from 100°C to 800°C.[21-25]

OBJECTIVE OF THE RESEARCH

The specific goal of the current study is to ascertain the durability, and ductility and strength properties of geopolymer concrete made of GGBS at varied alkaline activator ratios (1, 1.5, 2, and 2.5) and higher sodium hydroxide concentrations (14M and 16M) under exposed elevated temperature curing, which ranges from 100°C to 800°C. To provide a machine learning prediction tool to determine the mechanical characteristics of geopolymer concrete based on GGBS while taking into account factors like exposure, alkaline activator ratio, curing temperature, and concentration of sodium hydroxide.

2 Materials

To study the strength property of concrete, the properties of materials and mix proportion are to be ascertained. The following materials are used to prepare the geopolymer concrete for the current investigation.

- GGBS
- FA
- CA
- Alkaline Activators
- Water
- Super Plasticizer
- Ordinary Portland Cement (For Preparing Control Specimen)

3 Experimental Work

M25 grade concrete control specimens of mixture ratio 1:1.88:3.33:0.43 (Cement: Fine Aggregate: Coarse Aggregate: Water) with 1% Conplast are prepared based on IS 10262:2009. Then the mixtures are cast, compacted, de-moulded and water cured for 28days as per the requirement. After curing, the specimens are dried in electrical oven at 60°C for 24 hours to remove free water.

Mix Proportion

Table 1. Mix Proportions

Constituents	GGBS	Fine Aggregate	Coarse Aggregate	Alkaline Activator
Quantity (kg/m^3)	394	554	1294	158
Mix Proportion	1	1.40	3.28	0.4

Table 2. Mix Details of Geo-polymer concrete

Trial Mixture	Aggregates (kg)			GGBS (kg)	Alkaline Liquid (kg)	Alkaline Liquid Ratio	NaOH Solution	Sodium Silicate
	20mm	6mm	River Sand				Mass (kg)	Mass (kg)
GP14M1.0	776	518	554	394	158	1.0	31.86	78.80
GP14M1.5	776	518	554	394	158	1.5	25.49	94.56
GP14M2.0	776	518	554	394	158	2.0	21.24	105.07
GP14M2.5	776	518	554	394	158	2.5	18.21	112.57
GP16M1.0	776	518	554	394	158	1.0	35.02	78.80
GP16M1.5	776	518	554	394	158	1.5	28.01	94.56
GP16M2.0	776	518	554	394	158	2.0	23.35	105.07
GP16M2.5	776	518	554	394	158	2.5	20.01	112.57

Elevated Temperature Curing

The objective of the examination is to know the effect of increased temperature in the strength of geopolymer concrete. Hence the samples s which are already oven cured at 60°C for 24 hours and kept in ambient temperature for 24 hours exposed to elevated temperature curing by keeping it in a muffle furnace of 1000ºC capacity. The specimens are cured under different elevated temperatures starting from 100ºC, 200ºC, 400ºC, 600ºC and 800ºC and exposed for every one hour from up to 6 hours at the rate of heating 4.4ºC. The said specimens are tested for its physical and mechanical properties then the physical and mechanical properties have been investigated. The control specimens are also undergone same procedure after removal of free water by heating 60°C for 24 hours. Figure 3 shows the temperature curing of the specimens.

Fig.1. Temperature Curing of Specimens

The effect of elevated temperature curing on the strength characteristics is studied based on different factors. The factors considered for the strength characteristics evaluation are listed below.

a. Rise in Curing Temperature
b. Curing Time Exposure
c. Alkaline Ratio
d. Molar Concentration

The investigation is conducted with two different molar concentrations viz. 14M and 16M. Based on the molecular mass of NaOH, the solution is prepared (ex: for preparing14M concentration solution [14 x 40 (molecular mass of NaOH) = 560gm NaOH solid is used for One liter solution]. The addition of sodium silicate solution is depended on the ratio between $NaOH/Na_2SiO_3$ known as alkaline liquid ratio and four different ratios viz. 1, 1.5, 2 and 2.5 are used. To maintain the workability, 3% of water and 1% of super plasticizer are used in the mixture.

Table 3. Mechanical Properties of Control Concrete under Elevated Temperature of 100^0c

Series ID	Specimen ID	Curing Exposure (Hours)	Strength Properties (N/mm^2)		
			f_{ck}	f_t	f_{cr}
Control Concrete	CON01	1	31.70	3.00	5.80
	CON02	2	31.56	2.88	5.64
	CON03	3	31.50	2.70	5.48
	CON04	4	31.48	2.62	5.09
	CON05	5	31.46	2.50	5.00
	CON06	6	31.44	2.46	4.85

Table 4. Properties of Geopolymer Concrete under Temperature of 1000c Alkaline ratio 1.0

Series ID	Specimen ID	Curing Exposure (Hours)	Strength Properties (N/mm^2)		
			f_{ck}	f_t	f_{cr}
GP14M 100°C	GP14M01	1	32.00	3.02	6.23
	GP14M02	2	31.68	3.02	6.31
	GP14M03	3	31.60	2.98	6.35
	GP14M04	4	32.00	2.98	6.23
	GP14M05	5	32.64	3.00	6.27
	GP14M06	6	32.74	2.98	6.27
GP16M 100°C	GP16M01	1	30.69	2.90	6.48
	GP16M02	2	31.42	2.97	6.54
	GP16M03	3	31.54	2.98	6.54
	GP16M04	4	31.64	3.02	6.41
	GP16M05	5	31.94	3.02	6.53
	GP16M06	6	32.08	3.03	6.54

4 Application of Machine Learning Tools

Regression Analysis

Regression analysis is a tool to find the relationship between different variables and based on this relationship, the dependent variables results can be predicted. The relationships will be expressed in terms of statistical equation. The commonly used regression is linear regression. The study on simple regression technique is carried out to find out other mechanical properties using compressive strength as independent variable. The regression equation is

$$Y=AX+B$$

Where Y is dependent variable going to be predicted and X is the independent variable and A and B are constant.

Relationship between Split Tensile and Compressive Strengths under Elevated Temperatures:

Figures 2&3 portraits the linear relationship between (fck) and (ft) for GP14M and GP16M of alkaline ratios 1.0, 1.5, 2.0 and 2.5 and the equation have been developed. The ratio between ft / √fck has been called as _y‘ and it can be determined by the developed equation and compared with experimental results.

Relationship between Flexural and Compressive Strengths under Elevated Temperatures

Figures 2 to 3 portraits the linear relationship between (f_{ck}) and (f_{cr}) for GP14M and GP16M of alkaline ratios 1.0, 1.5, 2.0 and 2.5 and the equation have been developed. The ratio between f_{cr} / $\sqrt{f_{ck}}$ hasbeen called as ‗y' and it can be determined by the developed equation and compared with experimetal results.

PREDICTION OF MECHANICAL PROPERTIES USING MACHINE LEARNING

The current study intended to predict the structural properties of geopolymer concrete with supervised learning algorithms. This section has been discussing the step-by-step procedure of predicting flexural strengthusing linear regression and the respective python programming screenshots were enclosed for clear understanding.

Algorithm:

Step 1.Conversion of dataset from .xlsx to .csv.

Step 2. Uploading .csv file into panadas data frame.

Step 3. Input variables: "Temperature","Exposure_Time","Molarity","Alkaline Ratio" Target variables: "G25fck", ―G25ft‖, ―G25fcr‖

Step4. From sklearn.model_selection import of the training testing model using train_test_split with Ratio of test_data=0.25

Step 5.Importing of Linear Regression Model from sklearn. linear_model

Step 6.Model=Linear Regression().
Step 7.Fit our model.The model will be trained using independent and dependent variables to fit the linear regression model.
Step 8. Finally, predict the output

Prediction Equation= model intercept + coeffiient1*(Temperature)+coefficient2*(Exposure_time)+ coefficient3*(Molarity)+coefficient4*(Ratio)

The predicted Equation = Model Intercept + Coefficient 1 x (Temperature) + Coefficient 2 x (Exposure Time) + Coefficient 3 x (Molarity) – Coefficient 4 x (Alkaline Ratio)
Predicted f_{cr}= 6.52N/mm^2@100°C at Exposure Time 2hour.
Experimental Result f_{cr}= 6.54N/mm^2@100°C at Exposure Time 2hour.

The predicted result is show cased a highest compatibility with experimental result observed during testing. By adopting machine learning – linear regression all the GP16M 100°C mechanical properties are predicted and the same compared with experimental result observed and theoretical results derived earlier in the research. Figures 2 to 3 exhibits the comparison graphs of predicted results and experimental results. While seeing the curves it is very much clear that the machine learning predictions are almost accurate. Further the closeness of machine learning is on par with experimental results during the elevated temperature exposure curing especially later part where the safety become major concern for the researchers which lead them to do physical experiment and spending their valuable time and money.

This prediction is in line with the results of Shanmansouri et al. (2020), who predicted the compressive strength using Gene Expression Programming (GEP) with five parameters like age of specimen, NaOH concentration, combination of 3 different base materials and the prediction shown high accuracy with experimental results. Henceforth, the machine learning predictions are worthy to recommend identifying the interrelationships and finding simple solution.

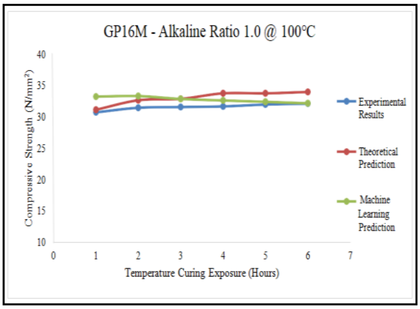

Fig.2. Experimental & Predicted Results of fck

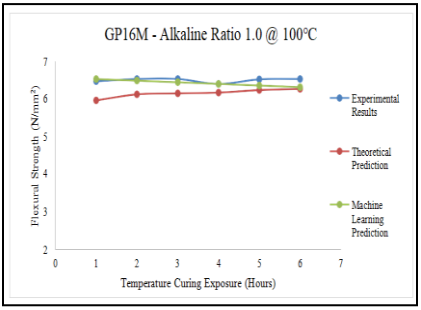

Fig.3. Experimental & Predicted Results of ft

5 Conclusions

The theoretical relationships between mechanical properties have been developed with respect to elevated temperature and derived equations for split tensile strength (0.52√fckfor both GP14M and GP16M) and flexural strength (1.03√fckfor GP14M and 1.08√fckfor GP16M). The said equation can be used as empirical equation for future studies. The future researchers can find split tensile and flexural strength based on their compressive strength tested results.

All the linear regression performed in theoretical investigations are synchronized with experimental results and the ratio between theoretical and experimental values are always more than 0.92 and R2 value also above 0.9 in all the cases of geopolymer specimen.

The normalized strengths of mechanical properties with respect to elevated temperatures prove an ideal relationship and safe. Hence the predicted relationship can help the researcher to determine the mechanical properties of GGBS based geopolymer concrete for different curing temperature. The linear regression equations are developed to predict normalized strengths and the R2 values of the said equations are higher than 0.8 in all the cases of geopolymer specimens.

Machine Learning concept has been adopted to predict the mechanical properties based on different dependent variables such as alkaline ratio, molar concentration, temperature exposure and elevated temperature. The predicted results are highly compatible with experimental and theoretical investigations. The predicted mechanical properties by machine learning are very much in line with experimental results especially under elevated temperature time exposure starting from 3 hours to 6 hours where the safety concern will be the major phenomena for any researchers. Now the proposed model can be used to predict the mechanical properties based on historical experimental data sets.

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