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Application of Response Surface Methodology in Predicting and optimizing the properties of Concrete containing Ground Scoria and Metakaolin blended Cement in Concrete

Abubakar Sabo Baba[1,*], Auwal Abdullahi Umar[1], Aliyu Abubakar[2], Terlumun Adagba[1]

[1] *Federal University Dutsinma, Department of Civil Engineering, Nigerai, (asbaba1@fudutsinma.edu.ng; aaumar1@fudutsinma.edu.ng; tadagba@fudutsinma.edu.ng.)*

[2] *Abubakar Tafawa Balewa University Bauchi, Department of Civil Engineering, Nigeria, aabubakar24@atbu.edu.ng.*

Abstract

The effect of Metakaolin and ground Scoria on various properties of concrete were investigated and optimised using Response Surfaces Methodology (RSM) in this study. Seven batches of concretes were cast at water to cement ratio of 0.5 and 5% fixed Metakaolin with 0, 5, 10, 15 and 20% Ground Scoria replaced cement. The resulting concrete then was tested for Slump. The Concrete cubes were cast and cured for 3, 7, 14, 28 and 60days before Water absorption and Compressive strength test were carried out. at all replacement levels of Metakaolin/Scoria content, Workability, Water absorption, Density and Compressive strength decreased when compared with the control concrete. However, Water absorption, Density and Compressive strength slightly increased with increase in curing age. The models developed were quite accurate as the percentages of error were in a good agreement and can explain the variability in Metakaolin/Ground Scoria concrete. Numerical method of optimisation was applied to determine the optimum mix proportions for Metakaolin/Ground Scoria. The optimum mix of concrete was obtained by addition of 8.60% GS after curing for 12-days with 0.8 desirability. Based on the result of optimisation, incorporating the optimum values of 13.6% (5%MK+8.6%GS) metakaolin and ground Scoria in concrete as cement substitute for every one kilogram of cement, can potentially result in reduction of CO2 emissions by 0.07-0.1224kg.

Keywords: *Optimization, Concrete, Response Surfaces, Metakaolin, Ground Scoria.*

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I. INTRODUCTION

Infrastructural development is the key indicator of level of growth and prosperity of any country. Concrete is major material used in construction of infrastructure such as Dams, Roads, Bridge, shelter and related amenities. Cement, a key ingredient of concrete production is the most expensive part in concrete and emit significant amount of CO2 to the atmosphere during its production, contributing to the environmental pollution [1]. This CO2 emission resulting from clinker production is a major concern to the environment. CO2 is a by-product of a chemical conversion process used in the production of clinker, a component of cement, in which limestone ($CaCO_3$) is disintegrated in the presence of heat to form lime and carbon dioxide [2]. In addition, CO_2 is also emitted during cement production by fossil fuel combustion. It is estimated the Carbon dioxide (CO_2) emission due to the cement production alone account for about 26% of the total industrial emissions [3]. For every one ton of Portland cement produced, 4000MJ of energy is used which result in discharge of about 800Kg of CO_2 to the atmosphere [4].

One way to minimise the excessive emission of greenhouse gases such as CO_2 which results in global warming with serious negative consequences to the environment is to reduce the amount of cement used in the construction industry, by use of alternative material to cement in concrete. consequently, the high energy consumption, greenhouse gas emission and high cost of cement has led researchers to use supplementary cementitious materials (SCMs) called pozzolanas to replace cement in concrete which improves the performance and lowers the cost of building material [5].

A large and growing body of literature have investigated the addition of SCMs to improve the performance of concrete such as: fly ash [6], ground granulated blast [7], silica fume [8], Calcined Termite mould [9], Pulverized Animal Bone and Animal Bone Ash [10], Metakaolin and Ground Scoria [11] etc. The use of SCMs in concrete has among other benefit of improving concrete properties such as workability, durability, strength, and low heat of hydration in concrete [11].

Metakaolin is produced by the calcination of kaolinite clay at temperature between 650℃ to 900℃ [11]. After the burning process is completed and allows cooling at room temperature, it grinds and sieves to desire fineness of 700 to 900 m^2/g [12]. It is capable of modifying the properties when added in concrete through conversion of calcium hydroxide in the cement paste to cementitious compound increasing the strength and reducing the permeability of concrete by refinement of the pore structure [12], [13] and also minimizing the autogenous shrinkage at early ages [14].

Scoria is a rock of volcanic origin which deposits can be found around volcanoes in many parts of the world [11]. Scoria can be found in Nigeria along the eastern part of Nigeria-Cameroon volcanic line in abundance in part of Jos and Biu Plateaus [15]. Scoria is porous, reddish or black in colour, lightweight and Pozzolanic when grinded to fine powdered [16], [11] and [17]. This paper reports the optimisation of metakaolin and Scoria substituted cement in concrete by application of response surface methodology (RSM).

The response surface methodology (RSM) consists of a collection of statistical and mathematical techniques applied for empirical model creation [18]. It is a sequential procedure that uses design of experiments (DOE) to minimise variances, least square method for empirical model fitting and application of desirability approach of Optimisation in the development, improvement, and process management in various industries [19].

The used of traditional experimental design method of one factor at a time to evaluate the influence of factor on different properties at different factor levels, results in large number of experimental runs, this is expensive and time consuming. RSM is robust experimental design tool capable of reducing the number of experimental runs; obtain an appropriate mathematical model and a highly effective tool for data analysis and interpretation, allowing efficiency and economy in the experimental process and scientific objectivity in the conclusions [20]. Researchers have used RSM modelled and optimise the properties of concrete containing admixtures.

[21] Have shown RSM as an effective tool for predicted the strength properties of concrete containing Calcined Black Cotton Soil (CBCS). Face-centered central composite design method of RSM with calcined Black Cotton Soil and curing age as independent variables was used in the experimental design. All the response surface models developed for water absorption, density and compressive strength were analysed at 95% level of significance. The models were accurate showed very good relationship between the variables and the responses with coefficients of determination, $R^2 > 0.94$.

[10] Have used RSM to developed models for prediction of mechanical properties of pulverized animal bone (PABAC) and animal bone ash (PABAC) replacement as cement in concrete. Face-Centred Central Composite Design (FCCCD) approach in RSM was used to design the experiment and Analysis of variance test (ANOVA) was utilised in accessing the statistical significance of the developed models. Based on ANOVA all the models were statistically significant at 95% level of significant and it was concluded that percentage of (PABC), percentage of (PABAC) and curing period can used as variables to predict the mechanical properties of PAB/PABA concrete which is economical and environmentally friendly.

II. MATERIAL AND METHOD

2.1 MATERIALS

A. Water

Tap water fit for drinking was used in the study; no test was conducted on the water.

B. Cement

Ashaka Portland cement was used in the study, claimed by the manufacturer having a specific gravity of 3.15, Bulk density of 1475 Kg/m^3, moisture content of 0.9% and PH value of 12.40. The oxide composition values of the Cement and other materials utilized as binders in this study are as shown in table 1.

TABLE 1: OXIDE COMPOSITION OF ASHAKA PORTLAND CEMENT, MK AND GS

Compounds	Values (%)		
	Cement	MK	GS
SiO_2	19.258	67.83	42.55
Al_2O_3	5.728	18.60	13.24
Fe_2O_3	2.380	1.15	11.87
CaO	62.238	1.71	10.24
Mn_2O_3	0.161	0.03	0.18
Na_2O	0.129	0.13	1.68
MgO	0.569	0.41	0.18
K_2O	0.955	0.67	0.67
SO_3	2.194	0.04	0.15
TiO_3	0.283	1.86	2.36
P_2O_5	0.193	0.08	0.58
Cl	0.006	--	--
LOI	--	6.12	4.08

C. Fine aggregate

The fine aggregate used was obtained from local supplier in Bauchi, Bauchi State Nigeria. The tests carried out on fine aggregate are specific gravity, bulk density and particle size distribution. The tests were conducted in accordance to [22], [23] and [24] specifications respectively. The test results are presented in Table 2.

D. Coarse aggregate

Coarse aggregate was procured from Triacta quarry site along Dass Tafawa Balewa road Bauchi State Nigeria. The physical properties of coarse aggregates determined were bulk density, specific gravity, particle size distribution, water absorption, aggregate impact value, and aggregate crushing value tests. The tests were conducted in accordance to [23], [22], [24] and [25] respectively. The test results are presented in Table 2.

TABLE 2: PHYSICAL PROPERTIES OF FINE AND COARSE AGGREGATES

Properties	Fine aggregate	Coarse aggregate
Specific gravity	2.64	2.66
Bulk density (Kg/m^3)	1525	1518
AIV (%)	-	14.95
ACV (%)	-	14.47
Water absorption (%)	-	0.15
Moisture content (%)	0.43	-

E. Ground Scoria (GS)

Natural volcanic scoria lumps deposits were collected from Kerang District of Mangu Plateau state Nigeria. The Scoria was then crushed manually using hammer in the size 2 to 10mm grind into powder using grinding machine and sieve through 150µm sieve. The tests conducted on the GS ware: specific gravity, pH and oxides composition determination using X-ray fluorescence (XRF) test in accordance with procedure in [26], and [27] specifications respectively. The test result indicates specific gravity of 1.74 and pH of 7.8. The XRF test result is presented in Table 1. From the table, the sum of silica (SiO_2), alumina (Al_2O_3) and iron oxide (Fe_2O_3) is 67.66%. For a suitable pozzolanas, ASTM C618 recommends the sum of the three oxides as weight percentage is required to have minimum value of 70%. Constant 5%MK of cement equivalent was added to supplement for the deficit in oxides [11].

F. Metakaolin (MK)

The metakaolin used in the study was obtained by procured Kaolin from Duguri, Alkaleri along Gombe-Bauchi Bauchi state Nigeria. It was calcined in a kiln to obtained metakaolin at about temperature band 650ºC to 900ºC. After cooling, the calcined Kaolin is grinded and sieved through 75µm sieve to obtained fine Metakaolin. Test results show specific gravity 2.78 and pH 7.6. The XRF test result is presented in Table 1.

2.2 Methods

2.2.1 Concrete Production and Specimens Testing

The normal concrete mix of 1:2:3 (grade 25) with water to cement ratio of 0.5 was used for cement production at fixed 5% MK and five levels of GS replacing cement by weight at 0, 5, 10, 15 and 20%. The calculated quantities of the concrete materials based on the mix ratio are used for batching. Concrete cubes of 100mm x100mm x 100mm sizes were cast and water cured for 3, 7, 14, 28 and 60 days before testing, as in the procedures of [28].

2.2.1 Experimental Design

The data utilized in this study were generated without the use of design of experiment method (DOE). Therefore, the data was analyzed based on the Historical Data Design (HDD) of the Design Expert Software. HDD provide the experimenter with flexibility to input number of factors, responses and data lines of existing data that were previously generated without the use of RSM design of experiment (DOE) method and are outside the control of the researcher [29], [30] and [31]. Ground Scoria at (5, 10, 15, and 20%) and curing age of (3, 7, 14, 28 and 60-days) are the input variables as presented in the Table 3. Table 4 presents input variables, responses, units and data ranges, the independent variables are represented as X1 and X2, while Y1, Y2, Y3 and Y4 represent the water absorption, density, compressive strength and flexural strength respectively.

TABLE 3: INPUT VARIABLES, RESPONSES, UNITS AND DATA RANGES

Designation	Data band
Ground Scoria (GS)	$5 \leq X1 \leq 20$
Curing age (days)	$7 \leq X2 \leq 60$
Water absorption (%)	$0.9 \leq Y1 \leq 3.23$
Density (Kg/m^3)	$1905 \leq Y2 \leq 2378$
Compressive strength (N/mm^2)	$6.12 \leq Y3 \leq 28.90$

TABLE 4: DETAILS VARIABLES COMBINATIONS, TEST RESULTS OF WATER ABSORPTION (%), DENSITY (KG/M^3) AND COMPRESSIVE STRENGTH (N/MM^2)

S/NO	A (X1)	B(X2)		Test results	
	SC (%)	CP (days)	W_a (Y1)	D_s (Y2)	C_S (Y3)
1	0	3	1.83	2378	7.45
2	5	3	1.52	2309	14.60
3	10	3	1.27	2256	15.99
4	15	3	1.26	2206	8.98
5	20	3	0.99	2156	6.12
6	0	7	2.83	2345	10.30
7	5	7	2.63	2269	16.50
8	10	7	2.74	2243	18.99
9	15	7	1.54	2143	12.76
10	20	7	1.47	2102	8.21
11	0	14	2.95	2324	16.56
12	5	14	2.72	2212	20.20
13	10	14	2.78	2198	22.56
14	15	14	1.98	2156	14.67
15	20	14	1.65	2065	10.51
16	0	28	3.08	2267	21.86
17	5	28	2.82	2123	23.80
18	10	28	2.85	2122	25.57
19	15	28	2.08	2097	17.23
20	20	28	1.98	1987	13.87
21	0	60	3.23	2208	24.60
22	5	60	2.98	2056	25.80
23	10	60	2.94	2002	28.99
24	15	60	2.67	1955	18.69
25	20	60	2.24	1905	14.56

III. III RESULTS AND DISCUSSIONS

3.1 Workability (Slump)

Slump test was used to measure the workability of the fresh concrete in accordance with the specifications in [32]. The result of slump values are presented in Table 4 and depicted in Figure 1. It can be seen from the figure, workability decreases with increase in GS replacement. This can be attributed to the low specific gravity of GS, 1.7 substituting cement with higher specific gravity, 3.15 resulting in more GS been added since the mix proportion is rational agreeing with the findings by [21]. [33] Reported addition of 5 to 10% MK in concrete mixture result in concrete with slightly higher slump than the control concrete. Result of slump value test result is presented in Table 5.

TABLE 5: RESULT OF SLUMP VALUE TEST

Designation	0%MK0%GS	5%MK0%GS	5%MK5%GS	5%MK 10%GS	5%MK 15%GS	5%MK 20%GS
Slump (mm)	85	70	60	48	33	20

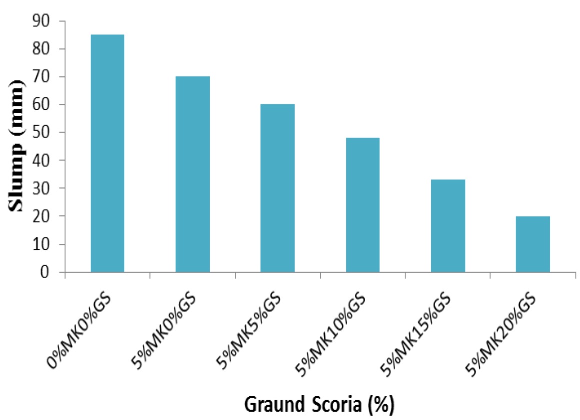


Figure 1: Slump (mm) of concrete against GS (%) contents

3.2 Modeling

The relations between factors and the responses water absorption; density and compressive strength were evaluated with the aid of the Design Expert software. Due to the nature of the dataset where each factor was varied individually, model fitting was performed by applying Backward Elimination Regression techniques with significance level alpha to remove, $\alpha = 0.1$. In Backward elimination techniques, all the model predictors are entered into the model. It then starts sorting out with the weakest predictor (model terms) and eliminate them one by one in every step. Regression is run until there is no any predictor which did not meet the specified condition of alpha to remove [33].

The model statistics summary for all responses is presented in Table 6. Analysis of variance (ANOVA) provide the rational values Fisher value (F-value), probability of significance (P-value), coefficient of determination (R^2) and adjusted coefficient of determination (Ajust R^2) of which determine the consistency of the system. It can be observed from the tables, all the model F-values which is the ratio of regression mean square and mean square error, have $P<0.05$ indicating they are statistically significant at $\alpha=0.05$. Furthermore, additional check for goodness of fit on the models shows the models coefficient of determination have $R^2 \geq 0.79$ and Adjust $R^2 \geq 0.7650$. The R^2 are close to Adjust R^2 and close to unit in each case. For a good model R^2 and Adjust R^2 difference should be within 0.2 [33]. The entire model shows Adjust R^2 is within 0.2 of R^2, indicating they are good models. The models for water absorption, density and compressive strength can explain 79.44, 90.09 and 92.32; variability in the properties MK-GS concrete respectively. The agreeable correlation between the experimental and predicted values are evident of the goodness of fit of the models as shown in parity plots of Figure 2(c), 3(c) and 4(c). In all the figures, the plotted points are observed to cluster around the diagonal fit line.

The signal to noise ratios for the four models water absorption, density, compressive strength and flexural strength shows adequate signals to noise ratio as can be deduced from the tables as 16.97, 28.512, 22.80 and 0000 respectively. [34] Suggested for a good RSM model, at least signal to noise ratios of greater than 4 is recommendable. It can be observed the entire models have signal to noise ratio greater than 4, therefore the models can be used to describe the properties of MK-GS concrete. The final model equations in terms of actual factors are presented in Equation 1, 2 and 3.

The inter relationship between the design factors and the responses (properties) of MK-GS concrete was done and presented using 3D, contour and parity plots of RSM in Figure 2, 3 and 4. It was observed from Figure 2 (a-b) and 3 (a-b) that there is clear interaction effect between the factor GS and CP in the property water absorption and density. The properties decreases with increases in GS% replacement and slightly increases with curing ages. This finding is in agreement with the results of ANOVA.

The effect of the interaction between GS and CP on the compressive strength of the concrete is illustrated in Figure 4 (a-b) and parity plot in (c). It was observed that the lower the proportions of GS% the higher the compressive strength and the higher the increase in CP the higher the compressive strength. The shape of 3D response surface and the contour of compressive strength show a significant interaction between the factors, the 3D response surface is steep at one side and the contour curved. The curved contour lines are indicating nonlinear relationships between factors. This finding is in agreement with the results of ANOVA.

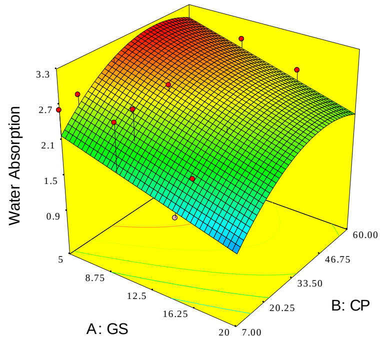
TABLE 6: SUMMARY OF MODEL STATISTIC FOR ALL THE RESPONSES

Responses	Type	R^2	Adjust R^2	P-value
Water absorption (%)	Quadratic	0.7944	0.7650	< 0.0001
Density (Kg/m^3)	Quadratic	0.9091	0.8961	< 0.0001
Compressive strength (N/mm^2)	Quadratic	0.9232	0.9030	< 0.0001

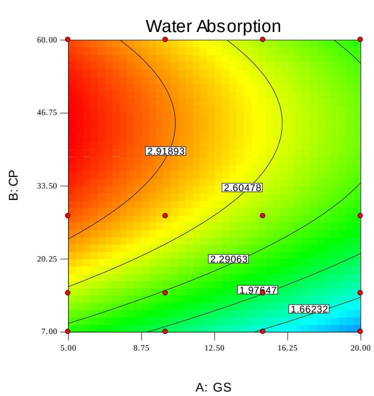
$$\text{Water-absorption}(\%)=+2.0800-0.0573GS+0.0614CP-7.1369CP^2 \quad \text{Eq.1}$$

$$\text{Density}(Kgm^3)=+2312.5937-11.5040GS-7.3359CP+0.0605CP^2 \quad \text{Eq.2}$$

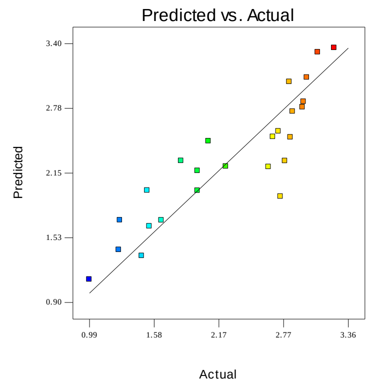
$$\text{Compressivestrength}(N/mm^2)=+7.5080+1.2905A+0.64792B6.7437GS.CP-0.0739GS^2-6.0366CP^2 \quad \text{Eq.3}$$



(a)

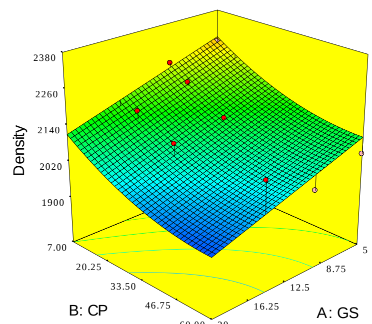


(b)

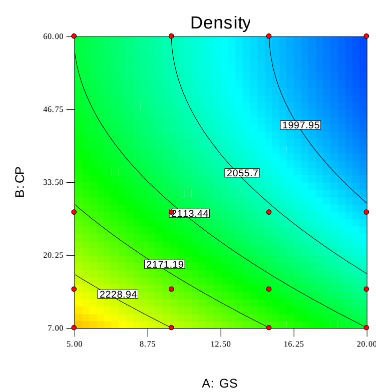


(c)

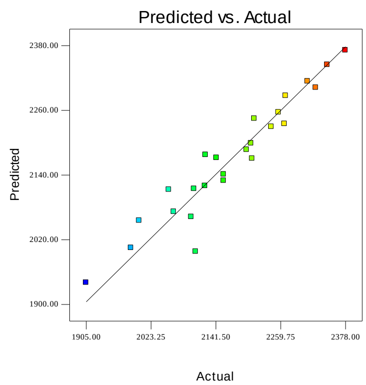
Figure 2: Response surfaces of 3D (a), contour (b) showing factors effect on the water absorption and parity plots (c).



(a)

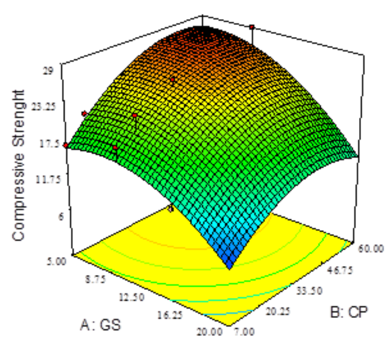


(b)

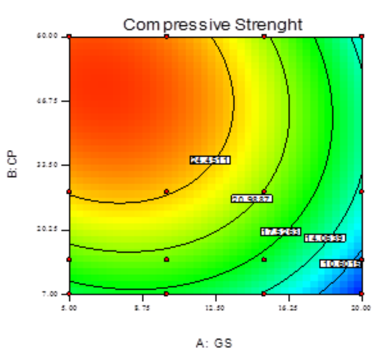


(c)

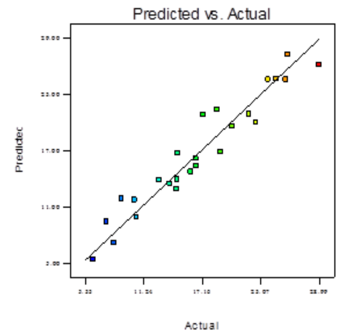
Figure 3: Response surfaces of 3D (a), contour (b) showing factors effect on the density and parity plots (c).



(a)



(b)



(c)

Figure 4: Response surfaces of 3D (a), contour (b) showing factors effect on the Compressive strength and parity plots (c)

3.3 Numerical Optimisation

The responses water absorption was minimized while density and compressive strength were maximized in range of values of factors studied. The goals and limits of the optimization are shown in Table 7. The optimum mix For Ground Scoria concrete was obtained by addition of 8.58% GS after curing for 11.75-days with 0.8 desirability as shown in the Ramp plot of Figure 5. The results obtained from the optimization are presented in Table 7.

Incorporating the optimum (5%MK+8.6%GS) 13.6% metakaolin and ground Scoria in concrete as cement substitute for every one kilogram of cement, can potentially result in reduction of CO2 emissions by 0.07-0.1224kg. [35] and [36] have reported for every 1Kg of cement produced, 0.5-0.9kg of CO2 is emitted into the atmosphere. Furthermore, it may improve sustainability by reducing the reliance on cement and enhanced performance of concrete since both MK and GS contribute to improvement in strength, durability, and workability of concrete, leading to longer lasting and more sustainable structures.

However, attempting to apply the optimized mix proportions from RSM to real-world construction projects may face with several potential challenges and limitations which include: variability in materials, site-specific conditions, practicality and feasibility, limited data points, time and resource constraints, expertise and training, stakeholder acceptance. Introducing optimized mix proportions derived from RSM may require convincing and gaining acceptance from various stakeholders, including contractors, clients, and regulatory authorities. Resistance to change and skepticism are both potential challenges faced when attempting to apply the optimized mix proportions Response Surface Methodology (RSM) to real-world construction projects.

TABLE 7: RESULT OF NUMERICAL OPTIMIZATION

Response	Limits	Goals	Optimum value
Ground Scoria (%)	5 - 25	In rage	8.50
Curing Age (days)	7 - 60	In range	11.75
Water absorption (%)	0.99 - 3.23	Minimize	2.25
Density (Kg/m^3)	1905 - 2378	Maximize	2218
Compressive strength (N/mm^2)	6.12 –28.99	Maximize	19.29

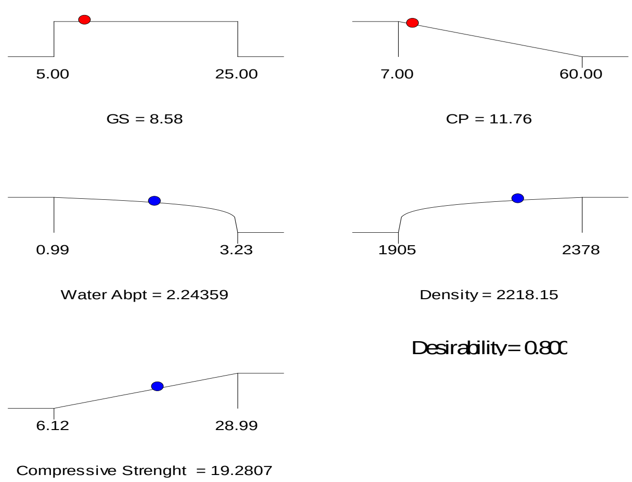


Figure 5: Ramp plot showing the optimum settings

IV. CONCLUSION

In this study, RSM was used to model the effect of substituting Metakaolin and ground Scoria with cement in concrete.

1. The effects of design factors on properties of concrete evaluated. The water absorption, density and compressive decreases with increase in GS% contents, and slightly increases with curing age.
2. The models for all four responses were statistically significant at a 95% confidence levels and all the p-value are less than α=0.05.
3. The optimum values of the responses were obtained by combining 8.58% GS and curing age of 12days with desirability of 0.8.
4. Incorporating metakaolin and ground Scoria in concrete, can potentially result in reduction of CO2 emissions by reducing the amount of cement needed, improved sustainability by reducing the reliance on cement and enhanced performance of concrete since both Metakaolin and ground Scoria contribute to improvement in strength, durability, and workability of concrete, leading to longer lasting and more sustainable structures.

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