

Recent Developments on Partial Replications of Response Surface Central Composite Designs: A Review

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Abstract: In this study, we take an extensive study of the second-order response surface central composite designs (CCDs). The partial replication of the central composite designs (CCDs) and its related studies are especially in focus. Earlier studies pertaining to the partial replication of the different portions of the CCD are examined and the findings highlighted. Even the later studies, which focused more on the properties and distribution of the prediction variance of the replicated variations of the CCD throughout the design region using graphical methods, were also reviewed. Research findings have shown that the optimum performance of the replicated variations of the CCD depends on the axial distance, α , and design region, cuboidal or spherical. No particular replicated variation of the CCD is consistently optimum in both design regions and for all the available axial distances utilized in exploring the second-order response surfaces using the CCD. However, replicating the star portion, in most cases, improves the designs' performances. Areas for further research and extension of the concept of partial replication of the CCD were also highlighted.

Keywords: Design efficiency, Design region, Graph, Orthogonality, Prediction variance, Rotatability

1 Introduction

The works of [1] laid the foundation for response surface methodology (RSM). According to [2], RSM is a combination of experimental design, regression technique and optimization theory which utilizes Taylor series approximations to describe the relationship between the response(s) of interest and the independent factor(s). Therefore, it is known as a collection of mathematical and statistical techniques for empirical model building: see, for example, [3] and [4]. By careful design of experiments, the objective of RSM is to optimize the response (output variable) of interest which is being influenced by several independent variables (input variables). Here, an experiment is a series of runs (or tests) in which changes made in the input variables help to ascertain the changes and reasons for the changes in the output variables.

RSM has been evolving over the years since its inception and has been very useful in numerous industrial and scientific revolutions. [5] reviewed developments in RSM from the Biometric perspective. [6] reviewed the progress made in RSM and suggested areas for further advancement. [7] and [8] made the more recent updates on the advancements on RSM. Furthermore, RSM has been extended to evaluating mixture experiments and experiments involving noise factors: see, for example, [9], [10] and [11].

RSM is a sequential procedure where the form of the actual relationship between the response variable, y , and independent variable(s), x_i , is unknown but could be approximated using low-order polynomial. Most often, the approximating function is the first-order model,

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \varepsilon \quad (1)$$

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$$\begin{array}{rcccccccc}
 & & \text{cube portion} & & \text{star portion} & & \text{centre} & \\
 x_1 & \pm 1 & \pm 1 & \pm 1 & \pm 1 & \pm \alpha & \underline{0} & \underline{0} & \underline{0} \\
 \mathbf{X}' = x_2 & \pm 1 & \pm 1 & \pm 1 & \pm 1 & \underline{0} & \pm \alpha & \underline{0} & 0 \\
 x_3 & \pm 1 & \pm 1 & \pm 1 & \pm 1 & \underline{0} & \underline{0} & \pm \alpha & 0
 \end{array}$$

Figure 1: Design Matrix of the CCD for $k = 3$ Factors

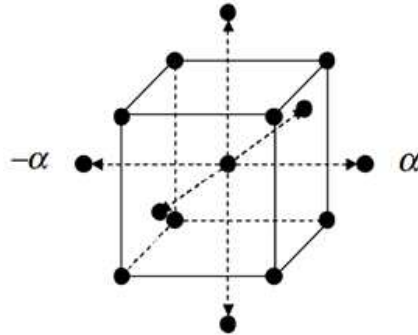


Figure 2: Geometric Structure of the CCD for $k = 3$ Factors

where β_0 and β_1 are the regression parameters, ε is the error and k is the number of experimental factors. If there is curvature, a higher degree polynomial, like the second-order model,

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_{ii}^2 + \sum_{i=1}^k \sum_{j>i}^k \beta_{ij} x_i x_j + \varepsilon, i = 1, 2, \dots, k; j > i \tag{2}$$

has to be used, where the symbols and notations take similar meanings as in equation (1). [8] gave three objectives for considering regression models in RSM and outlined steps to realizing these objectives.

Designs for fitting the second-order response surface models are called second-order response surface designs. These designs have desirable properties for a number of industrial experiments. However, a second-order response surface design is often chosen on the consideration of several criteria as identified by [12] and [13]. Among the numerous second-order response surface designs with their unique features, the central composite design is the most popular and useful in response surface exploration. The symmetry and flexibility offered by the structure of the design give substantial advantage in prediction capabilities and parameter estimation. The CCD exists for spherical and cuboidal regions and for $k \geq 2$, where k , a positive integer, is the number of factors.

According to [14], the structure of the CCD has three components: the factorial (cube) portion of at least resolution V , the star (axial) portion at distance, α , from the centre of the design along each axis, and the centre point located at the centre of the design space. A resolution V design is a design in which two-factor interactions are aliased with three-factor interactions but no main effect or two-factor interaction is aliased with another main effect or two-factor interaction. That is, main effects and the two-factor interactions do not have other main effects and two-factor interactions as their aliases. Hence, for a resolution V design, the shortest word in the defining relation must have five letters. The cube or factorial portion has full ($q = 0$) or fractional ($q > 0$) factorial number of runs, where q is an integer. The star portion has $2k$ number of runs augmented with n_0 centre points. Hence, the CCD uses a total of $N = f + 2k + n_0$ number of runs to estimate the $p = (k + 1)(k + 2)/2$ number of model parameters. The cube (factorial) portion has coordinates of the form, $(x_1, x_2, \dots, x_n) = (\pm 1, \pm 1, \dots, \pm 1)$; the star portion has coordinates of the form, $(\pm \alpha, 0, 0, \dots, 0), \dots, (0, 0, \dots, \pm \alpha)$ while the centre point is of the form, $(0, 0, \dots, 0)$. The design matrix and geometric structure of the CCD for $k = 3$ with $n_0 = 1$ are shown in Figures 1 and 2, respectively, with the vector, $\underline{0} = (0, 0, 0)$: see [15] and [4].

The three components of the CCD play important but different roles in parameter estimation. The resolution V full or fractional factorial component (the cube) contributes substantially to the estimation of the k linear terms and the $\frac{k(k-1)}{2}$ two-factor interaction terms. Only the factorial point contributes to the estimation of the interaction terms. The star points contribute to the estimation of the k quadratic terms. Without the star points, only the sum of the quadratic terms can be estimated. The star points do not contribute to the estimation of the interaction terms. The centre points contribute

towards the estimation of pure error and estimation of quadratic terms.

2 Evaluation of the Central Composite Design

Numerical and graphical methods of evaluating the CCD and other response surface designs exist. When fitting second-order models, optimal design methods include single-value criteria to construct designs for RSM. We focus on some of the criteria that use the variance characteristics of the design, the A - and D -efficiency criteria. The D -efficiency is a useful tool for quantifying the quality of the estimated model parameters and is defined as $D_{eff} = \{|\mathbf{X}'\mathbf{X}|^{1/p}/N\}100$. The power, $1/p$, takes account of the p parameter estimates being assessed when the determinant of the information matrix is being computed, N is the total number of design runs and \mathbf{X} is the design matrix extended to model form from which the information matrix, $M = \mathbf{X}'\mathbf{X}$, is obtained. The A -efficiency is given by $A_{eff} = 100p/\text{trace}[N(\mathbf{X}'\mathbf{X})^{-1}]$, and is directly related to minimizing the individual variances of the model parameters. According to [16] and [17], A - and D -efficiency measures represent the percentage number of runs required by a particular orthogonal design to achieve the same determinant and trace. While A -efficiency deals with the individual variances of the model parameters, D -efficiency considers the variances and covariances of the regression parameters. Furthermore, we also consider G -efficiency and V -criterion, which depend on the scaled prediction variance of the design. The scaled prediction variance is given by

$$SPV = Nf'(\mathbf{x})\mathbf{M}_{\xi}^{-1}f(\mathbf{x}) \quad (3)$$

where $\mathbf{M}_{\xi}^{-1}=(\mathbf{X}'\mathbf{X})^{-1}$ is the inverse of the information matrix of the design, ξ , whose design matrix is \mathbf{X} and $f'(\mathbf{x}) = (1, x_1, x_2, \dots, x_k; x_1^2, \dots, x_k^2; x_1x_2, \dots, x_{k-1}x_k)$ is the vector of design points in the design space expanded to model form by classifying the coordinates of the design points into linear, quadratic and mixed (interaction) components of the model. Therefore, the G -efficiency is given by $G_{eff} = 100p/[Nf'(\mathbf{x})\mathbf{M}_{\xi}^{-1}f(\mathbf{x})]$ while the V -criterion is given by $V = N[\text{trace}S(\mathbf{X}'\mathbf{X})^{-1}]$, where S is the matrix of region moments. The V -criterion minimizes the average of the scaled prediction variance. The values of A -, D - and G -efficiencies are in the interval, $[0, 1]$. However, for easy assessment and comparison, these values are converted to percentages by multiplying by 100. N is used to scale the results based on the overall size of the design. The higher the efficiency values, the better for A -, D - and G -efficiencies while the smaller the value, the better for the V -criterion.

When the practitioner is interested in understanding the prediction variance distribution, that is, to know if the prediction variance is stable throughout the entire design region or where in the region has the best and worst prediction variance, graphical methods offer the best approach for exploring the prediction properties of competing designs. As rightly pointed out by [13], single-value criteria, like the four alphabetic criteria considered here, do not effectively reflect the prediction capabilities of a design. Hence, graphical approach is necessary to obtain the complete prediction characteristics of the CCD throughout the entire design region. The two graphical approaches adopted here are the variance dispersion graphs (VDGs) by [18] and fraction of design space graphs (FDSGs) by [19].

3 Historical Review of Partial Replications of the CCD

Traditionally, it is only the centre point that is replicated n_0 times for the purpose of the estimation of pure error, test of model lack-of-fit and other tests of hypotheses with $n_0 - 1$ degrees-of-freedom: see, for example, [20]. However, there is increasing concern about replicating only at the centre of the design, as this may not give complete knowledge of the prediction capability of a design since there is no clear information on how the design will perform if there are replications at the cube and/or star points. Figure 3 shows the three different structures of a three-factor CCD with each component replicated twice.

The history of partial replication of the CCD dates back to [21] who argued that replicating only at the centre could be misleading since there is no assurance that the experimental error will be constant throughout the entire design region. He pointed out that variability might increase away from the centre of the design such that the estimate of the experimental error may be too small for proper evaluation of the coefficients of the second-order models, and therefore, it is a sound experimental strategy to obtain replicates over the experimental region in order to estimate error and provide reliable estimates of the experimental effects. In his work also, the cube and star portions of the CCD were examined through partial replication and suggestions made on possible advantages of replicating these portions of the design in the spherical region. Furthermore, he considered the cases of partially replicated orthogonally-blocked CCD and, from his analysis, concluded that replication of the star portion of the orthogonally-blocked CCD has better potential than replicating the

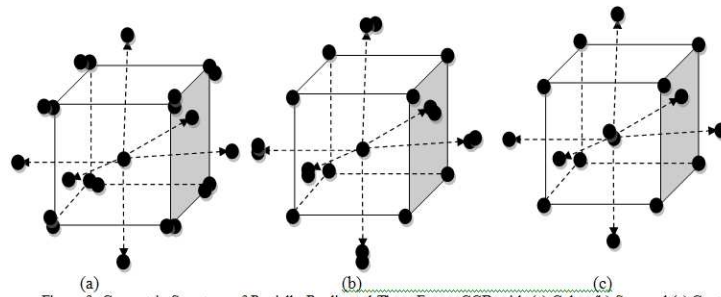


Figure 3: Geometric Structure of Partially Replicated Three-Factor CCD with (a) Cube, (b) Star and (c) Centre Point Replicated Twice

cube. For a CCD with the star portion replicated twice, [21] proposes the axial distance that ensures orthogonal blocking as

$$\alpha = \left\{ \frac{f(N - f - n_f)}{4(f + n_f)} \right\}^{1/2} \quad (4)$$

where $N = f + 4k + n_f + n_a$.

[20] examined the appropriate number of centre points that offers minimum prediction variance for central composite and Box-Behnken designs. Experimenters usually resort to various 'rules of thumb' for choosing number of replications of the centre point for design selection and test of model lack-of-fit. One of the 'rules of thumb', as pointed out in [20], is selecting enough centre points to create enough degrees-of-freedom for model lack-of-fit in the F-test. Another 'rule of thumb', still in [20], is to have at least two centre points and sufficient replications from other portions of the designs to obtain at least three degrees-of-freedom for pure error. Instead of resorting to the rule of thumb, he introduced the integrated variance criterion for determining the number of centre points suitable for using the CCD in response surface exploration. To achieve this, he considered three partially replicated options of the CCD, namely: (i) one cube plus two stars, (ii) one cube plus one star, and (iii) two cubes plus one star, for $k = 5, 6, 7$ and 8 factors. The designs are evaluated by varying the number of centre points to know the design option that minimizes the integrated variance function. Contrary to initial recommendations that more number of centre points is needed for evaluating these designs, the results show that fewer centre points are generally more appropriate.

[22] developed analytical procedure for plotting the VDGs and this procedure accommodates the replication of the star portion only. Secondly, he demonstrated the impact of replicating the star portion by plotting the VDGs for $k = 5$ and 6 factors where he used two star points ($4k$) for evaluation of the CCD in spherical region with axial distance, $\alpha = \sqrt{k}$. He concluded that replicating the star portion improves the spherical prediction variance characteristics of the CCD.

[17] evaluated the effects of replicating the cube, star and centre points of the CCD on the A -, D - and G -efficiencies and the V -criterion for the reduced models in the hypercube. The reduced model here implies the nature of the second-order model when either the quadratic term, x_i^2 , or the linear term, x_i , or the interaction term, $x_i x_j$, is removed from the model. The study considered seven versions of partially replicated CCD for the comparison. They are: $(0, 1, 1)$; $(2, 1, 1)$; $(4, 1, 1)$; $(0, 2, 1)$; $(2, 2, 1)$; $(0, 1, 2)$ and $(2, 1, 2)$, each being the realization values for (n_0, n_s, n_c) , where n_0 is the number of centre points, n_s is the number of star point replication and n_c is the number of cube replication, respectively. The points of zero values for the centre point represent the cases of missing values. [17] concluded that for the reduced models for the CCD, the partial replication of the CCD influences the optimality criteria in different ways. What improves one criterion may be detrimental to the other criterion and therefore, the decision rests with the experimenter based on professional experience and preferences.

4 Recent Developments in Evaluation of Partially Replicated CCD

In this section, we consider developments in the area of partial replication of the CCD in the last five years or thereabout. Earlier works did not pay much attention to the prediction variance properties of the partially replicated CCD options. The prediction variance performance of a design determines how well the design could predict responses with precision. Designs with smaller prediction variances predict responses with higher precision than designs with large prediction variances. [23] replicated the cube and star portions of the CCD for $k = 2, 3, 4$ and 5 factors to evaluate the performances of the CCD with respect to the rotatability and orthogonality properties of the designs. The pattern of replication by [20] was adopted and extended for the study. They utilized the D -optimality as the basis for comparison of the variations

of the partially replicated CCD. From their results, it was concluded that replicating the cube offer better D -optimality than replicating the star for both the rotatable and orthogonal CCDs. While the case of rotatable CCD may be true, the same may not be said of the orthogonal CCD due to the fact that the values of the axial distances used for the orthogonal CCD for which the function, $\alpha = \{[(2^k n_c)^{1/2} - 2^k n_c]/2n_s\}^{1/2}$, for partially replicated orthogonal CCD was derived is consistent with an earlier general expression for the orthogonal α for partial replications given by [24] as $\alpha = \{[N^{1/2} - (2^k n_c)^{1/2}]/4n_s^2\}^{1/4}$.

Usually, when the cube and star points are replicated the same number of times, the cube-replicated CCD will have more runs than the star-replicated CCD. However, in their study, [23] made cube- and star-replicated CCDs which are replicated equal number of times to have the same number of runs by augmenting the star-replicated option with excess number of centre points. This also influenced the outcome of their study. For instance, for the five-factor CCD, one of the replicated options, four cubes plus one star augmented with three centre points has a total of 141 design runs. The corresponding star-replicated option, four stars plus one cube, also has 141 runs. Normally, and based on the literature, the star-replicated option should have a total of 75 runs when equally augmented with the same three centre points. To achieve 141 runs for this design option, excess of 66 centre points were added. Put in another way, the centre point was replicated sixty-six times. The implications are obvious. First, the smaller number of design runs, which should be an advantage for the star-replicated CCDs, is not reflected. Secondly, the D -optimality values for the star-replicated design options are also expected to be affected since N , as earlier explained, is somewhat over-bloated.

The use of graphical methods to assist in evaluating the replicated design prediction potential has not received much attention in the previous works discussed so far. However, the importance of graphical techniques like the variance dispersion graphs and fraction of design space graphs earlier mentioned need not be over emphasized. Subsequent works presented here made consistent effort to utilize one or two of the graphical methods along with the alphabetic criteria to evaluate partially replicated CCD options. This gives a more general understanding of the design potentials than relying only on the alphabetic criteria, which as earlier pointed out do not reflect the overall performance of the design throughout the design region.

[25] considered variations of partially replicated central composite designs in the hypercube. The hypercube is a multi-dimensional cuboidal region with axial distance, $\alpha = 1$. They extended the [20] form of replication of the CCD. Hence the designs considered are (i) two cubes plus one star (C_2S_1); (ii) one cube plus two stars (C_1S_2); (iii) three cubes plus one star (C_3S_1); (iv) one cube plus three stars (C_1S_3); (v) four cubes plus one star (C_4S_1); and (vi) one cube plus four stars (C_1S_4). The prediction capabilities of the design options with respect to their prediction variances are evaluated using the G - and I -optimality criteria as single-value optimality criteria. The fraction of design space graphs are used to evaluate and compare the prediction variance performance of the replicated design options on a common scale and on a two-dimensional space. The performances of the design options are observed for $n_0 = 2$ and 3 centre points. The replication of the star point is recommended since the replicated-star options always give smaller G - and I -optimal values than the corresponding replicated-cube options with equal number of replications. The FDSGs show that star-replicated CCD options have more stable spread of small-scaled prediction variances throughout the entire design region, with the (C_1S_2) option being the best. The FDSGs for $k = 4$ and 5 factors are displayed in Figures 4 and 5.

There is increasing argument and consideration for the use of unscaled (standardized) prediction variance (UPV) in design evaluation when graphical methods are used while viewing the prediction variance performance of a given design throughout the design region. This argument is based on the fact that scaling the prediction variance which entails multiplying the prediction variance by N , the sample size or runs of the design, gives smaller designs undue advantage over larger designs. Smaller and larger designs here imply designs with smaller and larger sample sizes, respectively. According to [19] and [14], scaling penalizes larger designs over smaller ones. The rationale for scaling the prediction variance is to account for the cost of the design, represented by N , in comparing designs of various sizes. However, there is increasing awareness for the use of the UPV in design evaluation. [26] and [27] argue that larger designs often lead to smaller prediction variances and provide the experimenter with more useful information than scaling the prediction variance. Subsequent discussions will feature the unscaled prediction variance (UPV) among the veritable tools for the evaluation and comparison of the replicated design options.

[28] revisited the partially replicated CCD options in the hypercube for $k = 3$ to 6 experimental factors. In this case, graphical methods alone, VDG and FDSG, are used in the evaluation of the designs. The VDGs of the replicated design options are plotted for the scaled prediction variances (SPV) on a common scale while the FDSGs of the designs are plotted for the UPV but not on a common scale. The importance of this is to be able to ascertain the merit or lack of it of considering the UPV in design evaluation throughout the entire design region. The replicated options are considered for $n_0 = 1, 2$ and 3 centre points. This helped in monitoring the performances of the designs in the cuboidal region as the number of centre points increases from 1 to 3. The VDGs and FDSGs for $k = 6$ factors, and 3 centre points are displayed in Figures 6 and 7.

In general, the results have shown that the replicated-star designs displayed stability and no dispersion within the unit cube considering the VDG and smaller unscaled prediction variances for the FDSG. Therefore, the replicated-star options

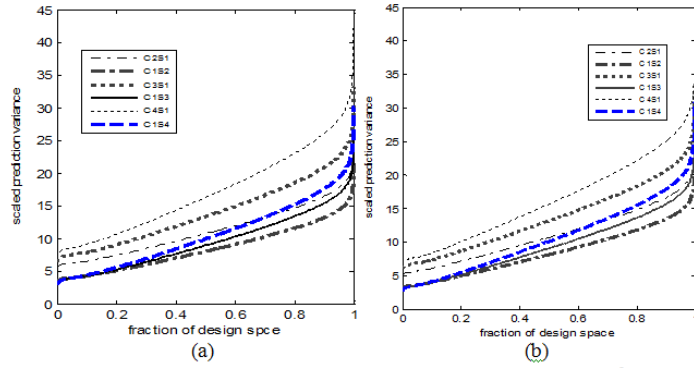


Figure 4: Fraction of Design Space Graphs for (a) $n_0 = 2$ and (b) $n_0 = 3$, $k = 4$ factors

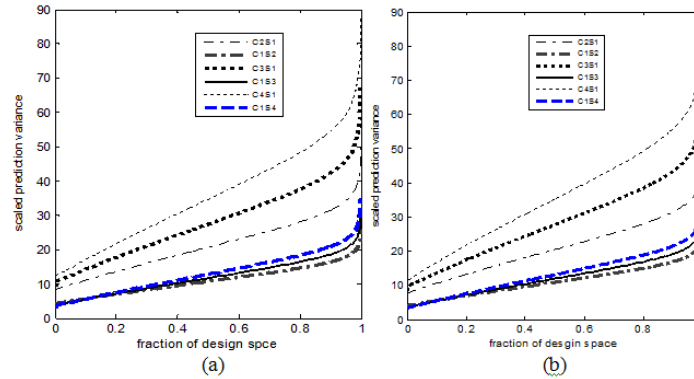


Figure 5: Fraction of Design Space Graphs for (a) $n_0 = 2$ and (b) $n_0 = 3$, $k = 5$ factors

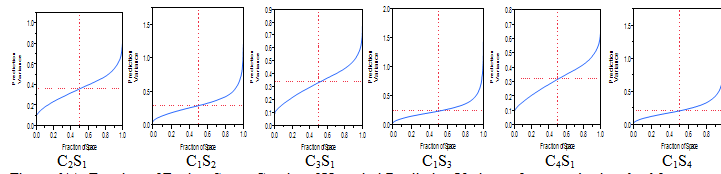


Figure 6(a): Fraction of Design Space Graphs of Unscaled Prediction Variance for $n_0 = 1$ when $k = 6$ factors

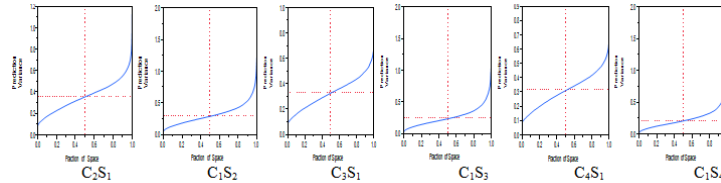


Figure 6(b): Fraction of Design Space Graphs of Unscaled Prediction Variance for $n_0 = 3$ when $k = 6$ factors

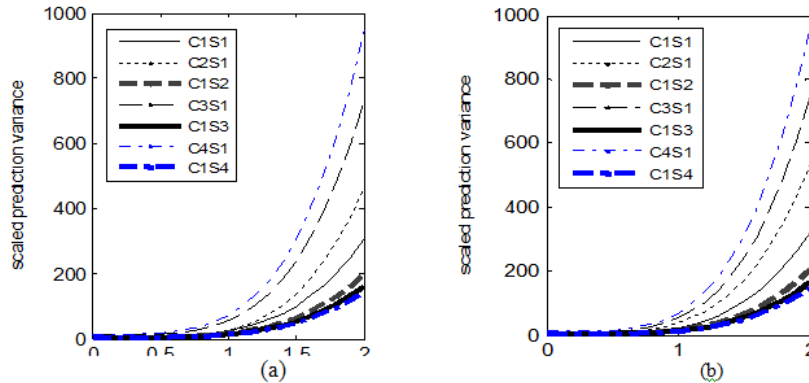


Figure 7: VDG of Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$ when $k = 6$ Factors

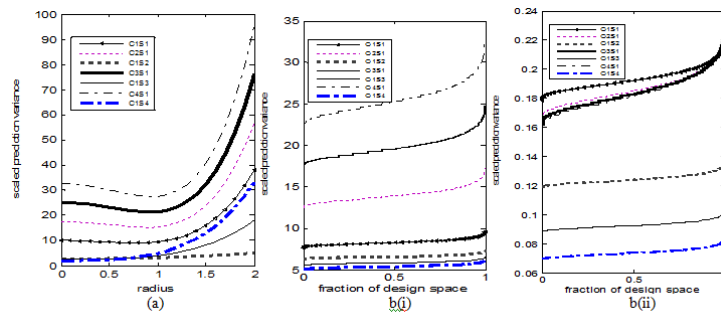


Figure 8: (a) VDGs and (b) FDS plots for (i) SPV and (ii) UPV for the replicated CCD, $k=5, n_0 = 3$

have higher prediction potentials in the hypercube. Also, the replicated-cube options showed some dispersion around the centre of the design region for the VDG and higher unscaled prediction variance for the FDSG which deteriorates rapidly away from the centre of the design region. However, the deterioration worsens as the replication of the cube portion increases. Moreover, the replicated-star designs have smaller number of runs than the replicated-cube designs which are replicated the same number of times. This makes the replicated-star designs more economically feasible than the replicated-cube designs.

Orthogonality is a very important geometric property of the CCD. The CCD is made orthogonal by the choice of axial distance, α . The orthogonality property of the CCD enables for uncorrelated estimates of the response model coefficients as well as minimizes the variances of the coefficients. The axial distance, α , for an orthogonal CCD is given by $\alpha = \{[(Nf)^{1/2} - f]/2\}^{1/2}$: see, for example, [29]. [24] showed that for an orthogonal CCD with the cube or star point replicated, the axial distance is given by

$$\alpha = \left\{ \frac{2^{k-q}n_c[N^{1/2} - (2^{k-q}n_c)^{1/2}]^2}{4n_s^2} \right\}^{1/4}, \tag{5}$$

where the symbols and notations of the alpha equations take their usual meanings highlighted earlier in this work.

[30] conducted extensive study on the prediction capabilities of partially replicated orthogonal central composite design. The D - and G -efficiencies are used to evaluate the performances of the designs for 3 to 6 factors in the spherical region while the VDG and FDSG are the graphical methods used to display the design prediction variances throughout the entire design region. Only the scaled prediction variance (SPV) was considered for the VDG while both SPV and UPV were considered for the FDSG. Furthermore, they evaluated the designs while assessing their performances as the number of centre points increases from 1 to 3. The six partially replicated design options of [25] are compared with the classical (unreplicated) CCD, one cube plus one star (C_1S_1). The VDG and FDSG show that for both the scaled and unscaled prediction variances, the replicated-star options display smaller and stable prediction variances than the replicate-cube options and the classical (unreplicated) CCD. The graphs for $k = 5$ with 3 centre points are displayed in Figure 8.

Rotatability is another important property of the CCD introduced by [31]. Rotatability is a reasonable basis for the selection of a response surface design in response surface optimization and it is wise to choose a design that provides equal precision of estimation in all directions. A design which variance, $V\{\hat{y}(\mathbf{x})\}$, of the predicted response, $\hat{y}(\mathbf{x})$, is constant at any given point, \mathbf{x} , in the design space such that equal information is obtained in all directions at equal distance from the centre of the design space is said to be rotatable. This means that for a rotatable design, $V\{\hat{y}(\mathbf{x})\}$ is the same at all points, \mathbf{x} , that are of the same distance from the centre of the design region. The CCD is made rotatable by the choice of α , the axial distance. This property is achieved by setting the star point at distance, $\alpha = (f)^{1/4}$, f being the factorial (cube) portion of the CCD. [32], [33], [34] and [4] offer further discussions on rotatability and measures of rotatability. If the cube is replicated n_c times and the star, n_s times, then, $\alpha = \{(n_c f)/n_s\}^{1/4}$ yields a rotatable CCD, where $f = 2^{k-q}$ is the number of factorial points in the design: see [24].

[35] discussed the prediction variance properties of rotatable partially replicated CCD in the spherical region for $k = 3$ to 10 factors. Full factorial portion of the CCD was used for $k = 3, 4$ and 5 factors. With the number of factors moderately increasing, one-half fraction of the factorial portion is considered for $k = 6$ and 7 factors while one-quarter fraction is considered for $k = 8, 9$ and 10 factors. Each design option is augmented with $n_0 = 3$ centre points. The D - and G -efficiencies as well as the V -criterion are used for the design evaluation while the FDSG is the graphical method considered in displaying the prediction variances of these designs in the design region. The choice of plotting the SPV or UPV is very important since comparisons are being made among designs of various sizes. If the experimenter is interested in obtaining efficient designs while considering the cost of adding an extra run to increase precision of prediction by the reduction of the prediction variance, plotting the SPV is preferable. In this case, C_1S_4 is recommended for $k = 3, 4, 5, 6,$

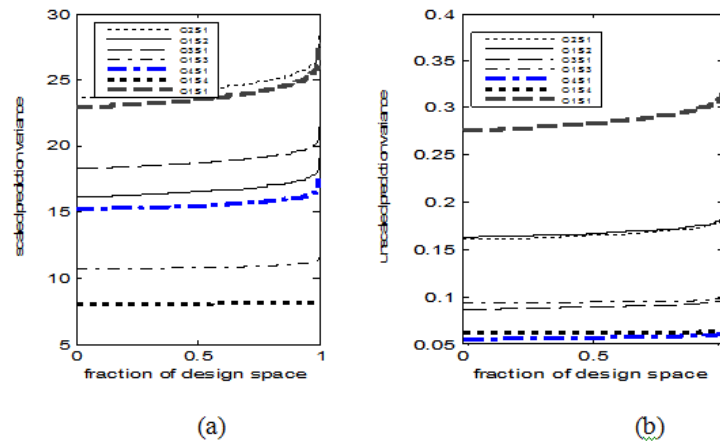


Figure 9: (a) SPV and (b) UPV for Eight-Factor Rotatable CCD

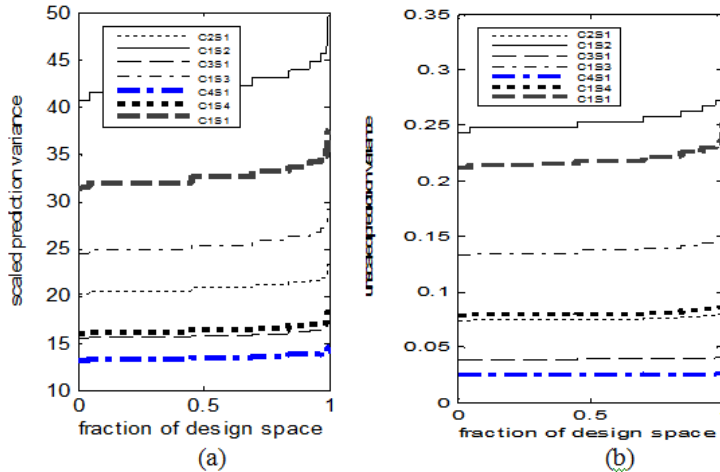


Figure 10: (a) SPV and (b) UPV for Nine-Factor Rotatable CCD

	Block 1							Block 2									
	cube							star									
	n_f							n_a									
x_1	1	1	1	1	-1	-1	-1	-1	0	α	$-\alpha$	0	0	0	0	0	0
x_2	1	1	-1	-1	1	1	-1	-1	0	0	0	α	$-\alpha$	0	0	0	0
x_3	1	-1	1	-1	1	-1	1	-1	0	0	0	0	0	α	$-\alpha$	0	0

Figure 11: Orthogonally Blocked Three-Factor CCD in Two Blocks with One Centre Point in each Block where the Factorial runs are in Block 1 and the Axial runs are in Block 2

7 and 8 factors for the rotatable CCD while C_4S_1 is recommended for $k = 9$ and 10 factors. Plotting the UPV is a better alternative if the experimenter is not restricted by cost but desires a design with high precision for prediction irrespective of the design's sample size. The various plots show that larger design runs yield smaller prediction variance since C_4S_1 and C_1S_4 , the higher replicated-cube and star-options with high number of runs, respectively, continuously yield small prediction variances. The graphs for $k = 8$ and 9 are displayed in Figures 9 and 10, respectively.

One of the cardinal advantages of the CCD is its amenability to be arranged in orthogonal blocks. The second-order response surface model with blocking effects is given by

$$Y_u = \beta_0 + \sum_{i=1}^k \beta_i x_{ui} + \sum_{i=1}^k \beta_{ii} x_{ui}^2 + \sum_{i < j} \beta_{ij} x_{ui} x_{uj} + \sum_{l=1}^b \delta_l (z_{ul} - \bar{z}_l) + \epsilon_u; u = 1, 2, \dots, N \tag{6}$$

where Y_u is the observed response values at the u^{th} experimental run, x_{ui} is the corresponding setting of the i^{th} input variable, x_{uj} is the corresponding setting of the j^{th} input variable, $i \neq j$, z_{ul} is the dummy variable with value one if the u^{th} observation is in l^{th} block and zero otherwise; δ_l is the l^{th} block effect, $\bar{z}_l = \frac{1}{N} \sum_u z_{ul}$ is the fraction of the total runs in

l^{th} block, $\beta_0, \beta_i, \beta_{ii}, \beta_{ij}$ are, respectively, the constant, first-order (linear), second-order (quadratic) and interaction model parameters and ε_u is random error. The block effects are orthogonal to the model parameters if $\sum_{u=1}^N x_{ui}(z_{ul} - \bar{z}_l) = 0$, $\sum_{u=1}^N x_{ui}x_{uj}(z_{ul} - \bar{z}_l) = 0$, for $i \neq j$ and $\sum_{u=1}^N x_{ui}^2(z_{ul} - \bar{z}_l) = 0$.

Orthogonal blocking of the central composite design (CCD) is possible due to the flexibility involved in the choice of the axial distance, α , and the number of centre points, n_0 . The orthogonal blocking of the CCD is such that the star portion forms a block while the cube (factorial portion) can be in one or more blocks depending on the number of factors, k . That is, the cube can be sub-divided into more than one block but the axial block can never be sub-divided. An illustration using a three-factor CCD arranged in two blocks with one centre point in each block is given in Figure 11. The number of centre points in the factorial block is n_f while n_a is the number of centre points in the axial block.

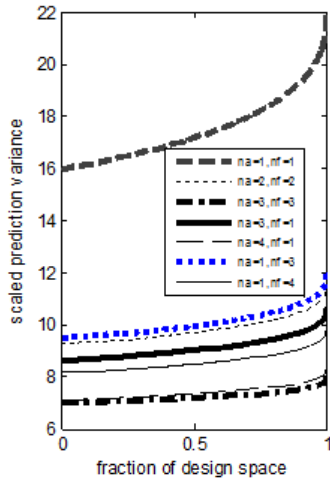


Figure 12: FDS plots for Five-Factor Orthogonally Blocked CCD in Two Blocks

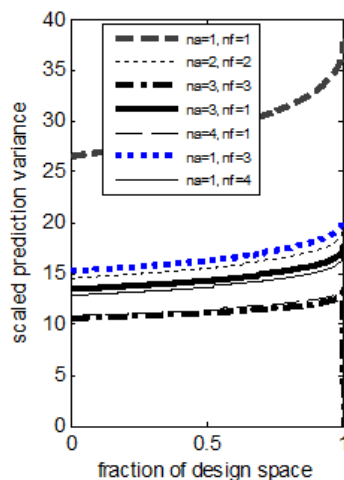


Figure 13: FDS plots for Five-Factor CCD in Two Blocks Involving Two Cubes Plus One Star

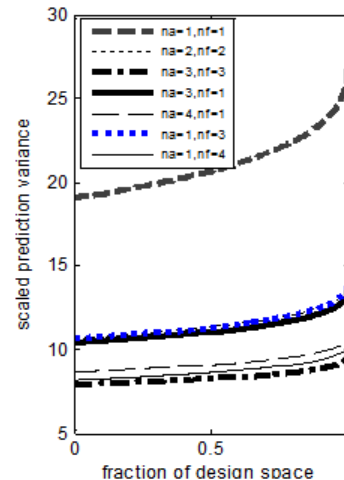


Figure 14: FDS plots for Five-Factor CCD in Two Blocks involving Two Stars Plus One Cube

For the orthogonally-blocked CCD, the block effects do not affect the estimates of the parameters of the response surface model: see, for example, [36]. [4] suggested that the number of centre points should be distributed equally among the blocks. The size of the experiment, N , changes as portions of the CCD is replicated. Replicating the centre, the cube or the star points increases N . [27] suggested that it is always a good idea for an experimenter designing an experiment to evaluate designs of different sizes.

Orthogonally-blocked CCD with partial replications of the cube and star components of the design are evaluated by [37]. In this study, they considered the central composite design with the cube being at least one block and n_a and n_f are not strictly distributed equally among the blocks. The values of n_a and n_f are varied in this study and their effects on the performances of the A -, D - and G -efficiencies and V -criterion are evaluated. Comparison of these design criteria when the cube and star portions of the CCD are partially replicated is the focus of the study. Graphical comparisons of the designs are made using FDSG to understand the prediction variance characteristics of these orthogonally-blocked and partially replicated design options. They deduced that the axial distance that ensures orthogonal blocking when the cube is replicated n_c times, and the star, n_s times, with the centre point, n_0 , augmentation is $\alpha = \left\{ \frac{F(N-F-n_f)}{2n_s(F+n_f)} \right\}^{1/2}$, where $N = F + 2n_s k + n_f + n_a$ and $F = n_c f$.

Also, from [37], it could be observed that the Partial replication of the CCD affects the location of the star points and the performances of the A -, D -, G -efficiencies and V -criterion. Replicating the cube portion increases α , thereby moving the star-points away from the centre of the design region, while replicating the star-portion reduces, α , thereby bringing the star points closer to the centre of the design region. Graphical evaluations of the designs show that increasing the centre points equally in the blocks or increasing the centre points in the star blocks more than the cube blocks consistently give stable distribution of small scaled prediction variance throughout the entire design region. Also, replicating the star while increasing n_f more than n_a , improves the designs prediction capability. The designs have better precision throughout the entire design region for predicting responses in spherical region when the star is replicated than when the cube is replicated. In general, replicating the centre points more in the star-blocks than the cube blocks enhances the prediction capabilities of orthogonally-blocked central composite designs. Typical FDSGs for $k = 5$ are presented in Figures 12, 13 and 14.

The spherical property of the CCD is achieved by setting $\alpha = \sqrt{k}$ which is called the spherical α . This puts all the factorial and star points on the surface of a sphere of radius, \sqrt{k} : see, for example, [22] and [4]. The spherical and rotatable alpha values have some significant drawbacks as the number of factors gets higher: the α values get larger and may attain

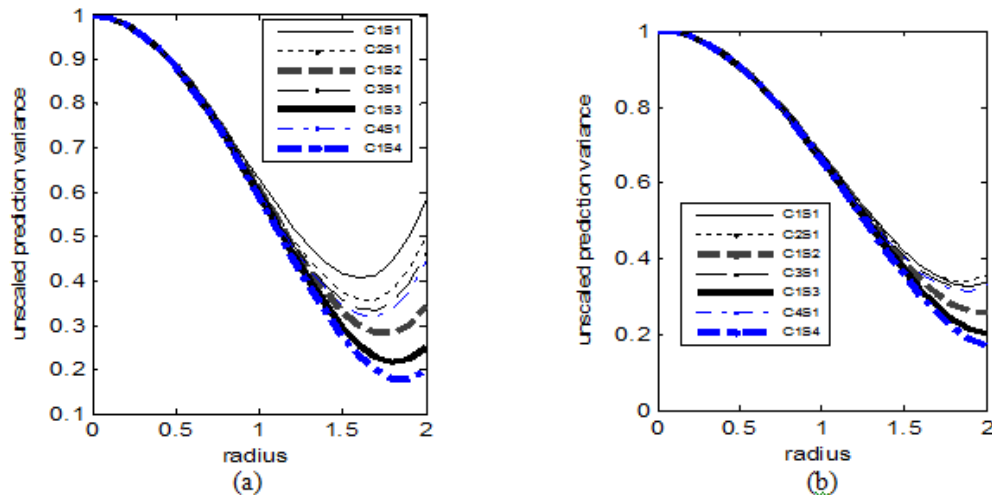


Figure 15: VDG of Unscaled Prediction Variance for (a) $k = 4$ and (b) $k = 5$ factors

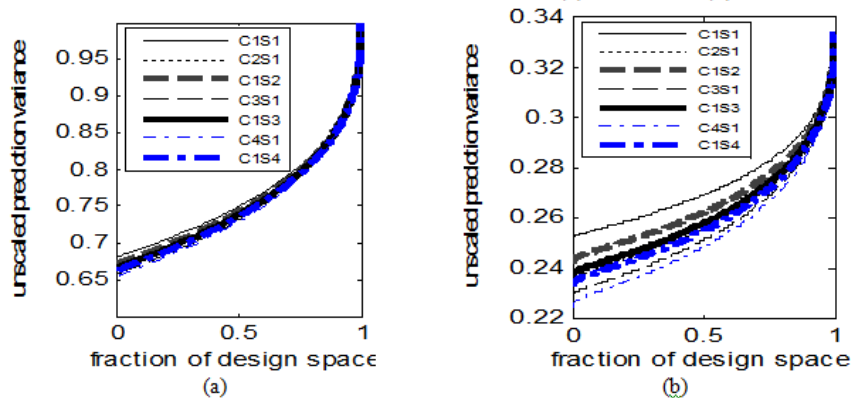


Figure 16: FDSG of Unscaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$ for $k = 5$ factors

an impractical level for the factors of interest. These values may also not be feasible in many experiments. For both the VDG and FDSG, the unscaled prediction variance is not recommended as metric for design evaluation and comparison for the spherical CCD because of the apparent instability in the spread of the prediction variances for the spherical CCD. The spherical CCDs display very high and unstable unscaled prediction variances which tend to converge at the extreme points. Additional centre points do not significantly improve the instability of the unscaled prediction variance. Illustrations are given in Figures 15 and 16 for $k = 4$ and 5 factors, respectively, with one and three centre point.

As earlier pointed out, as k increase, the spherical α attains impractical level that may be infeasible to apply in industrial experiments. For this reason, [38] proposed the practical alpha, $\alpha = k^{1/4}$, which is a compromise between the spherical α and the cuboidal alpha, $\alpha = 1$. The practical alpha has acceptable variance inflation factor (VIF) and provides design points that are less extreme as the number of factors increases. [39] considered the partially replicated options of the CCD when the axial distance, is $\alpha = k^{1/4}$ for $k = 3$ to 6 factors. The four alphabetic criteria, the A -, D - and G -efficiencies and V -criterion as well as the graphical methods, VDG and FDSG are used in the evaluation of the various replicated options of the practical CCD.

This study by [39] was performed for the spherical region. The results obtained show that replicating the cube is beneficial only up to C_3S_1 as the replications improve the performances of the alphabetic criteria. Beyond this, further replication causes the performances of the alphabetic criteria to begin to deteriorate. For $k = 5$, the more the star is replicated, the better the value of the V -criterion while the star-replicated CCD, C_1S_2 , gives the best value for A with or without additional centre points except for $k = 3$. Finally, the replication of the star ensures uniform distribution of the unscaled and scaled prediction variances throughout the entire design space for both the variance dispersion graphs and fraction of design space graphs and for all the number of factors considered.

[17] proposed exact functions for the four alphabetic criteria, A -, D - and G -efficiencies and the V -criterion for evaluation of the classical CCD. However, these exact functions do not accommodate the replications of the components

of the CCD. Hence, there is need to obtain exact functions that are robust to the replication of the cube and/or star portions of the CCD. [35], through matrix algebra and calculus, developed exact G -efficiency and V -criterion for $k > 1$ which are robust to the replication of the components of the CCD. They show that for the cube points, f , having multiplicity, n_c the star points, $2k$, having multiplicity n_s and with n_0 centre points; the subscripts, c , s and 0 representing cube, star and zero, respectively and $k > 1$, the exact G -efficiency is

$$G_{eff} = \frac{100 \times p}{N \max\{\mathbf{B}_0 + \mathbf{B}_1 \sum_{i=1}^k x_i^2 + \mathbf{B}_2 \sum_{i=1}^k x_i^4 + \mathbf{B}_3 \sum_{i < j}^{k(k-1)/2} x_i^2 x_j^2\}}, \tag{7}$$

where $\mathbf{B}_0 = \mathbf{A}_1$, $\mathbf{A}_1 = \frac{kF + 2n_s\alpha^4}{Q}$, $\mathbf{B}_1 = [\frac{1}{F + 2n_s\alpha^2} - \frac{2(F + 2n_s\alpha^2)}{Q}]$, $\mathbf{B}_2 = \frac{1}{2n_s\alpha^4 Q} [2n_s N\alpha^4 + (k + 1)\rho]$ and $\mathbf{B}_3 = [\frac{1}{F} - \frac{\rho}{n_s\alpha^4 Q}]$.

Furthermore, the V -criterion was obtained as

$$N[\frac{kF + 2n_s\alpha^4}{Q} - \frac{2k(F + 2n_s\alpha^2)}{3Q} + \frac{k}{s(F + 2n_s\alpha^2)} + \frac{k[9(2Nn_s\alpha^4) + 4(k - 1)\rho]}{45(2n_s\alpha^4 Q)} + \frac{k(k - 1)}{18F}] \tag{8}$$

which is the trace of the product of the matrix of region moments and the inverse of the information matrix. From the functions, $Q = 2Nn_s\alpha^4 + k\rho$ and $\rho = NF - (F + 2n_s\alpha^2)^2$.

The exact A - and D -efficiencies for the partially replicated CCD are also proposed by [40]. They show that for the CCD with the cube and/or star portions replicated, the A -efficiency is given by

$$A_{eff} = \frac{100 \times p}{N\{\mathbf{A}_1 + \frac{k}{F + 2n_s\alpha^2} + \frac{k[2n_s N\alpha^4 (k - 1)\rho]}{2n_s\alpha^4 Q} + \frac{k(k - 1)}{2F}\}} \tag{9}$$

For the exact D -efficiency, they obtained

$$D_{eff} = \frac{1}{N} \{(2n_s\alpha^4 Q)^{k-1} Q(F + 2n_s\alpha^2)^k F^{k(k-1)/2}\}^{1/p} \tag{10}$$

Some numerical results for the exact design criteria presented above for the partially replicated CCD are shown in Table 1 for three- to six-factor experiments involving the CCD in spherical region. The results are presented for the spherical axial distance of the CCD when $\alpha = \sqrt{k}$, otherwise called the spherical CCD. The results are displayed for $n_0 = 1$ and 3 to reflect the performance of the spherical CCD as the number of centre points increases. The cube and star replicated versions of the CCD considered are: (i) two cubes plus one star (C_2S_1), (ii) two stars plus one cube (C_1S_2), (iii) three cubes plus one star (C_3S_1), (iv) three star plus one cube (C_1S_3), (v) four cubes plus one star (C_4S_1), (vi) four stars plus one cube (C_1S_4). For proper judgment, these replicated versions were compared with the unreplicated CCD option, one cube plus one star (C_1S_1) in order to highlight the performance of the spherical CCD with every replication of the cube or star and with every additional centre point.

Results are presented for $n_0 = 1$ and 3 centre points to reflect the values of the alphabetic criteria as the number of centre points is increased. The replication of the cube and star does not improve A , D and G for all the factors. Also, replicating the centre point improves V but does not improve A , D and G . It could also be noticed that the deterioration in the values of A , D and G as n_0 increases is not significant and therefore, for the sake of appropriate degrees-of-freedom for pure error measurement and test of lack-of-fit, it is recommended that the centre is replicated rather than the cube or star.

Apart from the few results which are displayed in Table 1, research has shown that the performances of the replicated versions of the CCD depend on the axial distance, α , under consideration. Replicating the star is better in some cases for the orthogonal α , practical α and cuboidal α and the α for orthogonal blocking (see [10]; [28]; [30] and [37]). For the rotatable α , replicating the cube improves the performance of the CCD (see [35]).

5 Challenges and Suggestions for Future Studies

One of the major challenges facing research works and their outcomes is improper implementations. Most research findings, especially in Statistics and many other related areas, could not find their way to the industrial and industrialized world and therefore are limited to the pages of projects, journals and technical reports stashed away forever in University and Departmental archives. The most challenging aspect of industrial Statistics, like the RSM being discussed here, is in

Table 1: Exact Values of the Alphabetic Criteria for the Partially Replicated Spherical CCD

k	Design			$n_0 = 1$					$n_0 = 3$					
		F	$2n_2k$	α	N	D	A	G	V	N	D	A	G	V
3	C ₁ S ₁	8	6	1.7321	15	71.1	32.4	100.0	9.1055	17	70.1	63.6	89.0	4.9476
	C ₂ S ₁	16	6	1.7321	23	68.4	29.4	43.5	12.8026	25	70.3	53.3	77.7	6.0146
	C ₁ S ₂	8	12	1.7321	21	67.3	24.7	47.6	12.1310	23	68.6	41.7	75.6	6.0181
	C ₃ S ₁	24	6	1.7321	31	64.9	19.2	32.3	16.6118	33	68.1	38.3	64.9	7.2539
	C ₁ S ₃	8	18	1.7321	27	63.1	19.8	37.1	15.2917	29	64.1	35.0	60.5	7.1605
	C ₄ S ₁	32	6	1.7321	39	61.8	15.8	25.6	20.4484	41	65.6	33.1	55.6	8.5400
	C ₁ S ₄	8	24	1.7321	33	59.4	16.5	30.3	18.2786	35	62.5	30.3	57.1	8.3257
	C ₁ S ₁	16	8	2.0000	25	76.6	33.2	60.0	14.4442	27	76.4	52.3	95.2	7.2003
4	C ₂ S ₁	32	8	2.0000	41	53.2	26.6	36.6	21.8284	43	75.1	43.4	69.9	9.5164
	C ₁ S ₂	16	16	2.0000	33	73.5	29.1	45.6	25.0239	35	63.9	44.1	80.7	8.6526
	C ₃ S ₁	48	8	2.0000	57	69.3	17.0	26.3	29.3577	59	72.0	35.8	76.7	12.0335
	C ₁ S ₃	16	24	2.0000	39	69.1	20.8	36.6	22.4575	41	70.9	37.6	97.7	10.1762
	C ₄ S ₁	64	8	2.0000	73	61.7	13.7	20.6	34.2982	75	69.1	30.2	63.0	14.5987
	C ₁ S ₄	16	32	2.0000	49	65.1	17.6	30.6	26.5087	51	67.3	31.5	85.9	12.5511
	C ₁ S ₁	32	10	2.2361	43	80.2	21.2	48.8	25.7726	45	80.7	50.9	86.0	9.1771
	C ₂ S ₁	64	10	2.2361	75	75.2	18.6	28.0	30.0576	77	77.1	38.6	56.7	14.2796
5	C ₁ S ₂	32	20	2.2361	53	78.9	24.0	39.6	28.3568	55	80.1	44.8	89.2	10.5688
	C ₃ S ₁	96	10	2.2361	107	70.8	13.7	19.6	52.0312	109	73.3	30.4	42.2	19.4156
	C ₁ S ₃	32	30	2.2361	63	75.4	20.5	33.3	31.0938	65	77.0	39.3	78.9	12.0513
	C ₄ S ₁	128	30	2.2361	139	67.4	10.8	15.1	67.0459	141	70.0	25.0	33.6	24.5617
	C ₁ S ₄	32	40	2.2361	73	71.7	17.9	28.8	35.6925	75	73.6	34.8	70.7	13.5593
	C ₁ S ₁	32	12	2.4495	45	83.8	33.7	62.2	25.4624	47	83.5	55.8	94.9	12.2040
	C ₂ S ₁	64	12	2.4495	77	81.4	23.4	36.4	39.9974	79	82.5	45.8	69.7	16.8486
	C ₁ S ₂	32	24	2.4495	57	79.6	27.6	49.1	31.4863	59	79.9	47.3	79.9	14.5269
6	C ₃ S ₁	96	12	2.4495	109	78.1	17.7	25.7	54.7701	111	79.7	37.6	52.4	21.7898
	C ₁ S ₃	32	36	2.4495	69	74.2	23.2	40.6	37.5818	71	75.0	40.6	69.0	16.9329
	C ₄ S ₁	128	12	2.4495	141	75.1	14.2	19.8	69.6030	143	77.0	31.6	42.0	26.8075
	C ₁ S ₄	32	48	2.4495	81	69.3	20.0	34.6	43.6962	83	70.3	35.4	46.2	19.3628

the area of application. Many industries and companies that are expected to lead the way in utilizing these amazing research findings and sponsoring other major and extensive studies have unfortunately, backed out from this responsibility. The researcher is now saddled with the responsibility of finding areas of application to his/her research findings. For the ongoing discussion on partial replication of the portions of the CCD, [40] has given an example on the application of the results to improving local cassava content in bread production in Nigeria while maintaining desirable quality of loaf. In the same work, a computer program has been developed as an Excel Macro which gives the optimum replication of the cube, star and centre points of the CCD, making it easier for an experimenter to use. More real-life problems facing different aspects of the economy need to be examined and solutions proffered by the exploitation of the amazing properties of the CCD. RSM and in particular, the CCD has large potential applications in the health sector, painting industry (using Mixture experiments), automobile industry, financial sector, agricultural sector, manufacturing industry, food packaging, education, etc.

There are design evaluation criteria that have not been used in the literature to compare the variations of the CCD when the cube and star portions are replicated. Such evaluation (optimality) criteria should be considered in further studies to ascertain the performances of the replicated design options with respect to the design criteria and appropriate recommendations for the benefit of practitioners made. Further studies need to be done in deriving exact functions that accommodate replications of the portions of the CCD for the other regularly applied optimality criteria in design of experiments. Such optimality criteria like the E -optimality, D_s -optimality, and so on need to be investigated with respect to the partial replication of the CCD.

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