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A CONSTITUTIVE MODEL FOR FLY ASH-BASED GEOPOLYMER CONCRETE

Prabir SARKER*

* Department of Civil Engineering, Curtin University of Technology, Perth, WA 6845, Australia
E-mail address: *p.sarker@curtin.edu.au*

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Abstract
The conventional binding agent in concrete is Ordinary Portland cement (OPC). However, cement production is highly energy-intensive and involved in CO_2 emission to the atmosphere. Therefore, it is important to search for alternative low-emission binder for concrete in order to reduce the environmental impact caused by the production of cement. Geopolymer, also known as inorganic polymer, is an alternative binder that uses by-product material such as fly ash instead of cement. Recent research has shown that fly ash-based geopolymer concrete has suitable properties for its use as a construction material. Since the strength development mechanism of geopolymer is different from that of OPC, it is necessary to obtain a suitable constitutive model for geopolymer concrete. This paper has investigated the suitability of using an existing constitutive model originally proposed by Popovics for OPC concrete. It was found that the equation of Popovics can be used for geopolymer concrete with minor modification to the expression for the curve fitting factor. The modified expression provided better correlation between the experimental and calculated stress-strain curves. The modified constitutive model was then incorporated into a nonlinear analysis for reinforced concrete columns. A good correlation was achieved between the experimental and analytical ultimate loads and corresponding deflections for twelve slender test columns. This shows the suitability of using the modified constitutive model for geopolymer concrete to analyse structural members.

Streszczenie
Konwencjonalnym spoiwem betonu jest Cement Portlandzki Zwykły (CPZ). Produkcja cementu jest procesem pochłaniającym dużo energii i wiąże się z emisją dwutlenku węgla do atmosfery. Dlatego tak ważne jest poszukiwanie alternatywnego, nisko-emisyjnego spoiwa do betonu w celu ograniczenia wpływu środowiskowego spowodowanego produkcją cementu. Geopolimer, znany również jako polimer nieorganiczny, jest spoiwem alternatywnym które zamiast cementu jako materiał wykorzystuje produkt uboczny w postaci popiołu lotnego. Niedawne badania pokazały że geopolimerowy beton na bazie popiołów lotnych posiada właściwości odpowiednie do wykorzystania go jako materiału konstrukcyjnego. Ponieważ mechanizm osiągania wytrzymałości geopolimeru jest inny niż dla Cementu Portlandzkiego Zwykłego (CPZ), należy uzyskać odpowiedni model konstytutywny dla betonu geopolimerowego. W artykule przeanalizowano istniejący model zaproponowany przez Popovicsa dla CPZ. Uznano, że równanie Popovicsa może zostać zastosowane dla betonu geopolimerowego z małą modyfikacją wyrażenia dotyczącego współczynnika dopasowania krzywej. Zmodyfikowane wyrażenie zapewniło lepszą współzależność pomiędzy krzywymi naprężnie – odkształcenie otrzymanymi z badań i obliczonymi. Następnie zmodyfikowany model konstytutywny został zastosowany do nieliniowej analizy słupów żelbetowych. Osiągnięto dobrą korelację pomiędzy doświadczalnymi i obliczeniowymi obciążeniami niszczącymi, a odpowiadającymi ugięciami dla dwunastu badanych smukłych słupów. Wskazuje to na właściwe wykorzystanie zmodyfikowanego modelu konstytutywnego dla betonu geopolimerowego do analizy elementów konstrukcyjnych.

Keywords: **Column strength; Constitutive model; Geopolymer concrete; Fly ash; Inorganic polymer concrete.**

1. INTRODUCTION

Concrete is the most widely used construction material in the world. Ordinary portland cement (OPC) is traditionally used as the binding agent for concrete. The worldwide consumption of concrete is estimated to increase due to the increase of infrastructure especially in countries such as India and China [1]. The amount of carbon dioxide released during the manufacturing process of OPC is approximately one ton for every ton of OPC produced. Globally, the OPC production contributes about 7% of the world's carbon dioxide. Since it is important to control the trend of global warming by reducing the carbon dioxide emissions, it is appropriate to search for alternative low-emission binding agents for concrete. Geopolymer, also known as inorganic polymer, is one such alternative material that acts as the binding agent in concrete. The geopolymer binder uses by-product materials instead of cement and thus its use by the construction industry can reduce the carbon dioxide emission and the environmental impact of the manufacturing of cement.

Geopolymer is an alumino-silicate product obtained from the geochemistry process [2]. Geopolymer binders show good bonding properties and utilize a by-product material such as fly ash, slag or metakaolin as the source of Silicon and Aluminium. In fly ash-based geopolymer binder, fly ash is reacted with an alkaline solution to create an alumino-silicate binder. Geopolymer binders are used together with aggregates to produce geopolymer concrete. Fly ash based geopolymer concrete is a recently developed concrete in which no portland cement is used and the geopolymer paste acts as the only binder. The basic ingredients of fly ash-based geopolymer concrete are fly ash, sodium hydroxide, sodium silicate, fine aggregates and coarse aggregates. However, water and super plasticizer can be added to improve workability of the freshly mixed concrete.

Recent research works [3-9] have studied the properties of heat-cured fly ash based geopolymer concrete. The results of these studies have shown potential use of geopolymer concrete as a construction material. The studies have shown that geopolymer concrete has the properties of high compressive strength, very little drying shrinkage, low creep, good bond with reinforcing steel, good resistance to acid, sulphate and fire. It was also found from the experimental and analytical works that the performance of geopolymer concrete structural members such as beams and columns was similar to that of OPC concrete members. Other recent studies [10-12] have also reported similar engineering properties of geopolymer concrete which are favourable for its use as a construction material.

Calculation of strength and deflection of reinforced concrete members is dependent on the stress-strain relationship of concrete. Since the strength development mechanism of geopolymer concrete is different from that of OPC concrete, it is necessary to obtain a suitable expression for the constitutive model of geopolymer concrete. Past research works [10, 11, 13, 14] have determined the experimental values of geopolymer concrete elasticity modulus. The experimental results of complete stress-strain behaviour of geopolymer concrete were reported by Hardjito et al. [13]. This paper has evaluated the use of an existing stress-strain model originally proposed by Popovics [15] for OPC concrete to predict the experimentally determined stress-strain curves of geopolymer concrete. The slightly modified set of stress-strain equations was then incorporated into a nonlinear analysis of reinforced concrete columns [16] to analyze twelve geoppolymer concrete columns tested by Sumajouw et al. [9]. The calculated ultimate axial loads and corresponding deflections are compared with the experimentally determined values. Thus, the suitability of using the modified set of equations for the analysis of geopolymer concrete structural members is demonstrated.

2. MODULUS OF ELASTICITY

2.1. Test results on the modulus of elasticity of geopolymer concrete

The modulus of elasticity (E_c) of geopolymer concrete was determined by testing cylinder specimens and reported in literature by Fernandez-Jimenez et al. [10], Sofi et al. [11], Hardjito et al. [14]. These test results are shown in Fig. 1. There were some variations in these reported test results in terms of the ingredients of the test specimens and the test methods used. The test results of Fernandez-Jimenez et al. [10] were measured in accordance with Spanish Standard UNE 83316. These specimens were made using low calcium fly ash, 12.5 molar NaOH, Na_2SiO_3 of SiO_2 to Na_2O ratio of 3.4, and coarse and fine aggregates. The test data by Sofi et al. [11] and Hardjito et al. [14] were measured in accordance with Australian Standard 1012.17 [17]. The test specimens of Sofi et al. [11] were made using low calcium fly ash from three different sources, slag containing 40% CaO by mass and a combination of NaOH or KOH and Na_2SiO_3 as the alkaline liquid. The specimens did not have any coarse aggregates except for one corresponding to compressive strength of 39 MPa. The test specimens by Hardjito et al. [14] used low calcium fly ash, 14 molar NaOH, Na_2SiO_3 with SiO_2 to Na_2O ratio of 2, as well as coarse and fine aggregates. The type of coarse aggregates used in these specimens was granite. It can be seen that the ingredients and the mixture proportions varied in these reported test specimens. Because of the variation in the ingredients and their mixture proportions, scatter is observed in the test data presented in Fig. 1.

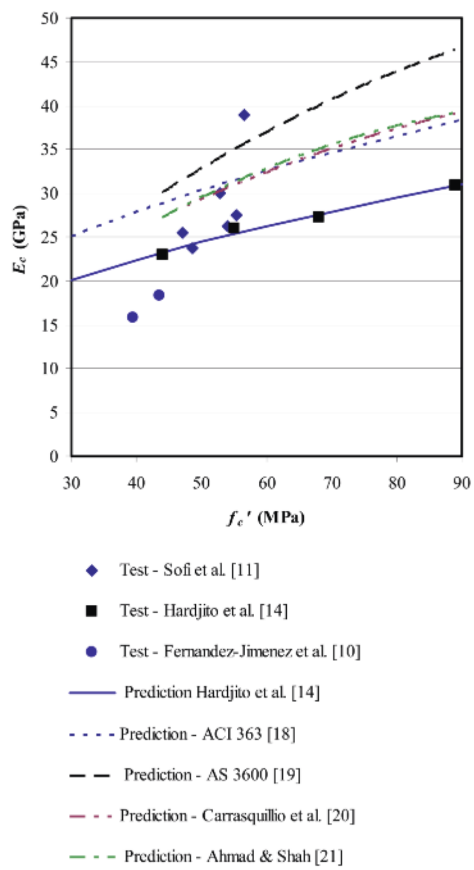

Figure 1.
Modulus of elasticity of geopolymer concrete

2.2. Equation to calculate the modulus of elasticity

While the modulus of elasticity of concrete varies depending on the type of aggregates, simplified empirical equations in terms of concrete compressive strength (f_c' or f_{cm}) and concrete density (ρ) are often used for normal-weight concretes. In this section, the values of the modulus of elasticity calculated by the empirical equations are compared with the test results of geopolymer concrete. Some empirical equations proposed for OPC concrete (Eqs. 1-4) and geopolymer concrete (Eq. 5) are given below.

American Concrete Institute, ACI 363 [18]:

$$E_c = 3320\sqrt{f_c'} + 6900 \quad (1)$$

Australian Standard, AS 3600 [19], within ± 20%:

$$E_c = 0.043\rho^{1.5}\sqrt{f_{cm}} \quad (2)$$

Carrasquilo et al. [20]:

$$E_c = 0.043\rho^{1.5}\sqrt{f_{cm}} \quad (3)$$

Ahmad and Shah [21]:

$$E_c = (3320\sqrt{f_c'} + 6900)(\rho/2320)^{1.5} \quad (4)$$

Hardjito et al. [14]:

$$E_c = 3.38\rho^{2.5}(\sqrt{f_c'})^{0.65} \times 10^{-5} \quad (5)$$

The equations for the modulus of elasticity of OPC concrete recommended by the Australian Standard AS 3600 [19], Carrasquillo et al. [20] and Ahmad & Shah [21] are functions of the density of concrete and the concrete compressive strength. The equation proposed by Hardjito et al. [14] for geopolymer concrete is similar to that given by the ACI 363 [18] with different values of the constants. These equations are relatively simple to use since they are expressed as function of concrete compressive strength only. Comparisons of the test values of the modulus of geopolymer concrete elasticity with those calculated by the above equations are shown in Fig. 1. The mean value of the compressive strengths obtained from cylinder tests were used in the calculation.

The trend lines through the calculated values of the test results by the five equations (Eqs. 1-5) are shown in Fig. 1. It can be seen that the equations of the ACI 363 [18], AS 3600 [19], Carrasquillo et al. [20] and Ahmad & Shah [21] overestimate most of the test results of geopolymer concrete. The prediction of the modulus of elasticity by Eq. 5 is close to the test results and is considered reasonable taking the variations of test specimens into consideration. Therefore, this equation was used to calculate the modulus of elasticity required for the stress-strain relationship of geopolymer concrete in the next section.

3. CONSTITUTIVE MODEL FOR GEOPOLYMER CONCRETE

Experimental data on the complete stress-strain curve of geopolymer concrete is scarce in literature. Hardjito et al. [13] reported the experimental stress-strain curves of three different mixes of geopolymer concrete. The experimental curves for Mixes 1, 2 and 3 are shown in Figs. 2, 3 and 4 respectively. The mixture proportions of the concrete are given in Table 1. The fly ash used was of Class F. The concentration of the NaOH solution of Mixes 1 and 2 was 8M and that of Mix 3 was 14M. All specimens were heat-cured for 24 hours and then left in ambient temperature until testing. The curing temperature for Mix 1 was 60 °C and that for Mixes 2 and 3 was 90 °C. The specimens were tested at the age of 90 days after casting.

The expression for the complete stress-strain response of conventional OPC concrete cylinders proposed by Popovics [15] was subsequently modified by Thorenfeldt et al. [22] by introducing a factor k in the equation to ensure a steeper descending part of the curve for high-strength concrete. This expression of Thorenfeldt et al. was selected to investigate the suitability of its use for geopolymer concrete.

The stress-strain relationship by Popovics, modified by Thorenfeldt et al. is given under the following expression:

$$\frac{f_c}{f_c'} = \frac{\varepsilon_c}{\varepsilon_c'} \cdot \frac{n}{n - 1 + \left(\frac{\varepsilon_c}{\varepsilon_c'}\right)^{nk}} \qquad (6)$$

where f_c = concrete compressive stress, ε_c = strain in concrete, f_c' = maximum compressive stress in concrete, ε_c' = strain when fc reaches f_c' and n = curve fitting factor. The factor k equals 1 when $\varepsilon_c / \varepsilon_c'$ is less than 1. Collins and Mitchell [23] suggested that k is given by Eq. 7 for $\varepsilon_c / \varepsilon_c'$ is greater than 1 and the curve fitting factor n is estimated by Eq. 8.

$$k = 0.67 + \frac{f_c'}{62} \quad \text{when} \quad \frac{\varepsilon_c}{\varepsilon_c'} > 1 \text{ in MPa unit} \qquad (7)$$

$$n = 0.8 + \frac{f_c'}{17} \text{ in MPa unit} \qquad (8)$$

Collins et al. [24] recommended that the strain at peak stress ε_c' can be found from Eq. 9 by knowing the value of the modulus of elasticity (E_c).

$$\varepsilon_c' = \frac{f_c'}{E_c} \cdot \frac{n}{n-1} \qquad (9)$$

Equations 6 to 9 were used to calculate the stress-strain curves for the test specimens of Hardjito et al. [14]. Equation 5 was used to calculate Ec. The calculated stress-strain curves are shown in Figs. 2 to 4. It can be seen from the figures that when the curve fitting factor n is calculated by Eq. 8, the strains corresponding to peak stress (ε_c') calculated with the use of Eq. 9 are slightly higher than the measured values and the post peak parts of the calculated stress-strain curves are pushed to the right from the measured curves for all three cases. It was therefore attempted to obtain a similar modified equation for the curve

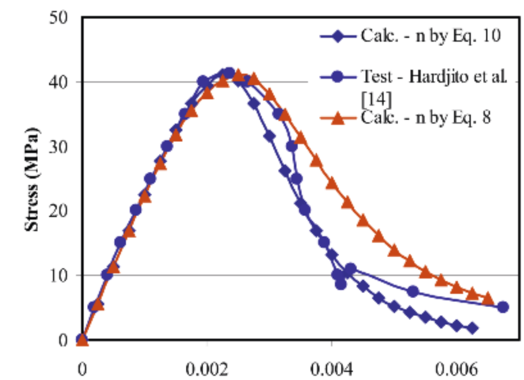

Figure 2.
Stress-strain curve of geopolymer concrete (Mix 1, f_c' = 41 MPa)

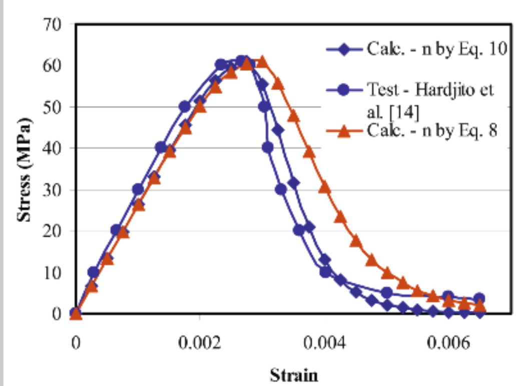

Figure 3.
Stress-strain curve of geopolymer concrete (Mix 2, f_c' = 61 MPa)

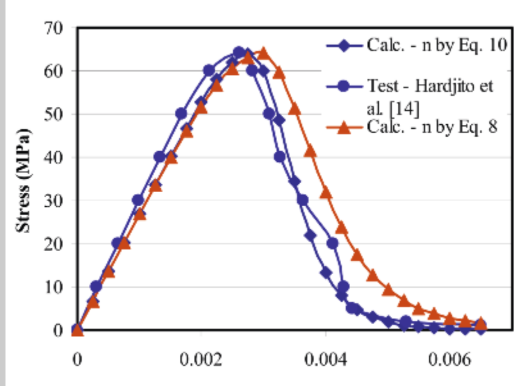

Figure 4.
Stress-strain curve of geopolymer concrete (Mix 3, f_c' = 64 MPa)

Table 1.
Mixture proportions (kg/m3) of concrete [13]

Mix	Fly ash	NaOH	Na_2SiO_3	Superplasticiser	Aggregates		
					10 mm	7 mm	Fine sand
1	408	55.4	103	6.1	554	647	647
2	408	41	103	6.1	554	647	647
3	408	41	103	8.2	554	647	647

fitting factor in order to obtain a better fit between the calculated and the measured stress-strain curves. Equation 10 was thus obtained from trials.

$$n = 0.8 + \frac{f_c'}{12} \text{ in MPa unit} \qquad (10)$$

The stress-strain curves calculated by using the curve fitting factor given by Eq. 10 are also shown in Figs. 2 to 4. From the comparison between the calculated and measured stress-strain curves, it can be seen that Eq. 10 provides better correlation between the experimental and calculated curves. Hardjito et al [13] obtained the mixture proportions of the specimens after many trials in the laboratory. Similar mixtures were also used to make large beams and columns in the laboratory. Therefore, Eq. 6, together with Eqs. 5, 7 and 10, were used to calculate the complete stress-strain curve of fly ash-based geopolymer concrete.

4. GEOPOLYMER CONCRETE COLUMN ANALYSIS USING THE CONSTITUTIVE MODEL

A method of analysis was developed for reinforced concrete columns under combined compression and uniaxial bending with equal or unequal load eccentricities at the ends. The method of analysis is based on the common assumptions for reinforced concrete members such as preservation of plain sections after bending, perfect bonding between concrete and steel, negligible tensile strength of concrete and initial straightness of the member with prismatic section along the length. The analytical method determines the ultimate axial load capacity of a column using the usual load-moment interaction diagram. The section capacity line and the loading line in the interaction diagram are constructed using the moment-thrust-curvature relationship of the cross-section and the load-deflection relationship of the column. The procedures of the development of moment-thrust-curvature and load-deflection relationships are similar to

Table 2.
Comparison between calculated and test results of geopolymer concrete columns

Specimen	Test [9]		Prediction		Test-prediction ratio	
	Ultimate load (kN)	Mid-height deflection (mm)	Ultimate load (kN)	Mid-height deflection (mm)	Ultimate load (kN)	Mid-height deflection (mm)
GCI-1	940	5.44	992	4.50	0.95	1.21
GCI-2	674	8.02	711	6.75	0.95	1.19
GCI-3	555	10.31	555	8.64	1.00	1.19
GCI-4	1237	6.24	1151	4.70	1.07	1.33
GCI-5	852	9.08	821	7.02	1.04	1.29
GCI-6	666	9.40	651	9.02	1.02	1.04
GCII-1	1455	4.94	1420	4.87	1.02	1.01
GCII-2	1030	7.59	990	7.22	1.04	1.05
GCII-3	827	10.70	758	9.74	1.09	1.10
GCII-4	1559	5.59	1442	4.64	1.08	1.20
GCII-5	1057	7.97	1014	7.25	1.04	1.10
GCII-6	810	9.18	792	9.32	1.02	0.98
Average					1.03	1.14
Standard deviation					0.05	0.11

those generally used for reinforced concrete columns [25, 26, 27]. The method uses the actual nonlinear stress distribution in the cross-section to calculate the section capacity. The load path of the column is obtained by calculating the actual deflected shape using the load eccentricities and column slenderness, and is not based on any simplified assumption regarding the deflected shape. Thus, both material and geometric nonlinearities are taken into account to determine the ultimate load capacity of the column. Since the method needs much iteration, it is conveniently solved by writing a computer program. The method of analysis is described in more details with numerical examples in References 16 and 28. Use of this analytical procedure provided good correlation between the test and calculated strength and deflection data of OPC concrete columns subjected to unequal load eccentricities at the end.

Since the use of geopolymer in reinforced concrete application is relatively new, very limited test data on geopolymer concrete column is available in literature. The twelve geopolymer concrete test columns available in literature [9] were analysed with the use of the method. The mixture proportions used for these specimens were similar to those used in the stress-strain test specimens by Hardjito et al [13]. Equation 6, together with Eqs. 5, 7, 9 and 10, was used as the constitutive model for fly ash-based geopolymer concrete. Reinforcing steel was assumed as an elastic-perfectly plastic material. Table 2 shows the comparison of the calculated and measured values of ultimate load and corresponding mid-height deflections for each test column. The mean value of the ratios of test to calculated ultimate axial loads for these twelve columns is 1.03 with a standard deviation of 5%. The mean value of the test – prediction ratios of corresponding mid-height deflections is 1.14 with a standard deviation of 11%. This is considered as good correlation between the experimental and analytical results of the test columns.

5. CONCLUSIONS

From the presented analytical works, the following conclusions are drawn:

(i) The stress-strain curves calculated by using Eq. 6, together with the proposed modification to the curve fitting factor (Eq. 10) correlated well with the test stress-strain curves of fly ash-based geopolymer concrete. This shows that the constitutive model used for OPC concrete (Eq. 6) can be used for geopolymer concrete with minor modification to the curve fitting factor (Eq. 10).

(ii) The ultimate axial loads of slender geopolymer concrete columns calculated with the use a nonlinear method developed originally for OPC concrete columns correlated well with the experimentally measured values. The mean value of the test-prediction ratios of ultimate loads is 1.03 with standard deviation of 5% for the 12 test columns. Calculated mid-height deflections at the ultimate loads correlated reasonably well with the corresponding test values. The mean value of test-prediction ratios of the deflections is 1.14 with standard deviation of 11%.

(iii) The good correlation between the experimental and analytical results of the test columns has shown the suitability of using the modified constitutive model (Eqs. 5, 6, 7, 9 and 10) for the analysis of fly ash-based geopolymer concrete structural members.

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