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Factors affecting the performance of metakaolin geopolymers exposed to elevated temperatures

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Abstract The effects of geopolymer binder systems exposed to elevated temperatures are examined. Geopolymers investigated were synthesized from metakaolin, activated by combinations of sodium/potassium silicate and sodium/potassium hydroxide. The specimens were then exposed to temperatures of 800 °C. The factors studied were: (1) calcining temperatures of kaolin; (2) Si/Al ratio of the geopolymer; (3) activator/metakaolin ratio; (4) curing temperature; and (5) alkali cation type. Altogether 30 geopolymer formulations were studied. The samples were subjected to compressive strength, thermogravimetry, and scanning electron microscopy tests. Results showed that Si/Al ratio has a significant influence on elevated temperature exposure deterioration. Lesser strength loss due to elevated temperature exposures were observed in geopolymer with high Si/Al ratios (>1.5). The geopolymer binders activated by potassium-based activators showed an enhanced post-elevated temperature exposure performance compared to sodium-based systems. The optimum calcining temperature of kaolin and curing temperatures for improved temperature performance are also reported.

Introduction

Geopolymers [1] are said to possess excellent strength, fire resistant, and chemical resistant properties. They are produced by synthesizing aluminosilicate source materials with alkaline silicate solutions [2]. A relatively low temperature (600–800 °C) is required for the thermal processing of aluminosilicates derived from kaolin sources to produce metakaolin. Alternatively, fly ash, typically Class F type, from coal-fired power stations can be used in geopolymer synthesis [3]. The production of raw materials for geopolymer does not require a high-energy consumption level. In fact, the energy consumption is considered to be 60% less than that required for ordinary Portland cement (OPC) production [4].

Research into geopolymer technology specific to cement and concrete applications has been gaining interest among researchers in recent years [5–7]. In particular, significant research work on geopolymer concrete has been reported by Rangan and his co-workers [8, 9] based on concrete made from fly ash in combination with sodium silicate and sodium hydroxide solution. These researchers observed that the mechanical properties of their geopolymer concrete were similar to conventional OPC concrete [10]. In elevated temperature exposure related studies, Cheng and Chiu [11] reported that the fire resistance of blast furnace slag-based geopolymer binders was enhanced by increasing the K_2O content. Similarly, Poon et al. [12] investigated the performance of metakaolin-blended OPC concrete at elevated temperatures and observed that the blended cement concrete suffered loss in strength with occurrence of explosive spalling. On the other hand, Duxson et al. [13] reported that the shrinkage and densification of Na-based metakaolin geopolymer are highly dependent on Si/Al ratio and gel structure. Overall, only very limited data have been

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published to date on elevated temperature response of geopolymers for cement and concrete applications, which this current study aims to address.

The fire resistance of geopolymer systems is known to be highly dependent on its constituent materials, particularly the kaolin source [14]. However, for the current study the kaolin used was limited to one source. The specific objective was to establish the correlation between metakaolin-based geopolymer mixture compositions and parameters that affect strengths of geopolymers in relation to fire performance. The study includes investigation of several physical, chemical, and microstructural changes that characterizes geopolymer systems after exposure to elevated temperatures.

Experimental work

Materials characterization

Metakaolin (MK) is a product of the calcination of kaolin (china) clay. The kaolin clay used in this paper was procured from Unimin Australia Ltd. The kaolin was of HR1-F grade with an average particle size of 38 μm. The chemical composition determined by X-ray Fluorescence (XRF) is given in Table 1.

Alkaline-silicate activators in the investigation consisted of silicate solutions and alkali hydroxide solutions, MOH (where M represents K or Na). Sodium silicate solution, Na_2SiO_3 was of laboratory grade D with a modular ratio (M_s) equal to 2 (where $M_s = SiO_2/Na_2O$, $Na_2O = 14.7\%$ and $SiO_2 = 29.4\%$) and potassium silicate solution, K_2SiO_3 was of Kasil 2040 with M_s equal to 2.02 (where $M_s = SiO_2/K_2O$, $K_2O = 13.3\%$ and $SiO_2 = 26.7\%$). These commercial silicate solutions were supplied by PQ Australia. Potassium hydroxide (KOH) flakes of 90% purity and sodium hydroxide (NaOH) micropearls of 98% purity were supplied by Redox Chemicals and Orica Chemicals respectively. All activator solutions were prepared 1 day prior to usage. Additional pure silica comprised of fumed silica (Aerosil 300) with an average particle size of 7 nm (supplied by Degussa Australia).

Table 1 Chemical composition of metakaolin

Chemical	Component (%)
Al_2O_3	37.2
SiO_2	55.9
CaO	0.11
Fe_2O_3	1.7
K_2O	0.18
MgO	0.24
Na_2O	0.27
P_2O_5	0.17
TiO_2	2.4
BaO	0.05
MnO	–
SrO	0.03
SO_3	0.02
ZrO_2	–
LOI[a]	0.8

[a] Loss on ignition

Specimen preparation procedures

Specimen processing and mix proportions

The MK source material utilized for specimen processing was obtained by conducting 6-h calcination of raw kaolin using an electrical furnace. The majority of the investigation involved a combination of 'Na_2SiO_3 with KOH' as the alkali-silicate activators. Other combinations involving 'Na_2SiO_3 with NaOH' and 'K_2SiO_3 with KOH' were also studied. All concentrations of MOH liquids were kept to a constant molarity of 7.0 M. A summary of the mixture composition is presented in Table 2.

The MK and alkaline silicate solution were hand-mixed for 10 min and a further 5 min with a mixer before casting into 25 mm × 25 mm × 25 mm cubic steel molds. Molded samples were vibrated to release any residual air bubbles. Subsequently, the samples were covered with a film and transferred to an airtight container to prevent moisture loss. Each sample batch was prepared in duplicates.

Curing regime and elevated temperature exposure

All specimens were cured undisturbed for 24 h at room temperature in sealed containers before being subjected to high temperature curing at 80 °C for a further 24 h. At the end of the curing regime, the specimens were removed from their moulds and allowed to cool before initial physical properties including dimensions, masses and densities were recorded.

After 3 days, the specimens were subjected to elevated temperature exposure which consisted of ramping-up furnace temperatures from ambient to 800 °C at rate of 4.4 °C/min. The target temperature (800 °C) was maintained for 1 h before the furnace was switched off. The specimens together with the furnace were allowed to cool naturally inside the furnace to room temperature. The reference, i.e., unexposed, specimens were left undisturbed at room temperature.

Table 2 Metakaolin-based geopolymer mixture composition

Mixture no	Calcining temperature (°C)	Si/Al ratio	M/Al ratio	Silicate type	Hydroxide type	Curing temperature (°C)
1	650	1.40	0.66	Na_2SiO_3	KOH	80
2	700	1.40	0.66	Na_2SiO_3	KOH	80
3	750	1.40	0.66	Na_2SiO_3	KOH	80
4	800	1.40	0.66	Na_2SiO_3	KOH	80
5	850	1.40	0.66	Na_2SiO_3	KOH	80
6	650	1.54	0.42	Na_2SiO_3	KOH	80
7	700	1.54	0.42	Na_2SiO_3	KOH	80
8	750	1.54	0.42	Na_2SiO_3	KOH	80
9	800	1.54	0.42	Na_2SiO_3	KOH	80
10	850	1.54	0.42	Na_2SiO_3	KOH	80
11	750	1.46	0.56	Na_2SiO_3	KOH	80
12	750	1.50	0.49	Na_2SiO_3	KOH	80
13	750	1.52	0.45	Na_2SiO_3	KOH	80
14	750	1.80	0.42	Na_2SiO_3	KOH	80
15	750	2.05	0.42	Na_2SiO_3	KOH	80
16	750	2.31	0.42	Na_2SiO_3	KOH	80
17	750	1.58	0.48	Na_2SiO_3	KOH	80
18	750	1.51	0.38	Na_2SiO_3	KOH	80
19	750	1.49	0.34	Na_2SiO_3	KOH	80
20	750	1.54	0.42	Na_2SiO_3	KOH	70
21	750	1.54	0.42	Na_2SiO_3	KOH	90
22	750	1.54	0.42	Na_2SiO_3	KOH	100
23	750	1.38	0.63	Na_2SiO_3	NaOH	80
24	750	1.51	0.40	Na_2SiO_3	NaOH	80
25	750	1.38	0.59	Na_2SiO_3	KOH	80
26	750	1.38	0.62	K_2SiO_3	KOH	80
27	750	1.43	0.50	K_2SiO_3	KOH	80
28	750	1.46	0.42	K_2SiO_3	KOH	80
29	750	1.48	0.37	K_2SiO_3	KOH	80
30	750	1.49	0.34	K_2SiO_3	KOH	80

Characterization tests

Compressive strengths

Compressive strength measurements of specimens were performed using a Mohr and Federhaff AG mechanical testing machine in load control mode with a loading rate of 20 MPa/min. The specimens were tested at the age of 3 days after casting.

Thermogravimetric analysis

Thermogravimetric analysis (TGA) was conducted using a Settaram TGA92 device to measure the mass loss, while specimens were exposed to gradually increasing temperatures. Powdered specimens were used in TGA to ensure thermal equilibrium during heating.

Electron microscopy

Scanning electron microscopy (SEM) imaging was performed to study the microstructure of geopolymers. The samples were cut from 25-mm diameter cylindrical specimens using a diamond saw and polished down gradually to a 0.1 µm diamond-paste finish. The samples were vacuum dried overnight prior to SEM. The samples were then mounted on the sample stubs and sputter-coated with gold–palladium alloy. Imaging was conducted using a Hitachi S-4700 SEM.

Results and discussions

Figure 1 shows the typical images of the specimens before and after temperature exposure. Some small lightening of color was noticed in samples that underwent temperature exposure. As can be seen in this figure, there are noticeable macrocracks of 0.1–0.2 mm width appearing on the surface of the specimen as a result of temperature exposure.

The following sections provide discussions on a number of factors that affect the strengths of MK-based geopolymers before and after exposure to elevated temperatures.

Effect of kaolin calcining temperature

The calcining temperatures investigated were 650, 700, 750, 800, and 850 °C, which involved Mixtures 1–10 of Table 2. Calcination was conducted using an electrical ceramic furnace for 6 h in accordance to the methods described by Davidovits [15]. For all mixtures, the activator/MK ratio was kept at 1.25, while the curing temperature was held constant at 80 °C. Figure 2 shows the effect of various kaolin calcining temperatures on the strength of geopolymers. The percentages indicated in Fig. 2 represent the percentages of residual strength remaining after temperature exposure. The Si/Al ratio of 1.40 and 1.54 were investigated along with the effects of calcining temperature.

Curve (a) of Fig. 2 (Si/Al = 1.40) shows that the calcining temperatures have no significant impact on either unexposed strengths or percentages of residual strengths after exposure. Curve (b) (Si/Al = 1.54) shows a similar behavior with strengths peaking at calcining temperatures of 750 °C, except for the 850 °C calcining temperature shows a different behavior. This suggests that the highest overall compressive strength could be achieved at this temperature.

In summary, calcining temperatures appear to have a marginal effect on elevated temperature performance of the samples. The percentages of residual strength, was observed to be consistent throughout the entire range of calcining temperatures investigated. However, the effect of calcining temperature was found to be highly dependent on the Si/Al ratio. Increasing the Si/Al ratio causes the overall strength and temperature-exposed residual strengths to increase significantly. The effect of Si/Al ratio will be further investigated in the next section.

Silica-to-alumina (Si/Al) ratio

The strengths of the geopolymer samples with Si/Al between 1.40 and 1.54 were investigated in greater detail by manipulation of the activating solution; involving Mixtures 2, 8, 11, 12, and 13 of Table 2. The kaolin was calcined at 750 °C and the activator/MK ratio was kept fixed at 1.25. All specimens underwent consistent curing temperature of 80 °C for a period of 24 h.

Unexposed specimens strengths increased when Si/Al ratio was increased from 1.40 to 1.54 as shown in Fig. 3. With increasing Si/Al ratio, more Si–O–Si bonds are formed, which are stronger in comparison to Si–O–Al and Al–O–Al bonds [16]. The microstructure of the matrix comprises of large interconnected pores and loosely structured precipitates which results in low mechanical strength especially for Si/Al < 1.40 [17]. Unexposed strengths decreased with increase in Si/Al ratios from 1.54 to 2.30. This differs from results by Duxson et al. [18] who reported peak strength at Si/Al ratio of 1.90. However, it should be noted that Duxson et al. [18] reported 7-day strength results as opposed to the 3-day strengths in this study. When specimens were subjected to an elevated temperature of 800 °C, there was deterioration in strength. Both exposed and unexposed strengths peaked at Si/Al ratio of 1.54.

The method used for varying silicon content within the alkali solutions as described earlier also had an influence. It would be recalled that fumed silica in the form of Aerosil 300 was introduced to the mixture of the geopolymer to increase the Si/Al ratio in Mixtures 14–16 (Table 2).

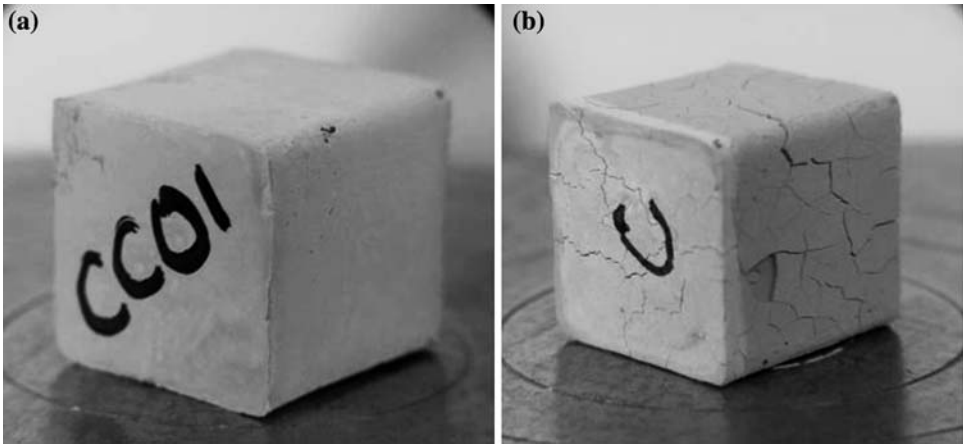


Fig. 1 Photographs of typical metakaolin-based geopolymer specimen (**a**) before and (**b**) after elevated temperature exposure

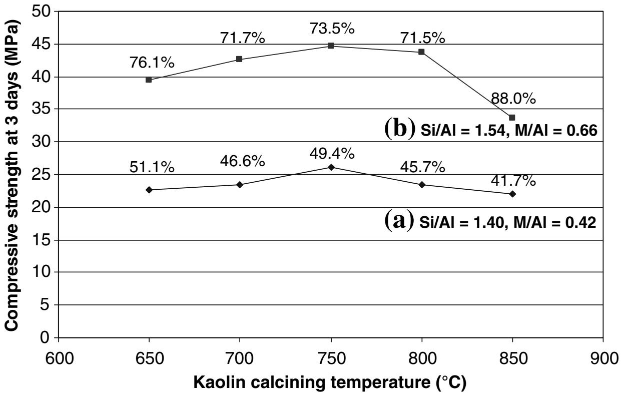


Fig. 2 Unexposed strengths of geopolymers with MK calcined at various temperatures. Percentages indicated at each data point represent residual strength percentages after temperature exposure

The strength of unexposed specimen decreased for Si/Al ratio exceeding 1.54, but the reduction in strength due to elevated temperature exposures were substantially reduced. Strength reductions of the temperature-exposed specimens from unexposed specimens for Si/Al > 1.54 are about 4–6% in comparison to 27–51% for Si/Al ≤ 1.54.

A possible explanation is that a major proportion of the added fumed silica remains unreacted, as suggested by Singh et al. [19]. Duxson et al. [17] also suggest that the binder is homogeneous and contains unreacted particles and small isolated pores when the Si/Al ratio exceeds 1.65. It is also evident in Fig. 4(a) that there are a large proportion of unreacted particles. When exposed to elevated temperature, sintering of these unreacted particles occurs (Fig. 4(b)). The sintering effect causes increase in strength by forming stronger bonds, countering the other thermal damages caused at elevated temperatures. As a result, the specimens with high Si/Al ratio (Si/Al > 1.54) demonstrate smaller strength reductions when exposed to elevated temperatures as compared specimens with low Si/Al ratio (Si/Al < 1.54). At lower magnification, a uniform-layered plate-like structure was observed with angular edges, as previously described by Steveson and Sagoe-Crentsil [20]. Notably, much fewer distinct layers were observed in the temperature-exposed specimens.

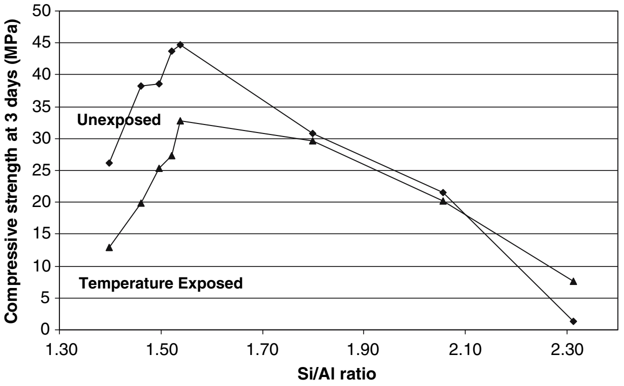


Fig. 3 Effect of the silica-to-alumina ratio on temperature-exposed and unexposed compressive strengths

Influence of activator-to-metakaolin ratio

Mixtures 8, 17, 18 and 19 of Table 2 was used this investigation. The plot of compressive strengths against activator/MK ratios in Fig. 5 shows that compressive strengths decrease when activator/MK ratios increase, with the exception being initial ratio of 1.00. The activator/MK ratio influences the porosity of the hardened geopolymers. Thus, this ratio affects the volume of voids in the pastes, which directly influences the strength of geopolymer binders.

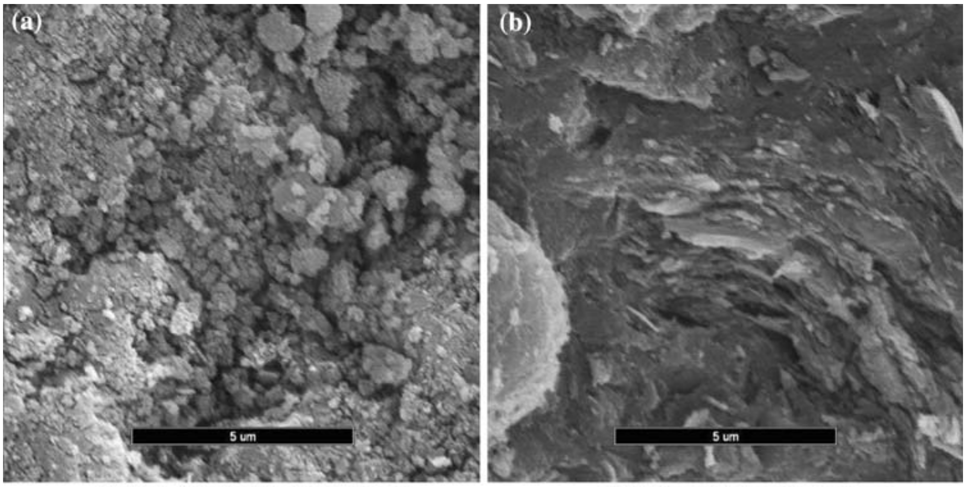
It was observed that the fresh paste became increasingly stiff as the activator/MK ratios decreased. At the lowest activator/MK ratio (1.00), the paste was very stiff with low workability. This low workability and resulting lack of compaction are the likely reason for the lower than the expected strength for the 1.00 ratio following the trend from the rest of the data.

Influence of curing temperature

Figure 6 shows the influence of curing temperatures studied on the compressive strengths for unexposed and exposed specimens using Mixtures 8, 20, 21, and 22 (Table 2). The parameters that were kept constant were kaolin calcination temperature of 750 °C, activator/MK ratio of 1.25 and Si/Al ratio of 1.54 while the curing temperatures were varied from between 70 and 100 °C. As shown, the unexposed strength peaked at 80 °C. However, the strength recorded dropped significantly at 90 and 100 °C. This is often associated with the excessive loss of water during curing at these high temperatures, causing the specimen to 'dry out'. Rapid water loss is observed at approximately 90°C as depicted by the TGA and DTG curves of Fig. 7. Although the specimens were sealed from interaction with the environment during curing, at higher temperature there is a greater tendency for 'dry out' to occur.

For the temperature-exposed specimens, there was a compressive strength gain with the increase in curing temperature. However, the loss in strength was insignificant beyond 90 °C curing temperature (i.e., the strength before and after exposure are almost the same). Moisture dissipation is the primary cause of damage to the geopolymer structure. 'Dried out' specimens, as previously mentioned, are not likely to lose much strength, as there is less moisture

Fig. 4 SEM images of geopolymers



before temperature exposure **after temperature exposure**

in the system. Since there is less moisture to begin with, damage would be limited to damage already sustained during the curing stages—unaffected by elevated temperature exposure (800 °C). This can be observed in the in Fig. 8 where moisture loss is less significant for 90 and 100 °C cured specimens when compared with 80 °C cured specimens in the early stages (<200 °C) of the elevated temperature exposure.

Curing temperatures are known to have a large effect on properties of geopolymers [21]. Investigation regarding the effects of varied temperatures has been previously reported by Alonso and Palomo [21] where temperatures studied were between the ranges of 35–60 °C. They observed that the geopolymerization reaction accelerated with increasing temperatures resulting in increased compressive strengths.

Effect of activator alkali cation type

Table 2 shows compositional ratios of Mixtures 18, 23, 24, and 25 using MK calcined at 750 °C and activator/MK ratio of 1.11. The NaOH-based activator test results are shown in Fig. 9 alongside with KOH-based activators results for comparison purposes. The severity of the thermal damage is presented in Fig. 9 as the percentage of strength loss relative to the reference samples.

NaOH-based geopolymer with lower Si/Al = 1.38 showed weaker elevated temperature resistance than the higher Si/Al ratio. As observed in Fig. 9(a), a 50% drop in strength was recorded after the NaOH-based specimens were exposed to elevated temperature whereas KOH-based geopolymers registered a drop of 25% after the same exposure. In contrast, at higher Si/Al = 1.51 shown in Fig. 9(b), NaOH-based specimens presented slightly better results than the KOH; a 16% reduction in strength losses after temperature exposure in NaOH-based specimens, as opposed to 21% for KOH-based specimens.

Previous studies [22–24] showed that Na is more effective in promoting aluminosilicate dissolution than K. The yield stress of the fresh Na-based geopolymer paste is greater than the K-based paste, meaning the Na-based paste is more viscous and harder to mix [23]. Although Na-based

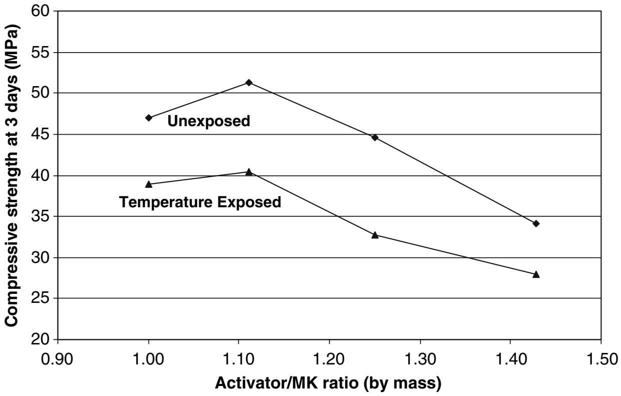


Fig. 5 Effect of the activator-to-MK ratio on temperature-exposed and unexposed compressive strengths

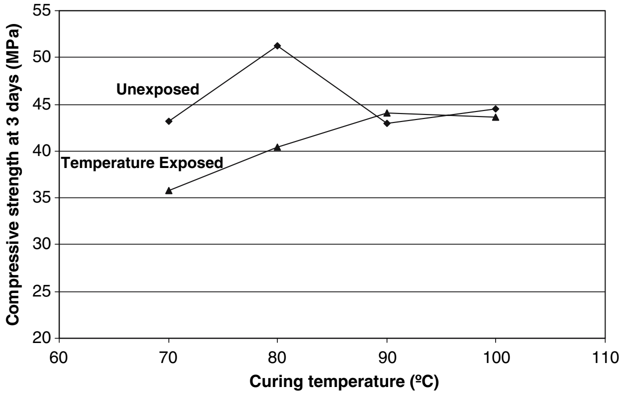


Fig. 6 Effect of the curing temperature on temperature-exposed and unexposed compressive strength

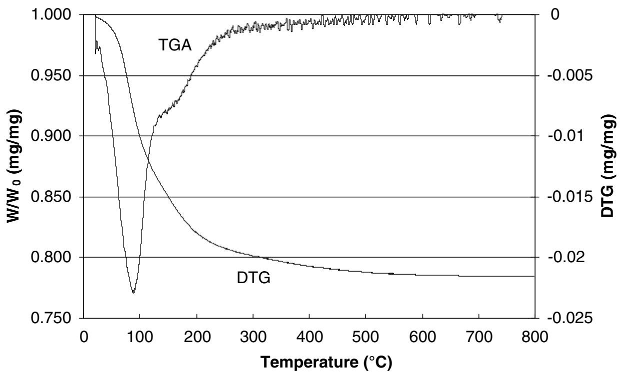


Fig. 7 TGA and DTG curves for 24 h ambient-cured metakaolin-based geopolymer subjected to elevated temperature of 800 °C

pastes showed better workability, KOH-based pastes provided better compressive strength. This finding is consistent with work conducted by Xu et al. [23]. Based on the above results, KOH-based specimens perform better than NaOH-based specimens, both at room temperature and after elevated temperature exposure.

Effect of alkali cation type of activator silicate component

The K_2SiO_3 with KOH combination was also investigated with Mixtures 26–30 of Table 2. The K_2SiO_3 strength performances are presented in Fig. 10. Lower strengths at room temperatures were attained when compared to the Na_2SiO_3 counterpart. However, the thermal damage (percentage of strength loss after elevated temperature exposure) in K_2SiO_3-based geopolymer was generally lower between Si/Al ratios of 1.38–1.49.

The sodium silicate-based geopolymer was found to be stronger than its potassium silicate-based equivalent. Rahier et al. [25] found that geopolymers synthesized with sodium silicate set at a faster rate than those synthesized with potassium silicate. Therefore, it is likely that the Na_2SiO_3-based geopolymer underwent further progression of geopolymerization reaction compared to the K_2SiO_3-based geopolymer, resulting in higher strength obtained.

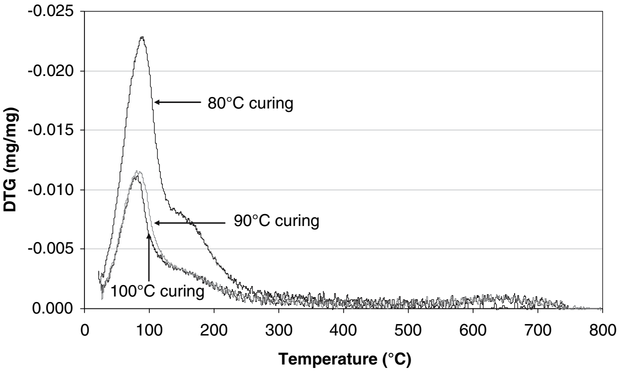


Fig. 8 DTG curves for metakaolin-based geopolymer cured at (**a**) 80 °C, (**b**) 90 °C, and (**c**) 100 °C for 24 h and further subjected to elevated temperature exposure of 800 °C

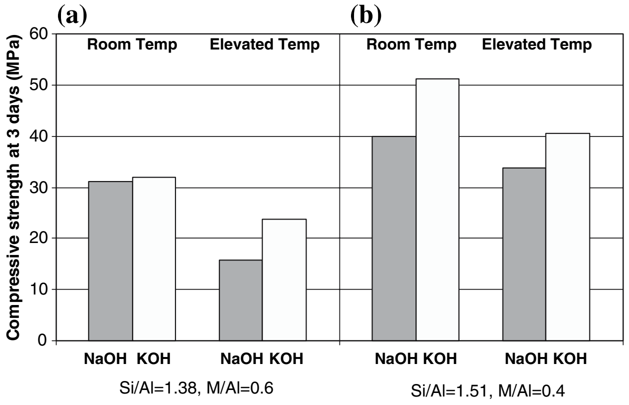


Fig. 9 NaOH versus KOH strength performances under ambient and elevated temperatures (Na_2SiO_3/MOH = 0.5 and 2.5)

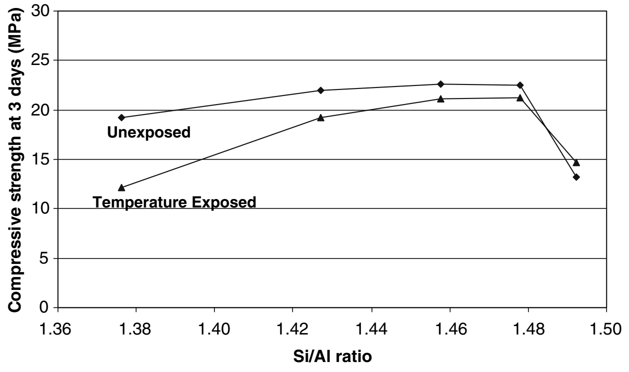


Fig. 10 Performance of geopolymers synthesized with potassium silicate and potassium hydroxide

Conclusions

This article presented results of the behavior of MK-based geopolymer paste exposed to elevated temperatures. The results demonstrate that:

1. The characteristic Si/Al ratio of the geopolymer remains the key parameter influencing the strength reductions observed after elevated temperature exposure to 800 °C. The strength deterioration due to temperature exposure reduced with increasing Si/Al ratio. This effect is very prominent at high Si/Al ratios (>1.5) where the strength reductions observed were very small of the order of 5%. This latter observation is attributed partly to sintering of unreacted Si-rich particles in the mixtures.

2. Calcining temperatures of kaolin appears to have a little influence on elevated temperature performance of mixture compositions investigated.
3. Geopolymer mixture curing temperatures above 80 °C showed good elevated temperature performance, however, room temperature performance was poor. This is evidently due to specimen "drying out" that appears to occur at during high temperature curing.
4. Potassium-based geopolymer (synthesized with potassium silicate and hydroxide) exhibited less strength regression after elevated temperature exposure compared to equivalent sodium-based geopolymer systems.
5. Alkaline solution selection and concentration ratio are shown to be critical parameters necessary for optimization of elevated temperature performance of metakaolin-based geopolymers.
6. It should be noted that the test trends observed are valid only for the type of geopolymers studied. Further, the effects of addition of aggregates or fillers are not considered in the study.

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