On the Prediction Variance Performance of Replicated Minimum-Run Resolution V Designs

F. I. Nsude[1, 2], E. C. Ukaegbu[3], and O. Elem-Uche[3]

The Minimum-run resolution V (MinResV) central composite designs used in response surface exploration offer a smaller number of experimental runs when compared to the standard central composite design (CCD), which is an advantage when considering the cost of experimentation. However, the evaluation of the MinResV design has focused on replicating only the centre point for error estimation. Replicating the other portions of the design and the implications have not yet been considered in previous related studies. The cube and star portions of the Minimum-run resolution V (MinResV) designs have been replicated, evaluated and compared using the A-, D-, G- and I-optimality criteria. The stability and prediction capabilities of the designs generated by partial replication of the portions of the MinResV designs are tracked using the fraction of design space (FDS) graph. In this study, these graphs were plotted for the scaled and unscaled prediction variances of the partially replicated variations of the MinResV designs in the spherical regions. For the k=6, 7, 8, 9 and 10 factors considered in this study, the MinResV CCDs with star-replicated designs performed better than the cube-replicated designs in terms of minimum spread of scaled and unscaled prediction variances.

Keywords: MinResV designs, partial replication, prediction variance, optimality criteria

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1.0 Introduction

Minimum-Run resolution V (MinResV) designs are equi-replicated two-level irregular fractions of resolution V, often used for screening and estimations. Oehlert and Whitcomb (2002) developed this class of response surface designs as a smaller alternative to standard Central Composite designs (CCD). Generally, CCDs are known to consist of regular fractions (called the "cube") of at least resolution V, axial runs (called the "star") and centre runs. In the construction of MinResV composite designs, the regular fraction or cube portion of the CCD is replaced by the MinResV fraction, but it still consists of the same number of star runs and centre points: see, for example, Li et al (2009). This design usually has a smaller number of experimental runs when compared to the standard CCD, especially as the number of factors, k, increases.

The design matrix, X, of the MinResV design for six factors with one centre point is given as

[1] Corresponding Email: ijelink@gmail.com

[2] Department of Maths/Statistics, Akanu Ibiam Federal Polytechnic Unwana
[3] State University of Medical and Applied Sciences, Igbo-Eno,Enugu State

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} = \overbrace{\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{matrix}}^{min\, resV fraction} \overbrace{\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -\alpha & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\alpha & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\alpha & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\alpha & \alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\alpha & \alpha & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\alpha & \alpha \end{matrix}}^{starrun} \overbrace{\begin{matrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{matrix}}^{centrerun}$$

Traditionally, only the centre point of the CCD is replicated n_0 times for the estimation of experimental error. However, in reality, by replicating only the centre point, variability may not be adequately accounted for since variability is not expected to be constant throughout the design region. As Dykstra (1960) rightly pointed out, if variability increases elsewhere aside from the centre of the design region, the associated experimental error may be too small to properly evaluate the model parameters. On this note, some authors have suggested replication at other portions of the design to adequately estimate the experimental error: see, for example, Giovannitti-Jensen and Myers (1989).

In this study, we focus on partially replicating the cube and star portions of the MinResV CCD for error estimation. The objective for the partial replication of the portions of this design in this study is to assess the behaviour of the design's scaled and unscaled prediction variances as well as the prediction capabilities when other portions of the, design except the centre point, are replicated. To achieve this, the maximum and average points of the scaled prediction variances of the designs were studied using the *G*- and *I*-optimality criteria, while the fraction of design space (FDS) graphs were used to track the scaled and unscaled prediction variances throughout the design space.

2. Literature Review

In this section, we start by introducing the model that is used to describe the relationship between the variables under study. Generally, the response surface model of equation (1) is used to describe the relationship between the response variable, y, and the k prediction variables. The model is given by

$$Y = X'\beta + e, \tag{1}$$

where Y = $N \times 1$ vector of responses, X = $N \times p$ design matrix expanded to model form and which is derived from the $N \times k$ design matrix, β = vector of the unknown p model parameters, and e = random error associated with y; e follows the normal distribution with zero mean and variance, σ^2 . Appropriately, each row of X represents an experimental observation involving the different levels of the factors, such that the total number of rows accounts for the total number of design runs. N, while each column of X represents a model parameter such that the total number of columns gives the total number of model parameters, p, to be estimated.

However, in many experimental situations, the relationship between the response and predictor variables is more adequately described by a second-order response surface model (see Ukaegbu and Chigbu, 2017),

$$y(x) = \beta_0 + x'\beta + x'Bx + e. \tag{2}$$

Here, x = point in the design space spanned by the design, and $B = k \times k$ matrix with the diagonal elements being the pure quadratic terms and the off-diagonal elements being the mixed quadratic or interaction terms.

Now, every point, x, in the design space, it has a prediction variance given by

$$Var[\hat{y}(x)] = \sigma^2 x'(X'X)^{-1}x. \qquad (3)$$

$x' = [1, x_1, x_2, \ldots, x_k; x_1^2, \ldots, x_k^2; x_1x_2, \ldots, x_{k-1}x_k]$ is the vector of points in the design space expanded to model form. The scaled prediction variance (SPV) is obtained by multiplying equation (3) by N and dividing by the process variance, σ^2. That is,

$$\frac{Nvar[\hat{y}(x)]}{\sigma^2} = Nx'(X'X)^{-1}x. \qquad (4)$$

It is known that the scaling is very useful when comparing competing designs of various sizes, and it penalises larger designs concerning the smaller ones. For further information on the scaling of prediction variance, see Anderson-Cook et al. (2009), Li et al. (2009) and Umegwuagu et al. (2020).

Some practitioners prefer the standardised or unscaled prediction variance (UPV) given in equation (5) for design evaluation and comparison. The UPV is

$$\frac{var[\hat{y}(x)]}{\sigma^2} = x'(X'X)^{-1}x. \qquad (5)$$

In this case, the quality of the designs under comparison is not considered as a function of cost; rather, the UPV is useful in comparing designs of different sizes in order to know if the variance of the predicted response is substantially reduced by increasing the number of runs of larger designs. Piepel (2009) and Goos (2009) presented further justification for the use of the UPV in design evaluation and comparison.

In this study, we explored the prediction capabilities of variations of the partially replicated MinResV CCDs by tracking the qualities of the SPV and UPV in the spherical region. The number of factors under consideration here is $k = 6$, 7, 8, 9 and 10.

3. Methods

3.1 Optimality Criteria

Two optimality criteria that are directly related to the measure of the scaled prediction variance of the design are used to study the maximum and average measures of the SPV. They are the *G*- and *I*-optimality criteria.

G-Optimality

The *G*-optimality criterion is known to minimise the maximum SPV of a design over the region of interest. Symbolically, the *G*-optimality is expressed as

$$G = minmax\left\{\frac{Nvar[\hat{y}(x)]}{\sigma^2}\right\}. \qquad (6)$$

I-Optimality

The *I*-optimality is also known as the *V*-optimality or *IV*-criterion and minimises the normalised average integrated SPV in the region R of interest. The *I*-optimality is defined as

$$I = min\frac{1}{k}\int_R V[\hat{y}(x)]dx. \quad (7)$$

3.2 Fraction of design space plots

The fraction of design space (FDS) graph, developed by Zahran et al (2003), is used as a tool for evaluating the spread of the prediction variances of any design throughout the design region. This graphical technique has been used extensively in robust design evaluations and designs with mixture components, see, for example, Ozol-Godfrey (2004), Anderson-Cook, Borror and Montgomery (2009) and Jang and Anderson-Cook (2011). The stability and prediction capability of a design is measured by the flatness of the graph so that, a design with flatter graphs has stronger stability and higher prediction capability.

3.3 Design replication

In this study, the cube was replicated n_c times and the star was replicated n_s, such that the MinResV CCD uses a total of $N = n_c f + 2n_s k + n_0$ observations or runs for model parameter estimation. The pattern of replication is that if the cube (C) is replicated, then the star (S) is not replicated and vice versa. In each case, the number of centre points used is $n_0 = 1$. Therefore, the first design variation is C_2S_1, in which there is the replication of the cube portion twice, and there is no replication of the star portion. The second design variation is C_1S_2, in which there is the replication of the star portion twice, but there is no replication of the cube portion. The other design variations include C_3S_1, C_1S_3, C_4S_1 and C_1S_4. These design variations were compared with the standard MinResV CCD, C_1S_1, where the cube and star portions are not replicated. The replication procedure adopted here is an extension of Draper (1982). For other forms of replication of the CCD and mixed resolution designs, see Dykstra (1960), Borkowski (1995), Borkowski and Lucas (1997), and Borkowski and Valeroso (2001).

4. Results and Discussion

In this section, we evaluate the prediction variances of the seven variations of the MinResV designs and compare the results using the two optimality criteria and FDS plots. Statistical package JMP (version 12) was used to obtain the values of the optimality criteria and the FDS graphs.

4.1 Comparison using *I*-optimality

The results of the *I*-optimality were presented in Table 1. For $k = 6$, 7, 8, 9 and 10 factors, the star-replicated MinResV CCD gave smaller values of *I*-optimalilty when compared with other design variations. The MinResV CCD with higher replication of the star portion, C_1S_3 and C_1S_4 have *I*-optimal values that compete favourably for all the factors under consideration. Though C_1S_4 have slightly smaller *I*-optimal values but C_1S_3 compensated for this with a smaller number of runs. The replicated cube designs and C_1S_1 have poor I-optimal values when compared with the star designs. The *I*-optimal values of these designs get worse as the replication and number of runs increase, making these designs undesirable.

Table 1: Summary Statistics for the Design Optimality Criteria

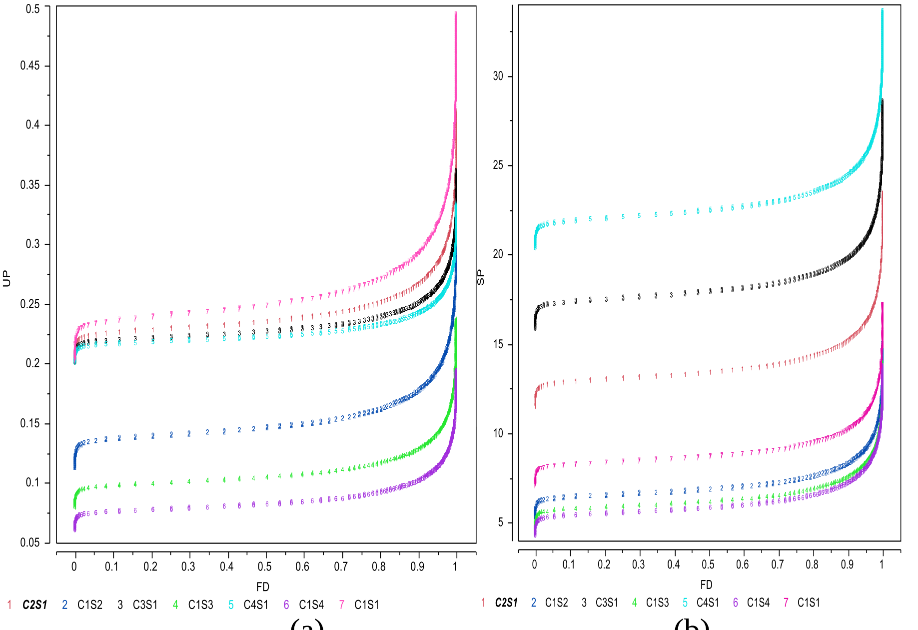
k	Design	N	*I*-Optimality	*G*-Optimality	*k*	Design	N	*I*-Optimality	*G*-Optimality
6	C_1S_1	35	12.16	17.25	9	C_1S_1	65	13.07	15.11
	C_2S_1	57	17.48	23.48		C_2S_1	111	20.44	22.67
	C_1S_2	47	10.20	15.08		C_1S_2	83	10.02	12.67
	C_3S_1	79	22.25	28.61		C_3S_1	157	28.17	30.67
	C_1S_3	59	9.35	14.02		C_1S_3	101	9.21	12.17
	C_4S_1	101	27.02	33.68		C_4S_1	203	36.32	39.85
	C_1S_4	71	**9.07**	**13.81**		C_1S_4	119	**8.81**	**12.15**
7	C_1S_1	45	10.77	12.49	10	C_1S_1	77	14.99	17.79
	C_2S_1	75	16.28	18.03		C_2S_1	133	23.88	27.25
	C_1S_2	59	8.68	10.77		C_1S_2	97	11.02	13.84
	C_3S_1	105	22.78	25.51		C_3S_1	189	32.19	35.49
	C_1S_3	73	7.90	**10.21**		C_1S_3	117	9.56	12.55
	C_4S_1	135	29.20	32.99		C_4S_1	245	40.73	44.31
	C_1S_4	87	**7.70**	10.40		C_1S_4	137	**8.94**	**12.22**
8	C_1S_1	55	12.57	15.20					
	C_2S_1	93	18.91	21.45					
	C_1S_2	71	9.57	12.11					
	C_3S_1	131	25.61	28.33					
	C_1S_3	87	8.77	11.67					
	C_4S_1	169	32.99	36.64					
	C_1S_4	103	**8.39**	**11.60**					

4.2 Comparison with *G*-optimality Criterion

The results for the *G*-optimality criterion are shown in Table 1. It could be observed that the three MinResV CCD with replication of the star portion have smaller values of the *G*-optimality criterion than the other design variations. Although these star-replicated MinResV CCDs compete favourably, C_1S_4 has the smallest *G*-optimal values for all the factors being studied. The replicated cube designs and C_1S_1 behave in a similar manner to the *I*-optimality criterion, with the *G*-optimal values increasing as the number of runs increases.

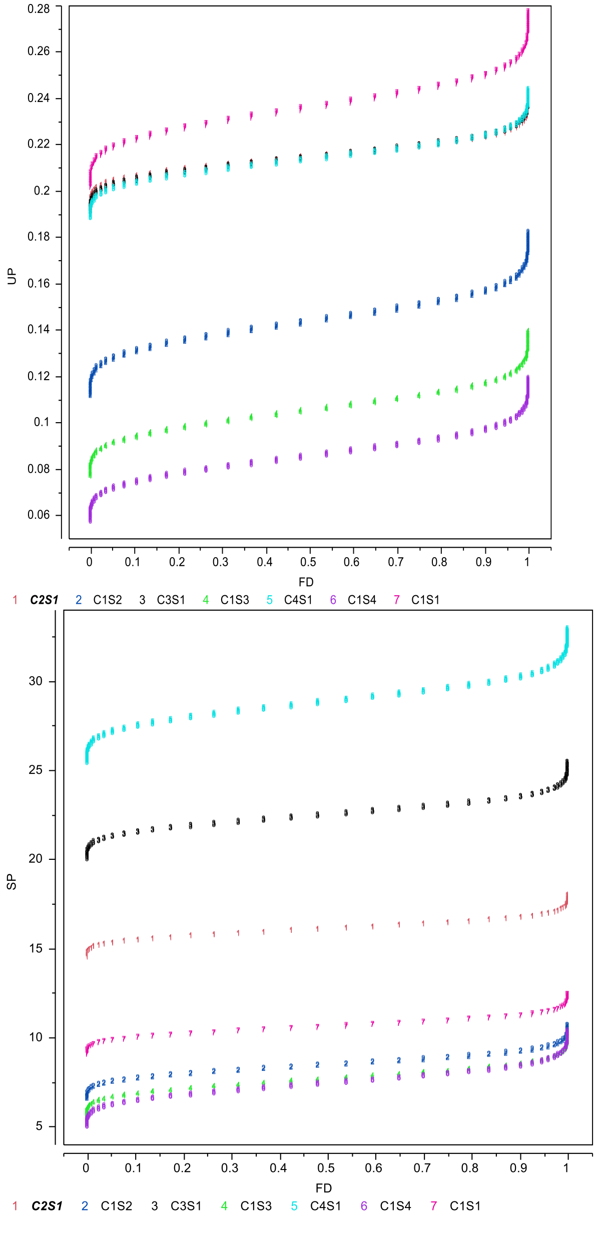
4.3 Comparison using fraction of design space plots

The FDS plots for the unscaled and scaled prediction variances are displayed in Figures 1, 2, 3, 4 and 5 for 6, 7, 8, 9 and 10 factors, respectively. For all the factors and both the scaled and unscaled prediction variances, the FDS plots show that star-replicated MinResV CCD options displayed flatter graphs closer to the horizontal line, which indicates the spread of minimum prediction variances for almost all the fractions of the design space. The FDS plots for the SPV of the higher replicated star designs, C_1S_3 and C_1S_4, show that these two designs compete favourably with little dispersion, though C_1S_4 tends to be better with smaller prediction variances.



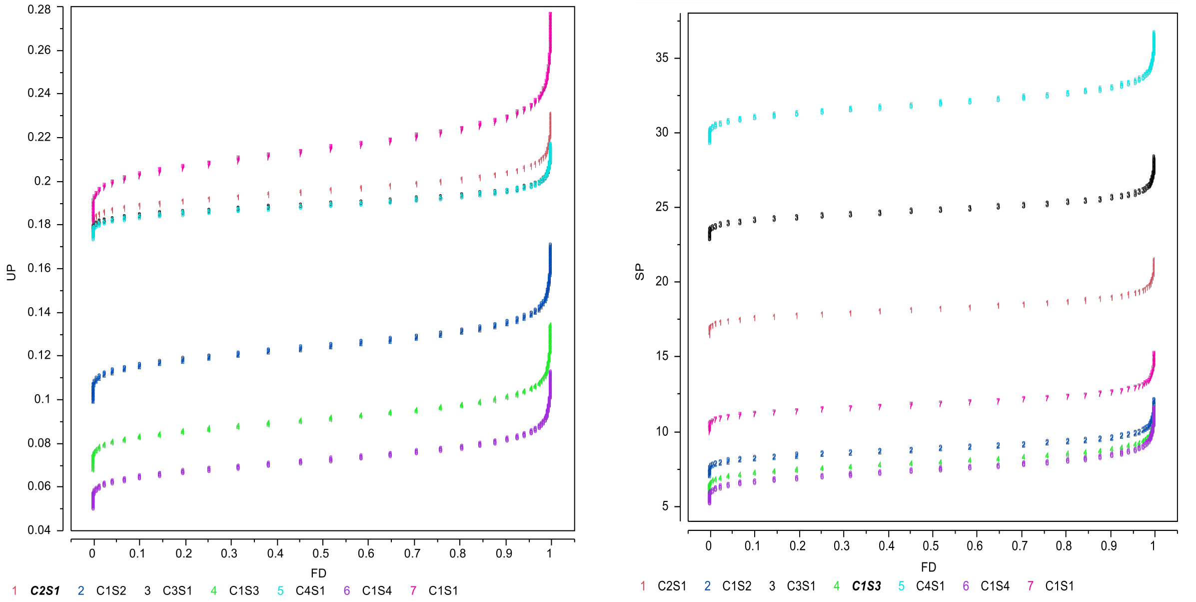
(a) (b)

Figure 1: FDS plots for (a) Unscaled and (b) Scaled Prediction Variances, $k = 6$ factors



(a) (b)

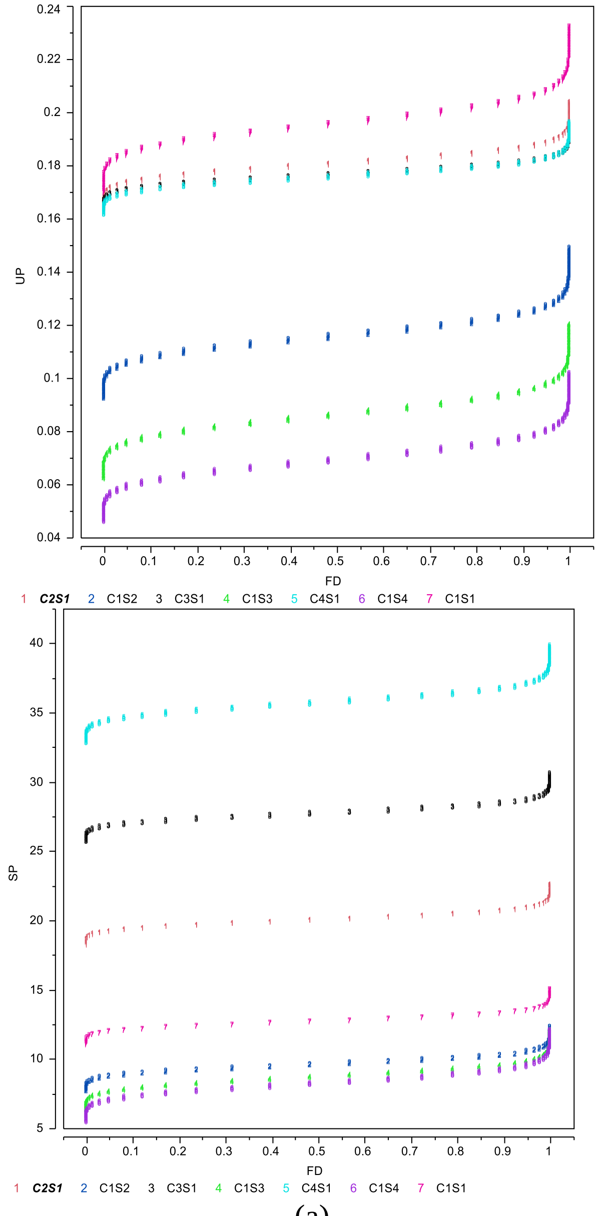
Figure 2: FDS plots for (a) Unscaled and (b) Scaled Prediction Variances, $k = 7$ factors



(a) (b)

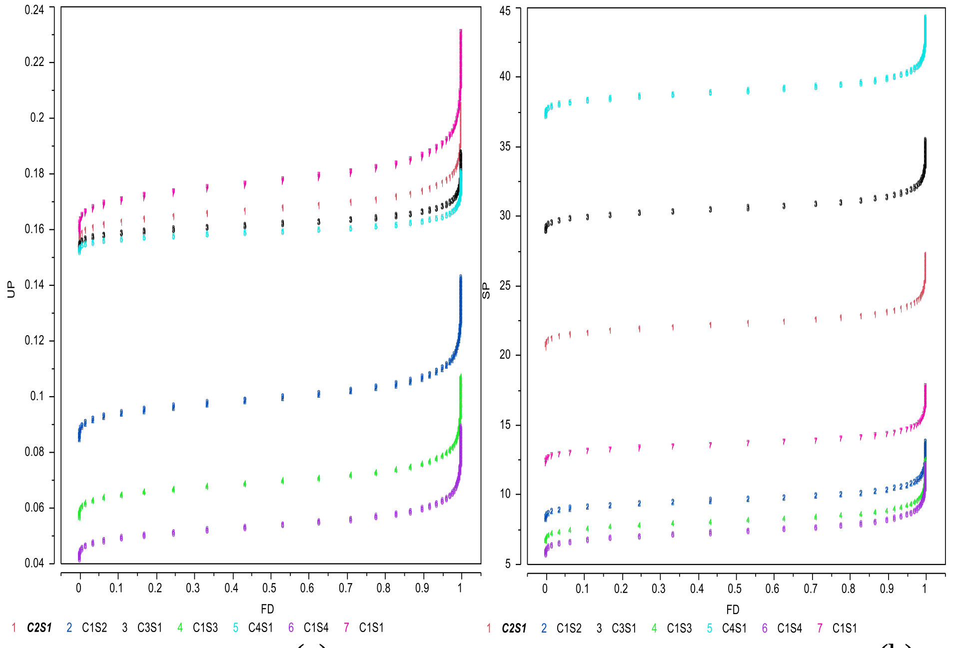
Figure 3: FDS plots for (a) Unscaled and (b) Scaled Prediction Variances, $k = 8$ factors.

On the other hand, the design, C_1S_1, seems to be the worst of the seven under the UPV FDS plots, but performs better than the replicated cube designs under the SPV FDS plots. The replicated cube designs display poor prediction capability for all the factors under consideration, with high prediction variances for the scaled and unscaled prediction variances. As can be seen from Figures 1, 2, 3, 4 and 5, the higher replicated cube designs, C_3S_1 and C_4S_1, tend to compete favourably for UPV but exhibit serious dispersions for SPV.



(a) (b)

Figure 4: FDS plots for (a) Unscaled and (b) Scaled Prediction Variances, $k = 9$ factors



(a) (b)

Figure 5: FDS plots for (a) Unscaled and (b) Scaled Prediction Variances, $k = 10$ factors

5. Summary and Recommendations

The star-replicated MinResV CCD options performed better than the other design variations when judged with the *G*- and *I*-optimality criteria. This is also true when evaluated using the FDS plots. The FDS graphs show that for all the factors under study, C_1S_3 and C_1S_4 displayed better stability and higher prediction capabilities than the other design variations. The design, C_1S_4, is recommended if the practitioner has the resources for the number of observations obtainable for the design. In terms of number of design runs, we recommend C_1S_3 since this design competes well with C_1S_4 for the three conditions under which the designs are judged. On the other hand, replicating the cube portion of the MinResV CCDs for $k = 6$ to 10 factors is not advantageous for all the factors under consideration.

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