Exact Calculation of Integrated Prediction Variance for Response Surface Designs on Cuboidal and Spherical Regions

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Over the years, design optimality evaluation of response surface designs focused mainly on D-optimality and G-optimality criteria. The apparent limited use of the IV-optimality criterion appears to be influenced by the computational challenges associated with the criterion. The lack of available computer code appears to be the main reason for limited use of the IV-optimality criterion. In addition, the IV-optimality criterion appears more difficult to code than the D-optimality criterion because of the integration required over the specified design region. In this paper, an efficient and exact method is presented for computing the IV-optimality criterion for selected response surface designs. The pseudo-code for the computer program is also presented. The investigation examines both spherical and cuboidal regions of interest. In addition, an analytical approach is outlined for computing the IV-optimality criterion for second-order split-plot designs. A particular feature of the analytical expressions is that they are derived using the design parameters. In addition, several comparisons of second-order response surface designs are illustrated for completely randomized designs and split-plot designs.

Key Words: Design Optimality; IV-Criterion; Region Moments; Restricted Randomization.

NOTICEABLY absent from the response surface literature are studies involving the use of the exact integrated prediction variance (IV) for response surface designs, particularly for spherical designs, where the computational time required increases exponentially. Myers et al. (1992) present some integrated prediction variance values for selected designs ($k \leq 5$) while evaluating the variance-dispersion properties of

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second-order response surface designs. However, they do not give any details on the computational procedure used to generate the IV values. Ozol-Godfrey et al. (2005) illustrate the use of the fraction of design-space plots for examining model robustness using G-optimality and IV-optimality criteria. However, the IV values presented are approximated values, which they argue are unbiased estimates of the true IV values. Hussey (1987) utilizes the IV-optimality criterion in a study on correlated simulation experiments but focuses only on first-order models, which are essentially cuboidal designs. Borkowski and Valeroso (2001) study design optimality criteria for reduced models but focus only on cuboidal designs and presented IV values for designs with $3 \leq k \leq 5$. An analytical approach is presented that computes the exact IV values for the central composite design (CCD). However, for other designs, the exact IV value is computed by evaluating the appropriate integrals, but this is time consuming. Haines (1987) and Borkowski (2003b) utilize the IV-optimality criterion in generating exact optimal designs, but its application is restricted to second-order models with 2 or 3 factors for the cuboidal region. Hardin and Sloane (1993) present an algorithm capable of generating IV-optimal designs for a number of "classical" situations, such as linear, quadratic, or cubic response surface designs with $1 \leq k \leq 12$ continuous variables in a cube or a sphere.

Borkowski (2003a) demonstrates the inaccuracies of computer packages in generating average prediction variance (APV) as an approximation of the IV-criterion for cuboidal designs. He gives a cautionary note that the practitioner should be careful in using APV values given by these computer packages to compare designs. A Monte Carlo approach is suggested for computing the IV-criterion, which is not necessarily exact but provides better approximation values than what is currently available in computer packages. However, this suggestion can still be time consuming, depending on the number of sampled points. The most obvious reason for the seemingly limited use of the IV-optimality criterion is the lack of available computer code to generate exact IV values. Even though published research work gives IV values for selected designs, there is no published work on how to efficiently compute the exact IV values without the need for numerical computation involving integration. It is the objective of this paper to present a method to obtain a closed-form expression for the IV-optimality criterion for second-order response surface designs.

General Form of the Second-Order Model

The split-plot model is developed as the general case and the completely randomized model is considered a specific instance of the split-plot model. The general form for split-plot models in matrix form is given as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\Theta} + \boldsymbol{\delta} + \boldsymbol{\varepsilon},$$

where $\mathbf{y}$ is an $N \times 1$ vector of responses, $\boldsymbol{\Theta}$ is a $p \times 1$ vector of unknown model parameters, $\mathbf{X}$ is the $N \times p$ matrix of the levels of the independent variables, and $\boldsymbol{\delta}$ and $\boldsymbol{\varepsilon}$ are $N \times 1$ vectors of random variables for whole-plot and subplot errors, respectively. It is assumed that $\boldsymbol{\delta} + \boldsymbol{\varepsilon} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$. The structure of the variance–covariance matrix, $\boldsymbol{\Sigma}$, is a block diagonal matrix in which the ith block matrix is of the form, $\boldsymbol{\Sigma}_i = \sigma_\delta^2 \mathbf{1}_{w_i \times 1}\mathbf{1}'_{1\times w_i} + \sigma_\varepsilon^2 \mathbf{I}_{w_i \times w_i}$, where w_i represents the number of subplot runs (whole-plot size) for the ith block matrix, σ_δ^2 is the covariance and whole-plot error variance, and σ_ε^2 is the subplot error variance. A split-plot design (SPD) is similar to that of a completely randomized design (CRD); the only difference is the variance–covariance matrix, $\boldsymbol{\Sigma}$. For a CRD, $\boldsymbol{\Sigma} = \sigma^2 \mathbf{I}_N$, where $\mathbf{I}$ is the identity matrix of dimension N.

IV-Optimality Criterion

Box and Draper (1959, 1963) were the pioneers of the IV-optimality criterion. They present the mean-squared deviation from the true response as the average over the region of interest, normalized by the design points and variance. The average mean-square error criterion is comprised of two main components. The first component is the "variance error" resulting from sampling errors, and the second component is the "bias error," which reflects the inadequacy of the fitted model. The first component is the IV-optimality criterion, which generates a single measure of prediction performance throughout the entire region of interest, Ξ. Computationally, this is accomplished by integrating the prediction variance $v(\mathbf{x})$ over Ξ. The standardized IV function for a CRD response surface design can be expressed as follows:

$$\begin{aligned} \mathrm{IV} &= \frac{1}{\Omega}\int_\Xi v(\mathbf{x})d\mathbf{x} \\ &= \frac{1}{\Omega}\int_\Xi f(\mathbf{x})'(\mathbf{X}'\mathbf{X})^{-1}f(\mathbf{x})d\mathbf{x} \\ &= \mathrm{trace}\left[(\mathbf{X}'\mathbf{X})^{-1}\frac{1}{\Omega}\int_\Xi f(\mathbf{x})'f(\mathbf{x})d\mathbf{x}\right], \end{aligned}$$

where $\Omega = \int_{\Xi} d\mathbf{x}$ is the volume of the region Ξ. The general form of the model vector for second-order designs is given as $f(\mathbf{x})' = [1 \mid x_1, \ldots, x_k \mid x_1x_2, \ldots, x_{k-1}x_k \mid x_1^2, \ldots x_k^2]$.

For many applications, the regions of interest, Ξ, in response surface methodology are either cuboidal or spherical. The difference is that, for a cuboidal region, the design variables are confined according to $-1 \leq x_i \leq 1$ for $i = 1, 2, \ldots, k$ such that all points are either positioned on or inside a hypercube; while for a spherical region, the design variables are confined according to $\sum_{i=1}^{k} x_i^2 \leq k$ such that all points are either positioned on or inside a hypersphere of radius $\sqrt{k}$. In addition, the volume of the respective region is given as follows:

$$\Omega = \begin{cases} 2^k & \text{for cuboidal region} \\ \dfrac{(\sqrt{\pi})^k}{\Gamma\left(\dfrac{k+2}{2}\right)} & \text{for spherical region.} \end{cases} \tag{1.1}$$

Computing the IV-optimality criterion numerically is challenging primarily because integration is required over the specified design region. Computation is less extensive for cuboidal regions than it is for spherical regions. However, computation time increases exponentially for both regions as the dimensionality of the problem increases. That is, as the number of factors increases, both the dimension of information matrix and the number of variables to integrate expand rapidly. In the case of the spherical region, the integration process is even more elaborate because the process involves converting from rectangular to hyperspherical coordinates, formulating the Jacobian due to change of variables, and integrating trigonometric functions. In addition, numerical computations are prone to numerical errors and error propagation. These issues are typically overcome when an analytical approach to the problem can be developed. In general, analytical computation is much more efficient than numerical computation and often reveals a clear relationship among the parameters governing the system and the system-optimality performance measure. Further, it is much easier to write computer codes for analytical expressions. These features of the analytical computational approach can then be exploited to design optimal systems or study the optimality of a system. The method presented in this paper eliminates the need for integrating trigonometric functions. In addition, the method is not only efficient computationally, but computes exact IV-optimality values.

Matrix of Region Moments

In response surface methodology, region moments of order two and four are required for second-order designs. Giovannitti-Jensen and Myers (1989) present expressions for these region moments when the region of interest is a spherical surface. They illustrated the matrix of region moments for the case of $k = 3$ for both the first- and second-order models. Haines (1987) also presents the matrix of region moments for $k = 2$ for a cuboidal region. Hussey et al. (1987) show a similar moment matrix but consider only first-order models.

In general, the matrix $\int_{\Xi} f(\mathbf{x})' f(\mathbf{x}) d\mathbf{x}$ is a $(p \times p)$ matrix of region moments $(\mathbf{M})$ of the form given in Equation (1.2). The variable p represents the number of model parameters and

$$\mathbf{M} = \left(\begin{array}{cc|c} \Omega & \mathbf{0} & \Omega\phi_1\mathbf{J}_k' \\ \mathbf{0} & \mathrm{diag}(\Omega m_i) & \mathbf{0} \\ \hline \Omega\phi_1\mathbf{J}_k & \mathbf{0} & \Omega\phi_2\mathbf{I}_k + \Omega\phi_3\mathbf{J}_k\mathbf{J}_k', \end{array}\right) \tag{1.2}$$

where Ω is as described in Equation (1.1), ϕ_1 represents region moment of order 2, while ϕ_2 and ϕ_3 represent region moments of order 4. Therefore, dividing the matrix of region moments $(\mathbf{M})$ by the volume of the region reduces the matrix of region moments to

$$\frac{\mathbf{M}}{\Omega} = \left(\begin{array}{cc|c} 1 & \mathbf{0} & \phi_1\mathbf{J}_k' \\ \mathbf{0} & \mathrm{diag}(m_i) & \mathbf{0} \\ \hline \phi_1\mathbf{J}_k & \mathbf{0} & \phi_2\mathbf{I}_k + \phi_3\mathbf{J}_k\mathbf{J}_k', \end{array}\right) \tag{1.3}$$

where

$$m_i = \begin{cases} \phi_1 & \text{for } 1 \leq i \leq k \\ \phi_3 & \text{for } k+1 \leq i \leq k + \dbinom{k}{2}. \end{cases}$$

After a careful study of the region moments for cuboidal designs, it became apparent that the second- and fourth-order moments are constants regardless of the number of factors. Therefore, only the dimensionality of the matrix $\mathbf{M}$ changes to reflect the number of parameters in the model. Thus, for a cuboidal region, the second- and fourth-order moments are given as

$$\phi_1 = \frac{1}{3}, \quad \phi_2 = \frac{4}{45}, \quad \text{and} \quad \phi_3 = \frac{1}{9}. \tag{1.4}$$

In the case of the spherical region, a unit sphere was considered. The investigation revealed that, unlike the cuboidal region, the second- and fourth-order moments are functions of k. Table 1 gives the values of these quantities for $2 \leq k \leq 6$.

TABLE 1. Spherical Second- and Fourth-Order Region Moments for $2 \le k \le 6$

k	Region moments ϕ_1	ϕ_2	ϕ_3
2	1/4	1/12	1/24
3	1/5	2/35	1/35
4	1/6	1/24	1/48
5	1/7	2/63	1/63
6	1/8	1/40	1/80

The values in Table 1 agree with the expressions

$$\phi_1 = \frac{1}{k+2}$$
$$\phi_2 = \frac{2}{(k+2)(k+4)} \quad \text{or} \quad 2\phi_3$$
$$\phi_3 = \frac{1}{(k+2)(k+4)} \tag{1.5}$$

as presented by Box and Draper (1959, 1963).

In terms of implementation, the computation of the exact value for the IV-optimality criterion is accomplished by simply taking the trace of $(\mathbf{X}'\mathbf{X})^{-1}$ and Equation (1.3). For a cuboidal region, the applicable second- and fourth-order region moments are given in Equation (1.4); while for a spherical region, the applicable second- and fourth-order region moments are given in Equation (1.5). The pseudo-code used to implement the MATLAB program for computing the exact integrated prediction variance is as follows:

1. Set $\mathbf{D}$ = design matrix
2. Set k = number of design factors
3. Set N = number of observations
4. Specify type of design region, whether cuboidal or spherical
5. If cuboidal region of interest
   (i) Set $\mathbf{X}$ = model matrix for $\mathbf{D}$ (2nd order model)
   (ii) Set $\mathbf{A}$ = information matrix $\mathbf{X}'\mathbf{X}$
   (iii) Set region moments as follows:
   $$\phi_1 = \frac{1}{3}, \quad \phi_2 = \frac{4}{45}, \quad \text{and} \quad \phi_3 = \frac{1}{9}$$
   (iv) Generate matrix of region moments ($\mathbf{M}$)
   (v) Go to step 7
6. If spherical region of interest
   (i) Scale design ($\mathbf{D}$) to be within a sphere of radius 1
   (ii) Set $\mathbf{X}$ = model matrix for $\mathbf{D}$ (second-order model)
   (iii) Set $\mathbf{A}$ = information matrix $\mathbf{X}'\mathbf{X}$
   (iv) Set region moments as follows:
   $$\phi_1 = \frac{1}{k+2}$$
   $$\phi_2 = \frac{2}{(k+2)(k+4)} \quad \text{or} \quad 2\phi_3,$$
   $$\phi_3 = \frac{1}{(k+2)(k+4)}$$
   (v) Generate matrix of region moments ($\mathbf{M}$)
   (vi) Go to step 7
7. Set $\mathbf{A}^*$ = inverse of $\mathbf{A}$
8. Set IV = trace of $(\mathbf{M} \times \mathbf{A}^*)$
9. Integrated prediction variance = IV
10. Scaled integrated prediction variance = $N*$ IV

It is important to point out that scaled optimality values are used to compare designs of different number of observations (N) that have the same number of factors. However, the standardized optimality values are appropriate for comparing designs with the same number of observations and factors.

The following section shows the results of the application of the MATLAB code in computing the integrated prediction variance for several types of designs for both spherical and cuboidal regions of interest. Interested persons can contact the author for the actual computer codes.

Integrated Prediction Variance for CRDs

Lucas (1974, 1976) examines design optimality properties for several second-order designs; however, his examination did not include integrated prediction variance. Park et al. (2005) study the prediction-variance properties of second-order designs for cuboidal regions. Their investigation focused on maximum prediction variance (G-optimal) and presented the average prediction variance for the outer edge of the design space. This approach will not give the exact value for the integrated prediction variance even though it can provide some insight into the behavior of the average-prediction variance over the selected set of points. Also, several of the saturated designs developed for second-order models focus on the generalized variance of the parameter estimates (D-optimality). Designs such as those

TABLE 2. Integrated Prediction Variance for Standard CCD and BBD—Spherical Designs

				IV	
k	Design	N	n_c	Standardized	Scaled
2	CCD	11	3	0.3611	3.9722
3	BBD	15	3	0.4619	6.9286
	CCD	17	3	0.3757	6.3862
4	BBD	28	4	0.3611	10.1110
	CCD	28	4	0.3611	10.1110
5	BBD	44	4	0.3360	14.7830
	CCD	29	3	0.4130	16.0498
6	BBD	52	4	0.4242	22.0590
	CCD	48	4	0.3887	20.3001
7	BBD	59	3	0.4423	26.0980
	CCD	81	3	0.3784	30.6480
8	CCD	84	4	0.3967	33.3200
9	BBD	128	0	0.3587	45.9080

developed by Hoke (1974), Box and Draper (1974), and Notz (1982) all use the generalized variance as the criterion for optimal designs. These designs may not be the best for prediction purposes because the designs are generated based on the variance of the parameter estimates, while the primary concern often is on prediction variance when choosing a second-order design.

According to the equivalence theorem of Kiefer–Wolfowitz (1959, 1961), D-optimal designs are also G-optimal in the limit of an infinite number of trials. Lucas (1974) discusses some of the merits of G-efficient designs. Table 2 presents the integrated prediction variance for the CCD and Box-Behnken designs (BBD) for $2 \leq k \leq 9$. For the CCDs on a spherical region, $\alpha = \sqrt{k}$. The number of center points, (n_c), used is also presented. The results indicate that, for $k = 3$, 5 and 6, the CCD performs better than the BBD. However, for $k = 7$, the BBD is a better design. Note that, for $k = 4$, both the BBD and CCD give the same average scaled-prediction variance because, in this case, the BBD is simply a rotation of the CCD design. Therefore, for $k = 4$, either design would produce the same level of confidence in terms of predicting new observations. However, it is important to point out that the spherical CCD provides additional degrees of freedom for lack of fit and for estimating pure cubic terms because of the fact that it is a 5-level design in comparison with a 3-level spherical BBD or even cuboidal designs. The data given for $k = 2$, 8, and 9 is presented for completeness.

For comparison purposes, the designs presented in Table 2 were evaluated using JMP version 7 up to $k = 8$, which is the limit of JMP's built-in design-generation feature. The results indicate that the average prediction variances for the CCDs are the same. However, the average prediction variance reported for the BBDs were different because the BBD designs were not scaled to be on a sphere of radius 1 in JMP. Compensating for the difference in scaling results in the same values of the IV criterion. To make fair comparisons among competing designs, the authors emphasize the need to scale the designs to the same spherical radius.

Hybrid and Small Composite Designs (SCD)

Giovannitti–Jensen and Myers (1989) and Myers et al. (1992) compare the hybrid and SCD designs for three factors using variance-dispersion graphs to study the properties of the prediction variance throughout the entire region for these designs. The information presented here complements the work done by these authors and confirms their findings. For details on the construction of these designs, see Roquemore (1976) and Hartley (1959). In computing and ranking the IV values for these designs, the number of center runs and the ranking system used by Myers et al. (1992) were utilized, as shown in Table 3. The ranking is done such that 1 and 4 represent the best and worst designs, respectively. The design matrices have been scaled such that the points in the design either lie on or inside a sphere of radius 1. The scaling factor used for each design is also given in Table 3. In terms of integrated prediction-variance properties, the design with the smallest scaled IV value is desirable. The results in Table 3 show that, for $k = 3$, the hybrid 311B with three center runs performs the best, followed by 311A. The SCD performs the worst as a result of having the largest scaled IV value. It is important to point out that scaled optimality values are used to compare designs of different number of observations, (N), that have the same number of factors. A similar ranking is obtained for $k = 4$, with the hybrid 416C with five center runs

TABLE 3. Comparison of IV Values for Near-Saturated Designs over Spherical Regions

Design	N	n_c	IV Standardized	IV Scaled	Ranked performance	Scaling factor
$k = 3$						
SCD $\alpha = \sqrt{k}$	13	3	0.798	10.369	4	0.57735
Hybrid						
310	12	2	0.670	8.034	3	0.64445
311A	12	2	0.576	6.911	2	0.44721
311B	13	3	0.519	6.745	1	0.40825
$k = 4$						
SCD $\alpha = \sqrt{k}$	19	3	0.816	15.503	4	0.50000
Hybrid						
416A	20	4	0.571	11.430	3	0.52244
416B	20	4	0.569	11.387	2	0.54189
416C	20	5	0.568	11.362	1	0.54865
$k = 6$						
1/2 fraction CCD $\alpha = 2.378$	48	4	0.389	18.659	1	0.42052
Hybrid						
628A	30	2	0.683	19.817	2	0.43301
628B	31	2	0.723	21.687	3	0.41547
$k = 7$						
1/2 fraction CCD $\alpha = 2.828$	81	3	0.378	30.648	1	0.35355
Hybrid						
746	47	2	1.311	61.601	2	0.30995

performing the best, followed by 416B. Again, the SCD performs the worst. These results agree with the rankings given by Myers et al. (1992). However, as pointed out by Myers et al. (1992), while the hybrid design outperforms the SCD in terms of prediction-variance properties, the SCD is useful particularly in situations where sequential experimentation and augmentation is desirable.

Table 3 also presents the comparison of the integrated prediction variance for hybrid and CCD for $k = 6$ and 7. According to the variance dispersion results presented by Myers et al. (1992) for $k = 6$, the hybrid design 628A performs much better than the half-fraction CCD over a considerable portion of the design region. However, it is clear from the scaled IV values given in Table 3 that the half-fraction CCD performs better but at a cost of over a 50% increase in design size. Therefore, depending on the interest of the practitioner, the most suitable design can be chosen. If the average variance is more of a concern, then the half-fraction CCD provides the better option. However, if cost constraints are more critical, then the hybrid 628A design is the better option. According to Roquemore (1976), the hybrid 746 design for $k = 7$ is not a near-saturated design but represents an economical alternative to the half=fraction CCD with $\alpha = 2.828$. The comparison of both designs in terms of their scaled IV values given in Table 3 indicate that the half-fraction CCD outperforms the hybrid 746. Therefore, the only time the hybrid 746 should be used is when very limited resources are available.

TABLE 4. Integrated Prediction Variance of Selected Cuboidal Designs

				IV	
k	Design	N	n_c	Standardized	Scaled
2	FCC	11	3	0.3260	3.5863
	Notz	9	3	0.4635	4.1716
	Box–Draper	7	1	0.6060	4.2417
3	FCC	16	2	0.3405	5.4483
	Notz	12	2	0.7073	8.4875
	Hoke	16	3	0.3524	5.6382
	SCD	10	0	1.0333	10.3330
	Box–Draper	12	2	0.4944	5.9327
4	FCC	25	1	0.3376	8.4397
	Notz	16	1	0.7430	11.8870
	Hoke	21	2	0.4918	10.3280
	SCD	16	0	1.0269	16.4300
	Box–Draper	18	3	0.5708	10.2740
5	FCC	26	0	0.4155	10.8030
	Notz	24	3	0.6213	14.9100
	Hoke	28	2	0.4382	12.2700
	SCD	21	0	1.9375	40.6880
	Box–Draper	24	3	0.8201	19.6820
6	FCC	44	0	0.3902	17.1670
	Notz	32	4	0.6788	21.7200
	Hoke	36	2	0.4883	17.5800
	Box–Draper	31	3	1.2146	37.6540
7	FCC	78	0	0.3840	29.9490
	Hoke	44	1	0.5768	25.3810
	Box–Draper	39	3	1.7784	69.3590
8	Hoke	53	0	0.6790	35.9870
	Box–Draper	48	3	2.5403	121.9400
9	Hoke	64	0	0.7814	50.0120
	Box–Draper	57	2	3.5967	205.0100
10	Hoke	76	0	0.9625	73.1530
	Box–Draper	68	2	4.8529	330.0000
11	Hoke	89	0	1.0813	96.2360
	Box–Draper	80	2	6.4077	512.6100

Comparison of Selected Cuboidal Designs

The exact IV-criterion for selected cuboidal designs was computed using 0 through 5 center points. The designs with the lowest scaled integrated prediction variance are presented in Table 4. The standardized values are also presented. Borkowski (2003b) presented similar results for cuboidal designs, as well as a discussion about exact versus approximate prediction-variance values. It is clear from the data presented in Table 4 that, for $2 \leq k \leq 6$, the face-centered cube (FCC) design is superior to the other cuboidal designs. For FCC designs with k equal to 4, 5, and 6, there are no degrees of freedom for lack of fit. Therefore, to facilitate the test for lack of fit, some form of replication would be needed. In terms of pure error calculation, 3 center runs are suggested. By adjusting the number of center runs to 2 and 3, respectively, the resulting scaled IV values are 8.45 and 8.53 for $k = 4$, 11.17 and 11.41 for $k = 5$, and 17.47 and 17.67 for $k = 6$. Even with these additional center runs, the FCC design maintains the advantage over the other designs, except for $k = 6$, when 3 center runs are used. For $k = 6$, the Hoke design offers a slightly better scaled IV value of 17.58. The Hoke design performs the best for $7 \leq k \leq 11$, even with the addition of 2 to 3 center runs. In general, the best saturated designs are the Hoke designs because they consistently outperform the Notz, Box and Draper, and the SCD designs. JMP 7 computes the exact average prediction variance for cuboidal designs such as the FCC. However, for the other designs in Table 4, a comparison could not be made because JMP 7 does not generate these designs.

Analytical Determination of Integrated Prediction Variance

It is understood that, for split-plot designs (SPDs), alphabetic optimality is dependent on an information matrix of the form $\mathbf{X}'\mathbf{\Sigma}^{-1}\mathbf{X}$. This situation suggests that optimal designs will depend on the variance ratio, $\eta = \sigma_\delta^2/\sigma_\varepsilon^2$. The standardized IV function for SPDs can be expressed as

$$\text{IV} = \text{trace}\left[(\mathbf{X}'\mathbf{R}^{-1}\mathbf{X})^{-1}\frac{1}{\Omega}\int_{\Xi} f(\mathbf{z},\mathbf{x})'f(\mathbf{z},\mathbf{x})d\mathbf{z}d\mathbf{x}\right],$$

where $\Omega = \int_{\Xi} d\mathbf{z}d\mathbf{x}$ is the volume of the region Ξ and $\mathbf{R}$ is the correlation matrix derived by dividing the variance–covariance matrix, $\mathbf{\Sigma}$, by $\sigma_\delta^2 + \sigma_\varepsilon^2$. The general form of the model vector for second-order SPD is given as

$$\begin{aligned} f(\mathbf{z},\mathbf{x})' = [1 \mid & z_1, \ldots, z_{wp} \mid x_1, \ldots, x_{sp} \mid \\ & z_1z_2, \ldots, z_{wp-1}z_{wp} \mid z_1x_1, \ldots, z_{wp}x_{sp} \mid \\ & x_1x_2, \ldots, x_{sp-1}x_{sp} \mid z_1^2, \ldots, z_{wp}^2 \mid \\ & x_1^2, \ldots, x_{sp}^2], \end{aligned}$$

where z and x are the whole-plot and subplot fac-

$$(\mathbf{X}'\mathbf{R}^{-1}\mathbf{X})^{-1} = \left(\begin{array}{cc|cc} \gamma_1 & \mathbf{0} & \gamma_2\mathbf{J}'_{wp} & \gamma_3\mathbf{J}'_{sp} \\ \mathbf{0} & \text{diag}(1/d_i) & \mathbf{0} & \mathbf{0} \\ \hline \gamma_2\mathbf{J}_{wp} & \mathbf{0} & \gamma_7(\mathbf{I}_{wp} - \gamma_4\mathbf{J}_{wp}\mathbf{J}'_{wp}) & \gamma_5[\mathbf{J}_{sp}\mathbf{J}'_{wp}]' \\ \gamma_3\mathbf{J}_{sp} & \mathbf{0} & \gamma_5\mathbf{J}_{sp}\mathbf{J}'_{wp} & \gamma_8(\mathbf{I}_{wp} - \gamma_6\mathbf{J}_{sp}\mathbf{J}'_{sp}) \end{array}\right) \quad (1.6)$$

tors, respectively, while wp and sp are the number of whole-plot and subplot factors, respectively.

To develop the analytical approach to compute IV-optimality of a design, the IV function is separated into two components. The first component is the inverse of the information matrix, $\mathbf{B} = (\mathbf{X}'\mathbf{R}^{-1}\mathbf{X})^{-1}$, and the second component is $\mathbf{M} = (1/\Omega)\int_\Xi f(\mathbf{z},\mathbf{x})'f(\mathbf{z},\mathbf{x})d\mathbf{z}d\mathbf{x}$, which is referred to as the matrix of region moments. Wesley et al. (2009) give a full discussion of the analytical characterization of $(\mathbf{X}'\mathbf{R}^{-1}\mathbf{X})^{-1}$ for both the CCD and BBD within a split-plot structure. The general form of $(\mathbf{X}'\mathbf{R}^{-1}\mathbf{X})^{-1}$ for the split-plot CCD and BBD is given as in Equation (1.6), where $\mathbf{0}$'s are zero matrices of appropriate sizes; $\mathbf{J}_{wp}$ and $\mathbf{J}_{sp}$ are unit vectors of $wp \times 1$ and $sp \times 1$, respectively; $\mathbf{I}_{wp}$ and $\mathbf{I}_{sp}$ are wp-dimensional and sp-dimensional identity matrices; γ_i are scalar quantities (see Appendix A); and diag$(1/d_i)$ is a diagonal matrix of which the diagonal elements correspond to the linear and interaction terms.

A similar characterization of the inverse of the information matrix for a (CRD) was presented by Borkowski (1995). However, by setting $\eta = 0$ and the whole plot size to 1 in the above results, the CRD characterization is obtained. Essentially, the split-plot design is the more general structure while the CRD actually represents a specific instance of the SPD. In the following section ,we examine the second component $\mathbf{M}$, the matrix of region moments.

It is important to point out that the matrix of region moments ($\mathbf{M}$) is not affected by restrictions on randomization and, thus, the variance ratio, η, will not have any impact on its structure. Therefore, the matrix of region moments for a CRD and an SPD are exactly the same. The whole-plot factor is simply seen as another variable in the design. To reflect the nature of the SPD, the matrix of region moments can be partitioned as

The following section presents the explicit functions that can be used to compute the integrated prediction variance for the split-plot CCD and the split-plot BBD. It is important to point out that the computation of IV values for second-order SPDs can also be easily computed by simply taking the trace of $(\mathbf{X}'\mathbf{R}^{-1}\mathbf{X})^{-1}$ and Equation (1.7), which is what Equation (1.8) represents.

IV for the Split-Plot CCD and BBD

Performing the necessary matrix multiplication, the IV-optimality criterion for both the CCD and BBD can be determined analytically as

$$\begin{aligned} \text{IV} = {} & \gamma_1 + \phi_1(wp\gamma_2 + sp\gamma_3)\sum_{i=1}^{k+\binom{k}{2}} \text{Diag}\left(\frac{m_i}{d_i}\right) \\ & + ([\phi_3(1 - wp\gamma_4) + \phi_2(1-\gamma_4)]\gamma_7 \\ & \quad + \phi_3 sp\gamma_5 + \phi_1\gamma_2)wp \\ & + ([\phi_3(1 - sp\gamma_6) + \phi_2(1-\gamma_6)]\gamma_8 \\ & \quad + \phi_3 wp\gamma_5 + \phi_1\gamma_3)sp. \qquad (1.8). \end{aligned}$$

Table 13 summarizes the scalar quantities γ_i for both the split-plot CCD and the split-plot BBD (see Appendix A). The expression in Equation (1.8) is general regardless of the shape of the region of interest. The distinction lies in the values for the region moments, ϕ_i. Tables 5 and 6 give the parameters used to characterize the split-plot CCD and BBD, respectively. Using these parameters and the pertinent constants (c_i) given in Tables 14 and 15, the IV value for the respective SPD can be calculated.

The computer codes generated for these analytical expressions are available upon request by emailing the first author. The following section shows the application of these functions in computing the integrated prediction variance for several types of SPDs for both spherical and cuboidal regions of interest.

$$\mathbf{M} = \left(\begin{array}{cc|cc} 1 & \mathbf{0} & \phi_1\mathbf{J}'_{wp} & \phi_1\mathbf{J}'_{sp} \\ \mathbf{0} & \text{Diag}(m_i) & \mathbf{0} & \mathbf{0} \\ \hline \phi_1\mathbf{J}_{wp} & \mathbf{0} & \phi_2\mathbf{I}_{wp} + \phi_3\mathbf{J}_{wp}\mathbf{J}'_{wp} & \phi_3[\mathbf{J}_{sp}\mathbf{J}'_{wp}]' \\ \phi_1\mathbf{J}_{sp} & \mathbf{0} & \phi_3\mathbf{J}_{sp}\mathbf{J}'_{wp} & \phi_2\mathbf{I}_k + \phi_3\mathbf{J}_k\mathbf{J}'_k \end{array}\right). \quad (1.7)$$

TABLE 5. Table of Notations for the Split-Plot CCD

Notations	Meanings
f	No. of factorial runs (2^k or 2_V^{k-m})
f_w	No. of whole-plot factor runs
w_i	ith whole plot size
a_i	No. of whole plots with size w_i
r_w	No. of repeated whole-plot axials
r_s	No. of repeated subplots axials
β	Whole-plot axial setting
α	Subplot axial setting
ζ	Factor-level setting

Integrated Prediction Variance for SPDs

In this section, we illustrate the utilization of the analytical method for computing integrated prediction variance values for second-order SPDs. The response surface designs considered are the CCD and the BBD for both spherical and cuboidal regions. These designs were developed within a split-plot structure by Vining et al. (2005) and Parker et al. (2006, 2007). The notation VKM is used to denote the Vining method of construction while MWP is used to denote the minimum whole-plot Parker method of construction. These designs were selected because they possess the equivalent estimation property indicating that the least-squares estimates are equivalent to the generalized least-squares estimates, making parameter estimation simple for practitioners. Equivalent designs allow for estimation of parameters using ordinary least squares instead of restricted maximum-likelihood estimation. One of the primary advantages of these designs is that the parameters of the mean model can be estimated separately from the whole-plot and subplot error terms, which are frequently not easy to estimate precisely. Several combinations of whole-plot and subplot factors are considered. Further, these designs were selected to demonstrate the flexibility of the methods presented and to show how easy it is to compute the IV values for large designs. Table 7 lists the split-plot designs selected for evaluation in this section. For details on these designs and others, visit the following link to access a reference catalog of split-plot designs: http://scholar.lib.vt.edu/theses/available/etd-0330 2005-194026/. The spherical designs are scaled such

TABLE 6. Table of Notations for the Split-Plot BBD

Notations	Meanings
f	No. of factorial runs per block (2^t)
f_c	No. of factorial runs at edge centers
w_i	ith whole-plot size
a_i	No. of whole plots with size w_i
r_w	No. of blocks within which a whole-plot factor appears
r_s	No. of blocks within which a subplot factor appears
t	No. of active subplot factors per block ($t \geq 1$)
λ_c	No. of edge centers
λ_w	No. of times a pair of whole plot factors appears in the same block ($\lambda_w \geq 1$)
λ_s	No. of times a pair of subplot factors appears in the same block
λ_{int}	No. of times a whole plot factor appears with a subplot factor in the same block
β	Whole-plot factor level setting
α	Factor-level setting

TABLE 7. Split-Plot Designs Selected for Evaluation

Design	Factor combination *wp*	Factor combination *sp*	Number of whole plots
Spherical region			
$k = 4$			
VKM BBD	1	3	5
MWP BBD	1	3	5
VKM BBD	2	2	11
VKM CCD	2	2	11
$k = 6$			
VKM CCD	2	4	11
MWP CCD	2	4	11
VKM BBD	2	4	11
Cuboidal region			
$k = 7$			
VKM CCD	3	4	17
MWP CCD	3	4	17

TABLE 8. Design Matrix for a Balanced VKM BBD with One Whole-Plot Factor and Three Subplot Factors

Whole plot	z_1	x_1	x_2	x_3	Whole-plot size
1	$-$**1**	$\pm$**1**	$\pm$**1**	**0**	4
	$-$**1**	$\pm$**1**	**0**	$\pm$**1**	4
	$-$**1**	**0**	$\pm$**1**	$\pm$**1**	4
2	**1**	$\pm$**1**	$\pm$**1**	**0**	4
	1	$\pm$**1**	**0**	$\pm$**1**	4
	1	**0**	$\pm$**1**	$\pm$**1**	4
3	**0**	$\pm$**1**	$\pm$**1**	**0**	4
	0	$\pm$**1**	**0**	$\pm$**1**	4
	0	**0**	$\pm$**1**	$\pm$**1**	4
4	**0**	**0**	**0**	**0**	12
5	**0**	**0**	**0**	**0**	12

TABLE 9. Design Matrix for a Balanced MWP BBD with One Whole-Plot Factor and Three Subplot Factors

Whole plot	z_1	x_1	x_2	x_3	Whole-plot size
1	-1	$\pm$**1**	**0**	**0**	2
	$-$**1**	**0**	$\pm$**1**	**0**	2
	$-$**1**	**0**	**0**	$\pm$**1**	2
	$-$**1**	**0**	**0**	**0**	7
2	**1**	$\pm$**1**	**0**	**0**	2
	1	**0**	$\pm$**1**	**0**	2
	1	**0**	**0**	$\pm$**1**	2
	1	**0**	**0**	**0**	7
3	**0**	$\pm$**1**	$\pm$**1**	**0**	4
	0	$\pm$**1**	**0**	$\pm$**1**	4
	0	**0**	$\pm$**1**	$\pm$**1**	4
	0	**0**	**0**	**0**	1
4	**0**	**0**	**0**	**0**	13
5	**0**	**0**	**0**	**0**	13

that the design points lie on or inside a sphere of radius 1. For each of the designs presented, both the standardized and scaled IV values are presented. Essentially, the standardized IV value is obtained using Equations (1.8). The standardized IV value is then multiplied by the design size (N) to obtain the scaled IV value. Because all the designs within a comparison have the same number of whole plots, scaling by the design size is appropriate. It is important to point out that scaled optimality values are used to compare designs of different number of observations (N) that have the same number of factors. However, the standardized optimality values are appropriate for comparing designs with the same number of observations and factors.

SPD With One Whole-Plot Factor and Three Subplot Factors

The first design type considered is the BBD. Tables 8 and 9 show the design matrices representing the structure of the balanced VKM BBD and MWP BBD, respectively. Their unbalanced counterparts would have the sizes of whole plots 4 and 5 reduced from 12 to 2 for the VKM and whole plots 4 and 5 reduced from 13 to 2 for the MWP. Table 10 gives the details of the design parameters used to compute the IV values for both the balanced and unbalanced designs.

Equation (1.8) is evaluated using the values of the parameters given in Table 10 and the expressions of the scalar quantities and pertinent constants for the split-plot BBD given in Tables 13, 14, and 15. The results are obtained for variance ratios 0.5, 1, and 10, which are used to compute the functions, Φ_i, as outlined in Appendix A. Table 11 summarizes the results obtained. It is important to note that smaller IV value indicates better design. It can be observed that the unbalanced MWP BBD design has the best scaled integrated prediction variance when compared with the other designs. The balanced MWP BBD design is the next best design, while the balanced VKM BBD design performs the worst. Because all the designs have the same number of whole plots, the unbalanced MWP design would be more cost effective and therefore the best design.

An investigation is also performed on the similarity between VKM CCD and VKM BBD with 4 factors. It is understood that, for a CRD in 4 factors, the BBD is just a rotation of the CCD. Therefore, both designs will give the same prediction variance results. The purpose of this investigation is to verify whether or not the VKM CCD and VKM BBD designs with 4 factors are equivalent. It was observed that, for the SPD, the condition of equivalency is dependent on the number of whole-plot and subplot factors. The details are presented only for the designs that are equivalent. The equivalent designs are balanced VKM CCD and VKM BBD; both with 2 whole-plot factors and 2 subplot factors. The scaled integrated prediction variance values for these designs are 14.31, 15.20, and 17.52 for variance ratios 0.5, 1, and 10, respectively. Both designs have whole-plot sizes of 4 observations, 11 whole plots, 2 of which

TABLE 10. Design Parameters for VKM BBD and MWP BBD with One Whole-Plot Factor and Three Subplot Factors

	VKM		MWP	
Parameters	Balanced	Unbalanced	Balanced	Unbalanced
f	4	4	2	2
f_c	4	4	2	2
t	2	2	1	1
a_1	3	3	3	3
a_4	2	2	2	2
w_1	12	12	13	13
w_4	12	2	13	2
wp	1	1	1	1
sp	3	3	3	3
N	60	40	65	43
r_w	6	6	13	13
r_s	6	6	6	6
λ_w	1	1	1	1
λ_s	3	3	2	2
λ_{int}	4	4	2	2
λ_c	3	3	2	2
β	0.57735	0.57735	0.70711	0.70711
α	0.57735	0.57735	0.70711	0.70711
p	15	15	15	15

are dedicated to center runs. The designs will also give the same result if the sizes of the two whole plots of center runs are increased or reduced. The results indicate that only SPD involving 2 whole-plot factors and 2 subplot factors will give the same prediction variance properties. Any other combination of whole-plot and subplot factors will result in different prediction variance properties, depending on the design type.

SPD With Two Whole-Plot Factors and Four Subplot Factors

We now consider the VKM and the MWP CCD with 2 whole-plot factors and 4 subplot factors. An examination of the results in Table 11 reveals that the unbalanced VKM CCD performs the best among the designs considered. The unbalanced VKM CCD has the lowest scaled integrated prediction variance across the variance ratios considered. The next best design is the unbalanced MWP CCD.

The VKM BBD given in Table 12 with 2 whole-plot factors and four subplot factors was also considered. A close examination of the design structure shows that subplot factor x_2 has a total of 48 settings at the ± 1 levels, while the remaining subplot factors have 24 settings at the ± 1 levels. Therefore, the design moments among the subplot factors are different and, as a result, the analytical method presented is not capable of computing the IV values for this design. However, the matrix manipulation method presented is used to compute the IV value. This method still represents an efficient and exact way of computing the IV values. The unbalanced structure of the design is a result of the size of the whole-plot centers reducing from eight to two. Table 11 gives the results, which indicate that the unbalanced design performs better than the balanced design. However, when compared with the IV results for VKM CCD with $k = 6$, the unbalanced VKM CCD performs better than the VKM BBD. This comparison is possible because both designs have the same number of whole plots and were scaled to be on a sphere of radius 1.

SPD With Three Whole-Plot Factors and Four Subplot Factors

The previous examples examined designs with spherical regions. However, the region of interest is often cuboidal. The cuboidal designs considered are

TABLE 11. Integrated Prediction Variance for Selected Split-Plot Designs

		Standardized IV				IV Scaled by design size			
		Balanced		Unbalanced		Balanced		Unbalanced	
Design	Variance ratio (η)	VKM	MWP	VKM	MWP	VKM	MWP	VKM	MWP
				Spherical region					
				$k = 4$					
BBD	0.5	0.658	0.373	0.686	0.397	39.453	24.270	27.431	17.075
1 *wp* 3 *sp*	1	0.827	0.404	0.848	0.425	49.629	26.246	33.932	18.261
	10	1.243	0.472	1.247	0.477	4.606	30.661	49.891	20.490
BBD & CCD	0.5	0.325	—	—	—	14.310	—	—	—
2 *wp* 2 *sp*	1	0.346	—	—	—	15.240	—	—	—
	10	0.398	—	—	—	17.521	—	—	—
				$k = 6$					
CCD	0.5	0.365	0.356	0.378	0.365	32.152	35.247	28.718	30.986
2 *wp* 4 *sp*	1	0.372	0.358	0.382	0.365	32.756	35.450	29.001	31.057
	10	0.389	0.360	0.391	0.361	34.236	35.601	29.697	30.714
BBD	0.5	0.441	—	0.453	—	38.780	—	34.441	—
2 *wp* 4 *sp*	1	0.490	—	0.499	—	43.110	—	37.944	—
	10	0.611	—	0.612	—	53.738	—	46.540	—
				Cuboidal region					
				$k = 7$					
CCD	0.5	0.323	0.262	0.339	0.267	43.956	40.010	41.986	37.160
3 *wp* 4 *sp*	1	0.362	0.277	0.375	0.282	49.288	42.406	46.536	39.189
	10	0.459	0.315	0.461	0.316	62.376	48.195	57.205	43.920

the VKM and MWP CCD, both having the same number of whole plots. Therefore, scaling these designs by the design size for comparison is a reasonable way of selecting the most efficient design. A comparison of the designs according to the IV values given in Table 11 indicates that the unbalanced MWP design performs the best among the designs for each of the variance ratios considered. The balanced MWP design is the next best design. Therefore, in this case, the MWP designs should be the design of choice rather than the VKM design, assuming that the cost of collecting the additional runs is feasible. The VKM and MWP designs are not the only cuboidal designs available. Draper and John (1998) and Goos and Vandebroek (2001) presented some split-plot cuboidal designs and D-optimal designs, respectively, but these designs do not satisfy the equivalent estimation criteria.

Conclusion

In most cases, the lack of available computer programs and the computational challenges encountered to compute the IV-optimality criterion have been a deterrent to most practitioners interested in using the criterion. Our investigation has led to the development of a computationally efficient method for computing the exact value of the IV-optimality criterion for second-order response surface designs. The methods presented are capable of dealing with com-

TABLE 12. Design Matrix for a Balanced VKM BBD with Two Whole-Plot Factors and Four Subplot Factors

Whole plot	z_1	z_2	x_1	x_2	x_3	x_4	Whole-plot size
1	**−1**	−1	**0**	±1	**0**	**0**	8
2	**−1**	**0**	**0**	±1	±1	**0**	4
	−1	**0**	±1	**0**	**0**	±1	4
3	**−1**	**1**	**0**	±1	**0**	**0**	8
4	**0**	−1	±1	**0**	±1	**0**	4
	0	−1	**0**	**0**	±1	±1	4
5	**0**	**0**	±1	±1	**0**	±1	8
6	**0**	**1**	±1	**0**	±1	**0**	4
	0	**1**	**0**	**0**	±1	±1	4
7	**1**	−1	**0**	±1	**0**	**0**	8
8	**1**	**0**	**0**	±1	±1	**0**	4
	1	**0**	±1	**0**	**0**	±1	4
9	**1**	**1**	**0**	±1	**0**	**0**	8
10	**0**	**0**	**0**	**0**	**0**	**0**	8
11	**0**	**0**	**0**	**0**	**0**	**0**	8

pletely randomized designs and split-plot designs for both spherical and cuboidal regions. An attractive feature of the derived analytical functions to compute the exact IV-optimality criterion for the CCD and the BBD is that they are functions of the design parameters. Therefore, the effect of changes in any of the design parameters can be easily evaluated without the need to generate the actual design.

The applications of these methods were demonstrated by the evaluation of several response surface second-order designs. With respect to completely randomized designs on spherical region, the results indicate that, for $k = 3$, 5, and 6, the CCD performs better than the BBD. However, for $k = 7$, the BBD is a better design. For saturated or near saturated designs on spherical region, the hybrid designs for $k = 3$ and 4 perform the best. However, for $k = 6$ and 7, the half-fraction CCD performs better than the hybrid designs. For a cuboidal region of interest, the FCC designs for $2 \le k \le 6$ are the best designs, while, for $7 \le k \le 11$, the Hoke designs are the best. In the case of split-plot designs, the results reveal that the unbalanced split-plot designs have a tendency to give better IV values when compared with the balanced split-plot designs. It was also shown that, for 4 factors, the CCD and BBD are only equivalent for situations involving two whole-plot factors and two subplot factors. Any other combination of whole-plot and subplot factors will result in two different designs, thus giving different optimality results.

The resulting equations and matrices presented provide an efficient and exact way of computing integrated prediction variance for certain second-order designs. Therefore, it is now possible for some of the software packages to present accurate results for integrated prediction variance without having to do extensive numerical computations. However, the method presented does not address the commonly used computer-generated designs for which design structure does not produce nice analytical forms for the prediction variance function. In these cases, the authors recommend the approach by Borkowksi (2003a), which performs an approximation by evaluating over a set of random points.

Appendix A
Scalar and Constant Quantities

According to the structure of SPD, there are four distinct categories of whole plots, denoted a_1 through a_4. These categories have whole-plot sizes of w_1 through w_4 for factorial, whole-plot axials, subplot axials, and center runs, respectively. In general, the functions (Φ_i) of the variance ratio and whole plot sizes are as follows:

$$\Phi_1 = \frac{1+\eta}{1+w_1\eta}$$

$$\Phi_2 = 1+\eta$$

$$\Phi_3 = -2\left(\frac{\eta(1+\eta)}{1+w_1\eta}\right) \text{ or } -2\left(\frac{\eta(1+\eta)}{1+w_3\eta}\right),$$

if unbalanced subplot axials.

$\Phi_4 = 1$ or Φ_2, if whole-plot axials are grouped with factorial whole plots.

$\Phi_5 = \Phi_2$ or Φ_1, if subplot axials are in separate whole plots, while Φ_3 is set to 0.

$$\Phi_6,\ \Phi_7, \text{ and } \Phi_8 = \frac{1+\eta}{1+w_i\eta} \text{ for } i = 2, 3, 4.$$

$$\Phi_9 = 0 \text{ or } 2\left(\frac{(1+\eta)^2}{1+w_3\eta}\right), \text{ if the centers are}$$

grouped with subplot axials.

Table 13 summarizes the scalar quantities represented by γ_i in the inverse of the information matrix for both the split-plot CCD and BBD. Tables 14 and 15 provide the details of the pertinent constants (c_i) for the split-plot CCD and BBD respectively.

TABLE 13. Table of Scalar Quantities for the Split-Plot CCD and BBD

Scalars	CCD expressions	BBD expressions
γ_1	$\frac{1}{c_{11}}$	$\frac{1}{c_{11}}$
γ_2	$-\frac{c_5}{c_{11}}$	$-\frac{c_5}{c_{11}}$
γ_3	$-\frac{c_9}{c_{11}}$	$-\frac{c_9}{c_{11}}$
γ_4	$\frac{c_1}{\Phi_6 2r_w\beta^4 + wpc_1} - \frac{\Phi_1 2r_w\beta^4(c_5)^2}{c_{11}}$	$\frac{c_1}{\Phi_1 f(r_w - \lambda_w)\beta^4 + wpc_1} - \frac{\Phi_6 f(r_w - \lambda_w)\beta^4(c_5)^2}{c_{11}}$
γ_5	$-\frac{\Phi_1 f\zeta^4}{c_2} + \frac{c_5c_9}{c_{11}}$	$-\frac{\Phi_1 f\lambda_{\text{int}}\alpha^4}{c_2} + \frac{c_5c_9}{c_{11}}$
γ_6	$c_7 - \frac{(\Phi_5 2r_s\alpha^4 + \Phi_9)(c_9)^2}{c_{11}}$	$c_7 - \frac{\Phi_5 f(r_s - \lambda_s)\alpha^4(c_9)^2}{c_{11}}$
γ_7	$\frac{1}{\Phi_6 2r_w\beta^4}$	$\frac{1}{\Phi_1 f(r_w - \lambda_w)\beta^4}$
γ_8	$\frac{1}{\Phi_5 2r_s\alpha^4 + \Phi_9}$	$\frac{1}{\Phi_5 f(r_s - \lambda_s)\alpha^4}$

TABLE 14. Table of Constant Quantities for CCD

Constants	Expressions
c_1	$\Phi_1 f_w\zeta^4 - \frac{(\Phi_1 f\zeta^4)^2 sp}{\Phi_5 2r_s\alpha^4 + \Phi_9 + sp(\Phi_4\Phi_1 f\zeta^4 + \Phi_3 2r_s\alpha^4)}$
c_2	$(\Phi_5 2r_s\alpha^4 + \Phi_9 + sp(\Phi_4\Phi_1 f\zeta^4 + \Phi_3 2r_s\alpha^4))(\Phi_6 2r_w\beta^4 + wpc_1)$
c_3	$\frac{\Phi_1 f_w\zeta^2 + \Phi_6 2r_w\beta^2}{\Phi_6 2r_w\beta^4 + wpc_1}$
c_4	$-\frac{\Phi_1 f\zeta^4(\Phi_1 f\zeta^2 + \Phi_7 2r_s\alpha^2)sp}{c_2}$
c_5	$c_3 + c_4$
c_6	$-\frac{\Phi_1 f\zeta^4(\Phi_1 f_w\zeta^2 + \Phi_6 2r_w\beta^2)wp}{c_2}$
c_7	$\frac{(\Phi_4\Phi_1 f\zeta^4 + \Phi_3 2r_s\alpha^4)c_2 - ((\Phi_5 2r_s\alpha^4 + \Phi_9)(\Phi_1 f\zeta^4)^2 wp)}{(\Phi_5 2r_s\alpha^4 + \Phi_9 + sp(\Phi_4\Phi_1 f\zeta^4 + \Phi_3 2r_s\alpha^4))c_2}$
c_8	$\frac{(\Phi_1 f\zeta^2 + \Phi_7 2r_s\alpha^2)(1 - c_7 sp)}{\Phi_5 2r_s\alpha^4 + \Phi_9}$
c_9	$c_6 + c_8$
c_{10}	$c_5(\Phi_1 f_w\zeta^2 + \Phi_6 2r_w\beta^2)wp + c_9(\Phi_1 f\zeta^2 + \Phi_7 2r_s\alpha^2)sp$
c_{11}	$a_1w_1\Phi_1 + a_2w_2\Phi_6 + a_3w_3\Phi_7 + a_4w_4\Phi_8 - c_{10}$

TABLE 15. Table of Constant Quantities for the Split-Plot BBD

Constants	Expressions
c_1	$\Phi_1 f\lambda_w\beta^4 - \dfrac{(\Phi_1 f\lambda_{\text{int}}\alpha^4)^2 sp}{\Phi_5 f(r_s-\lambda_s)\alpha^4 + sp(\Phi_1\Phi_4 f\lambda_s\alpha^4 + \Phi_3(f(r_s-\lambda_s)\alpha^4 + f_c\lambda_c\alpha^4))}$
c_2	$(\Phi_5 f(r_s-\lambda_s)\alpha^4 + sp(\Phi_1\Phi_4 f\lambda_s\alpha^4 + \Phi_3(f(r_s-\lambda_s)\alpha^4 + f_c\lambda_c\alpha^4)))(\Phi_1 f(r_w-\lambda_w)\beta^4 + wpc_1)$
c_3	$\dfrac{\Phi_1(fr_w\beta^2)}{\Phi_1 f(r_w-\lambda_w)\beta^4 + wpc_1}$
c_4	$-\dfrac{(\Phi_1 f)^2 r_s\alpha^2\lambda_{\text{int}}\alpha^4 sp}{c_2}$
c_5	$c_3 + c_4$
c_6	$-\dfrac{(\Phi_1 f)^2 r_w\beta^2\lambda_{\text{int}}\alpha^4 wp}{c_2}$
c_7	$\dfrac{(\Phi_1\Phi_4 f\lambda_s\alpha^4 + \Phi_3(f(r_s-\lambda_s)\alpha^4 + f_c\lambda_c\alpha^4))c_2 - (\Phi_5 f(r_s-\lambda_s)\alpha^4(\Phi_1 f\lambda_{\text{int}}\alpha^4)^2 wp)}{(\Phi_5 f(r_s-\lambda_s)\alpha^4 + sp(\Phi_1\Phi_4 f\lambda_s\alpha^4 + \Phi_3(f(r_s-\lambda_s)\alpha^4 + f_c\lambda_c\alpha^4)))c_2}$
c_8	$\dfrac{\Phi_1(r_s\alpha^2)(1-c_7 sp)}{\Phi_5(r_s-\lambda_s)\alpha^4}$
c_9	$c_6 + c_8$
c_{10}	$c_5\Phi_1 fr_w\beta^2 wp + c_9\Phi_1 fr_s\alpha^2 sp$
c_{11}	$a_1 w_1\Phi_1 + a_4 w_4\Phi_8 - c_{10}$

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