

# Comparison of Five Design Variables of Response Surface Designs in a Spherical Region Over a Set of Reduced Models

Boonorm Chomtee

## ABSTRACT

The research extended the work of Chomtee and Borkowski (2012) which compared response surface designs—central composite designs (CCDs), Box-Behnken designs (BBDs), small composite designs (SCDs), Plackett-Burman composite designs (PBDs) and uniform shell designs (USDs)—over a set of reduced models in a spherical design region for five design variables ( $k = 5$ ) based on the three alphabetic optimality criteria— $D$  and  $G$  where larger values imply a better design (on a per point basis) and  $IV$  (where a smaller value implies a better design). The results present a comparison of the design optimality criteria of the response surface designs across the full second order model and a set of reduced models (839 models) for five factors based on the three alphabetic optimality criteria. The results of the comparison ranking of the  $D$ ,  $G$  and  $IV$  criteria of reduced models showed that for small design sizes,  $N = 23, 25, 27$  and  $29$ , based on  $D$  and  $G$ , the SCD ( $n_0 = 1, 3$ ) are recommended over the PBD ( $n_0 = 1, 3$ ). For medium design sizes,  $N = 31, 33$  and  $35$ , based on  $D$  and  $G$ , the USD ( $n_0 = 1, 3$ ) are recommended over the PBD ( $r_s = 2, n_0 = 1, 3$ ), and when  $N = 35, 37$ , the SCD ( $r_s = 2, n_0 = 1$ ) is recommended over the PBD ( $r_s = 2, n_0 = 3$ ). For a large design size,  $N = 43$ , based on  $D$ , the CCD ( $n_0 = 1$ ) is recommended over the BBD ( $n_0 = 3$ ), and based on  $G$  and  $IV$ , the BBD ( $n_0 = 3$ ) is recommended over the CCD ( $n_0 = 1$ ).

**Keywords:** response surface design, design optimality criteria, spherical design region, reduced models, weak heredity

## INTRODUCTION

In practice, three to five factors are expected to affect a response variable and are often set to perform an experiment in various branches such as science, agriculture and industry. For response surface methodology (RSM), the second order model is widely used as an approximating model to the response model (Equation 1):

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{1 \leq i < j}^k \beta_{ij} x_i x_j + \varepsilon \quad (1)$$

where  $y$  is a response variable,  $\beta_0$  is a y-intercept,

$\beta$ 's are coefficients of  $x$ 's,  $x$ 's are factors or input variables expected in model,  $k$  is the number of input variables and  $\varepsilon$  is random error.

Chomtee and Borkowski (2012) compared central composite designs (CCDs), Box-Behnken designs (BBDs), small composite designs (SCDs), hybrid designs and uniform shell designs (USDs) when the designs are in a spherical region across sets of reduced models for three and four design variables ( $k = 3, 4$ ) consisting of 44 and 224 models, respectively. Hence, the purpose of this research was to extend the work of Chomtee and Borkowski (2012) by comparing

the response surface designs: CCDs, BBDs, SCDs, PBDs and USDs when  $k=5$  based three alphabetic optimality criteria— $D$  and  $G$  where larger values imply a better design (on a per point basis) and  $IV$  (where a smaller value implies a better design). This study used PBDs instead of hybrid designs because a hybrid design cannot be constructed when  $k=5$ .

## MATERIALS AND METHODS

### Design optimality criteria

Design optimality criteria are primarily concerned with the optimality properties of the  $\mathbf{X}'\mathbf{X}$  matrix for the design matrix  $\mathbf{X}$ . By studying the optimality criteria, the adequacy of proposed experimental design can be assessed prior to running it. If several alternative designs are proposed, their optimality properties can be compared to aid in the choice of design. However, Myers *et al.* (1989) pointed out that Kiefer and Box agree that design selection should be guided by more than one criterion because even if a design is the best among several designs by one optimality criterion, it may be poorer when evaluated by a different optimality criterion. Thus, the  $D$ ,  $G$  and  $IV$  design optimality measures (on a per point basis) were used in this research and calculated over the full second order model and a set of reduced models as Equations 2 to 4:

$$D\text{-efficiency} = 100 \frac{|\mathbf{X}'\mathbf{X}|^{1/p}}{N} \quad (2)$$

$$G\text{-efficiency} = 100 \frac{p}{N \hat{\sigma}_{\max}^2} \quad (3)$$

$$IV\text{-efficiency} = N \sigma_{ave}^2 \quad (4)$$

where  $\mathbf{X}$  is the design matrix,  $p$  is the number of model parameters,  $N$  is the design size,  $\hat{\sigma}_{\max}^2$  is the maximum of  $\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})$  approximated over the set of candidate points,  $\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}), \dots, f_p(\mathbf{x})]'$  is a vector of  $p$  real-values functions based on  $p$  parameter model terms,  $\sigma_{ave}^2$  is the average of  $\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})$  over the design space, and  $\mathbf{x}$  is any

point in the design region  $\mathbf{X}$ . The  $G$ -efficiency and the  $IV$ -efficiency are based on the scaled prediction variance function  $V(\mathbf{x}) = \mathbf{N}^p(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})$ . The evaluation of the  $G$  and  $IV$  are over a continuous design region. Thus, for a spherical region, the  $IV$ -efficiency  $= \omega^{-1} \int_{\mathbf{X}} V(\mathbf{x}) d\mathbf{x}$ , where  $\omega = \int_{\mathbf{X}} d\mathbf{x}$  is the volume of spherical design region  $\mathbf{X}$ . In the research, these design optimality measures were calculated using the Matlab software (Mathworks, 2010) for the response surface designs.

### Reduced models

In RSM, the second order model (Equation 1) is used as an approximating model. However, the final response surface model usually ends up with a reduced model. Thus, the research aimed to compare response surface designs across a set of reduced models. The set of reduced models is consistent with the definition of weak heredity given in Chipman (1996), that is: (i) a quadratic  $x_i^2$  term is in the model only if the  $x_i$  term is also in the model and (ii) an interaction  $x_i x_j$  term is in the model only if the  $x_i$  or  $x_j$  or both terms are also in the model. Based on a weak heredity structure, there are 839 models for  $k=5$ .

Let 1's and 0's indicate, respectively, the presence or absence of the term  $x_i$  in the reduced model,  $p$  indicate the number of model parameters,  $dv$  indicate the number of design variables present in the model, and  $l$ ,  $c$  and  $q$  indicate the number of linear, cross-product and quadratic terms in the model, respectively. An example of a set of reduced models for  $k=5$  is shown in Table 1.

### Spherical region

As mentioned in Myers *et al.* (2009), there is a variety of response surface designs in cuboidal, spherical and polyhedral regions. In this research, response surface designs in a spherical region were studied where  $\sum_{i=1}^k x_i^2 \leq k$ ,  $x$  is a design variable and  $k$  is the number of input variables. For  $k=5$ , all  $x_i$  values,  $i=1, 2, \dots, 5$  are inside a sphere of radius  $\alpha = \sqrt{5}$ .

**Table 1** Reduced models for  $k = 5$ .

| Model | $p$ | $dv$ | $l$ | $c$ | $q$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_{12}$ | $x_{13}$ | $x_{14}$ | $x_{15}$ | $x_{23}$ | $x_{24}$ | $x_{25}$ | $x_{34}$ | $x_{35}$ | $x_{45}$ | $x_{11}$ | $x_{22}$ | $x_{33}$ | $x_{44}$ | $x_{55}$ |
|-------|-----|------|-----|-----|-----|-------|-------|-------|-------|-------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1     | 21  | 5    | 5   | 10  | 5   | 1     | 1     | 1     | 1     | 1     | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        |
| 2     | 20  | 5    | 5   | 9   | 5   | 1     | 1     | 1     | 1     | 1     | 0        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        |
| 3     | 20  | 5    | 5   | 10  | 4   | 1     | 1     | 1     | 1     | 1     | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 0        | 1        | 1        | 1        | 1        |
| 4     | 19  | 5    | 4   | 10  | 4   | 0     | 1     | 1     | 1     | 1     | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 1        | 0        | 1        | 1        | 1        | 1        |
| ...   |     |      |     |     |     |       |       |       |       |       |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |
| 837   | 3   | 2    | 2   | 0   | 0   | 0     | 0     | 0     | 1     | 1     | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        |
| 838   | 3   | 1    | 1   | 0   | 1   | 0     | 0     | 0     | 0     | 1     | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 1        |
| 839   | 2   | 1    | 1   | 0   | 0   | 0     | 0     | 0     | 0     | 1     | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        | 0        |

$p$  = number of model parameters;  $dv$  = number of design variables present in the model;  $l$ ,  $c$  and  $q$  = number of linear, cross-product and quadratic terms in the model, respectively.

## RESULTS

In this research, one and three center points ( $n_0 = 1, 3$ ) CCDs, BBDs, SCDs, PBDs, USDs were considered for  $k = 5$  design variables. The three optimality criteria  $D$ ,  $G$  and  $IV$  were computed for the full second order model and a set of reduced models (a total of 839 models) assuming a spherical response surface design region.

The results for the full second order model are shown in Table 2 which indicates the following general results:

1. Replicating star points (increasing  $r_s$ ) tended to reduce the  $D$  and  $G$  criteria for CCDs, SCDs and PBDs and to increase the  $IV$  criterion for CCDs and SCDs.

2. Increasing center points (increasing  $n_0$ ) tended to increase the  $D$  and  $G$  criteria and to reduce the  $IV$  criterion for CCDs whether or not star points were replicated. However, for SCDs, increasing  $n_0$  tended to reduce the  $D$  criterion and to improve the  $G$  and  $IV$  criteria. For BBDs, increasing  $n_0$  tended to improve the  $D$ ,  $G$  and  $IV$  criteria. For PBDs, increasing  $n_0$  tended to reduce both  $D$  and  $G$ . For USDs, increasing  $n_0$  tended to improve the  $G$  criterion but not the  $D$  criterion.

### Design criteria comparison ranking

The comparison ranking based on the three criteria ( $D$ ,  $G$  and  $IV$ ) for CCDs, BBDs, SCDs, PBDs, and USDs when  $k = 5$  for the full second order model are summarized in Tables 3 and 4. The comparison is on a per point basis, that is, the optimality criteria are based on functions that are scaled by the design size  $N$ . Thus, any gains in the prediction variance properties are not offset by increased sample size.

For the comparison ranking for  $k = 5$ , each entry in Tables 3 and 4 contains the row rank that ranges from 1 (best) to 5 (worst) for  $D$  and  $G$ . The rank represents that design's rank relative to the other four designs. For  $IV$ , the row rank that ranges from 1 (best) to 3 (worst). The rank

**Table 2** Optimality criteria for the full second order model,  $k = 5$ .

| Design | $r_s$ | $n_0$ | $N$ | $D$ -eff | $G$ -eff | $IV$ -eff       |
|--------|-------|-------|-----|----------|----------|-----------------|
| CCD    | 1     | 1     | 43  | 80.159   | 48.837   | 62.0441         |
|        | 1     | 3     | 45  | 80.710   | 85.964   | 29.1527         |
|        | 2     | 1     | 53  | 78.883   | 39.622   | 74.1056         |
|        | 2     | 3     | 55  | 80.097   | 92.981   | 33.1745         |
| BBD    | -     | 1     | 41  | 79.628   | 51.219   | 59.8097         |
|        | -     | 3     | 43  | 80.002   | 92.221   | 28.5402         |
| SCD    | 1     | 1     | 27  | 80.020   | 77.777   | 43.3044         |
|        | 1     | 3     | 29  | 78.503   | 88.172   | 23.4557         |
|        | 2     | 1     | 37  | 73.127   | 56.756   | 56.7476         |
|        | 2     | 3     | 39  | 73.103   | 74.115   | 28.8082         |
| PBD    | 1     | 1     | 23  | 60.065   | 22.458   | Singular matrix |
|        | 1     | 3     | 25  | 58.228   | 20.662   | Singular matrix |
|        | 2     | 1     | 33  | 56.578   | 21.062   | Singular matrix |
|        | 2     | 3     | 35  | 56.210   | 19.858   | Singular matrix |
| USD    | -     | 1     | 31  | 65.455   | 1.500    | Singular matrix |
|        | -     | 3     | 33  | 64.790   | 1.700    | Singular matrix |

CCD = central composite design; BBD = Box-Behnken design; SCD = small composite design; PBD = Plackett-Burman composite design; USD = uniform shell design;  $r_s$  = Number of star points;  $n_0$  = Number of center points;  $N$  = Design size;  $D$ -eff =  $D$ -efficiency;  $G$ -eff =  $G$ -efficiency;  $IV$ -eff =  $IV$ -efficiency.

**Table 3** Design optimality criteria ( $D$ ,  $G$  and  $IV$ ) comparison ranking for the full second order model,  $k = 5$  and one center point ( $n_0 = 1$ ).

| Design<br>Criterion | CCD<br>( $N = 43$ ) | BBD<br>( $N = 41$ ) | SCD<br>( $N = 27$ ) | PBD<br>( $N = 23$ ) | USD<br>( $N = 31$ ) |
|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| $D$                 | 1                   | 3                   | 2                   | 5                   | 4                   |
| $G$                 | 3                   | 2                   | 1                   | 4                   | 5                   |
| $IV$                | 3                   | 2                   | 1                   | -                   | -                   |

CCD = central composite design; BBD = Box-Behnken design; SCD = small composite design; PBD = Plackett-Burman composite design; USD = uniform shell design;  $N$  = design size.

**Table 4** Design optimality criteria ( $D$ ,  $G$  and  $IV$ ) comparison ranking for the full second order model,  $k = 5$  and three center points ( $n_0 = 3$ ).

| Design<br>Criterion | CCD<br>( $N = 45$ ) | BBD<br>( $N = 43$ ) | SCD<br>( $N = 29$ ) | PBD<br>( $N = 25$ ) | USD<br>( $N = 33$ ) |
|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| $D$                 | 1                   | 2                   | 3                   | 5                   | 4                   |
| $G$                 | 3                   | 1                   | 2                   | 4                   | 5                   |
| $IV$                | 3                   | 2                   | 1                   | -                   | -                   |

CCD = central composite design; BBD = Box-Behnken design; SCD = small composite design; PBD = Plackett-Burman composite design; USD = uniform shell design;  $N$  = design size.

represents that design's rank relative to the other two designs. In case of ties, average ranks are shown.

For the full second order model and  $n_0 = 1$ , Table 3 indicates that based on  $D$ , the CCD ( $N = 43$ ) is the best design. However, if  $G$  and  $IV$  are considered, the SCD ( $N = 27$ ) is the best design. For the full second order model and  $n_0 = 3$ , Table 4 indicates that based on  $D$ , the CCD ( $N = 45$ ) is the best design. If  $G$  is considered, the BBD ( $N = 43$ ) is the best design. However, based on  $IV$ , the SCD ( $N = 29$ ) is the best design.

### Ranking comparison of design optimality criteria of reduced models

Tables 5–12 present the results of research related to the comparison of design optimality based on the  $D$ ,  $G$  and  $IV$  criteria of the spherical response surface designs for the set of reduced models (839 models) when  $k = 5$ .

For the comparison ranking tables, each row/column entry contains four ranks ( $r_0, r_1, r_2, r_3$ ). Each rank ranges from 1 (best) to the number of designs to be compared (worst). Ranks  $r_0, r_1, r_2$  and  $r_3$  represent a design's rank relative to the

**Table 5** Design criteria comparison ranking for  $k = 5, N = 23, 27$ .

| Design Criterion | PBD ( $n_0 = 1$ ), $N = 23$ | SCD ( $n_0 = 1$ ), $N = 27$ |
|------------------|-----------------------------|-----------------------------|
| $D$              | 2, 2, 2, 2                  | 1, 1, 1, 1                  |
| $G$              | 2, 2, 2, 2                  | 1, 1, 1, 1                  |

PBD = Plackett-Burman composite design; SCD = small composite design;  $n_0$  = Number of center points;  $N$  = design size;  $r_0, r_1, r_2, r_3$  = rank across 839, 736, 525, 289 models with  $q \geq 0, q \geq 1, q \geq 2, q \geq 3$ .

**Table 6** Design criteria comparison ranking for  $k = 5, N = 25, 27$ .

| Design Criterion | PBD ( $n_0 = 3$ ), $N = 25$ | SCD ( $n_0 = 1$ ), $N = 27$ |
|------------------|-----------------------------|-----------------------------|
| $D$              | 2, 2, 2, 2                  | 1, 1, 1, 1                  |
| $G$              | 2, 2, 2, 2                  | 1, 1, 1, 1                  |

PBD = Plackett-Burman composite design; SCD = small composite design;  $n_0$  = Number of center points;  $N$  = design size;  $r_0, r_1, r_2, r_3$  = rank across 839, 736, 525, 289 models with  $q \geq 0, q \geq 1, q \geq 2, q \geq 3$ .

**Table 7** Design criteria comparison ranking for  $k = 5, N = 25, 29$ .

| Design Criterion | PBD ( $n_0 = 3$ ), $N = 25$ | SCD ( $n_0 = 3$ ), $N = 29$ |
|------------------|-----------------------------|-----------------------------|
| $D$              | 2, 2, 2, 2                  | 1, 1, 1, 1                  |
| $G$              | 2, 2, 2, 2                  | 1, 1, 1, 1                  |

PBD = Plackett-Burman composite design; SCD = small composite design;  $n_0$  = Number of center points;  $N$  = design size;  $r_0, r_1, r_2, r_3$  = rank across 839, 736, 525, 289 models with  $q \geq 0, q \geq 1, q \geq 2, q \geq 3$ .

**Table 8** Design criteria comparison ranking for  $k = 5, N = 31, 33$ .

| Design Criterion | PBD ( $r_s = 2, n_0 = 1$ ), $N = 33$ | USD ( $n_0 = 1$ ), $N = 31$ |
|------------------|--------------------------------------|-----------------------------|
| $D$              | 2, 2, 2, 2                           | 1, 1, 1, 1                  |
| $G$              | 2, 2, 2, 1                           | 1, 1, 1, 2                  |

PBD = Plackett-Burman composite design; USD = uniform shell design;  $n_0$  = Number of center points;  $r_s$  = Number of star points;  $N$  = design size;  $r_0, r_1, r_2, r_3$  = rank across 839, 736, 525, 289 models with  $q \geq 0, q \geq 1, q \geq 2, q \geq 3$ .

other designs across the full set of reduced models (839 models), across the set of reduced models with  $q \geq 1$  (736 models), across the set of reduced models with  $q \geq 2$  (525 models) and across the set of reduced models with  $q \geq 3$  (289 models), respectively. In case of ties, average ranks are shown. However, some of these response surface designs for some reduced models had singular design matrices. Thus, the  $IV$  criterion cannot be computed for these response surface designs. Consequently, the response surface designs that have singular design matrices were not compared with other designs.

For Tables 5–7 and Table 11, the comparison ranking of the  $D$  and  $G$  of reduced models between the PBDs and SCDs shows that the SCDs are recommended over the PBDs. For Tables 8–10, the comparison ranking of the  $D$  of reduced models between the PBDs and USDs indicates that the USDs are recommended over the PBDs. If  $G$  is considered, for almost all of the reduced models, the USDs are better than PBDs except when  $q \geq 3$ . Table 12 indicates that based on  $G$  and  $IV$ , the BBD ( $n_0 = 3$ ) is better than the CCD ( $n_0 = 1$ ). If  $D$  is considered, the CCD ( $n_0 = 1$ ) is better than the BBD ( $n_0 = 3$ ) except when  $q \geq 3$ .

**Table 9** Design criteria comparison ranking for  $k = 5$ ,  $N = 33$ .

| Design Criterion | PBD ( $r_s = 2$ , $n_0 = 1$ ), $N = 33$ | USD ( $n_0 = 3$ ), $N = 33$ |
|------------------|---|-----------------------------|
| $D$              | 2, 2, 2, 2                              | 1, 1, 1, 1                  |
| $G$              | 2, 2, 2, 1                              | 1, 1, 1, 2                  |

PBD = Plackett-Burman composite design; USD = uniform shell design;  $n_0$  = Number of center points;  $r_s$  = Number of star points;  $N$  = design size;  $r_0, r_1, r_2, r_3$  = rank across 839, 736, 525, 289 models with  $q \geq 0, q \geq 1, q \geq 2, q \geq 3$ .

**Table 10** Design criteria comparison ranking for  $k = 5$ ,  $N = 33, 35$ .

| Design Criterion | PBD ( $r_s = 2$ , $n_0 = 3$ ), $N = 35$ | USD ( $n_0 = 3$ ), $N = 33$ |
|------------------|---|-----------------------------|
| $D$              | 2, 2, 2, 2                              | 1, 1, 1, 1                  |
| $G$              | 2, 2, 2, 2                              | 1, 1, 1, 1                  |

PBD = Plackett-Burman composite design; USD = uniform shell design;  $n_0$  = Number of center points;  $r_s$  = Number of star points;  $N$  = design size;  $r_0, r_1, r_2, r_3$  = rank across 839, 736, 525, 289 models with  $q \geq 0, q \geq 1, q \geq 2, q \geq 3$ .

**Table 11** Design criteria comparison ranking for  $k = 5$ ,  $N = 35, 37$ .

| Design Criterion | PBD ( $r_s = 2$ , $n_0 = 3$ ), $N = 35$ | SCD ( $r_s = 2$ , $n_0 = 1$ ), $N = 37$ |
|------------------|---|---|
| $D$              | 2, 2, 2, 2                              | 1, 1, 1, 1                              |
| $G$              | 2, 2, 2, 2                              | 1, 1, 1, 1                              |

PBD = Plackett-Burman composite design; SCD = small composite design;  $n_0$  = Number of center points;  $r_s$  = Number of star points;  $N$  = design size;  $r_0, r_1, r_2, r_3$  = rank across 839, 736, 525, 289 models with  $q \geq 0, q \geq 1, q \geq 2, q \geq 3$ .

**Table 12** Design criteria comparison ranking for  $k = 5$ ,  $N = 43$ .

| Design Criterion | CCD ( $n_0 = 1$ ) | BBD ( $n_0 = 3$ ) |
|------------------|-------------------|-------------------|
| $D$              | 1, 1, 1, 2        | 2, 2, 2, 1        |
| $G$              | 2, 2, 2, 2        | 1, 1, 1, 1        |
| $IV$             | 2, 2, 2, 2        | 1, 1, 1, 1        |

CCD = central composite design; BBD = Box-Behnken design;  $n_0$  = Number of center points;  $r_0, r_1, r_2, r_3$  = rank across 839, 736, 525, 289 models with  $q \geq 0, q \geq 1, q \geq 2, q \geq 3$  except for  $IV$  criterion.

## DISCUSSION

In the comparative study of response surface designs in a spherical region across a set of reduced models, some of the response surface designs for some reduced models have singular design matrices. Thus, the  $IV$  criterion cannot be computed for these response surface designs. Furthermore, both  $G$  and  $IV$  are optimality criteria based on the scaled prediction variance function. When the number of factors increases, both the number of reduced models and the dimensions of  $\mathbf{X}'\mathbf{X}$  increase. As a result, the computational time for the  $G$  and  $IV$  criteria increases substantially. Thus, for convenience and to save time, the comparison of any response surface designs may consider the  $G$  criterion instead of the  $IV$  criterion.

In the study, the comparison ranking was not the same when using different optimality criteria. Based on the three criteria:  $D$ ,  $G$  and  $IV$ ,  $D$  was able to assess the quality of estimation of the model parameters. Both  $G$  and  $IV$  were based on the scaled predictive variance. Thus, the advantage of the two criteria is in predicting a new observation at any location in the design space. When choosing an experimental design, one may think about which model is appropriate, and whether estimation of parameters or future prediction is most important.

In a previous study, Chomtee and Borkowski (2012) compared the seven 3-factor designs: CCDs, BBDs, SCDs, H310s, H311As, H311Bs, and USDs based on the three optimality criteria ( $D$ ,  $G$ , and  $IV$ ). It was found that based on the  $D$  criterion, the CCD was the superior design when  $n_0 = 1$ . However, based on the  $G$  and  $IV$  criteria, when  $n_0 = 1$ , the H311B and H310 were the superior designs, respectively. When  $n_0 = 3$  based on the  $D$  and  $G$  criteria, the CCD was the superior design. Based on the  $IV$  criterion, the H311A and H311B were the superior designs. Moreover, the eight 4-factor designs: CCDs, BBDs, SCDs, PBDs, H416As, H416Bs, H416Cs,

and USDs were also compared based on the  $D$ ,  $G$ , and  $IV$  criteria. For any number of center points, the four factor CCD and BBD are both rotatable designs and have identical efficiencies values. This is reflected in the identical rankings. Thus, the results indicated that when  $n_0 = 1$ , based on the  $D$  criterion, both CCD and BBD were the superior designs. However, the H416C was the superior design for the  $G$  criterion and the H416B was the superior design for the  $IV$  criterion. When  $n_0 = 3$ , the CCD and BBD were the superior designs for the  $D$  and  $G$  criteria. The H416B was the superior design for the  $IV$  criterion. Hence, it can be concluded that the CCDs were the superior designs based on the  $D$  criterion for  $k = 3, 4, 5$ ;  $n_0 = 1, 3$  over the full second order model and a set of reduced models except when  $q \geq 3$ . However, the results based on the  $G$  and  $IV$  criteria varied.

## CONCLUSION

To assist an experimenter to select a design, if several alternative designs are proposed, their optimality properties can be compared. Thus, the adequacy of a proposed experimental design can be assessed prior to running it. The results of comparison for central composite designs (CCDs), Box-Behnken designs (BBDs), small composite designs (SCDs), Plackett-Burman composite designs (PBDs) and uniform shell designs (USDs) when the center points are one and three over a set of reduced models in a spherical design region for  $k = 5$  based on  $D$ ,  $G$  and  $IV$  are summarized in Table 13. These results show that based on  $D$  and  $G$  criteria, for small ( $23 \leq N \leq 29$ ) and medium ( $35 \leq N \leq 37$ ) design sizes, the SCDs are recommended over the PBDs. For medium ( $31 \leq N \leq 35$ ) design sizes, the USDs are recommended over the PBDs as well. Based on  $D$ , for a large design size ( $N = 43$ ), the CCD ( $n_0 = 1$ ) is recommended over the BBD ( $n_0 = 3$ ). However, based on  $G$  and  $IV$  criteria, the BBD ( $n_0 = 1$ ) is recommended over the CCD ( $n_0 = 1$ ).



**Table 13** Summarized comparison of the response surface designs across a set of reduced models for  $k = 5$  and various numbers ( $N$ ) based on  $D$ ,  $G$  and  $IV$  criteria.

| $N$   | Choice of design  | Optimality criteria        |                            |                   |
|-------|---|----------------------------|----------------------------|-------------------|
|       |   | $D$                        | $G$                        | $IV$              |
| 23-29 | SCD ( $n_0 = 1, 3$ ),<br>PBD ( $n_0 = 1, 3$ )             | SCD ( $n_0 = 1, 3$ )       | SCD ( $n_0 = 1, 3$ )       | -                 |
| 31-35 | PBD ( $r_s = 2, n_0 = 1, 3$ ),<br>USD ( $n_0 = 1, 3$ )    | USD $n_0 = 1, 3$ )         | USD ( $n_0 = 1, 3$ )       | -                 |
| 35-37 | SCD ( $r_s = 2, n_0 = 1$ ),<br>PBD ( $r_s = 2, n_0 = 3$ ) | SCD ( $r_s = 2, n_0 = 1$ ) | SCD ( $r_s = 2, n_0 = 1$ ) | -                 |
| 43    | CCD ( $n_0 = 1$ ),<br>BBD ( $n_0 = 3$ )                   | CCD ( $n_0 = 1$ )          | BBD ( $n_0 = 3$ )          | BBD ( $n_0 = 3$ ) |

SCD = small composite design; PBD = Plackett-Burman composite design; USD = uniform shell design; CCD = central composite design; BBD = Box-Behnken design;  $n_0$  = Number of center points;  $r_s$  = Number of star points;  $N$  = design size.

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### LITERATURE CITED

- Chipman, H.A. 1996. Bayesian variable selection with related predictors. **The Canadian Journal of Statistics**. 24: 17–36.
- Chomtee, B. and J.J. Borkowski. 2012. Comparison of response designs in a spherical region. **Proceeding in International Conference on Mathematical, Computational, Statistical Sciences, Engineering**. Tokyo, Japan.

- Mathworks Inc. 2010. **Matlab Version 7.11**. Mathworks Inc. Natick, MA, USA.
- Myers, R.H., A.I. Khuri and W.H. Carter Jr. 1989. Response surface methodology: 1966-1988. **Technometrics** 31: 137-157.
- Myers, R.H., D.C. Montgomery and C.M. Anderson-Cook. 2009. **Response Surface Methodology Process and Product Optimization Using Designed Experiments**. (3rd ed.). Wiley. Hoboken, NJ, USA. 680 pp.