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Application of Simplex-Centroid Design Methodologies to Optimize the Proportions of Ternary Cementitious Blends in High Performance Concretes

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ABSTRACT

High performance concrete (HPC) mixtures often contain multiple cementitious components. Optimizing the proportion of these individual components to achieve the desired properties is extremely tedious requiring a large number of trial batches. This process is expensive and time consuming. The use of statistical mixture design technique provides a useful approach where in multiple outcomes can be met with fewer number of test runs. This is particularly true when multiple cementitious components are used in concrete. The research in progress here uses a statistical design of experiments approach - simplex-centroid design, with three cementitious components and seven minimum design points that represent specific mixture proportions. In this study, a ternary blend of portland cement, slag and Class F fly ash was used. The total cementitious content of the concrete was kept constant, although the individual proportions were varied. Fresh and hardened properties of concrete were evaluated, including mechanical properties such as compressive and split tensile strength and durability indicators such as rapid chloride-ion permeability and expansion due to alkali-silica reaction. Results from this study suggest that simplex-centroid method is a valuable tool in minimizing the number of trial batches needed to identify the optimal concrete proportions for achieving the desired properties.

INTRODUCTION

Portland cement concrete is a composite mixture consisting of individual components such as portland cement, aggregates, water, admixtures and supplementary cementing materials. The strength and durability properties of concrete are a function of the individual proportions of these materials. The strength and durability of concrete are challenged if the concrete is subjected to adverse environmental conditions (Fig 1). For this purpose, one or more SCMs may need to be used to achieve the desired strength and durability requirements. In order to develop concrete mixture proportions to meet these requirements, traditional approach of concrete mixture proportioning requires a systematic investigation by varying the proportions of the cementitious materials in small increments. This process is tedious, time-consuming and inefficient, particularly when the design requirements change.

(a) Alkali-Silica Reaction (b) Corrosion of steel reinforcement

(c) Freeze-Thaw Failure (d) Sulfate Attack on Concrete

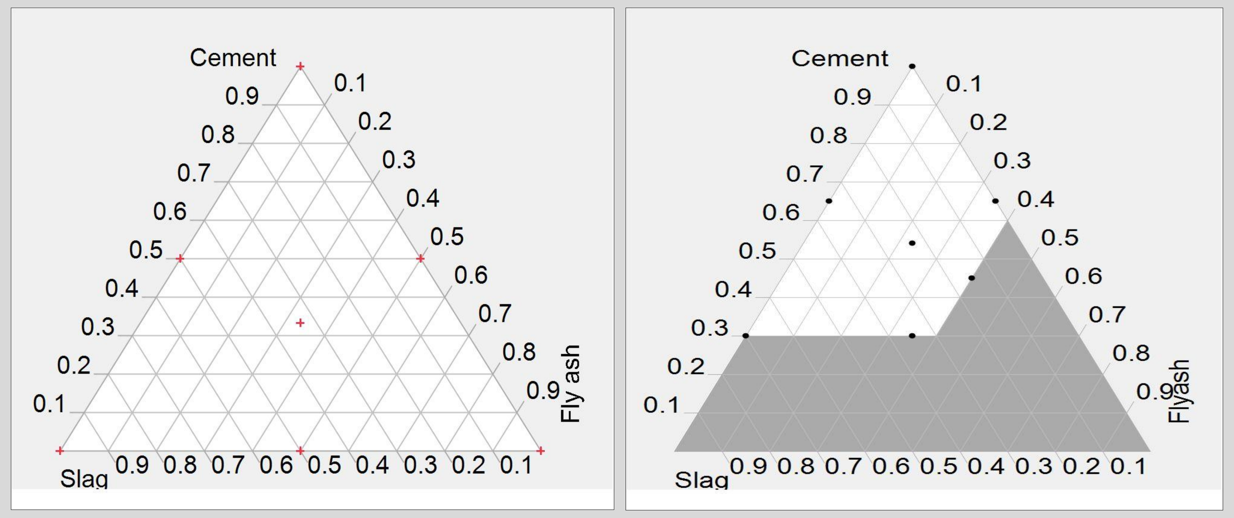
Figure 1: Major durability problems in concrete structures

The use of statistical design-of-experiment techniques can be beneficial in designing an experimental matrix that will achieve the desired outcomes with fewer trials. In this research study, effort has been made to optimize concrete mixtures to address various strength and durability requirements for specific job applications using Simplex-Centroid Design technique.

EXPERIMENTAL APPROACH

Different concrete mixtures were designed using ternary cementitious blends of cement, slag and Class F fly ash. The simplex-centroid mixture-design technique was adopted with seven (7) design points and five (5) validation points. Using seven (7) design points prediction equations were developed and response surfaces were generated within the simplex region. Five (5) new points were choose within the simplex region and validated by comparing actual test values with the predicted values from the simplex design model.

In this study, cement can be used 100% to create a test specimen, whereas slag and fly ash cannot be used 100% as they do not set and hold the test specimen together for the test. Thus, the upper limits for slag = 70% and fly ash = 40% has been employed in this study. The lower limit for cement = 30% is due to 70% slag, as the mixtures should add up to 100%. Fig 2 shows the regular simplex triangle and augmented simplex triangle with constrained design points.



(a) regular simplex triangle (b) augmented simplex triangle

Figure 2: Simplex-Centroid design triangle with constrained design points.

Concrete cylinders and prisms were cast to determine the strength and durability performance. Fig 3 shows the concrete test specimen dimensions. The performance parameters tested are listed below:

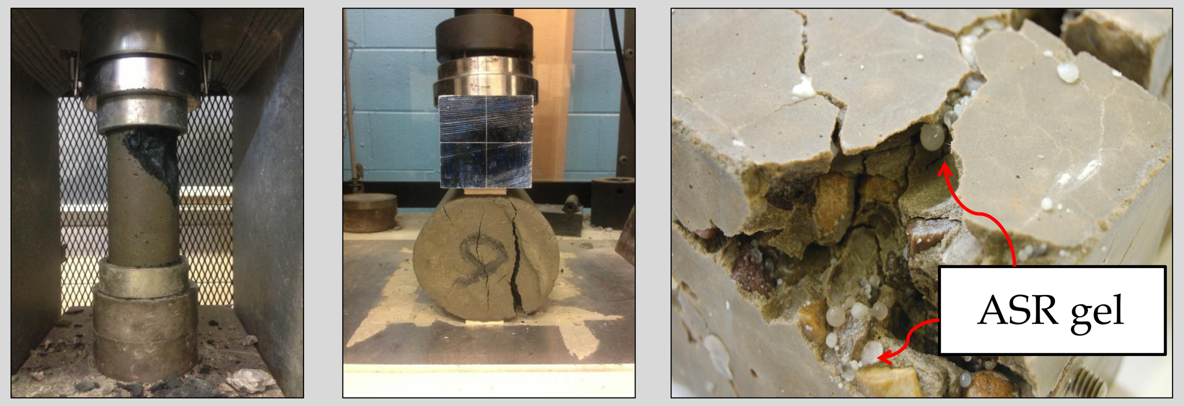
- For strength requirements compressive strength and split tensile strength of concrete was evaluated.
- For durability requirements chloride-ion permeability and alkali-silica reactivity of concrete was evaluated.

(a) 4″ x 8″ Cylinders (b) 2″ x 2″ x 11.25″ Prisms

Figure 3: Concrete specimens for strength and durability tests

RESULTS

The standard ASTM test procedures were used to determine the performance of concrete mixtures. Fig 4 shows the concrete testing procedure for determining strength and durability performance.



(a) Compression (b) Split tensile (c) Alkali-silica reaction

(d) Rapid chloride-ion permeability

Figure 4: Strength and Durability tests on concrete specimens

The strength and durability test results were used to develop performance prediction model with the 7 design points in the simplex region. An example model is shown below:

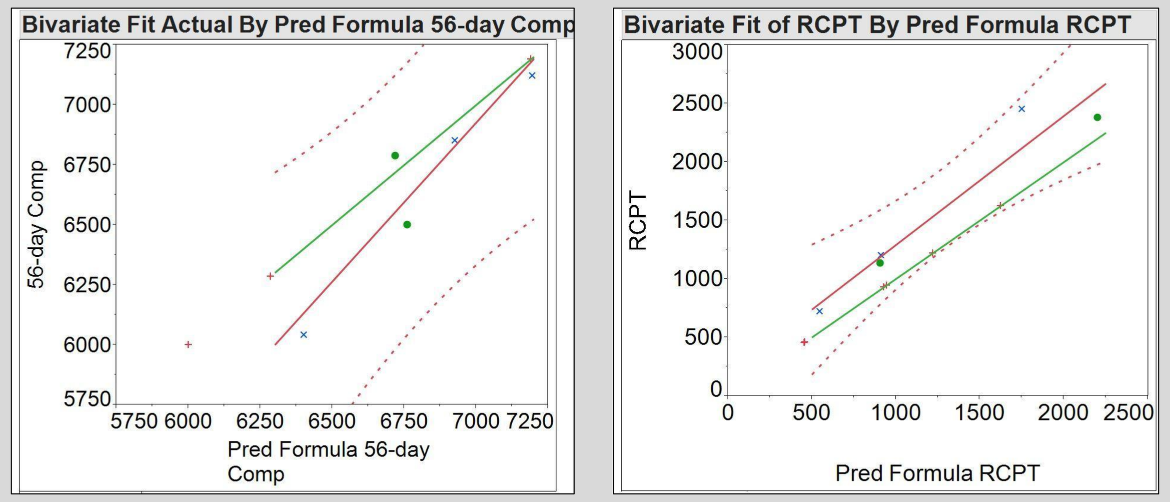
$$y = \beta_1 C + \beta_2 S + \beta_3 F + \beta_4 C{*}S + \beta_5 C{*}F + \beta_6 S{*}F + \beta_7 C{*}S{*}F$$

where, C, S, F are the mixtures components Cement, Slag and Fly Ash, respectively; and β is the coefficient that generates the response surface for any given performance parameter "y". Once the model was generated the predictability power of the model was validated.

Model Validation:

To validate the simplex-centroid design model, new data points within the simplex region were tested. The three following approaches were adopted to measure how well the model predicted the new data points:

1. The first approach was to estimate the squared correlation (R^2) of the actual and predicted values. An R^2 value closer to 1 is better. (Table 1)
2. The second approach was to estimate the slope (Actual/Unit Predicted). Slope value closer to 1 is better. An interval estimate of slope was used to determine if the slope was significantly different from 1.
3. The third approach was a visual assessment comparing, fitted actual vs. predicted line to the line of equality (slope = 1). The visual assessment shows the prediction ability (under or over prediction) of the fitted actual vs. predicted line w.r.t. the line of equality. (Fig 5)



(a) compressive strength (b) rapid chloride-ion permeability

Figure 5: Actual vs. Predicted fit w.r.t. the line of equality

Table 1: Summary fit for actual vs. predicted values

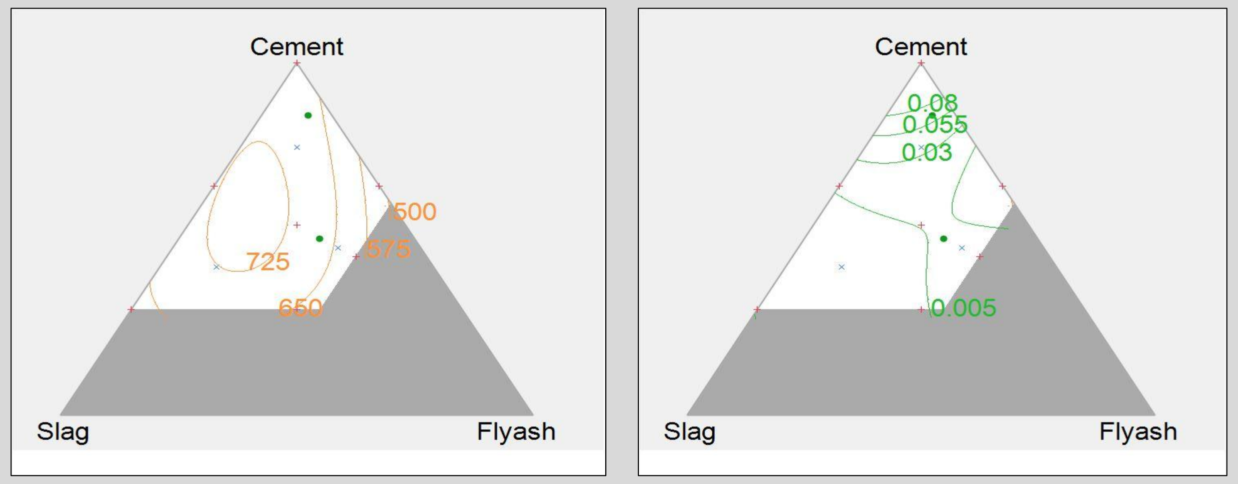
Compressive strength		Rapid Chloride-ion permeability	
R-Square	0.88	R-Square	0.93
R-Square Adjusted	0.84	R-Square Adjusted	0.90
Root Mean Square Error	162.30	Root Mean Square Error	244.73
Mean of Response	6661.4	Mean of Response	1580.2
Observations (Sum Wgts)	5	Observations (Sum Wgts)	5

Based on the validation studies, the concept of simplex centroid design model can be effectively applied to optimize concrete mixture proportions to meet both strength and durability requirements.

Response surface analysis:

The simplex triangle was analyzed using JMP statistical software and multiple response surfaces were generated for the performance parameters within the design space (Fig 6)

(a) compressive strength (psi) (b)chloride-ion permeability(coulomb)



(c) split tensile strength (psi) (d) alkali-silica expansion (percent)

Figure 6: Iso-contours developed for concrete performance parameters

The iso-contours developed for strength and durability performance parameters are overlapped and area within the simplex region is selected. The selected region has mixture proportions that will yield high performance concrete mixtures.

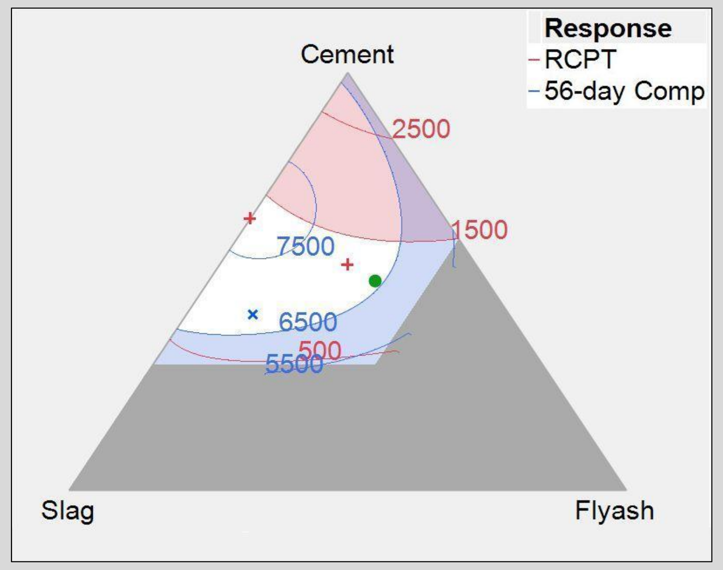


Figure 7: Compressive strength and rapid chloride-ion permeability iso-contours overlap

From Fig 7 the concrete mixtures in the un-shaded area (white region) represent the compressive strength values higher than 6500 psi and chloride-ion permeation value less than 1500 coulombs.

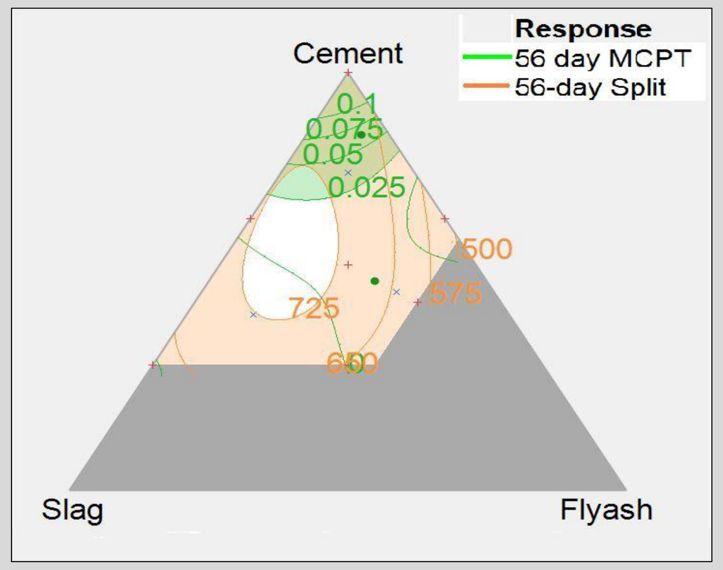


Figure 8: Split tensile strength and alkali-silica reaction expansions iso-contours overlap

From Fig 8 the concrete mixtures in the un-shaded area (white region) represent the split tensile strength values higher than 725 psi and alkali-silica reaction expansions below 0.025%

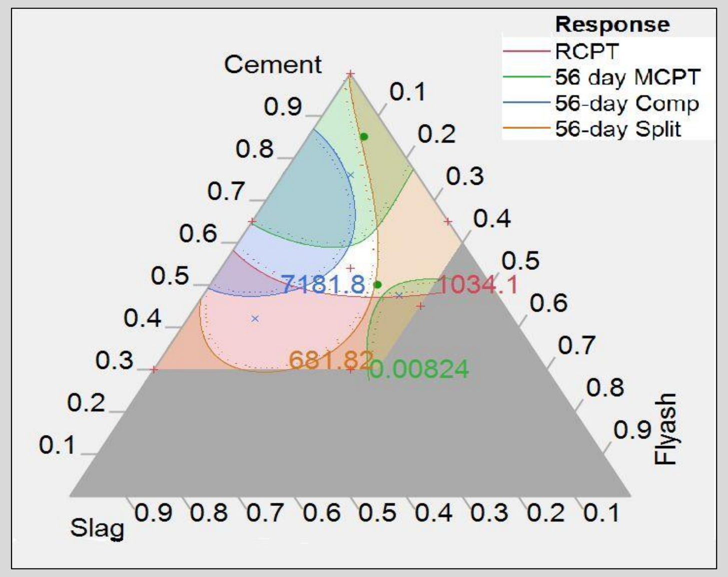


Figure 9: Superimposed multiple response surface contours

Multiple response surfaces were super-imposed within the simplex region and optimum mixture proportions were selected (Fig 9). The mixtures selected represent the desired strength and durability requirements of concrete for specific job applications. This concept of simplex-centroid design can be used to optimize concrete mixtures w.r.t. to other desired properties which are not discussed in this research study.

CONCLUSIONS

1. The mixture design techniques are effective in reducing the numerous test runs in laboratories and generate response surfaces to predict values.
2. The application of simplex-centroid design techniques proves to be helpful in optimizing concrete mixes while maintaining their strength and durability aspects.
3. The mixtures selected within the simplex region for concrete proportioning will reduce the total cement usage, which in turn decreases the embodied energy and carbon footprint of concrete structures.