Evaluation of Practical Central Composite Designs for Optimum Exploration of Response Surfaces

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The drawback of the spherical, α=√k, and rotatable, α=∜f, f=2^k axial distances of the central composite designs (CCD) is the extreme values of the axial distance as the number of experimental factors, k, increases, resulting in impractical axial distances beyond the bounds of the design region. The practical central composite design compensates for this drawback by providing more stable and less extreme axial distance irrespective of the size of k. This study focuses on the evaluation of partially replicated cube and star portions of the variations of the CCD with practical axial distance, α=∜k. By replicating the cube and star portions. The variation of the partially replicated central composite designs was evaluated using the following single-value optimality criteria: A-, D- and E-efficiencies and V-criterion. Fraction of design space graphs (FDSG) and variance dispersion graphs (VDG) were used to assess the scaled and unscaled prediction variances across the design regions. The replication of the star points yielded small and better distribution of the prediction variance across the design space and better results for the A-, G- and V-criterion.. On the contrary, The D-efficiency was not improved by the replication of the cube portion. Lack-of-fit, residual and pure error degrees of freedom of partially replicated CCD were ascertained.

Keywords: Axial distance, degrees of freedom, design efficiency, lack-of-fit, replication
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1.0 Introduction

In response surface methodology, most popular and commonly used response surface design is the CCD which was developed by Box and Wilson (1951). This design is characterized by three distinct components: the centre, the star (axial component) and the cube (factorial component). The coordinates of the cube portion is of the form, $(\pm 1, \pm 1, \dots, \pm 1)$ for the k independent variables, $(x_1, \dots, x_k)$. This iimplies that the cube has the highest value set at +1 and the lowest value set at -1 which defines the extreme regions of the unit cube. The star has coordinates of the form, $,(0,\ \pm\alpha,\ 0,\ \dots,\ 0), \dots, (0,\ 0,\ \dots,\ \pm\alpha)$, such that α defines the position of the star points in the design region. The highest value of the star points is at $+\alpha$ and lowest value at $-\alpha$. The centre component has coordinates of the form, $(0,\ 0,\ \dots,\ 0)$.

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Placing the star points on the axis of the design space defined by the CCD determines the distance of the star points from the centre of the design space and is important in the performance of the design with respect to prediction of responses. The axial distance, α, is the distance of the star points from the centre of the design space along the axes of the CCD. There are very important axial distances which exist in the literature for the CCD for different experimental conditions. One of such axial distances is the spherical alpha which puts the design points on a sphere of distance, $\alpha = \sqrt{k}$, from the centre of the design region. Another axial distance is the rotatable alpha, with distance, $\alpha = \sqrt[4]{f}$, from the centre of the design space, where $f = 2^k$ factorial runs, which gives a CCD that has equal precision at equal distance from the centre of the design region. Then, the cuboidal alpha at distance, $\alpha = 1$, puts the star points at the centre of the face of the unit cube, ensuring that the star points are distance $\alpha = 1\, from$ the centre of the cuboidal region.

The problem of the spherical and rotatable axial distances, as pointed out by Li et al (2009), is that as the number of factors increases, the values of the axial distances could be impracticable in response surface exploration. Consider, for example, an experiment involving k = 10, then, $\sqrt{10} = 3.1623$ and $\sqrt[4]{2^{10}} = 5.6569$, respectively, for the spherical and rotatable axial distances, which are not feasible values (see Table 1 for detailed results of the axial distances for k = 6 to 10). Therefore, Anderson and Whitcomb (2005) provided the practical axial distance, $\alpha = \sqrt[4]{k}$, which is a compromise between the spherical and cuboidal axial distances. The practical alpha, which is moderate and less extreme, also offers reasonable variance inflation factor (VIF) as the number of factors, k increased. Ukaegbu (2018) compared the prediction variances of the practical axial distance of the CCD with the prediction variances of the spherical, face-centred, rotatable and orthogonal axial distances for 3 to 6 design factors using variance dispersion graphs (VDG) and the fraction of design space (FDS) graphs.

In the present study, we employ the advantage that the practical alpha offers in evaluating the CCD with partial replications of the factorial and star portions. To enhance the evaluation and comparisons of the replicated designs variations, we used three popular single-value efficiency criteria, the *A*-, *D*- and *G*-efficiencies, and the *V*-criterion. Graphical methods employed in assessing and comparing the prediction variance properties of the partially replicated design variations are the variance dispersion graphs (VDG) and the fraction of design space (FDS) graphs. The number of factors under consideration is k = 3 to 6 factors.

2.0 Literature Review

Anderson-Cook et al. (2009) listed some of the properties of a good design for fitting second-order response surfaces, some of which include providing sufficient information to allow the test of model lack-of-fit; be robust to outliers in the data; be robust to errors in the control of design levels; provide a good distribution of the prediction variance throughout the design region; etc. (see Myers and Montgomery, 2002 and Anderson-Cook, 2005 for further references). The CCD with spherical and rotatable axial distances have limitations in attaining some of the properties as the number of factors increases due to resulting impractical axial distances.

As already stated, the practical alpha, $\alpha = \sqrt[4]{k}$, was presented by Anderson and Whitcomb (2005) as a compromise between the spherical and cuboidal axial distances. According to Anderson and Whitcomb (2005), this practical axial distance provides (i) acceptable variance inflation factor (VIF), and (ii) design points which are less extreme with an increase in the number of design factors. Generally, the VIF is a measure of how much the variances of estimated model parameters are inflated when compared to the predictor variables not being linearly related. This measure is very useful in detecting the presence of multicollinearity in regression models. Li et al. (2009) submitted that the practical axial distance results in near-rotatable central composite designs and offers stable scaled prediction variance across the design region. In the study by Li et al. (2009), the CCD with practical axial distance was shown to perform better than the other competing designs in the cuboidal region considering the scaled and unscaled prediction variances; the design with practical axial distance improved the prediction variance performance of the design throughout the design space by extending the axial points beyond the cuboidal region of interest.

In this study, the partially replicated variations of the CCD with practical axial distance was evaluated in the cuboidal region for k = 3 to 6 factors. These design variations were evaluated using *A*, *D*, *G* and *V* efficiency criteria and variance dispersion graphs (VDG) and fraction of design space (FDS) graphs used to measure the spread of the prediction variances.

3.0 Methods

3.1 Partial replications

The partially replicated variations of the central composite designs considered in this study, as provided by Draper (1982) 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). These partially replicated design variations are compared with the CCD without replication of the cube or star portions, that is, (vii). One cube plus one star (C_1S_1). Each design variation was augmented with n_0 centre points to effectively determine the effect of increasing the number of centre points on the prediction capabilities of the replicated designs.

3.2 Measures of Design Properties

The *D*-efficiency is a useful statistical tool for quantifying the quality of estimated model parameters, and is defined by $D_{eff} = \left\{|X'X|^{1/p}/N\right\} \times 100$, where $N = 2^{k-q}n_c + 2n_s k + n_0$, q is the fraction of 2^k, n_c = number of replications of the cube, n_s = number of replications of the star, n_0 = number of replications of the centre point and *k* is the number design factors. The power, $1/p$, is the inverse of the number of model parameter estimates, *p*, being assessed as the determinant of the information matrix is being computed. The *A*-efficiency, given by $A - eff. = 100p/\{trace[N(X'X)^{-1}]\}$, is obtained as a function of the trace of the inverse of the information matrix, $(X'X)^{-1}$. Also, the *G*-efficiency, given by $G - eff. = 100p/[N\, max\, v\,(x)]$, is obtained from the scaled maximum prediction variance of the design. For the *V*-criterion, a design is *V*-optimal if it minimizes the normalized integrated scaled prediction variance, $V - opt. = min\frac{1}{\Psi}\int_\Omega v(x)dx$, where $\Psi = \int_\Omega dx$ is the volume of the design space. For *A*-, *D*- and *G*-efficiencies, higher values are desirable, while smaller values are desirable for the *V*-criterion. MATLAB version 14 software was used to compute the efficiency criteria of the partially replicated designs.

3.3 Graphical methods for comparison

According to Anderson-Cook et al. (2009), single-value criteria such as the *D*- and *G*-efficiencies do not completely show the prediction variance characteristics of response surface designs. That is, the strengths and weaknesses of a response surface design under evaluation cannot be captured completely using such single-value criteria. On the other hand, graphical methods of prediction variance assessment can completely display the distribution of the prediction variances of a design throughout the design space. One of these graphical methods in the variance dispersion graph (VDG). Giovannitti-Jensen and Myers (1989) developed the VDG as a prediction variance-based graphical method which displays the spread of unscaled and scaled prediction variances of a multi-dimensional design region on a two-dimensional space. Prediction variance assessment using the VDG requires plotting the prediction variances against the radius, *r*, of the sphere from zero up to the outer region of the sphere covering the region of interest. Zahran et al (2003) developed the fraction of design space (FDS) graph to complement the VDG in prediction variance assessment of both spherical and cuboidal design regions. The FDS graphs display the characteristics of the scaled prediction variance (SPV) throughout a multi-dimensional region on a two-dimensional space with a single curve. The volume of the fraction of the design space is the key factor in the concept of the FDS criterion. The stability and prediction capability of a design are determined by how flat and closer to the horizontal line the graph is. The FDS graphs were computed and plotted using Design Expert version 12, while the VDGs were computed and plotted using MATLAB version 14.

4.0 Results and Discussion

4.1 Results of alphabetic criteria

For ease of use in this study, *A*, *D*, *G* and *V* were used to refer to the four single value criteria, *A*-, *D*- and *G*-efficiencies and *V*-criterion, respectively. In Table 1, the results for the single-value efficiency criteria and *V*-optimality are displayed. For k = 3 factors, the table shows that additional centre point improves *V* with smaller values and *A* with higher percentage efficiency values. Increasing the number of centre points is beneficial for *D* and *G* for the higher replication of the cube, three cubes plus one star and four cubes plus one star, which have higher efficiency values when the number of centre points increases. The best *D* efficiency values are obtained for the cube-replicated design, C_2S_1, which maintained the highest *D* efficiency values even as the number of centre points increases. The unreplicated CCD, C_1S_1, has the overall best values for *A*, *G* and *V* with the highest percentage efficiency values for *A* and *G* and smallest optimality value for *V*. Also, C_1S_1 is the best for *G* without an additional centre point. However, with increase in number of centre points, C_2S_1 has the best *G* efficiency value.

Table 1: Values of the *A*, *D*, *G* and *V* Criteria for the Partially Replicated Practical CCD

k	Design				$n_0 = 1$					$n_0 = 3$				
		F	$2n_sk$	α	N	D	A	G	V	N	D	A	G	V
3	C_1S_1	8	6	1.3161	15	55.3	37.5	89.1	5.9864	17	52.5	42.7	79.3	4.7882
	C_2S_1	16	6	1.3161	23	55.5	30.9	84.7	7.7480	25	54.8	38.3	83.9	5.5476
	C_1S_2	8	12	1.3161	21	51.4	34.2	69.6	6.1975	23	49.8	39.1	64.6	5.1268
	C_3S_1	24	6	1.3161	31	53.6	25.4	64.2	9.7021	33	54.0	32.8	67.7	6.5621
	C_1S_3	8	18	1.3161	27	47.6	30.2	57.5	6.6242	29	46.8	34.5	54.7	5.5637
	C_4S_1	32	6	1.3161	39	51.6	21.4	51.5	11.7102	41	52.5	28.3	56.5	7.6494
	C_1S_4	8	24	1.3161	33	44.5	26.8	49.1	7.1141	35	44.1	30.7	47.7	6.0216
4	C_1S_1	16	8	1.4142	25	58.1	41.8	63.0	7.5417	27	55.8	44.2	58.5	6.4203
	C_2S_1	32	8	1.4142	41	32.2	12.3	37.9	25.9217	43	32.0	13.2	37.0	23.8894
	C_1S_2	16	16	1.4142	33	55.0	42.7	75.6	7.0583	35	44.3	44.6	71.7	6.4323
	C_3S_1	48	8	1.4142	57	54.9	25.9	52.9	13.1066	59	54.9	30.3	54.6	9.8632
	C_1S_3	16	24	1.4142	39	51.2	39.9	63.4	7.1739	41	49.8	41.3	60.8	6.7236
	C_4S_1	64	8	1.4142	73	52.6	21.4	42.1	16.0643	75	53.0	25.4	43.9	11.8071
	C_1S_4	16	32	1.4142	49	47.8	36.8	54.7	7.4575	51	46.8	37.8	53.0	7.0890

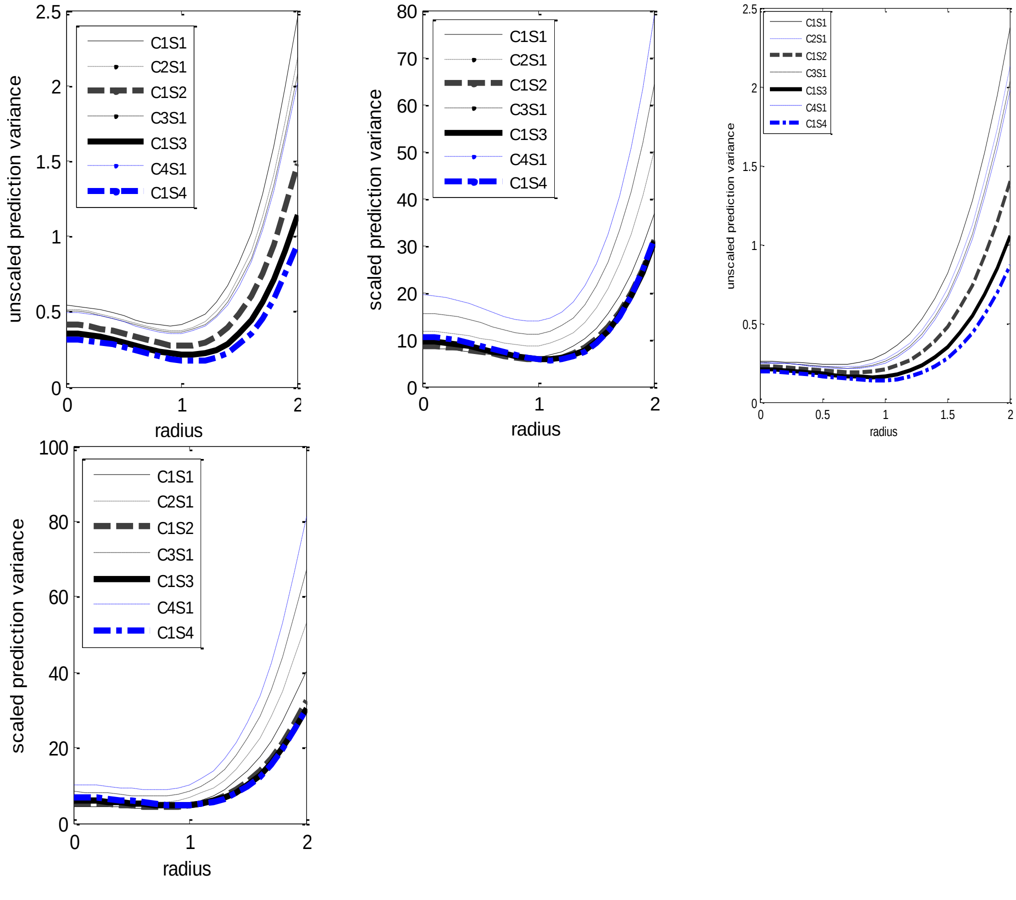
5	C_1S_1	32	10	1.4954	43	60.2	41.6	90.9	8.4625	45	58.7	43.8	90.9	7.1443
	C_2S_1	64	10	1.4954	75	57.7	29.8	55.1	13.0996	77	57.3	32.6	56.4	10.5355
	C_1S_2	32	20	1.4954	53	58.9	47.4	85.2	6.6552	55	57.5	48.4	82.2	6.0779
	C_3S_1	96	10	1.4954	107	54.8	22.9	39.4	17.8309	109	54.8	25.4	40.7	14.0473
	C_1S_3	32	30	1.4954	63	55.8	47.0	73.5	6.0707	65	54.6	47.4	71.4	5.7248
	C_4S_1	128	30	1.4954	139	52.3	18.5	30.7	22.5881	141	52.6	20.7	31.8	17.5922
	C_1S_4	32	40	1.4954	73	52.7	45.0	64.9	5.8222	75	51.7	45.2	63.3	5.5798
6	C_1S_1	32	12	1.5651	45	61.5	48.1	94.0	10.4743	47	59.6	48.6	90.0	9.7810
	C_2S_1	64	12	1.5651	77	61.1	37.4	68.0	13.9348	79	60.2	39.1	70.7	12.3548
	C_1S_2	32	24	1.5651	57	57.7	50.7	57.3	9.6140	59	56.1	50.4	73.9	9.4249
	C_3S_1	96	12	1.5651	109	59.0	29.7	50.5	17.7553	111	58.5	31.5	51.5	15.3747
	C_1S_3	32	36	1.5651	69	53.1	47.8	64.6	9.8328	71	51.9	47.4	62.9	9.7848
	C_4S_1	128	12	1.5651	141	57.0	24.6	39.5	21.6692	143	56.9	26.3	40.5	18.4661
	C_1S_4	32	48	1.5651	81	49.2	44.2	56.1	10.3236	83	48.2	43.8	54.8	10.3343

For the four-factor CCD, k = 4, additional centre point improves *A* and *V* but the effect is inconsistent for *D* and *G*, where, for the cube-replicated options, C_3S_1 and C_4S_1, additional points at the centre improves *D* and *G* which is not the case with the replication of the star. The best value for *A* and *G* are obtained with C_1S_2 even with additional centre point. However, the values of the four alphabetic criteria indicated that further replications of the star does not in any way improve the performances of the designs. The unreplicated CCD, C_1S_1, gives the best values for *D* even with additional point at the centre. Also, with additional centre point, C_1S_1 gives the best value for *V* but was outperformed by C_1S_2 when there is only one centre point. It is important to notice that replicating the cube portion from C_2S_1 to C_3S_1 improves the design's alphabetic criteria, which begins to deteriorate with further replication of the cube. For k = 3 and 4, further replication of the CCD does not improve any of the four alphabetic criteria.

The effects of additional centre point on the four alphabetic criteria for k = 3 and 4 factors are also true for k = 5 and 6. However, for k = 5, with or without additional centre point, C_1S_1 gives the best values for *D* and *G* while C_1S_2 offers the best values for *A*. Unlike the cases of k = 3 and 4, the higher the star is replicated, the better is the value of *V* with or without additional centre points. For k = 6, C_1S_1 gives the best for *G* with or without an additional centre point and also the best for *D* with one centre point, while C_2S_1 performs better with an additional centre point. Also, C_1S_2 gives the best *A* and *V* values with and without an additional centre point.

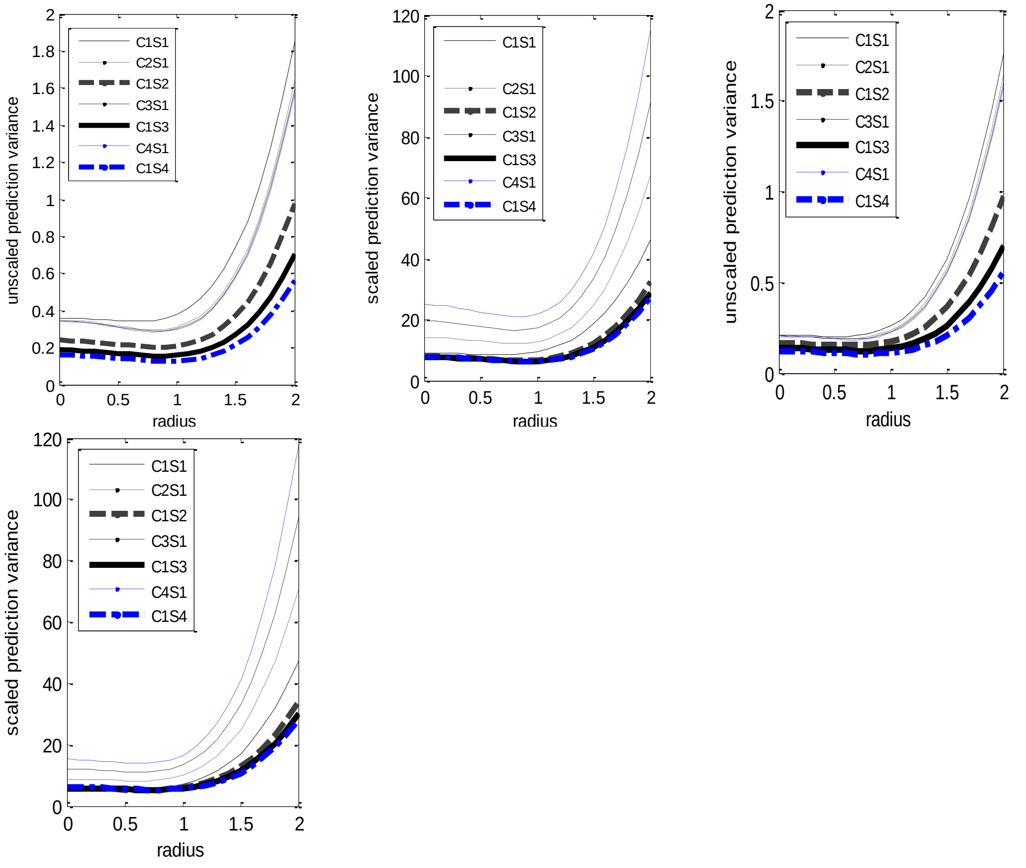
4.2 Results of graphical methods

If the interest of a practitioner is to understand the prediction variance distribution of a design throughout the entire design region, that is, to understand the stability of the prediction variance throughout the entire design region and/or where in the region the design has the best and worst prediction variance, the two graphical methods are formidable tools for exploring the prediction variance properties of competing designs. In this section, the VDG and FDS graphs were plotted for the unscaled and scaled prediction variances in the spherical region for n_0 = 1 and 3. The graphs are displayed in Figures 1 to 4 for the VDGs and Figures 5 to 9 for the FDS plots. The VDG and FDS graphs show that replicating the star resulted in minimum and stable spread of the prediction variances throughout the entire design space for both unscaled and scaled prediction variances. The VDGs show that the star-replicated practical CCD options have the lowest distribution of the unscaled and scaled prediction variances. All the designs maintain a slightly stable prediction variance from the origin up to the point where the radius, *r* = 1.0, then the prediction variance increases rapidly as *r* increases towards the extreme of the design region. An additional centre point tends to reduce the prediction variance for both the unscaled and scaled prediction variance.



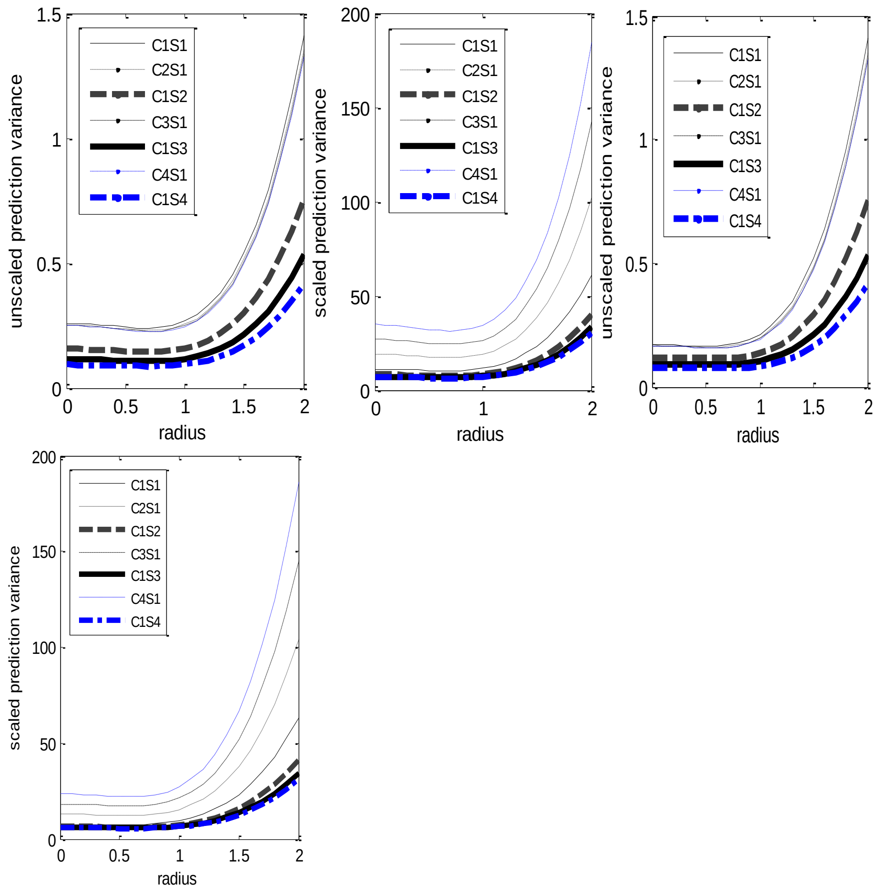
(a) (b)

Figure 1: VDG for Unscaled and Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$, and $k = 3$



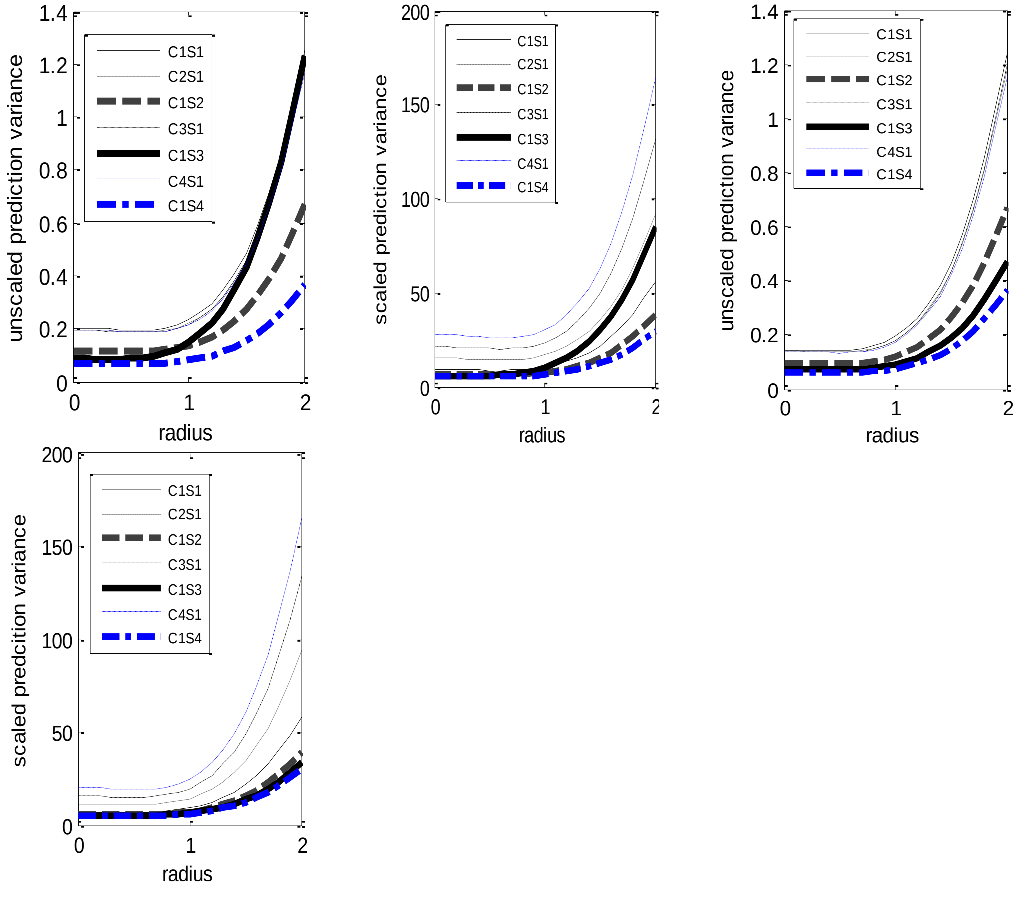
(a) (b)

Figure 2: VDG for Unscaled and Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$ and, $k = 4$



(a) (b)

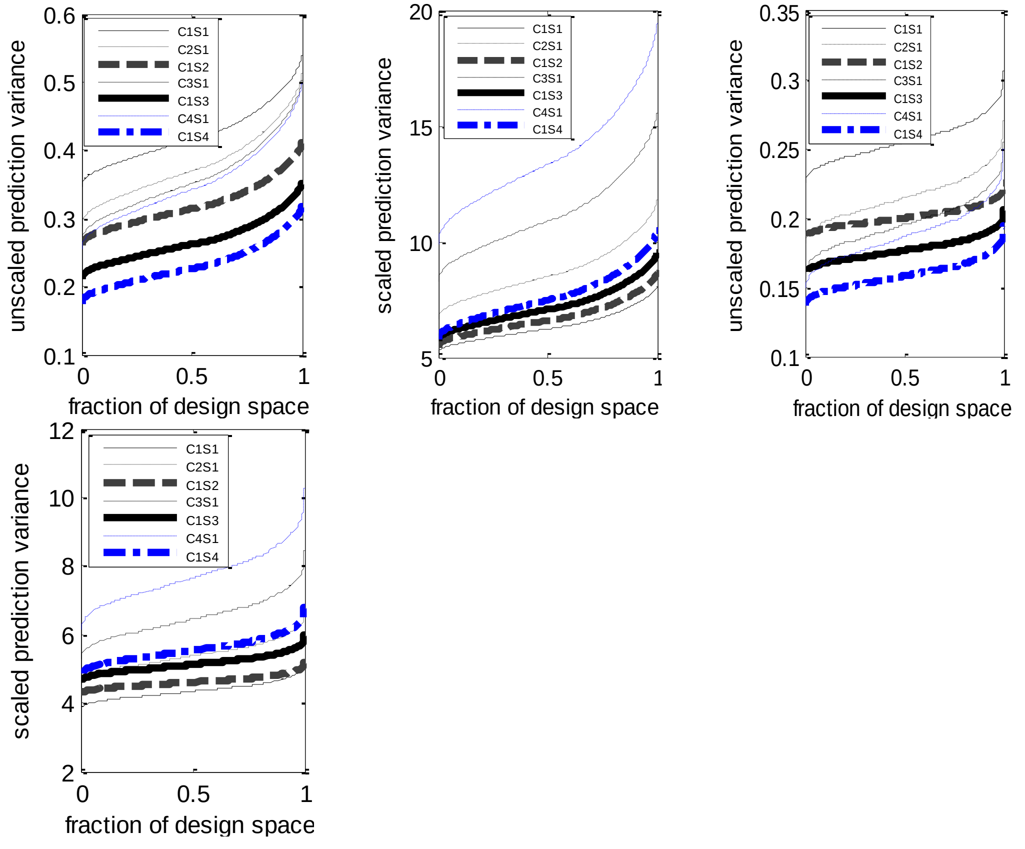
Figure 3: VDG of Unscaled and Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$, for $k = 5$



(a) (b)

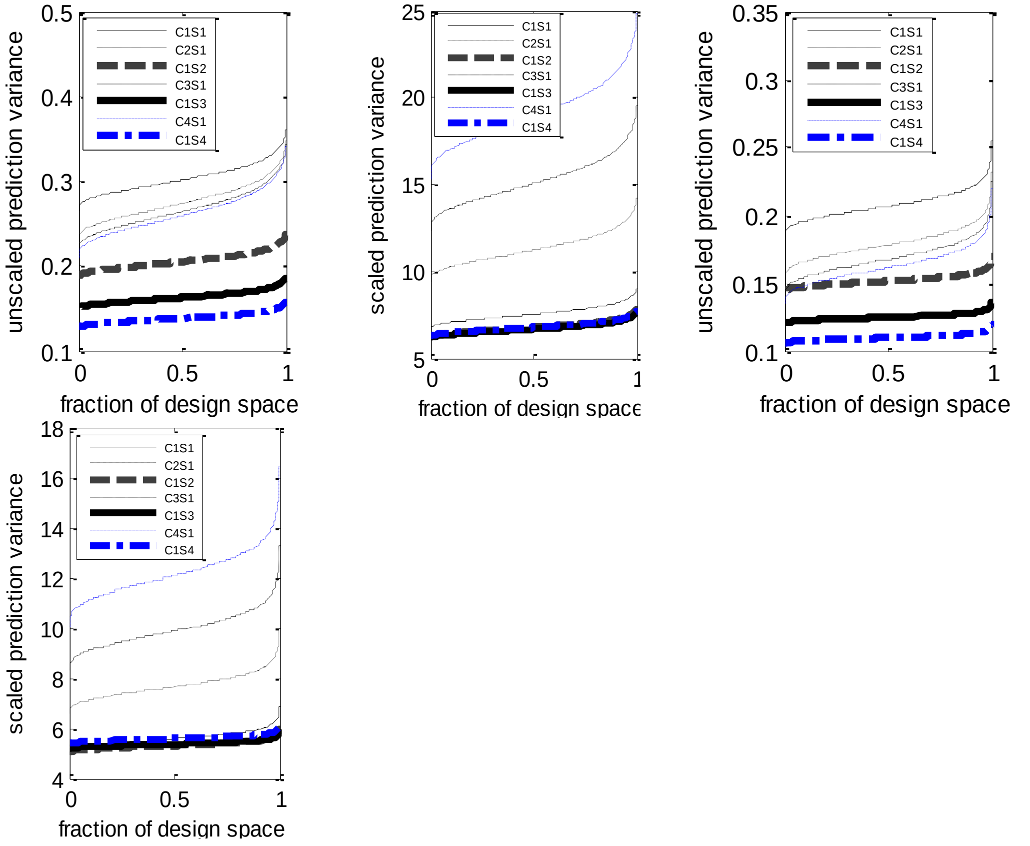
Figure 4: VDG for Unscaled and Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$, and $k = 6$

The FDS plots for $k = 3$ show unique results. The unreplicated CCD option, C_1S_1, have the worst unscaled prediction variance irrespective of the number of centre points. Scaling the prediction variance gives a design undue advantage over the others due to the smaller number of runs compared to the replicated options. Hence, the design has the smallest scaled prediction variance for the entire design space with or without additional centre points. The star-replicated options display the best (smallest) unscaled prediction variance, which improves with additional centre points. For $k = 4$, 5 and 6, the star-replicated options display the smallest and most stable unscaled and scaled prediction variance throughout the entire design space. The prediction variance of the star-replicated CCD options gets better with scaling and with additional centre points. Hence, the star-replicated designs are recommended for the prediction of responses involving practical CCD in the spherical region.



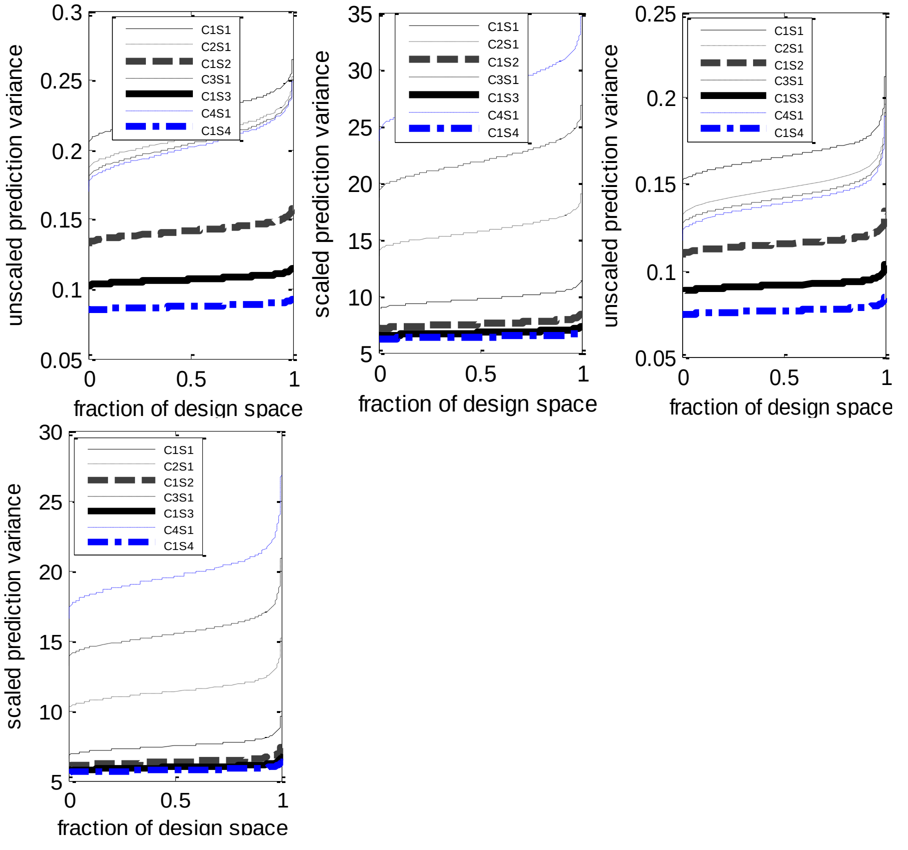
(a) (b)

Figure 5: FDS Graphs for the Unscaled and Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$, $k = 3$



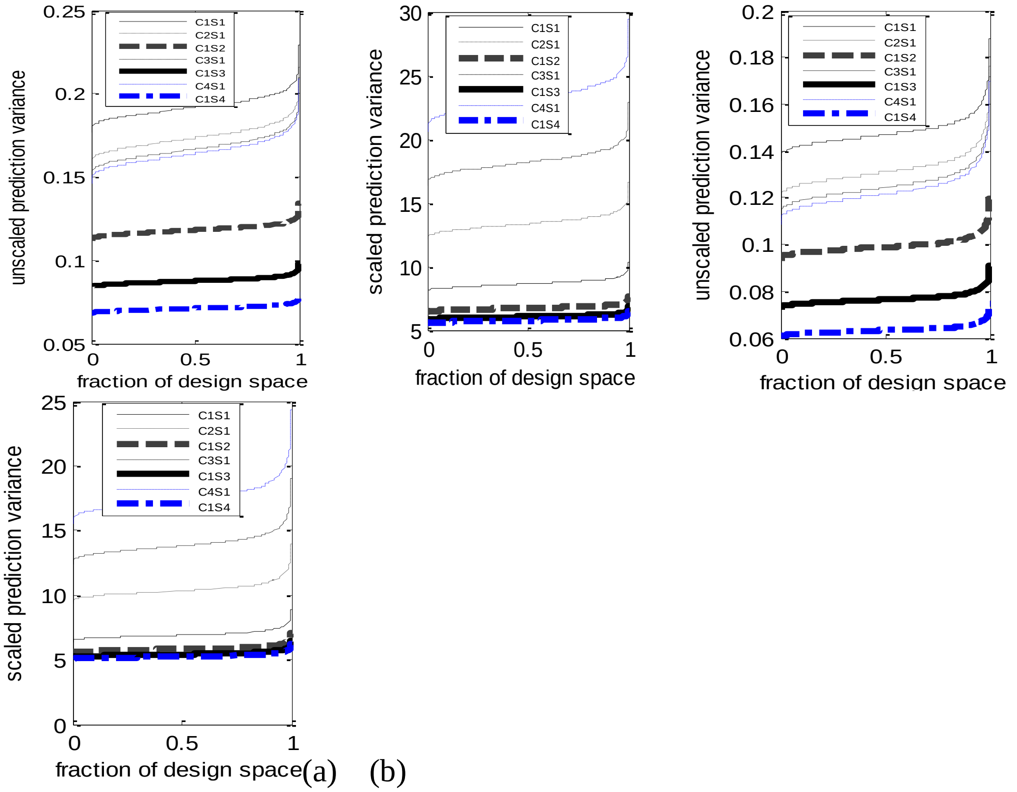
(a) (b)

Figure 6: FDS Graphs for Unscaled and Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$, $k = 4$



(a) (b)

Figure 7: FDS Graphs for Unscaled and Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$, $k = 5$



(a) (b)

Figure 8: FDS Graphs for Unscaled and Scaled Prediction Variance for (a) $n_0 = 1$ and (b) $n_0 = 3$, $k = 6$

4.3 Determination of Degrees of Freedom

According to Draper (1982) and Montgomery (2013), one of the reasons for replicating the centre point of a design was to obtain the required error degrees of freedom for the test of hypothesis. The recommendation from Montgomery (2013) is a minimum of three degrees of freedom for model lack-of-fit and four degrees of freedom for pure error. Fewer degrees of freedom will lead to a test that may not detect model lack-of-fit. In this section, we show that we can obtain the exact degrees of freedom required for pure error and test of model lack-of-fit by partially replicating the cube and sta portions of the CCD with practical axial distance and with or without replicating the centre point. According to Montgomery (2013), the total error sum of squares is calculated as the aggregate of the pure error sum of squares and the lack-of-fit sum of squares. Furthermore, the residual or total error degrees of freedom, RE_{df}, is calculated as the difference between the total number of runs, N, and the number of model parameters, p, being tested. That is

$$RE_{df} = N - p. \quad (1)$$

The pure error degrees of freedom, PE_{df}, is the sum over all the replicates of each run. That is

$$PE_{df} = \sum_{i=1}^{N}\left(N_{reps,i} - 1\right) = \sum_{i=1}^{F}\left(F_{rep,i} - 1\right) + \sum_{i=1}^{H}\left(H_{rep,i} - 1\right) + n_0 - 1 \ , \qquad (2)$$

$$= (n_c - 1)f + 2(n_s - 1)k + (n_0 - 1) \qquad (3)$$

where $N_{reps,i}$, = number of times the i^{th} run is replicated, $F_{rep,i}$ = the number of times the cube is replicated, $H_{rep,i}$ = the number of times the star is replicated, and $H = 2n_s k$. Therefore, any portion of the CCD that was not replicated does not contribute to the degrees of freedom. Therefore, the lack-of-fit degrees of freedom, LOF_{df}, is the difference between the residual degrees of freedom and the pure error degrees of freedom. That is,

$$LOF_{df} = RE_{df} - PE_{df}. \qquad (4)$$

The exact pure error and lack-of-fit degrees of freedom for some variations of the partially replicated practical CCD are presented in Table 2 for k = 3 to 6 factors.

Table 2: Exact Pure Error and Lack-of-Fit Degrees of Freedom for *k* = 3 to 6 Factors

k	Design	f	n_c	F	n_s	H	p	$n_0=1$			$n_0=3$		
								N	LOF_{df}	PE_{df}	N	LOF_{df}	PE_{df}
3	C_1S_1	8	1	8	1	6	10	15	5	0	17	5	2
	C_2S_1	8	2	16	1	6		23	5	8	25	5	10
	C_1S_2	8	1	8	2	12		21	5	6	23	5	8
	C_3S_1	8	3	24	1	6		31	5	16	33	5	18
	C_1S_3	8	1	8	3	18		27	5	12	29	5	14
	C_4S_1	8	4	32	1	6		39	5	24	41	5	26
	C_1S_4	8	1	8	4	24		33	5	18	35	5	20
4	C_1S_1	16	1	16	1	8	15	25	10	0	27	10	2
	C_2S_1	16	2	32	1	8		41	10	16	43	10	18
	C_1S_2	16	1	16	2	16		33	10	8	35	10	10
	C_3S_1	16	3	48	1	8		57	10	32	59	10	34
	C_1S_3	16	1	16	3	24		41	10	16	43	10	18
	C_4S_1	16	4	64	1	8		73	10	48	75	10	50
	C_1S_4	16	1	16	4	32		49	10	24	51	10	26
5	C_1S_1	32	1	32	1	10	21	43	22	0	45	22	2
	C_2S_1	32	2	64	1	10		75	22	32	77	22	34
	C_1S_2	32	1	32	2	20		53	22	10	55	22	12
	C_3S_1	32	3	96	1	10		107	22	64	109	22	66
	C_1S_3	32	1	32	3	30		63	22	20	65	22	22
	C_4S_1	32	4	128	1	10		139	22	96	141	22	98
	C_1S_4	32	1	32	4	40		73	22	30	75	22	32
6	C_1S_1	64	1	64	1	12	28	77	49	0	79	49	2
	C_2S_1	64	2	128	1	12		141	49	64	143	49	66
	C_1S_2	64	1	64	2	24		89	49	12	91	49	14
	C_3S_1	64	3	192	1	12		205	49	128	207	49	130
	C_1S_3	64	1	64	3	36		101	49	24	103	49	26
	C_4S_1	64	4	256	1	12		269	49	192	271	49	194
	C_1S_4	64	1	64	4	48		113	49	36	115	49	38

5. Summary and Recommendations

Additional centre points improved the *A* and *V* for all the factors considered. The unreplicated CCD, C_1S_1, offers the best values for the *A* and *V* for k = 3 factors. Replicating the cube is beneficial only up to C_3S_1, the replications improved the performances of the designs' alphabetic criteria, beyond which alphabetic criteria begin to deteriorate. For k = 5 factors, the higher the replication of the star, the smaller the *V* and the better the design; this characteristic is unique to k = 5 factors. Except for k = 3, the best value for *A* was obtained from the star-replicated CCD, C_1S_2, with or without an additional centre point.

In general, the higher the replication of the star portion of the CCD provided uniform the distribution of both the unscaled and scaled prediction variances throughout the entire design space. This is true using both the variance dispersion graphs and the fraction of design space graphs, and for all the factors considered in the study.

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