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Johnson-Mehl-Avrami-Kolmogorov equation for prediction of compressive strength evolution of geopolymer

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ABSTRACT

Geopolymers are cement-free constructional materials and for their production much lower greenhouse gases are emitted than traditional concrete. In this study, compressive strength of geopolymers was related to their degree of geopolymeric reactions. Then, the Johnson-Mehl-Avrami-Kolmogorov equation was applied to represent compressive strength evolution. The presented equation can be easily adopted for prediction of long-term compressive strength of geopolymers and even traditional cementitious systems. Johnson-Mehl-Avrami-Kolmogorov constants were shown to be higher for specimens with higher strengths while their corresponding exponents were smaller.

Keywords: Ceramic composites; Deformation and fracture; Alkali activated binders; Avrami solution

1. Introduction

Alkali activated binders (geopolymers) are amorphous cement free constructional materials which are normally produced from an aluminosilicate source [1]. Fly ash is the most attractive raw material which is widely used in production of geopolymers for construction [2, 3]. Alkali activation of fly ash is performed by a mixture of a silica-rich
source (such as sodium silicate or potassium silicate) and an alkali solution (such as sodium hydroxide (NaOH) or potassium hydroxide (KOH)) [4, 5].

Compressive strength of constructional materials is the most important property, which depends on the degree of reaction in cementitious system [6]. While hydration of ordinary Portland cement (OPC) is the main reason of strength evolution [6], strength gain in geopolymers is due to geopolymerization [7]. According to the utilized fly ash which is normally called by its CaO content, the main geopolymeric compounds are different. Formation of two common amorphous gels namely Calcium-(Sodium)-Alumino-Silicate-Hydrate [C-(N)-A-S-H] and Sodium-Alumino-Silicate-Hydrate [N-A-S-H] in class C and class F fly ash-based geopolymers respectively causes strength evolution. Class C and class F are classified according to the ASTM C618 for high and low calcium fly ash respectively. Compressive strength evolution of a specific geopolymeric mixture during the time of reaction, which is normally much longer for constructional materials, depends on the degree of reaction. The Johnson-Mehl-Avrami-Kolmogorov equation is the most attractive equation for representing degree of reaction in ceramics [8].

Although the Johnson-Mehl-Avrami-Kolmogorov equation is normally used for representing percentage of crystallization, some works have been conducted for prediction degree of amorphous nucleation [9]. Both C-(N)-A-S-H and N-A-S-H amorphous gels are formed widely in geopolymeric paste in nanoscale and act as reinforcements for the hardened paste. Higher amounts of these gels results in higher strengths. In this work, compressive strength evolution of geopolymers, which directly reflects the degree of reaction, has been predicted by the Johnson-Mehl-Avrami-Kolmogorov equation.

2. Materials and Methods

Two types of fly ashes were used in this study. Class C fly ash with the average
particle size of 15 μm and BET specific surface of 65.9 m²/g contained 40.2 wt.% SiO₂, 25.3 wt.% Al₂O₃, 5.8 wt.% Fe₂O₃, 22.9 wt.% CaO, 1.4 wt.% SO₃, 0.5 wt.% Na₂O while its loss on ignition (L.O.I) was 2.2 wt.%. Class F fly ash with the average particle size of 18 μm and BET specific surface of 46.2 m²/g consisted of 51.5 wt.% SiO₂, 30.3 wt.% Al₂O₃, 11.8 wt.% Fe₂O₃, 2.1 wt.% CaO, 2.5 wt.% SO₃, 0.2 wt.% Na₂O while its L.O.I was 0.9 wt.%. Alkali activation of both fly ashes was done by a mixture of NaOH with concentration of 8 M and sodium silicate containing 36.2 wt.% SiO₂ and 13.8 wt.% Na₂O. The sodium silicate to NaOH weight ratio was 2.5 by weight for both geopolymers. NaOH solution was obtained by dissolution of NaOH flakes into distilled water. After cooling NaOH solution to room temperature, it was introduced to sodium silicate.

Geopolymers were prepared by mixing fly ash and alkali activator for five minutes. The ratio of alkali activator to fly ash was 0.25. Geopolymeric pastes were poured into 50 mm cubic moulds. The content of fly ash, sodium silicate solution, NaOH solution and superplasticizer were 1520, 269 and 107 kg/m³ respectively for class C fly ash-based geopolymer. These contents were 1560, 304 and 122 kg/m³ respectively for class F fly ash-based geopolymer.

Pouring was performed in two layers where after pouring each layer, the mould was vibrated for 45 s to reduce air bubbles and achieve more compaction. The moulds then were covered by polythene sheets for 24 h at room temperature. After demoulding, specimens were oven-cured at 40, 70 and 90 °C for 16 h.

Compressive strength of specimens was achieved in accordance to the ASTM C109 standard by a hydraulic pressure jack with the maximum capacity of 100 tonne. Compressive strength of the specimens was conducted at 1, 3, 7, 28, 42 and 90 days of demoulding (16 h oven curing plus additional hours in ambient temperature). Each series of specimens were tested for three times and the average compressive strength was reported as the final strength.
3. Modelling

Compressive strengths as a function of curing time for both class C and class F fly ash-based geopolymers has been illustrated in Figure 1. Additionally, predicted values by the proposed following model have been included in these figures. According to Figure 1, compressive strength of geopolymers increases over time.

The Johnson-Mehl-Avrami-Kolmogorov equation is represented as following:

\[
f(t) = 1 - \exp(-kt^n)
\]

where \(f(t)\) is degree of reaction, \(t\) is time of reaction, \(k\) is constant and \(n\) is exponent.

According to Figure 1, and as it is an accepted rule in constructional materials, degree of reaction in cementitious systems is related directly to compressive strength. Therefore, Eq. (1) can be adopted for compressive strength of geopolymers as following:

\[
f_c = \alpha \left[1 - \exp(-kt^n)\right]
\]

where \(f_c\) is compressive strength and \(\alpha\) is constant.

Eq. (1) is solved while degree of reaction varies between 0 and 1. In Eq. (2), \(f_c\) is greater than 1 and hence for our case where strengths are below 100 MPa, we divide the strengths by 100. This normalized number can be included in the constant \(\alpha\). For specimens with higher strengths, one can divide them by a reference number.

To determine \(k\) and \(n\), Eq. (2) can be written as the following form:

\[
\ln\left(-\ln\left(1 - f_c\right)\right) = lnk + nlnt
\]

\(k\) and \(n\) can be easily found from intercept and slope of the line plotted in the form of \(\ln\left(-\ln\left(1 - f_c\right)\right)\) vs. \(lnt\) respectively. These lines for the whole considered geopolymeric systems considered in this study have been plotted in Figure 2. Calculated \(k\) and \(n\) and their corresponding equations have been given in Table 1. The predicted compressive strengths for all of the considered geopolymeric mixtures have been presented in Figure 1. As it is obvious, there is a strong relationship between the predicted strength and experimental ones.

Degree of completion of geopolymeric reactions can be considered as a function of
compressive strength. It is believed that for cementitious systems, 90 days of curing is enough to have the maximum capacity of strength evolution. This can be observed when compressive strength evolution vs. time is plotted in logarithmic scale. In this case, shape diagrams such as those illustrated in Figure 3 for the studied geopolymers in this paper are formed. Shape diagrams shows that at later ages, strength evolution tends to decrease with respect to early and middle ages of curing. Therefore, if by an accuracy of 95%, we can assume that maximum compressive strength of geopolymeric specimens are achieved, degree of completion of geopolymeric reaction at other ages can be found as following:

\[ f(t) = \frac{0.95t}{f_{c,90}} \]  

(4)

where \( f_{c,90} \) is compressive strength at 90 days of curing.

It is worthwhile to mention that the proposed formulation is based on the chemical composition of fly ash. There is not any relationship between chemical composition of fly ash and compressive strength of resultant geopolymer. Therefore, the whole modelling depends on the utilized fly ash and separate formulations should be provided for each mixture. A further work on determining the effect of chemical composition of fly ash on the proposed formulation is suggested for further works.

4. Conclusions

The Johnson-Mehl-Avrami-Kolmogorov equation was used as a basic formulation for prediction compressive strength of class C and class F geopolymers. Degree of reaction of geopolymers was supposed to be related directly to compressive strength and then Avrami constants and exponents were found for all geopolymers. It was shown that compressive strength evolution of geopolymers can be found by the proposed equations with an excellent approximation. Since logarithmic scale of compressive strength vs. time results in shape
diagrams, it was concluded that degree of reaction is easily accessible through the values of compressive strength at later ages of curing.

References


Table 1. Constant, exponent and equation of compressive strength evolution for class C and class F fly ash-based geopolymers

<table>
<thead>
<tr>
<th>Curing temperature (°C)</th>
<th>Class C fly ash-based geopolymers</th>
<th>Class F fly ash-based geopolymers</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( k )</td>
<td>( n )</td>
</tr>
<tr>
<td>40</td>
<td>0.137</td>
<td>0.31</td>
</tr>
<tr>
<td>70</td>
<td>0.172</td>
<td>0.27</td>
</tr>
<tr>
<td>90</td>
<td>0.211</td>
<td>0.25</td>
</tr>
</tbody>
</table>

(a)
Figure 1. Experimental and predicted compressive strength of a) class C and b) class F fly ash-based geopolymers.
Figure 2. Plots for determining $k$ and $n$ in a) class C and b) class F fly ash-based geopolymers
Figure 3. Compressive strength of a) class C and b) class F fly ash-based geopolymers in logarithmic scale.