

Efficient Mixture Designs using Galois Field

Poonam Singh¹, Vandana Sarin² and Neha Midha^{1*}

¹ Department of Statistics,
University of Delhi, Delhi 110007, India;
Email: pbs_93@yahoo.co.in

² Department of Statistics, Kirori Mal College,
University of Delhi, Delhi 110007, India;
Email: vandana_s_walia@yahoo.co.in

^{1*} Department of Statistics,
University of Delhi, Delhi 110007, India;

*Corresponding Author's Email: nehamidha1189@gmail.com

ABSTRACT

This paper proposes an algorithm for constructing mixture designs based on orthogonal arrays progressed by Galois Field. The algorithm can also be applied to constrained mixture experiments. The algorithm allows the generation of efficient mixture designs for Scheffé's canonical polynomials.

Keywords: Mixture experiments, Galois field, restricted region, G-efficiency.

Mathematics Subject Classification: 62K99; 05B15; 11T99; 12F10

1. INTRODUCTION

Experiments where the factors are the ingredients or the components of a mixture are called mixture experiments. The response in these experiments is assumed to depend only on the relative proportions of the components and not on the total amount in the mixture. Mixture experiments may be classified into standard mixture experiments and constrained mixture experiments.

In the standard mixture experiment, the proportions of the ingredients can vary between 0 and 1 and must sum up to unity. Suppose, we have a mixture experiment with q components, where, x_i is the proportion of the i^{th} component, $i = 1, 2, \dots, q$, then it must satisfy the following constraints:

$$0 \leq x_i \leq 1, \quad \sum_{i=1}^q x_i = 1 \quad (1.1)$$

Besides these constraints, there may be additional constraints imposed on the proportions of the i^{th} ingredients; $i = 1, 2, \dots, q$. The constraints may be in the form of upper (U_i) and/or lower (L_i) bounds,

$$0 \leq L_i \leq x_i \leq U_i \leq 1 \quad ; i = 1, 2, \dots, q \quad (1.2)$$

When mixture components are subject to additional constraints, such as a maximum and/or minimum value for each component, they are referred to as constrained mixture experiments.

Scheffé (1958,1963) developed simplex lattice and simplex centroid designs for fitting the canonical polynomial models:

$$\text{Linear model: } Y = \sum_{i=1}^q \beta_i x_i + \varepsilon \quad (1.3)$$

$$\text{Quadratic model: } Y = \sum_{i=1}^q \beta_i x_i + \sum_{i < j} \beta_{ij} x_i x_j + \varepsilon \quad (1.4)$$

$$\text{Special cubic model: } Y = \sum_{i=1}^q \beta_i x_i + \sum_{i < j} \beta_{ij} x_i x_j + \sum \sum_{i < j < k} \beta_{ijk} x_i x_j x_k + \varepsilon \quad (1.5)$$

McLean and Anderson (1966) established extreme vertices designs (EVD) which satisfy both the constraints (1.1) and (1.2). A partial solution to the restricted exploration problem was obtained by Thompson and Myers (1968) who considered an ellipsoidal region centred about a point of maximum interest. Saxena and Nigam (1977) explored the restricted mixture region using symmetric simplex design. Murthy and Murty (1983) discussed a method of construction of mixture designs for the exploration of the restricted region using factorials. Singh et al. (2018) generated mixture designs using Taguchi's fixed element orthogonal arrays. Bush (1952), Addelman and Kempthorne (1961), Rao (1946, 1947, 1949) and Bose and Bush (1952) constructed orthogonal arrays using Galois Fields and finite geometries.

In this paper, we present an algorithm for constructing mixture designs based on orthogonal arrays progressed by Galois Field. We have examined the designs constructed through this algorithm using the criterion of G-efficiency. The manageable number of design points help in reducing the cost and time in statistical experiments.

2. ORTHOGONAL ARRAYS BASED ON GALOIS FIELD

Rao (1946, 1947) defined orthogonal arrays as the extended versions of hypercubes of strength ' d '. An $N \times k$ array A with entries from S is said to be an orthogonal array $OA(N, k, s, t)$ with s levels, strength t and index λ (for some t in the range $0 \leq t \leq k$) if every $N \times t$ sub-array of A contains each t -tuple based on S exactly λ times as a row. If $\lambda = 1$, then such arrays are referred to as orthogonal arrays of index unity (Bush, 1952). Orthogonal arrays can be constructed using Galois field. Galois field, named after the French mathematician Evariste Galois, also known as Finite field, refers to a field that contains a finite number of elements. A field in which the number of elements is of the form p^n , where p is a prime and n is a positive integer, is called a Galois field and is denoted by $GF(p^n)$.

Design Criteria

If X denotes the $N \times k$ design matrix, then an advantageous criterion for evaluating the design is the minimum-maximum variance criterion. This refers to minimizing the maximum variance of prediction over the experimental region, where the prediction variance at the point x ($1 \times k$ row vector) is given by $\sigma^2 v$ and $v = x(X'X)^{-1}x'$. Computation of the maximum variance provides a criterion of how close is a design to optimality. The G-efficiency or Global efficiency of the design is given by,

$$G - \text{efficiency (percent of optimum)} = 100p/Nd$$

where, p is the number of model parameters, N is the number of design points and d is the maximum value of v over the experimental region.

As a practical rule of thumb, any design with a G – efficiency $\geq 50\%$ could be called good for practical purposes (Wheeler, 1972).

3. OABMD ALGORITHM

Let C be a $r \times q$ matrix with elements from $GF(m)$ such that $\rho(C) = g$. Let G be a $m^r \times r$ matrix with rows as ξ^T , where ξ^T is a $1 \times r$ vector with elements from $GF(m)$. If we consider any $m^r \times g$ submatrix of the array GC , then it contains every g tuple occurring equally often as a row. The resultant GC , under modulo m , is an $OA(m^r, q, m, g)$ as obtained by Bosh and Bush (1952).

We now present Orthogonal Array Based Mixture Design (OABMD) algorithm for constructing q component mixture designs using orthogonal arrays based on Galois Field.

Step 1: Construct an orthogonal array $OA(m^r, q, m, g)$ using the elements of $GF(m)$. Denote this matrix by A .

Step 2: Create a square matrix M of order $q \times q$ which is symmetrical but not orthogonal, having all elements as integers with sum of elements in each row and each column being zero. The choice of M is arbitrary and is useful in getting more vertices of the experimental region in the design as mentioned by Murthy and Murty (1983).

Step 3: Identify the minimum value in each column of $A \times M$ and subtract it from all the entries of that corresponding column to create a new matrix T .

Step 4: Obtain the row totals for matrix T . Divide the entries of each row of T by its corresponding row total to obtain a new matrix Z . The resultant matrix is a mixture design satisfying $0 \leq z_i \leq 1$ and $\sum_{i=1}^q z_i = 1$, z_i being the proportion for i^{th} component.

Further, if the mixture experiment has to be performed in the restricted region, where each component is bounded by lower or upper bounds, or both, then proceed as follows:

Step 5: Rank the components in order of their increasing ranges $R_i = (U_i - L_i)$ such that X_1 has the smallest range and X_q has the largest range, assuming range to be inversely proportional to the importance (in terms of cost, effectiveness, etc.) of the components in the experiment.

Step 6: Using the transformation given by Saxena and Nigam (1977), $X_i = L_i + (R_i \times z_i)$, compute the entries for the first $(q - 1)$ components of the design matrix X . The levels of X_q are obtained by $X_q = 1 - \sum_{i=1}^{q-1} X_i$.

Step 7: In case X_q lies beyond the specified bounds, generate candidate design points. There may be multiple candidate points corresponding to a given design point. The candidate points are generated by adjusting the level of one of the components by a quantity equal to the difference between the substituted upper or lower bound and the computed value for X_q . Additional points are produced only from those components whose adjusted levels remain within the limits of the components.

We have illustrated the OABMD algorithm for creating mixture designs using orthogonal arrays generated using Galois fields. These designs have been found to be efficient designs.

4. MIXTURE DESIGNS DEVELOPED USING GALOIS FIELDS

4.1 Construction I

Let $m \geq 2$ be a prime or prime power and let $r \geq 2$ be an integer. Then there exists an $OA(m^r, \frac{m^r-1}{m-1}, m, 2)$. (Bose and Bush, 1952).

For a given $A = OA(m^r, q, m, g)$ in Step 2 of the OABMD algorithm, a possible choice of M is $M = qI_q - J_{q,q}$, where I_q is an identity matrix of order q and $J_{q,q}$ is square matrix of order q with all elements equal to unity.

EXAMPLE 4.1.1

Consider a four-component mixture experiment, where all the components satisfy (1.1). Construct an orthogonal array $A = OA(9, 4, 3, 2)$ with four factors, using the elements of $GF(3)$.

$$A^T = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 1 & 2 & 1 & 2 & 0 & 2 & 0 & 1 \\ 0 & 2 & 1 & 1 & 0 & 2 & 2 & 1 & 0 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \end{pmatrix}$$

Multiply it with a symmetric and non-orthogonal matrix,

$$M = 4I_4 - J_{4,4} \quad (4.1.1)$$

having row sums and column sums as zero. Multiply A and M to obtain T ,

$$T^T = \begin{pmatrix} 5 & 1 & 0 & 6 & 5 & 4 & 7 & 9 & 8 \\ 5 & 5 & 8 & 6 & 9 & 0 & 7 & 1 & 4 \\ 5 & 9 & 4 & 6 & 1 & 8 & 7 & 5 & 0 \\ 6 & 6 & 9 & 3 & 6 & 9 & 0 & 6 & 9 \end{pmatrix}$$

Using step 4 of the OABMD algorithm, we obtain the design matrix Z for unrestricted region as follows:

$$Z^T = \begin{pmatrix} 0.238 & 0.047 & 0 & 0.286 & 0.238 & 0.190 & 0.333 & 0.429 & 0.381 \\ 0.238 & 0.238 & 0.381 & 0.286 & 0.429 & 0 & 0.333 & 0.047 & 0.190 \\ 0.238 & 0.429 & 0.190 & 0.286 & 0.047 & 0.381 & 0.334 & 0.238 & 0 \\ 0.286 & 0.286 & 0.429 & 0.142 & 0.286 & 0.429 & 0 & 0.286 & 0.429 \end{pmatrix}$$

We observe that $0 \leq z_i \leq 1$ and sum of the elements for each row is unity. This design matrix comprises of all distinct runs and has a G-efficiency of 72.72% for fitting (1.3). However, addition of extreme vertices, boundary points, edge centroids, face centroids or overall centroid allows for the fitting of higher order models. For instance, besides the nine design points in Z , incorporating $(1,0,0,0)$ and $(0,1,0,0)$ enables fitting of Scheffé's quadratic model with a G-efficiency of 90.90%. Similarly, addition of six design points, $(1,0,0,0)$, $(0,1,0,0)$, $(0,0,1,0)$, $(0,0,0,1)$, $(0.5, 0.5, 0, 0)$ and $(0, 0, 0.5, 0.5)$ to existing nine run design matrix Z , yields a G-efficiency of 93.33% for fitting (1.5).

Consider the constrained four component mixture experiment as discussed by McLean and Anderson (1966). In manufacturing one particular type of flare the chemical constituents are magnesium (x_1), sodium nitrate (x_2), strontium nitrate (x_3), and binder (x_4). Engineering experience has indicated that the following constraints (in order of increasing ranges) on a proportion by weight basis should be utilized:

$$0.03 \leq X_1 \leq 0.08, 0.40 \leq X_2 \leq 0.60, 0.10 \leq X_3 \leq 0.50 \text{ and } 0.10 \leq X_4 \leq 0.50$$

Using steps 5 and 6 of the OABMD algorithm, the constrained mixture design, X , is

$$X^T = \begin{pmatrix} 0.042 & 0.032 & 0.03 & 0.044 & 0.042 & 0.039 & 0.047 & 0.051 & 0.049 \\ 0.448 & 0.448 & 0.476 & 0.457 & 0.486 & 0.40 & 0.467 & 0.410 & 0.438 \\ 0.195 & 0.271 & 0.176 & 0.214 & 0.119 & 0.253 & 0.233 & 0.196 & 0.10 \\ 0.315 & 0.249 & 0.318 & 0.285 & 0.353 & 0.308 & 0.253 & 0.343 & 0.413 \end{pmatrix}$$

This design matrix comprises of all distinct runs and has a G-efficiency of 72.72% for fitting (1.3). Addition of two extreme vertices of the restricted region, $(0.03, 0.6, 0.1, 0.27)$ and $(0.08, 0.4, 0.1, 0.42)$ and six runs, $(0.03, 0.6, 0.1, 0.27)$, $(0.08, 0.4, 0.1, 0.42)$, $(0.055, 0.4, 0.2725, 0.2725)$, $(0.03, 0.5, 0.235, 0.235)$, $(0.08, 0.5, 0.21, 0.21)$ and $(0.055, 0.5, 0.2225, 0.2225)$, which comprises of extreme vertices of the constrained region, face centroid and the overall centroid, to the nine run

design matrix X , enables fitting of Scheffé's quadratic and special cubic models, yielding a G-efficiency of 90.90% and 93.33% for fitting (1.4) and (1.5) respectively.

Consider some other arbitrary choices of the matrix M as $M_1 = -M$,

$$M_2 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}, M_3 = -M_2, M_4 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}, M_5 = -M_4.$$

The G-efficiency values of unconstrained and constrained mixture designs corresponding to different choices of M for fitting Scheffé's canonical polynomials are listed in Table 1.

Table 1: G-efficiency of unconstrained and constrained mixture designs corresponding to different choices of M for fitting Scheffé's canonical polynomials.

Choice of M	G-efficiency for fitting (1.3) for Z and X	G-efficiency for fitting (1.4) for Z and X	G-efficiency for fitting (1.5)	
			Z	X
M	72.72%	90.90%	93.33%	93.33%
M_1	72.72%	90.90%	88.27%	93.33%
M_2	72.72%	90.90%	93.33%	93.33%
M_3	72.72%	90.90%	93.33%	93.33%
M_4	72.72%	90.90%	93.33%	93.33%
M_5	72.72%	90.90%	93.33%	93.33%

The G-efficiency of the unconstrained mixture design constructed using the orthogonal array $A = OA(9, 4, 3, 2)$ with any choice of M is 72.72% for fitting Scheffé's linear model and 90.90% for fitting (1.4). The same value of G-efficiency holds for the constrained four component mixture experiment as discussed above.

4.2 Construction II

Let $m \geq 2$ be a prime or prime power and let $g \geq 2$ be an integer. Then there exists an $OA(m^g, g + 1, m, g)$. (Bose and Bush, 1952)

EXAMPLE 4.2.1

Consider a four-component mixture experiment, where all the components satisfy (1.1). Construct an orthogonal array $A = OA(8, 4, 2, 3)$ with four factors, using the elements of $GF(2)$.

$$A^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$

Using a symmetric and non-orthogonal matrix, M , as stated in (4.1.1), yields the unconstrained mixture design Z ,

$$Z^T = \begin{pmatrix} 0.25 & 0 & 0 & 0 & 0.5 & 0.5 & 0.5 & 0.25 \\ 0.25 & 0 & 0.5 & 0.5 & 0 & 0 & 0.5 & 0.25 \\ 0.25 & 0.5 & 0 & 0.5 & 0 & 0.5 & 0 & 0.25 \\ 0.25 & 0.5 & 0.5 & 0 & 0.5 & 0 & 0 & 0.25 \end{pmatrix}$$

This design matrix consists of a repeat run and has a G-efficiency of 80% for fitting (1.3). Omitting the repeat run in Z , gives a G-efficiency of 88.88% for fitting the Scheffé's linear model. Subsequent addition of three points, $(1,0,0,0)$, $(0,1,0,0)$, $(0,0,1,0)$, to Z yields a 11-point design with a G-efficiency of 90.90% for fitting (1.4). Similarly, addition of four more points from the three-dimensional simplex, say, $(0,0,0,1)$, $(0.375, 0.125, 0.125, 0.375)$, $(0.125, 0.125, 0.375, 0.375)$ and $(0, 0.25, 0.25, 0.5)$, to the 11-point design matrix will yield a 15-point design matrix having a G-efficiency of 93.33% for fitting (1.5). Consider the constrained four component mixture experiment as discussed in Section 4.1. Using the OABMD algorithm, the constrained mixture design, X is

$$X^T = \begin{pmatrix} 0.0425 & 0.03 & 0.03 & 0.03 & 0.055 & 0.055 & 0.055 & 0.0425 \\ 0.45 & 0.4 & 0.5 & 0.5 & 0.4 & 0.4 & 0.5 & 0.45 \\ 0.2 & 0.3 & 0.1 & 0.3 & 0.1 & 0.3 & 0.1 & 0.2 \\ 0.3075 & 0.27 & 0.37 & 0.17 & 0.445 & 0.245 & 0.345 & 0.3075 \end{pmatrix}$$

This design also has a repeat runs and a G-efficiency of 80% for fitting (1.3). Considering only the seven distinct runs in X , yields a G-efficiency of 88.88% for fitting the Scheffé's linear model. Inclusion of two extreme vertices and the overall centroid of the constrained region, $(0.03, 0.6, 0.1, 0.27)$, $(0.08, 0.4, 0.1, 0.42)$ and $(0.055, 0.5, 0.2225, 0.2225)$, to X yields a 11-point design with a G-efficiency of 90.90% for fitting (1.4). Similarly, addition of four more points of the constrained region, say, $(0.055, 0.4, 0.2725, 0.2725)$, $(0.03, 0.5, 0.235, 0.235)$, $(0.08, 0.5, 0.21, 0.21)$ and $(0.055, 0.6, 0.1725, 0.1725)$, to the 11-point design matrix will yield a 15-point design matrix having a G-efficiency of 93.33% for fitting (1.5).

Other choices of M , as given in Section 4.1, along with the corresponding G-efficiency values of unconstrained and constrained mixture designs for fitting Scheffé's canonical polynomials are listed in Table 2.

Table 2: G-efficiency of unconstrained and constrained mixture designs corresponding to different choices of M for fitting Scheffé's canonical polynomials

Choice of M	G-efficiency for fitting (1.3) for Z and X	G-efficiency for fitting (1.4)		G-efficiency for fitting (1.5)	
		Z	X	Z	X
M	80%	90.90%	90.90%	93.33%	93.33%
M_1	80%	90.90%	90.90%	93.33%	93.33%
M_2	80%	55.29%	90.90%	93.33%	93.33%
M_3	80%	75.82%	90.90%	78.10%	93.33%
M_4	80%	85.91%	90.90%	80.13%	93.33%
M_5	80%	85.91%	90.90%	75.44%	93.33%

The G-efficiency of the unconstrained mixture design constructed using the orthogonal array $A = OA(8, 4, 2, 3)$ with any choice of M is 80% for fitting Scheffé's linear model. The flexibility in the choice of additional points to be incorporated in the design matrix gives many conceivable design. Out of the several possibilities, the design with a G-efficiency greater than or equal to 50%, may be chosen for

fitting higher order models. The same result holds for the constrained four component mixture experiment as discussed in Section 4.1.

4.3 Construction III

Let $m \geq 2$ be a prime or prime power. Then there exists an $OA(m^g, m+1, m, g)$ of index unity, where, $2 \leq g \leq m$. (Bose and Bush, 1952).

EXAMPLE 4.3.1

Consider a four-component mixture experiment, where all the components satisfy (1.1). Construct an orthogonal array $A = OA(27, 4, 3, 3)$ with four factors, using the elements of $GF(3)$.

$$A^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \\ 0 & 1 & 2 & 1 & 2 & 0 & 2 & 0 & 1 & 1 & 2 & 0 & 2 & 0 & 1 & 0 & 1 & 2 & 2 & 0 & 1 & 0 & 1 & 2 & 1 & 2 & 0 \\ 0 & 1 & 2 & 2 & 0 & 1 & 1 & 2 & 0 & 1 & 2 & 0 & 0 & 1 & 2 & 2 & 0 & 1 & 2 & 0 & 1 & 1 & 2 & 0 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \end{pmatrix}$$

Using a symmetric and non-orthogonal matrix M , as specified in (4.1.1), gives the unconstrained mixture design Z , with all twenty-seven distinct runs, as shown in Table A.1, having a G-efficiency of 72.72%, 64.51% and 56.36% for fitting (1.3), (1.4) and (1.5) respectively.

Consider the constrained four component mixture experiment as discussed in Section 4.1. Using the OABMD algorithm, the constrained mixture design X , consisting of all distinct runs is shown in Table A.1. It has a G-efficiency of 72.72%, 64.51% and 57.35% for fitting (1.3), (1.4) and (1.5) respectively.

Other choices of M , as given in Section 4.1, along with the corresponding G-efficiency values of unconstrained and constrained mixture design for fitting Scheffé's canonical polynomials are listed in Table 3.

Table 3: G-efficiency of unconstrained and constrained mixture designs corresponding to different choices of M for fitting Scheffé's canonical polynomials

Choice of M	G-efficiency for fitting (1.3) for Z and X	G-efficiency for fitting (1.4) for Z and X	G-efficiency for fitting (1.5)	
			Z	X
M	72.72%	64.51%	56.36%	57.35%
M_1	72.72%	64.51%	56.36%	57.35%
M_2	72.72%	64.51%	54.06%	53.11%
M_3	72.72%	64.51%	54.06%	53.11%
M_4	72.72%	64.51%	61.50%	55.22%
M_5	72.72%	64.51%	61.50%	55.22%

The G-efficiency of the unconstrained as well as constrained mixture design, with the set of constraints as given in Section 4.1, constructed using the orthogonal array $A = OA(27, 4, 3, 3)$ with any choice of M is 72.72% for fitting (1.3) and 64.51% for fitting (1.4).

If limitation of resources demands a reduction in the number of design points, we may use the method of normalization, as discussed by McLean and Anderson (1966). The operative idea is to compute a

normalized distance d_{ij} between points of the design and randomly omit points that are less than a certain minimum distance from other design points.

$$d_{ij} = \left(\sum_{r=1}^q \frac{(x_{ir} - x_{jr})^2}{b_r - a_r} \right)^{\frac{1}{2}}$$

Here, $b_r - a_r$ denotes the length of the constraint interval.

The design matrices, Z and X , corresponding to the unrestricted and restricted region constructed using M , stated in (4.1.1), consisting of just five design points, obtained using the above-mentioned technique are:

$$Z = \begin{pmatrix} 0 & 0.3333 & 0.3333 & 0.3334 \\ 0.4583 & 0.1250 & 0.1250 & 0.2917 \\ 0.1250 & 0.4583 & 0.1250 & 0.2917 \\ 0.3333 & 0 & 0.3333 & 0.3334 \\ 0.1250 & 0.4583 & 0.2917 & 0.1250 \end{pmatrix} \quad (4.3.1)$$

and

$$X = \begin{pmatrix} 0.04667 & 0.04666 & 0.1 & 0.38667 \\ 0.03625 & 0.45834 & 0.28333 & 0.22208 \\ 0.03625 & 0.42500 & 0.28333 & 0.25542 \\ 0.05292 & 0.42500 & 0.15000 & 0.37208 \\ 0.04458 & 0.42500 & 0.28334 & 0.24708 \end{pmatrix} \quad (4.3.2)$$

The design matrix Z in (4.3.1) and matrix X in (4.3.2) have a G-efficiency of 80% and 80.18% respectively for fitting (1.3).

In practical situations, fitting linear model is not always suitable. A higher model may provide a better fit to the given design. To facilitate the computation of G-efficiency for fitting higher order models as stated in (1.4) and (1.5), we may select at least 11 runs or 15 runs respectively from the available 27 runs, using the above-mentioned distance criteria.

For example, a 11-point design and a 15-point design for unconstrained region, constructed using M , as mentioned in (4.1.1), and using the distance criteria, yields a G-efficiency of 85.28% and 76.76% for fitting (1.4) and (1.5) respectively. Similarly, their constrained counterparts yield a G-efficiency of 90.90% and 93.33% for fitting Scheffé's quadratic and Scheffé's special cubic models respectively.

4.4 Construction IV

Let $m = 2^u$, $u \geq 1$, then there exists an $OA(m^3, m+2, m, 3)$ of index unity. (Bose and Bush, 1952).

EXAMPLE 4.4.1

Consider a four-component mixture experiment, where all the components satisfy (1.1). Construct an orthogonal array $A = OA(8, 4, 2, 3)$ with four factors, using the elements of $GF(2)$.

$$A^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \end{pmatrix}$$

Using a symmetric and non-orthogonal matrix, M , as stated in (4.1.1), yields the unconstrained mixture design Z ,

$$Z^T = \begin{pmatrix} 0.18 & 0 & 0 & 0 & 0.46 & 0.28 & 0.28 & 0.28 \\ 0.27 & 0.45 & 0.45 & 0.09 & 0.18 & 0.36 & 0.36 & 0 \\ 0.27 & 0.46 & 0.09 & 0.45 & 0.18 & 0.36 & 0 & 0.36 \\ 0.28 & 0.09 & 0.46 & 0.46 & 0.18 & 0 & 0.36 & 0.36 \end{pmatrix}$$

This design matrix consists of all distinct runs and has a G-efficiency of 80% for fitting (1.3).

Subsequent addition of three points, (1,0,0,0), (0,1,0,0), (0,0,1,0), to Z yields a 11-point design with a G-efficiency of 90.90% for fitting (1.4). Similarly, addition of four more points from the three-dimensional simplex, say, (0.5, 0.5, 0, 0), (0, 0.5, 0.5, 0), (0, 0, 0.5, 0.5) and (0.5, 0, 0, 0.5), to the 11-point design matrix will yield a 15-point design matrix having a G-efficiency of 93.33% for fitting (1.5).

Consider the constrained four component mixture experiment as discussed in Section 4.1. Using the OABMD algorithm, the constrained mixture design, X , is

$$X^T = \begin{pmatrix} 0.0425 & 0.03 & 0.03 & 0.03 & 0.055 & 0.055 & 0.055 & 0.0425 \\ 0.45 & 0.4 & 0.5 & 0.5 & 0.4 & 0.4 & 0.5 & 0.45 \\ 0.2 & 0.3 & 0.1 & 0.3 & 0.1 & 0.3 & 0.1 & 0.2 \\ 0.3075 & 0.27 & 0.37 & 0.17 & 0.445 & 0.245 & 0.345 & 0.3075 \end{pmatrix}$$

This design also has all distinct runs and a G-efficiency of 80% for fitting (1.3). Insertion of two more extreme vertices and the overall centroid of the restricted region, (0.03, 0.6, 0.1, 0.27), (0.08, 0.4, 0.1, 0.42) and (0.055, 0.5, 0.2225, 0.2225), to X yields a 11-point design with a G-efficiency of 90.90% for fitting (1.4). Similarly, addition of four more points of the constrained region, say, (0.055, 0.4, 0.2725, 0.2725), (0.03, 0.5, 0.235, 0.235), (0.08, 0.5, 0.21, 0.21) and (0.055, 0.6, 0.1725, 0.1725), to the 11-point design matrix will yield a 15-point design matrix having a G-efficiency of 93.33% for fitting (1.5). Other choices of M , as given in Section 4.1, along with the corresponding G-efficiency values of Z and X for fitting Scheffé's canonical polynomials are listed in Table 4.

Table 4: G-efficiency of unconstrained and constrained mixture designs corresponding to different choices of M for fitting Scheffé's canonical polynomials

Choice of M	G-efficiency for fitting (1.3) for Z and X	G-efficiency for fitting (1.4) for Z and X	G-efficiency for fitting (1.5) for Z and X
M	80%	90.90%	93.33%
M_1	80%	90.90%	93.33%
M_2	80%	90.90%	93.33%
M_3	80%	90.90%	93.33%
M_4	80%	90.90%	93.33%
M_5	80%	90.90%	93.33%

The G-efficiency of the unconstrained mixture design constructed using the orthogonal array $A = OA(8, 4, 2, 3)$ with any choice of M is 80% for fitting Scheffé's linear model, 90.90% for fitting Scheffé's quadratic model and 93.33% for fitting Scheffé's special cubic model. The same result holds for the constrained four component mixture experiment as discussed in Section 4.1.

EXAMPLE 4.4.2

Consider a six-component mixture experiment, where all the components satisfy (1.1).

Construct an orthogonal array $A = OA(4^3, 6, 2^2, 3)$ with six factors, using the elements of $GF(2^2)$. To generate unconstrained mixture design in six components with sixty-four distinct runs, we follow the OABMD algorithm with the choice of M as $M = 6I_6 - J_{6,6}$.

The six columns of A and Z are stated in Table A.2 of the appendix. The design matrix Z consists of all distinct runs and has a G-efficiency of 53.37%, 51.24% and 64.06% for fitting (1.3), (1.4) and (1.5) respectively. Following the steps of the OABMD algorithm, a constrained mixture design may also be fit.

Some other choices of the arbitrary matrix M are $M_1 = -M$, $M_2 = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$,

$M_3 = -M_2$, $M_4 = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$, $M_5 = -M_4$.

The G-efficiency values of unconstrained and constrained mixture designs corresponding to different choices of M for fitting Scheffé's canonical polynomials are listed in Table 5.

Table 5: G-efficiency of unconstrained mixture designs corresponding to different choices of M for fitting Scheffé's canonical polynomials.

Choice of M	G-efficiency for fitting (1.3) for Z	G-efficiency for fitting (1.4) for Z	G-efficiency for fitting (1.5) for Z
M	53.37%	51.24%	64.06%
M_1	53.37%	51.24%	64.06%
M_2	53.37%	51.24%	64.26%
M_3	53.37%	51.24%	64.26%
M_4	53.37%	51.24%	65.22%
M_5	53.37%	51.24%	65.22%

The G-efficiency of the unconstrained mixture design constructed using the orthogonal array $A = OA(4^3, 6, 2^2, 3)$ with any choice of M is 53.37% for fitting Scheffé's linear model and 51.24% for fitting Scheffé's quadratic model.

Using the method of normalization as discussed in Section 4.3, the G-efficiency for a 7-run design, 22-run design and a 42-run design for fitting (1.3), (1.4) and (1.5) are 85.71%, 75.70% and 84.14% respectively.

5. DISCUSSION AND CONCLUSION

The Constructions I, II, III and IV have been discussed for generating mixture experiments with four components, in both, unconstrained space as well in a constrained region.

For the unconstrained mixture experiment, the G-efficiency for fitting (1.3) using a 5-run design matrix, is observed to be higher in Construction IV, at 82.28%, as compared to Constructions I, II and III, at 80% each. Also, it is detected that the G-efficiency for fitting (1.4) using a 11-run design matrix is 90.90% each for Constructions I, II and IV in contrast to 85.28% for Construction III. Similarly, the G-efficiency for fitting (1.5) using a 15-run design matrix is 93.33% each for Constructions I, II and IV as compared to 76.76% for Construction III.

For constrained mixture experiments, the G-efficiency for fitting (1.3) using a 5-run design matrix, is seen to be more in Constructions III and IV, at 80.18% and 82.28% respectively, as compared to Constructions I and II, at 80% each. Also, it is noticed that the G-efficiency for fitting (1.4) and (1.5) using a 11-run and a 15-run design matrix is 90.90% and 93.33% respectively for all Constructions I, II, III and IV. On the other hand, the design points generated by the algorithm given McLean and Anderson (1966) have a G-efficiency of 80%, 90.90% and 93.33% for fitting (1.3), (1.4) and (1.5) respectively.

To summarize, the designs constructed through the proposed OABMD algorithm have a sufficiently high G-efficiency that make them suitable for practical purposes. These designs have manageable number of design points that help in reducing the cost and time in statistical experiments. Furthermore, the flexibility in choice of matrix M allows for enhanced variety of design points. When the region of interest is pre-defined, the proposed OABMD algorithm can be customized to explore a restricted region.

6. REFERENCES

- Addelman, S., Kempthorne, O., 1961, Some main-effect plans and orthogonal arrays of strength two. *Ann. Math. Stat.* **32**, 1167-1176.
- Bose, R.C., Bush, K.A., 1952, Orthogonal arrays of strength two and three. *The Annals of Mathematical Statistics* **23**, 508-524.
- Bush, K.A., 1952, Orthogonal arrays of index unity. *Ann. Math. Stat.* **23**, 426-434.
- McLean, R.A., Anderson, V.L., 1966, Extreme vertices design of mixture experiments. *Technometrics* **8(3)**, 447-454.
- Murthy, M.S.R., Murty, J.S., 1983, Restricted Region Simplex design for Mixture Experiments. *Communication in Statistics Theory and Methods* **12(22)**, 2605-2615.
- Rao, C.R., 1946, Hypercubes of strength " d " leading to confounded designs in factorial experiments. *Bulletin of the Calcutta Mathematical Society* **38**, 67-78.
- Rao, C.R., 1947, Factorial Experiments derivable from combinatorial arrangements of arrays. *Journal of Royal Statistical Society (Suppl.)* **9(1)**, 128-139.
- Rao, C.R., 1949, On a class of arrangements. *Proc. Edinburgh Math. Soc.* **8**, 119-125.
- Saxena, S.K., Nigam, A.K., 1977, Restricted Exploration of mixtures by Symmetric Simplex Design. *Technometrics* **19(1)**, 47-52.

Scheffé, H., 1958, Experiments with Mixtures. *Journal of the Royal Statistical Society. Series B (Methodological)* **20(2)**, 344-360.

Scheffé, H., 1963, The Simplex Centroid Design for Experiments with Mixtures. *Journal of the Royal Statistical Society, Series B (Methodological)* **25(2)**, 235-263.

Singh, P., Sarin, V., Midha, N., 2018, Construction of Mixture Designs Based on Taguchi's Fixed Element Orthogonal Arrays. *International Journal of Statistics and Reliability Engineering* **5(2)**, 89-95.

Thompson, W.C., Myers, R.H., 1968, Response surface designs for experiments with mixtures. *Technometrics* **10(4)**, 739-756.

Wheeler, R.E., 1972, Efficient experimental design presented at the Annual Meeting of the American Statistical Association, Montreal, August 1972.

APPENDIX

Table A.1: 27 runs of $OA(27, 4, 3, 3)$ for unconstrained and constrained design matrix

Run No.	Columns of Z				Columns of X			
	I	II	III	IV	I	II	III	IV
1	0.25	0.25	0.25	0.25	0.0425	0.45	0.2	0.3075
2	0.125	0.292	0.292	0.291	0.03625	0.45833	0.216667	0.28875
3	0	0.333	0.333	0.334	0.03	0.46667	0.23333	0.27
4	0.125	0.292	0.458	0.125	0.03625	0.45833	0.28334	0.22208
5	0.125	0.458	0.125	0.292	0.03625	0.49167	0.15	0.32208
6	0.125	0.125	0.292	0.458	0.03625	0.425	0.21667	0.32208
7	0.125	0.458	0.292	0.125	0.03625	0.49167	0.21667	0.25541
8	0.125	0.125	0.458	0.292	0.03625	0.425	0.28333	0.25542
9	0.125	0.292	0.125	0.458	0.03625	0.45833	0.15	0.35542
10	0.292	0.292	0.291	0.125	0.04458	0.45833	0.21667	0.28042
11	0.167	0.333	0.333	0.167	0.03833	0.46667	0.23333	0.26167
12	0.292	0.125	0.125	0.458	0.04458	0.425	0.15	0.38042
13	0.292	0.458	0.125	0.125	0.04458	0.49167	0.15	0.31375
14	0.292	0.125	0.292	0.291	0.04458	0.425	0.21667	0.31375
15	0.167	0.167	0.333	0.333	0.03833	0.43333	0.23334	0.295
16	0.292	0.125	0.458	0.125	0.04458	0.425	0.28334	0.24708
17	0.292	0.292	0.125	0.291	0.04458	0.45834	0.15	0.34708
18	0.167	0.333	0.167	0.333	0.03833	0.46667	0.16667	0.32833
19	0.333	0.333	0.333	0	0.04667	0.46667	0.23333	0.25333
20	0.458	0.125	0.125	0.292	0.05292	0.425	0.15	0.37208
21	0.333	0.167	0.167	0.333	0.04667	0.43333	0.16667	0.35333
22	0.458	0.125	0.292	0.125	0.05292	0.425	0.21667	0.30541
23	0.333	0.167	0.333	0.167	0.04667	0.43333	0.23333	0.28667
24	0.333	0.333	0	0.333	0.04667	0.46667	0.1	0.38667
25	0.458	0.292	0.125	0.125	0.05292	0.45833	0.15	0.33875
26	0.333	0.333	0.167	0.167	0.04667	0.46667	0.16666	0.32
27	0.333	0	0.333	0.333	0.04667	0.4	0.23333	0.32

Table A.2: 64 runs of $OA(4^3, 6, 2^2, 3)$ and unconstrained design matrix

Run No.	Columns of A						Columns of Z					
	I	II	III	IV	V	VI	I	II	III	IV	V	VI
1	0	0	0	0	0	0	0.166	0.166	0.167	0.167	0.167	0.167
2	0	1	3	2	1	0	0.069	0.153	0.319	0.237	0.153	0.069
3	0	2	1	3	2	0	0.056	0.222	0.139	0.305	0.222	0.056
4	0	3	2	1	3	0	0.042	0.291	0.208	0.125	0.292	0.042
5	0	1	2	3	0	1	0.069	0.153	0.237	0.319	0.069	0.153
6	0	2	1	1	1	1	0.083	0.250	0.167	0.167	0.167	0.166
7	0	3	3	0	2	1	0.042	0.292	0.291	0.042	0.208	0.125
8	0	2	0	2	3	1	0.056	0.222	0.056	0.222	0.306	0.138
9	0	2	3	1	0	2	0.056	0.222	0.306	0.138	0.056	0.222
10	0	3	0	3	1	2	0.042	0.292	0.042	0.291	0.125	0.208
11	0	0	2	2	2	2	0.056	0.056	0.222	0.222	0.222	0.222

12	0	1	1	0	3	2	0.069	0.153	0.153	0.069	0.319	0.237
13	0	3	1	2	0	3	0.042	0.292	0.125	0.208	0.042	0.291
14	0	2	2	0	1	3	0.056	0.222	0.222	0.056	0.139	0.305
15	0	1	0	1	2	3	0.069	0.153	0.069	0.153	0.237	0.319
16	0	0	3	3	3	3	0	0	0.250	0.250	0.250	0.250
17	1	1	1	1	0	0	0.194	0.194	0.194	0.194	0.112	0.112
18	1	2	2	3	1	0	0.125	0.208	0.208	0.292	0.125	0.042
19	1	3	0	2	2	0	0.139	0.305	0.056	0.222	0.222	0.056
20	1	2	3	0	3	0	0.125	0.208	0.291	0.042	0.292	0.042
21	1	2	3	2	0	1	0.125	0.208	0.292	0.208	0.042	0.125
22	1	3	0	0	1	1	0.167	0.333	0.083	0.083	0.167	0.167
23	1	2	2	1	2	1	0.125	0.209	0.208	0.125	0.208	0.125
24	1	3	1	3	3	1	0.083	0.250	0.083	0.250	0.250	0.084
25	1	3	2	0	0	2	0.139	0.306	0.222	0.055	0.056	0.222
26	1	2	1	2	1	2	0.125	0.208	0.125	0.208	0.125	0.209
27	1	1	3	3	2	2	0.083	0.083	0.250	0.250	0.167	0.167
28	1	0	0	1	3	2	0.153	0.069	0.069	0.153	0.319	0.237
29	1	2	0	3	0	3	0.125	0.208	0.042	0.292	0.042	0.291
30	1	3	3	1	1	3	0.083	0.250	0.250	0.083	0.084	0.250
31	1	0	1	0	2	3	0.153	0.069	0.153	0.069	0.237	0.319
32	1	1	2	2	3	3	0.083	0.083	0.167	0.167	0.250	0.250
33	2	2	2	2	0	0	0.222	0.222	0.222	0.222	0.056	0.056
34	2	3	1	0	1	0	0.237	0.319	0.153	0.069	0.153	0.069
35	2	0	3	1	2	0	0.222	0.056	0.306	0.138	0.222	0.056
36	2	1	0	3	3	0	0.208	0.125	0.042	0.292	0.292	0.041
37	2	3	0	1	0	1	0.237	0.319	0.069	0.153	0.069	0.153
38	2	2	3	3	1	1	0.167	0.167	0.250	0.250	0.083	0.083
39	2	1	1	2	2	1	0.209	0.125	0.125	0.208	0.208	0.125
40	2	0	2	0	3	1	0.222	0.056	0.222	0.056	0.305	0.139
41	2	0	1	3	0	2	0.222	0.056	0.139	0.305	0.056	0.222
42	2	1	2	1	1	2	0.208	0.125	0.208	0.125	0.125	0.209
43	2	2	0	0	2	2	0.222	0.222	0.056	0.056	0.222	0.222
44	2	3	3	2	3	2	0.125	0.208	0.208	0.125	0.209	0.125
45	2	1	3	0	0	3	0.208	0.125	0.292	0.042	0.042	0.292
46	2	0	0	2	1	3	0.222	0.056	0.056	0.222	0.138	0.306
47	2	3	2	3	2	3	0.125	0.209	0.126	0.208	0.125	0.208
48	2	2	1	1	3	3	0.167	0.167	0.083	0.083	0.250	0.250
49	3	3	3	3	0	0	0.250	0.250	0.250	0.250	0	0
50	3	2	0	1	1	0	0.319	0.237	0.069	0.153	0.153	0.069
51	3	1	2	0	2	0	0.306	0.139	0.222	0.056	0.222	0.055
52	3	0	1	2	3	0	0.292	0.042	0.125	0.208	0.291	0.042
53	3	2	1	0	0	1	0.319	0.237	0.153	0.069	0.069	0.153
54	3	3	2	2	1	1	0.250	0.250	0.167	0.167	0.083	0.083
55	3	0	0	3	2	1	0.291	0.042	0.042	0.292	0.208	0.125
56	3	1	3	1	3	1	0.250	0.083	0.250	0.083	0.250	0.084
57	3	1	0	2	0	2	0.306	0.138	0.056	0.222	0.056	0.222
58	3	0	3	0	1	2	0.291	0.042	0.292	0.042	0.125	0.208
59	3	3	1	1	2	2	0.250	0.250	0.083	0.083	0.167	0.167
60	3	2	2	3	3	2	0.209	0.125	0.125	0.208	0.208	0.125
61	3	0	2	1	0	3	0.291	0.042	0.208	0.125	0.042	0.292
62	3	1	1	3	1	3	0.250	0.083	0.083	0.250	0.084	0.250
63	3	2	3	2	2	3	0.208	0.125	0.208	0.125	0.125	0.209
64	3	3	0	0	3	3	0.250	0.250	0	0	0.250	0.250