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D- And A- Optimal Orthogonally Blocked Mixture Component-Amount Designs via Projections

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Abstract
Mixture experiments are usually designed to study the effects on the response by changing the relative proportions of the mixture ingredients. This is usually achieved by keeping the total amount fixed but in many practical applications such as medicine or biology, not only are the proportions of mixture ingredients involved but also their total amount is of particular interest. Such experiments are called mixture amount experiments. In such experiments, the usual constraint on the mixture proportions that they should sum to unity is relaxed. The optimality of the design strictly depends on the nature of the underlying model. In this paper, we have obtained D- and A- optimal orthogonally blocked mixture component-amount designs in two and three ingredients via projections based on the reduced cubic canonical model presented by Husain and Sharma [7] and the additive quadratic mixture model proposed by Husain and Parveen [3], respectively.

Keywords Additive quadratic mixture amount model, Reduced cubic mixture amount model, D-optimality, A-optimality, Latin squares, Mixture experiments.

AMS 2010 subject classifications 62K05, 62K10

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1. Introduction

A simple mixture experiment is assumed to involve only the proportions of the ingredients and not the total amount of the mixture but in some situations, the response is assumed to depend on the total amount of the mixture ingredients as well as on the ingredients' relative proportions. This type of experiment is called the mixture amount experiment where the experiment is carried out at various levels of the total amount. A common example is pharmaceutical drug which contains different proportions of salts. The experimenter wishes to know how much drug needs to be administered to the patients and also to investigate the best relative proportions of the constituents so that optimum result(s) may be obtained.

Several models have been proposed for fitting data arising from mixture-amount experiments. Piepel and Cornell [11] suggested designs for fitting models which include the proportions of the q ingredients subject to the condition $\sum_{i=1}^{q} x_i = 1$, and the levels of the total amount indexed by A. For example for q ingredients, a useful quadratic model is of the form

$$\eta = \sum_{i=1}^{q} \gamma_i^0 x_i + \sum_{i<j}^{q} \gamma_{ij}^0 x_i x_j + \sum_{k=1}^{2} (\sum_{i=1}^{q} \gamma_i^k x_i + \sum_{i<j}^{q} \gamma_{ij}^k x_i x_j) A^k \tag{1}$$

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Model (1) contains three second order Scheffé's polynomial in q ingredients, each multiplied by the powers of the total amount A, viz., A^0, A^1 and A^2. A drawback of this model is that when no mixture ingredients are applied, i.e, when $A = 0$, then equation (1) predicts a zero response, which is often inaccurate. This situation may arise when a control (i.e., placebo) is applied. To tackle the zero-amount situation, Piepel [10] suggested $\sum \gamma_i^0 = 1$. Prescott and Draper [12] presented an alternative model which uses the actual amounts of the ingredients rather than the proportions and hence makes the estimation of a placebo response feasible.

Piepel and Cornell [11] gave the relation between individual component amounts a_i and individual component proportions x_i for each level of the total amount A as $a_i = x_i A$, so that $a_1 + a_2 + ... + a_q = A$. An alternative polynomial model in the a_i, known as the component-amount model for a second degree fit is given in (2).

$$\eta = a_0 + \sum_{i=1}^{q} \alpha_i a_i + \sum_{i=1}^{q} (\alpha_{ii} a_i^2 + \sum_{i<j}^{q} \alpha_{ij} a_i a_j) \tag{2}$$

In this paper, we present the additive quadratic mixture model and reduced cubic canonical model in the a_i as our component-amount mixture model to fit the response. Additive quadratic mixture amount model in terms of a_i is as given in equation (3), while equation (4) presents reduced cubic canonical mixture amount model.

$$\eta_A = \alpha_0 + \sum_{i=1}^{q} \alpha_i a_i + \sum_{i=1}^{q} \alpha_{ii} a_i^2 + \sum \sum_{i<j} \alpha_{ij} a_i (a_i - a_j) \tag{3}$$

$$\eta_R = \alpha_0 + \sum_{i=1}^{q} \alpha_i a_i + \sum_{i=1}^{q} \alpha_{ii} a_i^2 + \sum \sum_{i<j} \alpha_{ij} a_i a_j |a_i - a_j| \tag{4}$$

Prescott and Draper [12] projected simplex-lattice and simplex-centroid designs for two or more ingredients to obtain sets of points at different levels of the total amount. They also projected D-optimal orthogonal block design in two blocks for three and four ingredients and obtained D-optimal orthogonal block designs in two blocks for two and three ingredients, respectively. Aggarwal *et al*. [1] obtained orthogonally blocked mixture component amount designs via projections of F-squares. Husain and Hafeez [2] obtained optimal orthogonally blocked mixture designs in three components for additive quadratic mixture model. Husain and Sharma [6] discussed about uniform designs based on F-squares. Husain and Parveen [4] obtained nearly D- and A-optimal orthogonally blocked designs for additive quadratic mixture model and reduced cubic canonical model in four components. Husain and Sharma [8] obtained efficient uniform designs based on F-squares for mixture experiments in three and four components. Husain and Parveen [5] obtained orthogonal blocks of two and three mixture component amount blends via projection of F- squares based design.

In Section 2, we have discussed orthogonally blocked mixture component-amount designs in two and three ingredients via projection of John's [9] three and four component mixture designs. Section 3 presents D- and A-optimal orthogonal block designs in two mixture component amount blends via projection of the designs considered in Section 2, while the same is obtained for three mixture component-amount blends in Section 4.

2. Orthogonally Blocked Mixture Component-Amount Designs

Since it is not always possible to carry out all the experimental runs in similar conditions, it might be useful to split the experiment into blocks. Orthogonal blocking leads to estimation of the model parameters independently of the estimation of block effects. Table 1 depicts the latin square based design given by John [9] for three mixture ingredients. Following Prescott and Draper's [12] approach, we obtain orthogonally blocked mixture component-amount designs in two blocks for two ingredients by projecting mixture designs for three ingredients in two orthogonal blocks.

Table 1. Block structure for three ingredient mixture design in two orthogonal blocks.

Design 1

$$B_1 = \begin{bmatrix} a & b & c \\ b & c & a \\ c & a & b \\ 1/3 & 1/3 & 1/3 \end{bmatrix} \qquad B_2 = \begin{bmatrix} a & c & b \\ b & a & c \\ c & b & a \\ 1/3 & 1/3 & 1/3 \end{bmatrix}$$

For three component mixtures, we need a design having seven distinct blends in order to estimate the seven parameters including one block parameter (consisting of 3 first order terms and 3 second order terms) for both the models η_A and η_R given in (3) and (4), respectively.

For the model η_A given in (3), we obtained blocking conditions given in (5) for the two blocks B_1 and B_2 .

$$u_1 = u_2 = u_3 = a + b + c + \frac{1}{3}$$

$$u_1^2 = u_2^2 = u_3^2 = a^2 + b^2 + c^2$$

$$u_{12} = u_{13} = u_{23} = a^2 + b^2 + c^2 - ab - bc - ca \tag{5}$$

For model η_R given in (4), we obtained blocking conditions given in (6) for the two blocks B_1 and B_2 .

$$k_1 = k_2 = k_3 = a + b + c + \frac{1}{3}$$

$$k_1^2 = k_2^2 = k_3^2 = a^2 + b^2 + c^2$$

$$k_{12} = k_{13} = k_{23} = ab^2 - a^2b + bc^2 - b^2c + c^2a - a^2c \tag{6}$$

Table 2. Block structure for four ingredient mixture design in two orthogonal blocks.

Design 2

$$B_1 = \begin{bmatrix} a & b & c & d \\ b & c & d & a \\ c & d & a & b \\ d & a & b & c \\ a & d & b & c \\ b & c & a & d \\ c & a & d & b \\ d & b & c & a \\ 1/4 & 1/4 & 1/4 & 1/4 \end{bmatrix} \qquad B_2 = \begin{bmatrix} a & d & c & b \\ b & a & d & c \\ c & b & a & d \\ d & c & b & a \\ a & c & b & d \\ b & d & a & c \\ c & b & d & a \\ d & a & c & b \\ 1/4 & 1/4 & 1/4 & 1/4 \end{bmatrix}$$

For four mixture components in the models η_A and η_R, we require 17 distinct runs to estimate 11 parameters including the block parameter (consisting of four pure mixture components and 6 binary blends). Table 2 presents John's [9] design in four mixture components based on pairs of mates of latin squares.

For model η_A given in (3), we obtained blocking conditions given in (7) for the two blocks B_1 and B_2.

$$u_1 = u_2 = u_3 = u_4 = 2(a + b + c + d)$$

$$u_1^2 = u_2^2 = u_3^2 = u_4^2 = 2(a^2 + b^2 + c^2 + d^2)$$

$$u_{12} = u_{14} = u_{23} = u_{34} = 2(a^2 + b^2 + c^2 + d^2) - ab - ac - 2ad - 2bc - bd - cd$$

$$u_{13} = u_{24} = 2(a^2 + b^2 + c^2 + d^2) - 2ab - 2ac - 2bd - 2cd \tag{7}$$

For model η_R given in (4), we obtained blocking conditions given in (8) for the two blocks B_1 and B_2.

$$k_1 = k_2 = k_3 = k_4 = 2(a + b + c + d)$$

$$k_1^2 = k_2^2 = k_3^2 = k_4^2 = 2(a^2 + b^2 + c^2 + d^2)$$

$$k_{12} = k_{14} = k_{23} = k_{34} = ab^2 - a^2b + 2bc^2 - 2b^2c + cd^2 - c^2d + 2ad^2 - 2a^2d + c^2a - a^2c + bd^2 - b^2d$$

$$k_{13} = k_{24} = 2(ac^2 - a^2c + bd^2 - b^2d + ab^2 - a^2b + cd^2 - c^2d) \quad (8)$$

In tables 1 and 2; a, b, c and d denote the mixture proportions between 0 and 1 and their sum is unity. Centroid points are added in order to remove the singularity of the design. We may obtain component-amount designs in q proportions by projection i.e., by eliminating any r columns from the original design. To illustrate the procedure, we begin with John's [9] orthogonally blocked mixture designs in three and four ingredients given in tables 1 and 2, respectively. The designs are based on two latin squares called mates with the blocks indexed by $Z = +1$ and $Z = -1$, where Z denotes the blocking variable.

Equation (9), (10), (11) and (12) depict the models $\eta_{A,3}$, $\eta_{A,4}$, $\eta_{R,3}$and $\eta_{R,4}$ in three and four ingredients for additive quadratic mixture model and reduced cubic canonical model, respectively. As mentioned earlier in Husain and Sharma's [7] paper, here also orthogonality conditions are satisfied when we take $a < b < c$ for model η_R. Here, the blocking parameter δ is estimated orthogonally to the mixture terms.

$$\eta_{A,3} = \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_{12}x_1(x_1 - x_2) + \beta_{13}x_1(x_1 - x_3) + \beta_{23}x_2(x_2 - x_3) + \delta z \quad (9)$$

$$\begin{aligned}\eta_{A,4} =& \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1(x_1 - x_2) + \beta_{13}x_1(x_1 - x_3) + \beta_{14}x_1(x_1 - x_4) \\ &+ \beta_{23}x_2(x_2 - x_3) + \beta_{24}x_2(x_2 - x_4) + \beta_{34}x_3(x_3 - x_4) + \delta z\end{aligned} \quad (10)$$

$$\eta_{R,3} = \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_{12}x_1x_2|x_1 - x_2| + \beta_{13}x_1x_3|x_1 - x_3| + \beta_{23}x_2x_3|x_2 - x_3| + \delta z \quad (11)$$

$$\begin{aligned}\eta_{R,4} =& \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1x_2|x_1 - x_2| + \beta_{13}x_1x_3|x_1 - x_3| + \beta_{14}x_1x_4|x_1 - x_4| \\ &+ \beta_{23}x_2x_3|x_2 - x_3| + \beta_{24}x_2x_4|x_2 - x_4| + \beta_{34}x_3x_4|x_3 - x_4| + \delta z\end{aligned} \quad (12)$$

2.1. Orthogonally Blocked Mixture Component-Amount Designs in Two Ingredients

We may obtain a mixture component amount-design for two ingredients in two orthogonal blocks by eliminating any one of the three columns say, x_3 from Design 1 and any two of the four columns say, x_3 and x_4 from Design 2, respectively. Here, we only show the block structure of two ingredients via projection of Design 1.

Table 3. Block structure for a two ingredient component-amount design in two orthogonal blocks via projection of Design 1.

B_1			B_2		
Component		Amount	Component		Amount
a_1	a_2	A	a_1	a_2	A
a	b	$a+b$	a	c	$a+c$
b	c	$b+c$	b	a	$b+a$
c	a	$c+a$	c	b	$c+b$
$1/3$	$1/3$	$2/3$	$1/3$	$1/3$	$2/3$

The additive quadratic mixture amount model (3) and reduced cubic mixture amount model (4) for two ingredients (a_1, a_2) are as given in (13) and (14), respectively.

$$\eta_{A,2} = \alpha_0 + \alpha_1a_1 + \alpha_2a_2 + \alpha_{11}a_1^2 + \alpha_{22}a_2^2 + \alpha_{12}a_1(a_1 - a_2) + \delta z \quad (13)$$

$$\eta_{R,2} = \alpha_0 + \alpha_1a_1 + \alpha_2a_2 + \alpha_{11}a_1^2 + \alpha_{22}a_2^2 + \alpha_{12}a_1a_2|a_1 - a_2| + \delta z \quad (14)$$

The **X** matrix for the additive quadratic mixture amount model $\eta_{A,2}$ obtained via projection of Design 1 is given in equation (15).

$$\mathbf{X} = \begin{bmatrix} 1 & a & b & a^2 & b^2 & a(a-b) & -1 \\ 1 & b & c & b^2 & c^2 & b(b-c) & -1 \\ 1 & c & a & c^2 & a^2 & c(c-a) & -1 \\ 1 & 1/3 & 1/3 & 1/9 & 1/9 & 0 & -1 \\ 1 & a & c & a^2 & c^2 & a(a-c) & 1 \\ 1 & b & a & b^2 & a^2 & b(b-a) & 1 \\ 1 & c & b & c^2 & b^2 & c(c-b) & 1 \\ 1 & 1/3 & 1/3 & 1/9 & 1/9 & 0 & 1 \end{bmatrix} \tag{15}$$

The **X** matrix for additive quadratic mixture amount model $\eta_{A,2}$ obtained via projection of Design 2 is given in equation (16).

$$\mathbf{X} = \begin{bmatrix} 1 & a & b & a^2 & b^2 & a(a-b) & -1 \\ 1 & b & c & b^2 & c^2 & b(b-c) & -1 \\ 1 & c & d & c^2 & d^2 & c(c-d) & -1 \\ 1 & d & a & d^2 & a^2 & d(d-a) & -1 \\ 1 & a & d & a^2 & d^2 & a(a-d) & -1 \\ 1 & b & c & b^2 & c^2 & b(b-c) & -1 \\ 1 & c & a & c^2 & a^2 & c(c-a) & -1 \\ 1 & d & b & d^2 & b^2 & d(d-b) & -1 \\ 1 & 1/4 & 1/4 & 1/16 & 1/16 & 0 & -1 \\ 1 & a & d & a^2 & d^2 & a(a-d) & 1 \\ 1 & b & a & b^2 & a^2 & b(b-a) & 1 \\ 1 & c & b & c^2 & b^2 & c(c-b) & 1 \\ 1 & d & c & d^2 & c^2 & d(d-c) & 1 \\ 1 & a & c & a^2 & c^2 & a(a-c) & 1 \\ 1 & b & d & b^2 & d^2 & b(b-d) & 1 \\ 1 & c & b & c^2 & b^2 & c(c-b) & 1 \\ 1 & d & a & d^2 & a^2 & d(d-a) & 1 \\ 1 & 1/4 & 1/4 & 1/16 & 1/16 & 0 & 1 \end{bmatrix} \tag{16}$$

The **X** matrix for the reduced cubic canonical mixture amount model $\eta_{R,2}$ via projection of Design 1 and Design 2 for two component mixture amount designs may be obtained similarly.

2.2. Orthogonally Blocked Mixture Component-Amount Designs in Three Ingredients

Table 4. Block structure of a component-amount design in three ingredients in two orthogonal blocks.

Block 1				Block 2			
Component			Amount	Component			Amount
a_1	a_2	a_3	A	a_1	a_2	a_3	A
a	b	c	$1-d$	a	d	c	$1-b$
b	c	d	$1-a$	b	a	d	$1-c$
c	d	a	$1-b$	c	b	a	$1-d$
d	a	b	$1-c$	d	c	b	$1-a$
a	d	b	$1-c$	a	c	b	$1-d$
b	c	a	$1-d$	b	d	a	$1-c$
c	a	d	$1-b$	c	b	d	$1-a$
d	b	c	$1-a$	d	a	c	$1-b$
$1/4$	$1/4$	$1/4$	$3/4$	$1/4$	$1/4$	$1/4$	$3/4$

Without loss of generality, we eliminate the fourth column, x_4 for obtaining the mixture component-amount designs in three ingredients. Equations (17) and (18) depict the models $\eta_{A,3}$ and $\eta_{R,3}$, respectively in three components in terms of a_i. Table 4 depicts the block structure for a three ingredient component amount design in two orthogonal blocks. The additive quadratic mixture amount model (3) and the reduced cubic mixture amount model (4) for three ingredients (a_1, a_2, a_3) and with a block difference 2δ are estimated orthogonally to all the mixture terms as shown in (17) and (18), respectively.

$$\begin{aligned}\eta_{A,3} = &\alpha_0 + \alpha_1 a_1 + \alpha_2 a_2 + \alpha_3 a_3 + \alpha_{11} a_1^2 + \alpha_{22} a_2^2 + \alpha_{33} a_3^2 + \alpha_{12} a_1(a_1 - a_2) \\ &+ \alpha_{13} a_1(a_1 - a_3) + \alpha_{23} a_2(a_2 - a_3)\end{aligned} \tag{17}$$

$$\begin{aligned}\eta_{R,3} = &\alpha_0 + \alpha_1 a_1 + \alpha_2 a_2 + \alpha_3 a_3 + \alpha_{11} a_1^2 + \alpha_{22} a_2^2 + \alpha_{33} a_3^2 + \alpha_{12} a_1 a_2 |a_1 - a_2| \\ &+ \alpha_{13} a_1 a_3 |a_1 - a_3| + \alpha_{23} a_2 a_3 |a_2 - a_3|\end{aligned} \tag{18}$$

The $\mathbf{X}$ matrix for the additive quadratic mixture amount model $\eta_{A,3}$ as well as for model $\eta_{R,3}$ via projection of Design 2 may be obtained in a similar manner as done earlier in Section 2.1.

3. D- and A- Optimal Design For Two Ingredients in Two Orthogonal Blocks

In order to obtain D- and A- optimality, we need to find the values of a, b and c that maximize $|\mathbf{X}'\mathbf{X}|$ and minimize T = trace $(\mathbf{X}'\mathbf{X})^{-1}$, respectively. For the model η_A given in equation (3), we obtain the same results on all the boundary points i.e., $a = 0, b = 0$ and $c = 0$. For model η_R discussed in equation (4), we attain the optimality at $a = 0$. The cases $b = 0$ and $c = 0$ are not feasible due to the restriction $a < b < c$.

3.1. Projection of Design 1

For model η_A, the general expression for $|\mathbf{X}'\mathbf{X}|$ is as given in (19) and the general expression of T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ is very lengthy, hence it is not discussed here.

$$|\mathbf{X}'\mathbf{X}| = \frac{32}{3}(a-b)^4(a-c)^4(b-c)^4(1-2b+a(-2+3b)-2c+3(a+b)c)^2 \tag{19}$$

We obtain the same optimality on all the boundary points. For case $c = 0$, the expressions of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ in terms of a alone are given in equations (20) and (21), respectively.

$$|\mathbf{X}'\mathbf{X}| = \frac{32}{3}(1-2a)^4(-1+a)^4 a^4 (1+3(-1+a)a)^2 \tag{20}$$

$$T = \frac{T_1}{T_2} \tag{21}$$

where,

$$\begin{aligned}T_1 = &448 - 4032a + 19829a^2 - 58996a^3 + 100640a^4 - 94374a^5 + 51324a^6 - 26748a^7 \\ &+ 18837a^8 - 8100a^9 + 1620a^{10}\end{aligned}$$

$$T_2 = 72(-1+a)^2 a^2 (-1+2a)^2 (1-3a+3a^2)^2$$

The graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ in two mixture components for the additive quadratic mixture amount model η_A are shown in Figure 1.

Numerically and graphically, we observe from Figure 1 that

1. $|\mathbf{X}'\mathbf{X}| = 0$ when $a = 0, 0.5$ and 1.
2. The curve of $|\mathbf{X}'\mathbf{X}|$ is an m-shaped curve. Its maximum (= 0.000266872) is attained when a = b, 1 - b, where b = 0.1685, 0.8315.
3. T attains its minimum (= 537.868) when a = b, 1 - b, where b = 0.20513, 0.79487.

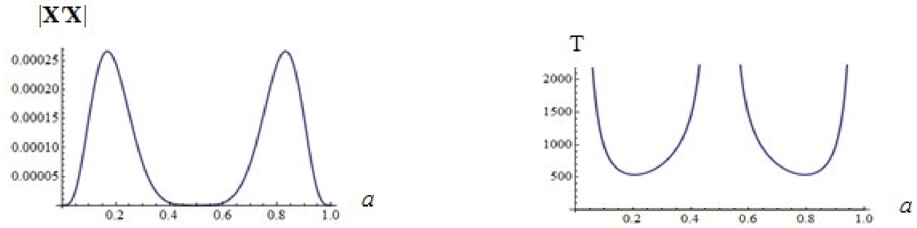


Figure 1. Graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ against a for two ingredients in two orthogonal blocks for model η_A obtained via projection of Design 1.

Since $a + b + c = 1$, we observe that equation (19) is same as that obtained by Prescott and Draper [12] for two component mixture amount designs based on Scheffé's quadratic model obtained via projection of three component mixture designs. Hence in this case, the optimal values as well as the D-optimality of the model (3) are exactly the same as that obtained by Prescott and Draper [12]. For model η_R, the general expression of $|\mathbf{X}'\mathbf{X}|$ is as given in (22) and the general expression of T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ is very lengthy, hence it is not discussed here.

$$\begin{aligned}|\mathbf{X}'\mathbf{X}| =& \frac{32}{27}(a-b)^4(a-c)^2(b-c)^4(a^3(-6+9b+9c)-(b-c)c(2-6c+b(-6+9c)) \\ &+a^2(2+6c-9(b^2+bc+2c^2))+a(b^2(6-18c)+b(-2+3(4-3c)c)+c(-4+6c+9c^2)))^2\end{aligned} \tag{22}$$

Without loss of generality, we have attained D- and A-optimality at $a = 0$ and presented the expressions of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ in terms of b alone as shown in the equations (23) and (24), respectively.

$$|\mathbf{X}'\mathbf{X}| = \frac{32}{27}(1-2b)^6(b-1)^4b^4(4+9(b-1)b)^2 \tag{23}$$

$$T = \frac{T_1}{T_2} \tag{24}$$

where,

$$\begin{aligned}T_1 &= 896+(b-1)b(9600+(b-1)b(45440+(b-1)b(122200+9(b-1)b(17383 \\ &\quad +24(b-1)b(173+90(b-1)b))))) \\ T_2 &= 24(1-2b)^4(b-1)^2b^2(4+9(b-1)b)^2\end{aligned}$$

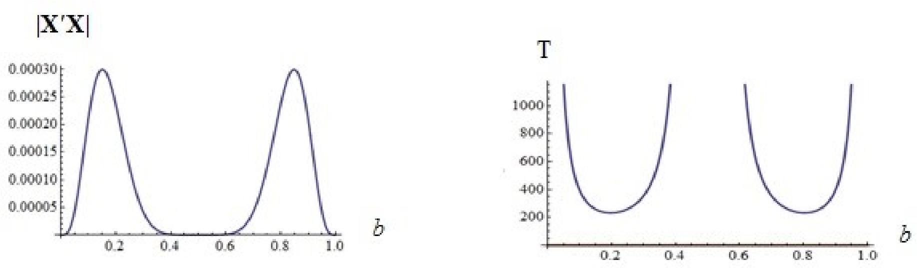


Figure 2. Graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ against b for two ingredients in two orthogonal blocks for model η_R obtained via projection of Design 1.

Numerically and graphically, we observe from Figure 2 that

1. $|\mathbf{X}'\mathbf{X}| = 0$ when $b = 0, 0.5$ and 1.

2. The curve of $|\mathbf{X}'\mathbf{X}|$ is an m-shaped curve. Its maximum (= 0.00029993) is attained when b = 0.151761 and c = 0.848239.
3. T attains its minimum (= 233.082) when b = 0.197271 and c = 0.802729.

The D-optimal component-amount design for two ingredients in two orthogonal blocks for model η_R obtained via projection of Design 1 is given in Table 5 and illustrated in Figure 3.

Table 5. D-optimal component-amount design for two ingredients in two orthogonal blocks for model η_R obtained via projection of Design 1.

B_1			B_2		
Component		Amount	Component		Amount
a_1	a_2	A	a_1	a_2	A
0.151761	0.848239	1.0	0.151761	0	0.151761
0.848239	0	0.848239	0.848239	0.151761	1.0
0	0.151761	0.151761	0	0.848239	0.848239
0.33	0.33	0.66	0.33	0.33	0.66

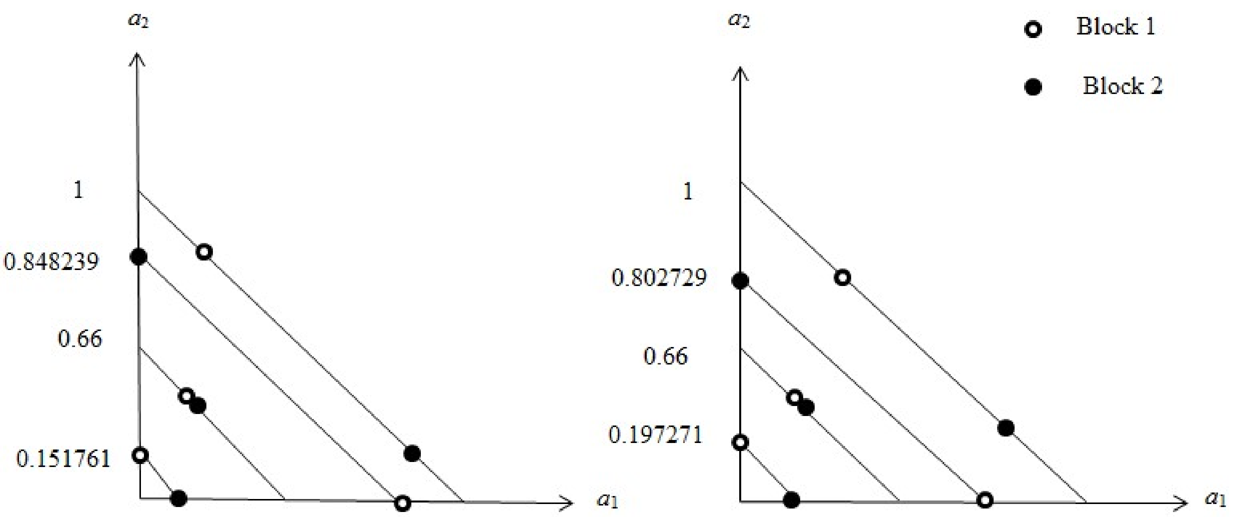


Figure 3. Two ingredient orthogonally blocked D- and A-optimal mixture component-amount design for model η_R obtained via projection of Design 1.

3.2. *Projection of Design 2.*

For model η_A, the general expressions of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ are very lengthy and hence not discussed here. We have attained optimality at $a = d = 0$, $b = 1 - c$ and $b = c = 0$, $a = 1 - d$. Here, we consider the case $a = d = 0$, $b = 1 - c$ and present the expressions of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ in terms of c alone as shown in equation (25) and (26), respectively.

$$|\mathbf{X}'\mathbf{X}| = 108(1-2c)^2(c-1)^4c^4(13+2(c-1)c(49+192(c-1)c(1+2(c-1)c))) \tag{25}$$

$$T = \frac{T_1}{T_2} \tag{26}$$

where,

$$
\begin{aligned}
T_1 &= 4416 + (c-1)c(50352 + (c-1)c(330611 + 16(c-1)c(82242 + (c-1)c(132085 \\
&\quad + 96(c-1)c)(135 + 64(c-1)c))))) \\
T_2 &= 144(1-2c)^2(c-1)^2c^2(13 + 2(c-1)c(49 + 192(c-1)c(1 + 2(c-1)c)))
\end{aligned}
$$

The graphs for $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ for the additive quadratic mixture amount model η_A obtained via projection of Design 2 are as shown in Figure 4.

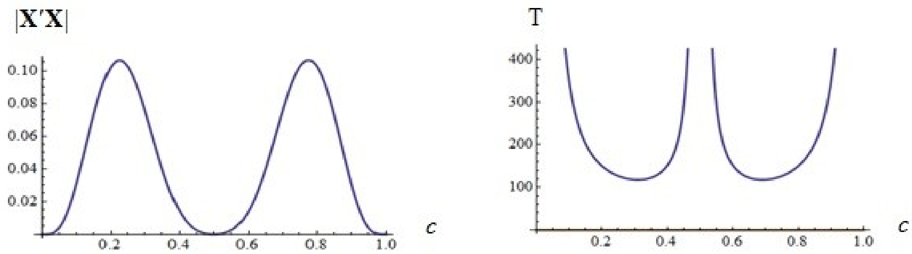


Figure 4. Graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ against c for two ingredients in two orthogonal blocks for model η_A obtained via projection of Design 2.

Numerically and graphically, we observe from Figure 4 that

1. $|\mathbf{X}'\mathbf{X}| = 0$ when $c = 0, 0.5$ and 1.
2. The curve of $|\mathbf{X}'\mathbf{X}|$ is an m-shaped curve. Its maximum (= 0.106183) is attained when c = b, 1 - b, where b = 0.225023, 0.774977.
3. T attains its minimum (= 118.073) when c = b, 1 - b, where b = 0.310061, 0.689939.

For model η_R, the general expressions of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ are very lengthy and hence Figure 4 not discussed here. We have obtained the optimality at a = b = 0, c = 1 - d. The expressions of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ are expressed in terms of d alone as shown in equations (27) and (28), respectively.

$$
|\mathbf{X}'\mathbf{X}| = \frac{405}{4}(1-2d)^4(d-1)^4d^4(18 + (d-1)d(147 + 16(d-1)d(31 + 48(d-1)d))) \tag{27}
$$

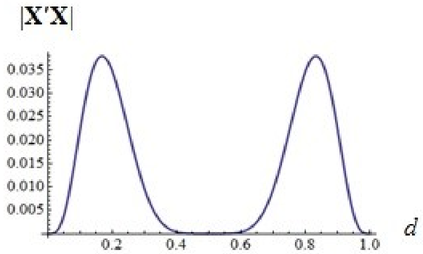
$$
T = \frac{T_1}{T_2} \tag{28}
$$

where,

$$
\begin{aligned}
T_1 &= 3888 + (d-1)d(37728 + (d-1)d(225171 + 4(d-1)d(203721 + 16(d-1) \\
&\quad d(17887 + 16(d-1)d(244 + 165(d-1)d))))) \\
T_2 &= 180(1-2d)^2(d-1)^2d^2(18 + (d-1)d(147 + 16(d-1)d(31 + 48(d-1)d)))
\end{aligned}
$$

The graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ for the reduced cubic canonical mixture amount model η_R obtained via projection of Design 2 are as shown in Figure 5.
Numerically and graphically, we observe from Figure 5 that

1. $|\mathbf{X}'\mathbf{X}| = 0$ when $d = 0, 0.5$ and 1.
2. The curve of $|\mathbf{X}'\mathbf{X}|$ is an m-shaped curve. Its maximum (= 0.0379108) is attained when c = 0.16763 and d = 0.83237.
3. T attains its minimum (= 150.248) when c = 0.19837 and d = 0.80163.



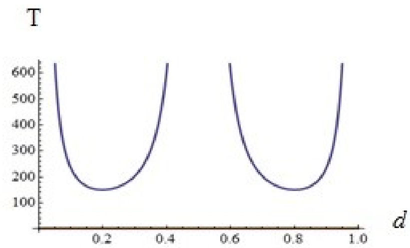


Figure 5. Graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ against d for two ingredients in two orthogonal blocks for model η_R obtained via projection of Design 2.

D-optimal component-amount design for two ingredients in two orthogonal blocks for model η_R obtained via projection of Design 2 is given in Table 6 and illustrated in Figure 6.

Table 6. D-optimal component-amount design for two ingredients in two orthogonal blocks for model η_R obtained via projection of Design 2.

B_1			B_2		
Component		Amount	Component		Amount
a_1	a_2	A	a_1	a_2	A
0	0	0	0	0.83237	0.83237
0	0.16763	0.16763	0	0	0
0.16763	0.83237	1	0.16763	0	0.16763
0.83237	0	0.83237	0.83237	0.16763	1
0	0.83237	0.83237	0	0.16763	0.16763
0	0.16763	0.16763	0	0.83237	0.83237
0.16763	0	0.16763	0.16763	0	0.16763
0.83237	0	0.83237	0.83237	0	0.83237
0.25	0.25	0.50	0.25	0.25	0.50

4. A Design For Three Ingredients in Two Orthogonal Blocks

We may obtain a mixture component-amount design for three ingredients in two orthogonal blocks by removing any one column from Design 2. Without loss of generality, we have dropped the fourth column from Design 2. Except for the centroid point, this design has no repeated blends either within the blocks or across the blocks. The **X** matrix in three ingredients for additive quadratic mixture amount model, η_A and reduced cubic canonical mixture amount model, η_R are already discussed in Section 2.2.

For model η_A, we have obtained the optimality at eight of the boundary points. Here, we consider the case $a = b = 0$, $c = 1 - d$ and present the expressions of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ in terms of d alone as given in (29) and (30), respectively.

$$|\mathbf{X}'\mathbf{X}| = 648(1-2d)^6(d-1)^{10}d^{10}(3+8(d-1)d)^2 \tag{29}$$

$$T = \frac{T_1}{T_2} \tag{30}$$

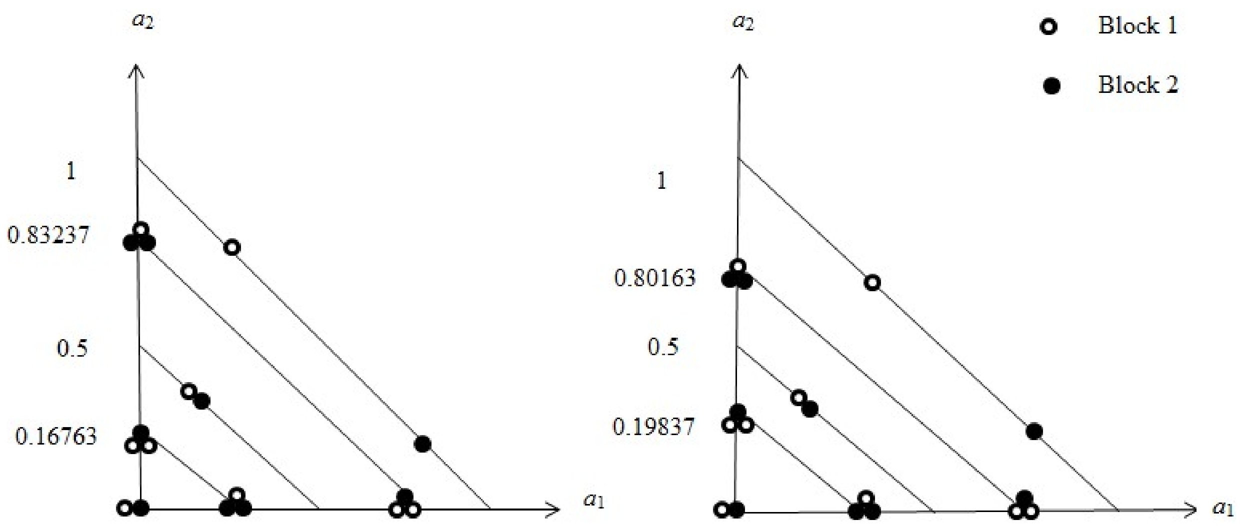


Figure 6. Two ingredient orthogonally blocked D- and A-optimal mixture component-amount design for model η_R obtained via projection of Design 2.

where,

$$T_1 = 5040 + (d-1)d(42552 + (d-1)d(146619 + 2(d-1)d(110685 + 16(d-1)\\ d(241 + 160(d-1)d))))$$
$$T_2 = 36(1-2d)^2(d-1)^2d^2(3+8(d-1)d)^2$$

Figure 7 shows the graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ against d in three mixture ingredients in two blocks for the additive quadratic mixture amount model η_A.

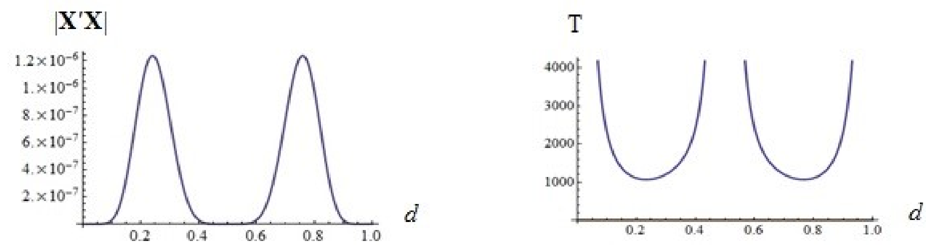


Figure 7. Graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ against d for three ingredients in two orthogonal blocks for model η_A obtained via projection of Design 2.

Numerically and graphically, we observe from Figure 7 that

1. $|\mathbf{X}'\mathbf{X}| = 0$ when $d = 0, 0.5$ and 1.
2. The curve of $|\mathbf{X}'\mathbf{X}|$ is an m-shaped curve. Its maximum (= 1.23976×10^{-6}) is attained at *d* = 0.240118, 0.759882.
3. T attains its minimum (= 1065.72) when *d* = 0.232843, 0.767157.

For model (3), D-optimality in the case of three mixture amount design obtained via projection of Design 2 matches with the D-optimality obtained by Aggarwal *et al*. [1] for F- square based three mixture component-amount design obtained via projection of four mixture components design for the case *a* = 0.

D-optimal component-amount design for three ingredients in two orthogonal blocks for the model η_A obtained via projection of Design 2 is given in Table 7.

Table 7. D-optimal component-amount design for three ingredients in two orthogonal blocks for model η_A obtained via projection of Design 2.

Block 1				Block 2			
Component			Amount	Component			Amount
a_1	a_2	a_3	A	a_1	a_2	a_3	A
0	0	0.240118	0.240118	0	0.759882	0.240118	1.0
0	0.240118	0.759882	1.0	0	0	0.759882	0.759882
0.240118	0.759882	0	1.0	0.240118	0	0	0.240118
0.759882	0	0	0.759882	0.759882	0.240118	0	1.0
0	0.759882	0	0.759882	0	0.240118	0	0.240118
0	0.240118	0	0.240118	0	0.759882	0	0.759882
0.240118	0	0.759882	1.0	0.240118	0	0.759882	1.0
0.759882	0	0.240118	1.0	0.759882	0	0.240118	1.0
0.25	0.25	0.25	0.75	0.25	0.25	0.25	0.75

For model η_R, the general expressions of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ are very lengthy and hence not discussed here. We have obtained the optimal design at *a* = *b* = 0 and shown the expression of determinant in terms of *d* alone as given in (31) and the expression of trace is not discussed here as again it is very lengthy.

$$|\mathbf{X}'\mathbf{X}| = 40(1-2d)^{10}(d-1)^{10}d^{10}(135+8(d-1)d(135+16(d-1)d(27+38(d-1)d))) \tag{31}$$

Figure 8 shows the graph of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ in three mixture ingredients in two blocks for model η_R.

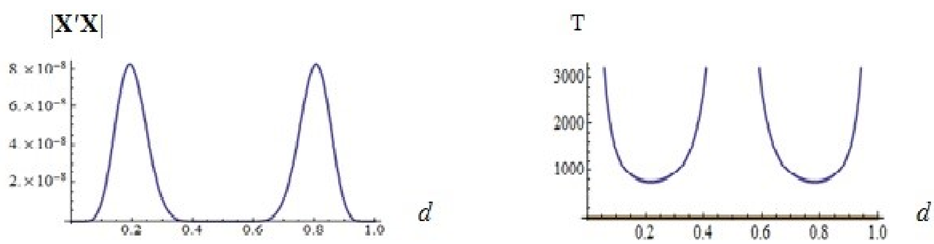


Figure 8. Graphs of $|\mathbf{X}'\mathbf{X}|$ and T = trace $(\mathbf{X}'\mathbf{X})^{-1}$ against d for three ingredients in two orthogonal blocks for model η_R obtained via projection of Design 2.

Numerically and graphically, we observe from Figure 8 that

1. $|\mathbf{X}'\mathbf{X}| = 0$ when $d = 0, 0.5$ and 1.
2. The curve of $|\mathbf{X}'\mathbf{X}|$ is an m-shaped curve. Its maximum (= 8.25203×10^{-8}) is attained when *c* = 0.19316 and *d* = 0.80684.
3. T attains its minimum (= 744.219) when *c* = 0.21745 and *d* = 0.78255.

D-optimal component-amount design for three ingredients in two orthogonal blocks for model η_R obtained via projection of Design 2 is given in Table 8 and illustrated in Figure 9.

Table 8. D-optimal component-amount design for three ingredients in two orthogonal blocks for model η_R obtained via projection of Design 2.

Block 1				Block 2			
Component			Amount	Component			Amount
a_1	a_2	a_3	A	a_1	a_2	a_3	A
0	0	0.19316	0.19316	0	0.80684	0.19316	1.0
0	0.19316	0.80684	1.0	0	0	0.80684	0.80684
0.19316	0.80684	0	1.0	0.19316	0	0	0.19316
0.80684	0	0	0.80684	0.80684	0.19316	0	1.0
0	0.80684	0	0.80684	0	0.19316	0	0.19316
0	0.19316	0	0.19316	0	0.80684	0	0.80684
0.19316	0	0.80684	1.0	0.19316	0	0.80684	1.0
0.80684	0	0.19316	1.0	0.80684	0	0.19316	1.0
0.25	0.25	0.25	0.75	0.25	0.25	0.25	0.75

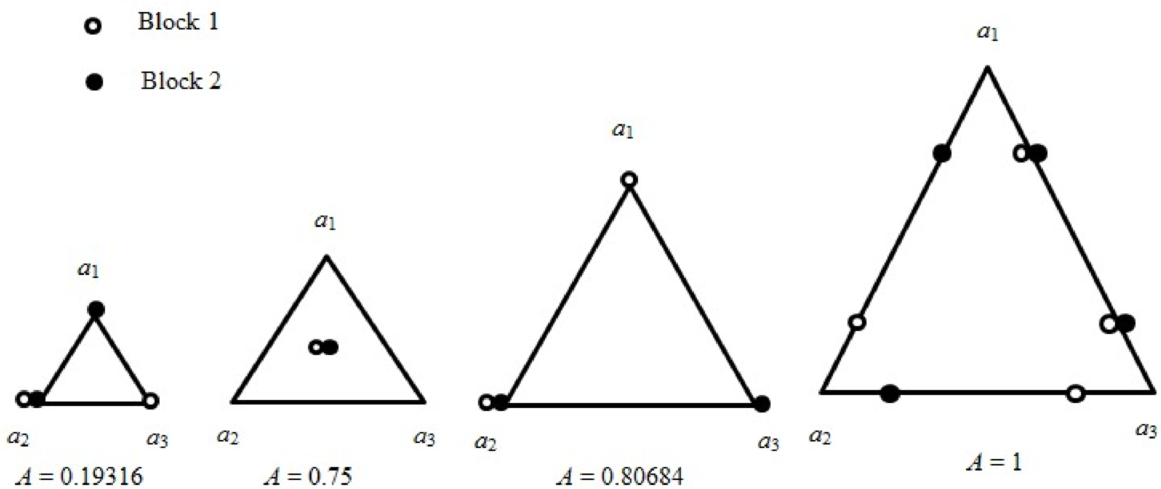


Figure 9. D-optimal orthogonal block structure for three ingredients in two orthogonal blocks for model η_R obtained via projection of Design 2.

5. Conclusion

In this paper, we have obtained D- and A- optimal orthogonally blocked designs via projection of three and four mixture designs based on John's [9] designs. The D- and A-optimality obtained for two ingredients via projection of Design 1 for the additive quadratic mixture amount model η_A and reduced cubic canonical mixture amount model η_R is same on all the boundary points. For model η_A, the D-optimality (0.000266872) for two components via projection of Design 1 is attained at a = 0.1685, b = 1 - a = 0.8315 and A-optimality (537.868) is attained at a = 0.20513, b = 1 - a = 0.79487, respectively. For model η_R, the D-optimality (0.00029993) for two components via projection of Design 1 is attained at b = 0.15176 and c = 0.848239 and A-optimality (128.883) is attained at b = 0.250318 and c = 0.749682, respectively. Next, we have obtained the D- and A- optimal orthogonally blocked mixture component amount designs in two ingredients via projection of Design 2 for models η_A and η_R, respectively. For model η_A, the D-optimality (0.106183) in two components via projection of Design 2 is attained at c = b, 1 - b, where b = 0.225023, 0.774977 and A-optimality (118.073) is attained at c = b, 1 - b, where b = 0.310061, 0.689939, respectively. For model η_R, the D-optimality (0.0379108) is attained at c = 0.16763 and d = 0.83237, and A- optimality (150.248) is attained at c = 0.19837 and d = 0.80163, respectively.

In Section 4, we have obtained D- and A- optimal orthogonally blocked mixture component amount designs in three components via projection of Design 2 for models η_A and η_R, respectively. For model η_A, the D-optimality (1.23976×10^{-6}) is attained at $d = c$, $1 - c$, where $c = 0.759882, 0.240118$ and A-optimality (1065.72) is attained at $d = c$, $1 - c$, where $c = 0.767157, 0.232843$, respectively. For model η_R, the D-optimality (8.25203×10^{-8}) is attained at $c = 0.19316$ and $d = 0.80684$ and A-optimality (744.29) at $c = 0.21745$ and $d = 0.78255$, respectively.

We conclude that for obtaining the mixture component designs in two components via projection of Design 1 and Design 2, Design 2 fares better as compared to Design 1 as regards both D- and A-optimality for both the models η_A and η_R.

As far as three ingredient mixture amount experiments are concerned, we observe that the additive quadratic mixture amount model is better in terms of D-optimality as compared to the reduced cubic canonical mixture amount model. However, reduced cubic canonical mixture amount model is better than additive quadratic mixture amount model when we compare the A-optimality.

Conflict of Interest:

All the Authors declare that they have no conflict of interest.

Ethical approval:

This article does not contain any studies with human participants or animals performed by any of the authors.

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