(12)

AD-A270 656

EDGEWOOD
RESEARCH,
DEVELOPMENT &
ENGINEERING
CENTER

ERDEC-TR-104

SHELL DESIGNS

Ronald B. Crosier

RESEARCH AND TECHNOLOGY DIRECTORATE

August 1993

Approved for public release; distribution is unlimited.

U.S. ARMY
CHEMICAL
AND BIOLOGICAL
DEFENSE AGENCY

Aberdeen Proving Ground, Maryland 21010-5423

Disclaimer

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorizing documents.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
1993 August

3. REPORT TYPE AND DATES COVERED
Final, 91 Jun - 92 Jul

4. TITLE AND SUBTITLE
Shell Designs

5. FUNDING NUMBERS
PR-10161102A71A

6. AUTHOR(S)
Crosier, Ronald B.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
DIR, ERDEC,* ATTN: SCBRD-RTM, APG, MD 21010-5423

8. PERFORMING ORGANIZATION REPORT NUMBER
ERDEC-TR-104

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES
*When this study was conducted, ERDEC was known as the U.S. Army Chemical Research, Development and Engineering Center, and the author was assigned to the Research Directorate.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The shell designs consist of two series of related designs (the uniform shell designs and the simplicial shell designs) that are used for fitting second-order response surfaces over spherical regions. The shell designs for two, four, six, and eight factors require fewer experimental runs than the central composite designs or the Box-Behnken designs, but they have not been used much because of their unequal treatment of the design factors. Rotations of the shell designs that provide an equal treatment of the factors are given. The rotated uniform shell designs have seven levels of each factor with the exception of the three-factor design (three levels) and the eight-factor design (five levels). An orthogonal blocking scheme is given for the uniform shell designs with an even number of factors. The simplicial shell designs have nine levels, except for the two-factor and seven-factor designs, which have seven levels, and the three-factor design, which has five levels but is singular. The simplicial shell designs have an orthogonal blocking scheme for any number of factors.

14. SUBJECT TERMS
Design rotation
Uniform shell design
Simplicial shell design
Response surface design

15. NUMBER OF PAGES
22

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

Blank

PREFACE

The work described in this report was authorized under Project No. 10161102A71A, Research in CW/CB Defense. This work was started in June 1991 and completed in July 1992.

The use of trade names or manufacturers' names in this report does not constitute an official endorsement of any commercial products. This report may not be cited for purposes of advertisement.

This report has been approved for release to the public. Registered users should request additional copies from the Defense Technical Information Center; unregistered users should direct such requests to the National Technical Information Service.

Blank

CONTENTS

LIST OF TABLES

SHELL DESIGNS

1. INTRODUCTION

In many industrial experiments the goal is to find the settings of process variables or factors $x_1, x_2, \ldots, x_k$ that will optimize some characteristic y of the product. A widely used strategy for such problems is to approximate the relationship between y and the process factors by a low-order polynomial. The coefficients of the polynomial are estimated from data collected during N experimental runs of the process; the settings of the x's for the N experimental runs are given by a response surface design. A response surface design for k factors is written as an $N \times k$ design matrix $\mathbf{D}$. To estimate the coefficients of the polynomial, the design matrix is expanded into an $N \times p$ model matrix $\mathbf{X}$ that has one column for each coefficient of the polynomial model. The estimate $\mathbf{b}$ of the coefficient vector $\boldsymbol{\beta}$ is then obtained from the least-squares formula

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}, \tag{1}$$

where $\mathbf{y}$ is an $N \times 1$ vector containing the response y for the N runs. Several classes of designs are available for fitting the second-order polynomial

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij} x_i x_j + \epsilon \tag{2}$$

over a spherical region. The most popular designs for fitting the second-order model (2) are the central composite designs of Box and Wilson (1951) and the designs of Box and Behnken (1960). For $k=2$, 4, 6, and 8, the uniform shell designs of Doehlert (1970) require fewer experimental runs than the central composite or Box-Behnken designs, but the uniform shell designs have not been widely used. Crosier (1991a) proposed generalizing the seven-factor Box-Behnken design to a new class of designs. These new designs have many properties (including the number of runs required) in common with Doehlert's (1970) uniform shell designs; the two series of designs will be referred to collectively as the shell designs.

The number of levels of the factors required by a design is sometimes cited as the reason for the lack of use of designs with many levels. Although designs with few levels are sometimes required, there are reasons to distrust the too-many-levels explanation of the unpopularity of some designs. First, the design points in a completely randomized design are run in a random order so that the factor levels must be reset frequently. Second, many experimenters who are not familiar with statistical designs use one-factor-at-a-time designs in which each factor is run at many levels (such individuals frequently *prefer* designs with many levels). Third, there is an inconsistency in the relationship of the popularity of a design to the number of levels of its factors. Doehlert and Klee (1972) show how to rotate the uniform shell designs to minimize the number of levels of the factors. Most of the rotated uniform shell designs have no more than five levels of any factor; yet the rotated designs are not as popular as the central composite designs, which have five levels of every factor. One reason for the lack of popularity of the shell designs proposed to date may be their lack of symmetry rather than the number of levels of the factors that they require. Section 2 discusses the difficulty of applying asymmetric designs to industrial problems.

The symmetry of popular designs is due to their use of regular geometric figures. The central composite designs have factorial points that lie at the vertices of a k-dimensional cube and star points that lie at the centers of the faces of another, larger cube. The Box-Behnken designs use only levels -1, 0, and 1 for the factors, so the design points must be centroids of $(k-m)$-dimensional faces of the k-dimensional cube, where m is the number of ± 1's in a design point.

A regular simplex is the geometric figure formed by $k+1$ equally spaced points in k-dimensional space; an equilateral triangle is a two-dimensional regular simplex. Both series of shell designs are constructed from regular simplexes. The shell designs are used for fitting a response surface to k independent factors over a spherical region, not for fitting a response surface to q proportions over a simplex, as in mixture experiments. [For symmetric mixture designs, see Crosier (1991b).] Simplexes do not have a unique, natural orientation that gives the best set of coordinates to any simplex-based design in any number of dimensions. Several orientations of simplexes yield symmetric design matrices for the shell designs, but the best orientation depends on both the design and the dimensionality. Section 3 presents a symmetric orientation for the uniform shell designs of Doehlert (1970).

Spendley, Hext, and Himsworth (1962) noted that the noncentral design points of the seven-factor Box-Behnken design are the midpoints of the edges of two simplexes. Crosier (1991a) proposed using the same construction for other numbers of factors and found symmetric, three-level designs for $k=11$ and $k=15$. Because of their relationship to the uniform shell designs and their construction from simplexes, Crosier (1991a) called these designs simplex-shell designs, but I now prefer to use the adjective *simplicial* and call them simplicial shell designs. Section 4 provides an alternative orientation of the simplicial shell designs that yields symmetric designs for all k. Section 5 examines the efficiency of the new designs.

The Appendix gives coordinates for the vertices, edge midpoints, and face centroids of simplexes and derives the symmetric orientations of the uniform shell designs and the simplicial shell designs.

2. PROBLEMS WITH ASYMMETRIC DESIGNS

Response surface designs are usually applied by scaling the coded factor ranges to the ranges of the experimental factors. A typical set of experimental factors and their ranges are blender speed (100-300 revolutions per minute, or rpm), mixing time (10-20 minutes), cooking temperature (180-200 degrees), and cooking time (40-60 minutes). There is no difficulty applying symmetric designs such as the Box-Behnken designs or central composite designs to problems such as this one. But consider the difficulties created by a design with unequal factor ranges, such as Doehlert's (1970) four-factor uniform shell design (Table 1).

In coded units, the first factor covers the interval $[-1,1]$, the second factor covers the interval $[-.866,.866]$, the third factor covers the interval $[-.816,.816]$, and the fourth factor covers the interval $[-.791,.791]$. Two methods of scaling the coded design factors to the experimental factors will be considered here; both methods have shortcomings for designs with unequal ranges for the coded factors.

Method A: Coded design diameter to experimental factor ranges. Because the noncentral design points of Doehlert's uniform shell design are at a radius of 1 in coded units, Doehlert and Klee (1972) suggested linearly transforming each column of the design matrix so that ± 1 in the design corresponds "to the limits of the region of interest of the natural variable in the experiment assigned to that column." An interpretation of this statement is that ± 1 in coded units would correspond to the low and high values given by the experimenter for each factor. Thus -1 would correspond to a blender speed of 100 rpm and 1 would correspond to a blender speed of 300 rmp. Likewise, -1 would correspond to a mixing time of 10 minutes and 1 would correspond to a mixing time of 20 minutes. As $-.866$ is the lowest coded value of the second factor, the lowest value of mixing time in the

Table 1. Doehlert's Four-Factor Uniform Shell Design

Point	x_1	x_2	x_3	x_4
1	1.	0.	0.	0.
2	−1.	0.	0.	0.
3	.5	.866	0.	0.
4	−.5	−.866	0.	0.
5	−.5	.866	0.	0.
6	.5	−.866	0.	0.
7	.5	.289	.816	0.
8	−.5	−.289	−.816	0.
9	−.5	.289	.816	0.
10	.5	−.289	−.816	0.
11	0.	−.577	.816	0.
12	0.	.577	−.816	0.
13	.5	.289	.204	.791
14	−.5	−.289	−.204	−.791
15	−.5	.289	.204	.791
16	.5	−.289	−.204	−.791
17	0.	−.577	.204	.791
18	0.	.577	−.204	−.791
19	0.	0.	−.612	.791
20	0.	0.	.612	−.791
21	0.	0.	0.	0.

experiment would be 10.67 minutes. Similarly, the highest value of mixing time would be 19.33 minutes. For cooking temperature, ±1 in coded units is assigned to the range 180-200 degrees, but the design has a range of ±.816 in coded units for the third factor, so that cooking temperature would be varied over the range 181.84-198.16 degrees in the experiment. The last factor, cooking time, would be varied over the range 42.09-57.91 minutes. Although this method of applying the design is consistent with the theory of optimal designs, the resulting design, with reduced ranges for most of the factors, is generally unacceptable to experimenters.

Method B: Coded factor ranges to experimental factor ranges. In method B, the coded range for each design factor is transformed to the range for the natural variable (experimental factor) assigned to that design column. Thus, −.866 for the second factor becomes 10 minutes of mixing time, .866 for the second factor becomes 20 minutes of mixing time, −.816 for the third factor becomes 180 degrees for cooking temperature, and so on. This alternative method of applying the design solves the problem of giving the experimenter a design with the specified ranges, but it distorts the configuration of the design points and changes the mathematical and statistical properties of the design; it is equivalent to rescaling each column of the design matrix to have a range of ± 1 in coded units. Because the statistical properties of the design with rescaled factors are unknown, statisticians have generally avoided applying asymmetric designs by Method B. Designs with unequal ranges in coded units leave the practitioner with the choice of a design with unacceptable ranges or a design with unknown statistical properties.

3. UNIFORM SHELL DESIGNS

Doehlert (1970) obtained the uniform shell designs from a regular simplex that has one vertex at the origin; subtracting each vertex of the simplex from every other vertex of the simplex yields the complete set of design points. In the orientation given by Doehlert (1970), the uniform shell designs have a different range for each factor. For $k = 3, 7, 11, \ldots$, Doehlert and Klee (1972) found symmetric, three-level rotations of the uniform shell designs. Doehlert and Klee (1972) give the 3- and 7-factor designs and Crosier (1991a) gives the 11- and 15-factor designs.

In the new orientation presented in this section, the uniform shell designs can be specified by a few points; the complete set of design points is obtained by generating all permutations of the factor levels for each basic point. Therefore it is clear that (a) for any point in the design, all permutations of the factor levels of that point are also points in the design, (b) for any point in the design, other points with the *cyclic* permutations of its factor levels are in the design, and (c) the design points can be grouped into sets with cyclic permutations of the factor levels. With these ideas in mind, examine the new orientation of the four-factor uniform shell design in Table 2. The symmetric rotation in Table 2 can be applied without the difficulties that the rotation in Table 1 generates. The symmetric rotation in Table 2 has an intuitive appeal based on the equal treatment of the factors: each factor has the same set of levels and the same relationship exists between any pair of factors. For k even, the uniform shell designs can be divided into two orthogonal blocks (as in Table 2). The same number of center points must be used with each block to make the blocks orthogonal. The orthogonal blocking for even k is a new discovery and is helpful because even k is the case for which the shell designs require fewer design points than the central composite or Box-Behnken designs.

Table 2. Four-Factor Uniform Shell Design

Point	x_1	x_2	x_3	x_4	Block
1	1	−1	0	0	1
2	0	1	−1	0	1
3	0	0	1	−1	1
4	−1	0	0	1	1
5	−1	1	0	0	2
6	0	−1	1	0	2
7	0	0	−1	1	2
8	1	0	0	−1	2
9	1	0	−1	0	1
10	0	1	0	−1	1
11	−1	0	1	0	2
12	0	−1	0	1	2
13	a	$-b$	$-b$	$-b$	2
14	$-b$	a	$-b$	$-b$	2
15	$-b$	$-b$	a	$-b$	1
16	$-b$	$-b$	$-b$	a	1
17	$-a$	b	b	b	1
18	b	$-a$	b	b	1
19	b	b	$-a$	b	2
20	b	b	b	$-a$	2
21	0	0	0	0	1
22	0	0	0	0	2

$a = (3-5^{1/2})/4 \simeq .191$
$b = (1+5^{1/2})/4 \simeq .809$

The uniform shell designs also have the property that if a point is in the design, so is the negative of that point. (Note that, in Table 2, points 11 and 12 are the negatives of points 9 and 10.) Hence it is only necessary to give half of the design points in a table. To show the pattern for odd k, Table 3 gives the five-factor uniform shell design. Note that for odd k, there is no cyclic group that contains its own negatives (as do points 9-12 in Table 2).

Table 3. Five-Factor Uniform Shell Design
Add negatives and center points.

Point	x_1	x_2	x_3	x_4	x_5
1	1	−1	0	0	0
2	0	1	−1	0	0
3	0	0	1	−1	0
4	0	0	0	1	−1
5	−1	0	0	0	1
6	1	0	−1	0	0
7	0	1	0	−1	0
8	0	0	1	0	−1
9	−1	0	0	1	0
10	0	−1	0	0	1
11	$-a$	b	b	b	b
12	b	$-a$	b	b	b
13	b	b	$-a$	b	b
14	b	b	b	$-a$	b
15	b	b	b	b	$-a$

$a = (4-6^{1/2})/5 \simeq .310$
$b = (1+6^{1/2})/5 \simeq .690$

To generalize the above construction method to any k, the k-factor uniform shell design is given by all permutations of the factor levels of the four points $(-1,1,0,0,\ldots,0)$, $(-a,b,b,\ldots,b)$, $(a,-b,-b,\ldots,-b)$, and $(0,0,\ldots,0)$, where $a = (k-1-(k+1)^{1/2})/k$ and $b = (1+(k+1)^{1/2})/k$. As a check on the values of a and b, notice that $a+b=1$. This rotation gives the uniform shell designs seven levels $(0,\pm a,\pm b,\pm 1)$ with the following exceptions: $k=3$, $a=0$, $b=1$, yielding a three-level design, and $k=8$, $a=b=.5$, yielding a five-level design. The two-factor design is a rotation of the well-known hexagon design and the three-factor design is the three-level design given by DeBaun (1959), Box and Behnken (1960), and Doehlert and Klee (1972). Note that the five levels (−1, −.5, 0, .5, and 1) of the eight-factor uniform shell design are equally spaced.

For seven factors, the three-level rotation given by Doehlert and Klee (1972) will usually be the preferred orientation. For completeness, I point out that the seven-factor uniform shell design has (at least) three symmetric orientations: the three-level design, the seven-level design given above (using a and b), and an alternative seven-level design that has equally spaced levels. When the levels are coded −3, −2, −1, 0, 1, 2, and 3, the design is given by the *cyclic* permutations of the four points (−3, 0, 1, −1, 1, 0, 2), (−3, 1, 0, 0, 1, 2, −1), (−3, 1, 1, 2, 0, −1, 0), and (2, 2, 1, 2, 1, 1, −1), their negatives, and center points.

4. SIMPLICIAL SHELL DESIGNS

Simplicial shell designs were obtained by Crosier (1991a) by generalizing the seven-factor Box-Behnken design. The design points are the origin, the midpoints of the edges of a regular simplex centered on the origin, and the negatives of the edge midpoints (which are edge midpoints of another simplex). The simplicial shell designs share many properties with the uniform shell designs, including $N=k(k+1)+n_0$ design points (where n_0 is the number of center points), construction from simplexes, and symmetric orientations given by the permutations of the factor levels of a few points. Unlike the uniform shell designs, the simplicial shell designs can be orthogonally blocked for any k: the midpoints of the edges of one simplex and center points form one block and the midpoints of the edges of the other simplex and center points form the second block. The same number of center points must be used in each block.

The midpoints of the edges of one simplex are given by all permutations of the factor levels of the two points $(-1,-1,q,q,\ldots,q)$ and $(-r,b,b,\ldots,b)$, where $q=2/(k-1+(k+1)^{1/2})$, $r=(k-1)/(k-1+(k+1)^{1/2})$, and b is as defined for the uniform shell designs: $b=(1+(k+1)^{1/2})/k$. Hence these points plus center points, (0,0,...,0), form one block; the second block consists of the negatives of the points in the first block. In this orientation, the simplicial shell designs for $k>3$ are nine-level designs. The two-factor design is a seven-level design because the levels $\pm q$ do not appear; the two-factor design differs from the uniform shell design only by a sign change of one factor. Table 4 gives the two-factor shell designs scaled to cover the range (−1,1). The two-factor uniform shell and simplicial shell designs are rotations of each other and therefore have the same orthogonal blocking pattern, whereas, for other numbers of factors, the uniform shell and simplicial shell designs are distinct and have different blocking patterns. The three-factor simplicial shell design has five levels but is singular.

For k=3, 7, 11, ..., symmetric, three-level rotations of the simplicial shell designs exist, but (a) the three-factor design is singular, (b) the seven-factor design

Table 4. Two-Factor Shell Designs

Uniform Shell			Simplicial Shell		
x_1	x_2	Block	x_1	x_2	Block
1.	.268	1	1.	−.268	1
−.268	−1.	1	−.268	1.	1
−.732	.732	1	−.732	−.732	1
0.	0.	1	0.	0.	1
−1.	−.268	2	−1.	.268	2
.268	1.	2	.268	−1.	2
.732	−.732	2	732	.732	2
0.	0.	2	0.	0.	2

is the Box-Behnken design, and (c) the 11- and 15-factor designs were given by Crosier (1991a).

Because of the similar constructions of the uniform shell and simplicial shell designs, it is possible to give both shell designs for a specific k in one table by redefining the constants in the table. Table 5 gives the shell designs for six factors. The points listed in Table 5 versus their negatives are an orthogonal blocking of the simplicial shell design, but for the uniform shell design it is necessary to change the signs in rows 16, 17, and 18 before assigning the points in Table 5 to one block and their negatives to the other block.

Like the uniform shell design, the seven-factor simplicial shell design has three (known) symmetric rotations: the three-level design given by Box and Behnken (1960), the nine-level design given by the construction method above, and a rotation with seven equally spaced levels. One block of the seven-level design consists of center points and the cyclic permutations of the four points (−3, 0, 0, −1, 0, −1, −1), (2, 1, 1, 1, 0, −2, −1), (2, 0, 1, −2, 1, −1, 1), and (2, 1, 0, −1, 1, 1, −2). The points in the second block are the negatives of the points in the first block. Designs with many levels have been recommended for computer experiments (Welch *et al* 1992), so the nine-level rotations of the simplicial shell designs might be useful for that purpose. The eight-factor simplicial shell design has the simple levels 0, ±.2, ±.5, ±.7, and ±1.

Table 5. Six-Factor Shell Designs
Add negatives and center points.

Point	x_1	x_2	x_3	x_4	x_5	x_6
1	−1	h	e	e	e	e
2	e	−1	h	e	e	e
3	e	e	−1	h	e	e
4	e	e	e	−1	h	e
5	e	e	e	e	−1	h
6	h	e	e	e	e	−1
7	−1	e	h	e	e	e
8	e	−1	e	h	e	e
9	e	e	−1	e	h	e
10	e	e	e	−1	e	h
11	h	e	e	e	−1	e
12	e	h	e	e	e	−1
13	−1	e	e	h	e	e
14	e	−1	e	e	h	e
15	e	e	−1	e	e	h
16	$-r$	b	b	b	b	b
17	b	$-r$	b	b	b	b
18	b	b	$-r$	b	b	b
19	b	b	b	$-r$	b	b
20	b	b	b	b	$-r$	b
21	b	b	b	b	b	$-r$

NOTE: The uniform shell design has $h=1$, $e=0$, $r=.392$, and $b=.608$; the simplicial shell design has $h=-1$, $e=.262$, $r=.654$, and $b=.608$.

5. DESIGN COMPARISONS

Lucas (1976) compared response surface designs, including the uniform shell designs, by their D- and G-efficiencies. The G-efficiency, which is based on the maximum prediction variance within the experimental region, is the more sensitive criterion: a design can have a high D-efficiency and a low G-efficiency, but not vice versa. As a practical rule, a design with a G-efficiency of 50% or more is good enough for use. Table 6 gives the number of noncentral design points and the G-efficiencies of the Box-Behnken designs, the central composite designs, and the

Table 6. $N-n_0$ and G-Efficiency (percent) for Designs

	Box Behnken		Central Composite		Uniform Shell		Simplicial Shell	
k	$N-n_0$	G	$N-n_0$	G	$N-n_0$	G	$N-n_0$	G
2			8	96.0	6	90.0	6	90.0
3	12	71.4	14	94.6	12	71.4	12	0.0
4	24	98.9	24	98.9	20	70.5	20	23.1
5	40	90.9	26	87.6	30	65.6	30	51.8
6	48	67.2	44	97.0	42	64.4	42	76.9
7	56	99.3	78	84.7	56	62.1	56	99.3
8			80	99.8	72	61.2	72	93.1

NOTE: The central composite designs (CCD's) for 5-7 factors use a 1/2 fractional factorial; the 8-factor CCD uses a 1/4 fractional factorial.

shell designs. The G-efficiencies in Table 6 were obtained using $n_0 = 2$ center points. The G-efficiency of a design is defined as $p / V(\mathbf{x})_{\max}$, where p is the number of parameters in the model and $V(\mathbf{x})_{\max}$ is the maximum value of $V(\mathbf{x}) = N\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}$ for any point $\mathbf{x}$ in the experimental region. The variance of $\hat{y}$ at $\mathbf{x}$ is $V(\mathbf{x})\,\sigma^2/N$, so the G-efficiency of a design compares the maximum value of $V(\mathbf{x}) = N\,Var[\hat{y}(\mathbf{x})]/\sigma^2$ within the experimental region to its theoretical minimum, which is p. The G-efficiencies of some of the uniform shell designs in Table 6 are slightly lower than the values reported by Lucas (1976) because a more thorough search was done for the point $\mathbf{x}$ at which the maximum value of $V(\mathbf{x})$ occurs. Based on the G-efficiency in Table 6, the four-factor simplicial shell design should not be used.

Both D- and G-efficiency are measures of information per point, which is supposed to allow a comparison of designs with different numbers of design points. From the experimenter's point of view, the efficiency of a design is primarily (perhaps exclusively) a function of the number of design points. Thus the mathematical efficiencies are not practical measures of how good a design is, but theoretical measures that indicate how well the points are arranged over the experimental region. The shell designs provide symmetric designs with fewer runs than the Box-Behnken or central composite designs for $k = 2$, 4, 6, and 8. For $k = 3$, the Box-Behnken design is the symmetric orientation of the uniform shell design; for $k = 5$, the central composite design based on a 2^{5-1} fractional factorial is the symmetric design with the fewest runs; and for $k = 7$, the Box-Behnken design is the base design from which the simplicial shell designs were derived.

6. SUMMARY

Response surface designs with equal ranges for the coded factors have been widely used, but designs with unequal ranges for the coded factors have not been used frequently. Asymmetric designs give the consultant the choice of obtaining a design whose factor ranges do not match the ranges specified by the client, or of distorting the design's geometric configuration and statistical properties to obtain the desired factor ranges.

Symmetric orientations were given for the uniform shell designs and the simplicial shell designs. Both series of designs have $N = k(k+1) + n_0$ design points, and are symmetric designs that require fewer design points than the central composite designs or the Box-Behnken designs for $k = 2$, 4, 6, and 8. An orthogonal blocking of the uniform shell designs was given for even k. The symmetric orientations of the uniform shell designs are generally seven-level designs, the exceptions being $k = 3$ (three-levels), $k = 8$ (five-levels), and the sequence $k = 7$, 11, 15 ... (for which both three-level and seven-level rotations exist).

The simplicial shell designs are a generalization of the seven-factor Box-Behnken design. The two-factor simplicial shell design differs from the uniform shell design only by a sign change of one factor. The three-factor design is singular and the four-factor design is too inefficient for use. The simplicial shell designs have an orthogonal blocking for all k, but the simplicial shell designs for $k > 4$ are nine-level designs except for $k = 7$, which has three-, seven-, and nine-level rotations, and the sequence $k = 11, 15, 19, \ldots$, which has both three-level and nine-level rotations.

APPENDIX: DERIVATION OF THE DESIGNS

Coordinates for Simplexes. The coordinates of the $k+1$ vertices of a k-dimensional simplex are expressed most conveniently as the rows of a $(k+1)\times(k+1)$ identity matrix $\mathbf{I}_{k+1}$. The distance between any two rows of $\mathbf{I}_{k+1}$ is $2^{1/2}$, thus showing that $\mathbf{I}_{k+1}$ does represent the vertices of a regular simplex. A simplex centered on the origin may be represented by $(k+1)\mathbf{I}_{k+1} - \mathbf{J}_{k+1}$, where $\mathbf{J}_{k+1}$ is a $(k+1)\times(k+1)$ matrix of 1's. The coordinates of the vertices of the simplex are therefore all permutations of the $k+1$ values $k, -1, -1, \ldots, -1$. After rescaling to integral values, the midpoints of the edges of the centered simplex may be expressed as all permutations of $(k-1, k-1, -2, -2, \ldots, -2)$ and the centers of the $(k-1)$-dimensional faces (hereafter, just *faces*) may be written as all permutations of $(-k, 1, 1, \ldots, 1)$. Notice that the rescaled face centroids are the negatives of the vertices (before scaling).

Thus designs based on simplexes are more naturally expressed by $k+1$ linearly dependent variables than by k independent variables. To obtain experimental designs, rotate the design matrix of $k+1$ linearly dependent variables so that one linearly dependent variable becomes a constant. The variable that has the constant value has no effect in calculating the distances between the points of the design; hence the other k variables correctly describe the geometric configuration and may be used as the experimental design. It is well known that multiplication by an orthogonal matrix $\mathbf{\Theta}$ corresponds to a rotation if the determinant of $\mathbf{\Theta}$ is equal to 1, and to a rotation followed by a reflection if $\det(\mathbf{\Theta})=-1$. To reduce the $k+1$ linearly dependent variables to the $N \times k$ design matrix $\mathbf{D}$, it is necessary that the orthogonal matrix contain a constant column. If the constant column is the last column of $\mathbf{\Theta}$, this process is written in matrix notation as

$$\left[\mathbf{D} \,|\, d\,\mathbf{1}\right] = \mathbf{M}\,\mathbf{\Theta}, \tag{A.1}$$

where $\mathbf{M}$ is the $N \times (k+1)$ matrix of the design in linearly dependent variables, $\mathbf{1}$ is an $N \times 1$ matrix (column vector) of 1's, and d is a constant; typically, $d=0$ because the linearly dependent variables sum to zero.

Uniform Shell Designs. For the uniform shell designs, the $N \times (k+1)$ matrix $\mathbf{M}$ consists of all permutations of $(-1,1,0,\ldots,0)$ and a row of 0's for the center point (Doehlert and Klee 1972). For $k \equiv 3 \pmod 4$ — meaning the remainder is 3 when k is divided by 4 — Doehlert and Klee (1972) obtained symmetric, three-level rotations of the uniform shell designs by using a normalized Hadamard matrix for the orthogonal matrix $\mathbf{\Theta}$ in equation (A.1). [A Hadamard matrix is a square matrix of 1's and −1's whose columns are orthogonal — that is, the model matrix of a saturated two-level Plackett and Burman (1946) design; the normalization consists of scaling the Hadamard matrix so that $\mathbf{H}'\mathbf{H}=\mathbf{I}$.]

The symmetric orientation of the uniform shell designs given in Section 3 is obtained by using the orthogonal matrix

$$\mathbf{P} = \begin{bmatrix} f\mathbf{J}_k - \mathbf{I}_k & c\mathbf{1} \\ -c\mathbf{1}' & c \end{bmatrix} \tag{A.2}$$

where $\mathbf{1}$ is a $k \times 1$ matrix (column vector) of 1's, $f = (1 + (k+1)^{-1/2})/k$, and $c = (k+1)^{-1/2}$, for $\boldsymbol{\Theta}$ in equation (A.1).

Simplicial Shell Designs. For simplicial shell designs, the matrix $\mathbf{M}$ of $k+1$ linearly dependent variables consist of all permutations of $(k-1, k-1, -2, -2, \ldots, -2)$, their negatives, and the origin (Crosier 1991a). The orientation given by the use of a normalized Hadamard matrix $\mathbf{H}$ for $\boldsymbol{\Theta}$ in equation (A.1) is the best rotation of these designs for $k=7$ (the Box-Behnken design), 11, and 15.

The symmetric orientation of the simplicial shell designs given in Section 4 is obtained by using the orthogonal matrix

$$\mathbf{Q} = \begin{bmatrix} \mathbf{I}_k - g\mathbf{J}_k & c\mathbf{1} \\ -c\mathbf{1}' & c \end{bmatrix} \tag{A.3}$$

where $g = (1 - (k+1)^{-1/2})/k$ and $c = (k+1)^{-1/2}$, for $\boldsymbol{\Theta}$ in equation (A.1). The orthogonal matrix $\mathbf{P}$ will also yield nine-level rotations of simplicial shell designs. The advantage of using $\mathbf{Q}$ rather than $\mathbf{P}$ to obtain the simplicial shell designs is that the diameter/range (D/R) ratio is larger when $\mathbf{Q}$ is used to obtain the designs than when $\mathbf{P}$ is used to obtain the designs. [See Crosier (1991a) for a discussion of the D/R ratio.] The D/R ratio of the simplicial shell designs for $3<k<11$ ranges from 1.48 to 1.51 for the orientation given by $\mathbf{Q}$, but it is less than 1.1 when $\mathbf{P}$ is used to obtain the designs. Similarly, the use of $\mathbf{Q}$ to obtain the uniform shell designs yields seven-level designs with a small D/R ratio. In the orientation given by $\mathbf{P}$, the uniform shell designs have a D/R ratio of $2^{1/2}$.

The rotations of the seven-factor shell designs that have seven equally spaced levels are obtained by using an orthogonal matrix $\mathbf{C}$ for $\boldsymbol{\Theta}$ in (A.1). To form the 8×8 matrix $\mathbf{C}$, start with the 7×7 matrix consisting of the cyclic permutations of (1, 0, 0, −2, 1, 1, 0). Then append a row of −1's to form an 8×7 matrix. Finally, append a column of 1's to form $\mathbf{C}$. Normalization of $\mathbf{C}$ so that $\mathbf{C}'\mathbf{C} = \mathbf{I}$ is unnecessary. The uniform shell design given by $\mathbf{C}$ has a D/R ratio of $4/3 = 1.33$ and the simplicial shell design given by $\mathbf{C}$ has a D/R ratio of $12^{1/2}/3 = 1.15$.

Curtailed Representation. Because the columns of **M** are linearly dependent, one column of **M** (usually the last) can be deleted without the loss of information. Denote this curtailed representation by $\mathbf{M}_k$; $\mathbf{M}_k$ is not a correct design for k factors because the distances among the rows of $\mathbf{M}_k$ are not the same as the distances among the rows of **M**. But the correct design matrix **D** can be obtained from $\mathbf{M}_k$. For the uniform shell designs, $\mathbf{D} = \mathbf{M}_k\mathbf{A}$, where $\mathbf{A} = \mathbf{I}_k - [(1+(k+1)^{1/2})/k]\mathbf{J}_k$ and $\mathbf{J}_k$ is a $k \times k$ matrix of 1's. For the simplicial shell designs, $\mathbf{D} = \mathbf{M}_k\mathbf{B}$, where $\mathbf{B} = \mathbf{I}_k + [1/(1+(k+1)^{1/2})]\mathbf{J}_k$. It is often easier to form **A** and **B** than the orthogonal matrices **P** and **Q** on electronic worksheets that have matrix capabilities. The curtailed representation of **C** is the matrix formed by the cyclic permutations of (2, 1, 1, −1, 2, 2, 1).

REFERENCES

Box, G. E. P. and Behnken, D. W. (1960), "Some New Three-Level Designs for the Study of Quantitative Variables," *Technometrics*, 2, 455-475.

Box, G. E. P. and Wilson, K. B. (1951), "On the Experimental Attainment of Optimum Conditions," *Journal of the Royal Statistical Society*, Ser. B, 13, 1-45.

Crosier, R. B. (1991a), "Some New Three-Level Response Surface Designs," technical report CRDEC-TR-308, U.S. Army Chemical Research, Development and Engineering Center.

Crosier, R. B. (1991b), "Symmetry in Mixture Experiments," *Communications in Statistics — Theory and Methods*, 20, 1911-1935.

DeBaun, R. M. (1959), "Response Surface Designs for Three Factors at Three Levels," *Technometrics*, 1, 1-8.

Doehlert, D. H. (1970), "Uniform Shell Designs," *Journal of the Royal Statistical Society*, Ser. C, 19, 231-239.

Doehlert, D. H. and Klee, V. L. (1972), "Experimental Designs Through Level Reduction of the *d*-Dimensional Cuboctahedron," *Discrete Mathematics*, 2, 309-334.

Lucas, J. M. (1976), "Which Response Surface Design is Best," *Technometrics*, 18, 411-417.

Plackett, R. L. and Burman, J. P. (1946), "The Design of Optimum Multifactorial Experiments," *Biometrika*, 33, 305-325.

Spendley, W., Hext, G. R., and Himsworth, F. R. (1962), "Sequential Application of Simplex Designs in Optimisation and Evolutionary Operation," *Technometrics*, 4, 441-461.

Welch, W. J., Buck, R. J., Sacks, J., Wynn, H. P., Mitchell, T. J., and Morris, M. D. (1992), "Screening, Predicting, and Computer Experiments," *Technometrics*, 34, 15-25.