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RESPONSE SURFACE DESIGN COMPARISONS

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Ronald B. Grosier

RESEARCH AND TECHNOLOGY DIRECTORATE

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PREFACE

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RESPONSE SURFACE DESIGN COMPARISONS

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1. INTRODUCTION

In many industrial experiments the goal is to investigate the relationship between the process variables or factors x_1, x_2, \dots, x_k and a quality 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 D . To estimate the coefficients of the polynomial, the design matrix is expanded into an $N \times p$ model matrix X that has one column for each coefficient of the polynomial model. The estimate b of the coefficient vector is then obtained from the least-squares formula

$$b = (X'X)^{-1}X'y. \quad (1)$$

Several classes of designs are available for fitting first- or second-order polynomials over spherical or cuboidal regions. This report will be limited to comparison of designs for fitting second-order polynomials over spherical regions.

2. BACKGROUND

The most popular designs for fitting a second-order polynomial are the central composite designs of Box and Wilson (1951) and the designs of Box and Behnken (1960). Crosier (1993a) examined the utility of the shell designs for fitting a second-order polynomial model. The shell designs are two series of related designs: the uniform shell designs (Doehlert 1970) and the simplicial shell designs, which are a generalization of the seven-factor Box-

Behnken design (Crosier 1991).

The central composite designs, the uniform shell designs, and the simplicial shell designs have geometric constructions that are uniform in all dimensions; the Box-Behnken designs are a collection of three-level designs that have various geometric constructions. The central composite designs consist of (a) factorial points, which are a 2^k design or 2^{k-f} fractional factorial design of at least resolution V, (b) star or axial points, which have each factor in turn set to its high and low levels and the other factors at their central level, and (c) center points, which have all factors set to their central level. The uniform shell designs are obtained from a regular simplex that has one vertex at the origin: subtracting each vertex from all other vertices produces the complete list of design points. The simplicial shell designs are obtained from a regular simplex centered on the origin: the midpoints of its edges, their negatives, and the origin are the design points. The Box-Behnken designs are obtained by combining balanced incomplete block (BIB) or partially balanced incomplete block (PBIB) designs with two-level factorial or fractional factorial designs. Crosier (1991) gave some additional designs generated by this method.

Design matrices are given in coded units that center the design on the origin and yield convenient numbers for the coded design levels. To apply a response surface design, the coded factor levels must be scaled to the ranges of the process variables (experimental factors). Two methods of converting the coded factor levels to the levels of the experimental factors will be considered in this report. In method A, the diameter of the coded design is scaled to the range of each experimental factor. Method A was recommended by Doehlert and Klee (1972) and is consistent with the theory of experimental design, which compares designs for spherical regions by scaling the designs to have the same diameter. In method B, the range of the coded factors is scaled to the ranges of the experimental factors. Method B is widely used, but allows spherical designs to have different diameters, thus invalidating the traditional design comparisons. Crosier (1991) therefore suggested that the diameter/range (D/R) ratio of a design is an important property of the design because the ratio indicates the size of design region.

Lucas (1976) compared response surface designs, including the uniform shell designs, by their D- and G-efficiencies. The D-efficiency of a design is the p th root of the ratio of $\det(X'X)/N^p$ to the maximum possible value of $\det(X'X)/N^p$ for any design covering the same region. The D-efficiencies in

Lucas (1976) are obtained by scaling the designs to have radius 1 (that is, the region is a sphere of radius 1). The G-efficiency of a design is defined as $p/V(x)_{\max}$, where p is the number of parameters in the model and $V(x)_{\max}$ is the maximum value of $V(x) = N x'(X'X)^{-1}x$ for any point x in the experimental region. The variance of \hat{y} at x is $V(x)\sigma^2/N$, so the G-efficiency of a design compares the maximum value of $V(x) = N \text{Var}[\hat{y}(x)]/\sigma^2$ within the experimental region to its theoretical minimum, which is p . G-efficiency is a more sensitive criterion than D-efficiency: a design can have a high D-efficiency and a low G-efficiency, but not vice versa.

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.

Box and Draper (1987, p.498) have criticized the use of single number design criteria, such as the D- and G-efficiencies, and have suggested examining the predictive ability of the design over the entire experimental region. For this purpose, Giovannitti-Jensen and Myers (1989) recommend using variance dispersion graphs, which show the minimum, average, and maximum values of $V(x)$ as a function of the distance of x from the center of the design. The variance dispersion graphs are similar to the variance profiles of Box and Behnken (1960), which give the minimum and maximum values of $V(x)$ as a function of the distance of x from the center of the design. Myers, Vining, Giovannitti-Jensen, and Myers (1992) discuss the scaling by N in the variance dispersion graphs.

3. DESIGN COMPARISONS

I wish to make a few points about design comparisons and will do so through two examples. The second example involves the scaling of the designs and the relevance of the two methods (A and B) of applying a design to design comparisons. But first I compare two designs that have the same number of design points, the same range for the coded factors, and the same diameter, so that the scaling issues are not involved in the comparison.

The first example compares the four-factor Box-Behnken design with two center points to the uniform shell design (as given by Crosier 1993a) with six center points. Both designs have $N = 26$ design points, a range of -1 to 1 for every factor, and a diameter of $2 \times 2^{1/2}$ in coded units. The Box-Behnken design has a G-efficiency of 98.9% and the uniform shell design, with six center points, has a G-efficiency of 59.7%. Thus on the basis of G-efficiency, the Box-Behnken design is to be preferred. Figure 1 gives the variance profiles of the designs. The Box-Behnken design is rotatable (another desirable property) so that its minimum and maximum $V(x)$ are the same at any given distance from the center of the design. Hence the Box-Behnken design has one line in Figure 1, whereas the uniform shell design has separate lines for the minimum and maximum values of $V(x)$. From Figure 1, the uniform shell design gives better prediction near the center of the region and the Box-Behnken design gives better prediction at the perimeter of the region.

Although these comparisons (efficiency, rotatability, and predictive ability over the experimental region) may favor the Box-Behnken design, the uniform shell design should be preferred because it provides adequate degrees of freedom (five for pure error, six for residual error) for testing lack of fit. With only one degree of freedom for pure error, the Box-Behnken design does not provide an adequate test for lack of fit. The significance of the model terms must be tested using the residual error, which might be inflated by (undetectable) lack of fit. Even worse is that the predictions of the model may be far from the true response, and that this bias in the predictions due to lack of fit cannot be detected. In contrast, the uniform shell design allows both a lack of fit test and, if necessary, testing the model terms versus the five degrees of freedom (df) for pure error; five df for error is adequate — see Wheeler (1974, 1975). An overemphasis on optimal design theory may lead to ignoring important design goals.

The second example compares the three-factor central composite design (CCD) with $n_0 = 3$ center points to the three-factor Box-Behnken design (BBD), also with $n_0 = 3$ center points. Myers *et al* (1992) compared these designs and concluded that "The BBD performs better near the design center while the CCD clearly performs better near the perimeter." Their conclusion is based on graphs of the minimum, average, and maximum of $V(x)$ versus the radius of x . Then they remove the scaling by N —plotting $V(x)/N = \text{Var}[\hat{y}(x)]/\sigma^2$ versus the radius of x —and state the result: ". . . the advantage of the BBD near the design center disappears while the advantage

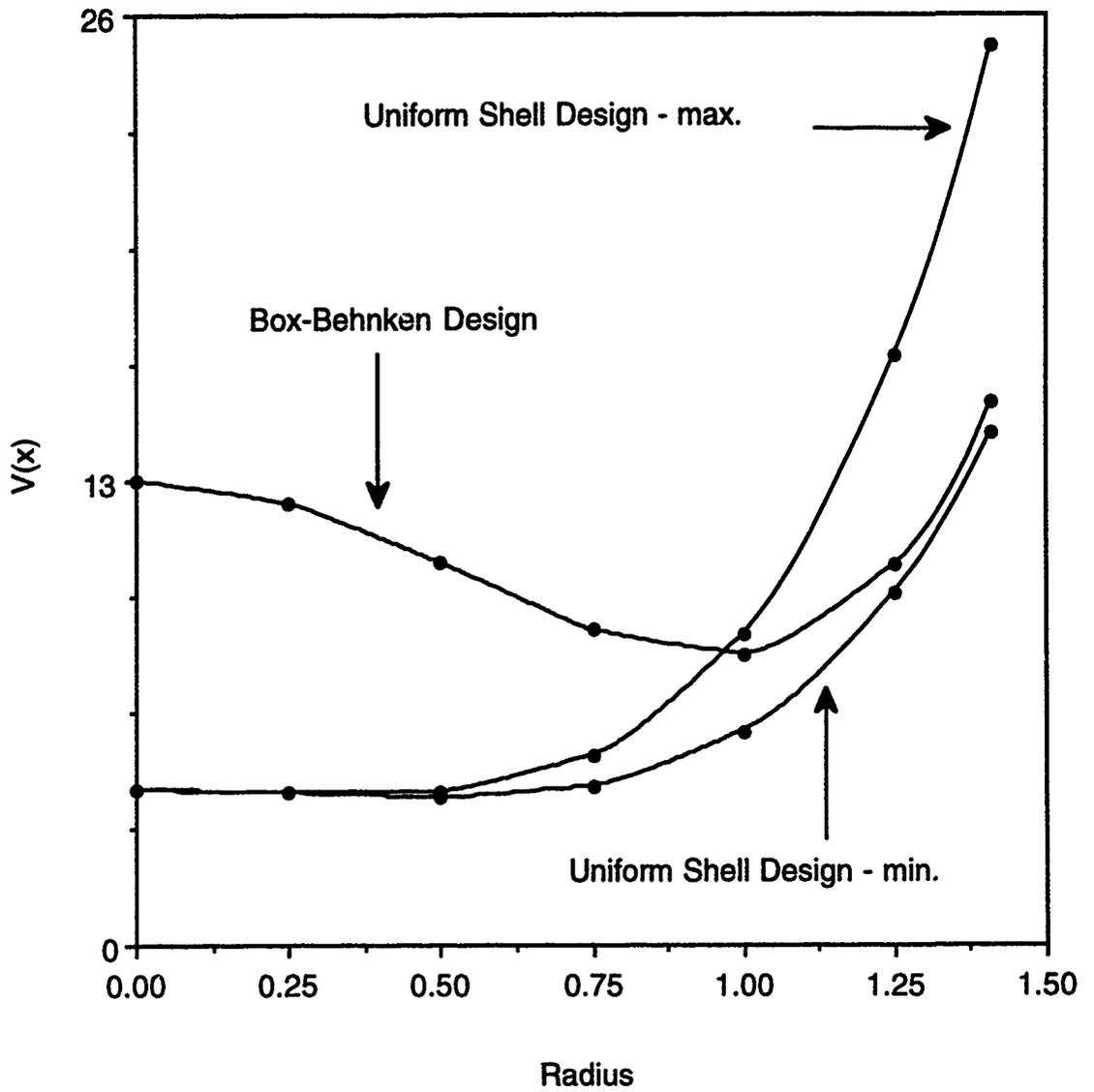


Figure 1. Variance Profiles for the Four-Factor Box-Behnken and Uniform Shell Designs.

of the CCD at the perimeter is even greater." These comparisons are based on scaling the designs to have the same diameter. Scaling the designs to have the same diameter for comparison is appropriate if the designs are applied by Method A.

To show what the same-diameter-scaling convention implies for statistical practice, I give the CCD and the BBD as applied to the three factors blender speed (100-300 rpm), mixing time (10-20 minutes), and cooking temperature (180-200°) by Method A in Tables 1 (the CCD) and 2 (the BBD).

Table 1. Three-Factor CCD Applied by Method A or Method B.

Point	Blender Speed	Mixing Time	Cooking Temperature
1	142.3	12.1	184.2
2	257.7	12.1	184.2
3	142.3	17.9	184.2
4	257.7	17.9	184.2
5	142.3	12.1	195.8
6	257.7	12.1	195.8
7	142.3	17.9	195.8
8	257.7	17.9	195.8
9	100	15	190
10	300	15	190
11	200	10	190
12	200	20	190
13	200	15	180
14	200	15	200
15	200	15	190

To save space, Tables 1 and 2 show only one center point. Because the diameter of the CCD is equal to the range of its coded factors, Methods A and B are equivalent for the CCD. For the BBD, Method A yields reduced ranges for the experimental factors because the range of the coded factors is less than the design diameter. I do not believe that the scaling in Table 2 reflects statistical practice—that is, I do not believe that the BBD would be applied by Method A. Table 3 gives the BBD applied by Method B. I believe that the scaling by Method B in Table 3 reflects statistical practice and is

Table 2. Three-Factor BBD by Method A.

Point	Blender Speed	Mixing Time	Cooking Temperature
1	129.3	11.5	190
2	270.7	11.5	190
3	129.3	18.5	190
4	270.7	18.5	190
5	129.3	15	182.9
6	270.7	15	182.9
7	129.3	15	197.1
8	270.7	15	197.1
9	200	11.5	182.9
10	200	18.5	182.9
11	200	11.5	197.1
12	200	18.5	197.1
13	200	15	190

therefore the correct scaling to use for making design comparisons. However, the literature on optimal designs uses scaling by Method A to compare designs. Box and Draper (1987) note the sensitivity of optimal design criteria to the scaling of the designs and state (in a footnote on page 499) "It is important to be aware that the apparent superiority of one design over another will often disappear if the method of scaling the design is changed." Their comment needs more emphasis in the applied statistical literature.

To make a realistic comparison between the CCD and the BBD, code the designs listed in Tables 1 and 3 by the equations:

$$x_1 = (\text{blender speed} - 200) / 100 \quad (2)$$

$$x_2 = (\text{mixing time} - 15) / 5 \quad (3)$$

and

$$x_3 = (\text{cooking temperature} - 190) / 10 \quad (4)$$

Equations 2-4 are typical of the scaling equations given in many textbooks on the design of experiments, but, apparently, the use of the same set of

Table 3. Three-Factor BBD by Method B.

Point	Blender Speed	Mixing Time	Cooking Temperature
1	100	10	190
2	300	10	190
3	100	20	190
4	300	20	190
5	100	15	180
6	300	15	180
7	100	15	200
8	300	15	200
9	200	10	180
10	200	20	180
11	200	10	200
12	200	20	200
13	200	15	190

equations to scale two designs that are to be compared is not common practice. When the designs in Tables 1 and 3 are coded by equations 2-4, both designs have the range -1 to 1 for the coded factors, but the diameters of the designs are different. Figure 2 shows the maximum and minimum values of $V(x)/N$ versus the radius of x for the CCD and the BBD when the designs are scaled to have the range -1 to 1 . The superiority of the CCD at its design perimeter has now disappeared, and there are two design perimeters—at a radius of 1 for the CCD and at a radius of $2^{1/2}$ for the BBD.

Because response surface designs are usually applied by Method B, the optimal design criteria based on Method A scaling apply to design regions of varying sizes. Specifically, the D- and G-efficiencies of the CCD apply to a sphere of radius 1 and the D- and G-efficiencies of the three-factor BBD apply to a sphere of radius $2^{1/2}$. Crosier (1991a) introduced the diameter/range (D/R) ratio as a measure of the size of a spherical design; when a design is scaled so that the factors cover the interval $[-1, 1]$, the D/R ratio is equal to the radius of the noncentral design points.

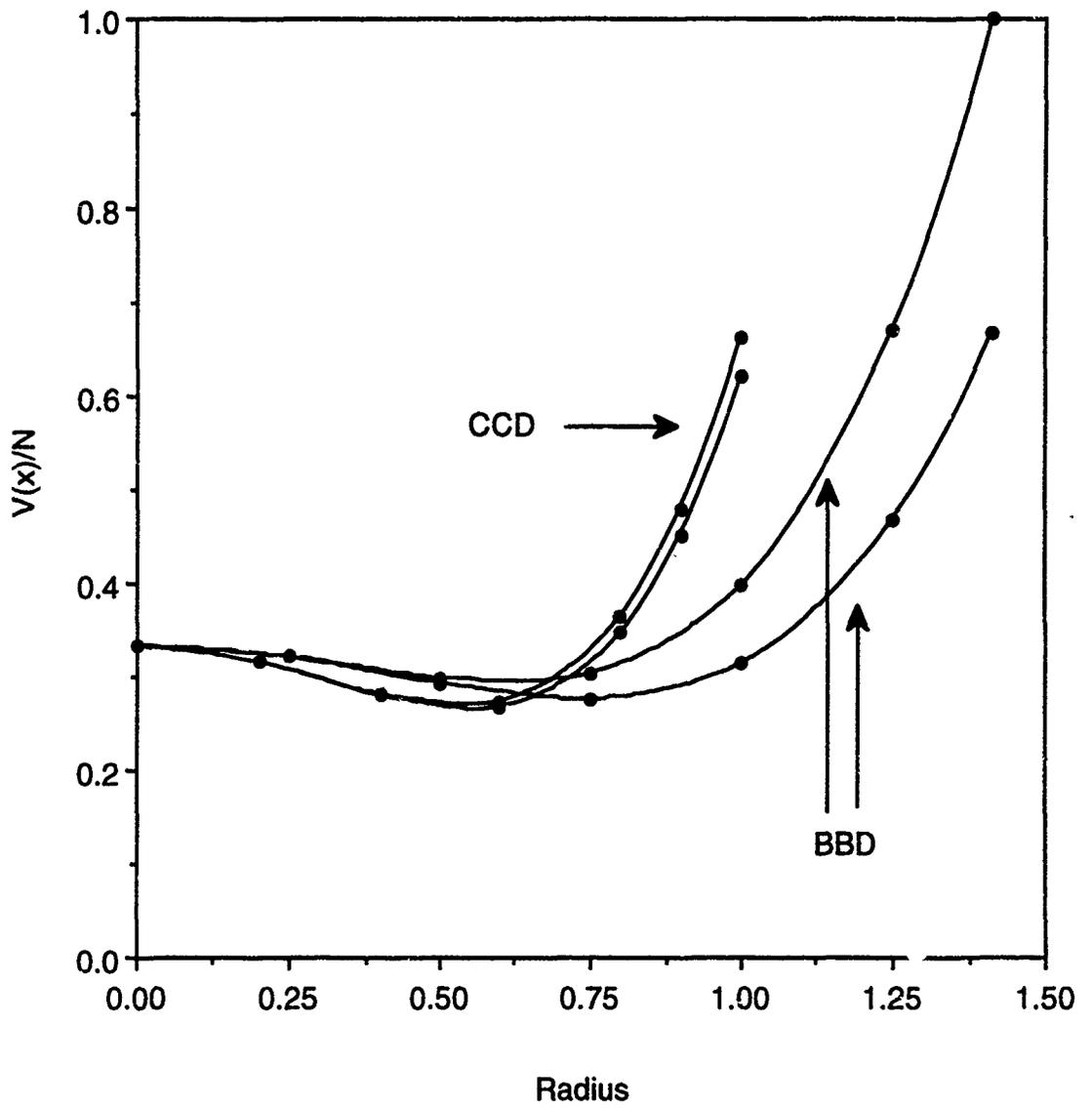


Figure 2. $V(\mathbf{x}) / N$ for the Three-Factor Central Composite and Box-Behnken Designs.

Experimentation over a large region gives more precise estimates of the polynomial coefficients than experimentation over a small region, but a polynomial model will approximate an unknown function better over a small region than over a large region. I believe that spherical designs with a D/R ratio greater than one are a reasonable compromise between the small spherical region of the central composite designs (D/R=1) and the large cuboidal region of the face centered cube designs. Also, it seems intuitive that a polynomial will approximate an unknown function better over a spherical region than over a cuboidal region of the same volume.

Rotating a first- or second-order response surface design does not change its D- and G-efficiencies, so design rotations have been ignored. But rotating a response surface design can change the number of levels of the factors and the ranges of the coded factors (and hence the diameter of the design region if the design is applied by method B). Comparisons of response surface designs therefore need to specify the orientations of the designs because characteristics of practical importance (such as the number of levels) depend on the orientation of a design. Table 4 gives the number of noncentral design points, the number of levels, the number of orthogonal blocks, the diameter/range ratio (D/R), and the G-efficiencies of the central composite (CC) designs, the Box-Behnken (BB) designs, the uniform shell (US) designs, the simplicial shell (SS) designs, and some additional three-level designs [denoted by (P)BIB+2^m to indicate their construction] given by Crosier (1991). For $k > 8$, only three-level designs are given in Table 4. The central composite designs for even k are given in two orientations in Table 4; first is the standard orientation and second are the new orientations given by Crosier (1991, 1993b). The factorial point versus axial point blocking of the central composite designs can be made orthogonal by proper choice of the axial point distance and the number of center points in the two blocks. The G-Efficiencies in Table 4 are for unblocked designs with two center points. The G-efficiencies of some of the uniform shell designs in Table 4 are slightly lower than the values reported by Lucas (1976) because a more thorough search was done for the point x at which the maximum value of $V(x)$ occurs. The uniform shell and simplicial shell designs in Table 4 are in the symmetric orientations discussed by Crosier (1991, 1993a). In the orientation given by Doehlert (1970), the uniform shell designs have coded factors with different ranges. Such asymmetric designs are difficult to apply (Crosier 1993a, 1993b) and so are not included in Table 4. Some comments on the designs in Table 4 appear after Table 4.

Table 4. Some Properties of Symmetric Designs.

Design	k	$N-n_0$	Levels	Blocks	D/R	G-Eff.(%)
CC	2	8	5	2e	1.	96.0
CC	2	8	5	2e	1.082	96.0
US=SS	2	6	7	2e	1.035	90.0
CC	3	14	5	2	1.	94.6
BB=US	3	12	3e	-	1.414	71.4
SS	3	12	3e	2e	1.	0.0
SS	3	12	5e	2e	1.5	0.0
CC	4	24	5e	3e	1.	98.9
BB=CC	4	24	3e	3e	1.414	98.9
US	4	20	7	2e	1.414	70.5
SS	4	20	9	2e	1.514	23.1
CC	5	26	5	2	1.	87.6
BB	5	40	3e	2e	1.414	90.9
US	5	30	7	-	1.414	65.6
SS	5	30	9	2e	1.513	51.8
CC	6	44	5	2	1.	97.0
CC	6	44	5	2	1.414	97.0
BB	6	48	3e	2e	1.732	67.2
US	6	42	7	2e	1.414	64.4
SS	6	42	9	2e	1.508	76.9
CC	7	78	5	2	1.	84.7
BB=SS	7	56	3e	2e	1.732	99.3
SS	7	56	9	2e	1.502	99.3
SS	7	56	7e	2e	1.155	99.3
US	7	56	3e	-	2.	62.1
US	7	56	7	-	1.414	62.1
US	7	56	7e	-	1.333	62.1
CC	8	80	5	2	1.	99.8
CC	8	80	5	2	1.414	99.8
US	8	72	5e	2e	1.414	61.2
SS	8	72	9	2e	1.497	93.1
BB	9	120	3e	10e	1.732	83.2
BIB+2 ³	9	96	3e	8e	1.732	92.9

BB	10	160	3e	2e	2.	68.6
PBIB+2 ⁵⁻¹	10	160	3e	-	2.236	41.8
BB	11	176	3e	-	2.236	80.9
US	11	132	3e	-	2.449	56.9
SS	11	132	3e	2e	2.236	80.6
BB	12	192	3e	2e	2.	89.2
BIB+2 ⁴	13	208	3e	2e	2.	94.5
US	15	240	3e	-	2.828	56.2
SS	15	240	3e	2e	2.646	71.9
BB	16	384	3e	12e	2.	85.0

NOTE: The e indicates equally spaced levels or equal-size blocks.

For $k = 2, 4,$ and $6,$ the uniform shell designs require fewer runs than the central composite or Box-Behnken designs, but require seven levels of the factors. The three-factor simplicial shell design is singular and the four-factor simplicial shell design is too inefficient for use. The nine-factor design designated by BIB+2³ has eight orthogonal blocks: the four blocks given by Crosier (1991) can be divided into eight blocks by using the three-way interaction of the 2³ design to separate the design points. $V(x)_{\max}$ for the 10-factor design denoted PBIB+2⁵⁻¹ is worse than $V(x)_{\max}$ for the 10-factor Box-Behnken design at every radius up to 2.236. Hence the Box-Behnken design is to be preferred. However, the 11-factor shell designs require fewer runs than the 10-factor Box-Behnken design. Thus one would usually use one of the 11-factor shell designs for 10 factors by ignoring one of the design columns. In comparing the three-level rotations of the shell designs (for $k = 7, 11,$ and $15,$), there is only a trivial difference in $V(x)_{\max}$ between the uniform shell designs and the simplicial shell designs, with the uniform shell designs being slightly better at the design perimeters and the simplicial shell designs being slightly better closer to the center of the design region. The benefit of the larger region of the uniform shell designs (more precise estimates of the coefficients) only compensates for the lower efficiencies of the uniform shell designs and does not provide any real advantage over the simplicial shell designs. I would therefore prefer the simplicial shell designs to the uniform shell designs (for $k = 7, 11,$ and $15,$) because of the orthogonal blocking of the simplicial shell designs and because the smaller region of the simplicial shell designs reduces the bias due to lack of fit.

4. SUMMARY

Response surface designs are often compared by optimal design theory criteria, such as the D- and G-efficiencies. For designs over spherical regions, such criteria are calculated by scaling the designs to have the same diameter. But, in practice, designs are applied by scaling the coded factor ranges (not the diameter) to the ranges of the factors in the experiment. The result of this discrepancy between theory and practice is that the mathematical efficiencies may apply to regions of different sizes. Further, there are practical objectives, such as minimizing the number of runs or testing for lack of fit, that are ignored by optimal design theory. Two examples were given to show the limitations of comparisons of designs by optimal design theory criteria. For many symmetric second-order designs, a table listing the following items was provided: number of noncentral design points, number of levels, number of orthogonal blocks, D/R ratio, and G-efficiency.

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