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Predictive Optimisation Model for Commercial Geopolymer Cement Manufacturing

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Abstract

Our invention/paper relates to the use of a kaolin source material that is mixed with a pozzolanic material in the absence of water, to form a geopolymer cement binder material. It relates to the industrial scale processes that these two major materials go through as they are prepared by special manufacturing processes to obtain optimised raw material constituent materials first and then when they mixed by large scale/commercial processes to obtain products of uniform quality. A geopolymer cement product capable of achieving a compressive strength of 104 Mpa with a compressive strength after a chemical attack of 100.74 Mpa and a thermal expansion of 0,2mm can be achieved after producing the input raw materials into this GPC cement at a Pyro processing temperature of 681 Degrees Celsius resulting in an aluminium material phase of 4.01 and silica to alumina ratio of 2.26. This product should be ground to a particle surface area of 6863 parts/cm^2 with an alkali activator of 18,78%.

Keywords: metakaolin; pozzolanic materials; geopolymer cement; material phase; optimisation

Introduction

Different Geopolymer inputs have different physical and chemical characteristics depending on source or process from which they are made [8, 2, 4]. High physical and chemical quality variability of materials even from the same source were noticed due to variations within raw material sources [1, 3]. Different grindability of materials means different particle sizes for various materials in same product after grinding [5]. Current Pyro-processing and Grinding process has limitations to achieve same particle size after grinding for optimized chemical reaction [12]. Product strength/Quality can only be determined after hydration. - (Destructive Testing) [9, 6, 7]. Current manufacturing process/system has a poor response to rapid changes in raw material quality and process conditions. (Rigid Manufacturing Processes) [1]. Current manufacturing processes producing product that is economically incompetent and is only used for specialised applications [8, 10, 11]. Poor Early Day Strength Statistical Compliance and product rejection by structural engineers despite having better characteristics after 28 Days of natural curing [9, 13, 14].

Methodology

The following methodology was used in the development of the geopolymer cement production model.

1. process that are critical to the model development were identified.
2. process and quality ranges for these identified inputs processes/parameters were determined.
3. the desired GPC product outcomes were fixed within prescribed output limits.
4. the processes are then allowed to run in the algorithms and the optimised results are recorded.

silica/alkali ratio

Raw material chemistry the following results were obtained after inputs geopolymer materials are selected and mixed to produce the desired silica/alumina ratios in the material chemistry after an XRF-analysis of the inputs is done. they are then ground to the required surface area by a ball mill that also acts as a mixing tool. further mixing is done by a blending system for 4 hours that allows the particles to be uniformly distributed. the required final blending ration for the input materials is 1. this means the material chemistry quality of successive samples is the same. it therefore guarantees the availability of all the required mineral elements to be in close proximity to each other at the time of reaction.

alkali

The alkali of potassium or sodium hydroxide is used to activate the process. it is also used to balance the charges during the reaction processes. it initiates the reaction between the silica and alumina molecules during the geopolymerisation process. A 1molar solution of potassium or sodium hydroxide was used at mass ratios of between 12% to 20% of total expected geopolymer mass.

Pyro processing temperature

The pyro processing temperature is important in the model because this temperature determines the material phase that is obtained by the alumina and silica components. the objective is to get these two main elements to be in the best reactive state as possible. the higher the alumina and silica phase state they will be the more reactive and hence the better the strength development of the final finished GPC product. this temperature is controlled in the kiln or metakaolin preparation phase. the silica is also subjected to this process so that it gets activated and converts the non-reactive silica at room temperature to activated silica at the optimised pyro processing temperature. the maximum pyro processing temperature that is used in the preparation of the metakaolin is used i the material quality identification and naming, i.e. mk 750, mk 850 denotes the operating temperature of 750 degrees Celsius or 850 degrees Celsius respectively, at which the metakaolin was formed and quenched at. a temperature range of between 400 and 850 degrees Celsius was used for this experiment. temperatures above 850 degrees are characterised by a creation of sintered materials. these materials are unreactive as the reactive components would have already combined during the sintering process. they are therefore not ideal for the geopolymerisation processes.

Material phase

The material phase is determined by the maximum pyro processing temperature that is reached during material preparation. it is also influenced by the quenching method that is used. rapid air cooling is preferred to get the metakaolin and silica into the amorphous phases. for aluminium the phases range from al 2+ to al 5+. the +5 phase is the most unstable of the phases and hence the most reactive. sor silica, the most reactive phase is the silica 4 + phase. this instability in molecular structure induced by the temperature as it activates/excites the atomic structure is what provides the reactivity required for improved strength development. the method of cooling or quenching is also very important. when the materials are rapidly cooled, the materials are not given enough time to change their phases to the more stable states when crystallisation is allowed to proceed slowly. blasts of cold air are used quench these materials in the amorphous states that we require for maximum reactivity. so ideally the most reactive states of these materials that can be obtained at room temperature is required for the purposes of our experiment. the remainder of the crystallisation process is then

allowed to proceed when the strength development process is initiated.

surface area

The surface area of the reacting elements has a direct bearing on GPC compressive and tensile strength development and the minimum temperature that is required to activated the geopolymerisation process. the finer the input raw materials the lower the temperature requirements and also the stronger the finished GPC product that is formed. surface area ranges of 5800 to 7000 ppm/cm^2 were selected for this experiment. to achieve this fine surface area, a special high speed hammer crusher was developed to attain this very fine Blaine. this is because the current existing crushing methods cannot sustainably crush to this required fitness in a cost-effective manner. current processes have very high specific energy requirements as shown in the power consumption comparison.so a model that produces geopolymer cement of a specified compressive strength range of between 100mpa and 104mpa, a chemical resistance percentage of between 98% and 100% and a thermal expansion of between 0.2 and 1.2 % was developed. this was achieved after controlling the pyro processing temperature between 400 and 850 degrees Celsius, a alumina material phase in metakaolin of between 2+ and 5+, with geopolymer cement surface area between 5800 - 7000ppm/cm^2. the alkali activator of between 12 and 20% was used with the material chemistry having a silica/alumina ratio of between 2 and 2.4.

Control logic Schematic Diagram

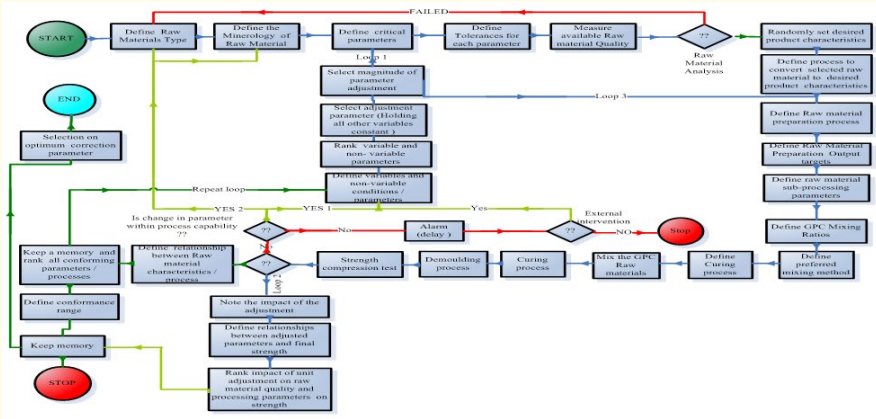


Figure 1: Control Logic Schematic Diagram.

Model System Equations

Equation 1: Pyro processing Temperature

$$\textit{Pyro-processing Temperature} = +2675.79 + 4.24A - 23.88\,B - 147.05\,C \quad (1)$$

Equation 2: Material Phase

$$\text{Material Phase} = +24.11 - 0.025\,A - 0.17\,B - 1.11\,C \quad (2)$$

Equation 3: GPC Surface area

$$\textit{GPC Surface area} = -12128.83 + 113.50\,A + 71.39\,B - 14.53\,C \quad (3)$$

Equation 4: Silica/Alumina Ratio

$$\textit{Silica/Alumina Ratio} = 2.47 - 0.00043\,A - 0.0014\,B - 0.046\,C \quad (4)$$

Equation 5: Alkali

$$Alkali = -44.32 + 0.038\ A + 0.59\ B - 1.065\ C \quad (5)$$

Where:

A = Compressive Strength.
B = Chemical Resistance.
C = Thermal Expansion.

overview design of the cement plant

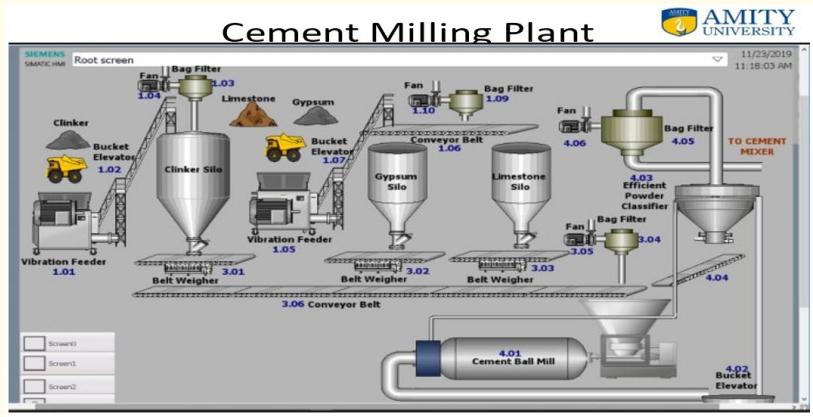


Figure 2: The Scada system design of the cement plant.

Results

The following results were obtained after a series of tests were done 20 (tests in total). these results show the required control parameters at which the geopolymer manufacturing process should be operating at to produce the desired or predetermined geopolymer cement that has the ability to produce the desired compressive strength, the desired acid resistance and the desired thermal expansion. The Table 1 shows the test data and the results obtained from each set of results.

Discussion of results

Results in fig 1 show 2D surfaces response of model parameters that GPC surface area, pyro processing temperature, alkali, silica and alkali ratio, desirability, material phase.

Std	Run	Factor 1 A: Accomp Strength Mpa	Factor 2 B: Chemical resistance Mpa	Factor 3 C: thermal expansion %	Response 1 Pyro process-ing Degrees Celsius	Response 2 Material Phase Number	Response 3 GPC Surface area Parts/cm2	Response 4 Silica/Alkali Ratio Number	Response 5 Alkali %
13	1	102	100	-0.274986	850	5	6500	2.3	20
4	2	104	102	0.1	800	5	7000	2.2	19
1	3	100	98	0.1	750	5	6500	2.3	20
3	4	100	102	0.1	700	4	6750	2.4	19
2	5	104	98	0.1	650	4	7000	2.3	18
17	6	102	100	0.65	600	4	7000	2.1	19
14	7	102	100	1.57499	550	3	7000	2.2	20
7	8	100	102	1.2	500	3	7000	2.2	17
15	9	102	100	0.65	450	2	7000	2.3	18
20	10	102	100	0.65	400	2	7000	2.4	19
8	11	104	102	1.2	400	2	7000	2.4	20
10	12	105.364	100	0.65	450	2	6900	2.4	20
9	13	98.6364	100	0.65	500	3	5800	2.3	17
5	14	100	98	1.2	550	3	5900	2.3	18
12	15	102	103.364	0.65	600	4	6200	2	19
16	16	102	100	0.65	650	4	6100	2.4	20
19	17	102	100	0.65	700	4	6300	2.1	15
11	18	102	96.6364	0.65	750	5	6200	2.13	13
18	19	102	100	0.65	800	5	6000	2.15	12
6	20	104	98	1.2	850	5	6400	2.12	13

Table 1: Shows the test data and the results obtained from each set of results.

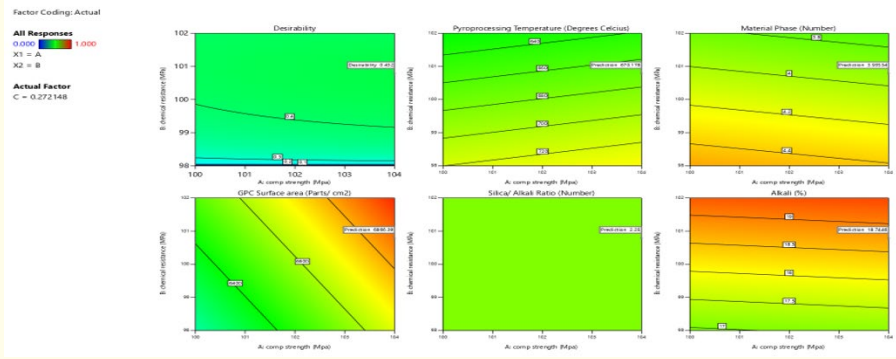


Figure 3: 2D Surface Response of the model parameters.

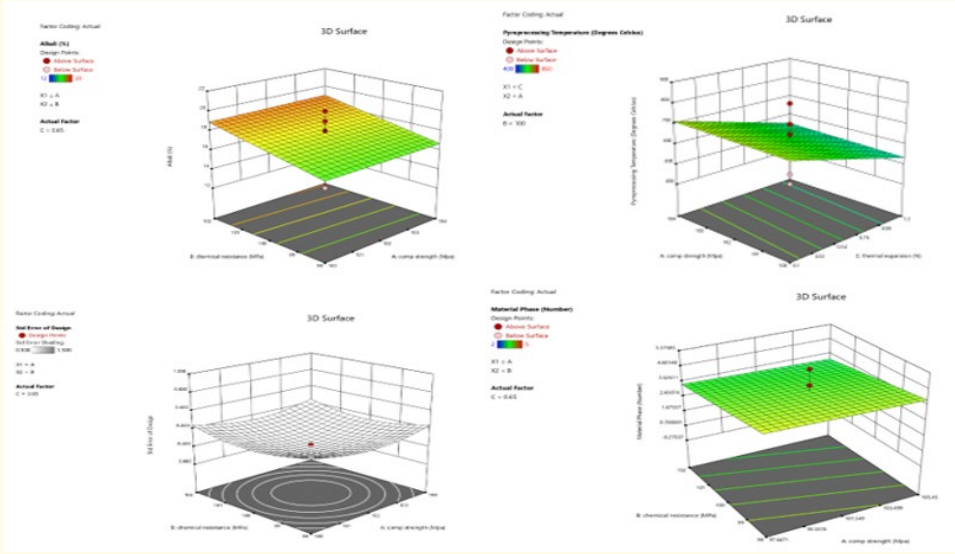


Figure 4: Summary of results.

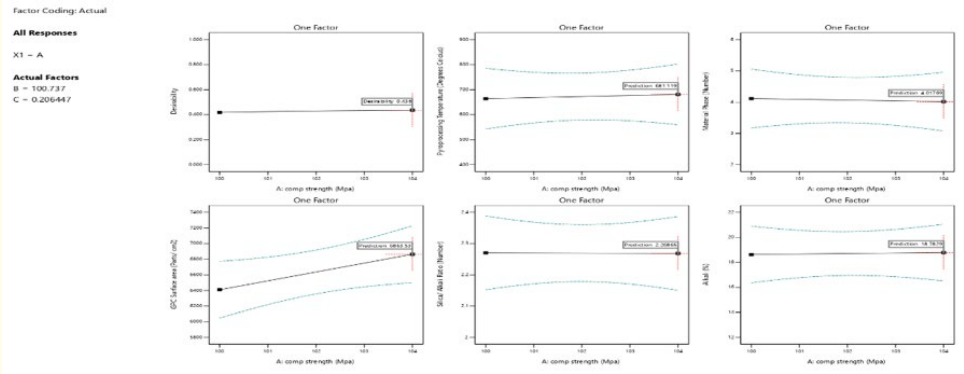


Figure 5: 3D Surface Response for Model parameters.

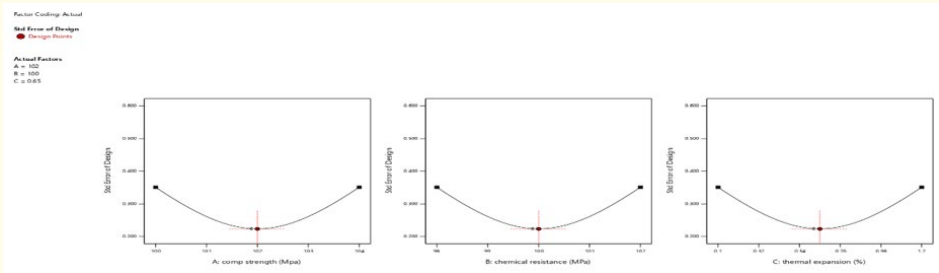
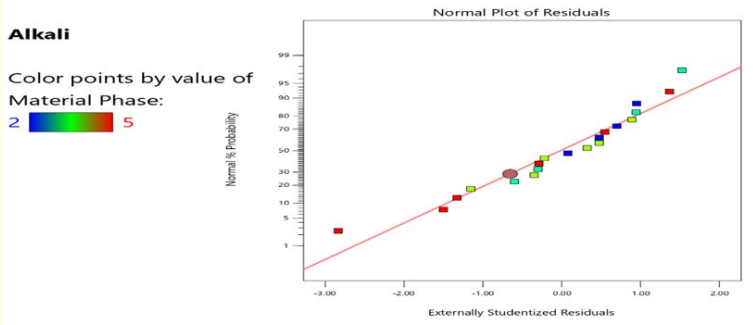


Figure 6: Standard error designs comp strength, chemical resistance, thermal expansion.



Pyro processing temperature

The temperature data obtained had a standard deviation of 134, a mean of 625 and a co-efficiency of variance of 21.58.

The optimum pyro processing temperature is given by the equation below

Pyro processing temperature = +2675.79 + 4.24 *comp strength* -23.88 *chemical resistance* -147.05 *thermal expansion*.

Material phase

The equation below is used to define the material phase of the geopolymer cement.

Material phase = +24.11 -0.02 *compressive strength* - 0.17 *chemical resistance* -1.11 *thermal expansion*

The model produced geopolymer cement with an alumina material phase of 3.7, coefficient of variance of 28, standard deviation of 1.04 and a root mean square of 0.936.

The equation in terms of actual factors can be used to make predictions about the response for given levels of each factor. Here, the levels should be specified in the original units for each factor. This equation should not be used to determine the relative impact of each factor because the coefficients are scaled to accommodate the units of each factor and the intercept is not at the centre of the design space.

GPC surface area.

Gpc surface area = -12128.83+ 113.50 comp strength +71.39 chemical resistance -14.53 thermal expansion.

The model produces surface area with a mean of 403cm^2/g, a standard deviation of 403, a coefficiency of variance of 6.14 with a root mean square of 0.86.

Silica/alumina ratio

Silica/alumina ratio = 2.47 -0.0004 *compressive strength* -0.0014 *chemical resistance* -0.0464 *thermal expansion*

The equation in terms of coded factors can be used to make predictions about the response for given levels of each factor. By default, the high levels of the factors are coded as +1 and the low levels are coded as -1. The coded equation is useful for identifying the relative impact of the factors by comparing the factor coefficients.

Alkali

$$Alkali = -44.32 + 0.04\ comp\ strength + 0.59\ chemical\ resistance - 1.07\ thermal\ expansion$$

The equation in terms of actual factors can be used to make predictions about the response for given levels of each factor. Here, the levels should be specified in the original units for each factor. This equation should not be used to determine the relative impact of each factor because the coefficients are scaled to accommodate the units of each factor and the intercept is not at the centre of the design space.

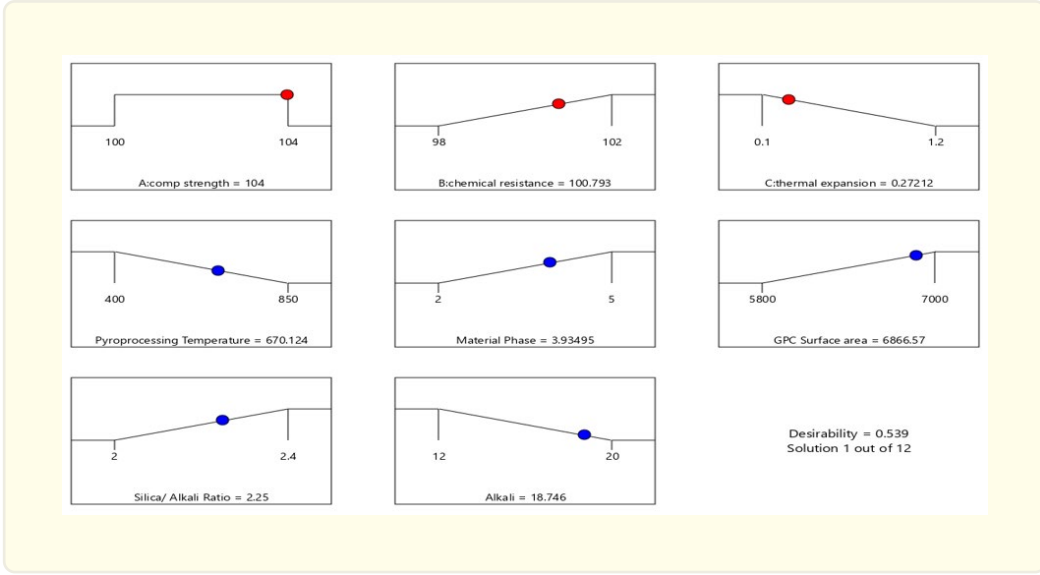
$$Silica/alkali\ ratio = +2.25 - 0.0009a - 0.0028b - 0.0255c$$

Were

A = compressive strength.
B = chemical resistance.
C= thermal expansion.

The model produces geopolymer cement at an optimised silica/alkali ratio with a mean of 2.25, a coefficiency of varience of 5.82, a standard deviation of 0.013 and a root mean square of 0.91.

Summary of Results



The geopolymer model developed produced a geopolymer cement with a compressive strength of 104 Mpa, with a chemical resistance of 100.79, a thermal expansion of 0.27212 with a surface area of 6866 cm^2/g. a pyro processing temperature of 670 degrees is required on the materials and an alumina material phase of 3.93, a silica to alumina ratio of 2.25, an alkali ratio of 18.746 at a surface area of 6866 cm^2/g.

Conclusion

From the research done it can be safely concluded that geopolymer cement material can be successfully produced under optimized conditions to produce a cement that has improved strengths of up to 104 Mpa with very low thermal expansion, very good chemical resistance using very cheap raw materials and a less heat intensive system as compared to the current limestone based cement which gives an Ordinary Portland Cement target strength of 52.5 Mpa.

References

1. Otto Labahn. “Cement Engineers Handbook”. 2nd Edition.
2. C Yeh. “Generalization of strength versus water-cementitious ratio relationship to age”. Cement and Concrete Research 36.10 (2006): 1865-1873.
3. Fernando Castro. “Employment of sodium aluminate waste solutions for the processing of fly-ash based geopolymers containing industrial wastes”. Geopolymer Camp (2017).
4. A Guilladucii., et al. “Artificial additions for cement: Reproduction in Laboratory of Fluidised Bed Ash”. Procedia Materials Science 9 (2015): 285-291.
5. H Wang, H Li and F Yan. “Reduction in wear of metakaolinite-based geopolymer composite through filling of PTFE”. Wear 258.10 (2005): 1562-1566.
6. RE Lyon., et al. “Fire resistant aluminosilicate composites”. Fire Mater 21.2 (1998): 67-73.
7. J Davidovits. “Geopolymers — inorganic polymeric new materials”. J. Therm. Anal 37.8 (1991): 1633-1656.
8. A Palomo., et al. “Chemical stability of cementitious materials based on metakaolin”. Cem. Concr. Res 29.7 (1999): 997-1004.
9. P Duxson, GC Lukey and JSJ van Deventer. “Thermal conductivity of metakaolin geopolymers used as a first approximation for determining gel interconnectivity”. Ind. Eng. Chem. Res 45.23 (2006): 7781-7788.
10. Basil S Al-Shathr, Tareq S Al-Attar and Zaid A. “Optimization of Geopolymer Concrete Based on Local Iraqi Metakaolin”. The Second International Conference on Buildings, Construction and Environmental Engineering (2015).
11. Metwally abd allah Abd elaty. “Compressive strength prediction of Portland cement concrete with age using a new model”. HBRC Journal 10.2 (2014): 145-155.
12. Provis, John L., and Jan Stephanus Jakob Van Deventer, eds. “Geopolymers: structures, processing, properties and industrial applications”. Elsevier (2009).
13. Ali Nazarin and Jay G Sanjayan. “Modelling of compressive strength of geopolymer paste, mortar and concrete by optimized support vector machine”. Ceramics International 41.9 Part B (2015): 12164-12177.
14. Provis, John L., and Jan Stephanus Jakob Van Deventer, eds. “Geopolymers: structures, processing, properties and industrial applications”. Elsevier (2009).