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Effect of Combined Different Sources of Alumina Silicate on Mechanical Properties and Carbonation Depth of Environmentally Friendly Geopolymeric Composite Based on Metakaolin

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ABSTRACT

Today, concrete is the most widely used building material. Cement production releases about 7% of carbon dioxide gas into the atmosphere and increases greenhouse gases, so it seems necessary to use an alternative to Portland cement. In recent years, geopolymers (mineral polymers) have been proposed as a new environmentally friendly cement. Metakaolin, bentonite, zeolite, iron blast furnace slag and fly ash can be mentioned as aluminosilicate sources. In the field of geopolymer concrete construction, few articles have been working on the composition and effect of replacing aluminosilicate sources. In this experimental study, the effect of replacing slag aluminosilicate sources, class F fly ash and bentonite with proportions of 5-45% with metakaolin on the mechanical properties and durability of geopolymer concrete based on metakaolin was investigated. After making the samples, compressive, bending, tensile and carbonation tests were performed on the geopolymer concrete samples to obtain the optimal strength and carbonation depth of the samples. Also, to determine the validity of the tests, machine learning estimation analysis was performed on the samples. The findings showed that bentonite leads to a decrease in strength, while fly ash and slag lead to an increase in strength. The predicted R^2 values showed the highest matching of the correlation matrix (more than 93%) for the pressure samples. In addition, the results of the tests showed that the metakaolin-based geopolymer concrete sample replaced with fly ash (35%) had a lower penetration depth (carbonation) and higher mechanical properties than other samples.

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1. INTRODUCTION

The World Environment Commission has defined the concept of sustainable development as the ability to meet our current needs without compromising the ability of future generations to meet their needs. This definition requires us to consider all aspects of a particular industry through raw material supply, energy consumption and reuse or recycling. As the main component of ordinary concrete, Portland cement is the most widely used cement material in the construction industry [1, 2]. But the production of Portland cement has major environmental disadvantages, including: high energy consumption, consumption of primary resources, and carbon dioxide emissions [3, 4]. So that the production of one ton of Portland cement causes the release of approximately one ton of carbon dioxide into the environment and the consumption of 1.5 tons of raw materials [5-8]. On the other hand, pollution and global warming have become the most important concerns of developed countries [1]. The main cause of the global warming phenomenon is the emission of greenhouse gases, and carbon dioxide plays the biggest role in the global warming phenomenon [9]. In the process of producing each ton of Portland cement, on average, 125 liters of fossil fuel and 118 kilowatt hours of electricity are consumed, and polluting gases enter the environment due to the burning of fuel oil and electricity consumed in cement factories [10]. In recent years, in order to produce environmentally friendly building materials,

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geopolymers have been proposed as a green cement element and a suitable alternative to Portland cement all over the world. Geopolymer was first introduced in the late 1970s by Davidovits, a prominent French chemist, as a new binder from the inorganic polymer family. The use of geopolymer cement can reduce carbon dioxide emissions by 44-64% compared to Portland cement [11]. Also, geopolymer concrete makes optimal use of available waste, which has a positive impact on the environment [12]. In terms of properties, geopolymer concretes have better mechanical and chemical properties than conventional concretes, including higher compressive, tensile and flexural strengths [13-15], faster hardening [13, 16], longer durability [17], resistance to fire, and high temperatures [18-20], less permeability and resistance to attack by salts and acids [21, 22] and less creep [23, 24]. Geopolymers are inorganic aluminosilicate materials obtained from the polymerization reaction between a silica-rich aluminosilicate source (SiO_2) and alumina (Al_2O_3) with an alkaline activating solution [1, 2]. Geopolymerization is a rapid chemical reaction in alkaline conditions between Si and Al elements, which causes the formation of a three-dimensional Si-O-Al polymer chain [3, 4]. In this article, metakaolin was used as the main source of aluminosilicate. Blast furnace slag, which is called a slag for short, is a by-product of the iron blast furnace, which is one of the most potential sources of aluminosilicate due to its structural nature.

The alkaline activating solution, as one of the two main parts of geopolymers, plays an important role in breaking down and forming the crystal structure of Si and Al, and it is usually selected based on sodium or potassium, which are soluble alkaline metals. The most common alkaline activator solution used in polymerization is a combination of sodium hydroxide (NaOH) or potassium hydroxide (KOH) solution with sodium or potassium silicate solution [4]. The source of aluminosilicate, which is known by other names, such as the source of polymerization, base material, and adhesive, as a supplier of Si and Al, plays the most important role in geopolymer cements. Aluminosilicate sources can be natural, such as bentonite; industrial, such as: metakaolin; Or waste materials or by-products [5], the most common of which are fly ash [6] and iron blast furnace slag [7-12]. The type of source, the content of source elements, molecular structure and crystalline degree of the source, alkali substances in the source, Si/Al ratio in the source, etc. are some of the influencing parameters in the strength of geopolymer concretes. Metakaolin is one of the aluminosilicate sources . Fly ash is a by-product of coal-fired power plants, which can be one of the best primary sources of geopolymerization due to its amorphous structural nature [10, 13]. Fly ash is classified into two classes: C (containing high amounts of calcium oxide) and F (containing low amounts of calcium oxide). Bentonite is another source of aluminosilicate. It is a type of fine-grained clay that has at least 85% of montmorillonite clay. Bentonite is a material from the category of clays and consists of swelling minerals, which are mainly montmorillonite and a small amount of beadlite. Most bentonites are formed by the weathering and alteration of volcanic ash, often in the presence of water, and their source rock is the most basic [14, 15]. In this article, class F fly ash, bentonite and slag were used as aluminosilicate sources to replace metakaolin to make geopolymer concrete.

Some researches have been done in the field of the composition of aluminosilicate sources, which will be briefly discussed. Zhang et al. [16] studied on the thermal resistance of geopolymers used in combination of metakaolin and fly ash. They have concluded that the replacement of fly ash by 50% increases the compressive strength. Fernández et al. [17] also reported similar results. Rajamma et al [18]observed the positive effects of replaced fly ash up to 40% instead of metakaolin. Bernal et al. [19], in research using the slag and metakaolin combination, concluded that 40% of slag is used instead of metakaolin, which causes a significant increase in the compressive strength of geopolymer concrete. Yip et al. [20] also concluded in their research that the combination of slag (below 40%) and metakaolin increases the compressive strength and durability of concrete and also improves the microstructure of geopolymer cement. Esparham [21] in research on geopolymer cement paste, used the combination of metakaolin and zeolite in different replacement percentages as a source of aluminosilicate. In a research on geopolymer cement paste, they used the combination of metakaolin and zeolite in different replacement percentages as a source of aluminosilicate. These researchers concluded that replacing zeolite instead of metakaolin increases the compressive strength of geopolymer concrete. Cheng et al. [22] also reported similar results in their research.

Soft Programming, Machine Learning (ML) and Artificial Neural Networks (ANNs) are new methods to predict the mechanical behavior of concrete. Currently, engineers prefer to practice using computer programming including machine studying, data mining, and other types to forecast concrete mechanical properties. Computer prediction techniques can reduce time and material. Furthermore, classical programming can transfer equations to commuter programs, and algorithms to find the precise outcomes [23-31] Topçu and Saridemir [32] investigated the prediction of concrete mixture with extra fly ash through ANNs and FL techniques separately. They concentrated on aggregate diameter to forecast the mechanical properties of concrete. At the end, their outcomes showed that the R^2 was extra than 0.9, and their method turned into reliable. Another researcher, Kashyzadeh et al. [33] also applied Data Mining to predict the concrete mechanical properties based on the mechanical properties of aggregate. They found that features of data mining of aggregate properties affect compressive strength. Data mining can predict the mechanical properties of concrete. Kumar et al. [34] used ML techniques, Gaussian Progress Regression (GPR), Support Vector Machine Regression (SVMR), and Ensemble Learning (EL) to predict lightweight-concrete mechanical properties. They concluded that R^2 was 0.98 for GPR forecasting. In another example, Hematibahar et al. [35] used classical programming to predict compressive strength They used classical programming to forecast the compressive strength and compressive stress-strain of concrete. Their results show that R^2 was more than 0.97. Hasanzadeh et al. [36] studied the prediction of the mechanical properties of concrete with ML. Their results showed that the Polynomial Regression (PR) for basalt fibred high-performance concrete can predict mechanical properties (R^2>0.99).

In this experimental study, the role of the combination of fly ash, bentonite and slag with metakaolin on the compressive, flexural and tensile strength and depth of carbonation of geopolymer concrete was investigated. Because, the research conducted on the effect of the combination of different sources of alumina silicate on the mechanical properties and durability of concrete Geopolymer is low and insufficient. In this experimetal investigation research, fly ash, slag and bentonite - types of aluminosilicate sources - were used instead of metakaolin (geopolymer concrete based on metakaolin) in ratios of 5, 10, 15, 20, 25, 30, 35, 40 and 45, respectively. Then the samples were tested in terms of compressive strength, indirect tensile strength and three-point bending at the age of 7 and 28 days, and also to obtain the carbonation depth, 7 and 14 day carbonation tests were performed on the samples. The correlation matrix was used to determine the relationship between the mechanical properties of concrete. Finally, the results were collected, analyzed and presented.

2. MATERIALS AND METHODS

2. 1. Materials The main source of aluminosilicate in this study was metakaolin. Also, the fly ash was of class F type. Bentonite used was in this study as well. XRF of these 4 materials are presented in Table 1. The alkaline activator solution in this research was sodium hydroxide with 98% purity and liquid sodium silicate solution with a ratio of SiO_2 to Na_2O equal to 2. The chemical breakdown of these two substances is summarized in Table 2. Consumable sand is also obtained from mines. Around Tehran, the sand used was broken sand, which was sieved according to ASTM C33 standard [37] and granulated. In this research, specific gravity and water absorption test were performed according to ASTM standard C127 [38]. It was taken from used sand. This test was performed on the used sand according to ASTM standard C128 [39]; whose results are provided in Table 3. Also, the coefficient of softness of sand according to ASTM standard C136 [40] equal to 8.2, the amount rejected from sieve No. 200, 9.0% and the value of sands was also measured according to ASTM D2419 standard [41]. The water used was the tap water of Tehran city. The superplasticizer used was polycarboxylate with a specific weight of 1.1 grams per cubic centimeter the detailed of sand and gravels are shown in Figure 1 and Table 3.

TABLE 1. XRF of mineral materilas

Chemical analysis		SiO_2	Al_2O_3	CaO	Fe_2O_3	Na_2O	K_2O	MgO	MnO	SO_3	Cl	LOI
Slag	**wt.%**	15.4	7.3	20.4	38.20	0.62	0.68	9.8	5.19	1.2	0.23	0.5
Metakaolin	**wt.%**	54.98	17.54	5.40	5.33	0.95	0.86	0.20	0.12	-	-	1.4
Fly ash	**wt.%**	70.7	21.1	1.13	3.9	0.26	1.09	0.77	0.05	-	-	1.8
Bentonite	**wt.%**	68.93	11.14	2.68	1.08	0.41	0.59	2.54	-	-	-	15.06

TABLE 2. Chemical Analysis of Sodium Hydroxide and Sodium Silicate

NaOH			KOH		
Chemical substance	**Result**	**Unit**	**Chemical substance**	**Result**	**Unit**
NaOH	98	%	**NaOH**	90.7	%
Na_2CO_3	1	%	**Na_2CO_3**	0.2	%
NaCl	200	ppm	**NaCl**	0.006	ppm
Fe	6	ppm	**Fe**	0.2	ppm
SiO_2	15.7	ppm	**SiO_2**	0.6	ppm
Appearance	**White flake**		**Appearance**	**White flake**	

2. 2. Experimental Methods The main aluminosilicate source in this study was metakaolin. Also, the fly ash was of class F type. The bentonite used was natural bentonite and clinoptilolite. XRF analysis of these 4 materials is presented in Table 1.

The alkaline activating solution in this research was sodium hydroxide with 98% purity and liquid sodium silicate solution with a ratio of SiO_2 to Na_2O equal to 2.

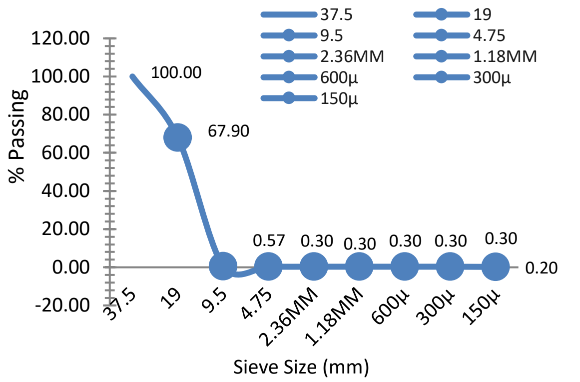

Figure 1. Gradation curves of fine and coarse aggregates

TABLE 3. Water absorption, specific density of aggregates and Fineness modulus

	Specific density of aggregates (g/cm^3)	Water absorption (%)	Fineness modulus
Gravel	2.69	0.8	6.5
Sand	2.65	2.2	1.2

The chemical analysis of these two materials is summarized in Table 2. The used sand was broken sand, which after preparation, was granulated by ASTM C33 [37] standard sieve. In this research, sand with a maximum diameter of 12.5 mm was used. The test of specific gravity and water absorption according to ASTM C127 standard [38] was taken from the used sand. This test was carried out using sand according to ASTM C128 standard [39], the results of which are presented in Table 3. Also, the softness coefficient of sand according to ASTM C136 [40] standard was equal to 2.8, the amount rejected from sieve No. 200 was 0.9% and the sand value was also measured according to ASTM D2419 [41] standard, 74. The water used was the tap water of Tehran city. The superplastiziter used was polycarboxylate with a specific weight of 1.1 grams per cubic centimeter.

After conducting preliminary tests and using the results of previous research [42], the geopolymer concrete mixing plan based on metakaolin was selected and metakaolin was replaced with slag, fly ash and bentonite in proportions of 5, 10, 15-45%. Mixing schemes are presented in Table 4. To make the samples, the alkaline activating solution was first prepared. For this purpose, first, sodium hydroxide solution with a concentration of 12 M was mixed with sodium silicate solution and supreplaseter according to the mixing plans. In the day of the test, first, dry materials including: sand, sand, metakaolin, slag, bentonite and fly ash were poured into the concrete mixer according to the mixing plans and mixed for 3 minutes in order to distribute evenly. Then, alkaline activator solution and additional water were added to the mixer and the concrete mixture was mixed for 2 minutes. After finishing the mixing, concrete compressive, tensile and bending samples were molded. The samples were compacted for 10 seconds on the vibrating table. Then the samples were processed for 24 hours in an oven at a temperature of 80 degrees Celsius. After the processing, the samples were removed from the oven and placed at ambient temperature. 7 and 28 days compressive, tensile and bending strength tests were taken from the samples. It is worth mentioning that the dimensions of compression samples were 10x10x10 and bending 50x10x10 cm. Also, the dimensions of the cylindrical tensile samples were 10 x 20 cm. In this term, the concrete cylinder has been locked between four steels, and at the moment of of the failure splitting in two parts (see Figure 2).

The tests performed on concrete samples include: compressive strength test based on Part 116: BS1881, indirect tensile test (Brazilian) based on ASTM C496 [43] and three-point bending strength test based on ASTM C293.

TABLE 4. The mixture of the first part

Mix ID	Metakoalin	Fly ash	Slag	Bentonite	NaOH	Na_2SiO_3	Coarse aggregates	Fine sand	SP	Unit
M	350	0	0	0	140	210	840	840	10	**kg/m^3**
MF5	3320.5	17.5	0	0	140	210	840	840	10	**kg/m^3**
MF10	315	35	0	0	140	210	840	840	10	**kg/m^3**
MF15	297.5	52.5	0	0	140	210	840	840	10	**kg/m^3**
MF20	280	70	0	0	140	210	840	840	10	**kg/m^3**
MF25	262.5	87.5	0	0	140	210	840	840	10	**kg/m^3**
MF30	245	105	0	0	140	210	840	840	10	**kg/m^3**
MF35	227.5	122.5	0	0	140	210	840	840	10	**kg/m^3**
MF40	210	140	0	0	140	210	840	840	10	**kg/m^3**

MF45	192.5	192.5	0	0	140	210	840	840	10	**kg/m³**
MS5	3320.5	0	17.5	0	140	210	840	840	10	**kg/m³**
MS10	315	0	35	0	140	210	840	840	10	**kg/m³**
MS15	297.5	0	52.5	0	140	210	840	840	10	**kg/m³**
MS20	280	0	70	0	140	210	840	840	10	**kg/m³**
MS25	262.5	0	87.5	0	140	210	840	840	10	**kg/m³**
MS30	245	0	105	0	140	210	840	840	10	**kg/m³**
MS35	227.5	0	122.5	0	140	210	840	840	10	**kg/m³**
MS40	210	0	140	0	140	210	840	840	10	**kg/m³**
MS45	192.5	0	192.5	0	140	210	840	840	10	**kg/m³**
MB5	3320.5	0	0	17.5	140	210	840	840	10	**kg/m³**
MB10	315	0	0	52.5	140	210	840	840	10	**kg/m³**
MB15	297.5	0	0	52.5	140	210	840	840	10	**kg/m³**
MB20	280	0	0	70	140	210	840	840	10	**kg/m³**
MB25	262.5	0	0	87.5	140	210	840	840	10	**kg/m³**
MB30	245	0	0	105	140	210	840	840	10	**kg/m³**
MB35	227.5	0	0	122.5	140	210	840	840	10	**kg/m³**
MB40	140	0	0	210	140	210	840	840	10	**kg/m³**
MB45	157.5	0	0	192.5	140	210	840	840	10	**kg/m³**

Figure 2. Tensile, flexural, and compression samples made

2. 3. Machine Learning An AI calculation generally works by taking a gander at a great deal of information to sort out the principles, new encounters, and information (the "preparing process") prior to utilizing these guidelines, encounters, and information to tackle and foresee future issues (the "testing process"). As a result, developing a database is a crucial and essential step in the development of machine learning.

The types of materials and their properties were the subjects of the input data in this kind of database. The experimental data that led to the collection of these data. The target of this strategy was found the compressive strength by means of polynomial relapse. The data set was split into two parts: one for training and one for testing. Note that Equation (1) shows that the kinds of polynomial relapse (PR) which can anticipate the compressive strength.

According to the current study, the polynomial regression has been provided to predict the compressive, tensile and flexural strengths, the polynomial regression equeation followed by :

$$y_{(x)} = a_n x^n + a_{n-1} x^{n-1} + a_{n-2} x^{n-3} + \ldots + a_1 x^1 + a_0 , \qquad (1)$$

The a_n , is the coefficient of a polynomial function has different value at various conditions. As well as, the a_0 , is the Y-intercept of polynomial function or constant value [44]. Where a known as the polynomial function coefficient, x is variable, and $y_{(x)}$ is dependent variables to x in Equation (1).

The machine learning method was performed according by Python and Spyder Plugin. In this regard, the concrete experimental results has been classification and next divided to “train and test”. The “polynomial regression” has been imported from”skylearn”. Finally the polynomial regression has been applied to data.

To find the verify of prediction, the Correlation Coefficient (R^2), Mean Absolute Errors (MAE) and Root Mean Squared Errors (RMSE) have been established. Equation (2) illustrates the R^2 formula:

$$R^2 = 1 - \frac{\sum^{n}(y-\hat{y})^2}{\sum^{n}(y-\bar{y})^2} \tag{2}$$

where y, ˆy, and −y are the actual, predicted, and mean of the actual value, respectively.

The MAE equation is equal the sum of the numerical differences of the values of community set divided by whole numbers (Equation (2)). The MAE equation is defined as (Equation (3)):

$$MAE = \frac{1}{n}\sum^{n}\left|y-\hat{y}\right| \tag{3}$$

RMSE calculate the average deviation of each actual data point and the predicted results (Equation (4)):

$$RMSE = \sqrt{\frac{1}{n}\sum^{n}(y-\hat{y})^{2}} \tag{4}$$

2. 4. Deep Learning An idea in machine learning called deep learning is based on artificial neural networks. Deep learning models perform better than basic machine learning models and conventional data analysis techniques for many applications. The structure is deeper and includes a perceptron with multiple hidden layers and multiple layers of layers. By combining low-level features to discover distributed feature representations of data, deep learning creates more abstract attribute categories of high-level representation or features.

The correlation matrix can able to find the maximum relationship among the properties of the materials of concrete with deep learning and machine learning.

This article found the correlation matrix between mechanical properties and the properties of concrete.

2. 5. Carbonation One of the most important failures of reinforced concrete is steel corrosion in concrete. Corrosion starts for two reasons, one is carbonation in concrete and the other is the penetration of chloride ions into concrete.

Due to the alkalinity of the concrete, the steels in the concrete have a thin surface layer on them, and the carbonation process begins when this surface layer that protects the concrete against corrosion is destroyed and the pH of the concrete reach below 9.

The phenomenon of carbonation in concrete is one of the main reasons for the corrosion of reinforcements.

To carry out carbonation tests, a special device has been installed that reduces the time required to measure the depth of carbonation of concrete with the increase in the concentration of carbon dioxide gas. The procedure is as follows: two chambers were made to place a small cylindrical sample with a length of 20 cm and a diameter of 5 cm, which are placed in a closed circuit. In the mentioned closed circuit, a flow of a mixture of 50% air and 50% carbon dioxide gas is established. Considering that water is produced in the carbonation reactions of concrete, the relative humidity will change, for this reason, chemical dryers (moisture absorbent silicate gel) are used in the mentioned circuit to achieve relative humidity. It is accompanied by an increase by placing the above-mentioned chambers inside the water tanks, controlled and kept constant at around 27 degrees Celsius by circulating the water at a lower temperature and adjusting its heigh

2. 5. 1. Determining the Depth of Carbonation of Concrete According to the RILEM CPC-18 standard, first the selected samples are placed lengthwise in the force application device and divided into two halves like the Brazilian test. Then, a solution of phenolphthalein and ethyl alcohol is sprayed on the fracture surface, and the distance between the purple color and no color change compared to the outer surface of the sample is reported as the carbonation depth of the geopolymer concrete sample [45-48].

3. RESULTS

3. 1. Compressive Strength The results of the compressive strength test of the samples and the effect of replacing fly ash, bentonite and slag are presented in Figure 5. As shown in Figure 5, the 7- and 28-day compressive strength of sample M (100% metakaolin) is 18 and 26 MPa was measured. The replacement of 5% fly ash (MF5) increased the compressive strength by approximately 12%. Also, with a further increase in the replacement percentage of fly ash up to 35% (MF15, MF10, and... MF35), the compressive strength of the samples also increased. So that in the ratio of 35%, the maximum compressive strength of 7 and 28 days of MF35 sample reached more than 25.9 and 37 MPa with a 30% increase compared to M. In the case of replacement with slag, it can be seen that the compressive strength increases in general, so that the maximum compressive strength of 7 and 28 days corresponds to the MS15 sample (containing 15% slag and 85% metakaolin), which were measured as 25.2 and 36 MPa, respectively. (approximately 12% increase compared to 100% metakaolin). By replacing 35% more slag (MS35), the process of improving the compressive strength compared to sample M (100% metakaolin) also increased and the 7 and 28 days compressive strength of this sample was measured as 19.6 and 28 MPa. But with more slag replacement of 35% (MS35), (unlike fly ash), the compressive strength of the sample decreased with respect to M. Yet, on account of bentonite, the outcomes were unique. According to the findings, the samples' compressive strength decreased by 100% (M) when bentonite was substituted for metakaolin, from 5 to 45%. For instance, the 7-day compressive strength of the MB30 design was measured at 13.8 MPa, while the 28-day compressive strength was measured at 23.46 MPa, which is approximately 8% lower than the M sample (see Figures 3 and 5).

3. 2. Tensile Strength The tensile strength test results of the samples are also presented in Figures 4 and 6. As the results of Figure 6 show, the 7- and 28-day tensile strength of sample M was measured as 2.26 and 2.7 MPa, respectively. Replacing 15-45% fly ash instead of metakaolin increased the 28-day tensile strength by approximately 4-19% compared to design M; so that the maximum 7 and 28-day tensile strength was observed in design MF35 with values of 2.7 and 3.22. In the samples replaced with slag (up to 35 observations of replacement), the tensile strength of the samples has increased so that at 15% replacement (MS 15) the tensile strength reached to its maximum (7 and 28 days resistances were 2.66 and 3.15 MPa, respectively). But by replacing 40% and 45% more slag instead of metakaolin, similar to the compressive strength, the 28-day tensile strength compared to M, also decreased by 10% and 12%, respectively. The replacement of bentonite instead of metakaolin, similar to the

Figure 3. Failure sample of geopolymer concrete

Figure 4. Failure sample of geopolymer concrete

compressive strength in all replacement ratios, decreased the 7 and 28 day tensile strength of the samples compared to the M plan. For example, at 5% replacement ratio (MB5), the tensile strength at 7 and 28 days, it faced a very slight reduction compared to the M plan. Also, with an increase in the replacement percentage from 10 to 45%, the tensile strength of the samples gradually decreased. So that the tensile strength of 7 and 28 days of sample MB45 was measured as 1.91 and 2.50 MPa, respectively, which is approximately 26 and 15% less than that of sample M (see Figures 4 and 6).

3. 3. Flexural Strength The trend of bending strength results was similar to the trend of compressive and tensile strength. Specimen M (100% metakaolin) had a flexural strength of 4.18 and 4.9 MPa at days 7 and 28, as shown in Figure 7, when fly ash was replaced with 5 to 45% metakaolin, the flexural strength increased, so that the greatest increase in strength in 7 and 28 days was related to the replacement of 35% with fly ash compared to other samples (flexural strength of 7 days, 4.98 MPa and 28 days, 5.96 MPa, respectively). Similar to the compressive and tensile strength results, in the replacement of metakaolin with 15% slag, the highest flexural strength of 7 and 28 days was obtained (4.92 and 5.88 MPa, respectively). In replacement of 40 and 45% with slag, compared to the 100% sample of metakaolin (M), the resistance was determined at 7 and 28 days.

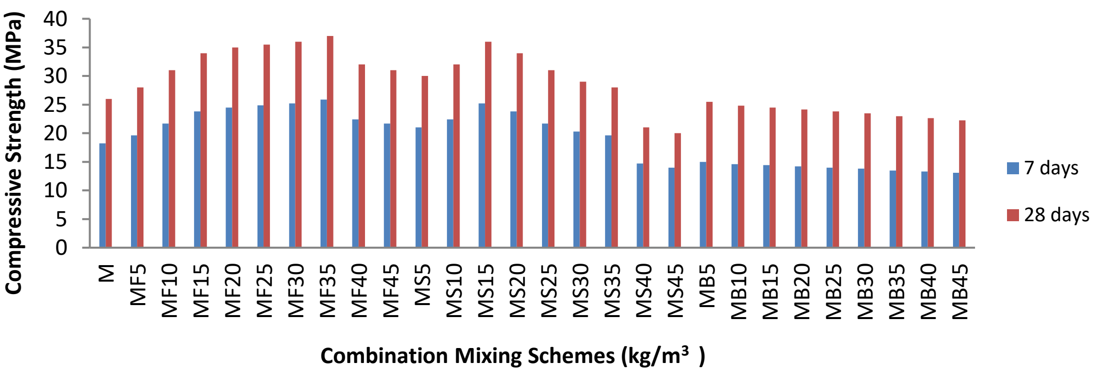

Figure 5. Compressive Strength results

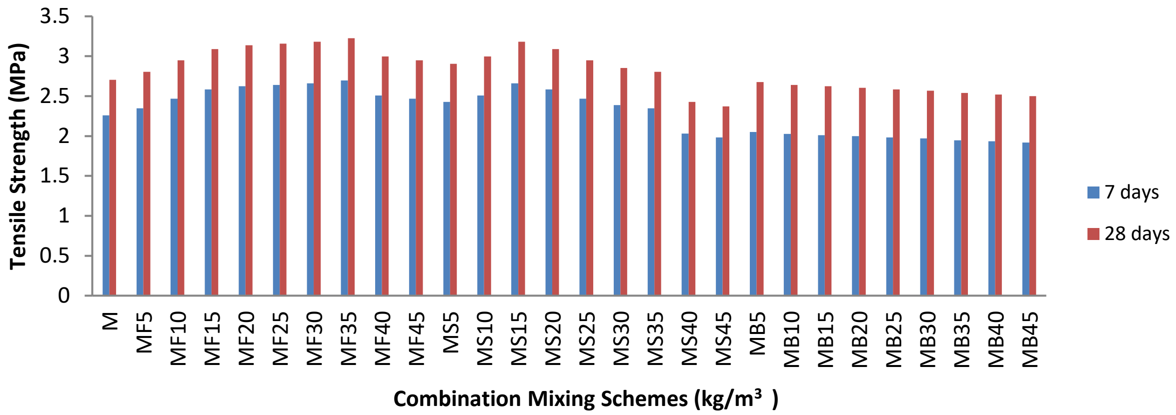

Figure 6. Tensile Strength results

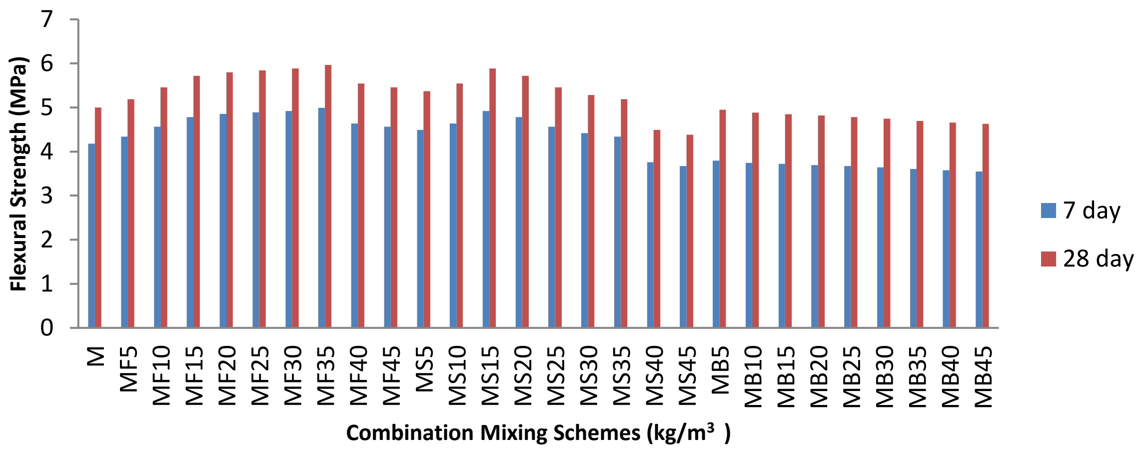

Figure 7. Flexural Strength results

Fasting decreased by 11 to 14%. In replacing metakaolin with bentonite, the tensile strength values faced a gradual decreasing trend, so that the greatest amount of reduction in tensile strength in 7 and 28 days occurred in 45% replacement with bentonite (approximately 12 to 13%) (see Figure 7).

3. 4. Machine Learning The results show a good polynomial regression for all strengths between the predictive data and the experimental data. It can be the experimental data overestimated or underestimated than predicted results in each types of results (Figures 8-11).

The R^2 RMSE, and MAE results has been shown in Table 5. According to Table 5 the Polynomial regression had the best results for compressive strength and next, flexural strength. The results shows that the compressive strength was experimental and prediction results was similar together.

The tensile strength prediction according to machine learning is illustrated in Figure 9, the results show that the R^2 was more than 0.8 and the closet sample was MB25 to experimental results. MAE, and RMSE results was 1.2 and 3.4 respectively

The flexural strength shows that the close relationship between experimental results and predictably results the R^2 was more than 0.75. In fact the polynomial function was able to predict the flexural strength with 75% accuracy (Figure 10).

The results can be provided for the other type of concrete and other type of consept as well. For example Hasanzadeh et al [36] has been predicted the compressive, tensile and flexural strengths with 99% for basalt fibred high performace concrete via polynomial regression.

3. 5. Correlation Regarding the relationship between the compressive, tensile and flexural strength, the correlation matrix is provided by the Python Software Spyder extension (Figure 11). Based on the results, the compressive strength with tensile and flexural strength is more than 0.96 and 0.93%, respectively. In the mortar, fly ash had a large Impact with more than 60%

compressive strength, followed by slag with 33%. Bentonite and methicillin had -77 and -20% effect on compressive strength.

According to samples and experimental results, the relationship between compressive strength and tensile strength (Equation (5)) and flexural strength (Equation (6)) has been provided.

$$f_t' = 0.3f_c' + 0.96 \tag{5}$$

$$f_f' = 0.011f_c' + 0.3 \tag{6}$$

where f'_c is compressive strength, f'_f is flexural strength and f'_t is tensile strength. Tables 6 and 7 shows the tensile and flexural strengths for 28 days for prediction and experimental results.

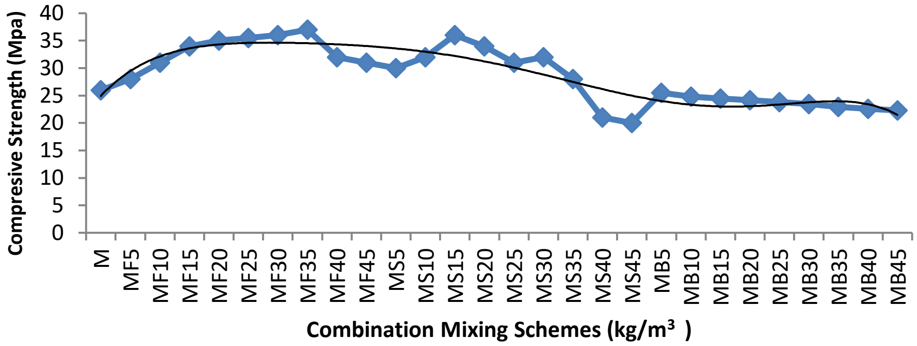

Figure 8. Polynomial prediction for compressive strength

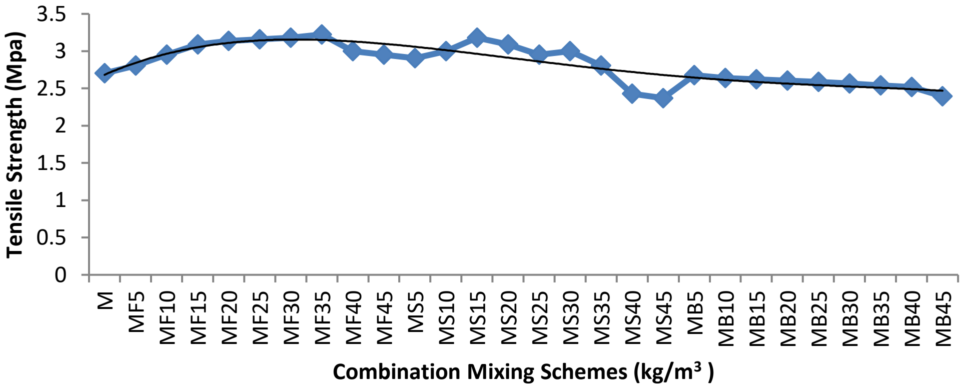

Figure 9. Polynomial prediction for tensile strength

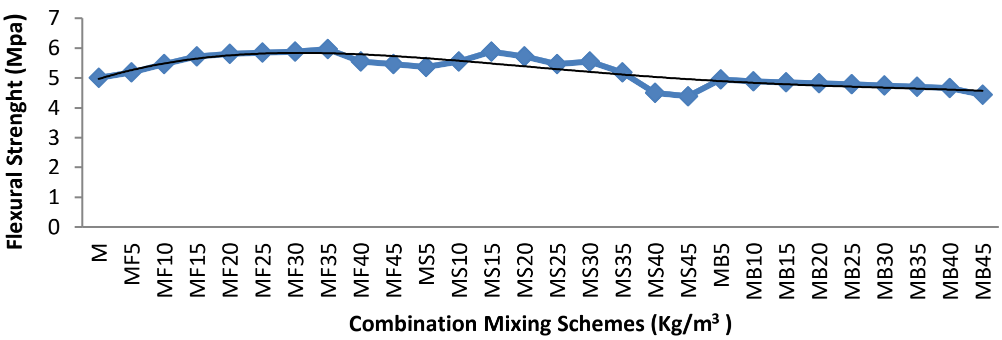

Figure 10. Polynomial prediction for Flexural strength

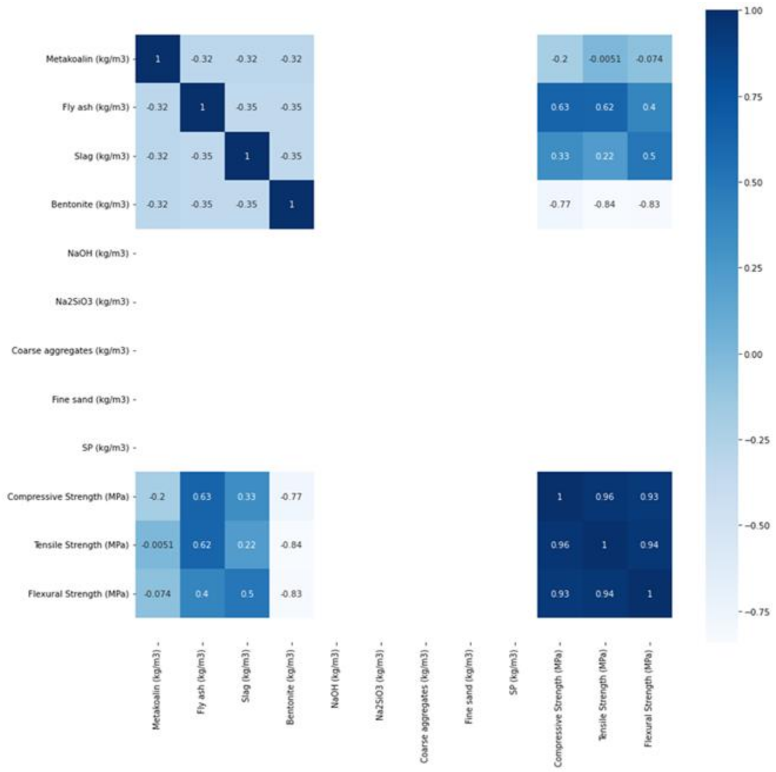

Figure 11. The correlation matrix of geopolymer concret

TABLE 5. R^2, RMSE, MAE results

	R^2(MPa)	RMSE(MPa)	MAE(MPa)
Compressive (MPa)	0.93	1.4	4.2
Tensile (MPa)	0.8	1.2	3.4
Flexural (MPa)	0.75	0.9	3.2

TABLE 6. The results of prediction tensile strength according to Equation (5)

Mix ID	Prediction	Experimental	Errors
M	1.8869	1.955	0.0681
MF10	2.06515	2.185	0.11985
MF15	2.1721	1.725	0.4471
MF20	2.20775	2.3	0.09225
MF25	2.225575	2.07	0.15558
MF30	2.2434	2.415	0.1716
MF35	2.27905	2.0125	0.26655
MS10	2.07104	1.9075	0.16354
MS15	2.20992	1.8857	0.32422
MS20	2.14048	2.0165	0.12398
MS25	2.03632	2.0056	0.03072
MS30	2.07104	1.962	0.10904
MS35	1.93216	1.8857	0.04646
MB10	1.58062	1.001	0.57962
MB15	1.594725	0.9646	0.63013
MB20	1.60883	0.9919	0.61693
MB25	1.63704	0.9828	0.65424
MB30	1.69346	1.08	0.61346
MB35	1.72167	1.025	0.69667

TABLE 7. The results of prediction flexural strength according to Equation (6)

Mix ID	Prediction	Experimental	Errors
M	1.8869	3.5085	0.0585
MF10	2.06515	3.819	0.254
MF15	2.1721	3.9225	0.346
MF20	2.20775	3.97425	0.23675
MF25	2.225575	4.026	0.254
MF30	2.2434	4.1295	0.1045
MF35	2.27905	3.5256	0.7294
MS10	2.07104	3.9288	0.4188
MS15	2.20992	3.7272	0.0552
MS20	2.14048	3.4248	0.3552
MS25	2.03632	3.5256	0.384
MS30	2.07104	3.1224	0.8196

MS35	1.93216	2.1018	1.8726
MB10	1.58062	2.14275	0.56775
MB15	1.594725	2.1837	0.5637
MB20	1.60883	2.2656	0.5556
MB25	1.63704	2.4294	0.5394
MB30	1.69346	2.5113	0.4863
MB35	1.72167	2.3	0.23

3. 6. Durability (Carbonation Test) Carbonation test was done as durability test. Carbonation of concrete is a chemical reaction between carbon dioxide permeated into concrete and alkaline products resulting from the hydration of cement in concrete and the production of calcium carbonate. The penetration of CO_2 reduces the alkalinity of concrete and destroys the alkaline protective layer around the reinforcement, and as a result, the rebars are exposed to corrosion. Carbonation test results of the selected mixture designs (M, MF35, MS15, MB5) are shown in graphs of Table 8 below.

4. DISCUSSION

4. 1. Analysis of Compressive, Tensile and Flexural Strengths According to the summary of the obtained results, it can be said that the replacement of fly ash instead of metakaolin increased the compressive, tensile and bending strength of the samples compared to the 100% metakaolin sample. This issue can be related to various reasons. The first parameter is the degree or degrees of amorphous crystallization of the aluminosilicate source. This parameter is ignored in most cases, but it is one of the important conditions of the source of aluminosilicate. due to lack of reactivity and having a strong and regular crystal structure, they cannot effectively participate in the geopolymerization process, because breaking the structures of SiO_2 and Al_2O_3 to become SiO_4 and AlO_4 monomers in these sources is done less and harder [10]. Structurally, fly ash has a more suitable structure than metakaolin for making geopolymer. As a result, replacing fly ash instead of metakaolin increases the geopolymerization process and increases the mechanical resistance of geopolymer concrete [8-12].

TABLE 8. The results carbonation of selected mixture designs

Sample	80°C Carbonation Depth (mm) 28 days	80°C Carbonation Depth (mm) 14 days	Density (M)
M	10.4	8.2	12
MF35	7.3	6.5	
MS15	9.1	7.6	
MB5	16.8	12.8	

On the other hand, another important and influencing parameter on the mechanical strength of geopolymeric concrete is the Al/Si ratio of the aluminosilicate source. Many researchers consider the Al/Si ratio as the most effective parameter in the compressive strength of geopolymer concrete. These researchers have reported the optimal value of this ratio between 3.3 and 5.3, which results in achieving the highest compressive strength [7, 13, 45, 46]. Al/Si ratio in metakaolin used in this research was equal to 1/8. This ratio is 35.3 in fly ash. In fact, with the addition of fly ash instead of metakaolin, in addition to the amorphousness of the cement material, the Al/Si ratio also increases and approaches the optimal level (3.3 to 5.3). As a result, the compressive, tensile and flexural strength increases and also with the increase of the replacement ratio, the increase and improvement of the compressive, tensile and flexural strength also increases. The optimal amount of fly ash replacement in this research was measured at 25%.

Regarding replacing slag instead of metakaolin, the summary of the obtained results showed that replacing slag also increased the mechanical resistance of geopolymer concrete based on metakaolin. This issue can have various reasons. One of the reasons similar to fly ash is the more amorphous and reactive structure of slag compared to metakaolin. But other reasons can be different from fly ash. Although the Al/Si ratio of slag is equal to 3 and similar to fly ash, it can increase the mechanical resistance of concrete, but there are other important parameters that cause differences in the results of replacing slag with fly ash. Another influential parameter is the CaO content of the aluminosilicate source. According to the results of this article and our previous research [10] this parameter has a significant role on the compressive strength of geopolymer concrete. In a research on geopolymers, van Jaarsveld et al. [46] concluded that the characteristics of the aluminosilicate source, especially the amount of calcium oxide CaO, determines the properties of the geopolymer. Xu et al. [47] also consider the amount of CaO of the aluminosilicate source, along with the parameters of the alkaline solution and the Al/Si ratio, as one of the important and influencing factors on the properties and mechanical resistance of geopolymers. In the case of using fly ash and metakaolin, considering that both materials have a very low percentage of CaO (13.1 percent in fly ash and 3.1% in metakaolin), so the role of CaO in the mechanical resistance of geopolymer concrete is not key. But regarding slag, due to the high percentage CaO in slag (37%), this role can be important and influential. Replacing slag up to 20%, due to having large amounts of CaO and increasing the Si/Ca ratio, as well as the potential of CaO for ion geopolymerization and chain formation with this ion [34, 35] leads to an increase in the compressive, tensile and bending strengths of $+Ca_2$ Geopolymer concrete.

On the other hand, with a further increase in the replacement ratio of slag from 25 to 35%, the mechanical resistance of concrete decreased compared to the case of 25% slag replacement. The reason for this issue can be another important parameter of the sources in the source [34]. Likewise, the amount of Al in the aluminosilicate $2O_3$, which was mentioned and the results of this article showed, with the increase in the amount of CaO (Si/Ca) in the aluminosilicate source, the compressive and tensile strengths and the bending of geopolymer concrete increases, but on the other hand, in aluminosilicate sources with a high CaO, the amount of Al_2O_3 in the source is very important. In these aluminosilicate sources, if there are large amounts of Al2O3, scale is also produced. This substance reacts with Ca and causes the formation of +3 calcium aluminate compounds next to the geopolymer network and H-S-C gel, which reduces the compressive strength of the geopolymer [13, 14]. As can be seen in Table 1, metakaolin has large amounts Al_2O_3 is (2.30%). As a result, when using the combination of metakaolin and slag, if the amount of slag is too much (35%), the mechanical resistance of geopolymer concrete will decrease. As a result, the optimal amount of slag replacement for the greatest effect in improving compressive and tensile strengths flexural in this research was measured at 25%. Regarding the replacement of bentonite instead of metakaolin, the summary of the results showed that the replacement of this material instead of metakaolin has caused a significant reduction in the compressive, tensile and bending strengths of geopolymer concrete compared to the case of using 100% metakaolin. The reason for this can be related to the structure of bentonite. bentonite has a strong crystal structure [49] and among the aluminosilicate sources used in this article, it has the strongest crystal structure, and as mentioned, the aluminosilicate source must have a suitable amorphous structure. Compared to metakaolin, bentonite has a more crystalline structure. As a result, replacing a material with a higher crystalline degree instead of a material with a lower crystalline degree causes a relative decrease in the geopolymerization process and, as a result, a decrease in compressive, tensile and bending resistances. On the other hand, with the increase of bentonite replacement percentage from 5 to 45%, the reduction of compressive, tensile and flexural strengths of the samples slightly increased. The reason for this increase in resistance can be related to the tetrahedral structure of clinoptilolite, which strengthens the metakaolin geopolymer matrix [15, 49, 50].

4. 2. Analysis of Durability (Carbonation Test)

According to the carbonation test results, it can be seen that the composite samples with fly ash(MF15) and slag(MS25) have a lower carbonation depth compared to the control sample based on metakaolin (M). This can be due to the increase in the amount of calcium oxide in the aluminosilicate source and help in the formation of gel C-S-H, which itself causes the denser and improved microstructure of the samples combined with fly ash and thermally slag. It can also be seen that the lowest amount of carbonation depth belongs to sample MF15 (28 days-7.3 mm and 14 days -6.5 mm). On the other hand, it can be seen that by combining metakaolin with bentonite(MB5), the degree of crystallization of the aluminosilicate source has increased and the amorphous ratio(SI/AL) has decreased, which itself causes a decrease in geopolymerization, as a result, the depth of carbonation increases. According to the results, it can be concluded that corrosion potential Rebar in metakaolin geopolymer concrete samples combined with fly ash and slag decreases and samples combined with bentonite increases [13, 14, 49, 51].

5. CONCLUSION

In this experimental research, an attempt was made to study the role of replacing F-class fly ash, natural clinoptilolite bentonite, and slag of the slag furnace instead of metakaolin on the compressive, tensile, and bending strengths of geopolymer concrete based on metakaolin. In this regard, after conducting related experiments and data analysis, the following are presented as specific results of this article.

1. The replacement of class F fly ash instead of metakaolin in the composition of geopolymer concrete increased the compressive, tensile and flexural strengths of concrete. The optimal amount of fly ash replacement in this research was measured as 35%, which caused an increase of approximately 25.9 and 37 and in the 7 and 28 days gor compressive strength of geopolymer concrete.
2. The replacement of slag instead of metakaolin in the composition of geopolymer concrete increased the compressive, tensile and flexural strengths of concrete. The optimal amount of slag replacement in this research was measured to be 15%, which caused an increase of approximately 25.2, and 36 for compressive strength in 7 days and 28 days .
3. The replacement of bentonite instead of metakaolin in the composition of geopolymeric concrete caused a significant decrease in the compressive, tensile and flexural strength.
4. The correlation matrix shows that the compressive strength with tensile and flexural strength had more than 90% relationship. Moreover, the strength of materials has related to fly ash more than other addictive.

5-The Machine learning results shows that the compressive strength R^2 was more than 0.93, tensile strength was more than 0.8 and flexural strength was more than 0.75.

6. The carbonation depth was decreased when fly ash and slag were used to replace metakaolin (metakaolin-based geopolymer concrete). The lowest carbonation penetration depth was associated with a 35% replacement with fly ash. However, substituting bentonite for metakaolin resulted in a deeper carbonation.

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Persian Abstract

چکیده

امروزه بتن پرمصرف ترین مصالح ساختمانی است .تولید سیمان باعث انتشار حدود ۷ درصد گاز دی اکسید کربن در جوو افزایش گازهای گلخانه ای میباشد بنابراین استفاده از جایگزینی برای سیمان پرتلند ضروری به نظر می رسد. در سال های اخیر ژئوپلیمرها (پلیمرهای معدنی)، به عنوان یک عنصر سیمانی جدید مطرح شده است. متاکائولین، بنتونیت، زئولیت، سرباره کوره بلند آهن و خاکستر بادی (بقایای نیروگاه های حرارتی) را می توان به عنوان منابع آلومینوسیلیکات نام برد. در زمینه ساخت بتن ژئوپلیمری، مقالات کمی در مورد ترکیب و اثر جایگزینی منابع آلومینوسیلیکات کار شده است. در این مطالعه آزمایشگاهی، تأثیر جایگزینی منابع آلومینوسیلیکات: سرباره، خاکستر بادی کلاس F و بنتونیت با نسبت‌های ۱۰، ۱۵، ۲۰، ۲۵، ۳۰، ۳۵، ۴۰ و ۴۵ درصد با متاکائولین بر خواص مکانیکی و دوامی(کربناتسیون)بتن ژئو پلیمری بر پایه متاکائولین مورد بررسی قرار گرفت. پس از ساختنمونه ها، آزمایش های فشاری، خمشی ، کششی و کربناتاسیون بر روی نمونه های بتن ژئوپلیمری انجام شد تا مقاومت بهینه و عمق کربناسیون نمونه ها به دست آید. همچنین برای تعیین اعتبار آزمون ها، تحلیل تخمین یادگیری ماشین بر روی نمونه ها انجام شد. در این بخش به دلیل دقت بالا، رگرسیون چندلیلی انتخاب شده است. یافته ها نشان داد که بنتونیت منجر به کاهش استحکام می شود در حالی که خاکستر بادی و سرباره منجر به افزایش استحکام می شود. مقادیر R2 پیش‌بینی بیش از ۹۳ درصد برای نمونه‌های فشاری، بیش از ۸۰ درصد برای نمونه‌های کششی، و بیش از ۷۵ درصد برای نمونه‌های خمشی با ماتریس همبستگی مطابقت دارند. علاوه بر این، نتایج آزمایشات نشان داد که نمونه بتن ژئوپلیمری ۳۵ MF(متاکائولین جایگزین شده با خاکستر بادی (۳۵٪)) نسبت به سایر نمونه‌ها ، عمق نفوذ کمتر(کربناته شدن) و خواص مکانیکی بالاتری داشت.