An Ideal Four-Factor Components Mixture Experiment Design Based on Prominent Optimality Criteria at Level Two

ABSTRACT

Aim: *Mixture experiment designs are essential tools that need to be determined prior to conducting any mixture experiment in any field of study. The primary goal of these types of experiments are optimization that is either maximizing the profit/produce or minimizing the cost of production.*

Study Design: *Any researcher anticipating to do any research work on the mixture experiment will not evade to talk about the design that he or she is likely to use. The common of such designs being either Simplex Lattice Design (SLD) or Simplex Centroid Design (SCD).*

Methodology: *The choice of such design is wholly based on the optimality criteria employed. The classical of these criteria include on D-Determinant criterion, A-Average variance criterion, E- Eigen value criterion and T- Trace optimality criterion usually denoted as D-, A-, E- T- criteria. They are also known as prominent criteria.*

Results: *This paper considered four-factor components at order two. The penalized moment matrices obtained from the information matrices whose primary source was the design points gave the values of the criteria aforementioned. These values were ranked independently with the least average rank termed as the best design.*

Conclusion: *The {4,4} Simplex Lattice Design had the lowest rank value of 1.0 as compared to the other designs. This design is therefore to be used in any research work considering four factors when only two of factors are to be employed.*

Keywords**:** *Mixture experiment, optimization, design, Simplex-Lattice, Simplex-Centroid, optimality criteria, prominent, average rank value*.

1. INTRODUCTION.

Optimal designs are standard ways that are mathematically proven to be meeting certain minimal threshold that often times give unique solutions. They are essential as to compare to non-optimal designs in that they aid in familiarising with the experiment before the actual study is done. They provide also crucial information like probable cost of the research, the overall outline of the experiment, the factors to be encompassed in the experiment and the runs/plots thereof among others. Additionally, optimizing refers to the process of maximizing or minimising something depending with the output of interest. The common instance of optimizing is minimising the cost and maximizing the yield/profit.

A design is usually selected based on certain criterion. The common criteria that are used in optimization include; D-optimality, E-optimality, A- optimality, T- optimality, G-optimality, I-optimality, MV-optimality among others. (Ashish, 2002)

Let X be $n * p$ matrix that is constructed to obtain the desired matrix. This indicates that to obtain the information matrix is given as X^TX. Dividing information matrix by N yields $(\frac{X^TX}{N})$ which is moment matrix, where N is the total number of runs/plots and tend to equalize the design. The information matrix is crucial since it provides essential properties pertaining the response of interest i.e., it has statistical properties. D-optimality is taken to be the one that has the maximum or highest value of determinant or the minimum value of inverse of the information matrix. To standardize and to remove outliers in a given design, D-Efficiency is usually, D-efficiency = $(\frac{100}{N})*|X^TX|^{1/p}$, where N is the total number of runs, in a given experiment and p is the total number of parameters in a given model. A –optimality is the design that has maximum value of average-variance in information matrix (or the minimum value of average variance of inverse of information matrix). Like the D optimality, it has to be standardized, thus A efficiency = $\frac{100p}{trace[N(X'X)^{-1}]}$. (Lawson, 2011)

Criteria that are commonly in use include determinant (D-optimality), average-variance (A-optimality), Eigen value (E-optimality) and trace (T-optimality) criterion. These criteria are usually referred to as classical or prominent criteria. To obtain such values, according to Pukelsheim (2006) we have the following;

D-optimality= (det $(X^TX))^{1/}$p of which the minimum value takes 0. p is the number of parameters that tend to penalize the design

A-optimality = $(\frac{1}{p}*\text{trace }(X^TX)^{-1})^{-1}$ of which the minimal value is taken. Usually, it is -1

E- Optimality = $\lambda_{min}(X^TX)$. The minimum is usually $-\infty$

T- optimality = $\frac{1}{p}*(X^TX)$, the minimum is 1.

Optimal designs provide useful information depending on the interest of a given design. Some provide information about the model, prediction inside the lattice space, the general layout of the design and the probable number of runs that might be considered among others. For a given moment matrix, say, M it is usually given as M = $(\frac{X^TX}{N})$, taking determinant i.e., |M| = $(\frac{|X^TX|}{N^p})$. There is a close relationship between moment matrix and variance-covariance matrix. D-optimality design maximizes |M| = $(\frac{|X^TX|}{N^p})$ and also maximizes trace of M, i.e., |M| = $(\frac{|X^TX|}{N})$. Thus, moment matrix is a key player in the determination of the design based on optimality criteria. (Cook, 2009).

2. METHODOLOGY

2.1 Useful equations in Mixture Experiment

Mathematically speaking, suppose that are q constituents in the study then to get the i[th] constituent in the mixture represented as x_i, is given by

$$Xi \geq 0, \ i = 1, 2, 3, \dots q \qquad (1)$$

(For this study q = 4)

The nonnegative constituents must sum to one as indicated in equation 2.

$$\sum_{i=1}^{q} Xi = X1 + X2 + X3 + X4 = 1 \qquad (2)$$

The main objective of this research was to establish the best mixture design that will be employed in any four-factor mixture experiment that will yield maximally holding all factors constant.

Equation (2) above is very vital because all proportions that makes part of the mixture experiment will be restricted by it. Furthermore, it can represent single component that is a pure mixture or fractions of components under test all adding to one. Scheffe (1963)

In this study, let $X1$, $X2$, $X3$ and $X4$ represent component 1, component 2, component 3 and component 4 respectively.

2.2 The Simplex Lattice Design

A lattice may have a special correspondence to a specific polynomial equation. To support a polynomial model of degree *m* in *q* components over the simplex, the lattice, referred to as a $\{q, m\}$ Simplex-Lattice Design, consists of points whose coordinates are well-defined by the following combinations of the component proportions: the proportions assumed by each component take the *m* + 1 equally spaced values from 0 to 1, that is,

$$X_i = 0, 1/m, 2/m, 3/m, \dots, 1 \qquad (3)$$

and the *{q, m)* simplex-lattice consists of *all* possible combinations (mixtures) of the components where the proportion(s) for each constituent are used. (Cornell 2002)

In this research, four components were considered. This implies that the component system will be containing all the possible mixture in the entire factor space which is a tetrahedron. Its four vertices will be representing the pure mixture denoted by Xi = 1, j = 0 for i, j = 1, 2, 3 and 4, i ≠ j. The edges represent blend between any two given constituents, say, Xij , i < j. In addition, the internal central points of the simplex will be representing the mixture of the four manures under consideration of which non is missing.

In the simplex-lattice design, usually denoted as $\{q, m\}$, we can come up with a number of designs and design points that will be used as runs (plots) to give the response of interest. In this case, the maximum component is four, q = 4. Therefore, we vary the value of m to either 2, 3, or 4 so as to come up with 3 different types of simplex-lattice design which eventually will have different experimental points as discussed in detailed as below. In the design $\{q, m\}$, m does not take the value of one (1) because all other designs will always have to contain it. When m = 1, this represents single-mixture experiment.

2.2.1 Experimental points of {4, 2} Simplex Lattice Design.

To obtain this design we let the value of m to 2, m = 2, in equation (3) above. This will result into three (3) equally spaced proportions of 0, 0.5 and 1. These proportions will be used to indicate the experimental points within which response of interest is to be determined at. Thus, {4, 2} SLD will be having 10 design points to be considered independently. Among the 10 points four are pure mixtures while six are two component mixtures.
The design is as shown below:

Table 1. The layout of experimental points in {4, 2} Simplex-Lattice Design

Experimental Points	Mixture Type	{4, 2} design Components X1	X2	X3	X4	Observed Response
1	Pure	1	0	0	0	Y1
2	Pure	0	1	0	0	Y2
3	Pure	0	0	1	0	Y3
4	Pure	0	0	0	1	Y4
5	Binary	0.5	0.5	0	0	Y12
6	Binary	0.5	0	0.5	0	Y13
7	Binary	0.5	0	0	0.5	Y14
8	Binary	0	0.5	0.5	0	Y23
9	Binary	0	0.5	0	0.5	Y24
10	Binary	0	0	0.5	0.5	Y34

2.2.2 Experimental points of {4, 3} Simplex Lattice Design.

To come up with {4, 3} SLD, we let the value of m =3. Using equation 3 above, we will have four points that are all equidistant from each other within the simplex factor space in the aforementioned tetrahedron. These points are 0, 0.33, 0.67 and 1. Fixing these design points will result into the following layout, which has four pure mixture, twelve double mixture and four triple mixture design points summing to 20 experimental points.
Table 2 gives the experimental design points of {4, 3} SLD;

Table 2. The layout of experimental points in {4, 3} Simplex-Lattice Design

	{4, 3} design				
Experimental Points	Components				Observed Response
	X1	X2	X3	X4	
1	1	0	0	0	Y1
2	0	1	0	0	Y2
3	0	0	1	0	Y3
4	0	0	0	1	Y4
5	0.33	0.67	0	0	Y12
6	0.33	0	0.67	0	Y13
7	0.33	0	0	0.67	Y14
8	0	0.33	0.67	0	Y23
9	0	0.33	0	0.67	Y24
10	0	0	0.33	0.67	Y34
11	0.67	0.33	0	0	Y12*
12	0.67	0	0.33	0	Y13*
13	0.67	0	0	0.33	Y14*
14	0	0.67	0.33	0	Y23*
15	0	0.67	0	0.33	Y24*
16	0	0	0.67	0.33	Y34*
17	0.33	0.33	0.33	0	Y123
18	0.33	0.33	0	0.33	Y124
19	0.33	0	0.33	0.33	Y134
20	0	0.33	0.33	0.33	Y234

* Implies the second time a particular set of components is mixed at a given proportion different from the first case.

2.2.3 Experimental points of {4, 4} Simplex Lattice Design.

Similarly, to come up with {4, 4} Simplex Lattice Design is also obtained using the same application as of the prior designs above. In this scenario, m = 4, substituting the value of m in the equation 3 above we will obtain five different particular points that are to be combined so as to come with the required design. These five points are 0, 0.25, 0.5, 0.75 and 1. Table 3 gives all the possible combination of components present summing up to unity when each one at a time is considered. The design will have 35 different experimental points (plots), which are autonomous. Out of the 35 plots, four (4) are of pure mixture, eighteen (18) are of double mixture component, twelve (12) are of triple mixture component and only one (1) is four-mixture component.

Table 3. The layout of experimental points in {4, 4} Simplex-Lattice Design

{4, 4} design

Experimental Points	Components				Observed Response
	X1	X2	X3	X4	
1	1	0	0	0	Y1
2	0	1	0	0	Y2
3	0	0	1	0	Y3
4	0	0	0	1	Y4
5	0.25	0.75	0	0	Y12
6	0.25	0	0.75	0	Y13
7	0.25	0	0	0.75	Y14
8	0	0.25	0.75	0	Y23
9	0	0.25	0	0.75	Y24
10	0	0	0.25	0.75	Y34
11	0.75	0.25	0	0	Y12*
12	0.75	0	0.25	0	Y13*
13	0.75	0	0	0.25	Y14*
14	0	0.75	0.25	0	Y23*
15	0	0.75	0	0.25	Y24*
16	0	0	0.75	0.25	Y34*
17	0.5	0.5	0	0	Y12**
18	0.5	0	0.5	0	Y13**
19	0.5	0	0	0.5	Y14**
20	0	0.5	0.5	0	Y23**
21	0	0.5	0	0.5	Y24**
22	0	0	0.5	0.5	Y34**
23	0.25	0.25	0.5	0	Y123
24	0.25	0.25	0	0.5	Y124
25	0.25	0	0.25	0.5	Y134
26	0.25	0.5	0.25	0	Y123*
27	0.25	0.5	0	0.25	Y124*
28	0.25	0	0.5	0.25	Y134*
29	0	0.25	0.25	0.5	Y234
30	0	0.25	0.5	0.25	Y234*
31	0.5	0.25	0.25	0	Y123**
32	0.5	0.25	0	0.25	Y124**
33	0.5	0	0.25	0.25	Y134**
34	0	0.5	0.25	0.25	Y234**
35	0.25	0.25	0.25	0.25	Y1234

* Implies the second time yield of a particular set of components is mixed at a given proportion different from the first case while ** is its third appearance.

In summary, combining all the three types of simplex-lattices designs so far discussed above, we will have the following layout. This structure shows experimental points, type of mixture, the four components under consideration and the expected response.

From the summary table 4, the total number of runs/plots to be looked at stands at 57. Out of which 4 are of pure mixture, 36 are of double-component experiment, 16 are of triple-component mixture and only 1 quinary i.e., contain all the four types of components, all at the same proportion equidistant from the centre of the tetrahedron. However, after final determination of the criteria, one and only one of the above designs will be used that meet the minimum threshold.

Table 4. The layout of all experimental points in overall 4-factor component Simplex-Lattice Design

Exp. Points	Type	{4, 2} design Components				{4, 3} design Components				{4, 4} design Components				Obs. Resp
		X1	X2	X3	X4	X1	X2	X3	X4	X1	X2	X3	X4	
1	Pure	1	0	0	0	1	0	0	0	1	0	0	0	Y1
2	Pure	0	1	0	0	0	1	0	0	0	1	0	0	Y2
3	Pure	0	0	1	0	0	0	1	0	0	0	1	0	Y3
4	Pure	0	0	0	1	0	0	0	1	0	0	0	1	Y4
5	Binary	0.5	0.5	0	0	0.33	0.67	0	0	0.25	0.75	0	0	Y12
6	Binary	0.5	0	0.5	0	0.33	0	0.67	0	0.25	0	0.75	0	Y13
7	Binary	0.5	0	0	0.5	0.33	0	0	0.67	0.25	0	0	0.75	Y14
8	Binary	0	0.5	0.5	0	0	0.33	0.67	0	0	0.25	0.75	0	Y23
9	Binary	0	0.5	0	0.5	0	0.33	0	0.67	0	0.25	0	0.75	Y24
10	Binary	0	0	0.5	0.5	0	0	0.33	0.67	0	0	0.25	0.75	Y34
11	Binary					0.67	0.33	0	0	0.75	0.25	0	0	Y12*
12	Binary					0.67	0	0.33	0	0.75	0	0.25	0	Y13*
13	Binary					0.67	0	0	0.33	0.75	0	0	0.25	Y14*
14	Binary					0	0.67	0.33	0	0	0.75	0.25	0	Y23*
15	Binary					0	0.67	0	0.33	0	0.75	0	0.25	Y24*
16	Binary					0	0	0.67	0.33	0	0	0.75	0.25	Y34*
17	Binary									0.5	0.5	0	0	Y12**
18	Binary									0.5	0	0.5	0	Y13**
19	Binary									0.5	0	0	0.5	Y14**
20	Binary									0	0.5	0.5	0	Y23**
21	Binary									0	0.5	0	0.5	Y24**

22	Binary					0	0	0.5	0.5	Y34**
23	Ternary	0.33	0.33	0.33	0	0.25	0.25	0.5	0	Y123
24	Ternary	0.33	0.33	0	0.33	0.25	0.25	0	0.5	Y124
25	Ternary	0.33	0	0.33	0.33	0.25	0	0.25	0.5	Y134
26	Ternary					0.25	0.5	0.25	0	Y123*
27	Ternary					0.25	0.5	0	0.25	Y124*
28	Ternary					0.25	0	0.5	0.25	Y134*
29	Ternary	0	0.33	0.33	0.33	0	0.25	0.25	0.5	Y234
30	Ternary					0	0.25	0.5	0.25	Y234*
31	Ternary					0.5	0.25	0.25	0	Y123**
32	Ternary					0.5	0.25	0	0.25	Y124**
33	Ternary					0.5	0	0.25	0.25	Y134**
34	Ternary					0	0.5	0.25	0.25	Y234**
35	Quinary					0.25	0.25	0.25	0.25	Y1234

* Implies the second time yield of a particular set of components is mixed at a given proportion different from the first case while ** is its third appearance.

2.3 Experimental points of Simplex-Centroid Design

Considering a q-component simplex-centroid design, the numeral of distinct points is $2^q - 1$.
These points correspond to q permutations of (1, 0, 0, . . ., 0) or q single-component blends, the $\binom{q}{2}$ permutations of *(½, ½*, 0, ..., 0) or all binary mixtures, the $\binom{q}{3}$ permutations of ($1/3$, $1/3$, $1/3$, 0, ..., 0), . . ., and so on, with finally the overall centroid point *($1/q$, $1/q$, …, $1/q$)* or q-nary mixture. Cornel (2002).

From the understanding of the above explanation on how to obtain Simplex-Centroid Design, it can be seen that components to be contained in the design must always appear in equal proportions. The experimental points are all located within the simplex designs that are dimensionally (q-1). At the autonomous experimental points in the simplex-centroid design, the response of interest will be collected and a polynomial equation modeled to explain the effects of each component type singly or in their combination. In this research work, the all-out number of variables is 4. Hence an appropriate model that will explain the effect of single component, double-component parameter, triple-component parameter and lastly one with all the four types of components considered. Just like the simplex-lattice design, the simplex-centroid will be having four component systems as its entire factor space which is also a tetrahedron. Table 5 illustrates the experimental points by use the centroid study design.

The design gives a total of 15 experimental points out of which 4 are of single-component, 6 are of double-component, 4 are of triple-component and 1 quinary-component, i.e., contains all the four types of components in equal proportions.

Table 5. The layout of all experimental points in Simplex-Centroid Design

Experimental Points	Mixture Type	Simplex-Centroid Design Components				Exp. Response
		X1	X2	X3	X4	
1	Pure	1	0	0	0	Y1

2	Pure	0	1	0	0	Y2
3	Pure	0	0	1	0	Y3
4	Pure	0	0	0	1	Y4
5	Binary	0.5	0.5	0	0	Y12
6	Binary	0.5	0	0.5	0	Y13
7	Binary	0.5	0	0	0.5	Y14
8	Binary	0	0.5	0.5	0	Y23
9	Binary	0	0.5	0	0.5	Y24
10	Binary	0	0	0.5	0.5	Y34
11	Ternary	0.33	0.33	0.33	0	Y123
12	Ternary	0.33	0.33	0	0.33	Y124
13	Ternary	0.33	0	0.33	0.33	Y134
14	Ternary	0	0.33	0.33	0.33	Y234
15	Quinary (All)	0.25	0.25	0.25	0.25	Y1234

3. RESULTS AND DISCUSSION

3.1 Designs

Two main types of mixture experiment designs, simplex-lattice and simplex-centroid designs, were put into consideration in regard to their respective criteria values. There was a need to do these prior so as the best design was to be obtained and implemented for any mixture experiment study that has to put into consideration four components.

3.1.1 The {4, 2} Simplex-Lattice Design

With the help of experimental points in Table 1, the following is the information matrix obtained from the resultant matrix i.e., $M = X^T X$. The information matrix of {4, 2} Simplex-Lattice Design is given as bellow;

$$M = \begin{pmatrix} 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.50 & 0.50 & 0.00 & 0.00 & 0.25 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.50 & 0.00 & 0.50 & 0.00 & 0.00 & 0.25 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.50 & 0.50 & 0.00 & 0.00 & 0.00 & 0.00 & 0.25 & 0.00 & 0.00 \\ 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.50 & 0.00 & 0.00 & 0.50 & 0.00 & 0.00 & 0.25 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.50 & 0.00 & 0.50 & 0.00 & 0.00 & 0.00 & 0.00 & 0.25 & 0.00 \\ 0.00 & 0.00 & 0.50 & 0.50 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0..25 \\ 0.00 & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \end{pmatrix}$$

The moment matrix for this design given as $\mathbf{N = M^{-1}M/}p$, where p is the number of plots or runs is given below as indicated. Thus,

$$N = \begin{pmatrix}
0.1750 & 0.0250 & 0.0250 & 0.0250 & 0.0125 & 0.0125 & 0.0125 & 0.0000 & 0.0000 & 0.0000 \\
0.0250 & 0.1750 & 0.0250 & 0.0250 & 0.0125 & 0.0000 & 0.0000 & 0.0125 & 0.0125 & 0.0000 \\
0.0250 & 0.0250 & 0.1750 & 0.0250 & 0.0000 & 0.0125 & 0.0000 & 0.0125 & 0.0000 & 0.0125 \\
0.0250 & 0.0250 & 0.0250 & 0.1750 & 0.0000 & 0.0000 & 0.0125 & 0.0000 & 0.0125 & 0.0125 \\
0..0125 & 0.0125 & 0.0000 & 0.0000 & 0.0063 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0125 & 0.0000 & 0.0125 & 0.0000 & 0.0000 & 0.0063 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0125 & 0.0000 & 0.0000 & 0.0125 & 0.0000 & 0.0000 & 0.0063 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0125 & 0.0125 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0063 & 0.0000 & 0.0000 \\
0.0000 & 0.0125 & 0.0000 & 0.0125 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0063 & 0.0000 \\
0.0000 & 0.0000 & 0.0125 & 0.0125 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0063
\end{pmatrix}$$

Thus, Determinant criterion, D-optimality = $\phi_0 (N) = (\det(N))^{1/p} = 5.960464e-18$, where p is the number of parameters that tend to penalize the design.

Average variance criterion, A-optimality = $\phi_{-1} (N) = (\frac{1}{p}*\text{trace} (N)^{-1})^{-1} = 148$

Smallest Eigen value Criterion, E- Optimality = $\phi_{-} (N) = \lambda_{min} (N) = 0.002462692$.
T- Optimality = $\frac{1}{p}*$ trace(N) = 0.073750.

3.1.2 The {4, 3} Simplex-Lattice Design

Table 2 shows the experimental design points of {4, 3} Design that was used to come up with the following information matrix and its resultant moment matrix i.e., $M = X^TX$.
The information matrix of {4, 3} SLD is given as follows;

$$M = \begin{pmatrix}
1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.6667 & 0.3333 & 0.0000 & 0.0000 & 0.2222 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.3333 & 0.6667 & 0.0000 & 0.0000 & 0.2222 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.6667 & 0.0000 & 0.3333 & 0.0000 & 0.0000 & 0.2222 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.3333 & 0.3333 & 0.3333 & 0.0000 & 0.1111 & 0.1111 & 0.0000 & 0.1111 & 0.0000 & 0.0000 \\
0.0000 & 0.6667 & 0.3333 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2222 & 0.0000 & 0.0000 \\
0.3333 & 0.0000 & 0.6667 & 0.0000 & 0.0000 & 0.2222 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.3333 & 0.6667 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2222 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.6667 & 0.0000 & 0.0000 & 0.3333 & 0.0000 & 0.0000 & 0.2222 & 0.0000 & 0.0000 & 0.0000 \\
0.3333 & 0.3333 & 0.0000 & 0.3333 & 0.1111 & 0.0000 & 0.1111 & 0.0000 & 0.1111 & 0.0000 \\
0.0000 & 0.6667 & 0.0000 & 0.3333 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2222 & 0.0000 \\
0.3333 & 0.0000 & 0.3333 & 0.3333 & 0.0000 & 0.1111 & 0.1111 & 0.0000 & 0.0000 & 0.1111 \\
0.0000 & 0.3333 & 0,3333 & 0.3333 & 0.0000 & 0.0000 & 0.0000 & 0.1111 & 0.1111 & 0.1111 \\
0.0000 & 0.0000 & 0.6667 & 0.3333 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2222 \\
0.3333 & 0.0000 & 0.0000 & 0.6667 & 0.0000 & 0.0000 & 0.2222 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.3333 & 0.0000 & 0.6667 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2222 & 0.0000 \\
0.0000 & 0.0000 & 0.3333 & 0.6667 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2222 \\
0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000
\end{pmatrix}$$

Its respective moment matrix is given as follows below; that is **N= M^{-1}M/**p**,** where p is the number of plots or runs. Hence,

$$N = \begin{pmatrix} 0.1500 & 0.0333 & 0.0333 & 0.0333 & 0.0148 & 0.0148 & 0.0148 & 0.0019 & 0.0019 & 0.0019 \\ 0.0333 & 0.1500 & 0.0333 & 0.0333 & 0.0148 & 0.0019 & 0.0019 & 0.0148 & 0.0148 & 0.0019 \\ 0.0333 & 0.0333 & 0.1500 & 0.0333 & 0.0019 & 0.0148 & 0.0019 & 0.0148 & 0.0019 & 0.0148 \\ 0.0333 & 0.0333 & 0.0333 & 0.1500 & 0.0019 & 0.0019 & 0.0148 & 0.0019 & 0.0148 & 0.0148 \\ 0.0148 & 0.0148 & 0.0019 & 0.0019 & 0.0062 & 0.0006 & 0.0006 & 0.0006 & 0.0006 & 0.0000 \\ 0.0148 & 0.0019 & 0.0148 & 0.0019 & 0.0006 & 0.0062 & 0.0006 & 0.0006 & 0.0000 & 0.0006 \\ 0.0148 & 0.0019 & 0.0019 & 0.0148 & 0.0006 & 0.0006 & 0.0062 & 0.0000 & 0.0006 & 0.0006 \\ 0.0019 & 0.0148 & 0.0148 & 0.0019 & 0.0006 & 0.0006 & 0.0000 & 0.0062 & 0.0006 & 0.0006 \\ 0.0019 & 0.0148 & 0.0019 & 0.0148 & 0.0006 & 0.0000 & 0.0006 & 0.0006 & 0.0062 & 0.0006 \\ 0.0019 & 0.0019 & 0.0148 & 0.0148 & 0.0000 & 0.0006 & 0.0006 & 0.0006 & 0.0006 & 0.0062 \end{pmatrix}$$

From this moment matrix above, the following values for the optimality are obtained.
D-optimality = ϕ_0 (N) = $(\det(N))^{1/p}$ = 6.82364e-19
Average variance criterion, A-optimality = ϕ_{-1} (N) = $(\frac{1}{p}*\text{trace } (N)^{-1})^{-1}$ = 94.41073
Smallest Eigen value Criterion, E- Optimality = ϕ_{-} (N) = λ_{min} (N) = 0.001923614
Trace criterion, T- Optimality = $\frac{1}{p}$* trace(N) = 0.0398148

3.1.3 The {4, 4} Simplex-Lattice Design

From Table 3 showing the experimental design points of {4, 4} SLD, information matrix and its resultant moment matrix i.e., M = X^TX is as shown below.

The information matrix for this design is also given as: -

$$
N = \begin{bmatrix}
1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.7500 & 0.2500 & 0.0000 & 0.0000 & 0.1875 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.5000 & 0.5000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.2500 & 0.7500 & 0.0000 & 0.0000 & 0.1875 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.7500 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.1875 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.5000 & 0.2500 & 0.2500 & 0.0000 & 0.1250 & 0.1250 & 0.0000 & 0.0625 & 0.0000 & 0.0000 \\
0.2500 & 0.5000 & 0.2500 & 0.0000 & 0.1250 & 0.0625 & 0.0000 & 0.1250 & 0.0000 & 0.0000 \\
0.0000 & 0.7500 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.1875 & 0.0000 & 0.0000 \\
0.5000 & 0.0000 & 0.5000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.2500 & 0.2500 & 0.5000 & 0.0000 & 0.0625 & 0.1250 & 0.0000 & 0.1250 & 0.0000 & 0.0000 \\
0.0000 & 0.5000 & 0.5000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 \\
0.2500 & 0.0000 & 0.7500 & 0.0000 & 0.0000 & 0.1875 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.2500 & 0.7500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.1875 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 1.000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.7500 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.1875 & 0.0000 & 0.0000 & 0.0000 \\
0.5000 & 0.2500 & 0.0000 & 0.2500 & 0.1250 & 0.0000 & 0.1250 & 0.0000 & 0.0625 & 0.0000 \\
0.2500 & 0.5000 & 0.0000 & 0.2500 & 0.1250 & 0.0000 & 0.0625 & 0.0000 & 0.1250 & 0.0000 \\
0.0000 & 0.7500 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.1875 & 0.0000 \\
0.5000 & 0.0000 & 0.2500 & 0.2500 & 0.0000 & 0.1250 & 0.1250 & 0.0000 & 0.0000 & 0.0625 \\
0.2500 & 0.2500 & 0.2500 & 0.2500 & 0.0625 & 0.0625 & 0.0625 & 0.0625 & 0.0625 & 0.0625 \\
0.0000 & 0.5000 & 0.2500 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.1250 & 0.1250 & 0.0625 \\
0.2500 & 0.0000 & 0.5000 & 0.2500 & 0.0000 & 0.1250 & 0.0625 & 0.0000 & 0.0000 & 0.1250 \\
0.0000 & 0.2500 & 0.5000 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.1250 & 0.0625 & 0.1250 \\
0.0000 & 0.0000 & 0.7500 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.1875 \\
0.5000 & 0.0000 & 0.0000 & 0.5000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.0000 \\
0.2500 & 0.2500 & 0.0000 & 0.5000 & 0.0625 & 0.0000 & 0.1250 & 0.0000 & 0.1250 & 0.0000 \\
0.0000 & 0.5000 & 0.0000 & 0.5000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 \\
0.2500 & 0.0000 & 0.2500 & 0.5000 & 0.0000 & 0.0625 & 0.1250 & 0.0000 & 0.0000 & 0.1250 \\
0.0000 & 0.2500 & 0.2500 & 0.5000 & 0.0000 & 0.0000 & 0.0000 & 0.0625 & 0.1250 & 0.1250 \\
0.0000 & 0.0000 & 0.5000 & 0.5000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2500 \\
0.2500 & 0.0000 & 0.0000 & 0.7500 & 0.0000 & 0.0000 & 0.1875 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.2500 & 0.0000 & 0.7500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.1875 & 0.0000 \\
0.0000 & 0.0000 & 0.2500 & 0.7500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.1875 \\
0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000
\end{bmatrix}
$$

The moment matrix for this design is given as below;

$$
N = \begin{pmatrix}
0.1375 & 0.0375 & 0.0375 & 0.0375 & 0.0156 & 0.0156 & 0.0156 & 0.0031 & 0.0031 & 0.0031 \\
0.0375 & 0.1375 & 0.0375 & 0.0375 & 0.0156 & 0.0031 & 0.0031 & 0.0156 & 0.0156 & 0.0031 \\
0.0375 & 0.0375 & 0.1375 & 0.0375 & 0.0031 & 0.0156 & 0.0031 & 0.0156 & 0.0031 & 0.0156 \\
0.0375 & 0.0375 & 0.0375 & 0.1375 & 0.0031 & 0.0031 & 0.0156 & 0.0031 & 0.0156 & 0.0156 \\
0.0156 & 0.0156 & 0.0031 & 0.0031 & 0.0059 & 0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0001 \\
0.0156 & 0.0031 & 0.0156 & 0.0031 & 0.0010 & 0.0059 & 0.0010 & 0.0010 & 0.0001 & 0.0010 \\
0.0156 & 0.0031 & 0.0031 & 0.0156 & 0.0010 & 0.0010 & 0.0059 & 0.0001 & 0.0010 & 0.0010 \\
0.0031 & 0.0156 & 0.0156 & 0.0031 & 0.0010 & 0.0010 & 0.0001 & 0.0059 & 0.0010 & 0.0010 \\
0.0031 & 0.0156 & 0.0031 & 0.0156 & 0.0010 & 0.0001 & 0.0010 & 0.0010 & 0.0059 & 0.0010 \\
0.0031 & 0.0031 & 0.0156 & 0.0156 & 0.0001 & 0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0059
\end{pmatrix}
$$

Similarly, as in the case of the above seen designs, the following values were obtained from this moment matrix of the {4, 4} SLD. They include,

Determinant Criterion, D-optimality = ϕ_0 (N) = $(\det(N))^{1/p}$ = 1.246503e-19

Average variance criterion, A-optimality = ϕ_{-1} (N) = $(\frac{1}{p}*\text{trace }(N)^{-1})^{-1}$ = 66.57143

Smallest Eigen value Criterion, E- Optimality = ϕ_{-} (N) = λ_{min} (N) = 0.001554355

Trace criterion, T- Optimality = $\frac{1}{p}*\text{trace}(N)$ = 0.016728

<u>3.1.4 The Simplex-Centroid Design</u>

For simplex-centroid design, the components to be contained in the design must always appear in equal proportions. The experimental points are all located within the simplex designs that are dimensionally (q-1) spaced. At the experimental points in the simplex-centroid design, the response of interest will be collected and a polynomial modeled to explain the effects of each component type singly or in their combination if the design is selected. In this study, the maximum number of variables is 4. Hence fit model that will explain the effect of single component, double-component parameter, triple-component parameters and lastly one with all the four types of components. Just like the simplex-lattice design, the simplex-centroid will be having four component systems as its entire factor space which is also a tetrahedron. The information matrix for the simplex-centroid design of the four-component mixture design is given as below;

$$M = \begin{pmatrix}
1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.5000 & 0.5000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.5000 & 0.0000 & 0.5000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.5000 & 0.0000 & 0.0000 & 0.5000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.5000 & 0.5000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 & 0.0000 \\
0.0000 & 0.5000 & 0.0000 & 0.5000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2500 & 0.0000 \\
0.0000 & 0.0000 & 0.5000 & 0.5000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.2500 \\
0.3300 & 0.3300 & 0.3300 & 0.0000 & 0.1089 & 0.1089 & 0.0000 & 0.1089 & 0.0000 & 0.0000 \\
0.3300 & 0.3300 & 0.0000 & 0.3300 & 0.1089 & 0.0000 & 0.1089 & 0.0000 & 0.1089 & 0.0000 \\
0.3300 & 0.0000 & 0.3300 & 0.3300 & 0.0000 & 0.1089 & 0.1089 & 0.0000 & 0.0000 & 0.1089 \\
0.0000 & 0.3300 & 0.3300 & 0.3300 & 0.0000 & 0.0000 & 0.0000 & 0.1089 & 0.1089 & 0.1089 \\
0.2500 & 0.2500 & 0.2500 & 0.2500 & 0.0625 & 0.0625 & 0.0625 & 0.0625 & 0.0625 & 0.0625
\end{pmatrix}$$

The moment matrix of the simplex-centroid design is given as below, i.e., $\mathbf{N} = \mathbf{M}^{-1}\mathbf{M}/p$,

$$N = \begin{pmatrix} 0.1426 & 0.0354 & 0.0354 & 0.0354 & 0.0142 & 0.0142 & 0.0142 & 0.0034 & 0.0034 & 0.0034 \\ 0.0354 & 0.1426 & 0.0354 & 0.0354 & 0.0142 & 0.0034 & 0.0034 & 0.0142 & 0.0142 & 0.0034 \\ 0.0354 & 0.0354 & 0.1426 & 0.0354 & 0.0034 & 0.0142 & 0.0034 & 0.0142 & 0.0034 & 0.0142 \\ 0.0354 & 0.0354 & 0.0354 & 0.1426 & 0.0034 & 0.0034 & 0.0142 & 0.0034 & 0.0142 & 0.0142 \\ 0.0142 & 0.0142 & 0.0034 & 0.0034 & 0.0060 & 0.0011 & 0.0011 & 0.0011 & 0.0011 & 0.0003 \\ 0.0142 & 0.0034 & 0.0142 & 0.0034 & 0.0011 & 0.0060 & 0.0011 & 0.0011 & 0.0003 & 0.0011 \\ 0.0142 & 0.0034 & 0.0034 & 0.0142 & 0.0011 & 0.0011 & 0.0060 & 0.0003 & 0.0011 & 0.0011 \\ 0.0034 & 0.0142 & 0.0142 & 0.0034 & 0.0011 & 0.0011 & 0.0003 & 0.0060 & 0.0011 & 0.0011 \\ 0.0034 & 0.0142 & 0.0034 & 0.0142 & 0.0011 & 0.0003 & 0.0011 & 0.0011 & 0.0060 & 0.0011 \\ 0.0034 & 0.0034 & 0.0142 & 0.0142 & 0.0003 & 0.0011 & 0.0011 & 0.0011 & 0.0011 & 0.0060 \end{pmatrix}$$

The criteria values for the Simplex-Centroid Design with the four factor components are given as;
Determinant Criterion, D-optimality = ϕ_0 (N) = $(\det(N))^{1/}p$ = 7.45E-19
Average variance criterion, A-optimality = ϕ_{-1} (N) = $(\frac{1}{p}$*trace $(N)^{-1})^{-1}$ = 113.7022
Smallest Eigen value Criterion, E- Optimality = ϕ_{-} (N) = λ_{min} (N) = 0.002907049
Trace criterion, T- Optimality = $\frac{1}{p}$*(X^TX) = 0.0404335.

3.2 Selection of Design.

From the output of the above designs in regard to their respective optimal values, each of the criterion is ranked independently. To obtain the design to be used, average rank is of key. The design that has the least average rank value shall be employed any research work which four factors at level two . The simplex- Lattice Design {4, 4} had the smallest value of 1.00 on average of ranking as shown in the table below. Hence this design was selected to be used in this research work.

Table 6. The Obtained Features of the Criterion and their respective ranking

Criterion	Simplex-Lattice Design			Simplex-Centroid Design
	{4, 2} Design	{4, 3} Design	{4, 4} Design	
D	5.960464e-18	6.82364e-19	1.246503e-19	7.45E-19
Rank	4	2	1	3
A	148	94.41073	66.57143	113.7022
Rank	4	2	1	3
E	0.002462692	0.001923614	0.001554355	0.002907049
Rank	3	2	1	4
T	0.073750.	0.0398148	0.016728	0.0404335
Rank	4	2	1	3
Average Rank	3.75	2.00	1.00	3.25

4. CONCLUSION

The study began by comparing all the possible combination of Simplex Lattice Designs (SLD) and Simplex Centroid Design (SCD) with four factors under consideration. With the help of their respective standard matrices (information matrices) obtained from their respective experimental points, moments matrices were formed. From the resultant moment matrices; determinants, average variance, smallest Eigen values and trace values were obtained. These obtained features of the criterion were ranked accordingly with the smallest average rank value being the best.

According to D-, A-, E-, T-optimality criterion, {4.4} SLD had the least average value upon ranking of 1.0. This design met the minimum required threshold and is therefore recommended to be used in any four-factor component research work at level two.

Disclaimer (Artificial intelligence)

Author(s) hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc.) and text-to-image generators have been used during writing or editing of manuscripts.

REFERENCE

[1] Amalina, N., Bakar, M., Kormin, F., Linatoc, A., & Mohamed, M. (2018). Application of statistically simplex-centroid mixture design to optimize the TPC and TFC on the Proportion of Polyherbal Formulation used by Jakun Women. *Journal of Engineering and Applied Sciences*, *13*(9), 6996-7002. Doi: 10.3923/jeasci.2018.6996.7002

[2] Anderson-Cook, C., Borror, C., & Montgomery, D. (2009). Response surface design evaluation and comparison. *Journal of Statistical Planning Inference*, 139(2),629-641. DOI: 10.1016/j.jspi.2008.04.004

[3] Belay, Z., Caleb, O., Mahajan, P., Fröhling, A., & Opara, U. (2019). A simplex lattice design to optimize active modified atmosphere for storing pomegranate (cv. Wonderful) arils: Part II, determining optimum gas for maintaining quality attributes. *Biosystems Engineering*, *178*, 322-335. Doi: 10.1016/j.biosystemseng.2018.11.009

[4] Bondari, K. (2005). Mixture experiments and their application in agricultural research. *Statistics and Data Analysis.* Retrieved from https://support.sas.com/resources/papers/proceedings/proceedings/sugi30/209-30.pdf

[5] Cornell, J. A. 2002. *Experiment with Mixtures: Designs, Models, and the Analysis of Mixture Data, 3rd Edition,* 680 pages, John Wiley & Sons, Inc., USA.

[6] Das, A. (2002). An Introduction to Optimality Criteria and Some Results on Optimal Block Design. Design Workshop Lecture Notes ISI, Kolkata, November, 25-29, 2002, pp. 1-21.

[7] Marquardt, D.W and Snee, R. D. (1974). Test Statistics for Mixture Models. Technometrics, 16(4) 533-537

[8] Myers, R.H., Montgomery, D.C. and Anderson-Cook, C.M. (2009). Response Surface Methodology: Process and Product Optimization using Design Experiments. John Wiley & Sons, Inc., Hoboken, New Jersey.

[9] Myers, H.R., Montgomery, D.C. & Cook, C.M.A. (2009). Response Surface Methodology-Process and Product Optimization Using Designed Experiments. John Wiley & Sons, Inc., Hoboken, New Jersey. 3rd Ed.

[10] Patel, M., Shaikh, F., Patel, V., & Surti, N. (2017). Application of simplex centroid design in formulation and optimization of floating matrix Tablets of metformin. *Journal of Applied Pharmaceutical Science*, *7*(4), 23- 30. Doi: 10.7324/japs.2017.70403

[11] Pukelsheim, F. (2006). Optimal Design of Experiments. John Wiley & Sons, Inc., New York. Chapter 6, p. 135.

[12] Rady, E. A., A. M. M. E. El-Monsef, and M. M. Seyam, "Relationships among Several Optimality Criteria", *Interstat*, vol. 15, issue 6, 2009.

[13] Roelof Coetzer, Linda M. Haines, *The construction of D- and I-optimal designs for mixture experiments with linear constraints on the components, Chemometrics and Intelligent Laboratory System,* Volume 171,2017, pages 112-124, ISSN 0169-7439, https://doi.org/10.1016/j.chemolab.2017.10.007.

[14] Scheffe, H. 1963. Simplex-centroid designs for experiments with mixtures. *Journal of Royal Statistical Society, Series B,* 25: 235-263.

[15] Upendra Kumar Pradhan, Krishan Lal, Sukanta Dash & K. N. Singh (2017) Design and analysis of mixture experiments with process variable, Communications in Statistics - Theory and Methods, 46:1, 259-270, DOI: 10.1080/03610926.2014.990104.