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Comparison of Mixture Designs Obtained Through Projections

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SUMMARY

Box and Hau [4] and Prescott [18] discussed projection designs for mixture experiments. In this paper, we consider the projections of four types of standard three - level designs into the mixture simplex and provide efficiency measures for the resulting mixture designs when Scheffe's quadratic model and Darroch's quadratic models are fitted. We also tabulate and compare the uniformity measures for these designs.

Key words : Mixture experiments, Projection designs, Box-Behnken designs, Central composite designs, Small composite designs, Augmented pair designs, D-efficiency, A-efficiency, G-efficiency, Discrepancy.

1. Introduction

In experiments with mixtures, the response depends only on the proportions of the q components present in the mixture and not on the total amount of the mixture. As a result, the factor space reduces to a regular $(q-1)$-dimensional simplex

$$S_{q-1} = \left\{ x : (x_1, x_2, x_3 \ldots x_q) \left| \sum_{i=1}^{q} x_i = 1, x_i \geq 0 \right. \right\} \tag{1.1}$$

Mixture experiments are widely used in agricultural, horticultural, and industrial situations. Batra *et al.* ([1], [2]) used mixture experiments in analysis of agricultural experiments involving fixed quantity of fertilizer applied in splits at different crop growth stages. Deka *et al.* [9] applied methodology of mixture experiments for quality evaluation of mixed fruit juice/pulp ready to serve (RTS) beverages.

Scheffé ([20], [21]) was the first to introduce models and designs for experiments with mixtures. Murty and Das [17] have developed symmetric-simplex designs so that the design points are scattered uniformly over S_{q-1}.

In practice, physical and economic considerations often impose additional constraint in the form of lower (L_i) and upper (U_i) bounds

$$0 \le L_i \le x_i \le U_i \le 1 \tag{1.2}$$

on the level of some or all the x_i's in the mixture. In such cases, the experimental region is a part of the simplex S_{q-1}. Batra *et al.* ([1], [2]) observed that in experiments involving split application of fertilizer, constrained mixture designs are more appropriate. For exploring the restricted region, Mclean and Anderson [15] introduced extreme vertices designs (EVD). Saxena and Nigam [19] gave a transformation that provides designs constructed through symmetric simplex designs. Cornell [7] gives an excellent review on the problem of experiment with mixtures. In this paper, we consider the following two models : the quadratic model due to Scheffé [20]

$$\text{Model I}: \; E(Y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{1 \le i \le j \le q} \beta_{ij} x_i x_j \tag{1.3}$$

and the additive model due to Darroch and Waller [8]

$$\text{Model II}: \; E(Y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q} \beta_{ii} x_i (1 - x_i) \tag{1.4}$$

The Model I is the most commonly used model in mixture experiments and is appropriate for the well behaved systems. The Model II is additive in mixture components and is suitable for the design of industrial or agricultural products where mixture components have additive effects on response function. Chan [6] describes the study and design of solder plate used in surface-mount technology in electronic manufacturing as an example where this model can be applied and Scheffé's quadratic model is not a suitable model.

Box and Hau [4] and Prescott [18] discussed the construction of projection designs for mixture experiments by projecting the standard designs such as two-level factorials and central composite design. They also showed that some useful properties of the generating designs, such as orthogonal blocking and rotatability are retained in projected designs which make these designs suitable for mixture experiments. Prescott [18] also discussed the case when some ingredients are restricted to small values. Box and Hau [4] discussed some second order mixture designs generated by two-level factorials.

For a second order response surface model the designs involving three equally spaced levels are popular choices. In this paper, we have used the projections of well-known three-level response surface designs to obtain mixture designs for 3 to 5 mixture components. The four families of three-level designs considered here in this context are- the central composite designs of Box and Wilson [5], the Box and Behnken [3] plans, the small composite designs of Draper and Lin [11] and the augmented pair designs of Morris [16]. The D-, A- and G- efficiencies are also tabulated and compared when we fit Model I

Model II to these designs. The uniformity measure centered L_2-discrepancy (CD_2) is also tabulated and compared for these designs. We also construct designs for restricted exploration of mixtures, using the transformation given by Saxena and Nigam [19] with a slight modification. The method is illustrated with the help of examples.

In Section 2, we give the optimality criteria and uniformity measure used for evaluating and comparing designs. In Section 3, we briefly describe the four families of three-level designs considered here. Section 4 describes the construction of projection designs. In Section 5 we illustrate the construction of projection designs using a three component mixture experiment. The efficiencies and discrepancies of the mixture designs obtained by projecting the four families of designs are also tabulated and compared for 3 to 5 mixture components. The restricted exploration of mixtures that is when (1.2) is satisfied is discussed in Section 6.

2. *Design Evaluating Criteria*

After considering practical constraints design optimality criteria are often used to evaluate a proposed experimental design. The design optimality measures that we use to compare different designs are D-, A- and G-efficiencies given by

$$\mathrm{D-eff} = 100\left(\frac{|X'X|^{1/p}}{n}\right), \quad \mathrm{A-eff} = 100\left(\frac{p}{n\ \mathrm{trace}\,(X'X)^{-1}}\right)$$

$$\mathrm{G-eff} = 100\left(P/nd\right) \tag{2.1}$$

where n = number of design points in the design; p = number of parameters in the model; and d = max $\{v = x\,(X'X)^{-1}x'\}$ over a specified set of design points (the row vectors) x in X' where X is the extended design matrix depending on model to be fitted. Corresponding to Model I and Model II, we have p = q (q + 1)/2 and p = 2q respectively in (2.1). The efficiencies are generated using Matlab software and are simply denoted by D, A, and G for convenience.

In recent years uniformity concept is also applied for evaluation of designs. Fang and Wang [12] describes uniform designs in which the points are scattered uniformly over the experimental domain. Hickernell [14], gave centered L_2-discrepancy (CD_2) as a measure to find uniform design

$$(CD_2\,(P))^2 = \left(\frac{13}{12}\right)^s - \frac{2}{n}\sum_{k=1}^{n}\prod_{j=1}^{s}\left(1+\frac{1}{2}\left|x_{kj}-0.5\right|-\frac{1}{2}\left|x_{kj}-0.5\right|^2\right)$$

$$+\frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\left(1+\frac{1}{2}\left|x_{ki}-0.5\right|+\frac{1}{2}\left|x_{ji}-0.5\right|-\frac{1}{2}\left|x_{ki}-x_{ji}\right|\right) \tag{2.2}$$

where $P = \{x_1, x_2, \ldots x_n\}$ be a set of n points in $[0, 1]^s$.

The centered L_2-discrepancy (CD_2) considers the uniformity of P not only over C^s but also of all the projection uniformity of P over C^u where u is a non empty subset of coordinate indices $S = \{1, 2, 3, \ldots, s\}$.

The maximum value of D, A and G and the minimum value of CD_2 is desirable.

3. The Three-level Designs

For response surface model of order two, three-level designs are popular choices. Since the full factorial designs using factors with three levels require many experimental runs therefore, alternative designs with fewer runs are typically used in practice. We now briefly describe the four families of three level designs we are going to study in this paper.

1. The central composite designs (CCD) are given by Box and Wilson [5]. These designs are five level factorial experiments with levels denoted by $\pm\alpha, \pm 1, 0$. We take $\alpha = 1$, so that only three experimental levels are required.

2. Hartley [13] pointed out that the nonsingular composite designs can also be constructed using smaller fractional factorials, provided two factor interaction are not aliased with other two factor interactions following which, Westlake [23], Draper [10] and Draper and Lin [11] introduced other catalogues of small composite designs (SCD). The SCD employed here are taken from Draper and Lin [11].

3. In Box-Behnken designs (BBD) of Box and Behnken [3], The "gross" structure of the design is determined by selecting an incomplete block design (IBD) in q treatments and b blocks. A one-to-one relation is established between the treatments of the IBD and the factors of response surface problem. Then for each block of the IBD, the "fine" structure of the response surface design is determined by selecting a two-level factorial or fractional factorial in the factors associated with these treatments and assigning the value of 0 to all other factors in these runs.

4. The augmented pairs designs (APD) given by Morris [16] are obtained by augmenting the first order designs to provide second order designs. The three groups of points are (a) a two-level first-order design, preferably orthogonal; (b) for each pair of runs (x_r, x_s), $r < s$ in (a) add a new run x_{rs} by setting $x_{rs} = -(x_r + x_s)/2$; (c) a number n_0 of center points (0, 0, ..., 0).

4. Projection Designs

Box and Hau [4] and Prescott [18] discussed the construction of projection designs for situations when the design variables are subject to linear constraints. The idea of the construction is to project an appropriate unconstrained design onto the constrained space. Suppose we are interested in the construction of a design with q factors $x_1, x_2, x_3, \ldots, x_q$ subject to m constraints

$$\mathbf{Cx} = \mathbf{c} \tag{4.1}$$

where $\mathbf{C}$ is an $m \times q$ matrix and $\mathbf{c}$ is an $m \times 1$ column vector. Suppose $\mathbf{x}^0$ is the chosen origin for the levels of the experimental design then $\mathbf{Cx}^0 = \mathbf{c}$. Let the region of interest be the neighborhood $x_j^0 \pm r_j$ around $\mathbf{x}^0$ where r_j's are some positive numbers, then the coded variables

$$\xi_i = \frac{x_j - x_j^0}{ar_j} \tag{4.2}$$

satisfy the constraints

$$A\xi = \mathbf{0} \tag{4.3}$$

where ξ is a $q \times 1$ vector of coded variables ξ_i's, $\mathbf{A} = (a_{ij})$ is an $m \times q$ matrix of constraints with $a_{ij} = r_j c_{ij}$ and $\mathbf{0}$ is an $m \times 1$ vector of 0's and a is the scaling constant used by the experimenter to modify the overall coverage of the design, and is chosen to be the largest number such that all the entries of the matrix $\mathbf{aD}_\xi$ are between -1 and 1.

Let $\mathbf{D}_z$ be an $n \times q$ matrix of some unconstrained generating design and $\mathbf{D}_\xi$ be that of the corresponding constrained design obtained by projection to satisfy (4.3) then

$$D_\xi = D_Z P \tag{4.4}$$

where $\mathbf{P} = \mathbf{I} - \mathbf{A}'(\mathbf{AA}')^{-1}\mathbf{A}$ is an idempotent projection matrix of order $q \times q$ then $\mathbf{D}_\xi \mathbf{A}' = \mathbf{D}_z \mathbf{PA}' = \mathbf{0}$ and the levels of the design $\mathbf{D}_x$ may be obtained from

$$x_i = ar_j \xi_j + x_j^0 \tag{4.5}$$

where 'a' is the number such that all the entries of $\mathbf{aD}_\xi$ are between -1 and 1.

5. Evaluation of Mixture Designs Obtained Through Projections

In the simplest case of a three component mixture with $0 \le x_i \le 1$ for $i = 1, 2, 3$ let $\mathbf{x}^o = (1/3, 1/3, 1/3)$ be a point which satisfies $x_1 + x_2 + x_3 = 1$.

Let the region of interest be the neighborhood $x_j^0 \pm r_j$ around $\mathbf{x}^0$ where $r_j = 1/3$; $j = 1, 2, 3$. The response surface designs $\mathbf{D}_z$ for the four families of designs are given in Table 1 and are denoted here by $\mathbf{D}_{CCD}, \mathbf{D}_{BBD}, \mathbf{D}_{SCD}$ and $\mathbf{D}_{APD}$.

Table 1. Standard three-level designs in three factors

$\mathbf{D}_{CCD}$			$\mathbf{D}_{BBD}$			$\mathbf{D}_{SCD}$			$\mathbf{D}_{APD}$		
–1	–1	–1	–1	–1	0	–1	–1	–1	1	–1	–1
–1	–1	1	–1	1	0	1	1	–1	–1	1	–1
–1	1	–1	1	–1	0	1	–1	1	–1	–1	1
–1	1	1	1	1	0	–1	1	1	1	1	1
1	–1	–1	–1	0	–1	–1	0	0	0	0	1
1	–1	1	–1	0	1	1	0	0	0	1	0
1	1	–1	1	0	–1	0	–1	0	–1	0	0
1	1	1	1	0	1	0	1	0	1	0	0
–1	0	0	0	–1	–1	0	0	–1	0	–1	0
1	0	0	0	–1	1	0	0	1	0	0	–1
0	–1	0	0	1	–1	0	0	0	0	0	0
0	1	0	0	1	1	0	0	0	0	0	0
0	0	–1	0	0	0	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0

We may note that here we have used ½-replicate for the design APD. A full replicate will produce a large number of augmenting point, therefore a ½-replicate is taken. Use of other ½-replicate produces APD, which is same as SCD. Now the idea is to project the center (0,0,0) of the design D_Z onto the center $\mathbf{x}^0 = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$ of $\mathbf{D}_x$.

The projection matrix $\mathbf{P} = \mathbf{I} - \mathbf{A}'(\mathbf{A}\mathbf{A}')^{-1}\mathbf{A}$ is a matrix of order 3 × 3 where $A = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$. Following the method described in Section-3, we get mixture designs $\mathbf{PD}_{CCD}, \mathbf{PD}_{BBD}, \mathbf{PD}_{SCD}$ **and** $\mathbf{PD}_{APD}$ given in Table 2 for four families of designs considered in Table 1.

To illustrate, let us consider the design $\mathbf{D}_{CCD}$ given in Table 1 as the response surface design to be projected into the simplex S_2. The projection matix $\mathbf{P}$ is

$$P = \frac{1}{3}\begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}$$

so that

$$\mathbf{D}_\xi = \mathbf{D}_{\mathbf{CCD}}\ \mathbf{P} = \begin{bmatrix} 0.000 & 0.000 & 0.000 \\ -0.667 & -0.667 & 1.333 \\ -0.667 & 1.333 & -0.667 \\ -1.333 & 0.667 & 0.667 \\ 1.333 & -0.667 & -0.667 \\ 0.667 & -1.333 & 0.667 \\ 0.667 & 0.667 & -1.333 \\ 0.000 & 0.000 & 0.000 \\ -0.667 & 0.333 & 0.333 \\ 0.667 & -0.333 & -0.333 \\ 0.333 & -0.667 & 0.333 \\ -0.333 & 0.667 & -0.333 \\ 0.333 & 0.333 & -0.667 \\ -0.333 & -0.333 & 0.667 \\ 0.000 & 0.000 & 0.000 \end{bmatrix}$$

The largest absolute value of the entries of the design $\mathbf{D}_\xi$ is 1.333, so we take the scale factor a = 1/1.333 = 0.750 and the coordinates of the points of $\mathbf{PD}_{\mathbf{CCD}}$ in the mixture simplex are now obtained using the equation (4.5) and are given in Table 2.

Table 2. Mixture designs obtained through projections of three-level designs

$\mathbf{PD}_{\mathbf{CCD}}$			$\mathbf{PD}_{\mathbf{BBD}}$			$\mathbf{PD}_{\mathbf{SCD}}$			$\mathbf{PD}_{\mathbf{APD}}$		
0.333	0.333	0.333	0.222	0.222	0.556	0.333	0.333	0.333	0.667	0.167	0.167
0.167	0.167	0.667	0.000	0.667	0.333	0.500	0.500	0.000	0.167	0.667	0.167
0.167	0.667	0.167	0.667	0.000	0.333	0.500	0.000	0.500	0.167	0.167	0.667
0.000	0.500	0.500	0.444	0.444	0.111	0.000	0.500	0.500	0.333	0.333	0.333
0.667	0.167	0.167	0.222	0.556	0.222	0.167	0.417	0.417	0.250	0.250	0.500
0.500	0.000	0.500	0.000	0.333	0.667	0.500	0.250	0.250	0.250	0.500	0.250
0.500	0.500	0.000	0.667	0.333	0.000	0.417	0.167	0.417	0.167	0.417	0.417
0.333	0.333	0.333	0.444	0.111	0.444	0.250	0.500	0.250	0.500	0.250	0.250
0.167	0.417	0.417	0.556	0.222	0.222	0.417	0.417	0.167	0.417	0.167	0.417
0.500	0.250	0.250	0.333	0.000	0.667	0.250	0.250	0.500	0.417	0.417	0.167
0.417	0.167	0.417	0.333	0.667	0.000	0.333	0.333	0.333	0.333	0.333	0.333
0.250	0.500	0.250	0.111	0.444	0.444	0.333	0.333	0.333	0.333	0.333	0.333
0.417	0.417	0.167	0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333
0.250	0.250	0.500	0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333
0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333	0.333

We obtain mixture designs for 3 to 5 component mixtures by projecting the four families of designs in 3 to 5 factors. To save space we have not given mixture designs obtained through projections for four and five mixture components. These are available with the authors. We obtain uniformity measures for these designs. We fit Model I and Model II to these designs and obtain efficiency measures using efficiency criteria given in Section 2. We give the uniformity measures and the efficiency measures in Table 3.

Table 3. Discrepancies and efficiencies of the mixture designs obtained through projection

Generating Design	q	p	n	n_0	CD_2	Model I			Model II		
						D	A	G	D	A	G
BBD	3	6	15	3	0.374712	1.171	0.208	56.545	1.475	0.344	56.445
	4	10	27	3	0.688893	0.224	0.033	64.516	0.509	0.081	60.377
	5	15	46	3	1.100210	0.055	0.009	67.541	0.217	0.027	60.757
SCD	3	6	11	1	0.418501	0.468	0.051	58.995	0.589	0.064	58.995
			13	3	0.438016	0.419	0.045	50.264	0.527	0.055	50.264
			15	5	0.456852	0.378	0.040	43.730	0.477	0.048	43.730
	4	10	17	1	0.747609	0.094	0.011	60.890	0.247	0.028	52.173
			19	3	0.762765	0.086	0.010	54.580	0.228	0.025	46.725
	5	15	23	1	1.144800	0.024	0.002	67.115	0.096	0.005	50.904
			25	3	1.156502	0.022	0.002	61.775	0.090	0.005	46.840
			28	6	1.729070	0.020	0.002	55.180	0.083	0.004	41.829
CCD	3	6	15	1	0.392521	0.781	0.120	53.887	0.984	0.191	53.887
			17	3	0.410163	0.722	0.115	47.626	0.910	0.175	47.626
	4	10	24	0	0.713594	0.159	0.023	63.393	0.342	0.046	58.244
			25	1	0.719362	0.155	0.022	60.931	0.334	0.045	55.921
			27	3	0.730859	0.147	0.022	56.579	0.318	0.043	51.787
			29	5	0.742001	0.139	0.021	52.761	0.303	0.040	48.220
	5	15	27	1	1.132990	0.041	0.006	58.942	0.130	0.012	48.329
			28	2	1.138052	0.039	0.006	56.864	0.127	0.012	46.630
			29	3	1.430620	0.038	0.006	54.925	0.123	0.012	45.044
			31	5	1.152825	0.036	0.005	51.412	0.117	0.011	42.168
APD	3	6	11	1	0.417679	0.468	0.056	58.995	0.589	0.072	58.995
			13	3	0.437388	0.419	0.050	50.264	0.527	0.062	50.264
			15	5	0.456352	0.378	0.041	43.730	0.477	0.054	43.730
	4	10	36	0	0.750375	0.103	0.013	38.800	0.238	0.028	39.171
			37	1	0.753682	0.270	0.101	37.909	0.234	0.028	38.160
			39	3	0.760291	0.256	0.097	36.204	0.226	0.027	36.275
	5	15	27	1	1.153238	0.025	0.003	49.415	0.089	0.007	42.181
			39	3	1.160336	0.024	0.003	47.128	0.084	0.006	39.126
			41	5	1.167236	0.023	0.003	45.002	0.083	0.006	38.197
			42	6	1.170595	0.022	0.003	43.999	0.081	0.006	37.310

n_0 denotes the number of center points, n is total number of points inclusive of n_0.

For both Model I and Model II, the designs obtained by projecting BBD is better than other three classes of designs in terms of uniformity and all the three efficiency criteria. The G-efficiencies of projected APD's in general are poor and the design also requires a larger number of points, but for three components mixtures, the G-efficiency of projected APD is same as the G-efficiency of projected SCD in case of 11 point design. This is highest among G-efficiencies for three component mixtures.

Here for all the designs obtained in Table 2, we have taken the scale factor 'a' to be the inverse of the largest absolute value of the entries of the design $\mathbf{D}_\xi$. However if we use different scale factor a = 0.666667(say) for APD in three factors, it produces a projected design for APD which fills the simplex with bounds 0 and 1. This of course changes the efficiency criteria values to D-efficiency = 2.4021, A-efficiency = 0.7227 and G-efficiency = 43.7301 for Model I and D-efficiency = 3.0265, A-efficiency = 0.8820 and G-efficiency = 43.7300 for Model II and this makes mixture design obtained through the projection of APD better than those obtained using CCD, BBD and SCD in terms of D- and A-efficiencies. The uniformity measure for this design is $CD_2 = 0.383782$ which makes it better than those obtained through projections of CCD and SCD.

6. Restricted Exploration of Mixtures

For restricted exploration of mixtures i. e., when (1.2) is satisfied Saxena and Nigam [19] gave a transformation that provides designs constructed through symmetric simplex designs. Their transformation works well when some say $t\ (\leq q-1)$ components satisfy (1.2). Prescott [18] discussed the case when some components have small values in the form of upper bounds and has illustrated this using three components example. We use the transformation given by Saxena and Nigam but with a slight modification to generate the design points through mixture designs based on projections of three-level designs. We suggest the following steps.

Step-1 : Rank the components in order of their increasing ranges $(U_i - L_i)$. X_1 has the smallest range and X_q has the largest range.

Step-2 : Consider a mixture design Z satisfying (1.1). We can select this from the four families of mixture designs obtained through projection in Section 5.

Step-3 : Compute B and B', the minimum and maximum proportions of any component Z_i in the design so that $0 \leq B \leq z_i \leq B' \leq 1$ for all Z_i.

Step-4 : Make the transformation as given by Saxena and Nigam [19] i.e. $x_{iu} = \lambda_i + \mu_i z_{iu}$, $i = 1, 2, \ldots t;\ u = 1, 2, \ldots n$

where

$$\lambda_i = \frac{L_i B' - U_i B}{B' - B} \text{ and } \mu_i = \frac{U_i - L_i}{B' - B}$$

$$\text{and } x_{iu} = \frac{\left(1 - \sum_{h=1}^{t} x_{hu}\right)}{\left(1 - \sum_{h=1}^{t} z_{hu}\right)} \quad i = t+1, \ldots q; u = 1, 2, \ldots n$$

where $t \le (q-1)$ is the number of components constrained by (1.2).

This transformation works well when some say $t (\le q-1)$ components satisfy (1.2). When all the components are constrained by (1.2) then the levels of x_q may be obtained by $x_q = 1 - (x_1 + x_2 + \ldots + x_{q-1})$.

Step-5 : While determining the value of x_q in Step 4, if in any point x_q lies outside the range $L_q \le x_q \le U_q$, it can be adjusted by setting x_q equal to the violated bound and adjusting the level of x_{q-1} so that (1.2) is satisfied. Repeat this with x_{q-2} and so on. Every point out of range of x_q can generate a maximum of q – 1 adjusted points.

Step-6 : The design points from Step-4 combined with different combinations of adjusted points result in a number of designs. The design that is optimal with certain optimality criteria is taken as the best design.

We now illustrate the steps given above with the help of example of three components mixtures. Let us consider a three components given in Snee and Marquardt [22] with components ranked in order of their increasing ranges. Here all components are constrained by (1.2).

Example : $0.1 \le x_1 \le 0.6$

$0.1 \le x_2 \le 0.7$

$0.0 \le x_3 \le 0.7$

To obtain design for Example, let us consider the four mixture designs given in Table 2 as our generating designs in Step 2 given above. The bounds B and B' on the design points are 0 to 2/3 for $\mathbf{D_{CCD}}$ and $\mathbf{D_{BBD}}$, 1/4 to 2/3 for $\mathbf{D_{APD}}$ and 0 to 1/2 for $\mathbf{D_{SCD}}$. Making transformation given in Step 4, we obtain four sets of points S_I, S_{II}, S_{III} and S_{IV} given in Table 4 using four mixture designs given in Table 2.

Table 4. The four sets of points obtained through transformation from designs given in Table 2

No.	S_I (CCD)			S_{II} (BBD)			S_{III} (SCD)			S_{IV} (PAD)		
1	0.350	0.400	0.250	0.267	0.300	0.433	0.433	0.500	0.067	0.600	0.100	0.300
2	0.225	0.250	0.525	0.100	0.700	0.200	0.600	0.700	-0.300*	0.100	0.700	0.200
3	0.225	0.700	0.075	0.600	0.100	0.300	0.600	0.100	0.300	0.100	0.100	0.800*
4	0.100	0.550	0.350	0.433	0.500	0.067	0.100	0.700	0.200	0.267	0.300	0.433
5	0.600	0.250	0.150	0.267	0.600	0.133	0.267	0.600	0.133	0.183	0.200	0.617
6	0.475	0.100	0.425	0.100	0.400	0.500	0.600	0.400	0.000	0.183	0.500	0.317
7	0.475	0.550	-0.025*	0.600	0.400	0.000	0.517	0.300	0.183	0.100	0.400	0.500
8	0.350	0.400	0.250	0.433	0.200	0.367	0.350	0.700	-0.050*	0.433	0.200	0.367
9	0.225	0.475	0.300	0.517	0.300	0.183	0.517	0.600	-0.117*	0.350	0.100	0.550
10	0.475	0.325	0.200	0.350	0.100	0.550	0.350	0.400	0.250	0.350	0.400	0.250
11	0.413	0.250	0.338	0.350	0.700	-0.050*	0.433	0.500	0.067	0.267	0.300	0.433
12	0.288	0.550	0.163	0.183	0.500	0.317	0.433	0.500	0.067	0.267	0.300	0.433
13	0.413	0.475	0.113	0.350	0.400	0.250	0.433	0.500	0.067	0.267	0.300	0.433
14	0.288	0.325	0.388	0.350	0.400	0.250	0.433	0.500	0.067	0.267	0.300	0.433
15	0.350	0.400	0.250	0.350	0.400	0.250	0.433	0.500	0.067	0.267	0.300	0.433

When CCD, BBD and APD are used as generating designs, in points 7, 11 and 3 respectively x_3 lies outside the bounds $0.0 \leq x_3 \leq 0.7$ and when SCD is used, in points 2, 8 and 9, x_3 lies outside the bounds $0.0 \leq x_3 \leq 0.7$. Using step 5 we get two designs when CCD, BBD or APD is used as generating design and eight designs when SCD is used. We calculate the uniformity measures CD_2 for each of these designs and select the most uniform design for each of the four families. These are denoted here by $D_{II}(CCD)$, $D_{II}(BBD)$, $D_{II}(SCD)$, and $D_{II}(APD)$ and are given in Table 5. The values of uniformity measure CD_2 are given in Table 6.

Table 5. Most uniform mixture designs for example

No.	D_{II} (CCD)			D_{II} (BBD)			D_{II} (SCD)			D_{II} (APD)		
1	0.350	0.400	0.250	0.267	0.300	0.433	0.433	0.500	0.067	0.600	0.100	0.300
2	0.225	0.250	0.525	0.100	0.700	0.200	0.600	0.400	0.000	0.100	0.700	0.200
3	0.225	0.700	0.075	0.600	0.100	0.300	0.600	0.100	0.300	0.200	0.100	0.700
4	0.100	0.550	0.350	0.433	0.500	0.067	0.100	0.700	0.200	0.267	0.300	0.433
5	0.600	0.250	0.150	0.267	0.600	0.133	0.267	0.600	0.133	0.183	0.200	0.617
6	0.475	0.100	0.425	0.100	0.400	0.500	0.600	0.400	0.000	0.183	0.500	0.317
7	0.475	0.520	0.000	0.600	0.400	0.000	0.517	0.300	0.183	0.100	0.400	0.500
8	0.350	0.400	0.250	0.433	0.200	0.367	0.300	0.700	0.000	0.433	0.200	0.367
9	0.225	0.475	0.300	0.517	0.300	0.183	0.517	0.483	0.000	0.350	0.100	0.550
10	0.475	0.325	0.200	0.350	0.100	0.550	0.350	0.400	0.250	0.350	0.400	0.250
11	0.413	0.250	0.338	0.300	0.700	0.000	0.433	0.500	0.067	0.267	0.300	0.433
12	0.288	0.550	0.163	0.183	0.500	0.317	0.433	0.500	0.067	0.267	0.300	0.433
13	0.413	0.475	0.113	0.350	0.400	0.250	0.433	0.500	0.067	0.267	0.300	0.433
14	0.288	0.325	0.388	0.350	0.400	0.250	0.433	0.500	0.067	0.267	0.300	0.433
15	0.350	0.400	0.250	0.350	0.400	0.250	0.433	0.500	0.067	0.267	0.300	0.433

Again we fit Model I and Model II and calculate the efficiency measures D, A and G for these designs. These are given in Table 6.

Table 6. Discrepancies and Efficiencies for constrained mixture designs for example

Generating Design	q	p	n	n_0	CD_2	Model I			Model II		
						D	A	G	D	A	G
BBD	3	6	15	3	0.407418	0.702	0.098	54.059	0.831	0.134	53.843
CCD	3	6	15	1	0.440807	0.447	0.048	51.980	0.563	0.077	91.980
SCD	3	6	15	5	0.541108	0.254	0.006	42.083	0.320	0.009	42.083
APD	3	6	15	5	0.464157	0.401	0.038	43.765	0.506	0.051	43.765

We observe that design obtained using BBD as generating design is most uniform and most efficient for both the models.

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REFERENCES

[1] Batra, P.K., Prasad, R., and Khanduri, O.P. (1999). Some statistical studies relating to Design and Analysis of Experiments involving fixed quantity of inputs. *Technical Report*, IASRI, New Delhi.

[2] Batra, P.K., Prasad, R., Gupta, V. K., and Khanduri, O.P. (1999). A strategy for analysis of experiments involving split application of fertilizer. *Statistics and Applications*, **1(2)**, 175-187.

[3] Box, G. E. P. and Behnken, D. W. (1960). Some new three level designs for the study of quantitative variables. *Technometrics*, **2**, 455-475.

[4] Box, G. E. P. and Hau, I. (2001). Experimental designs with one or more factor constraints. *Journal of Applied Statistics*, **28(8)**, 973-989.

[5] Box, G. E. P. and Wilson, K. B. (1951). On the experimental attainment of optimum conditions. *Jour. Roy. Statist. Soc.*, **B13**, 1-45.

[6] Chan, L. Y., Meng, J. H., Jiang, Y. C. and Guan, Y. C. (1998). D-optimal axial designs for quadratic and cubic additive mixture model. *Australian and New Zealand Journal of Statistics*, **40**, 359-371.

[7] Cornell, J. A. (2002). *Experiments with Mixtures*. 3rd ed. Wiley, New York.

[8] Darroch, J. N. and Waller, J. (1985). Additivity and interactions in three-component experiments with mixtures. *Biometrika*, **72,** 153-163.

[9] Deka, B.C., Sethi, V., Prasad, R., and Batra, P.K. (2001). Use of experiments with mixture methodology for quality evaluation of mixed fruit juice/pulp RTS beverages. *Journal of Food Science and Technology*, **38(6)**, 615-618.

[10] Draper, N. R. (1985). Small composite designs. *Technometrics*, **27**, 173-180.

[11] Draper, N.R. and Lin, D. K. J. (1990). Small response surface designs. *Technometrics*, **32**, 187-194.

[12] Fang, K. T. and Wang, Y. (1994). *Number-theoretic Methods in Statistics*. Chapman & Hall, London.

[13] Hartley, H. O. (1959). Smallest composite designs for quadratic response surfaces. *Biometrics*, **15**, 611-624.

[14] Hickernell, F. J., (1998). A generalised discrepancy and quadrature error bound. *Math. Comp.*, **67**, 299-322.

[15] Mclean, R. A. and Anderson, V. L. (1966). Extreme vertices design of mixture experiments. *Technometrics*, **8**, 447-454.

[16] Morris, M. D. (2000). A class of three-level experimental designs for response surface modeling. *Technometrics*, **42(2)**, 111-122.

[17] Murty, J. S. and Das, M. N., (1968). Design and analysis of experiments with mixtures. *Ann. Math. Statist.*, **39**, 1517-1539.

[18] Prescott, P. (2000). Projection designs for mixture experiments in orthogonal blocks. *Commu. Stat. - Theory and Methods*, **29,** 2229-2253.

[19] Saxena, S. K. and Nigam, A. K. (1977). Restricted exploration of mixtures by symmetric-simplex design. *Technometrics*, **19,** 47-52.

[20] Scheffé, H. (1958). Experiments with mixtures. *Jour. Roy. Statist. Soc.*, **B20,** 344-360.

[21] Scheffé, H., (1963). Simplex-centroid designs for experiments with mixtures. *Jour. Roy. Statist. Soc.*, **B25,** 235-263.

[23] Snee, R. D. and Marquardt, D. W. (1974). Extreme vertices designs for linear mixture models. *Technometrics*, **16,** 399-408.

[24] Westlake, W. J. (1965). Composite designs based on irregular fractions of factorials. *Biometrics*, **21**, 324-336.