Comparison of the central composite design with augmented alternative designs for response surface exploration

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The cardinal objective of response surface methodology is reliability and quality improvement through well designed experiments. The choice of response surface design that satisfies this objective has been the subject of many studies on response surface explorations. The standard central composite design (CCD) remains popular choice among practitioners but offers high number of experimental runs with increase in number of factors. In this study, we propose augmented Minimum-run resolution V CCDs (MinResV CCD) as useful alternatives to the standard CCD in response surface exploration. The standard CCD and the augmented MinResV CCD are evaluated and compared with some alphabetic and graphical criteria in spherical and cuboidal design regions. Some augmented versions of the MinResV CCDs displayed better potentials for quality improvement and with smaller design runs in most cases than the standard CCD.

Keywords: Design augmentation, Design size, Fraction of design space graph, Prediction variance, Spherical region

1. Introduction

The central composite design (CCD) of Box and Wilson (1951) was developed for exploration of response surfaces with curvature and the design exists for $k \geq 2$ factors, where k is a fixed positive integer for both spherical and cuboidal response surfaces. The structure of the central composite design which consists of the cube (factorial) portion, the star (axial) portion and the centre point makes it flexible and adaptable. The number of runs, N, of the CCD increases rapidly as k increases, especially for $k \geq 6$. This has serious implication on the cost of experimentation, as some practitioners cannot afford to use the design for response surface exploration. For this reason, the small central composite design (SCD) by Hartley (1959) and minimum-run resolution V (MinResV) design by Oehlert and Whitcomb (2002) were developed as smaller alternatives to the CCD. The SCD and MinResV designs are readily available for $k \geq 2$ like the CCD but are more useful for higher number of factors, especially for $k \geq 6$. Both designs also exist for the cuboidal and spherical regions. However, unlike the CCD, the two smaller designs do not possess the orthogonality and rotatability properties.

The three designs, CCD, SCD and MinResV CCD, are made up of the same three components: the cube, the star and the centre point. The difference between them lies in the structure of their cubes. The cube component of the CCD is at least of resolution V. To obtain the SCD, the cube component of the CCD is replaced with a resolution III factorial design. The minimum-run resolution V CCD is obtained by replacing the resolution V factorial component of the CCD with a minimum-run resolution V design which gives fewer runs than the standard CCD (see, for example,

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Li et al, 2009 and Montgomery, 2013). Hence, the CCD, SCD and MinResV CCD have the same runs at the star and centre portions but different runs at the cube portion for any given value of *k*.

According to Li et al. (2009), minimum-run resolution V designs are equireplicated two-level irregular fractions of resolution V with each factor having equal number of low and high levels. These are constructed using *D*-criterion and columnwise-pairwise exchange algorithm by Li and Wu (1997). In practice, the MinResV designs can be used as stand-alone designs or serve as the factorial component of the CCD; an approach adopted in this study. Typical six-factor full factorial standard CCD with one centre point has 77 design runs while a MinResV CCD with the same number of factors and one centre point has 35 design runs.

The performance characteristics of these designs have been evaluated and compared with the aim of recommending, under some conditions, which of the designs will be most desirable. Li et al (2009) used box plots and fraction of design space plots as graphical tools to evaluate the prediction variance properties of the CCD, SCD and MinResV designs. The number of factors, *k*, considered in the study is from 6 to 10. Their results showed that for the scaled and unscaled prediction variances, the CCD offers substantial advantage in prediction with precision over the smaller alternatives, followed by the MinResV CCD. Li et al. (2009) recommended that, where the experimenter may not be able to afford the high number of runs for the CCD, the MinResV CCD should be used because of the reasonable prediction capability. The SCD displayed the worst prediction variance characteristics for all the cases considered and therefore, was not considered in this work.

In this study, we consider the scenario whereby if a practitioner can afford the standard CCD for response surface exploration, could there exist versions of the MinResV CCD that perform better than or compete favourably with the standard CCD but with relatively smaller number of runs as useful alternative to the standard CCD? Therefore, we propose augmented versions of the MinResV CCD which in most cases performed better than or competed favourably with the standard CCD under some evaluation criteria while offering smaller number of runs.

2. Preliminaries

2.1. Augmentation of the MinResV CCD

The pattern of augmentation adopted for this study is such that either the cube or star portion is included as additional set of runs to the MinResV CCD, as the case may be. Let C_i, $i = 1, 2, \ldots, n$, represent the cube portion(s) and S_j, $j = 1, 2, \ldots, m$, represent the star portion(s). For every *i*, $j = 1$ and for every *j*, *i* = 1 such that the first case gives the cube-augmented MinResV CCD options (M-C_iS_1) while the second case gives the star-augmented MinResV CCD options (M-C_1S_j). To avoid unnecessarily large design runs, the highest value of *n* and *m* used is such that the cube-augmented design options considered are M-C_2S_1, M-$C_3S_1$and M-C_4S_1. The star-augmented options considered are M-C_1S_2, M-C_1S_3 and M-C_1S_4.The standard CCD which was compared with the augmented MinResV CCD options is denoted in this study by C_1S_1. Half-fraction of the factorial portion of the standard CCD was used for *k* = 6 and 7 factors while one-quarter fraction of the factorial portion was used for *k*= 8, 9 and 10 factors. The structure of six-factor MinResV CCD augmented with one star is shown in Figure 1. The factorial, star and centre components of Figure 1 constitute the original six-factor MinResV CCD while the augmented star component is used to improve the design's quality.

$$\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{array} = \begin{array}{cccccccccccccccccc} \multicolumn{5}{c}{\text{factorial}} & \multicolumn{6}{c}{\text{star}} & \text{centre} & \multicolumn{6}{c}{\text{augmented star}} \\ \pm1 & . & . & . & \pm1 & \pm\alpha & 0 & 0 & 0 & 0 & 0 & 0 & \pm\alpha & 0 & 0 & 0 & 0 & 0 \\ \pm1 & . & . & . & \pm1 & 0 & \pm\alpha & 0 & 0 & 0 & 0 & 0 & 0 & \pm\alpha & 0 & 0 & 0 & 0 \\ \pm1 & . & . & . & \pm1 & 0 & 0 & \pm\alpha & 0 & 0 & 0 & 0 & 0 & 0 & \pm\alpha & 0 & 0 & 0 \\ \pm1 & . & . & . & \pm1 & 0 & 0 & 0 & \pm\alpha & 0 & 0 & 0 & 0 & 0 & 0 & \pm\alpha & 0 & 0 \\ \pm1 & . & . & . & \pm1 & 0 & 0 & 0 & 0 & \pm\alpha & 0 & 0 & 0 & 0 & 0 & 0 & \pm\alpha & 0 \\ \pm1 & . & . & . & \pm1 & 0 & 0 & 0 & 0 & 0 & \pm\alpha & 0 & 0 & 0 & 0 & 0 & 0 & \pm\alpha \end{array}$$

Figure 1: Augmented Six-Factor MinResV CCD with One Centre Point

2.2. Methods for Evaluation and Comparisons

Two evaluation methods, alphabetic and graphical criteria, were utilized in evaluating and comparing the designs. The first approach is the use of the four popular alphabetic criteria, the *A*-, *D*- and *G*-efficiencies and *V*-criterion. The *A*-efficiency aims at the proper estimation of model parameters by utilizing the individual variances of the model coefficients which appear on the diagonals of $(\mathbf{X}'\mathbf{X})^{-1}$ which is the inverse of the information matrix, $\boldsymbol{X}'\boldsymbol{X}$, of a design with design matrix, $\boldsymbol{X}$. Numerically, the *A*-efficiency criterion is given by $A_{eff} = 100p/N\{trace(\mathbf{X}'\mathbf{X})^{-1}\}$, where $trace(\mathbf{X}'\mathbf{X})^{-1}$ is trace or sum of the variances of the coefficients of the regression model. Atkinson and Donev (1992) symbolically presented the trace as $\sum_{i=1}^{p} \lambda_i^{-1}$, where λ_i is the ith diagonal element (variance) of $(\mathbf{X}'\mathbf{X})^{-1}$.

The *D*-efficiency makes use of the determinant, $|\mathbf{X}'\mathbf{X}|$, of the information matrix. Under the standard normality assumptions, $|\mathbf{X}'\mathbf{X}|$ is inversely proportional to the square of the volume of the confidence region of the regression coefficients. The volume of the confidence region is relevant because it reflects how well the set of coefficients are estimated. Therefore, the larger the determinant of $\boldsymbol{X}'\boldsymbol{X}$ is, the better the estimation of the model parameters. On the other hand, small $|\mathbf{X}'\mathbf{X}|$ and hence large $|(\mathbf{X}'\mathbf{X})^{-1}|$ implies poor estimation of the set of model parameters. The *D*-efficiency is a useful tool for quantifying the quality of the estimated model parameters and is defined as (see, for example, Borkowski and Valeroso, 2001), $D_{eff} = \left(|\mathbf{X}'\mathbf{X}|^{1/p} \times 100\right)/N$. The power, $1/p$, takes account of the p parameter estimates being assessed when the determinant of the information matrix is being computed.

The *G*-efficiency is one of the design criteria that are based on the scaled prediction variance (SPV) property of the design. The *G*-efficiency uses the maximum SPV given by, $\max\{\mathrm{N}\mathrm{f}'(\mathrm{x})(\mathbf{X}'\mathbf{X})^{-1}\mathrm{f}(\mathrm{x})\}$, in design evaluation and intuitively protects the experimenter against the worst-case scenario of the prediction variance being too undesirable since the user may wish to predict new responses anywhere in the design space. An interesting and important characteristic of the *G*-efficiency is that the lower bound for the maximum scaled prediction variance is equal to *p*, the number of model parameters. Therefore, when $\max\{Nf'(x)(\mathbf{X'X})^{-1}f(x)\} = p$, then the design is 100% *G*-efficient. Therefore, the *G*-efficiency is given as $G_{eff} = 100p/\max\{Nf'(\mathbf{x})\boldsymbol{M}_{\xi}^{-1}f(\mathbf{x})\}$.

Another optimality criterion that is based on the prediction variance of a design is the *V*-optimality criterion. This optimality criterion is designed to overcome a major disadvantage of the *G*-optimality, which is that, at each point in the design space, the experimenter needs to calculate the worst prediction variance. By averaging the prediction variances over the entire design region, the *V*-optimality eliminates the problem. Therefore, a design is said to be *V*-optimal if it minimizes the normalized integrated scaled prediction variance, $V_{opt} = \min \frac{N}{\Psi}\int_{\Omega} \mathrm{var}[y(\mathbf{x})]dx$, where $\Psi = \int_{\Omega} dx$ is the volume of the design space, Ω.For ease of usage, these alphabetic criteria will be simply denoted *D* and *G*, respectively.

The second approach is the use of the fraction of design space graphs (FDSG). According to Anderson-Cook et al. (2009), alphabetic criteria are single-value criteria which do not completely reflect the prediction variance characteristics of competing designs. The points of strength and weaknesses of competing designs are not effectively revealed by single-value criteria. The FDSG, on the other hand, displays the prediction variance characteristics of the partially replicated MinResV designs and the CCD throughout the entire design region for both the scaled and unscaled prediction variances. Further details on the FDSG could be found in Zahran et al.(2003) and Ozol-Godfrey et al (2005). The closer the graph is to the horizontal axis, the smaller the design's prediction variance and the better the prediction capability of the design.

The axial distance, α defines the distance of the star points from the centre of the design region and is known to influence the designs' performance characteristics (see Li et al, 2009). Three axial distances, α, common to the standard CCD and MinResV CCD, namely the spherical axial distance with $\alpha = \sqrt{k}$, the cuboidal axial distance with $\alpha = 1$ and the practical axial distance with $\alpha = \sqrt[4]{k}$, are considered for each design. Designs were evaluated for n_0 = 1 to 4 centre points but to avoid the tables and graphs being cumbersome, only the results for n_0 = 1 and 3 centre points were presented.

3. Evaluation and Comparison of the Designs

3.1. Evaluation using Alphabetic Criteria

In this section, the results of the A-, *D*- and *G*-efficiencies and V-criterion are presented in Tables 1, 2 and 3 for the practical ($\alpha = \sqrt[4]{k}$), cuboidal ($\alpha = 1$) and spherical ($\alpha = \sqrt{k}$) axial distances, respectively. The total number of runs, *N*, of each design option provides additional and important role in determining the viability of the design option based on the criterion. The recommended values of the respective design evaluation criteria are indicated in the Tables using bold fonts.

Table 1 shows the results for the practical axial distance. The standard CCD gives the best values for *D* for all the factors and also best results for *A*, *G* and *V* for *k* = 6 where the design possesses the smallest *N* among competing designs. This is also true for *k* = 8 factors with the CCD providing the best results for all the criteria. For *k* = 7, the design, M-C_1S_2, is recommended over the standard CCD for *A* and *V*. Though, the values of these two criteria for the CCD are slightly better than those of M-C_1S_2, this marginal advantage is achieved with additional 20 design runs when the 79 runs of the CCD is compared with the 59 runs of the M-C_1S_2.This is considered not to be cost effective. The design, M-C_2S_1, offers the best *G* values for the increasing number of centre points and this is also achieved with smaller number of design runs when compared with the CCD. The same is true for *k* = 9 where M-C_1S_2 is considered superior to the standard CCD in terms of *A* and *V* while M-C_2S_1 is better in terms of *G*. These results are achieved with 83 runs for M-C_1S_2 and 111 runs for M-C_2S_1 against the 147 runs for the CCD. For *k* = 10, M-C_1S_2 gives the best values for *A* and *V* (with a difference of 180 runs when compared with the 277 runs of the CCD). Also, M-C_2S_1 with 133 runs gives the best values for *G* (with a gain of 144 runs when compared to the CCD).

Table 1: Values of Alphabetic Criteria for Comparison of Augmented MinResV Design and the CCD for Practical Alpha

k	Design	*Cube*	Star	α	$n_0 = 1$					$n_0 = 3$				
					N	*D*	*A*	*G*	*V*	*N*	*D*	*A*	*G*	*V*
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**
	M-C_2S_1	44	12	1.5651	57	55.4	36.9	86.8	13.8987	59	54.2	37.6	88.0	12.9201
	M-C_1S_2	22	24	1.5651	47	48.9	40.1	63.6	11.6637	49	47.2	39.4	61.1	11.6919
	M-C_3S_1	66	12	1.5651	79	54.3	31.6	65.8	16.4721	81	53.6	32.9	51.8	14.8864
	M-C_1S_3	22	36	1.5651	59	44.1	36.2	51.6	12.3669	61	42.9	35.6	50.0	12.4676
	M-C_4S_1	88	12	1.5651	101	53.0	27.5	52.3	19.1444	103	52.6	28.9	52.9	16.9832
	M-C_1S_4	22	48	1.5651	71	40.3	32.6	43.5	13.2724	73	39.4	32.1	42.4	13.3986
7	C_1S_1	64	14	1.6266	79	**63.3**	43.6	86.5	14.2137	81	**62.2**	44.4	86.6	13.2031
	M-C_2S_1	60	14	1.6266	75	55.1	36.4	**87.8**	16.7908	77	51.1	36.7	**87.8**	15.9348
	M-C_1S_2	30	28	1.6266	59	48.6	**40.0**	71.5	**14.8497**	61	47.2	**42.3**	69.6	**14.0050**
	M-C_3S_1	90	14	1.6266	105	54.1	31.5	62.7	19.7008	107	53.5	30.9	65.3	18.2650
	M-C_1S_3	30	42	1.6266	73	42.3	30.8	59.1	17.4125	75	41.3	30.2	63.9	17.6470
	M-C_4S_1	120	14	1.6266	135	52.8	27.5	51.3	22.7922	137	52.4	28.3	52.0	20.8112
	M-C_1S_4	30	56	1.6266	87	39.9	30.4	50.5	17.3672	89	39.2	29.9	49.0	17.5943
8	C_1S_1	64	16	1.6818	81	**64.6**	**48.6**	**97.8**	**15.0200**	83	**63.4**	**48.8**	**95.5**	**14.3792**
	M-C_2S_1	76	16	1.6818	93	54.4	34.8	88.2	20.9033	95	53.5	34.9	86.6	20.1946
	M-C_1S_2	38	32	1.6818	71	48.0	36.5	67.4	18.7366	73	46.8	35.7	74.8	18.9788
	M-C_3S_1	114	16	1.6818	131	53.5	30.4	63.8	24.2171	133	52.9	30.8	64.5	22.9634
	M-C_1S_3	38	48	1.6818	87	43.3	32.8	63.1	20.1641	89	42.4	32.2	51.6	20.4552
	M-C_4S_1	152	16	1.6818	169	52.3	26.7	51.0	27.7367	171	52.0	27.2	50.8	25.9764
	M-C_1S_4	38	64	1.6818	103	39.4	29.5	47.9	21.8490	105	38.7	29.1	52.7	22.1507
9	C_1S_1	128	18	1.7321	147	**65.4**	40.7	72.5	21.1389	149	**63.8**	41.2	72.8	20.0633
	M-C_2S_1	92	18	1.7321	111	52.7	32.7	**90.2**	25.7119	113	51.9	32.6	**90.0**	25.1445
	M-C_1S_2	46	36	1.7321	83	46.2	**38.8**	75.2	**22.2643**	85	45.2	**39.2**	72.8	**22.6087**
	M-C_3S_1	138	18	1.7321	157	51.9	29.0	65.1	29.2718	159	51.5	29.6	66.7	27.8372
	M-C_1S_3	46	54	1.7321	101	41.6	29.3	61.6	26.4573	103	40.9	28.8	62.1	26.8388
	M-C_4S_1	184	18	1.7321	203	50.9	25.8	51.8	33.1182	205	50.6	26.1	52.3	38.9939
	M-C_1S_4	46	72	1.7321	137	37.9	25.8	50.6	31.0189	139	37.4	25.4	49.9	35.4484
10	C_1S_1	256	20	1.7783	277	**64.6**	30.9	47.0	32.1642	279	**64.3**	31.4	43.3	30.4235
	M-C_2S_1	112	20	1.7783	133	52.4	30.9	**85.5**	31.8710	134	51.7	30.8	**91.1**	31.3999
	M-C_1S_2	56	40	1.7783	97	46.2	**31.6**	71.3	**29.8301**	99	45.4	31.1	68.6	**30.2375**
	M-C_3S_1	168	20	1.7783	189	51.7	27.5	66.1	35.9967	191	51.3	27.6	65.7	35.0299
	M-C_1S_3	56	60	1.7783	117	41.7	28.6	65.2	32.2445	119	41.0	28.1	60.0	32.6766
	M-C_4S_1	224	20	1.7783	245	50.7	24.6	51.5	40.4091	247	50.5	24.8	52.1	38.9939
	M-C_1S_4	56	80	1.7783	137	40.3	32.6	43.5	33.2774	139	39.4	**32.1**	42.4	33.3986

For the cuboidal axial distance, the results of the design evaluation criteria are presented in Table 2. From the table, the standard CCD gives the best *D* values for all the sets of factors considered. The design option, M-C_2S_1, offers the best values for *G* for all the factors and with different numbers of centre points except for k = 8 where the CCD is superior to the other design options in terms of *G* and possesses the smallest number of design runs. The star-augmented design options, M-C_1S_2, M-C_1S_3 and M-C_1S_4, give *A* and *V* values which are very close and better than those of the CCD for all the sets of experimental factors. However, M-$C_1S_2$with the smallest number of design runs is recommended among them in terms of *A* and *V*. There is substantial gain in recommending M-C_1S_2 for *A* and *V* over the CCD in terms of cost of experimentation. Apart from k = 6 where M-C_1S_2 has two runs more than the CCD, the design saves the experimenter 20 additional runs for k = 7; 10 additional runs for k = 8; 64 additional runs for k = 9 and 180 additional runs for k = 10 over the CCD.

Table 2: Values of Alphabetic Criteria for Comparison of Augmented MinResV Design and the CCD for Cuboidal Alpha

k	Design	*Cube*	Star	α	$n_0 = 1$					$n_0 = 3$				
					N	*D*	*A*	*G*	*V*	*N*	*D*	*A*	*G*	*V*
6	C_1S_1	32	12	1.0000	45	**44.8**	19.0	92.0	17.2985	47	**43.2**	18.3	88.1	17.6710
	M-C_2S_1	44	12	1.0000	57	40.5	14.8	**95.1**	22.9885	59	39.1	14.3	**92.4**	23.2995
	M-C_1S_2	22	24	1.0000	47	34.1	**23.0**	61.6	**16.8279**	49	32.9	**22.1**	59.1	**17.4259**
	M-C_3S_1	66	12	1.0000	79	39.7	11.4	68.6	28.5774	81	39.0	11.2	68.8	28.6138
	M-C_1S_3	22	36	1.0000	59	30.3	22.7	49.7	17.4381	61	29.4	22.1	48.1	17.9612
	M-C_4S_1	88	12	1.0000	101	38.8	09.3	54.3	34.3535	103	38.3	09.1	54.7	34.1554
	M-C_1S_4	22	48	1.0000	71	27.4	21.7	41.7	18.4644	73	26.7	21.2	40.6	18.9383
7	C_1S_1	64	14	1.0000	79	**46.0**	12.9	89.6	30.0270	81	**45.1**	12.6	89.1	30.3017
	M-C_2S_1	60	14	1.0000	75	39.8	12.5	**90.8**	32.1233	77	39.0	12.3	**92.1**	32.5219
	M-C_1S_2	30	28	1.0000	59	34.0	**20.8**	64.6	**22.2747**	61	33.0	**20.2**	66.7	**22.9298**
	M-C_3S_1	90	14	1.0000	105	39.3	09.6	67.3	40.8220	107	38.7	09.4	67.3	40.9521
	M-C_1S_3	30	42	1.0000	73	28.9	19.1	57.2	25.4424	75	28.2	18.6	51.7	26.0944
	M-C_4S_1	120	14	1.0000	135	38.5	07.7	52.7	49.7754	137	38.1	07.6	53.0	49.6878
	M-C_1S_4	30	56	1.0000	87	27.2	19.8	45.3	24.5501	89	26.6	19.4	44.3	25.0777
8	C_1S_1	64	16	1.0000	81	**46.9**	13.4	**96.7**	35.2893	83	**45.9**	13.1	**94.4**	35.7933
	M-C_2S_1	76	16	1.0000	93	39.2	11.0	93.1	44.6324	95	38.5	10.8	92.2	45.1715
	M-C_1S_2	38	32	1.0000	71	33.6	**18.8**	67.1	**29.8536**	73	32.8	**18.3**	67.5	**30.6061**
	M-C_3S_1	114	16	1.0000	131	38.8	08.3	63.3	57.1270	133	38.3	08.2	67.9	57.4067
	M-C_1S_3	38	48	1.0000	87	29.9	19.0	53.5	30.5953	89	29.3	18.6	57.8	31.2500
	M-C_4S_1	152	16	1.0000	169	38.0	06.7	52.4	69.9345	171	37.7	06.6	52.8	69.9980
	M-C_1S_4	38	64	1.0000	103	26.9	18.4	49.5	32.2904	105	26.4	18.0	47.5	32.8853
9	C_1S_1	128	18	1.0000	147	**47.7**	08.5	74.2	64.7292	149	**47.2**	08.4	74.1	65.0985
	M-C_2S_1	92	18	1.0000	111	38.2	09.8	**96.0**	59.3011	113	37.5	09.7	**95.5**	59.9852
	M-C_1S_2	46	36	1.0000	83	32.6	**17.0**	67.4	**39.2230**	85	31.8	**16.6**	66.3	**40.0904**
	M-C_3S_1	138	18	1.0000	157	37.9	07.4	69.5	75.6737	159	37.4	07.3	68.7	76.6377
	M-C_1S_3	46	54	1.0000	101	28.9	17.2	56.8	40.2451	103	28.4	16.8	54.8	40.9997
	M-C_4S_1	184	18	1.0000	203	37.1	05.9	53.5	93.5264	205	36.8	05.9	53.6	93.7439
	M-C_1S_4	46	72	1.0000	137	26.3	15.6	49.8	42.5870	139	25.6	16.2	46.9	43.2750
10	C_1S_1	256	20	1.0000	277	**47.5**	05.0	47.6	127.176	279	**47.2**	05.0	47.7	27.3329
	M-C_2S_1	112	20	1.0000	133	38.1	08.8	**93.9**	78.7324	134	37.6	08.7	**96.0**	79.5510
	M-C_1S_2	56	40	1.0000	97	32.7	**15.7**	69.3	**50.4932**	99	32.1	**15.4**	67.9	**51.4625**
	M-C_3S_1	168	20	1.0000	189	37.7	06.6	68.7	101.656	191	37.4	06.5	68.6	102.212
	M-C_1S_3	56	60	1.0000	117	29.1	16.0	60.0	51.1425	119	28.7	15.7	56.4	51.9779
	M-C_4S_1	224	20	1.0000	245	37.1	05.3	53.2	125.051	247	36.9	05.2	53.7	125.399
	M-C_1S_4	56	80	1.0000	137	26.3	15.6	49.8	53.6003	139	25.9	15.3	48.7	54.3574

The performances of the designs for spherical axial distance are displayed in Table 3. As obtainable in the cases of cuboidal and practical axial distances, the standard CCD gives the best *D* values for all the sets of factors. Also, increasing the number of centre points substantially improves the performances of the *A*, *G* and *V* for all the design options under comparison. With additional centre points, the CCD has overall best values for the four alphabetic criteria for all the sets of factors. Exceptions are values of *V* for *k* = 7, 8 and 10 where M-C_1S_2 is superior while *G* has the best value for *k* = 10.With one centre point, the CCD has the best *A*, *G* and *V* for *k* = 6, the best *A* for *k* = 8 and best *V* for *k* = 9. On the other hand,M-C_1S_2 offers the best results for *A*, *G* and *V* for *k* =7 and 10, best *A* and *G* for *k* = 9and best *G* and *V* for *k* = 8.The best results for M-C_1S_2 are achieved at very substantial gain in cost of experimentation in terms of number of design runs. Obviously, augmenting with the cube of the MinResV CCD offers no advantage for the spherical axial distance.

Table 3: Values of Alphabetic Criteria for Comparison of Augmented MinResV Designs and the CCD for Spherical Alpha

k	Design	*Cube*	Star	*A*	$n_0=1$					$n_0=3$				
					N	*D*	*A*	*G*	*V*	*N*	*D*	*A*	*G*	*V*
6	C_1S_1	32	12	2.4495	45	**83.8**	**33.7**	**62.2**	**25.4624**	47	**83.5**	**55.8**	**94.9**	**12.2040**
	M-C_2S_1	44	12	2.4495	57	76.0	26.9	49.1	32.2950	59	76.4	45.3	77.2	15.3640
	M-C_1S_2	22	24	2.4495	47	70.6	27.6	59.6	28.4433	49	70.4	41.4	84.6	14.6512
	M-C_3S_1	66	12	2.4495	79	73.4	21.5	35.4	42.5574	81	74.5	39.5	66.0	18.8348
	M-C_1S_3	22	36	2.4495	59	64.6	22.6	47.5	34.8107	61	65.0	34.8	54.0	17.3142
	M-C_4S_1	88	12	2.4495	101	71.0	17.8	27.7	52.8513	103	72.4	34.8	54.2	22.3621
	M-C_1S_4	22	48	2.4495	71	59.5	19.1	39.4	41.2457	73	60.2	29.9	62.9	20.0569
7	C_1S_1	64	14	2.6458	79	**85.5**	28.1	45.6	41.9131	81	**85.9**	**51.6**	**83.7**	18.2884
	M-C_2S_1	60	14	2.6458	75	75.5	25.8	48.0	42.5361	77	75.8	42.6	81.5	20.2037
	M-C_1S_2	30	28	2.6458	59	70.1	**27.6**	**61.0**	**36.5567**	61	69.9	38.4	72.8	**17.2054**
	M-C_3S_1	90	14	2.6458	105	73.3	20.7	34.3	56.2895	107	74.1	37.6	62.9	24.7502
	M-C_1S_3	30	42	2.6458	73	62.5	21.3	50.0	44.4907	75	62.7	30.7	62.0	23.1741
	M-C_4S_1	120	14	2.6458	135	71.0	17.2	26.7	70.1132	137	72.2	33.4	51.3	29.3999
	M-C_1S_4	30	56	2.6458	87	59.1	18.8	41.4	51.8540	89	59.6	28.2	60.2	25.9235
8	C_1S_1	64	16	2.8284	81	**87.9**	**28.1**	55.6	44.0550	83	**87.9**	**56.0**	**98.6**	19.9354
	M-C_2S_1	76	16	2.8284	93	74.7	25.2	48.4	53.3882	95	74.9	40.5	78.8	25.6845
	M-C_1S_2	38	32	2.8284	71	69.1	26.3	**63.4**	**44.8608**	73	68.8	37.1	72.5	**19.5419**
	M-C_3S_1	114	16	2.8284	131	72.6	20.3	34.4	70.8074	133	73.3	36.0	62.4	31.4958
	M-C_1S_3	38	48	2.8284	87	63.1	22.1	51.7	53.6649	89	63.3	31.7	55.0	27.8690
	M-C_4S_1	152	16	2.8284	169	70.6	16.9	26.6	88.2919	171	71.5	32.0	50.6	37.4035
	M-C_1S_4	38	64	2.8284	103	58.0	19.0	43.7	62.5871	105	58.3	27.6	48.7	31.9135
9	C_1S_1	128	18	3.0000	147	**87.9**	24.9	37.4	**44.0550**	149	**88.5**	**56.0**	**98.6**	**19.9354**
	M-C_2S_1	92	18	3.0000	111	72.2	24.3	49.6	65.1962	113	72.4	37.4	82.0	32.1454
	M-C_1S_2	46	36	3.0000	83	66.4	**24.9**	**66.3**	54.8003	85	66.1	33.6	77.8	30.3760
	M-C_3S_1	138	18	3.0000	157	70.5	19.9	35.0	86.1381	159	71.0	33.8	62.4	39.0774
	M-C_1S_3	46	54	3.0000	101	60.6	21.0	54.5	65.1289	103	60.6	28.8	66.6	35.2219
	M-C_4S_1	184	18	3.0000	203	68.8	16.7	26.8	107.187	205	69.5	30.4	50.5	46.1534
	M-C_1S_4	46	72	3.0000	137	55.6	18.1	46.2	75.6030	139	55.8	25.1	56.4	40.2251
10	C_1S_1	256	20	3.1623	277	**86.2**	17.6	23.8	135.557	279	**87.0**	**37.9**	48.3	52.2161
	M-C_2S_1	112	20	3.1623	133	71.7	23.6	49.6	79.1559	134	71.8	35.8	**85.1**	39.5489
	M-C_1S_2	56	40	3.1623	97	66.1	**24.8**	**68.1**	**64.9684**	99	65.8	33.1	72.6	**36.3880**
	M-C_3S_1	168	20	3.1623	189	70.0	19.3	34.9	104.7890	191	70.5	32.2	62.5	48.1734
	M-C_1S_3	56	60	3.1623	117	60.4	21.2	56.4	76.4313	119	60.4	28.7	76.6	41.7734
	M-C_4S_1	224	20	3.1623	245	68.4	16.3	26.9	130.4786	247	69.0	29.1	51.2	56.8949
	M-C_1S_4	56	80	3.1623	137	55.5	18.4	48.2	88.1116	139	55.6	25.2	63.8	47.3890

Furthermore, we make critical comparison of the selected superior designs based on their axial distances. The results have already shown that the CCD has superior values for *D* for the three axial distances. We now compare the CCD with practical alpha (CCD-practical) with the CCD with cuboidal alpha (CCD-cuboidal) and the CCD with spherical alpha (CCD-spherical). In general, the best values for *D* are obtained using the spherical alpha. Therefore, CCD-spherical is superior to

CCD-practical and CCD-cuboidal for the sets of factors considered irrespective of number of centre points. Also, M-C_1S_2-practical offers the best results for *V*-criterion for all the sets of factors irrespective of the number of centre points and is therefore, superior to M-C_1S_2-cuboidal and M-C_1S_2-spherical in evaluating responses using *V*.

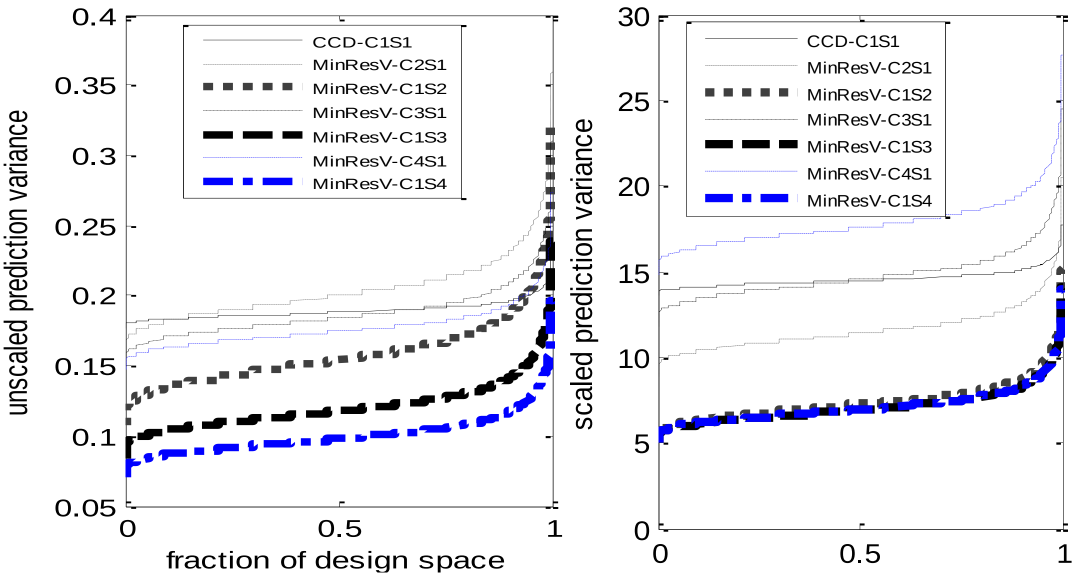
For the *A*-efficiency, CCD-practical has superior values for k = 6 and 8 factors while M-C_1S_2-practical has the best values for k = 7, 9 and 10 factors at $n_0 = 1$centre point. At$n_0 > 1$, CCD-spherical has superior *A* values for k = 6, 7, 8 and 9 factors while M-C_2S_1-sphericalhas superior value for k = 10 factors. Though the CCD-spherical gave *A* value that is slightly higher than that of M-C_2S_1-spherical for k = 10, the 5.9 percent gain in efficiency by the CCD-spherical over the M-C_2S_1-spherical is achieved with 145 additional design runs which makes recommending the CCD-spherical untenable.

For the *G*-efficiency, M-C_2S_1-cuboidal offers superior values for k = 6, 7, 9 and 10 factors at $n_0 = 1$centre point while CCD-practical gave highest value for k = 8 factors. For$n_0 > 1$, M-C_2S_1-cuboidal is superior for k = 7, 9 and 10 factors while CCD-spherical is superior for k = 6 and 8 factors. The M-C_2S_1-cuboidal is recommended over the CCD-spherical for k = 9 factors despite the later having slightly higher *G*-efficiency value than the augmented alternative design. However, the 3.3 percent gain in efficiency by the CCD-spherical is achieved at the expense of additional 37 design runs. This may not augur well for expensive industrial experiments.

3.2. Evaluation with Fraction of Design Space Graphs

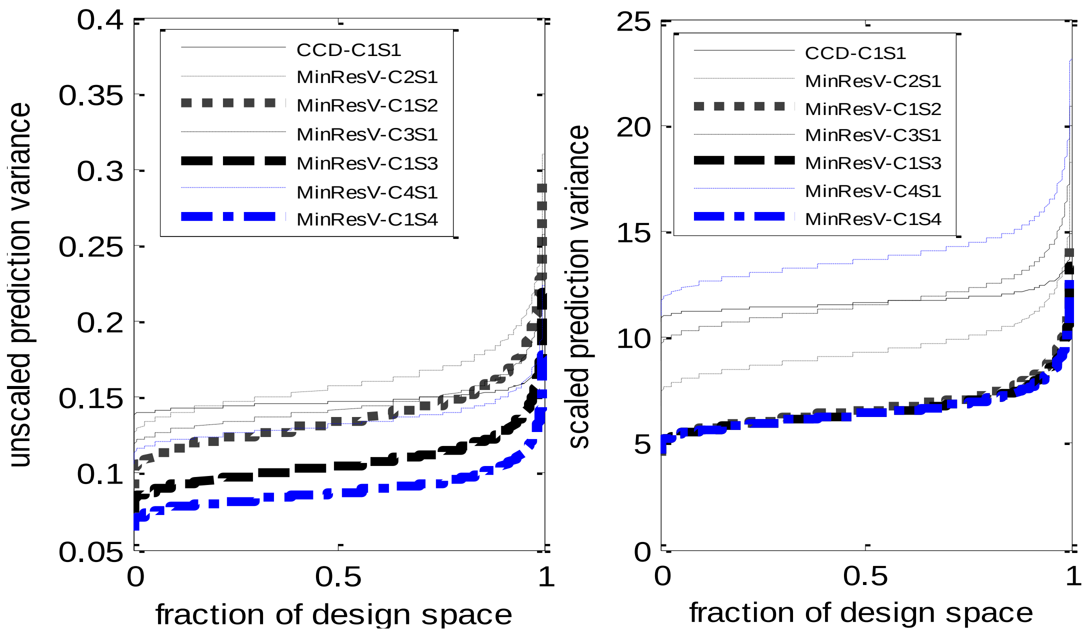
One of the major objectives of design evaluation and comparison is to identify the design that could be used to predict responses with the most precision among several competing designs. Therefore, improving the prediction capability of the designs is a good experimental strategy. When the practitioner is interested in understanding the prediction variance distribution throughout the design region; 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 precision, graphical methods offer the best approach for exploring the prediction properties of competing designs. The fraction of design space graphs (FDSG) are used to display the prediction variance characteristics of the augmented MinResV designs and the standard CCD throughout the entire design region for the scaled and unscaled prediction variances. The unscaled prediction variance is given as $f'(x)(X'X)^{-1}f(x)$. Since the prediction variance results for each specific axial distance are the same for all the factors, only the graphs for k = 6factors are presented for the practical and spherical axial distances while graphs for k = 7 factors are presented for the cuboidal axial distance for illustration.

The graphs are displayed in Figures 2 and 3 for k = 6 factors for the practical axial distance. In general, for $6 \le k \le 10$ factors, the star-augmented MinResV CCDs, M-C_1S_2, M-C_1S_3 and M-C_1S_4, displayed the best minimum scaled and unscaled prediction variances throughout the entire design region. Figure 2(a) shows the graphs of the CCD and augmented variations of the MinResVCCD for the unscaled and scaled prediction variances, with one centre point, respectively. The direction of the lines shows the spread of the prediction variances in the design region. The closer the line is to the horizontal axis, the smaller the prediction variance and the better the prediction capability of the design while the farther away the line is from the horizontal axis, the higher the values of the prediction variances and the poorer the prediction capability of the design. The design, M-C_1S_4, is preferred for the UPV while M-C_1S_2 is recommended for the SPV.



(a) (b)

Figure 2: FDSG of (a) Unscaled and (b) Scaled Prediction Variances for $k = 6$ at $n_0 = 1, \alpha = \sqrt[4]{k}$

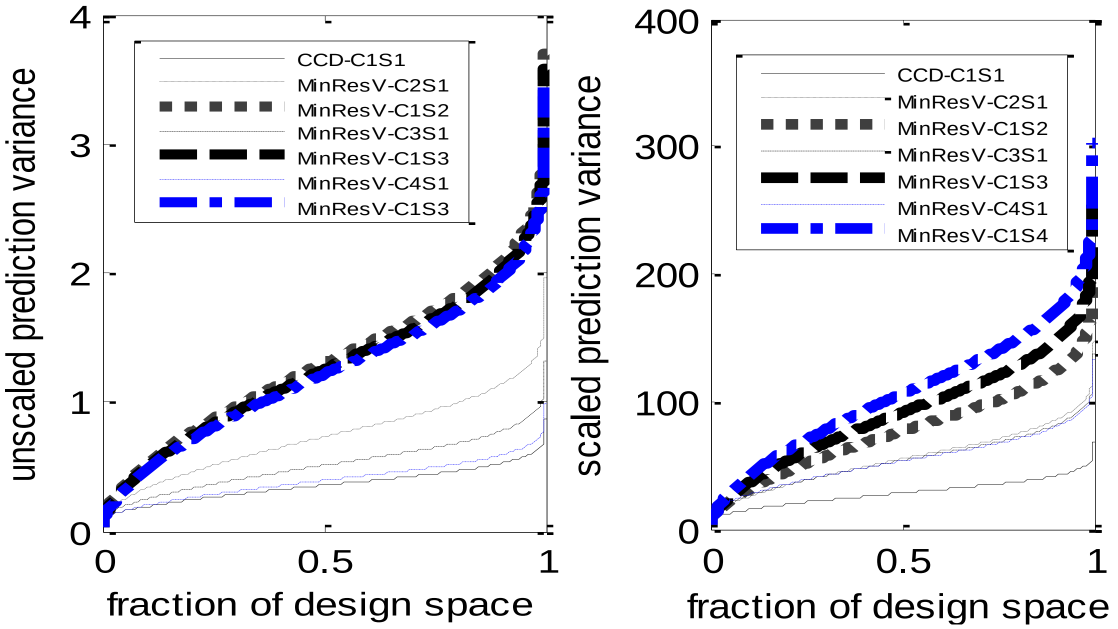


(a) (b)

Figure 3: FDSG of (a) Unscaled and (b) Scaled Prediction Variances for $k = 6$ at $n_0 = 3, \alpha = \sqrt[4]{k}$

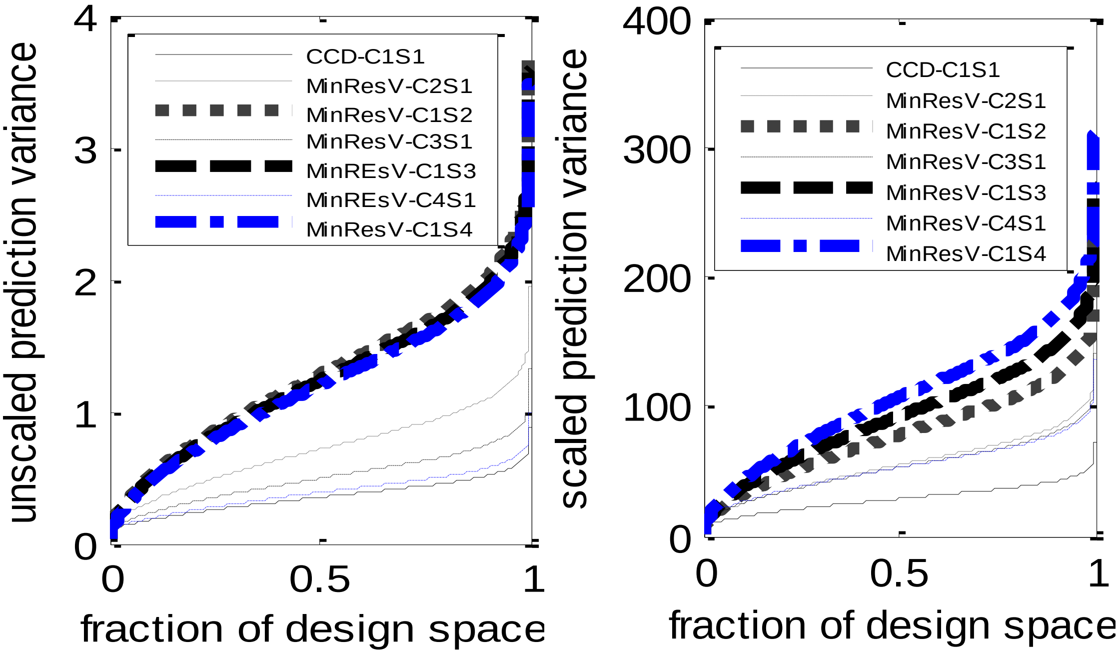
For the cube-augmented MinResV CCD variations, scaling affects their prediction variance performances as the higher the augmentation (which entails higher design runs and cost), the higher the prediction variance. The case is different when the star is used for augmentation. Scaling makes the designs to have almost the same small but stable prediction variances. The MinResV CCD option, M-C_1S_4, for the unscaled prediction variance is recommended if the experimenter is more interested in minimum variance of prediction than the cost of experimentation. However, if the experimenter is restricted by cost, the design option, M-C_1S_2, with minimum scaled prediction variance is recommended for predicting responses with precision.

The FDS plots for k = 7 factors for the cuboidal axial distance are presented in Figures 4 and 5 for unscaled and scaled prediction variances. In general, the standard CCD has the most stable and minimum prediction variance spread across the entire design region for the unscaled and scaled prediction variances and for all the factors considered. Hence, for the cuboidal axial distance, augmentation of the MinResV CCD is not necessary and the CCD is recommended over the other design options for predicting responses in the cuboidal region.



(a) (b)

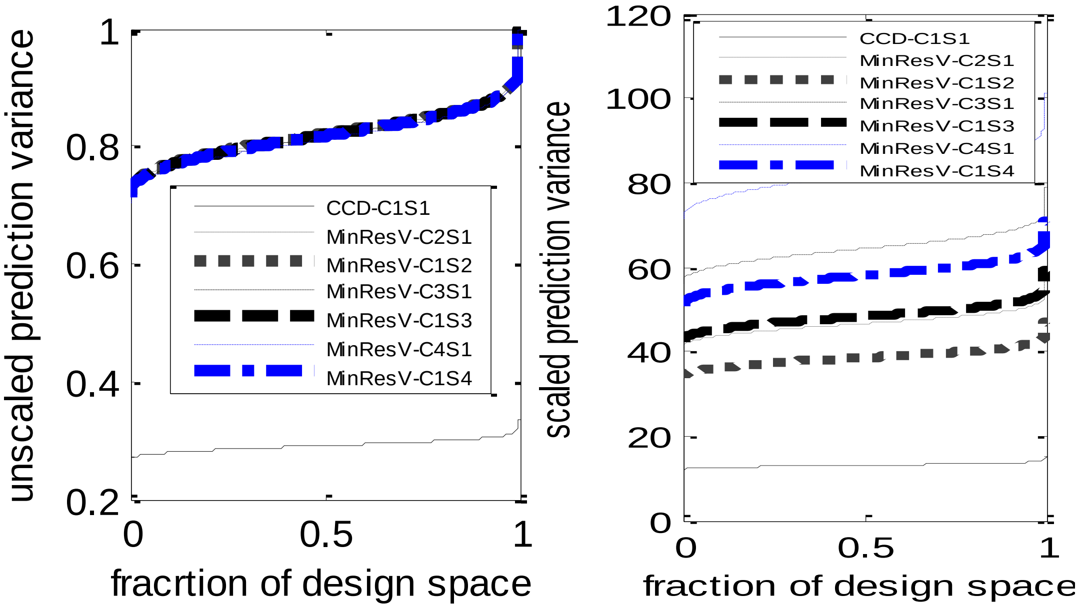
Figure 4: FDSG of (a) Unscaled and (b) Scaled Prediction Variance for k = 7 at $n_0 = 1$, $\alpha = 1$



(a) (b)

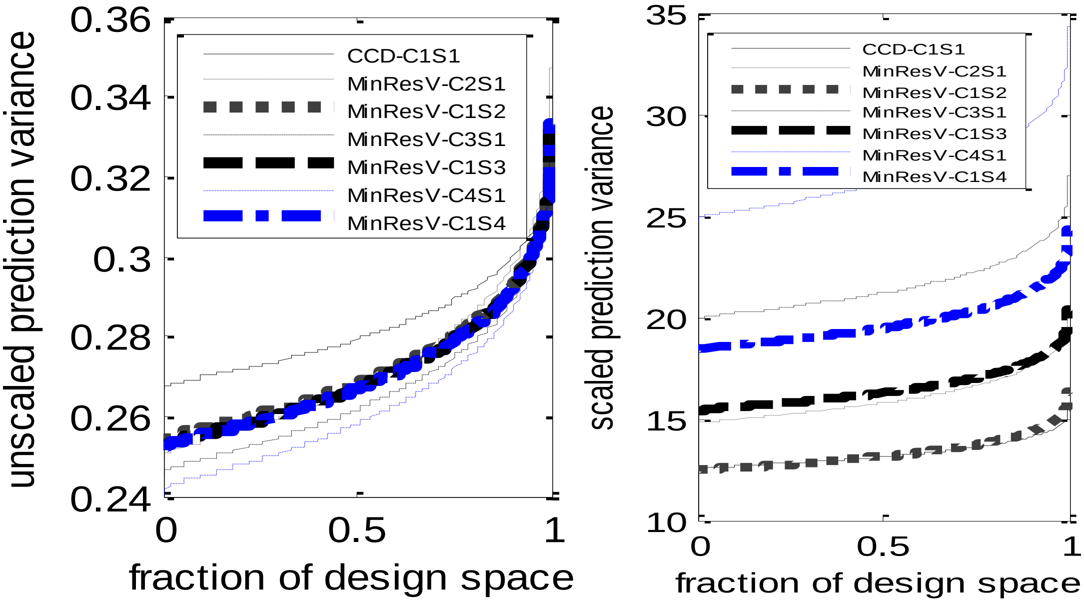
Figure 5: FDSG of (a) Unscaled and (b) Scaled Prediction Variance for k = 7 at $n_0 = 3$, $\alpha = 1$

For spherical axial distance, the FDS plots for k = 6 are displayed in Figures 6 and 7 for the unscaled and scaled prediction variances. Except for k = 6, where the standard CCD gives the best spread of minimum scaled and unscaled prediction variances for $n_0 = 1$ centre point, the MinResV CCD option, M-C_1S_2, is the best in terms of uniform spread of minimum scaled prediction variances throughout the entire design region. The unscaled prediction variances are very unstable and cannot be recommended for design evaluation involving spherical alpha. Therefore, the design option, $M - C_1S_2$, which consistently has substantial smaller number of runs than the standard CCD is recommended over the other designs for predicting responses.



(a) (b)

Figure 6: FDSG of (a) Unscaled and (b) Scaled Prediction Variance for k = 6 at $n_0 = 1$, $\alpha = \sqrt{k}$



(a) (b)

Figure 7: FDSG of (a) Unscaled and (b) Scaled Prediction Variance for k = 6 at $n_0 = 3$, $\alpha = \sqrt{k}$

We further compare some of the designs with superior prediction variance properties according to their axial distances. First, we consider M-C_1S_4-practical which we recommended for unscaled prediction variance because of its superior performances with practical axial distance. This design is compared with CCD-cuboidal and CCD-spherical for k = 6 factors. The comparison is aided by the fact that these designs are superior for their respective axial distances for the unscaled prediction variance criterion where number of runs is trivial. The fraction of design space plots are presented in Figure 8. The graph shows that M-C_1S_4-practical displays the smallest and stable prediction variance properties throughout the entire design region. Therefore, the M-C_1S_4-practical design option is recommended over the CCD-cuboidal and CCD-spherical for k = 6 experimental factors when the number of design runs is not relevant.

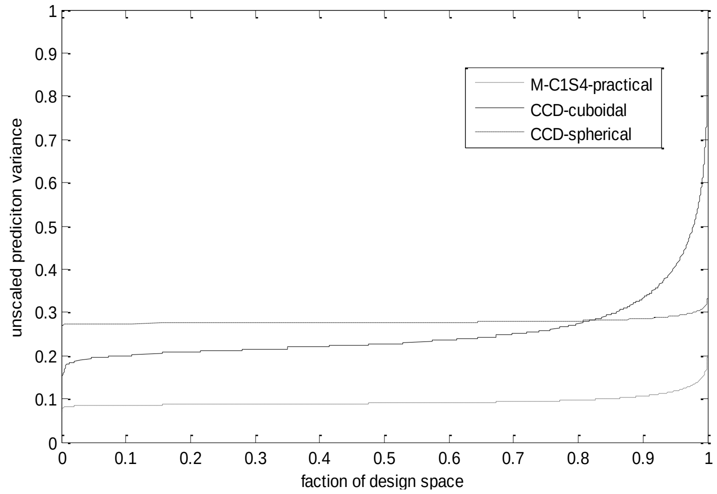


Figure 8: FDSG of M-C_1S_4-practical, CCD-cuboidal and CCD-spherical for k = 6 Factors, $n_o = 1$

It has already been known in this work that the standard CCD has superior scaled and unscaled prediction variance properties when $\alpha = 1$ and therefore requires no further consideration. We focus on the practical and spherical axial distances where the design options, M-C_1S_2-practical and M-C_1S_2-spherical, respectively, offer best scaled prediction variance properties for all the sets of experimental factors under consideration when $n_0 \geq 1$. The fraction of design space graphs show that for k = 6, 7, 8, 9 and 10 factors, the MinResV CCD option, M-C_1S_2-practical, consistently displays smaller scaled prediction variances throughout the design region. The graphs for k = 7 and 8 are displayed in Figures 9 and 10, respectively, for further illustration. Therefore, M-C_1S_2-practical is recommended over the M-C_1S_2-spherical which has the same number of experimental runs as the M-C_1S_2-practical for all the factors.

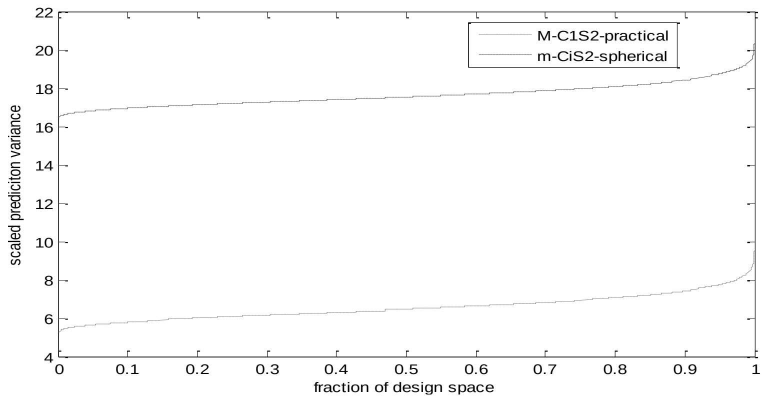


Figure 9: FDSG of M-C_1S_2-practical and M-C_1S_2-spherical for k =7, $n_0 = 1$

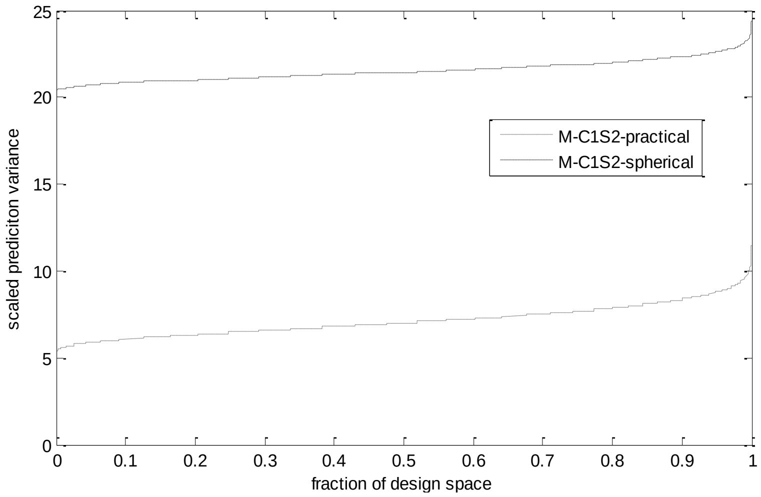


Figure 10: FDSG of M-C_1S_2-practical and M-C_1S_2-spherical for k =8, $n_0 = 3$

4. Conclusion and Recommendations

From the foregoing, there are merits in augmenting the MinResV CCD in comparison with the standard CCD. Except for k = 6 and 8 factors with practical alpha where the standard CCD offers the best values for the four alphabetic criteria, the MinResV CCD options, M-C_2S_1, offers superior performances for *G*-efficiency for $n_0 \geq 1$ centre points with smaller number of runs than the CCD in most cases. The M-C_1S_2 has superior values for *A*-efficiency and *V*-criterion in most cases for all the axial distances and best *G*-efficiency values for spherical alpha with $n_0 = 1$ and with the smallest number of runs. The standard CCD offers the best values for *D*-efficiency across the axial distances and for $n_0 \geq 1$.

Further comparisons of the designs based on their axial distances show that the best *D*-efficiency values are obtained with the spherical axial distance, $\alpha = \sqrt{k}$. Therefore, CCD-spherical is recommended for estimating the *D*-efficiency. Also, best (lowest) values for the *V*-criterion are obtained using M-C_1S_2 having the practical axial distance. Hence, M-C_1S_2-practical is recommended for estimating the *V*-criterion. The design, M-C_1S_2-practical is recommended for estimating *A*-efficiency while M-C_2S_1-cuboidal is recommended for estimating the *G*-efficiency for some sets of factors. In most cases, the augmented design alternatives are recommended over the standard CCD with substantial gain in cost of experimentation depicted by the number of experimental runs, *N*.

Attempts made to harness the advantages of the graphical evaluation of response surface designs over single-value criteria yielded some interesting results. The fraction of design space plots of the scaled and unscaled prediction variances show that the star-augmented MinResV CCD options consistently give stable spread of minimum scaled and unscaled prediction variances in spherical region. Among the star-augmented designs, M-C_1S_2 displays the best minimum scaled prediction variance properties while M-C_1S_4 has the best unscaled prediction variances for the practical axial distance. However, the standard CCD is superior to the augmented design options in the cuboidal region with $\alpha = 1$ irrespective of number of centre points. If an experimenter can afford the standard CCD, it is better to use the MinResV CCD option, M-C_1S_2, with practical and spherical axial distances, and which has the extra advantage of smaller design runs in most cases than the CCD. The exception is in the cuboidal region.

Further graphical comparisons across axial distances, especially for the designs with equal number of design runs show that the design, M-C_1S_2-practical consistently displayed superior scaled prediction variance characteristics and is recommended over M-C_1S_2-spherical. Overall, augmenting the MinResV CCD with one star improves the designs performances and offers formidable alternative with smaller experimental runs than the standard central composite design in most cases. Exception is the cuboidal region where augmentation of the MinResV CCD does not improve the design's prediction variance characteristics.

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