Restricted Mixture Designs for Three Factors

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ABSTRACT

Draper and Lawrence (1965 a) have given mixture designs for three factors when all the mixture components can vary on the entire factor space so that the region of interest is an equilateral triangle in two dimensions. In this paper their work is extended to the cases when the region of interest is an echelon, parallelogram, pentagon or hexagon, because of the restrictions imposed on some or all of the mixture components. The principles used in the choice of appropriate designs are those originally introduced by Box and Draper(1959). It is assumed that a response surface equation of first order is fitted, but there is a possibility of bias error due to presence of second order terms in the true model. Minimum bias designs for several cases of restricted regions of interest are illustrated.

Key Words: Mixture components, Region of interest, All-bias designs, Restricted mixture designs, Region moments, Design moments.

1. Introduction

Mixture experiments are those for which the response depends upon the proportions of the different components under study and not on the total amount of the mixture. If q components $(q \geq 3)$ are present in the mixture system under study, then

$$0 \leq z_i \leq 1 \quad (i=1, 2, \ldots, q), \quad \sum_{i=1}^{q} z_i = 1 \tag{1}$$

where z_i is the proportion of the ith component in the mixture. The possible factor space is thus a regular $(q-1)$-dimensional simplex.

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In many practical situations, additional constraints are placed on some or all of the components because of economic considerations, present physical requirements or informations obtained from previous experiments. In any case, such constraints might be expressed as

$$0 \leq a_i \leq z_i \leq b_i \leq 1 \quad (1 \leq i \leq q), \quad \sum_{i=1}^{q} z_i = 1, \tag{2}$$

and the resulting factor space is a $(q-1)$-dimensional irreqular convex polyhedron, which is usually more complicated in form than $(q-1)$-dimensional simplex.

When three components z_1, z_2, z_3 form a mixture, the constraints in (2) make the factor space to be such figures as equilateral triangle, echelon, parallelogram, pentagon and hexagon. Let A be the possible factor space

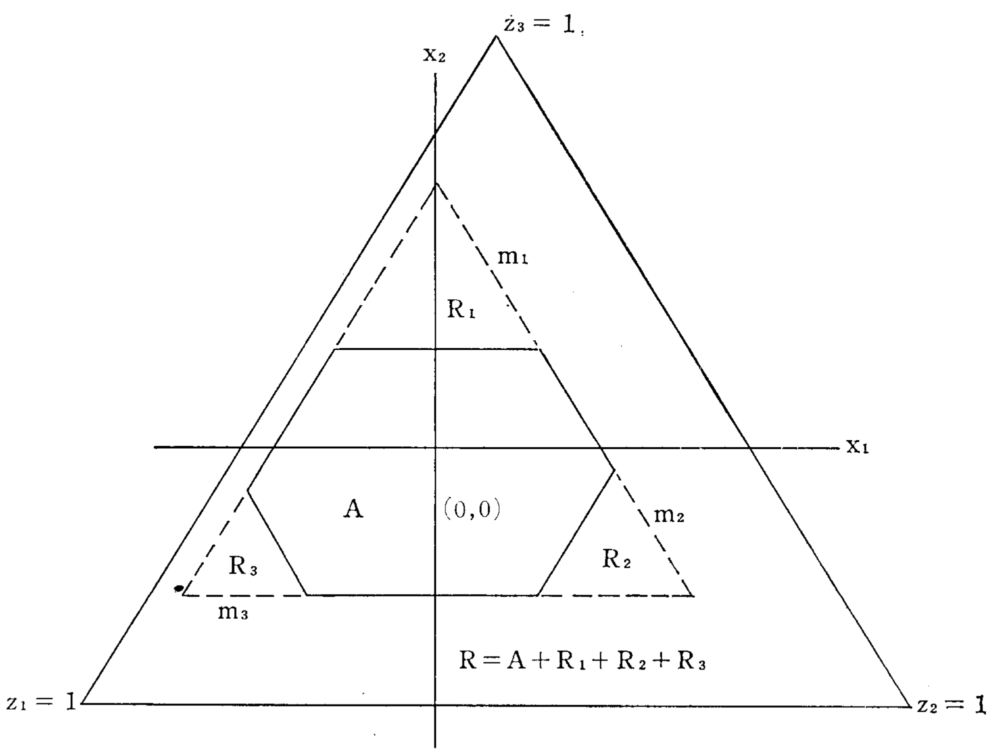

Figure 1. General Layout

resulting from (2). This region A is often called the region of interest to the experimenter. This region can be thought as polygons generated by cutting out small equilateral triangles from a large one. Figure 1 shows the general hexagon case attached by equilateral triangles R_1, R_2 and R_3. The number of equilateral triangles being attached might be one or two or three possibly. Let $R=A+R_1+R_2+R_3$.

If we choose new axes (x_1, x_2) instead of (z_1, z_2, z_3) for the equilateral triangle R so that one vertex lies on the line $x_1=0$, the other vertices are symmetrical about $x_1=0$ and the centroid is at $(0,0)$ as shown in Figure 1, we can move between the two representations by

$$x_1=\frac{1}{2}(-z_1+z_2)-\frac{1}{2}(-a_1+a_2),$$

$$x_2=\frac{\sqrt{3}}{6}(-z_1-z_2+2z_3)-\frac{\sqrt{3}}{6}(-a_1-a_2+2a_3),$$

$$x_3=z_1+z_2+z_3=1.$$

Or, equivalently,

$$z_1=\frac{1}{3}(-3\,x_1-\sqrt{3}\,x_2+1)+\frac{1}{3}(2\,a_1-a_2-a_3),$$

$$z_2=\frac{1}{3}(3\,x_1-\sqrt{3}\,x_2+1)+\frac{1}{3}(-a_1+2\,a_2-a_3),$$

$$z_3=\frac{1}{3}(2\sqrt{3}\,x_2+1)+\frac{1}{3}(-a_1-a_2+2\,a_3).$$

We now work in the coordinates (x_1, x_2) and assume that m is the length of side of the equilateral triangle R, and m_i for R_i, $i=1,2,3$. The coordinates of the vertices of R are

$$\left(0,\ \frac{1}{\sqrt{3}}m\right),\ \left(\frac{1}{2}m, -\frac{\sqrt{3}}{6}m\right) \text{ and } \left(-\frac{1}{2}m, -\frac{\sqrt{3}}{6}m\right).$$

We suppose that, although it is assumed that within the region of interest A a polynomial of degree d_1 is used, in fact the true function may be a polynomial of higher degree $d_2>d_1$. Let $\widehat{y}(\underline{x})$ be the value of the estimated response at the point $\underline{x}=(x_1, x_2)$, where this value is obtained by the least squares fitting of the polynomial of degree d_1 using a design containing N points. Let $\eta(\underline{x})$ be the true response at this point given exactly by the polynomial of higher degree d_2 and let σ^2 be the experimental error variance.

We shall determine the appropriate experimental designs which minimize the bias error which arises due to the possibility that the order d_1 of the model is inadequate.

Following the development of Box and Draper(1959), average squared bias error over the region A will be defined as

$$B=N\Omega\sigma^{-2}\int_A \{\hat{E}y(\underline{x})-n(\underline{x})\}^2\, dx_1dx_2 \tag{3}$$

where

$$\Omega^{-1}=\int_A dx_1dx_2.$$

A theorem by Box and Draper(1959) states that the average squared bias B will be minimized by choosing the design in such a way that

$$M_{11}^{-1}M_{12}=u_{11}^{-1}u_{12} \tag{4}$$

where M_{11} and M_{12} are matrices of design moments and u_{11} and u_{12} are matrices of region moments up to order d_1+d_2. One way to make (4) hold is to choose a design for which

$$M_{11}=u_{11} \text{ and } M_{12}=u_{12}. \tag{5}$$

Thus equating design moment matrices to region moment matrices represents a solution to the problem of minimizing B. Draper and Lawrence(1965a, 1965b) used these ideas to develop the all-bias designs for the unrestricted mixture system, defined by (1) and (5).

In this paper the all-bias designs of the restricted mixture experiments for three factors satisfying (2) and (5) will be investigated. Graphically, Draper and Lawrence(1965a) searched for designs over an equilateral triange R, but we will search for designs over A which can be an echelon, parallelogram, pentagon or hexagon. In particular we will assume that the response is fitted by a linear model($d_1=1$), and there is a possibility of error due to presence of second degree terms ($d_2=2$) in the true model. The case for $d_1=2$ and $d_2=3$ could be similarly approached in the same manner.

Briefly, literature on mixture designs needs to be reviewed. Scheffé(1958, 1963) did the pioneering work for experimenting with mixtures. Since then, the designs developed by Draper and Lawrence(1965a, 1965b), Murty and

Das(1968), Lambrakis(1969), Becker(1970), Paku, Manson and Nelson (1971) and Saxena and Nigam(1973) are useful in those situations where all the components can vary on the entire factor space. These designs can be applied to the restriced region of interest, if the region is an equilateral triangle. For general restricted regions of interest A as in Figure 1, McLean and Anderson(1966) explored extreme vertices design, Snee and Marquardt (1974) proposed an algorithm which selects a subset of the extreme vertices for fitting the linear model, Snee(1975) presented a similar algorithm to support the fit of a quadratic model, and Saxena and Nigam(1977) developed a transformed symmetric-simplex design.

So far, minimum bias designs for restricted regions of interest have not been explored. Hopefully, this paper will add a new dimension to the restricted mixture designs.

2. Moment Requirements

Suppose that the true response relationship is

$$E(y)=\underline{x}_1'\underline{\beta}_1+\underline{x}_2'\underline{\beta}_2$$

where

$$\underline{x}_1'=(1,\ x_1, x_2),\quad \underline{x}_2'=(x_1^2,\ x_2^2,\ x_1x_2)$$

and $\underline{\beta}_1$ and $\underline{\beta}_2$ are the corresponding vectors of regression coefficients. The fitted equation is

$$\widehat{y}(\underline{x})=\underline{x}_1'\widehat{\underline{\beta}}_1.$$

Then the design moment matrices are expressed as

$$M_{11}=N^{-1}(X_1'X_1),\quad M_{12}=N^{-1}(X_1'X_2),$$

where

$$X_1=\begin{pmatrix} x_{11} & x_{21} \\ x_{12} & x_{22} \\ \vdots & \vdots \\ x_{1N} & x_{2N} \end{pmatrix} \qquad X_2=\begin{pmatrix} x_{11}^2 & x_{21}^2 & x_{11}x_{21} \\ x_{12}^2 & x_{22}^2 & x_{12}x_{22} \\ \vdots & \vdots & \vdots \\ x_{1N}^2 & x_{2N}^2 & x_{1N}x_{2N} \end{pmatrix}.$$

The region moments are obtained from the following equations:

$$u_{11}=\rho^{-1}\int_A \underline{x}_1\underline{x}_1'd\underline{x} \quad u_{12}=\rho^{-1}\int_A \underline{x}_1\underline{x}_2'd\underline{x}$$

where

$$\rho=\frac{\sqrt{3}}{4}(m^2-m_1^2-m_2^2-m_3^2).$$

Using $A=R-R_1-R_2-R_3$, the moment of $x_1^u x_2^v$ (u, v are integers≥ 0) is

$$\rho^{-1}\int_A x_1^u x_2^v dx_1 dx_2$$

$$=\rho^{-1}\left\{\int_R-\int_{R_1}-\int_{R_2}-\int_{R_3}\right\}x_1^u x_2^v dx_1 dx_2,$$

which is expressed more precisely as follows:

$$\rho^{-1}\left\{\int_{-a}^{2a}\int_{-b}^{b}-\int_{a_1}^{2a}\int_{-b}^{b}-\int_{-a}^{a_2}\int_{b_2}^{b}-\int_{-a}^{a_3}\int_{-b}^{b_3}\right\} x_1^u x_2^v dx_1 dx_2,$$

and

$$a=\frac{\sqrt{3}}{6}m \quad , \qquad b=\frac{1}{3}(m-\sqrt{3}\,x_2),$$

$$a_1=\frac{\sqrt{3}}{6}(2m-3m_1), \qquad b_2=\frac{1}{3}(2m-3m_2+\sqrt{3}\,x_2),$$

$$a_2=-\frac{\sqrt{3}}{6}(m-3m_2), \qquad b_3=\frac{1}{3}(2m-3m_3+\sqrt{3}\,x_2).$$

$$a_3=-\frac{\sqrt{3}}{6}(m-3m_3),$$

The details of the evaluation of the integral (6) are given in the Appendix. The general formulas to obtain the region moments are summarized in Table 1. In this table we have $p_i=m_i/m$, $i=1,2,3$. The values of the associated coefficients in the foumulas, $K(u,v)$ and $k_i(u,v)$, are also summarized in Table 2.

Table 1. Formulas for Region Moments

region	formulas ($0\leq u$, $v\leq 3$)	
R	0	if u odd
	$2\rho^{-1}K(n,v)\sum_{i=0}^{v} k_i(u,v)(-1)^{v-i}$	if u even
R_1	0	if u odd
	$2\rho^{-1}K(u,v)\sum_{i=0}^{v} k_i(u,v)(2-3p_1)^{v-i}p_1^{u+2+i}$	if u even

region	formulas $(0\leq u,\ v\leq 3)$
R_2	$\rho^{-1}K(u, v)\ \sum_{i=0}^{v} k_i(u, v)(-1)^v\{(1-p_2)^{u+2+i}(1-3p_2)^{v-i}$ $[(-1)^{i+1}-1]+(-1)^i+(1-2p_2)^{u+2+i}\}$
R_3	$\rho^{-1}K(u,v)(-1)^v \sum_{i=0}^{v} k_i(u, v)\ (-1)^v\ \{(1-p_3)^{u+2+i}(1-3p_3)^{v-i}$ $[(-1)^{i+1}-1]+(-1)^i+(1-2p_3)^{u+2+i}]$

$$* \ K(u, v)=\left(\frac{m}{2}\right)^{u+v+2}\left(\frac{1}{3}\right)^{v-1}$$

$$k_i(u, v)=\frac{u!}{(u+2+i)!}(v)_i 3^i, \quad \text{where } (M)_n=M(M-1)\ldots(M-n+1)$$

Table 2. The values of $K(u, v)$ and $k_i(u, v)$, $i=0,\ldots,v$

u	v	$K(u, v)$	$k_i(u, v)$			
			$i=0$	$i=1$	$i=2$	$i=3$
0	0	$\frac{\sqrt{3}}{4}m^2$	$\frac{1}{2}$			
1	0	$\frac{\sqrt{3}}{8}m^3$	$\frac{1}{6}$			
0	1	$\frac{1}{8}m^3$	$\frac{1}{2}$	$\frac{1}{2}$		
2	0	$\frac{\sqrt{3}}{16}m^4$	$\frac{1}{12}$			
1	1	$\frac{1}{16}m^4$	$\frac{1}{6}$	$\frac{1}{8}$		
0	2	$\frac{\sqrt{3}}{48}m^4$	$\frac{1}{2}$	1	$\frac{3}{4}$	
3	0	$\frac{\sqrt{3}}{32}m^5$	$\frac{1}{20}$			
2	1	$\frac{1}{32}m^5$	$\frac{1}{12}$	$\frac{1}{20}$		
1	2	$\frac{\sqrt{3}}{96}m^5$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{3}{20}$	
0	3	$\frac{1}{96}m^5$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{9}{4}$	$\frac{27}{20}$

The values of the elements of matrices μ_{11} and μ_{12} are given in Table 3 and the matrices μ_{11} and μ_{12} are given in Table 4. Marginal letters indicate the arrangement of moments within the matrices; e.g., the moment at the intersection of the x_1 row and the x_2^2 colum is

$\rho^{-1}\int_A x_1 x_2^2 dx_1 dx_2$.

The matrices of design moments are of the form given in Table 4; marginal letters have been included as in the case of the matrices of the region moments. For example,

$$|122| = N^{-1} \sum_{u=1}^{N} x_{1u} x_{2u}^2.$$

In order to obtain design points, the conditions (5) must be solved. We have, then, nine equations of very complicated forms including up to cubic terms. The conditions to be satisfied in this case are the following:

$$\begin{array}{ll} \sum x_1 = c_1 & \sum x_1^3 = c_6 \\ \sum x_2 = c_2 & \sum x_1^2 x_2 = c_7 \\ \sum x_1^2 = c_3 & \sum x_1 x_2^2 = c_8 \\ \sum x_1 x_2 = c_4 & \sum x_2^3 = c_9 \\ \sum x_2^2 = c_5 & \end{array}$$

where all summations are from 1 to N, and c_i is a constant which is N times the associated region moment, $i=1,\dots,9$.

We now restrict the class of possible designs by imposing the following symmetry conditions on the desgin moments:

$$|1| = |12| = |111| = |122| = 0. \tag{8}$$

Table 3. Region Moments on A

u	v	region moments of A
1	0	$r_1 = -\frac{1}{2}\mathrm{Km}\,[p_2^2(1-p_2) - p_3^2(1-p_3)]$
0	1	$r_2 = \frac{\sqrt{3}}{6}\mathrm{Km}\,[-2p_1^2(1-p_1) + p_2^2(1-p_2) + p_3^2(1-p_3)]$
2	0	$r_{11} = \frac{1}{24}\mathrm{Km}^2\,[1 - p_1^4 - p_2^4 - p_3^4 - 6p_2^2(1-p_2)^2 - 6p_3^2(1-p_3)^2]$
1	1	$r_{12} = \frac{\sqrt{3}}{12}\mathrm{Km}^2\,[p_2^2(1-p_2)^2 - p_3^2(1-p_3)^2]$
0	2	$r_{22} = \frac{1}{24}\mathrm{Km}^2\,[1 - p_1^4 - p_2^4 - p_3^4 - 8p_1^2(1-p_1)^2 - 2p_2^2(1-p_2)^2 - 2p_3^2(1-p_3)^2]$
3	0	$r_{111} = -\frac{1}{16}\mathrm{Km}^3\,[2p_2^2(1-p_2)^3 - 2p_3^2(1-p_3)^3 + p_2^4(1-p_2) - p_3^4(1-p_3)]$

u	v	region moments on A
2	1	$r_{112}=-\frac{\sqrt{3}}{360}Km^3[1-p_1^5-p_2^5-p_3^5-15p_2^2(1-p_2)^3-15p_3^2(1-p_3)^3+5p_1^4(1-p_1)$ $-2.5p_2^4(1-p_2)-2.5p_3^4(1-p_3)]$
1	2	$r_{122}=-\frac{1}{48}Km^3[2p_2^2(1-p_2)^3-2p_3^2(1-p_3)^3+p_2^4(1-p_2)-p_3^4(1-p_3)]$
0	3	$r_{222}=\frac{\sqrt{3}}{360}Km^3[1-p_1^5-p_2^5-p_3^5-40p_1^2(1-p_1)^3+5p_2^2(1-p_2)^3+5p_3^2(1-p_3)^3$ $-15p_1^4(1-p_1)+2.5p_2^4(1-p_2)+2.5p_3^4(1-p_3)]$

* $K=(1-p_1^2-p_2^2-p_3^2)^{-1}$

Table 4. The matrices of region and design moments

$$\mu_{11}=\begin{array}{cccc} 1 & x_1 & x_2 & \\ \left(\begin{matrix} 1 \\ r_1 \\ r_2 \end{matrix}\right. & \begin{matrix} r_1 \\ r_{11} \\ r_{12} \end{matrix} & \left.\begin{matrix} r_2 \\ r_{12} \\ r_{22} \end{matrix}\right) & \begin{matrix} 1 \\ x_1 \\ x_2 \end{matrix} \end{array} \qquad \mu_{12}=\begin{array}{cccc} x_1^2 & x_2^2 & x_1x_2 & \\ \left(\begin{matrix} r_{11} \\ r_{111} \\ r_{112} \end{matrix}\right. & \begin{matrix} r_{22} \\ r_{122} \\ r_{222} \end{matrix} & \left.\begin{matrix} r_{12} \\ r_{112} \\ r_{122} \end{matrix}\right) & \begin{matrix} 1 \\ x_1 \\ x_2 \end{matrix} \end{array}$$

$$M_{11}=\begin{array}{cccc} 1 & x_1 & x_2 & \\ \left(\begin{matrix} 1 \\ [1] \\ [2] \end{matrix}\right. & \begin{matrix} [1] \\ [11] \\ [12] \end{matrix} & \left.\begin{matrix} [2] \\ [12] \\ [22] \end{matrix}\right) & \begin{matrix} 1 \\ x_1 \\ x_2 \end{matrix} \end{array} \qquad M_{12}=\begin{array}{cccc} x_1^2 & x_2^2 & x_1x_2 & \\ \left(\begin{matrix} [11] \\ [111] \\ [112] \end{matrix}\right. & \begin{matrix} [22] \\ [122] \\ [222] \end{matrix} & \left.\begin{matrix} [12] \\ [112] \\ [122] \end{matrix}\right) & \begin{matrix} 1 \\ x_1 \\ x_2 \end{matrix} \end{array}$$

These require that the possible designs be symmetric about x_2 axis. Unless such conditions are imposed the excessive number of moments that must be determined makes a search for a suitable design prohibitive. Hence, it is desirable for the restrited factor space to be symmetrical about x_2 axis, which can be achived if $m_2=m_3$.

In order to find the all-bias designs, it is convenient to consider point sets satisfying the assumptions (8). Table 5 shows typical examples of point sets which satisfy (8). The contribution of each point set to the sum $\sum x_1^u x_2^v$ is given for each moment. The individual point sets in Table 5 do not by themselves provide desgns since the equations (7) are not satisfied with four points or less. The designs, however will be formed by combining point sets so that all nine equations are satisfied.

Table 5. Point sets in two demensions

Set number	1	2	3	4
parameters	a, b △	c, d ▽	e, f ◇	g, h, i □

# of points in set	3	3	4	4
Σx_1	0	0	0	0
Σx_2	3β	3β	4β	4β
Σx_1^2	$2a^2$	$2c^2$	$2f^2$	$2(g^2+i^2)$
Σx_1x_2	0	0	0	0
Σx_2^2	$2b^2+(2b+3\beta)^2$	$2d^2+(3\beta-2d)^2$	$e^2-2\beta^2+(2\beta-e)^2$	$2h^2+2(2\beta-h)^2$
Σx_1^3	0	0	0	0
$\Sigma x_1^2x_2$	$-2a^2b$	$2c^2d$	$2\beta f^2$	$2g^2h+2i^2(2\beta-h)$
$\Sigma x_1x_2^2$	0	0	0	0
Σx_2^3	$(2b+3\beta)^3-2b^3$	$d^3+(3\beta-2d)^3$	$2\beta^3+e^3+(2\beta-e)^3$	$2h^3+2(2\beta-h)^3$

* $\beta\equiv r_2$, r_2 in Table 3.

Set number 1: Vertices of an isosceles triangle, oriented as R centroid at $(0, \beta)$; $(\pm a, -b)$, $(0. 2b+3\beta)$

Set number 2: Vertices of an isosceles triangle, inverted with respect to R, centroid at $(0, \beta)$; $(\pm c, d)$, $(0. 3\beta-2d)$

Set number 3: Points on the line $x_1=0$ or $x_2=\beta$, symmetrical about x_2 axis; $(\pm f, \beta)$, $(0, e)$, $(0, 2\beta-e)$

Set number 4: Vertices of an equilateral echelon, centroid at $(0, \beta)$; $(\pm g, h)$, $(\pm i, 2\beta-h)$

For example, set number 1 consists of three vertices of an isosceles triangle, which are parametrized by a and b. This set does not satisfy (7) but (8). Similar arguments follow for set number 2, parametrized by c and d. But if we consider them simultaneously as design points, these six points can satisfy both (7) and (8); i.e., it is possible to generate an all-bias design.

Let (i, j) denote the combinaton of point sets i, j from Table 5. The set combinations containing four unknown parameters or more all provide designs with six or more points, including additional center points possibly. The set combinations (1, 2), (1, 3), (2, 4), etc., are the simple examples. It can be shown that to find design using the set combination (1, 2) with a center point is equivalent to use the set combination (1, 3) or (2, 3), etc.. Hence it is quite useful to search for optimal designs using the set combination

(1, 2) with r center points ($r\geq 0$).

3. A General Result of $(6+r)$-point Designs

Consider the set combination (1, 2) with r center points which will provide $(6+r)$-point designs. As a matter of convenience, let

$$\beta=r_2,\ C_1=r_{11},\ C_2=r_{22},\ C_3=r_{112},\ C_4=r_{222}$$

where r_2, r_{11}, r_{22}, r_{112}, r_{222} are elements of the matrices of region moments on A in Table 3. The conditions to be satisfied are obtained by equating design moments and region moments up to and including moments of third order:

$$\begin{aligned}
&2a^2+2c^2=(6+r)C_1,\\
&2b^2+(2b+3\beta)^2+2d^2+(\beta-2d)^2+r\beta^2=(6+r)C_2,\\
&-2a^2b+2c^2d=(6+r)C_3,\\
&-2b^3+(2b+3\beta)^3+2d^3+(3\beta-2d)^3+r\beta^3=(6+r)C_4,
\end{aligned}$$

which are equivalent to

$$\begin{aligned}
&a^2+c^2=\left(3+\frac{r}{2}\right)C_1,\\
&(b^2+d^2)+2\beta(b-d)=\left(1+\frac{r}{6}\right)C_2-\left(3+\frac{r}{6}\right)\beta^2,\\
&a^2b-c^2d=-\left(3+\frac{r}{2}\right)C_3,\\
&(b^3-d^3)+6\beta(b^2+d^2)+9\beta^2(b-d)=\left(1+\frac{r}{6}\right)C_4-\left(9+\frac{r}{6}\right)\beta^3.
\end{aligned} \tag{9}$$

Let $b-d=u$ and $bd=v$. Then the second and third equations in (9) bocome the following:

$$\begin{aligned}
&u^2+2\beta u+2v=\left(1+\frac{r}{6}\right)C_2-\left(3+\frac{r}{6}\right)\beta^2,\\
&u^3+6\beta u^2+3(v+3\beta^2)u+12\beta v=\left(1+\frac{r}{6}\right)C_4-\left(9+\frac{r}{6}\right)\beta^3.
\end{aligned} \tag{10}$$

Or. equivalently,

$$v=\frac{1}{2}\left\{\left(1+\frac{r}{6}\right)C_2-\left(3+\frac{r}{6}\right)\beta^2-u^2-2\beta u\right\},$$

$$u^3+6\beta u^2+\left\{\left(15+\frac{r}{2}\right)\beta^2-\left(3+\frac{r}{2}\right)C_2\right\}u \tag{11}$$

$$+\left(18+\frac{5}{3}r\right)\beta^3-(12+2r)\beta C_2+\left(2+\frac{r}{3}\right)C_4=0.$$

Let $y=u+2\beta$. If we substitute y for u in the second equation in (10), then we have a reduced cubic of the form

$$y^3+\left(3+\frac{r}{2}\right)(\beta^2-C_2)y+\left(2+\frac{r}{3}\right)(2\beta^3-3\beta C_2+C_4)=0. \tag{12}$$

This cubic equation in y is easily solved by the trigonometric method [MacDuffee(1959)]. Let

$$k=\sqrt{2\left(2+\frac{r}{3}\right)(C_2-\beta^2)}.$$

Then the desired solution of the equation(12) will be

$$y=k\cos(A+240°),$$

where

$$A=\frac{1}{3}\cos^{-1}\left(-\frac{2(2\beta^3-3\beta C_2+C_4)}{(C_2-\beta^2)k}\right).$$

The roots of (10) are readily obtained fıom the root of y of (12). Hence we get

$$u=y-2\beta,$$

$$v=\left(\frac{1}{2}+\frac{r}{12}\right)C_2-\left(\frac{3}{2}+\frac{r}{12}\right)\beta^2+\beta y-\frac{1}{2}y^2.$$

Since $b=d+u$, the quadratic equation $d^2+ud-v=0$ gives

$$d=\frac{1}{2}(-u+\sqrt{u^2+4v}),$$

and, so that

$$b=\frac{1}{2}(u+\sqrt{u^2+4v}).$$

Finally, from the first two equations in (9)

$$c=\sqrt{\left(3+\frac{r}{2}\right)\frac{bC_1+C_3}{b+d}},$$

and

$$a=\sqrt{\left(3+\frac{r}{2}\right)\frac{dC_1-C_3}{b+d}}.$$

Therefore the design consists of the following $(6+r)$ points:

$(\pm a, \quad -b)$,

$(\pm c, \quad d)$,

$(0, \ 2b+3\beta)$,

$(0,\ 3\beta-2d)$,

$r(0,\ \beta)$.

4. 5-point Designs

In this section the method of obtaining 5-point designs are derived, not using the point set combinations but assuming more concrete symmetric conditions. General solutions of 5-point designs are not obtained easily. If we assume, however, that three of the five points lie on the coordinate axis and the remaining two are symmetrical about the coordinate axis, finding the 5-point designs resolves itself into solving the symmetric equations up to cubic order.

The coordinates of the five points assumed are the following:

$$(\pm u, v),\ (0, w_1),\ (0, w_2),\ (0, w_3).$$

The equations to be solved in this case, which are obtained by equating design moments to region moments, are:

$$w_1+w_2+w_3+2v=5\beta, \tag{13}$$

$$2u^2=5C_1, \tag{14}$$

$$w_1^2+w_2^2+w_3^2+2v^2=5C_2, \tag{15}$$

$$2u^2v=5C_3, \tag{16}$$

$$w_1^3+w_2^3+w_3^3+2v^3=5C_4, \tag{17}$$

where β, C_1, C_2, C_3, C_4 are defined in the previous section.

From (14)

$$u=\sqrt{\frac{5}{2}C_1}$$

is readily obtained and using this result into (16), we get

$$v=\frac{C_3}{C_1}.$$

Until now the values of w_1, w_2, w_3 are unknown to us. Since u and v are known values, if we arrange (13), (15) and (17) in w_1, w_2, w_3, then we have

$$w_1+w_2+w_3=s_1,$$
$$w_1^2+w_2^2+w_3^2=s_2, \tag{18}$$
$$w_1^3+w_2^3+w_3^3=s_3,$$

where

$$s_1=5\beta-2v,$$
$$s_2=5C_2-2v^2,$$
$$s_3=5C_4-2v^3.$$

By applying Newton's formula about symmetric equations [MacDuffee (1959)], it is deduced that x_1, x_2, x_3 are the roots of the following function f in x:

$$f(x)=x^3-s_1x^2+\frac{s_1^2-s_2}{2}x+\frac{-2s_3+3s_1s_2-s_1^3}{6}=0. \tag{19}$$

The values of w_1, w_2, w_3 are, then, obtained by transforming (19) into the reduced cubic and using the trigonometric method used in section 3. Let $x=y+s_1/3$. Then

$$y^3+\frac{s_1^2-3s_2}{6}y-\frac{2}{27}s_1^3+\frac{1}{3}s_1s_2-\frac{1}{3}s_3=0 \tag{20}$$

holds. If we let

$$k=\frac{1}{3}\sqrt{6s_2-2s_1^2},$$
$$q=-\frac{1}{27}(2s_1^3-9s_1s_2+9s_3),$$

and if we compute the following:

$$A_1=\frac{1}{3}\cos^{-1}\left(\frac{-4q}{k^3}\right),$$
$$A_2=A_1+120°,$$
$$A_3=A_2+120°,$$

then the roots y_1, y_2, y_3 of (20) are obtained as follows:

$$y_i=k\cos A_i, \quad i=1,2,3.$$

So that, we have

$$w_i=y_i+\frac{s_1}{3}, \quad i=1,2,3.$$

Even though there might be several designs beside this, they are hardly solvable compared with the design derived as above.

5. Examples

In this section we will deal with the real examples. The knowledge of the exact values of m_1, m_2, m_3 and m are required to find the values of the region moments. The values of them can be given by using the lower and upper bounds and they are listed in Table 6. Table 6 includes the general case of unsymmetrical polygons.

The following three cases are considered: (i) $m_1 \neq 0$, $m_2 = m_3 = 0$, (ii) $m_1 = 0$, $m_2 = m_3$, $m_2 \neq 0$, (iii) $m_1 \neq 0$, $m_2 = m_3$, $m_2 \neq 0$.

Table 6. General Foumulas for m_1, m_2, m_3, and m

	$m_1 \neq 0,\ m_2 = m_3 = 0$	$m_1 = 0,\ m_2 \neq 0,\ m_3 \neq 0$	$m_1 \neq 0,\ m_2 \neq 0,\ m_3 \neq 0$
m_1	$\frac{1}{2}(-a_1+b_1-a_2+b_2)$	0	$1-a_1-a_2-b_3$
m_2	0	$1-a_1-b_2-a_3$	$1-a_1-b_2-a_3$
m_3	0	$1-b_1-a_2-a_3$	$1-b_1-a_2-a_3$
m	$1-a_1-a_2-b_3$	$1-a_1-a_2-a_3$	$1-a_1-a_2-a_3$

5.1 Designs for the case $m_1 \neq 0$, $m_2 = m_3 = 0$

Assume that the factor space is determined by the following constraints:

$$\begin{aligned} .2 \leq z_1 \leq .7 \\ .1 \leq z_2 \leq .6 \\ .2 \leq z_3 \leq .6 \end{aligned} \tag{21}$$

In this case we get $m = .5$ and $m_1 = .1$. The graphical representation is given in Figure 2 (dotted area).

The general for mulas of the corresponding region moments for the echelon case are given in Table 7. For (21) the parameters p_1 and K have the values .2 and 1.0416667 respectively. Accordingly the constants of the region moments needed are:

$\beta = -.0096225$

$C_1 = \ .0108333$

$C_2 = \ .0086111$

$C_3 = -.0006303$

$C_4 = \ .0001010.$

By using the results of section 4, a 5-point all-bias design has the following coordinates and their graphical representatinis given in Figure 3.

$(\pm .165, \ -.058)$

$(.0 \quad , \quad .137)$

$(.0 \quad , \quad .053)$

$(.0 \quad , \ -.122)$

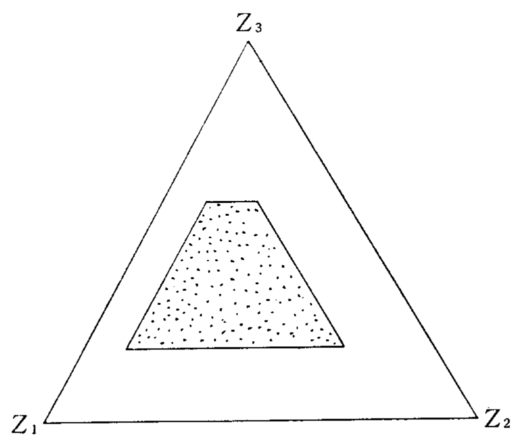

Figure 2. Graphical Representation of (21)

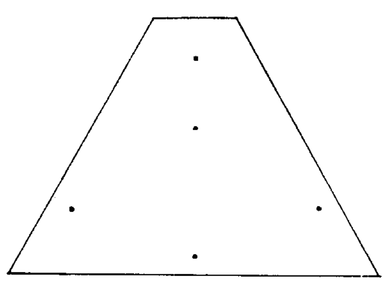

Figure 3. A 5-point design

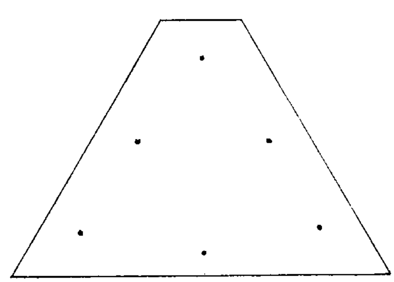

Figure 4. A 6-point design

Table 7. Region moments when $m_1 \neq 0$, $m_2 = m_3 = 0$

u	v	region moments
1	0	0
0	1	$-\frac{\sqrt{3}}{3} \mathrm{Km}\, p_1^2(1-p_1)$
2	0	$\frac{1}{24} \mathrm{Km}^2(1-p_1^4)$
1	1	0
0	2	$\frac{1}{24} \mathrm{Km}^2(1-p_1^4-8p_1^2(1-p_1)^2)$

Table 7. (continued)

3	0	0
2	1	$-\frac{3}{360} \mathrm{Km}^3(1-p_1^5+5p_1^4(1-p_1))$
1	2	0
0	3	$\frac{3}{360} \mathrm{Km}^3(1-p_1^5-15p_1^4(1-p_1)-40p_1^2(1-p_1)^3)$

* $K=(1-p_1^2)^{-1}$

A 6-point design using the set combination (1, 2) without center points (i.e $r=0$) consists of the following points and their graphical representation is shown in Figure 4:

(±.158, −.087)
(±.086, .040)
(.0 , −.109)
(.0 , .146)

A 7-point design using the set combination (1, 2) with one center point (i.e. $r=1$) consists of the following points and their graphical representation is shown in Figure 5:

(±.169, −.093)
(±.007, .046)
(.0 , .157)
(0 , −.120)
(0 , −.010)

As an another example, an 8-point design with two center points (i.e. $r=2$) consists of the following points and their graphical

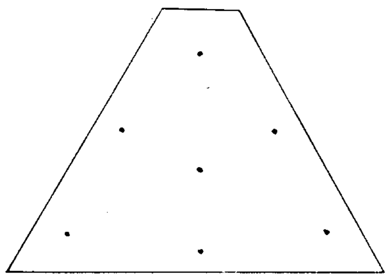

Figure 5. A 7-point design

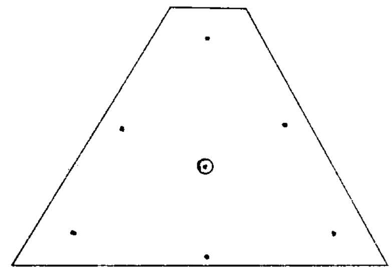

Figure 6. An 8-point design

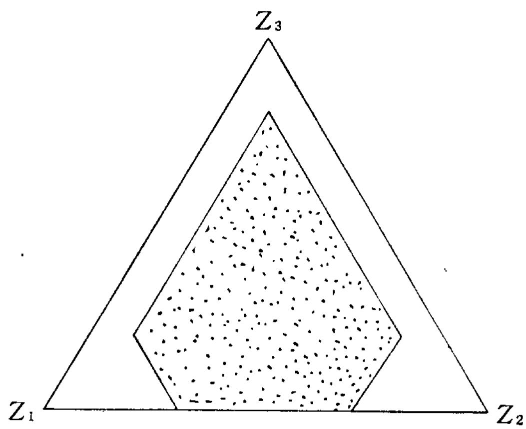

Figure 7. Graphical Representation of (22)

representation is shown in Figure 6:

$$
\begin{array}{l}
(\pm.178, \ -.098)\\
(\pm.107, \ \ .051)\\
(\ .0\ , \ \ .166)\\
(\ .0\ , \ -.130)\\
2(\ .0\ , \ -.010).
\end{array}
$$

Of course, designs with nine or more points are also possible in this manner.

5.2 Design for the case $m_1=0$, $m_2=m_3$, $m_2\neq 0$

Let the factor space be defined as follows:

$$
\begin{aligned}
.1 &\leq z_1 \leq .7 \\
.1 &\leq z_2 \leq .7 \qquad (22) \\
.0 &\leq z_3 \leq .8
\end{aligned}
$$

The restricted region of (22) is shown in Figure 7 (dotted area), and the values of m and m_2 are .8 and .2 respectively. The general formulas of the region moments in this pentagon case are given in Table 8.

The values of the region moments for (22) are:

$$
\begin{aligned}
\beta &= .0247435 \\
C_1 &= .0173809 \\
C_2 &= .0259524 \\
C_3 &= -.0005416 \\
C_4 &= .0035933.
\end{aligned}
$$

Table 8. Region moments when $m_1=0$, $m_2=m_3$, $m_2\neq 0$

u	v	region moments
1	0	0
0	1	$\frac{\sqrt{3}}{3}\mathrm{K}m^2(1-p)$
2	0	$\frac{1}{24}\mathrm{K}m^2[1-2p^4-12p^2(1-p)^2]$
1	1	0
0	2	$\frac{1}{24}\mathrm{K}m^2[1-2p^4-4p^2(1-p)^2]$
3	0	0
2	1	$-\frac{\sqrt{3}}{360}\mathrm{K}m^3[1-2p^5-30p^2(1-p)^3-5p^4(1-p)]$
1	2	0
0	3	$-\frac{\sqrt{3}}{360}\mathrm{K}m^3[1-2p^5+10p^2(1-p)^3+5p^4(1-p)]$

* $P\equiv P_2$, and $K=(1-2p^2)^{-1}$

A 5-point design is introduced to compare with the extreme vertices design and an 8-point design is considered as an another example. For the 5-point design, the coordinates of the points are:

$$
\begin{aligned}
&(\pm .208,\ -.031) \\
&(\ .0\ ,\ \ .290) \qquad (23)
\end{aligned}
$$

$$(\;.\; 0, \quad .087)$$
$$(\;.\; 0, \; -.191)$$

Extreme vertices design consists of the five vertices, or in our notation the points

$$\left(\;.0, \; \frac{1}{\sqrt{3}} m \right)$$
$$\left(\pm\left(\frac{m}{2} - \frac{m_2}{2}\right), \; -\frac{\sqrt{3}}{6}(m - 3m_2) \right)$$
$$\left(\pm\left(\frac{m}{2} - m_2\right), \; -\frac{\sqrt{3}}{6} m \right).$$

Extreme vertices design is actually the all-variance design as mentioned earlier, thus it is not appropriate for situations where both variance and bias exist. It should be noted that long edges occur frequently in extreme vertices design so that the uniformity cannot be achieved. Our design is able to overcome this possible disadvantage. Further it is customary that the region of interest is made around current operating levels. Hence the fact that extreme vertices design always gives the design points on the boundary is another disadvantage. This drawback remains althought the centroids are included. But our design gives the design points within the feasible region and the design points might be determined in many ways by combining various point sets and special points possibly. Therefore, that the experimenter is able to determine locations of design points within the region of interest as one pleases is the second advantage of our design to extreme vertices design.

An 8-point design with a repetition of the center point consists of the following coordinates:

$$\begin{array}{l} (\pm .209, \; -.126) \\ (\pm .161, \quad .130) \\ (\;.\; 0, \quad .326) \\ (\;.\; 0, \; -.186) \\ 2(\;.\; 0, \quad .025) \end{array} \tag{24}$$

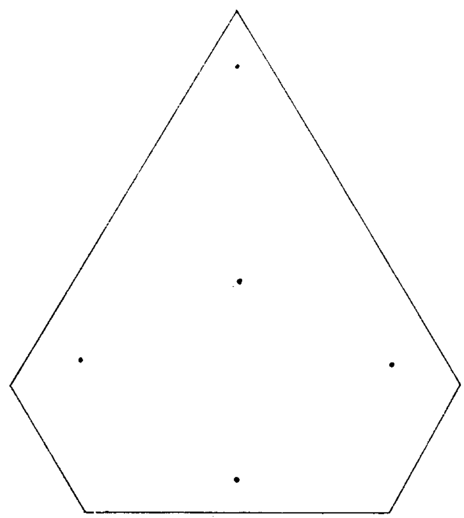

Figure 8. A 5-point design

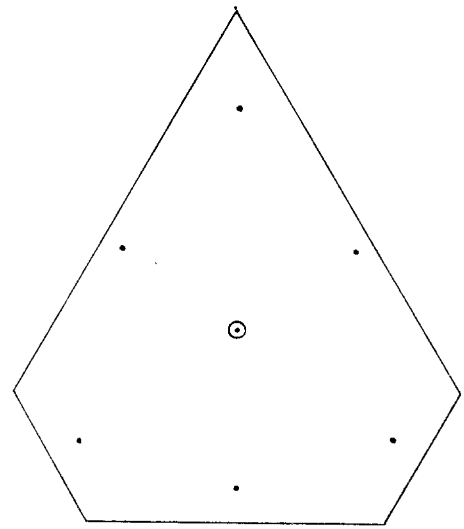

Figure 9. An 8-point design

The graphical representations (23) and (24) are given in Figures 8 and 9 respectively.

5.3 Designs for the case $m_1 \neq 0$, $m_2 = m_3$, $m_2 \neq 0$

Let the factor space be defined as follows:

$$
\begin{aligned}
.1 &\leq z_1 \leq .8 \\
.0 &\leq z_2 \leq .7 \qquad\qquad (25) \\
.1 &\leq z_3 \leq .6
\end{aligned}
$$

The region of (25) is shown in Figure 10 (dotted area) and the values of m_1, m_2 and m are .3, .1 and .8, respectively. The foumulas of region moments in this hexagon case can be deduced from Table 3 by letting $p_2 = p_3$. The values of the region moments for (25) are:

$$
\begin{aligned}
\beta &= -.0413948 \\
C_1 &= .0269261 \\
C_2 &= .0158569 \\
C_3 &= -.0021989 \\
C_4 &= -.0013696.
\end{aligned}
$$

A 7-point design is considered and the coordinates are:

$$
\begin{array}{ll}
(.255, & -.138) \\
(.171, & .043) \\
(.0\ \ , & .152) \\
(.0\ \ , & -.211) \\
(.0\ \ , & -.041).
\end{array}
\tag{26}
$$

The graphical representation of (26) is shown in Figure 11.

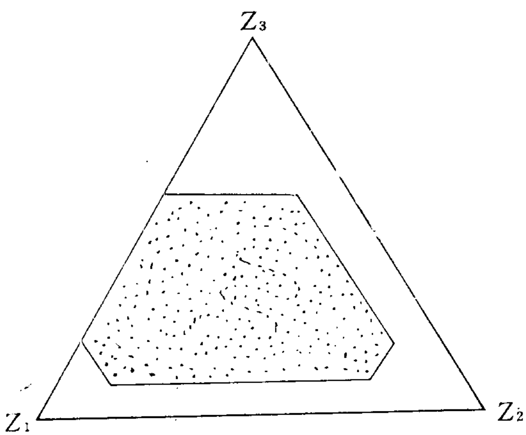

Figure 10. Graphical Representation of (25)

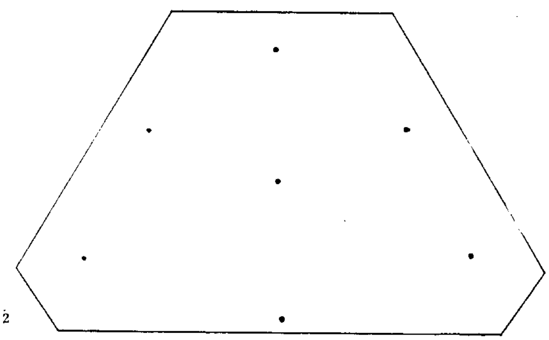

Figure 11. A 7-point design

In this case extreme vertices design consists of the six vertices and one centroid, whose coordinates are:

$$
\begin{array}{ll}
\left(\pm\frac{m_1}{2}, & \frac{\sqrt{3}}{6}(2m-3m_1)\right) \\
\left(\pm\left(\frac{m}{2}-\frac{m_2}{2}\right), & -\frac{\sqrt{3}}{6}(m-3m_2)\right) \\
\left(\pm\left(\frac{m}{2}-m_2\right), & -\frac{\sqrt{3}}{6}(m-3m_2)\right) \\
\left(\ .0, & \frac{\sqrt{3}}{6}(m_2-m_1)\right).
\end{array}
\tag{27}
$$

The coordinate of the centroid, the fourth of (27), is exactly (.0. —.046) so that the centroid is slightly below the center point.

Since the generated hexagon has the narrow edges toward the base, our discussions in Section 5.2 can be applied properly and our design is more practical than any other design ever proposed for the restricted mixture system. These facts will be seen more precisely if we let b_3, the upper bound of z_3, be .3 or .2, etc..

6. Concluding Remarks

The all-bias designs that we have derived seem to be excellently suited to the restricted mixture system. For the case of first order designs studied here, the designs consisting of five or more points have been easily obtained by using the theories of equations such as the Newton's foumula for symmetric equations and the trigonometric method for reduced cubic.

However, much remains to be done. First, if the number of factors are four or more, it would be difficult to obtain the region moments so that more robust symmetry conditions should be introduced. Second, if the second order designs are desired when the true polynomial is of order three, we must solve very complicated quintic equations, probably by use of an electronic computer, since it is known to us that the existence of the roots can only be approximately obtained.

We have considered the cases when the shapes of the generated polygons are symmetric about x_2 axis. Unless such conditions are imposed, we have to solve the nine equations in (7), and the excessive number of moments that must be determined will make a search for a suitable design prohibitive. However, a slight control of the lower and upper bounds could make the shapes of the generated polygons be symmetrical. The echelon case is symmetric by nature, but the pentagon and the hexagon are not such. Hence, the following procedures, for example, are recommended to preserve the symmetry of the polygons. That is, for the unsymmetrical pentagon;

(1) if $0 \ll m_i \ll m_j$ relatively, then adjust m_j to be m_i.

(2) if $0 = m_i \ll m_j$ relatively, then let m_i be zero and consider this case as the echelon one, where $i, j = 2, 3$.

For the unsymmetrical hexagon; if $0 \ll m_k$, k=1, 2, 3, respectively, then choose m_i and m_j such that $|m_i - m_j|$ is minimized where $i \neq j$ and reduce m_j to be m_i if $m_i < m_j$, etc.. It is, however, noteworthy that all design points in our all-bias designs lie on the interior of the region of interest, so that it can be inferred that all points might be within the original region even though the region will be more or less augmented.

The difficulties discussed above should be overcome in the future studies.

7. Acknowledgements

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Appendix

Integral Evaluation for the Region Moments

Suppose that an integral of the following form is given:

$$\left\{\int_R - \int_{R_1} - \int_{R_2} - \int_{R_3}\right\} x_1^u x_2^v dx_1 dx_2 \tag{28}$$
$$= \left\{\int_{-a}^{2a}\int_{-b}^{b} - \int_{a_1}^{2a}\int_{-b}^{b} - \int_{-a}^{a_2}\int_{b_2}^{b} - \int_{-a}^{a_3}\int_{-b}^{b_3}\right\} x_1^u x_2^v dx_1 dx_2,$$

where the values of all the parameters are given in (6). Noting that b is a function of x_2, the evaluation of (28) requires that we should solve that integral of the following form primarily:

$$\int (s-ty)^{u+1} y^v dy. \tag{29}$$

Let

$$I(c,d) \equiv \int (s-ty)^{u+1+c} y^{v+d} dy.$$

Then (29) can be expressed as $I(0,0)$. By the iterative procedures, the followings hold.

$$I(0,0) = -y^v \frac{1}{(u+2)t}(s-ty)^{u+2} + \frac{v}{(u+2)t} I(1,-1),$$
$$I(1,-1) = -y^{v-1} \frac{1}{(u+3)t}(s-ty)^{u+3} + \frac{v-1}{(u+3)t} I(2,-2), \tag{30}$$

$$I(2,-2)=-y^{v-2}\frac{1}{(u+4)t}(s-ty)^{u+4}+\frac{v-2}{(u+4)t}I(3,-3),$$
$$\vdots$$
$$I(v,-v)=-\frac{1}{(u+2+v)t}(s-ty)^{u+2+v}.$$

Hence $I(0,0)$ can be obtained from (30). That is,

$$\begin{aligned}I(0,0)=&-y^{v}\frac{1}{(u+2)t}(s-ty)^{u+2}\\&-y^{v-1}\frac{1}{(u+3)t}(s-ty)^{u+3}\frac{v}{(u+2)t}\\&-y^{v-2}\frac{1}{(u+4)t}(s-ty)^{u+4}\frac{v}{(u+2)t}\ \frac{v-1}{(u+3)t}\\&\ \vdots\\&-y^{v-v}\frac{1}{(u+2+v)t}(s-ty)^{u+2+v}\frac{v}{(u+2)t}\ \frac{v-1}{(u+3)t}\\&\cdots\frac{1}{(u+1+v)t}\\=&\sum_{i=0}^{v}y^{v-i}\frac{(u+1)!(v)_i}{(u+2+i)!t^{i+1}}(s-ty)^{u+2+i}.\end{aligned}$$

For convenience' sake, we will evaluate the integral (28) according to the order of R, R_1, R_2, and R_3. Further let

$$K(u,v)=\left(\frac{m}{2}\right)^{u+v+2}\left(\frac{1}{\sqrt{3}}\right)^{v-1},$$

and

$$k_i(u,v)=\frac{u!(v)_i}{(u+2+i)!}\ 3^i.$$

1. For R

On the region R, the value of the integral

$$\int_{-a}^{2a}\int_{-b}^{b}x_1^u x_2^v dx_1 dx_2 \tag{32}$$

is obviously zero whenever u is an odd integer. Otherwise, (32) becomes

$$\frac{2}{u+1}\left(\frac{1}{3}\right)^{u+1}\int_{-a}^{2a}(m-3x_2)^{u+1}x_2^v dx_2. \tag{33}$$

Using (31) we can evaluate (33) as follows:

$$2\left(\frac{m}{2}\right)^{u+v+2}\left(\frac{1}{\sqrt{3}}\right)^{v-1}\sum_{i=0}^{v}(-1)^{v-i}\frac{(v)_i u!}{(u+2+i)!}\ 3^i$$

which finally becomes

$$2\,K(u,v)\sum_{i=0}^{v}k_i(u,v)(-1)^{v-i}$$

whenever u is an even integer.

2. For R_1

Similarly as above, the integral (34)

$$\int_{a_1}^{2a}\int_{-b}^{b}x_1{}^u x_2{}^v dx_1 dx_2$$

attains zero whenever u is odd. If u is even, then (34) becomes

$$\frac{2}{u+1}\left(\frac{1}{3}\right)^{u+1}\int_{a_1}^{2a}(m-\sqrt{3}\,x_2)^{u+1}x_2{}^v dx_2$$

$$=2\left(\frac{m}{2}\right)^{u+v+2}\left(\frac{1}{\sqrt{3}}\right)^{v-1}\sum_{i=0}^{v}\frac{(v)_i u!}{(u+2+i)}3^i(2-3\,p_1)^{v=i}\,p_1{}^{u+2+i}$$

$$=2\,K(u,v)\sum_{i=0}^{v}k_i(u,v)(2-3\,p_1)^{v-i}\;p_1{}^{u+2+i},$$

where $p_1=m_1/m$.

3. For R_2

The double intergral

$$\int_{-a}^{a_2}\int_{b_2}^{b}x_1{}^u x_2{}^v dx_1 dx_2$$

becomes

$$\frac{1}{u+1}\int_{-a}^{a_2}x^v\left[\frac{m-3\,x_2{}^{u+1}}{3}-\frac{2\,m-3\,m_2+3\,x_2{}^{u+1}}{3}\right]dx. \tag{35}$$

The first part of (35) finally becomes as follows:

$$K(u,v)\sum_{i=0}^{v}k_i(u,v)(-1)^{v-i}\{1-(1-p_2)^{u+2+i}(1-3\,p_2)^{v-i}\}, \tag{36}$$

The second one gives

$$K(u,v)\sum_{i=0}^{v}k_i(u,v)(-1)^{v+1}\{(1-p_2)^{u+2+i}(1-3\,p_2)^{v-i} \\ -(1-2\,p_2)^{u+2+i}\}. \tag{37}$$

By combining (36) and (37), the following formula can be attained:

$$K(u,v)\sum_{i=0}^{v}k_i(u,v)(-1)^{v}\{(1-p_2)^{u+2+i}(1-3\,p_2)^{v-i}[(-1)^{i+1}-1] \\ +(-1)^i+(1-2\,p_2)^{u+2-i}\},$$

where $p_2=m_2/m$.

4. For R_3

Similarly as above, the double integral

$$\int_{-a}^{a_3}\int_{-b}^{b_3} x_1^u x_2^v dx_1 dx_2$$

becomes

$$(-1)^u \frac{1}{u+1}\left(\frac{1}{3}\right)^{u+1}\int_{-a}^{a_3} \{(m-\sqrt{3}\,x_2)^{u+1}$$
$$-(2m-3m_3+\sqrt{3}\,x_2)^{u+1}\}x_2^v dx_2$$
$$=(-1)^u K(u,v)\sum_{i=0}^{v} k_i(u,v)(-1)^v\{(1-p_3)^{u+2+i}(1-3p_3)^{v-i}$$
$$\cdot[(-1)^{i+1}-1]+(-1)^i+(1-2p_3)^{u+2+i}\}.$$

where $p_3=m_3/m$.

References

Becker, N.G. (1970). Mixture designs for a model linear in the proportions. Biometrika, 57, 329-338.

Box, G.E.P. and Draper, N.R. (1959). A basis for the selection of a response surface design. J. Amer. Statist. Assoc., 54, 622-654.

Draper, N.R. and Lawence, W.E. (1965a). Mixture designs for three factors. J. Roy. Statist. Soc., B-27, 450-465.

Draper, N.R. and Lawrence, W.E. (1965b). Mixture designs for four factors. J. Roy. Statist. Soc., B-27, 473-478.

Lambrakis, D.P. (1969). Experiments with mixtures: An alternative to the simplex-lattice design. J. Roy. Statist. Soc., B-21, 234-245.

MacDuffee, C.C. (1959). Theory of Equations, John Wiley & Sons, Inc., New York.

McLean, R.A. and Anderson, V.L. (1966). Extreme vertices design of mixture experiments. Technometrics, 8, 447-454.

Murty, J.S. and Das, M.N. (1968). Design and analysis of experiments with mixtures. Ann. Math. Statist., 39, 1527-1539.

Paku, G. A., Manson, A.R. and Nelson, L.A. (1971). Minimum bias estimation in the mixture problem. North Carolina State Univ. Inst. of Statistics Mimeo. Series, No. 757. Releigh, N.C.

Saxena, S.K. and Nigam, A.K. (1973). Symmetric-simplex block designs for mixtures. J. Roy. Statist. Soc., B-35, 466-472.

Saxena, S.K. and Nigam, A.K. (1977). Restricted exploration of mixture by symmetric-simplex designs. Technometrics, 19, 47-52.

Scheff'e, H. (1958). Experiments with mixture, J. Roy. Statist. Soc., B-20, 344-360.

Scheff'e, H. (1963). The simplex-centroid design for experiments with mixtures. J. Roy. Statist. Soc., B-25, 235-263.

Snee, R.D. (1975). Experimental designs for quadratic models in constrained mixture spaces. Technometrics, 17, 149-159.

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