Strength prediction and mix design procedures for geopolymer and alkali activated cement mortars comprising a wide range of environmentally responsible binder systems

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This research presents a mix design methodology for geopolymer (GP) and alkali activated (AA) mortars based on metakaolin and industrial waste products activated using potassium silicate. The aim is to enable a wide range of mix designs to be specified to given compressive strength, consistency and environmental footprints to facilitate their adoption as a Portland cement (PC) alternatives in the construction industry in applications such as fibre reinforced building cladding systems. The impact of the work is timely as literature quantifying effects of mix parameters on broad families of GP and AA materials is limited, and no standardised performance-based methodology exists. Initially, effects of binder composition on mechanical and environmental properties is presented for a standard GP mix design using contoured ternary plots for a range of material blends. Next, effects of altering mixture parameters such as liquid/solid, silica/alumina and activator/binder ratios are quantified for three selected binder compositions before a preliminary mix design methodology is presented allowing initial selection of mixture proportions. Finally, correlation analysis is used to identify multiple mix variables strongly correlating with strength, and regression modelling used to present predictive tools with average errors <6%.

Keywords: Geopolymer; alkali activated, metakaolin; industrial wastes; mixture design; performance prediction

**Introduction**

There is a significant need for change in the way buildings are designed, constructed and consume energy. The materials currently used are increasingly unable to meet demands for levels of thermal performance, fire safety and finish to be achieved with increasingly limited environmental impact, greenhouse gases and energy allowances (Jones, 2011; Benhelal et al, 2013). In recognition of this, the EU plan to invest around €40 billion a year through schemes like the €5.9 billion horizon 2020 project focused on renovating existing buildings, making construction projects more sustainable and making all new builds energy independent by 2020 (European commission, 2014).

To help address this issue, the underlying focus of this research is to investigate and advance the application of geopolymer (GP)- and alkali activated (AA) cement solutions; families of materials offering innovative, high-performance and low environmental impact construction solutions relative to, for instance, existing Portland cement (PC)-based alternatives. GPs and AAs can be designed to form, cure and gain strength rapidly in ambient temperatures by combining water, user friendly alkaline reagents and alumina/silicate source materials that are either commercially produced, such as metakaolin, or industrial wastes, such as slags and ashes. The result are strong, durable, solid matrices that behave similar to PC concrete (Zeobond group, 2012). Geopolymers offer the potential for high strength (over 20 and 100 N/mm2 at 4-hours and 28-days respectively), fire protection and chemical resistance. Crucially, this is coupled with up to 90% reductions in embodied carbon relative to PC-based materials via the use of 100% recycled waste-based binders (Davidovits, 2013; Banah UK, 2014; Geopolymer Institute, 2016).

Despite these benefits, a key barrier to the widespread industrial adoption of geopolymer as a replacement for PC is the lack of recognised mixture proportioning methodologies capable of producing materials with specified performance levels (Lahoti et al., 2017). Manufacturing geopolymer systems depends on mixing a suitable activator with one or more alumina-silicate powders. However, deciding the proportions required is not straight forward. While literature regarding geopolymer cement concrete design exists, the importance of various mixture parameters on compressive strength has not been fully quantified, with previous work limited in terms of scope (Lahoti et al., 2017). Previous related research has focussed on exclusive binder types or combinations and/or single proportioning ratios such as silica/alumina (S/A), activating solution to binder powder (A/B) or liquid to solid (L/S); an approach analogous to the water/cement ratio in PC-based concrete (Aughenbaugh, 2015; Austroads, 2016). The ratio most commonly reported to directly affect geopolymer concrete mechanical strength and microstructure is S/A. Other common ratios reported are sodium or potassium to alumina, water to sodium and sodium to silica. In the majority of cases, existing studies focus on specific materials such as fly ash-based systems, with empirical models reported to strongly relate to reactivity,based on the fly ash vitreous content, loss on ignition and mean particle size (Diaz-Loya et al, 2013; Austroads, 2016). As fly ash systems typically require curing at elevated temperatures, these methods are of limited relevance to wider groups of ambient-cured GP/AA binder systems that provide the greatest potential for embodied CO2 reduction (Aughenbaugh, 2015; Timakul, 2015). The vast majority of existing geopolymer studies use sodium based activating solutions, with very few papers considering potassium silicate activation (Austroads, 2016). No previous papers considering the use of iron silicate in geopolymer systems and associated mixture design procedures exist. While selective existing studies have investigated multiple parameters synergistically to create empirical formulas and neural networks to predict strength (e.g. Wilson, 2015), existing work describing generic relationships between strength and key mix design parameters for various binder types is limited.

Against this background, the aim of this study is to produce simplified, preliminary mix design methods allowing preliminary proportioning of GP and AA materials. The unique feature of this work is a methodology enabling strength prediction for potassium silicate activated mortars comprising a wide range of binder combinations and mix parameters. In this way, the intention is to facilitate adoption of these systems as a high performance, low impact alternative to PC-based materials in buildings. The work is presented in three phases. In the first, the effect of a wide range of binder composition on performance is initially investigated by holding all other components of a control mix constant. The second phase of work proceeds to investigate the influence of additional key mixture variables and proposes a preliminary mix design method based on liquid/solid ratio for a wide range of binder compositions. In the final phase, the synergistic effects of a more comprehensive suite of mixture variables is investigated for selective binder compositions and a more robust mixture proportioning model based on regression analysis, albeit for selective binder compositions, is presented.

**Experimental methodology**

***Materials***

A range of binder materials was investigated as part of this research to facilitate widespread national/international adoption of the methodologies presented and beneficial reuse of prevalent local waste streams. Metastar 501 metakaolin (MK) from Imerys UK was used as the primary binder due its commercial availability, consistent and highly amorphous nature and its rapid dissolution and geopolymerization at ambient temperatures (Provis, 2015). While MK has a low environmental impact compared to PC, partially or fully replacing it with industrial waste products has been shown to both significantly reduce this impact and provide reduced setting times and increased strength and flow values (Austroads, 2016). As such, the industrial waste materials used in this study included: ground granulated blastfurnace slag (GGBS) from ECOCEM Ireland; silica fume (SF) from Elkem; fly ash (FA) from Kilroot power station in Northern Ireland; and iron silicate (IS) fines from Aurubis Bulgaria. Iron silicate is a low impact by-product of copper production and novel in its usage as a geopolymer source material. GGBS geopolymers require a much smaller amount of activator solids and, therefore, have lower environmental impact than metakaolin systems, which have a lower Si:Al ratio necessitating a greater amount to be used for full dissolution to occur (Komnitsas, 2011). SF has been shown in the literature (Austroads, 2016) to increase the Si:Al of the binder and thereby provide increased strength development between 7 and 28 days, especially at around 20% binder mass. Measured chemical compositions and published embodied CO2 values for the binder materials considered are presented in Table 1, together with typical values for PC for comparative purposes.

Geosil, a commercially available activating solution with a potassium silicate solids content of 45% by mass was sourced from Woellner and used in all mix designs. Potassium, rather than sodium, silicate activator was chosen due to its reactivity and emergence as a cost-effective solution for geopolymer production (Davidovits, 2017). Mortar mixes were studied in this work, with locally sourced lough-dredged sand from Stanley Emerson & Sons Ltd. used as fine aggregate.

***Sample preparation and testing sequence***

All samples for compressive strength testing were cast in 50 mm cubes, covered with plastic for 24 hours to ensure uniform drying conditions and then stored in sealed containers until testing at 7 and 28 days in accordance with BS EN 1015-11:1999. Ambient laboratory temperatures of approximately 200C were provided over this casting and curing period. Relative workability was determined using flow table testing in accordance with BS EN 1015-3:1999 to ensure minimal void creation when casting. While this method specifies a 250 mm-wide flow table, this was identified as too small for comparing high flows created during the binder variation studies. As such, the flow exhibited by many of the mixes produced in Phase I could not be compared accurately.

**Results and discussion**

***Phase I: Influence of binder composition***

From Table 1, it is evident that significant variation existed in the major oxide contents of the various binder materials considered, suggesting potential to achieve geopolymer mixes with a wide range of performance and embodied CO2 levels. To investigate the impact of binder composition in this regard, a base MK only GP control mix with liquid/solid (L/S) and paste/sand ratios of 0.51 and 0.84 respectively was initially developed as part of a preliminary research phase. This mix was then held constant and replicated with the exclusive variation being binder powder composition, enabling investigation of effects on mortar compressive strength, flow and environmental impact (see Figure 1). Binder combinations considered in this way included MK/GGBS/FA, MK/GGBS/SF and MK/GGBS/IS, with full ranges of unary, binary and ternary binders considered for each by considering respective binder increments of 20% in the range 0-100% by mass. By adopting this approach, it was recognised that performance levels were likely to vary considerably and potentially beyond limits of suitability. MK-based mixes, for instance, are reported to require more liquids than fly ash or slag geopolymers to ensure monomer transport, full dissolution and reorganisation (Lahoti, 2017).

In terms of mortar flow, results varied significantly for the binder combinations considered and, at almost all increments of MK replacement, were in excess of 250 mm. As such, flow rates were generally too high for accurate measurement and meaningful comparison. While this high range was clearly influenced by the L/S ratio of the base mix used (0.51), the ability of industrial waste materials to increase flow was considered a positive finding in terms of industrial-scale cladding panel production, for example; a factory-based precast production process demanding high-flow and high-strength materials.

Based on the mixes considered, Figure 2 presents contoured ternary plots illustrating the significant influence of binder powder composition on both 7- and 28-day mortar strength. Represented at the pinnacle of each ternary plot in Figure 2, the 100% MK mix attained 7 and 28-day strengths of 41.5 and 46 N/mm2 respectively. At both 7 and 28 days, GGBS was proven to be a successful replacement for MK, with respective strengths of 69.5 and 85 N/mm2 recorded for the binary 20%MK/80%GGBS combination. Indeed, this binder blend outperformed the 100%GGBS mortar, suggesting that in these mixes geopolymer gels and CASH hydration products formed simultaneously, bonding well together as the latter expanded into the pores of the former to create a homogenous microstructure. While at 7 days (Figures 2a-c), the 20%MK/80%GGBS combination delivered the highest strength of all combinations considered (69.5 N/mm2), at 28 days this was achieved by the 20%SF/80%GGBS binary blend (106 N/mm2). As suggested previously these performance levels reflect increasing quantities of Si-O-Si bonds present due to associated increasing silica to alumina ratios.

In comparison to these maximum binary combinations, similar general trends were noted from the three ternary plots considered at both 7 and 28 days (MK/GGBS/SF, MK/GGBS/FA and MK/GGBS/IS), with strengths steadily decreasing as levels of MK and GGBS were replaced with increasing levels of either SF, FA or IS. While this was perhaps unexpected given the significant disparity of the chemical compositions of these binders, it confirmed the dominance of GGBS and MK in resultant geopolymerisation reactions and performance levels. Overall from Figure 2, it can be seen that compressive strength values ranged from 4-69.5 and 5-106 N/mm2 at 7 and 28 days respectively across the range of binder combination considered, offering significant performance and mix design flexibility moving forward.

Overlaid on the 28-day strength ternary plots (Figures 2d-f) are embodied CO2 contents for each binder combination based on published values, enabling both environmental- and performance-informed decision making. Clearly from these plots, embodied CO2 values generally decrease with corresponding reductions of MK; reflecting the fact that it is commercially mined and calcined, as opposed to a by-product from other industrial activities. Of particular significance from these combined plots in Figure 2(d-f) is the fact that, for the binder combinations considered, improving levels of compressive strength generally correspond with reducing levels of embodied CO2. This is contrary to trends typical of conventional PC-based concrete mixes.

***Phase II: Influence of singular mixture proportioning ratios***



*Mix designs*

While Phase I was effective in identifying the influence of binder composition on geopolymer mortar performance, this was established for one mix design only, with other important and inter-relating mix parameters not considered. As such, the following three binder powder blends were selected for further investigation in Phase II: 100% MK base mix; 80%GGBS/20%MK and 80% GGBS/20% SF. The latter two were chosen as they achieved the highest strength at 7 and 28 days respectively from Phase I. As shown in Table 2, a face centred central composite mix design approach was used to consider three mortar component variables (binder powder, activator and free water content) across three levels (-1, 0, +1) for each selected binder blend.

In Phase I, the L/S solid of 0.51 used provided a wide range of flow across the different binder types considered, with pure MK geopolymers exhibiting significantly lower values than hybrid or GGBS-based blends. This is due to the fact that the MK geopolymers require higher L/S and A/B ratios than fly ash or slag geopolymers for full dissolution, monomer transport and reorganisation to take place. This trend was addressed in Phase II by lowering the binder mass and increasing water mass for the 100%MK mixes in order to maximise the potential of forming homogenous geopolymers. Ranges of binder powder, activator and free water content considered for the MK mixes were 490-590, 400-500 and 100-160 kg/m3 respectively, while for the GGBS/MK and GGBS/SF mixes corresponding ranges were 550-650, 400-500 and 70-130 kg/m3. In this way, the intention was to further investigate influences of the following key relationships presented in the literature (Kim, 2012; Wilson, 2015; Provis, 2015; Austroads, 2016; Lahoti, 2017) as significant for geopolymers: S/A, L/S and A/B. Via the variables and ranges considered as part of the central composite design adopted, values of A/B and L/S ranged from 0.76-1.02 and 0.46-0.57 respectively for the 15 MK mixes. Corresponding ratio ranges for the GGBS/MK and GGBS/SF mixes were 0.62-0.91, 0.35-0.52.

*Compressive strength results*

The 7-day compressive strength results achieved by the geopolymer mortar mixes considered as part of Phase II are presented in Table 2. As expected and reflecting the mix constituent ranges introduced as part of the experimental design, broad ranges of strength were recorded for each binder combination investigated. For the 100%MK, 80%GGBS/20%MK and 80%GGBS/20%SF combinations, these were 33.0-58.0, 67.5-86.0 and 34.5-68.5 N/mm2 respectively. Of the 15 mix compositions considered for each binder blend, mix 4 was perhaps expected to produce the greatest compressive strength as it had the lowest L/S ratio, highest mass of binder powder and the lowest amount of activating solution and free water. This was provided, of course, that sufficient activating solids existed in the mix for full dissolution to occur without leaving unreacted binder to act as microdefects. Indeed, for the 100%MK mix 4 (as well as for mixes 8 and 11) this proved not to be the case, with the material failing to set and gain any appreciable strength.

Alternatively, all of the GGBS/MK and GGBS/SF mixes successfully broke down the binder powder and had sufficient liquidity for monomer transport and reorganisation, allowing homogeneous hardened geopolymer mortar to form in all 15 mix iterations irrespective of the lower ratio values considered. This suggests that the amount of activator solids required for geopolymers based on these industrial waste materials is significantly lower. As this is likely to be the most significant portion of these geopolymer mixtures from both an economic and environmental standpoint, the benefits of partially replacing the MK with these is obvious.

*Relationships between singular mixture proportioning ratios and strength*

As illustrated in Figure 3, work progressed to explore if clear relationships existed between the strength results obtained and the aforementioned ratios reported as being significant for geopolymer mix design (i.e. S/A, L/S and A/B). Figure 3 plots these ratios versus 7-day compressive strength for all 15 mixes considered for the three binder combinations under investigation. The S/A ratio of source materials used to create geopolymers dictates molecular- and nano-scale structures formed and, theoretically, there should be a direct correlation between silica content and strength due to increasing quantities of stronger Si-O-Si bonds. With that said, owing to other impacting mixture proportioning parameters such as L/S or activating solution composition, optimum levels of S/A reported by researchers vary (Kim, 2012; Austroads, 2016;). In this study, however, the influence of S/A ratio on 7-day strength was not as significant as previously reported, with insignificant R2 values of 0.06, 0.28 and 0.07 noted for the MK, GGBS/MK and GGBS/SF mixes respectively.

A/B ratio is reported to be one of the most important factors in the successful design of geopolymer mixes, enabling full dissolution and reorganisation of the mortar without defects from unreacted binder powder (Wilson, 2015). As mentioned previously, three of the 100%MK mortar mixes (4, 8 and 11) were unable to form geopolymer products owing to insufficient activator solids in the mix to break down the binder powder. With no release of silica and alumina monomers and chemically bound water, dry, sandy mortars lacking any cohesion or liquidity were formed. All MK mixes with an A/B ratio less than 0.75, or an activator solid to binder ratio of 0.34 reacted in this way. While vital to geopolymer formation, this ratio was found to be of little relevance in trying to predict strength, with R2 values ranging from 0.07 to 0.28.

L/S ratio in geopolymer materials (calculated by dividing the mass of solid materials in the binder and activator by that of the liquid portion of the activator and free water) is reported to be analogous to the water/cement (W/C) ratio in PC concrete mix designs in terms of its impact on properties such as flow and compressive strength. In PC-based materials, compressive strength is negatively proportional to W/C. Similar, albeit varying and diminished relationships were noted for the three geopolymer binder blends considered, reflecting the probable influence of other key mix variables not present in PC concrete. The R2 values noted in this case ranged from 0.41-0.72, indicating a more significant correlation between L/S ratio and strength.

In conclusion from Figure 3, it appears that no principal mix proportioning ratio can be considered in isolation to accurately predict 7-day compressive strength. With that said, of the three considered, L/S emerged as the most significant; albeit with differing relationships apparent for the different binder compositions investigated. Against this background, the data presented in Figure 3 was manipulated further in an attempt to investigate and develop generic relationships of performance versus L/S ratio and to explore its applicability to a wide range of geopolymer binder types. To this end, further laboratory work was undertaken to assess flow and compressive strength performance of additional selected representative binder types across a range of L/S ratios (0.35-0.61). Binder combinations considered in this way included: 100% MK; 100%GGBS; 80%GGBS/20%MK; and 60%GGBS/20%MK/20%SF. Primary data was additionally supplemented by performance versus L/S ratios published in the literature (Gao et al. 2013; Kumar, 2015; Shivaranjan, 2016; Lahoti, 2017; Guzman-Aponte, 2017). The findings of this work with respect to compressive strength are presented in Figure 4. From Figure 4(a), it is evident that while clearly distinctive and somewhat inconsistent relationships exist for individual mix types (determined by differences in binder types, associated geopolymerisation reactions, testing times, experimental variables, etc. used), families of generic relationships are identifiable. While recognised not to closely fit all primary and secondary data sets compiled in Figure 4(a), a proposed normalisation of this observation is presented in Figure 4(b) for use within a preliminary mixture proportioning methodology. Similar normalised relationships for flow versus L/S ratio are presented in Figure 5(a&b).

*Simplified preliminary mix design methodology*

Combining the results presented to this point, a simplistic mix design procedure is proposed for geopolymer mortar mixes comprising any binder combination of MK/GGBS/FA (see Figure 6). This methodology is intended to be reproducible for the other material combinations considered. Included in Figure 6 are values of embodied CO2 and 7-day compressive strength for mixes with L/S ratio of 0.51, as well as generic relationships linking both 7-day compressive strength and flow with L/S ratio in the range 0.30-0.65. In this way, the figure enables estimations of approximate mixture proportions for specified values of compressive strength and/or flow.

In the example presented, initial mix design requirements include a maximum value of embodied CO2 content (0.15 kgCO2/kg) and 7-day strength (50 N/mm2). Using Figures 6(a) and (b), the 7-day strength can be estimated for geopolymer cement mortar comprising a suitable binder combination and L/S ratio of 0.51. In the example shown, a value of 35 N/mm2 is predicted for a 30%MK/50%GGBS/20%FA binder combination. This value can then be transposed onto Figure 6(c) to enable an estimation of the required L/S ratio to achieve the required 7-day strength of 50 N/mm2. In the example shown, a L/S value of 0.38 is estimated, leading to an approximate flow value of 260 mm. It is recognised that by not accounting for other mix design criteria, such as aggregate size/type/properties and paste/aggregate ratio, this mix design procedure is by no means the finished article for geopolymer cement mortar/concrete. With that said, provided is a simplistic provisional methodology enabling rapid estimation of performance for a wide range of low impact binder material options.

***Phase III: Synergistic influence of multiple mixture proportioning ratios***

While the mixture proportioning method presented in Phase II was capable of providing preliminary mixture proportions for a variety of GP/AA materials, its limitations were recognised given the method’s sole reliance on L/S ratio as a predictor of performance. As such, work in this phase proceeded to ascertain if combinations of several mix parameters could be used synergistically with more success. Based on the 7-day compressive strength results presented in Table 2, correlation analysis was initially carried out to determine mix parameters most closely linked with performance. Parameters considered included binder mass (B), activator solution mass (A), free water mass (FW), sand mass (S), activator solids mass (AS), total water content (TW), A/B ratio, free water to activating solution (FW/A) ratio, free water to binder (FW/B) ratio, L/S ratio and S/A ratio. While the aim at the outset was to generate a generic model capable of predicting the performance of any binder combination, this was found not to be possible within acceptable limits of accuracy. As a result, independent variables were identified from the above list for each binder combination considered (100%MK; 80%GGBS/20%MK; and 80%GGBS/20%SF) separately. Strength prediction models were then generated for each based on intercept and slope coefficients generated from related regression analysis. Predicted compressive strength results for the 15 mixes for each binder blend were compared to corresponding experimental results to quantify the modelling accuracy. Comparing outputs such as adjusted R2, significance, f and p values, allowed the most accurate prediction of strength possible from the data sets available.

Results from this analysis are presented in Table 3, which shows modelling parameters and predictions for each of the three binder blends. For the 100%MK-based model, for instance, the key mix parameters identified included binder mass (B), free water mass (FW), FW/B and FW/A. Based on these, 7-day compressive strength predictions were possible with an average error of 3.12%, adjusted R2 value of 0.91 and statistical significance, f of 1.9×10-4. In comparison, for mixes comprising 100%GGBS/20%MK, modelling parameters used included binder mass, free water mass, FW/A, FW/B, S/A and L/S ratios, with an average modelling error, adjusted R2 and significance, f, value of 2.34%, 0.7 and 9.5×10-3 respectively. For the 100%GGBS/20%SF mixes, the singular modelling variable FW/A ratio produced the most accurate strength predictions with average error, adjusted R2 and significance, f values of 5.8%, 0.77 and 5.8×10-5 respectively.

Based on these findings, regression analysis of multiple mix parameters has provided a novel approach for AA/GP strength predictions; albeit that the models presented in Table 3 are only valid for mixes with activator to binder ratios appropriate to ensure full geopolymerisation. Moving forward, future development is clearly required, however, to improve model accuracy and significance by expanding their remit to encompass broader ranges of binder compositions.

**Conclusions**

The goal of the work reported in this paper was to develop mix design methodologies capable of reliably producing potassium silicate-activated geopolymer mortars – based on MK and a range of industrial by-products – with specified levels of strength, flow and/or embodied carbon content. In this way, the broader aim of the work was to facilitate adoption of alkali-activated and geopolymer cement systems as low impact replacements for conventional PC-based building components.

For a given geopolymer mix design (i.e. constant binder, water and activator contents), the influence of binder composition on the resulting reactions and corresponding values of strength gain has been shown to be significant. High performance AA and GP mortars were developed, exhibiting high flow and 7 and 28-day strengths of up to 87 and 106 N/mm2 respectively; the latter using a binder system comprising 100% by-product materials. Indeed, many of the highest performing mortars investigated had embodied CO2 binder levels around 30% lower than corresponding PC-based mixes when the activating solution is taken into account. This is deemed to be a major benefit of geopolymers, where a broad range of structural performance levels can be attained using various combinations of, ideally, locally available, low impact binders. Further improvements to performance are possible for geopolymer mixes via further adjustments to mixture proportioning parameters, such as the mass of activating solids, as these are the costly component and levels are unnecessarily high in binders without MK. While the CO2 savings reported in this paper are modest compared to some published in the literature (Davidovits, J (b) 2013), if geopolymer systems were used to replace all PC-based materials, the theoretical reduction in total global carbon emission would be approximately 2.1% (Jones, 2011; Benhelal, 2013).

This study confirmed that the use of single proportioning ratios is not the optimum approach for accurate strength prediction and that combinations of mixture design parameters can have a bearing on performance. Of the single ratios studied, L/S ratio appeared to show the greatest correlation with strength, albeit that mixes with low L/S values did not consistently provide the greatest strength in the mix designs studied. Those with the lowest L/S ratios often also had the lowest A/B ratio, causing samples to be unable break down the binder powder sufficiently to form a homogenous geopolymer without unreacted materials acting as a microdefect. In MK based mortars, A/B ratios below 0.75 produced dry, sandy mortars with no cohesion due to the lack of activating solids present causing incomplete dissolution.

For the various sets of MK-, GGBS/MK- and GGBS/SF-based mortar mixes studied, a suite of regression models was developed to predict compressive strength at 7 days. With average prediction errors across the binder combinations considered below 5.8%, the methods developed were relatively successful and indicate potential for future improvements. Future research will focus on improving predictions by widening the range of mix parameters and compositions studied and increasing the data sets on which they are based. The ultimate aim is to develop a single model suitable for accurately predicting the performance of any geopolymer binder type.

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Table 1. Composition and environmental impact of source materials used in this study

Table 2. Phase II experimental design methodology and resultant 7-day strength results

Table 3. Regression statistics and formulas

Figure 1. Phase I mix design methodology

Figure 2. Ternary plots (a-c) of 7-day strength results and combined ternary plots of 28-day strength results and embodied CO2 (d-f)

Figure 3: Geopolymer proportioning ratios vs 7-day compressive strength

Figure 4. Relationships between 7-day strength and L/S ratio for various binder combinations

Figure 5. Relationships between flow and L/S ratio for a range of binder combinations

Figure 6. Indicative mix design worked example

Table 1. Composition and environmental impact of source materials used in this study

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Material | Chemical composition (% by mass) | | | | Embodied carbon (kgCO2/kg) |
| SiO2 | Al2O3 | CaO | Fe2O3 |
| PC | 20 | 4.6 | 64.6 | 3.8 | 0.73+ |
| MK | 55 | 40 | 0.3 | 1.4 | 0.33+ |
| GGBS | 36.5 | 10.4 | 42.4 | 0 | 0.083+ |
| SF | 96 | 0.8 | 0.5 | 0.8 | 0.064++ |
| FA | 57 | 24 | 3.9 | 6 | 0.008+ |
| IS | 27 | 3.2 | 1.8 | 46 | 0.057++ |

+ Jones, C. (2011); ++Values provided by Elkem and Aurubis

Table 2. Phase II experimental design methodology and resultant 7-day strength results

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Mix | Central composite design variables | | | | 7-day compressive strength (N/mm2) | | |
| A | B | C |  | Binder combination: + | | |
| 1 | 2 | 3 |
| 1 | -1 | -1 | -1 | 42.5 | 75 | 48 |
| 2 | -1 | 1 | -1 | 42 | 69 | 53.5 |
| 3 | 1 | 1 | -1 | 58 | 86 | 60 |
| 4 | 1 | -1 | -1 | - | 82.5 | 68.5 |
| 5 | -1 | 1 | 1 | 38 | 67.5 | 38.5 |
| 6 | 1 | 1 | 1 | 39 | 79 | 51 |
| 7 | -1 | -1 | 1 | 33 | 72 | 34.5 |
| 8 | 1 | -1 | 1 | - | 79.5 | 44.5 |
| 9 | 0 | 0 | 0 | 42 | 77.5 | 55.5 |
| 10 | 0 | 1 | 0 | 41.5 | 73.5 | 54.5 |
| 11 | 0 | -1 | 0 | - | 71 | 52.5 |
| 12 | -1 | 0 | 0 | 35 | 75 | 50.5 |
| 13 | 1 | 0 | 0 | 46.5 | 82.5 | 57 |
| 14 | 0 | 0 | -1 | 51 | 85 | 52.5 |
| 15 | 0 | 0 | 1 | 39 | 79 | 47 |
| +1: 100%MK; 2: 80%GGBS/20%MK; 3: 80%GGBS/20%SF | | | | | | | |

Table 3. Regression statistics and formulas

|  |  |  |  |
| --- | --- | --- | --- |
| Key modelling equation parameters identified | Coefficients | t Stat | P-value |

|  |
| --- |
| *Binder 1: 100%MK* |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Intercept | -94.36 | -2.31 | | 5.413x10-2 |
| Binder | 0.3073 | 3.981 | | 5.317x10-3 |
| Free water (FW) | -1.046 | -3.26 | | 1.385x10-2 |
| Free water/ Binder (FW/B) | 459.03 | 2.738 | | 2.899x10-2 |
| Free water/Activator (FW/A) | -13.51 | -0.48 | | 6.466x10-1 |
| **7-day strength =**  **-94.36 + (Binder\*0.3173) + (FW\*-1.046) +**  **(FW/A\*-13.51) + (FW/B\*459.03)** | | | *Adjusted R2 = 0.91*  *Significance, f = 1.9x10-3*  *Average error = 3.1%* | |

|  |
| --- |
| *Binder 2: 80%GGBS/20%MK* |

|  |  |  |  |
| --- | --- | --- | --- |
| Intercept | -33.88 | -0.15 | 8.844x10-1 |
| Binder | 0.4905 | 1.717 | 1.244x10-1 |
| Total water (TW) | -280.4 | -2.11 | 6.823x10-2 |
| Free water/Binder (FW/B) | -1153 | -2.23 | 5.631x10-2 |
| Free water/ Activator (FW/A) | -0.7 | -1.42 | 1.927x10-1 |
| S/A ratio | -168.8 | -2.6 | 3.156x10-2 |
| L/S ratio | 2554 | -2.412 | 4.235x10-2 |
| **7-day strength =**  **-33.88 + (Binder\*0.4905) + (TW\*-280.4) + (FW/B\*-1153) + (FW/A\*-0.7) + (S/A\*-168.8) + (L/S\*2554)** | | *Adjusted R2 = 0.70*  *Significance, f = 9.5x10-3*  *Average error = 2.3%* | |

|  |
| --- |
| *Binder 3: 80%GGBS/20%SF* |

|  |  |  |  |
| --- | --- | --- | --- |
| Intercept | 5.3752 | 0.343 | 7.373x10-1 |
| Binder | 0.1117 | 4.431 | 8.195x10-3 |
| Free water/Activator (FW/A) | -94.54 | -5.41 | 1.572x10-3 |
| **7-day strength =**  **5.38 + (Binder\*0.1117) + (FW/A\*-94.54)** | | *Adjusted R2 = 0.77*  *Significance, f = 5.8x10-5*  *Average error = 5.9%* | |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Material quantities (kg/m3) | | | | L/S ratio | Paste/sand ratio |
| Binder | Activator | Water | Sand |
| 542 | 453 | 134 | 1340 | 0.514 | 0.843 |

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Mix  no. | Binder composition: (% by mass) | | | |  |  |  | | --- | --- | --- | | Binder combination: | | | | A | B | C | | Fly ash | MK | GGBS | | Silica Fume | MK | GGBS | | Iron Silicate | MK | GGBS |   Binder A  Binder B  Binder C |
| Binder A | Binder B | Binder C |
| 1 | 0 | 100 | 0 |
| 2 | 0 | 80 | 20 |
| 3 | 20 | 80 | 0 |
| 4 | 20 | 60 | 20 |
| 5 | 0 | 60 | 40 |
| 6 | 40 | 60 | 0 |
| 7 | 0 | 40 | 60 |
| 8 | 60 | 40 | 0 |
| 9 | 20 | 40 | 40 |
| 10 | 40 | 40 | 20 |
| 11 | 40 | 20 | 40 |
| 12 | 20 | 20 | 60 |
| 13 | 60 | 20 | 20 |
| 14 | 0 | 20 | 80 |
| 15 | 80 | 20 | 0 |
| 16 | 0 | 0 | 100 |
| 17 | 100 | 0 | 0 |
| 18 | 20 | 0 | 80 |
| 19 | 40 | 0 | 60 |
| 20 | 60 | 0 | 40 |
| 21 | 80 | 0 | 20 |

Figure1. Phase I mix design methodology



Figure 2. Ternary plots of 7-day strength (a-c) and combined ternary plots of 28-day strength and embodied CO2 (d-f)



(a) (b) (c)

Figure 3. Silica/Alumina, Liquid/Solid and Activating solution to Binder powder ratios vs 7-day compressive strength



1. (b)

Figure 4. Relationships between 7-day strength and L/S ratio for various binder combinations



(a) (b)

Figure 5. Relationships between flow and L/S ratio for various binder combination



Figure 6. Indicative mix design worked example