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# Generalized Review on EVD and Constraints Simplex Method of Materials Properties Optimization for Civil Engineering

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**Abstract**

Extreme vertex design (EVD) has been adapted to be used in the modeling of the behavior of mixture experiments in civil engineering. This method has been in use since the 1970s and has be prevalent in the field of medical science. Various other methods of design of experiments have been used in engineering but neither has EVD being used particularly in civil engineering. This review is presented to serve as a hub or guide for subsequent exercise where concrete production, asphalt production or modification, soils stabilization and concrete improvement or water treatment would be studied with the help EVD. Its ability to fix design points and centroids has been reviewed in this work. EVD operates with various algorithms and depends on the order or condition of problems to be solved. The XVERT algorithm working on Minitab and Design Expert platform was adopted in this review work because of its efficiency in handling quadratic model problems like the four cases reviewed in the present work. From the four special cases, it can be asserted that there is a confidence in the use of EVD to develop the constraints, design the experimental factor space, design the mix proportions, and validate the models resulting from these procedures after experimental specimens are tested to determine the responses.

*Keywords:* Extreme Vertex Design; MATLAB-MINITAB-DesignExpert; Optimization; CONSIM Algorithms; XVERT and XVERT1 Algorithms; Soil-Concrete-Asphalt-Water Treatment; Constraints Simplex Experimental Region.

## 1. Introduction

A mixture experiment is an experiment in which the response depends on the proportions of the components, not the total amount [1]. There are two main constraints of mixture experiments. First, the proportion of a component is between 0 and 1. Second, the sum of proportions of all components is unity.

$$\sum_{i=1}^{q} x_i = 1 \qquad (i = 1, 2, 3 \ldots q) \tag{1}$$

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Both constraints at the upper and lower regions affect the entire experimental region. The experimental region becomes a (q-1) simplex. An overview of the mixture experiment methodology was given by Cornell [2]. Furthermore, additional constraints on proportions, such as lower bounds ($L_b$), upper bounds ($U_b$), will affect the shape of the experimental region.

$$0 \leq L_b \leq X_i \leq U_b \leq 1, (i = 1,2,3 \dots . q) \tag{2}$$

The experimental region becomes a regular or irregular shape. Design points of the irregular shape of the mixture experiment of more than three components are difficult to determine by hand. It is needed for a computational approach. To determine the design points of an irregular mixture experiment is needed for a computational approach. Algorithms have been developed to select design points, planes, edges, vertices and centroids of experimental regions. One of such algorithms includes the XVERT algorithm developed to find the design points in the linear model by Snee [3]. The XVERT algorithm can be used for selecting a subset of extreme vertices when the number of candidate vertices is large [3, 4]. The linear model can be described by Scheffe [5].

$$\hat{y}(x) = \sum_{i=1}^{q} \text{Ɣ}_1 x_i \tag{3}$$

Subsequently, the XVERT algorithm to find the design points in the quadratic model was developed by Snee [3]. The mixture design for a quadratic model produces large experimental runs. The centroids are calculated by averaging various subsets of vertices. The quadratic model Scheffe can be described by:

$$\hat{y}(x) = \sum_{i=1}^{q} \text{Ɣ}_i x_i \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} \text{Ɣ}_{ij} x_i x_j \tag{4}$$

And,

$$p = \frac{q(q+1)}{2} \tag{5}$$

Equation 5 is the number of parameter in the quadratic model.

A design which minimizes the determinant of variance (Ɣ) or maximizes the determinant of the information matrix [M] is called D-optimal design. The D-optimality criterion is defined as

$$D = max\ |M| = max|X^T X| \tag{6}$$

Algorithms start with writing $2^{q-1}$ combinations of upper and lower bounds for all but one factor which is left blank as in Mclean [4]. The extreme vertices also can be computed using the XVERT Algorithm steps and sequences describe below;

- Rank the components in order of increasing $U_i - L_i$, $X_1$ ranges has the smallest range and $X_q$ has the largest range.
- Consider first components q-1 with the smallest ranges. Form a two-level design from the lower - upper bounds of these $q$-1 components. There are $2^{q-1}$ combinations.
- Determine the level of the omitted component $X_q$ with each of the $2^{q-1}$ combination in step 2 using $X_q = 1 - \sum_{i=1}^{q} x_i$
- If this computed value lie within the constraint limits it is an extreme vertex called as core point. If it falls outside the constraint limits of the corresponding component it is called as the candidate point. For the points which are outside of the constraint limits, set $X_q$ equal to the upper or lower limit, whichever is closest to the computed value
- Additional points are generated from the candidate points. Find the difference between computed value and substituted upper or lower limit. Adjust this difference to one of the $q$-1 components. The generated point is an extreme vertex if the level after adjustment remains within the limits of the components. Thus maximum $q$-1 points can be generated from one candidate point.

In general, extreme vertices method has been used in various fields of science of experimentation and mixture blending and more prominent in this effort is the medical sciences. Recently it has been adopted in the production and blending of cementing materials like the geopolymer cement [6-9]. This work has targeted adapting this method in various fields of design of experiments in civil engineering which include; concrete production and modification, soil stabilization, asphalt production, and water treatment. To accomplish these tasks in civil engineering, components are blended in proportion utilizing both primary and secondary components depending on the conditions of the blending. Four technical cases were reviewed in this work; (i) a 5- component experimental mixture for concrete production utilizing water proportion, cement proportion, palm bunch ash proportion, fine aggregate proportion, and coarse aggregate proportion. The blending of components form an experimental space called the simplex as shown in Figure 1. This forms the space within which the behavior of the homogenous blend resulting from the mixing of the experimental components are distributed.

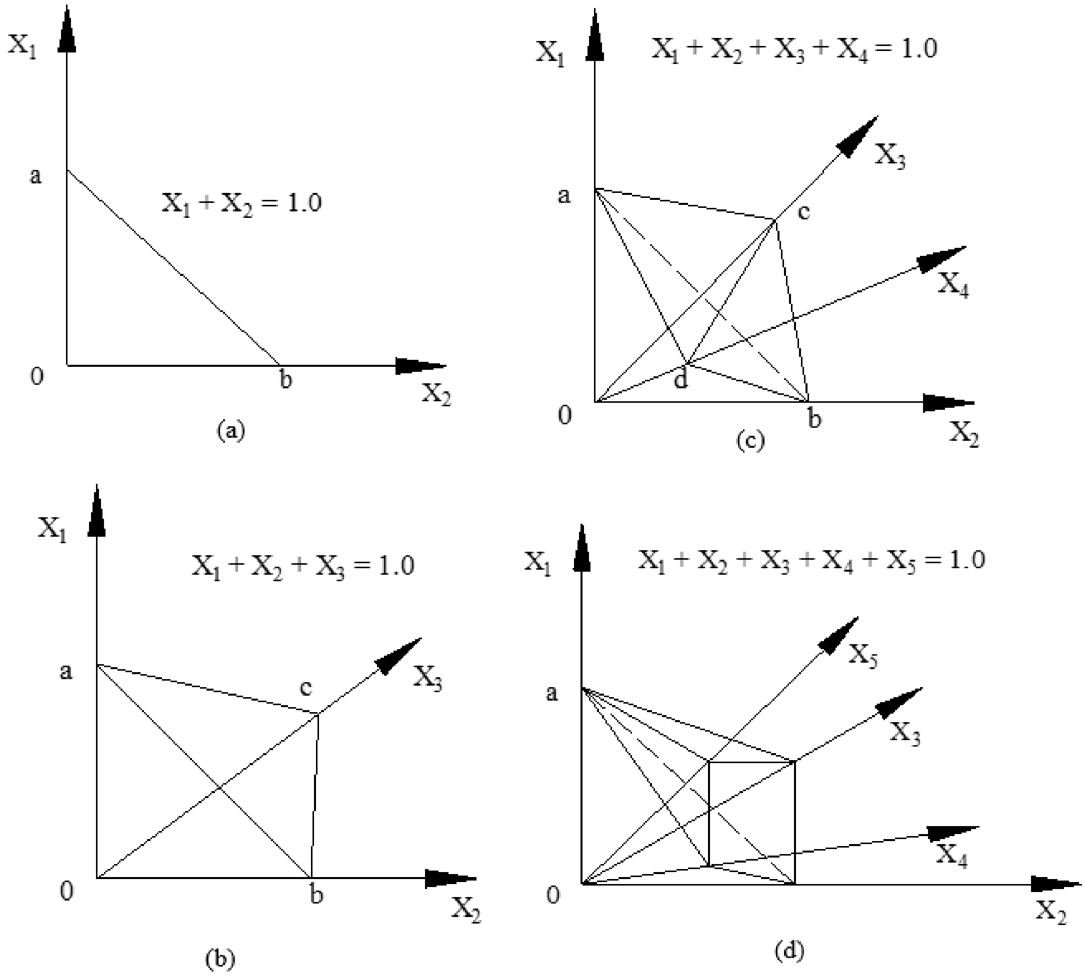


**Figure 1. Extreme vertices for; (a) 2-component simplex, (b) 3- component simplex, (c) 4- component simplex and (d) 5- component simplex**

## 2. Formulation of Constraints and Design of Factor Space

### 2.1. Constraints Formulation

Constraints are regions of lower and upper bounds established by the properties of the components that make up an experimental blend. As soon as these components are decided on based on intended results, the constraints that would define the experimental region are selected from available resources. In most cases and in practice, physical and economic considerations impose most often the lower and upper limits. Snee [3] had proposed general constraints equation as follows;

$$0 \le L_i \le X_i \le U_i \; 1 \; (i = 1, 2, 3 \ldots q) \tag{7}$$

Where; $L_i$ equals lower bound, $U_i$ equals upper bound, $X_i$ equals the $i^{th}$ component and q is the number of components in the mixture. Snee [3] also suggested an equation for multiple variable constraints for the form;

$$C_j \le A_{1j}X_1 + A_{2j}X_2 + \ldots + A_{qj}X_q \le D_j \tag{8}$$

Which are also found in experimentation and design of mixture where $C_j = D_j$ for all j = 1, 2, 3 …, m are scalar constants specified by multicomponent mixture and j designate the minor component proportion.

A consideration of some selected cases found in practice in various civil engineering disciplines are discussed as follows;

**Case 1**: Constraints of a five (5) component experimental mixture for concrete production: the multicomponent constraints in Eqns. 9-14 have been developed from concrete production literature references and end conditions from earlier research results on the utilization of additives as partial replacement for ordinary cement or as an enhancer of concrete mixes in concrete production [10-17]. Under the conditions of an additive serving as partial replacement for cement with cementing or pozzolanic properties, it is considered a minor component in a mixture of mixture experiment

(MME).

$$0.6 \leq X_4 + X_5 \leq 0.75 \quad (9)$$

$$0.1 \leq X_2 + X_3 \leq 0.35 \quad (10)$$

$$0.1 \leq X_1 \leq 0.15 \quad (11)$$

$$0.45 \leq \frac{X_1}{X_2+X_3} \leq 0.55 \quad (12)$$

$$0.05 \leq \frac{X_3}{X_2} \leq 0.25 \quad (13)$$

$$X_1 + X_2 + X_3 + X_4 + X_5 = 1 \quad (14)$$

Where; $X_1$ equals water proportion, $X_2$ equals cement proportion, $X_3$ equals palm bunch ash proportion, $X_4$ equals fine aggregate proportion, and $X_5$ equals coarse aggregate proportion.

**Case 2**: Constraints of a four (4) component experimental mixture for asphalt production: in a similar operation the multicomponent constraints in Eqns. 15-18 have been developed from asphalt production and modification literature references and end conditions from research results on the utilization of crushed waste glasses based geopolymer cement as a modifier [18-19]. In this case, the modifier is a proportion of the major cementing material in asphalt production i.e. the asphalt cement particularly shown in Equation 17.

$$0.01 \leq X_1 \leq 0.05 \quad (15)$$

$$0.75 \leq X_2 + X_3 \leq 0.95 \quad (16)$$

$$0.15 \leq \frac{X_4}{X_1} \leq 0.45 \quad (17)$$

$$X_1 + X_2 + X_3 + X_4 = 1.0 \quad (18)$$

Where; $X_1$ equals asphalt cement proportion, $X_2$ equals coarse aggregate proportion, $X_3$ equals fine aggregate proportion and $X_4$ equals crushed waste glasses based geopolymer cement (asphalt concrete modifier) proportion.

**Case 3**: Constraints of a three (3) component experimental mixture for soil treatment: in soil stabilization protocols, materials are blended with the treated soil to improve on its engineering properties. The utilization of quarry dust as an admixture has been in use in various circumstances and reported in many literatures [20-23]. The results achieved from the above operation have been helpful in the formulation of the multicomponent constraints as in Equations 19-21.

$$0.1 \leq \frac{X_1}{X_3} \leq 0.9 \quad (19)$$

$$0.1 \leq X_2 \leq 0.15 \quad (20)$$

$$X_1 + X_2 + X_3 = 1.0 \quad (21)$$

Where; $X_1$ equals quarry dust proportion, $X_2$ equals water content and $X_3$ equals test soil proportion.

**Case 4**: Constraints of a two (2) component experimental mixture of homogenous blend for example the improvement of freshly mixed concrete properties with freshly synthesized quarry dust based geopolymer cement. In a similar way, the constraints as in Equations. 22-24 have been proposed from earlier research works. It is important to also note that the synthesized quarry dust based geopolymer cement functions as a minor component in a partial replacement technique for the concrete or another case could serve as an additive in a side by side utilization as a major component for the improvement of certain properties in concrete for example durability, heat resistance, sulphate resistance, shrinkage resistance and cracking resistance [24, 25].

$$X_1 \leq 1.0 \quad (22)$$

$$0.1 \leq \frac{X_1}{X_2} \leq 0.55 \quad (23)$$

$$X_1 + X_2 = 1.0 \quad (24)$$

Where; $X_1$ equals the homogenous freshly mixed concrete proportion and $X_2$ equals the homogenous freshly synthesized geopolymer cement.

## 2.2. Design of Simplex and Factor Space

## 2.3. (5) Component Simplex and Factor Space for Concrete Production

The design of factor spaces from hyper-polyhedron simplexes begins with the testing and screening of the components constraints giving rise to an experimental points within the defined or constrained space. In the case of the 5- component factor space under review considerations, multicomponent constraints were developed from literatures on concrete production and modification. These constraints were used to test and evaluate the degrees of freedom (df) in the 5 factors component design experiment shown in Table 1. A recommendation is a minimum of 3 lack of fit df and 4 df for pure error. This ensures a valid lack of fit test. Fewer df will lead to a test that may not detect lack of fit (26, 27).

**Table 1. Design Matrix Evaluation for Mixture Quadratic Model 5 Factors: A, B, C, D, E**

| Mixture Component Coding is U_Pseudo. | |
|---|---|
| **Degrees of Freedom for Evaluation** | |
| Model | 14 |
| Residuals | 10 |
| Lack of Fit | 5 |
| Pure Error | 5 |
| Corr Total | 24 |

Power calculations test was also conducted on the developed constraints using the design expert and the Minitab software to establish the deviations and variances on the design planes and vertexes and edges contained in the simplex on 5% alpha level shown in Table 2 [26, 27].

**Table 2. Power at 5 % alpha level on 5- component for concrete production**

| Term | StdErr | VIF | Ri-Squared | Std. Dev. |
|---|---|---|---|---|
| **A** | 8.18 | 80.41 | 0.9876 | 5.5 % |
| **B** | 1.50 | 7.50 | 0.8666 | 9.8 % |
| **C** | 6.52 | 62.76 | 0.9841 | 5.7 % |
| **D** | 2.41 | 14.50 | 0.9311 | 8.8 % |
| **E** | 0.70 | 1.82 | 0.4503 | 10.3 % |
| **AB** | 14.27 | 22.58 | 0.9557 | 8.0 % |
| **AC** | 17.28 | 15.72 | 0.9364 | 7.0 % |
| **AD** | 14.76 | 19.62 | 0.9490 | 7.8 % |
| **AE** | 14.31 | 16.33 | 0.9388 | 8.0 % |
| **BC** | 11.28 | 16.25 | 0.9385 | 9.9 % |
| **BD** | 6.73 | 4.40 | 0.7725 | 19.0 % |
| **BE** | 4.13 | 2.36 | 0.5759 | 41.8 % |
| **CD** | 11.82 | 13.97 | 0.9284 | 9.4 % |
| **CE** | 12.43 | 13.01 | 0.9232 | 9.0 % |
| **DE** | 5.83 | 3.05 | 0.6726 | 23.7 % |

Basis Std. Dev. = 1.0

Approximate DF used for power calculations operate under the following condition;

- Standard errors should be similar within type of coefficient. Smaller is better.
- The ideal VIF value is 1.0. VIFs above 10 are cause for concern. VIFs above 100 are cause for alarm, indicating coefficients are poorly estimated due to multicollinearity.
- Ideal Ri-squared is 0.0. High Ri-squared means terms are correlated with each other, possibly leading to poor models.
- For mixture designs the proportions of components must sum to one.
- This is a constraint on the system and causes multicollinearity to exist, thus increasing the VIFs and the Ri-squareds, rendering these statistics useless.

The software further developed the conditions of the 5- component simplex shown in Figs. 2 & 3 and the results are presented in Table 3. The 25 runs were to improve on the optimality or efficiency of the model operation. Lack of fit was never recorded on any of the vertex points of the design space as shown in Table 3 rather on either the interior or plane points. This in effect raises concern for more design points to be located on the interior and plane spaces of the simplex to reduce the lack of fit effect on the experimental space [26, 27].

**Table 3. Measures derived from the information matrix on 5- component for concrete production**

| Run | Leverage | Space Type | Build Type |
|---|---|---|---|
| **1** | 0.2731 | Interior | Lack of Fit |
| **2** | 0.8503 | Edge | Model |
| **3** | 0.2550 | Plane | Replicate |
| **4** | 0.4124 | Plane | Lack of Fit |
| **5** | 0.2550 | Plane | Lack of Fit |
| **6** | 0.4771 | Edge | Replicate |
| **7** | 0.7860 | Edge | Model |
| **8** | 0.3999 | Plane | Model |
| **9** | 0.3999 | Plane | Replicate |
| **10** | 0.3989 | Plane | Replicate |
| **11** | 0.8193 | Vertex | Model |
| **12** | 0.9334 | Vertex | Model |
| **13** | 0.8727 | Vertex | Model |
| **14** | 0.4901 | Vertex | Model |
| **15** | 0.8335 | Vertex | Model |
| **16** | 0.4901 | Vertex | Replicate |
| **17** | 0.8508 | Vertex | Model |
| **18** | 0.4175 | Interior | Lack of Fit |
| **19** | 0.7665 | Edge | Model |
| **20** | 0.8631 | Vertex | Model |
| **21** | 0.3989 | Plane | Model |
| **22** | 0.8293 | Vertex | Model |
| **23** | 0.9410 | Vertex | Model |
| **24** | 0.4771 | Edge | Model |
| **25** | 0.5091 | Plane | Lack of Fit |
| **Average =** | 0.6000 | | |

However, watch for leverages close to 1.0 because they appear to be located on the vertexes and edges and consider replicating these points or make sure they are run very carefully. The software generates lots of other data that would be used to test the multicollinearity of the design, the G-efficiency and the scaled D- optimality. These information and results are needed when comparing designs.

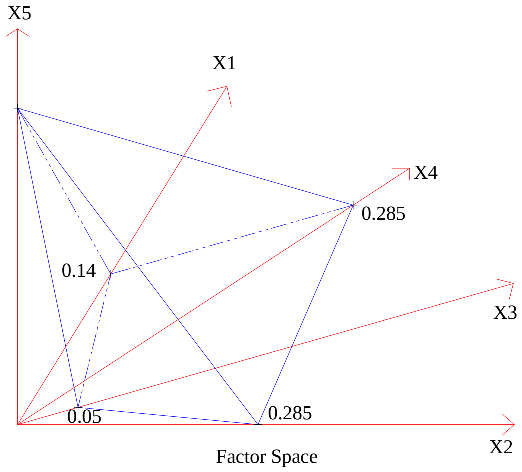


**Figure 2. Factor space simplex of a 5- component mixture experiment for concrete production**

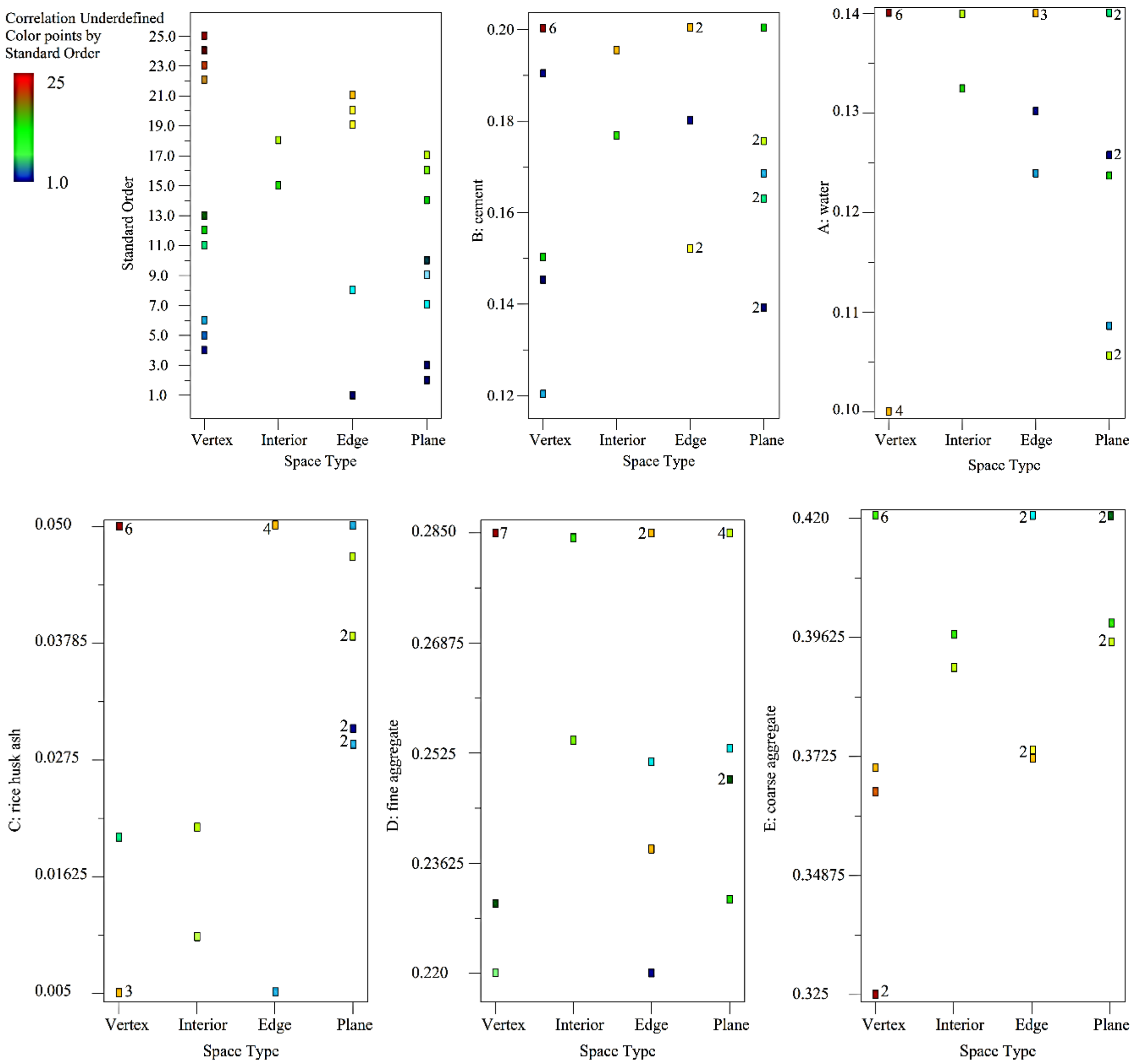


**Figure 3. Experimental factor space of the components in a 5- component mixture space for concrete production**

## 2.4. (4) Component Simplex and Factor Space

Table 4 shows the design evaluation for the four component mixture quadratic model conducted with the multicomponent constraints developed from literature to determine the degree of freedom for the experimental procedure of an asphalt production and modification exercise. A recommendation is a minimum of 3 lack of fit df and 4 df for pure error. This ensures a valid lack of fit test. Fewer df will lead to a test that may not detect lack of fit.

**Table 4. Design Matrix Evaluation for Mixture Quadratic Model 4 Factors: A, B, C, D with U_Pseudo Mixture Component Coding [26, 27]**

| Degrees of Freedom for Evaluation | |
|---|---|
| Model | 9 |
| Residuals | 15 |
| Lack of Fit | 8 |
| Pure Error | 7 |
| Corr Total | 24 |

Power calculations test was also conducted on the developed constraints using the design expert and Minitab software to find the standard deviations and variances on the design planes and vertexes and edges contained in the simplex on 5% alpha level shown in Table 5 [26, 27].

**Table 5. Power at 5 % alpha level on 4- component for asphalt production**

| Term | StdErr | VIF | Ri-Squared | Std. Dev. |
|---|---|---|---|---|
| **A** | 14.56 | 208.97 | 0.9952 | 5.1 % |
| **B** | 1.42 | 9.63 | 0.8961 | 5.4 % |
| **C** | 0.62 | 2.52 | 0.6034 | 5.3 % |
| **D** | 34.51 | 510.91 | 0.9980 | 5.0 % |
| **AB** | 21.04 | 64.80 | 0.9846 | 6.5 % |
| **AC** | 20.97 | 73.79 | 0.9864 | 6.5 % |
| **AD** | 43.66 | 35.04 | 0.9715 | 5.3 % |
| **BC** | 3.38 | 2.76 | 0.6377 | 60.1 % |
| **BD** | 44.85 | 145.55 | 0.9931 | 5.3 % |
| **CD** | 43.28 | 132.19 | 0.9924 | 5.3 % |

Basis Std. Dev. = 1.0

Approximate DF used for power calculations functions under the following;

- Standard errors should be similar within type of coefficient. Smaller is better.
- The ideal VIF value is 1.0. VIFs above 10 are cause for concern. VIFs above 100 are cause for alarm, indicating coefficients are poorly estimated due to multicollinearity.
- Ideal Ri-squared is 0.0. High Ri-squared means terms are correlated with each other, possibly leading to poor models.
- For mixture designs the proportions of components must sum to one.
- This is a constraint on the system and causes multicollinearity to exist, thus increasing the VIFs and the Ri-squareds, rendering these statistics useless.

The software further developed the conditions of the 4- component simplex shown in Figs. 4 & 5 and the results are presented in Table 6. The 25 runs were to improve on the optimality or efficiency of the model operation. Lack of fit was recorded on one vertex point of the design space in this case as shown in Table 6 and on the third edge and axial points [26, 27]. This in effect raises concern for more design points to be located on the third edge and axial spaces of the simplex to reduce the lack of fit effect on the experimental space [26, 27].

**Table 6. Measures derived from the information matrix on 4- component for asphalt production**

| Run | Leverage | Space Type | Build Type |
|---|---|---|---|
| 1 | 0.3356 | ThirdEdge | Lack of Fit |
| 2 | 0.1901 | Center | Center |
| 3 | 0.3344 | ThirdEdge | Replicate |
| 4 | 0.5196 | Vertex | Model |
| 5 | 0.1901 | Center | Center |
| 6 | 0.3344 | ThirdEdge | Model |
| 7 | 0.4232 | ThirdEdge | Model |
| 8 | 0.1901 | Center | Center |
| 9 | 0.3225 | ThirdEdge | Model |
| 10 | 0.4148 | CentEdge | Model |
| 11 | 0.83257 | Vertex | Model |
| 12 | 0.1747 | AxialCB | Lack of Fit |
| 13 | 0.4417 | Vertex | Lack of Fit |
| 14 | 0.3368 | TripBlend | Model |
| 15 | 0.3884 | Vertex | Replicate |
| 16 | 0.5385 | Vertex | Model |
| 17 | 0.3884 | Vertex | Model |
| 18 | 0.7909 | Vertex | Model |
| 19 | 0.3030 | PlaneCent | Model |
| 20 | 0.3562 | ThirdEdge | Lack of Fit |
| 21 | 0.4232 | ThirdEdge | Replicate |
| 22 | 0.3030 | PlaneCent | Replicate |
| 23 | 0.3241 | ThirdEdge | Lack of Fit |
| 24 | 0.3368 | TripBlend | Replicate |
| 25 | 0.807231 | Vertex | Model |
| **Average =** | 0.4000 | | |

However, watch for leverages close to 1.0 because they appear to be located on the vertexes and edges and consider replicating these points or make sure they are run very carefully. The software generates lots of other data that would be used to test the multicollinearity of the design, the G-efficiency and the scaled D- optimality [26, 27]. These information and results are needed when comparing designs.

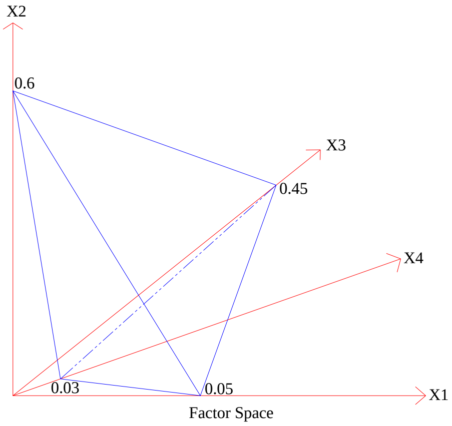


**Figure 4. Factor space simplex of a 4- component mixture experiment for asphalt production**

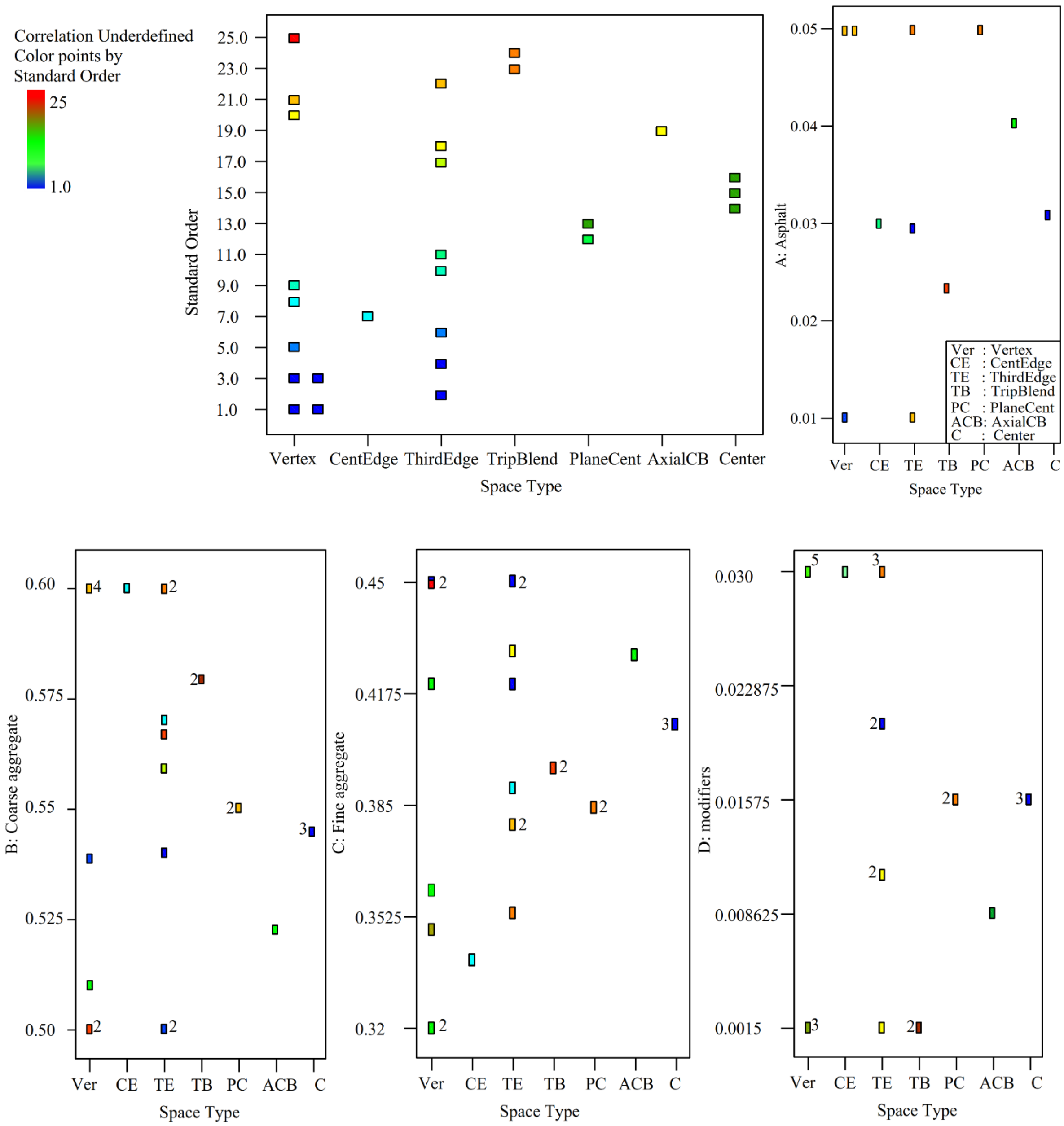


**Figure 5. Experimental factor space of the components in a 4- component mixture space**

## 2.5. (3) Component Simplex and Factor Space

The design evaluation for the three component mixture quadratic model conducted with the multicomponent constraints developed from literature to determine the degree of freedom for the experimental procedure of a soil stabilization protocol is as presented in Table 7. A recommendation is a minimum of 3 lack of fit df and 4 df for pure error. This ensures a valid lack of fit test. Fewer df will lead to a test that may not detect lack of fit [26, 27].

**Table 7. Design Matrix Evaluation for Mixture Quadratic Model 3 Factors: A, B, C with L_Pseudo Mixture Component Coding [26, 27]**

| Degrees of Freedom for Evaluation | |
|---|---|
| Model | 5 |
| Residuals | 19 |
| Lack of Fit | 7 |
| Pure Error | 12 |
| Corr Total | 24 |

Power calculations test was also conducted on the developed constraints using the design expert and minitab software to find the standard deviations and variances on the design planes and vertexes and edges contained in the simplex on 5% alpha level shown in Table 8

**Table 8. Power at 5 % alpha level on 3- component for soil treatment**

| Term | StdErr | VIF | Ri-Squared | Std. Dev. |
|---|---|---|---|---|
| A | 0.52 | 2.42 | 0.5860 | 6.4 % |
| B | 11.15 | 131.86 | 0.9924 | 5.3 % |
| C | 1.81 | 13.14 | 0.9239 | 6.1 % |
| AB | 16.13 | 64.60 | 0.9845 | 7.6 % |
| AC | 4.11 | 7.48 | 0.8663 | 45.5 % |
| BC | 16.55 | 45.85 | 0.9782 | 7.5 % |

Basis Std. Dev. = 1.0

Approximate DF used for power calculations functions as follows;

- Standard errors should be similar within type of coefficient. Smaller is better.
- The ideal VIF value is 1.0. VIFs above 10 are cause for concern. VIFs above 100 are cause for alarm, indicating coefficients are poorly estimated due to multicollinearity.
- Ideal Ri-squared is 0.0. High Ri-squared means terms are correlated with each other, possibly leading to poor models.
- For mixture designs the proportions of components must sum to one.
- This is a constraint on the system and causes multicollinearity to exist, thus increasing the VIFs and the Ri-squareds, rendering these statistics useless.

The software further developed the conditions of the 3- component simplex shown in Figs. 6 & 7 and the results are presented in Table 9. The 25 runs were to improve on the optimality or efficiency of the model operation [26, 27]. Lack of fit was recorded on three interior points of the design space in this case as shown in Table 9 and on two edge points [26, 27]. This in effect raises concern for more design points to be located on these spaces of the simplex to reduce the lack of fit effect on the entire experimental space [26, 27].

**Table 9. Measures derived from the information matrix on 3- component for soil treatment**

| Run | Leverage | Space Type | Build Type |
|---|---|---|---|
| 1 | 0.1200 | Interior | Lack of Fit |
| 2 | 0.3614 | Vertex | Model |
| 3 | 0.1314 | Center | Center |
| 4 | 0.2745 | Vertex | Model |
| 5 | 0.2377 | Edge | Model |
| 6 | 0.2477 | Edge | Model |

| | | | |
|---|---|---|---|
| 7 | 0.3614 | Vertex | Model |
| 8 | 0.1185 | Interior | Lack of Fit |
| 9 | 0.3364 | Vertex | Model |
| 10 | 0.2745 | Vertex | Replicate |
| 11 | 0.4050 | Vertex | Model |
| 12 | 0.1314 | Center | Center |
| 13 | 0.2745 | Vertex | Model |
| 14 | 0.3364 | Vertex | Replicate |
| 15 | 0.1314 | Center | Center |
| 16 | 0.2460 | Edge | Replicate |
| 17 | 0.2477 | Edge | Replicate |
| 18 | 0.2418 | Edge | Replicate |
| 19 | 0.2418 | Edge | Model |
| 20 | 0.1332 | Interior | Lack of Fit |
| 21 | 0.2460 | Edge | Lack of Fit |
| 22 | 0.1314 | Center | Center |
| 23 | 0.1314 | Center | Center |
| 24 | 0.2335 | Edge | Lack of Fit |
| 25 | 0.4050 | Vertex | Model |
| **Average =** | 0.2400 | | |

However, watch for leverages close to 1.0 because they appear to be located on none of the design points in this case. The software generates lots of other data that would be used to test the multicollinearity of the design, the G-efficiency and the scaled D- optimality. These information and results are needed when comparing design.

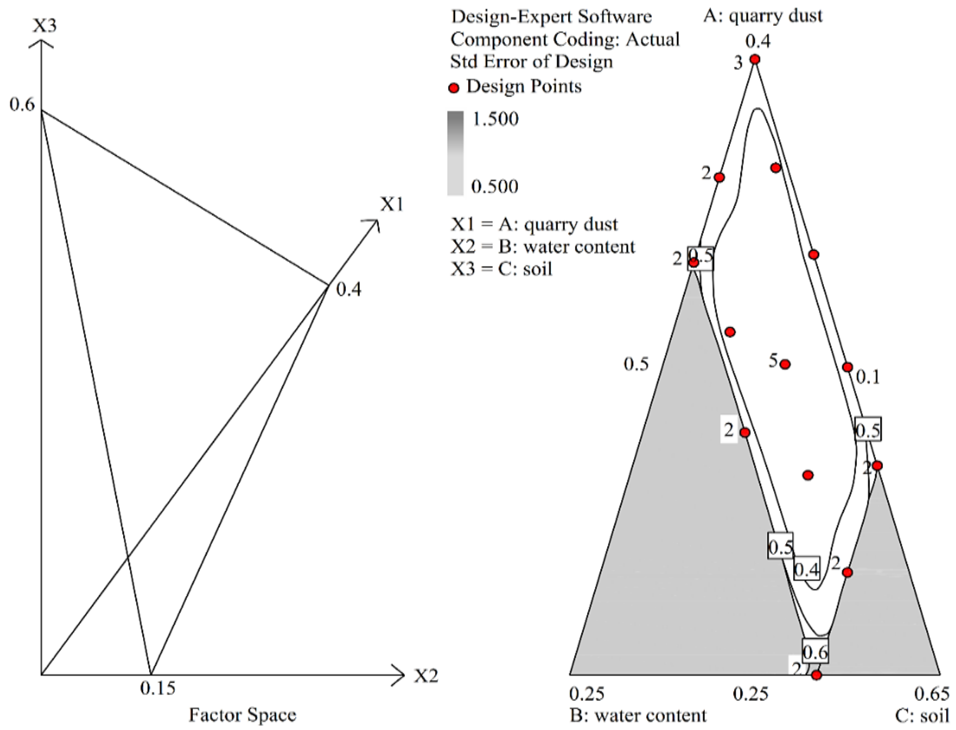


**Figure 6. Factor space simplex and contour space of a 3- component mixture experiment for soil stabilization**

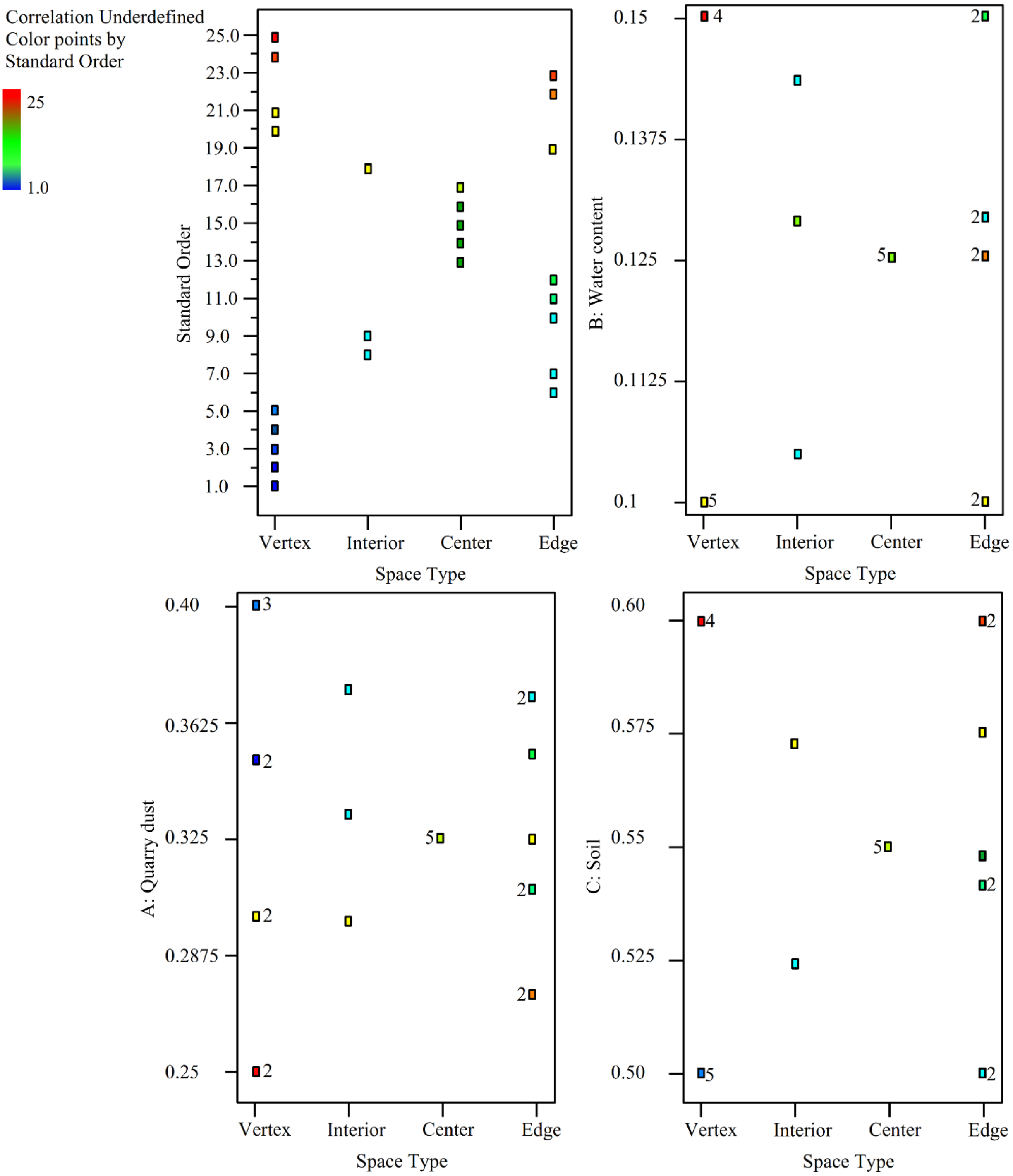


**Figure 7. Experimental factor space of the components in a 3- component mixture space**

## 2.6. (2) Component Simplex and Factor Space

In the final case scenario being reviewed, the design evaluation for the two component mixture quadratic model conducted with the multicomponent constraints developed from literature to determine the degree of freedom for the experimental procedure of a two homogenous mixture concrete modification protocol is as presented in Table 10. As usual, a recommendation is a minimum of 3 lack of fit df and 4 df for pure error. This ensures a valid lack of fit test. Fewer df will lead to a test that may not detect lack of fit [26, 27].

**Table 10. Design Matrix Evaluation for Mixture Quadratic Model 2 Factors: A, B with L_Pseudo Mixture Component Coding [26, 27]**

| Degrees of Freedom for Evaluation | |
|---|---|
| Model | 2 |
| Residuals | 4 |
| Lack of Fit | 4 |
| Pure Error | 0 |
| Corr Total | 6 |

Power calculations test was also conducted on the developed constraints using the design expert and minitab software to find the standard deviations and variances on the design planes and vertexes and edges contained in the simplex on 5% alpha level shown in Table 11 [26, 27].

**Table 11. Power at 5 % alpha level on 2- component for homogeneous mixtures**

| Term | StdErr | VIF | Ri-Squared | Std. Dev. |
|---|---|---|---|---|
| A | 0.92 | 2.07 | 0.5174 | 24.7 % |
| B | 0.92 | 2.07 | 0.5174 | 24.7 % |
| AB | 3.83 | 3.40 | 0.7055 | 36.0 % |

Basis Std. Dev. = 1.0

Approximate DF used for power calculations.

- Standard errors should be similar within type of coefficient. Smaller is better.
- The ideal VIF value is 1.0. VIFs above 10 are cause for concern. VIFs above 100 are cause for alarm, indicating coefficients are poorly estimated due to multicollinearity.
- Ideal Ri-squared is 0.0. High Ri-squared means terms are correlated with each other, possibly leading to poor models.
- For mixture designs the proportions of components must sum to one.
- This is a constraint on the system and causes multicollinearity to exist, thus increasing the VIFs and the Ri-squareds, rendering these statistics useless.

The software further also developed the conditions of the 2- component simplex shown in Fig. 8 and the results are presented in Table 12. The 7 runs were to improve on the optimality or efficiency of the model operation. Lack of fit was not recorded on any of the design points [26, 27].

**Table 12. Measures derived from the information matrix on 2- component**

| Run | Leverage | Space Type |
|---|---|---|
| 1 | 0.2815 | Center |
| 2 | 0.8525 | Vertex |
| 3 | 0.2524 | AxialCB |
| 4 | 0.2544 | ThirdEdge |
| 5 | 0.2524 | AxialCB |
| 6 | 0.2544 | ThirdEdge |
| 7 | 0.8525 | Vertex |
| **Average =** | 0.4286 | |

Watch for leverages close to 1.0. Consider replicating these points or make sure they are run very carefully. This case was observed on the 7$^{th}$ run located on the vertex of the experimental space. The software generates lots of other data that would be used to test the multicollinearity of the design, the G-efficiency and the scaled D-optimality [26, 27]. These information and results are needed when comparing designs.

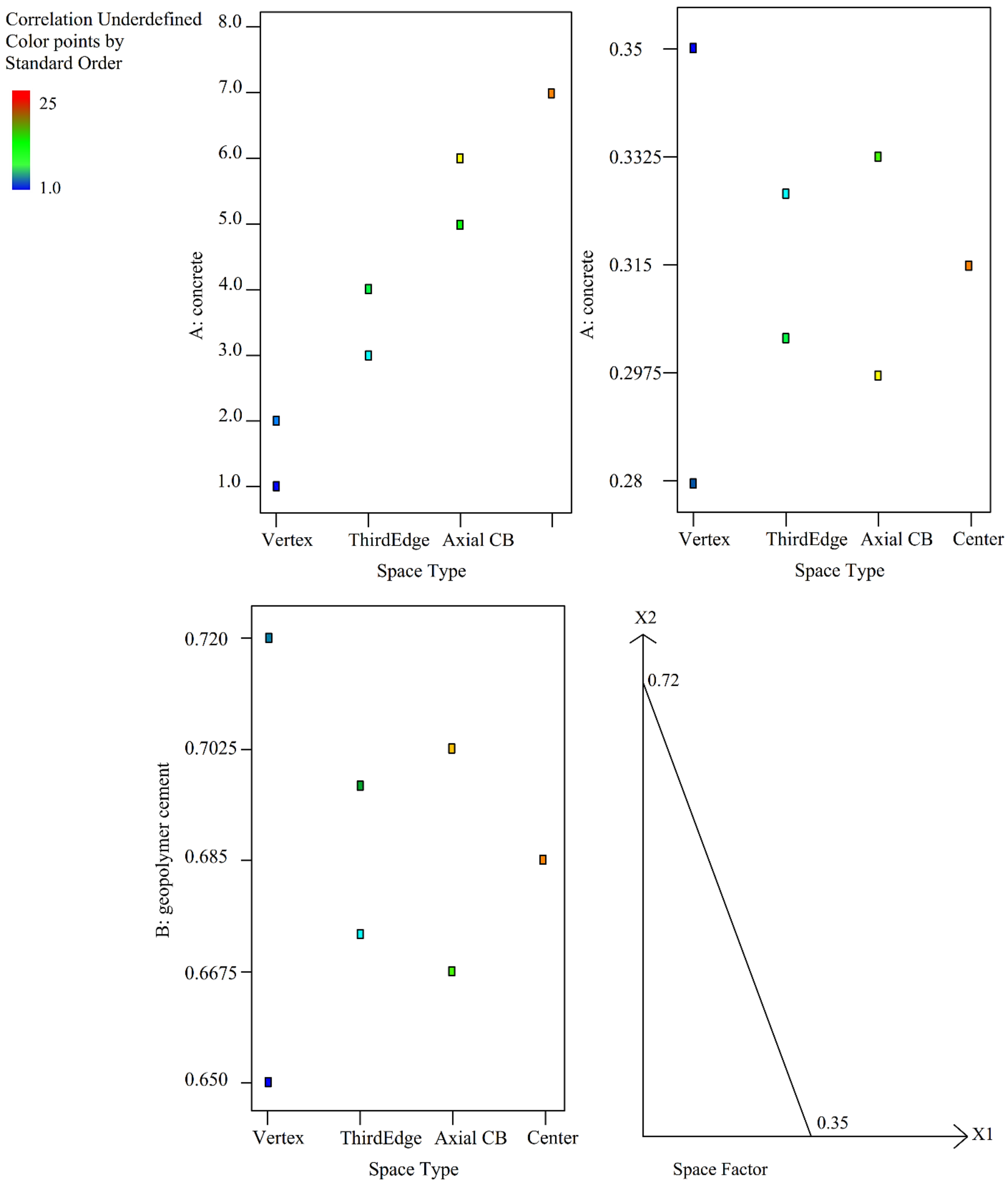


**Figure 8. Experimental simplex and factor space of the components in a 2- component mixture space**

## 3. Design of Experimental Mix Proportions

Tables 13, 14, 15 and 16 present the mixes and runs for the 5-, 4-, 3-, and 2- component multiconstraints experimental design. These mixes guide the preparation of specimens to be tested in the laboratory to achieve the responses. The number of runs can be increased to check and screen for errors and reduce lack of fit effects within the experimental space. The specimens are prepared with the actual components mix proportions of the different components that make the test blend. Figures. 9-15 show the factor spaces, traces and deviations and contour of the different multicomponent constraints mixture of mixture experiments. It would be appropriate that in a model exercise, the full simulation of the behavior of the tested specimens are observed and shown graphically to enable engineers monitor the performance and life service of such infrastructures. These designed mixes would guide from experimental stage to achieve laboratory responses that enable the establishment of model equations that would determine the overall behavior of the modelled facility. Experimental responses are key to validating and testing the accuracy of mathematical modeling exercise as this under review. This research is confident that it serves as a hub to direct and guide exercises in the field of civil engineering in adapting extreme vertex design in all mixture experimental and composite formulations in civil engineering and even in industrial and materials mechanical engineering.

**Table 13. 5- Component experimental mix proportions [26, 27]**

| Runs | Actual Components | | | | | Response | Pseudo Components | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | z1 | z2 | z3 | z4 | z5 | | x1 | x2 | x3 | x4 | x5 |
| 1 | 0.132 | 0.177 | 0.010 | 0.284 | 0.396 | Y1 | 0.080 | 0.246 | 0.417 | 0.009 | 0.248 |
| 2 | 0.124 | 0.200 | 0.005 | 0.251 | 0.420 | Y2 | 0.170 | 0.000 | 0.474 | 0.356 | 0.000 |
| 3 | 0.106 | 0.175 | 0.039 | 0.285 | 0.395 | Y3 | 0.361 | 0.261 | 0.113 | 0.000 | 0.265 |
| 4 | 0.124 | 0.200 | 0.047 | 0.231 | 0.398 | Y4 | 0.171 | 0.000 | 0.031 | 0.571 | 0.227 |
| 5 | 0.106 | 0.175 | 0.039 | 0.285 | 0.395 | Y5 | 0.361 | 0.261 | 0.113 | 0.000 | 0.265 |
| 6 | 0.140 | 0.152 | 0.050 | 0.285 | 0.373 | Y6 | 0.000 | 0.507 | 0.000 | 0.000 | 0.493 |
| 7 | 0.130 | 0.180 | 0.050 | 0.220 | 0.420 | Y7 | 0.104 | 0.212 | 0.000 | 0.684 | 0.000 |
| 8 | 0.126 | 0.139 | 0.030 | 0.285 | 0.420 | Y8 | 0.150 | 0.643 | 0.207 | 0.000 | 0.000 |
| 9 | 0.126 | 0.139 | 0.030 | 0.285 | 0.420 | Y9 | 0.150 | 0.643 | 0.207 | 0.000 | 0.000 |
| 10 | 0.140 | 0.163 | 0.029 | 0.249 | 0.420 | Y10 | 0.000 | 0.394 | 0.223 | 0.384 | 0.000 |
| 11 | 0.140 | 0.200 | 0.005 | 0.285 | 0.370 | Y11 | 0.000 | 0.000 | 0.474 | 0.000 | 0.526 |
| 12 | 0.100 | 0.200 | 0.050 | 0.230 | 0.420 | Y12 | 0.421 | 0.000 | 0.000 | 0.579 | 0.000 |
| 13 | 0.140 | 0.120 | 0.050 | 0.270 | 0.420 | Y13 | 0.000 | 0.842 | 0.000 | 0.158 | 0.000 |
| 14 | 0.140 | 0.200 | 0.050 | 0.285 | 0.325 | Y14 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 |
| 15 | 0.100 | 0.145 | 0.050 | 0.285 | 0.420 | Y15 | 0.421 | 0.579 | 0.000 | 0.000 | 0.000 |
| 16 | 0.140 | 0.200 | 0.050 | 0.285 | 0.325 | Y16 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 |
| 17 | 0.100 | 0.200 | 0.050 | 0.285 | 0.365 | Y17 | 0.421 | 0.000 | 0.000 | 0.000 | 0.579 |
| 18 | 0.140 | 0.195 | 0.021 | 0.254 | 0.390 | Y18 | 0.001 | 0.050 | 0.307 | 0.324 | 0.318 |
| 19 | 0.140 | 0.200 | 0.050 | 0.238 | 0.372 | Y19 | 0.000 | 0.000 | 0.000 | 0.492 | 0.508 |
| 20 | 0.140 | 0.150 | 0.005 | 0.285 | 0.420 | Y20 | 0.000 | 0.526 | 0.474 | 0.000 | 0.000 |
| 21 | 0.140 | 0.163 | 0.029 | 0.249 | 0.420 | Y21 | 0.000 | 0.394 | 0.223 | 0.384 | 0.000 |
| 22 | 0.140 | 0.200 | 0.020 | 0.220 | 0.420 | Y22 | 0.000 | 0.000 | 0.316 | 0.684 | 0.000 |
| 23 | 0.100 | 0.190 | 0.005 | 0.285 | 0.420 | Y23 | 0.421 | 0.105 | 0.474 | 0.000 | 0.000 |
| 24 | 0.140 | 0.152 | 0.050 | 0.285 | 0.373 | Y24 | 0.000 | 0.507 | 0.000 | 0.000 | 0.493 |
| 25 | 0.109 | 0.168 | 0.050 | 0.253 | 0.420 | Y25 | 0.331 | 0.333 | 0.000 | 0.336 | 0.000 |

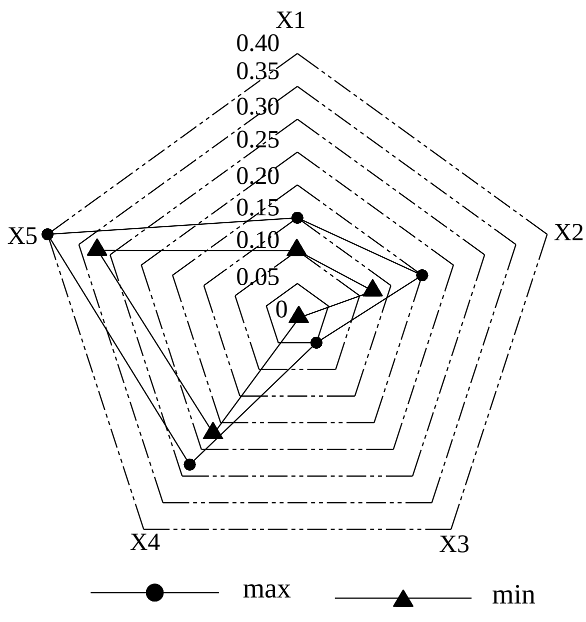


**Figure 9. Array factor space of the 5- component simplex of concrete production**

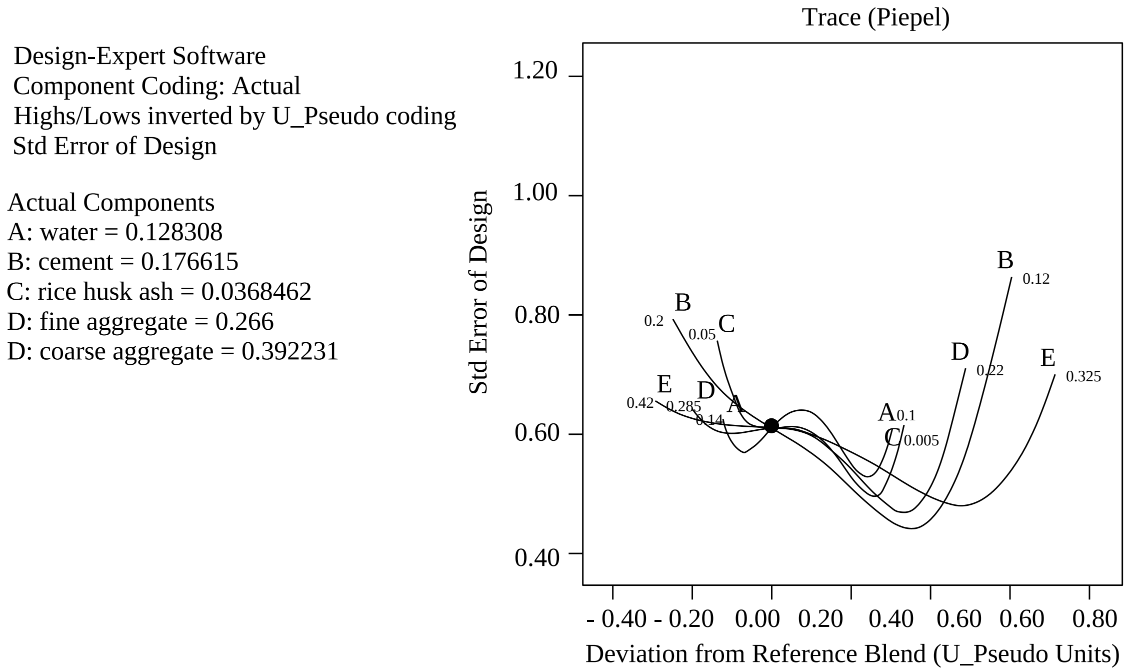


**Figure 10. Trace and deviation factor space of the 5- component mixture for concrete production**

**Table 14. 4- Component experimental mix proportions [26, 27]**

| Runs | Actual Components | | | | Response | Pseudo Components | | | |
|---|---|---|---|---|---|---|---|---|---|
| | z1 | z2 | z3 | z4 | | x1 | x2 | x3 | x4 |
| 1 | 0.010 | 0.540 | 0.420 | 0.030 | Y1 | 0.308 | 0.462 | 0.231 | 0.000 |
| 2 | 0.031 | 0.545 | 0.409 | 0.016 | Y2 | 0.147 | 0.424 | 0.319 | 0.110 |
| 3 | 0.030 | 0.500 | 0.450 | 0.021 | Y3 | 0.158 | 0.769 | 0.000 | 0.073 |
| 4 | 0.010 | 0.539 | 0.450 | 0.002 | Y4 | 0.308 | 0.473 | 0.000 | 0.219 |
| 5 | 0.031 | 0.545 | 0.409 | 0.016 | Y5 | 0.147 | 0.424 | 0.319 | 0.110 |
| 6 | 0.030 | 0.500 | 0.450 | 0.021 | Y6 | 0.158 | 0.769 | 0.000 | 0.073 |
| 7 | 0.010 | 0.600 | 0.379 | 0.011 | Y7 | 0.308 | 0.000 | 0.546 | 0.146 |
| 8 | 0.031 | 0.545 | 0.409 | 0.016 | Y8 | 0.147 | 0.424 | 0.319 | 0.110 |
| 9 | 0.010 | 0.570 | 0.390 | 0.030 | Y9 | 0.308 | 0.231 | 0.462 | 0.000 |
| 10 | 0.030 | 0.600 | 0.340 | 0.030 | Y10 | 0.154 | 0.000 | 0.846 | 0.000 |
| 11 | 0.050 | 0.500 | 0.420 | 0.030 | Y11 | 0.000 | 0.769 | 0.231 | 0.000 |
| 12 | 0.040 | 0.522 | 0.429 | 0.009 | Y12 | 0.074 | 0.597 | 0.165 | 0.164 |
| 13 | 0.010 | 0.600 | 0.360 | 0.030 | Y13 | 0.308 | 0.000 | 0.692 | 0.000 |
| 14 | 0.023 | 0.580 | 0.396 | 0.002 | Y14 | 0.205 | 0.158 | 0.418 | 0.219 |
| 15 | 0.050 | 0.600 | 0.320 | 0.030 | Y15 | 0.000 | 0.000 | 1.000 | 0.000 |
| 16 | 0.010 | 0.510 | 0.450 | 0.030 | Y16 | 0.308 | 0.692 | 0.000 | 0.000 |
| 17 | 0.050 | 0.600 | 0.320 | 0.030 | Y17 | 0.000 | 0.000 | 1.000 | 0.000 |
| 18 | 0.050 | 0.600 | 0.349 | 0.002 | Y18 | 0.000 | 0.000 | 0.781 | 0.219 |
| 19 | 0.050 | 0.550 | 0.384 | 0.016 | Y19 | 0.000 | 0.385 | 0.506 | 0.110 |
| 20 | 0.010 | 0.559 | 0.430 | 0.002 | Y20 | 0.308 | 0.315 | 0.158 | 0.219 |
| 21 | 0.010 | 0.600 | 0.379 | 0.011 | Y21 | 0.308 | 0.000 | 0.546 | 0.146 |
| 22 | 0.050 | 0.550 | 0.384 | 0.016 | Y22 | 0.000 | 0.385 | 0.506 | 0.110 |
| 23 | 0.050 | 0.567 | 0.353 | 0.030 | Y23 | 0.000 | 0.256 | 0.744 | 0.000 |
| 24 | 0.023 | 0.580 | 0.396 | 0.002 | Y24 | 0.205 | 0.158 | 0.418 | 0.219 |
| 25 | 0.050 | 0.500 | 0.449 | 0.002 | Y25 | 0.000 | 0.769 | 0.012 | 0.219 |

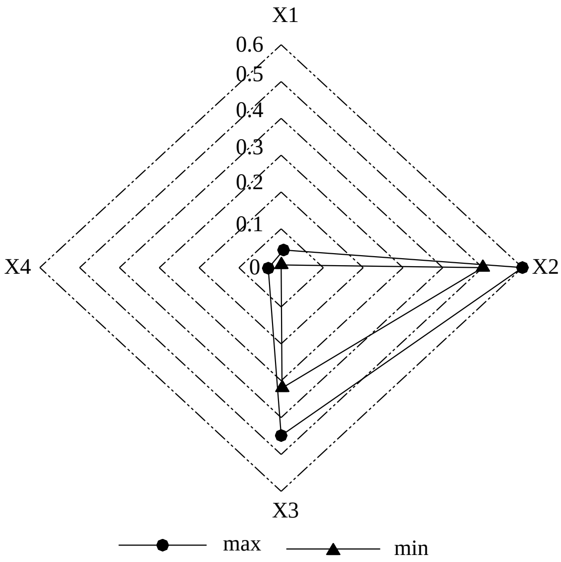


**Figure 11. Array factor space of the 4- component simplex of asphalt production**

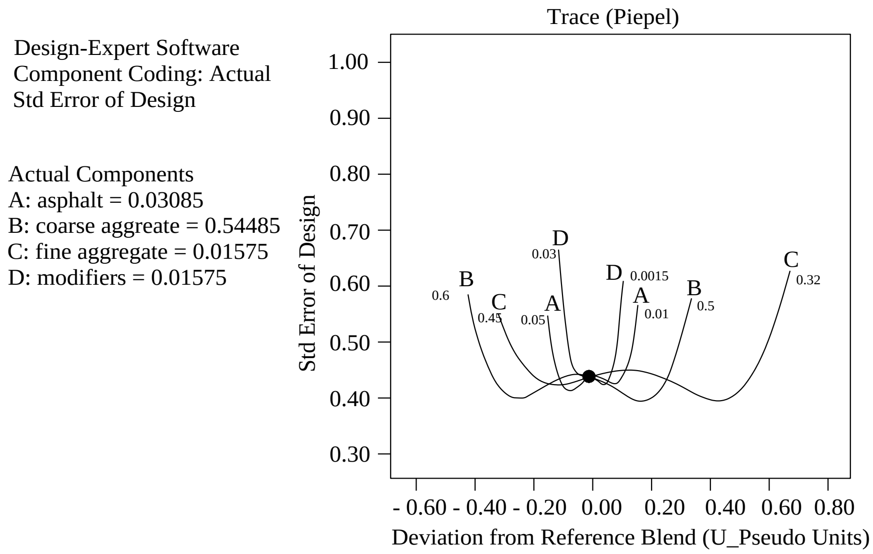


**Figure 12. Trace and deviation factor space of the 4- component mixture for asphalt production**

**Table 15. 3- Component experimental mix proportions for soil stabilization [26, 27]**

| Runs | Actual Components | | | Response | Pseudo Components | | |
|---|---|---|---|---|---|---|---|
| | z1 | z2 | z3 | | x1 | x2 | x3 |
| 1 | 0.333 | 0.143 | 0.524 | Y1 | 0.551 | 0.289 | 0.159 |
| 2 | 0.300 | 0.100 | 0.600 | Y2 | 0.333 | 0.000 | 0.667 |
| 3 | 0.325 | 0.125 | 0.550 | Y3 | 0.500 | 0.167 | 0.333 |
| 4 | 0.400 | 0.100 | 0.500 | Y4 | 1.000 | 0.000 | 0.000 |
| 5 | 0.352 | 0.100 | 0.548 | Y5 | 0.679 | 0.000 | 0.321 |
| 6 | 0.371 | 0.129 | 0.500 | Y6 | 0.804 | 0.196 | 0.000 |
| 7 | 0.300 | 0.100 | 0.600 | Y7 | 0.333 | 0.000 | 0.667 |
| 8 | 0.298 | 0.129 | 0.573 | Y8 | 0.322 | 0.193 | 0.485 |
| 9 | 0.350 | 0.150 | 0.500 | Y9 | 0.667 | 0.333 | 0.000 |
| 10 | 0.400 | 0.100 | 0.500 | Y10 | 1.000 | 0.000 | 0.000 |
| 11 | 0.250 | 0.150 | 0.600 | Y11 | 0.000 | 0.333 | 0.667 |
| 12 | 0.325 | 0.125 | 0.550 | Y12 | 0.500 | 0.167 | 0.333 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 13 | 0.400 | 0.100 | 0.500 | Y13 | 1.000 | 0.000 | 0.000 |
| 14 | 0.350 | 0.150 | 0.500 | Y14 | 0.667 | 0.333 | 0.000 |
| 15 | 0.325 | 0.125 | 0.550 | Y15 | 0.500 | 0.167 | 0.333 |
| 16 | 0.275 | 0.125 | 0.600 | Y16 | 0.165 | 0.169 | 0.667 |
| 17 | 0.371 | 0.129 | 0.500 | Y17 | 0.804 | 0.196 | 0.000 |
| 18 | 0.308 | 0.150 | 0.542 | Y18 | 0.390 | 0.333 | 0.277 |
| 19 | 0.308 | 0.150 | 0.542 | Y19 | 0.390 | 0.333 | 0.277 |
| 20 | 0.373 | 0.105 | 0.522 | Y20 | 0.818 | 0.032 | 0.149 |
| 21 | 0.275 | 0.125 | 0.600 | Y21 | 0.165 | 0.169 | 0.667 |
| 22 | 0.325 | 0.125 | 0.550 | Y22 | 0.500 | 0.167 | 0.333 |
| 23 | 0.325 | 0.125 | 0.550 | Y23 | 0.500 | 0.167 | 0.333 |
| 24 | 0.325 | 0.100 | 0.575 | Y24 | 0.497 | 0.000 | 0.503 |
| 25 | 0.250 | 0.150 | 0.600 | Y25 | 0.000 | 0.333 | 0.667 |

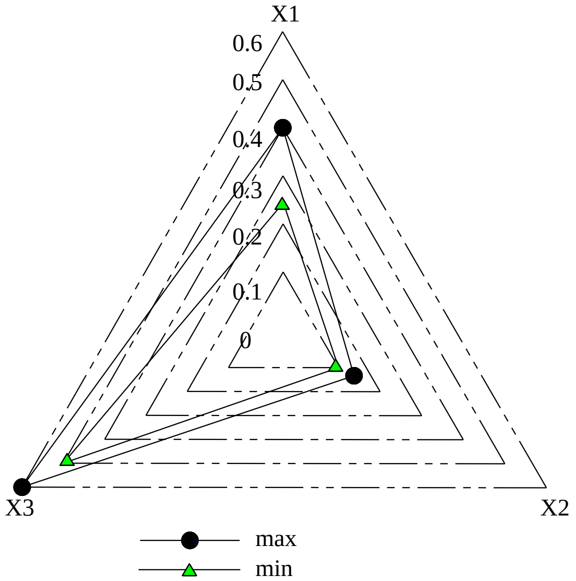


**Figure 13. Array factor space of the 3- component simplex of soil stabilization**

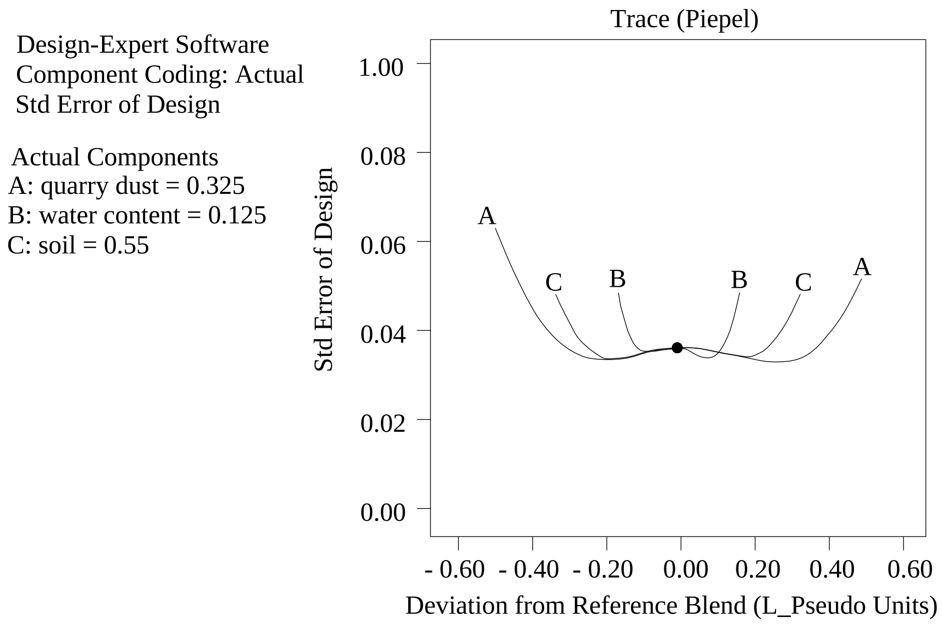


**Figure 14. Trace and deviation factor space of the 3- component mixture for soil stabilization**

**Table 16. 2- Component experimental mix proportions for concrete modification [26, 27]**

| Runs | actual components | | response | pseudo components | |
|---|---|---|---|---|---|
| | z1 | z2 | | x1 | x2 |
| 1 | 0.315 | 0.685 | Y1 | 0.500 | 0.500 |
| 2 | 0.280 | 0.720 | Y2 | 0.000 | 1.000 |
| 3 | 0.333 | 0.668 | Y3 | 0.750 | 0.250 |
| 4 | 0.303 | 0.697 | Y4 | 0.333 | 0.667 |
| 5 | 0.298 | 0.703 | Y5 | 0.250 | 0.750 |
| 6 | 0.327 | 0.673 | Y6 | 0.667 | 0.333 |
| 7 | 0.350 | 0.650 | Y7 | 1.000 | 0.000 |

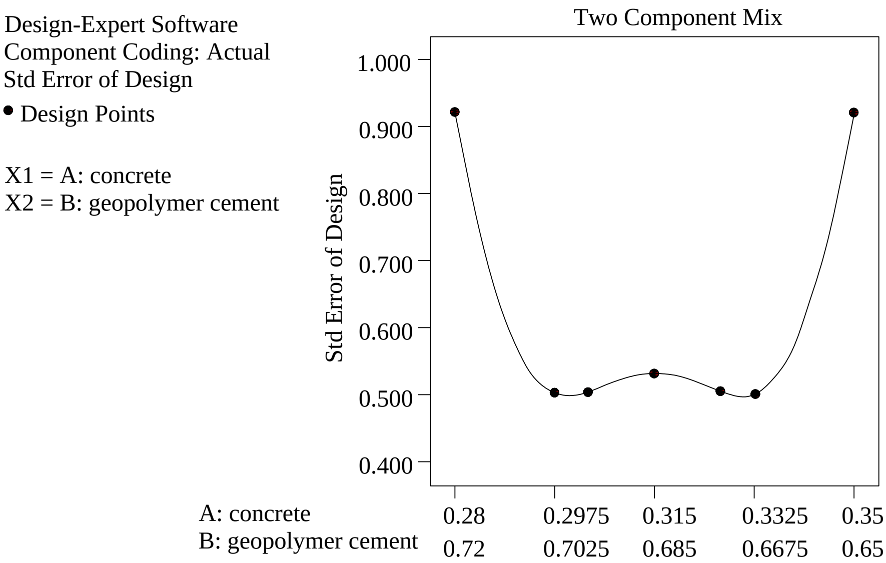


**Figure 15. Trace and deviation factor space of the 2- component mixture for homogenous mixtures**

## 4. Experimental Program

This is the laboratory investigation phase of the optimization exercise where the component mixes or mix proportions generated from the Minitab and design-expert manipulation of the constraints situations of the different combinations would be used to prepare laboratory specimens according to the number of runs and replicates. The tables of mix proportions are the fundamental guide in the operation. For the purpose of exactness and error proof exercise, the specimens are to be replicated three over and an average value estimated in the end. This value becomes the responses to be utilized in the future modeling exercises. To begin with, all the materials characterization investigations are to be carried out to enable proper materials classification and behavioral observation. The four cases being reviewed in this work have their peculiar characteristics. Soils stabilization, concrete production study, asphalt production and concrete improvement or water treatment exercises have been cited as special and general case scenarios in civil engineering works and this serves as a hub and guide to all other works of component mixture experimentation design in civil engineering.

## 5. Results Validation and Adequacy Tests

The analysis of variance (ANOVA) is the tool to be adopted to test for validity and adequacy of the experimental and mathematical modeling operation. With a tested hypothesis under 95% confidence level, the design of experimental protocol would be validated or not [26, 27]. The test for adequacy of the model is usually done using Fischer test at 95% confidence level on the behavioral properties being studied. In this test, two hypotheses would be set as follows:

Null Hypothesis: this states that “there is no significant difference between the laboratory tests and model predicted and the Alternative Hypothesis: states as follows “there is a significant difference between the laboratory test and model predicted”. A two-tail test (inequality) will be conducted in this case and if t Stat < -t Critical two-tail or t Stat > t Critical two-tail, we reject the null hypothesis [26, 27]. In ANOVA validation of designs, if F > F crit, we reject the null hypothesis [26, 27]. The developed models can also be tested by writing a representative MATLAB program and observe the running efficiency of the program.

## 6. Conclusion

This work has reviewed the use of extreme vertex design in the modeling of the behavior of multicomponent mixture of mixture experiments in civil engineering and composite materials formulation of mechanical engineering designs. Four special cases were cited which were 5-, 4-, 3-, and 2- component mixture experiments of concrete production, asphalt production, soil stabilization and concrete improvement or water treatment exercises. It has shown that these cases can be extrapolated to deal with similar cases in not only civil engineering designs but also in materials engineering, agricultural and bio-resources engineering, chemical engineering, mechanical engineering, polymer and textile engineering, optimization of most production operations in engineering, etc. The cases reviewed yielded results that would eventually guide future users of this optimization technique in civil engineering works and other mixture component modeling works as a hub. The development of constraints is an interesting part of this exercise because it helped in defining the factor space within which experimental points are to be studied for optimal mixture effects.

## 7. Funding

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## 8. Conflict of Interests

The authors declare no conflict of interest.

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