The Impact of Increasing Centre Points on Three-Factor Spherical N-Point Design Using Full Quadratic Model

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Abstract

The study considered the Impact of increasing center points on three-factor spherical N-point Designs using quadratic model. The research considered how the increase in center points will affect the D-optimality, Sum of square errors, Grand Means of the designs as well as the Akaike information and Schwarz' Bayesian Criteria. The center point's addition considered were 1-5 inclusive. It was found that the D-optimality of the designs were maximized at 1 center point with the central composite circumscribed design (CCCD) having the highest value. This shows that the CCCD is the best three factor design on the basis of D-optimalty. The study shows that the Box-Behnken design (BBD) has the smallest sum of square error from 1 to 3 center points, while from 4 to 5 center points the CCCD recoreded the smallest sum of square error. The grand mean of Doehlert design and Central composite inscribed design increases for increasing center poins, while BBD decreases from 1 to 4 center points. The CCCD proves to be the best design based on AIC and SBC criteria, followed by CCID.

Key words: *Three-factor design, Box Behnken design, Doehlert design and Central Composite design*

1. Introduction

Box Behnken designs take three equally spaced levels which are: -1, 0 and +1, of the factors into consideration. These designs are more economical as compared to other 3k designs due to the reduced number of experimental trials in the design. The number of experimental trials is computed using the formula; $N = 2k(k-1) + cp$ where N is the number of trials, k is the number of factors and cp is the number of replicates for the centre points. All the experimental points are present in the form of a hyper sphere and are placed equidistant from the central point. Such designs have been used in optimization studies involving enzyme assays, emulsion formation.

Box-Behnken design is a second class of experimental designs for modelling quadratic response function which was introduced in 1960 by Box and Behnken. Assuming $k \geq 3$, most of the Box-Behnken designs (BBD) are constructed by conjoining two-level factorial designs with balanced incomplete block designs (BIBD) associated with every BIBD, and hence, every BBD considered, have the following parameters:

k = the number of design variables.

b = the number of blocks in the BIBD.

t = the number of design variables per block.

r = the number of blocks in which a design variable appears.

λ = the number of times that each pair of design variables appear in the same block.

Central Composite Design (CCD), is the most popular of all second-order designs or the Box Wilson Design. This design consists of the following parts: i) a complete (or a fractional of) $2k$ factorial design whose factors' settings are coded as (Low = −1, High = 1); this is called the factorial portion; ii) an additional design, star points, which provides justification for selecting the distance of the star points from the centre; the CCD always contains twice as many star points as there are factors in the design ($2k$); iii) $n0$ central point. Thus, the total number of design points in a CCD is $n = 2k + 2k + n0$. A CCD is obtained by augmenting the first-order design of a $2k$ factorial with additional experimental runs, the $2k$ axial points, and the $n0$centre-point replications. This design is consistent with the sequential nature of a response surface investigation. The analysis starts with a first-order design and a fitted first-degree model, followed by the addition of design points to fit a higher second-degree model. The first-order design in the preliminary phase gives initial information about the response system and assesses the importance of the factors in a given experiment. . In the CCD, the values of α and $n0$, are chosen for their desirable properties, where α is the axial point and $n0$ the number of centre point replicates. For instance, to ensure that a CCD has a rotatable, orthogonal, and uniform precision property, all three factors are studied at five levels $(-\alpha,-1,0,+1,+\alpha)$. The orthogonality of a second-order design is achieved when the quadratic model is expressed in terms of orthogonal polynomials. The value of $n0$ can be determined for a rotatable CCD to have either the additional orthogonality property or the uniform precision property.
Doehlert Design was proposed in 1970 by Doehlert. It starts from k=2 factors from an equilateral triangle of length 1 unit to construct a regular hexagon with a centre point (0, 0). (Suleiman, 2017). The designs that are popular in fitting second-order model are the Central Composite and the Box-Behnken designs. Another design that was found comparable with the above-mentioned designs was the Doehlert design. (Verdooren, 2017).This design requires fewer experimental runs as compared to the CCD and BBD. It is also a spherical design.

This study is aimed at investigating the impact of increasing centre points in three factor designs. The designs considered are the Central Composite (inscribed, circumscribed), Doehlert and the Box-Behnken designs.

Over the years, researchers have sought knowledge on the effect of increasing the addition of centre points to second-order two factor designs thereby giving so much interest on two factor designs of Central Composite, Box-Behnken and Doehlert designs in the literatures, Such as those studied by Ukaegbu & Chigbu, (2015), Oyejola & Nwanya, (2015), Iwundu & Onu (2017), Onu, *et al.* (2021) and Iwundu, (2016 a & b). Verdooren, (2017) studied the Use of Doehlert Designs for Second-order Polynomial Models, where the D-optimal design of the Doehlert Design was compared with the D-optimal designs of the Box-Behnken and Central Composite Designs. The study did not consider estimation of parameters of these designs, Onu et al (2022) studied estimation of parameters and optimality of second-order spherical designs using quadratic function relative to non-spherical face centred CCD. The parameters and optimalities of second-order designs were estimated for increasing centre points from 1 to 10 inclusive. It was only considered for two factor designs. This study will investigate the impact of increasing centre points on three factor designs of central composite circumscribed design (CCCD), central composite inscribed design (CCID), Doehlert design (DD)and Box-Behnken design (BBD), with emphasis placed on the D-optimality, Sum of square errors, Akaike Information criterion (AIC) and Schwarz' Bayesian Criterion (SBC) and Grand means of the designs.

Shruti & Padma (2017), while studying the selection of a design for Response Surface, compared Box-Behnken, Central Composite, D-optimal and I-optimal designs using statistical tools. Nitin & Vivek (2019) presented Box-Behnken Design as a basis of optimization to evaluation of the effect of some process parameters.

Xiaoxia & Guang (2020) used single-factor experiments and response surface methodology that is based on a Box-Behnken Design, such that two most commonly experimental design methods were used to optimize the extraction conditions of Pectin.

Satriani et al. (2013) stated that in order to predict the optimal point, a second-order polynomial function be fitted to correlate the relationship between input variables and the output variable.

Suliman, (2017), also studied Box-Behnken and Central Composite designs estimated Eigen values and other optimality. Iwundu (2016), and Onu *et al.* (2021) studied Equiradial designs for changing model parameters, while Iwundu considered Equiradial Design of radius of 1.0 for one centre point, Onu et al. considered Equiradial Design for radius of 1.0 and 1.414 for centre points from 1 to 5 inclusive.The use of Doehlert design for optimizing the digestion of beans for multi-element, was considered by Wagna et al., (2008), it was observed that the mineral composition of food legumes is a more-or-less variable factor and influenced by a number of interrelated factors like climate change, genetic diversity. Suliman, (2017) stated that it is essential to have a choice of control variables that have main effects because it is not possible to detect the effects of all potential control variables. As an alternative, the process of factorial design may be utilized for this purpose. Brandley, (2009), noted that the design of response surface models starts with the estimation of parameters, pure error, and lack of fit. Anup & Saiket (2018), stated that Design of Experiment is an integral chemometric tool for process optimization. William & Alain (2018), said that Design of experiment is a method used for planning experiments and analyzing the information obtained.

2.1 Obtaining Parameters of Second-Order Spherical Designs for full Model for increasing centre points

2.1.1 Obtaining parameters of Box-Behnken Design for increasing centre points

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_{12} + \beta_{13} x_{13} + \beta_{23} x_{23} + \beta_{11} \beta_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \varepsilon \quad (2.1)$$

which is a Quadratic Model having all the variables present,the model in (2.1) can be written in matrix form as:

$$y = X\beta + \varepsilon \qquad (2.2)$$

Where X is an $N \times P$ matrix, y is an $N \times 1$ vector of observed responses, $\boldsymbol{\beta}$ is the $P \times 1$ vector of unknown parameters and $\varepsilon \sim N(0, \delta^2)$ is the error term which is randomly distributed. From (2.1) ϕ is not known and represents real functional relationship between the response y and the explanatory variables $(x_1, x_2, \ . \ . \ . \ , x_n)$.

The model in (2.1) will be applied throughout this study in obtaining Design Matrices for Box-Behnken, Central Composite (Circumscribed and inscribed) and Doehlert Designs. The parameters of these models will be estimated together with their Sum of Square Errors and D-Optimality Criterion for increasing centre points from 1-5 inclusive.

The design points for Box-Behnken design are: (-1 1 -1 1 0 0 0 0 -1 1 -1 1 0 0 0 0 0 0 0 0 -1 1 -1 1 0, -1 -1 1 1 0 0 0 0 0 0 0 0 -1 1 -1 1 -1 1 -1 1 0 0 0 0 0, 0 0 0 0 -1 1 -1 1 0 0 0 0 -1 -1 1 1 0 0 0 0 -1 -1 1 1 0).

For the full model in equation (2.1), we obtain the design matrix, X, The design matrix obtained from the model will be used to obtain the transpose, X', then by multiplication of X' by X gives the information matrix, because of unequal design sizes, the information matrices obtained will be normalized to enable the comparisons of designs with varying design sizes.

Normalizing the, $\frac{X'X}{N}$ which cancels out the effect of design sizes in a design for the reason of comparing two or more designs with different design sizes.

The least square equation which will be used in the estimation of the parameters for the model is given as

$$\underline{\hat{\beta}} = \left(\frac{X'X}{N}\right)^{-1} X'Y \qquad (2.3)$$

Where $\underline{\hat{\beta}}$ is an $\mathrm{N} \times 1$ vector, given as $(\beta_0, \ \beta_1, \ \beta_2, \ \beta_{12} \ldots, \ \beta_{11}, \ \beta_{22} \ldots)'$ and $\left(\frac{X'X}{N}\right)^{-1}$ is the inverse of the normalized information matrix and N is the number of Design size. The Design Matrix X is obtained from the Quadratic Model in (2.1) as seen in Iwundu (2016a &b), Oyejola and Nwanya (2015), Iwundu and Onu (2017), Onu et al (2021) and Onu et al (2022).

2.1.2 Obtaining parameters of Central Composite Designs for increasing centre points

The design points of Circumscribed Central Composite Design are: (1 1 1 1 -1 -1 -1 -1 1.414 -1.414 0 0 0 0 0, 1 1 -1 -1 1 1 -1 -1 0 0 1.414 -1.414 0 0 0, 1 -1 1 -1 1 -1 1 -1 0 0 0 0 1.414 -1.414 0), and that of CCD Inscribed are (1 1 1 1 -1 -1 -1 -1 0.707 -0.707 0 0 0 0 0, 1 1 -1 -1 1 1 -1 -1 0 0 0.707 -0.707 0 0 0, 1 -1 1 -1 1 -1 1 -1 0 0 0 0 0.707 -0.707 0), these sets of points are used to obtain the Design matrix for full and reduced models and all the processes above will be followed.

The Design points for Doehlert Design are: (10 1 0 -1 -0.5 0.5 0.5 -0.5 -0.5 0.5 0.5 -0.5 0, -1 0 1 1 -0.5 -0.5 0.5 0.5 -0.5 -0.5 0.5 0.5 0, 0 0 0 0 0.707 0.707 0.707 0.707 -0.707 -0.707 -0.707 -0.707 0), these points are used to obtain design matrix for full model of (2.1). All other processes stated above are followed strictly to obtain the parameters of the two models.

2.2 Obtaining the D-optimality of Box-Behnken, Central Composite and Doehlert Designs for increasing centre points

D-optimality:

The D-Optimality of any Design is given as

D-Opt.= $Min\ det(M^{-1}) \equiv Max\ det(M)$ (2.4)

The design that has the highest determinant of the normalized information matrix is considered the best design under this criterion. Equation (3.5) will be applied to all the four studied three factor second-order designs, for centre points from 1 to 5, to see the design and for what centre points and for which model gave the highest determinant. The study applied MATHLAB software for this computation.

2.3 Obtaining the Sum of Square Error (SSE)for increasing centre points

From each of these designs with each centre point, the estimate of the regression sum of square subject in (2.1), gives

$\varepsilon = (y - \hat{y}\ )$, for changing values of y given as $y_i$and corresponding values of $\hat{y}$ given as $\hat{y}_i$ gives

$$\varepsilon_i = (y_i - \hat{y}_i) \quad (2.5)$$

Summing and squaring (2.5), we obtain the error sum of square for both the quadratic model and it is given as

$$\sum \varepsilon_i^2 = \sum (y_i - \hat{y}_i)^2 \quad (2.6)$$

In obtaining these errors sum of square of the regression equations, EXCEL software package was used.

2.4 Model Adequacy Criteria for increasing centre points

The model adequacy criteria to be employed in this work are the Akaike Information Criterion (AIC) and the Schwarz Bayesian Criterion (SBC).

2.4.1 Akaike Information Criterion (AIC) for increasing centre points

The AIC is given as seen in Kutner et al (2005), Onu, et al. (2021) as.

$$AIC = nInSSE - nInn + 2p \quad (2.7)$$

The first term of (2.7) which is $nInSSE$ decreases as the number of model parameters P increases, while the second term is fixed for a given sample size n and the third term increases with the number of parameters, P. The models with small SSE perform better by this criterion, as long as the penalties 2P for AIC is concerned. The smaller the value of the AIC, the better the model.

2.4.2 Schwarz' Bayesian Criterion (SBC) for increasing centre points

This criterion is given as:

$$SBC_P = n \ln SSE - n \ln n + [\ln n]p \qquad (2.8)$$

Note that the smaller the SBC the better the model.

3.1 Analysis of the Parameters, D-optimality and Sum of Square Errors of Three Factors Second-Order Designs for Full Quadratic Model for increasing centre points

3.1.1 Estimation of Parameters of Three Factors Second-Order Designs for Full Quadratic Model for increasing centre points

The Design Matrix of Box-Behnken Design for Full Quadratic Model for 1 centre point is given as:

$$X = \begin{pmatrix}
1 & -1 & -1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\
1 & 1 & -1 & 0 & -1 & 0 & 0 & 1 & 1 & 0 \\
1 & -1 & 1 & 0 & -1 & 0 & 0 & 1 & 1 & 0 \\
1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\
1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 1 & 1 \\
1 & 0 & 1 & -1 & 0 & 0 & -1 & 0 & 1 & 1 \\
1 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 1 & 1 \\
1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\
1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & -1 & 0 & -1 & 0 & 1 & 0 & 1 & 0 & 1 \\
1 & 1 & 0 & -1 & 0 & -1 & 0 & 1 & 0 & 1 \\
1 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & 1 \\
1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

The determinant was obtained as:

$$\left|\frac{X'X}{25}\right| = 5.0468\text{e} - 006$$

The inverse of the normalized information matrix was obtained as:

$$\left(\frac{X'X}{25}\right)^{-1} = \begin{pmatrix} 7.3529 & 0 & 0 & 0 & 0 & 0 & 0 & -4.4118 & -4.4118 & -4.4118 \\ 0 & 2.0833 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.0833 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.0833 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6.2500 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6.2500 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6.2500 & 0 & 0 & 0 \\ -4.4118 & 0 & 0 & 0 & 0 & 0 & 0 & 5.1471 & 2.0221 & 2.0221 \\ -4.4118 & 0 & 0 & 0 & 0 & 0 & 0 & 2.0221 & 5.1471 & 2.0221 \\ 7.3529 & 0 & 0 & 0 & 0 & 0 & 0 & -4.4118 & -4.4118 & -4.4118 \\ 0 & 2.0833 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The parameters were obtained as shown below:

$$\underline{\hat{\beta}} = \begin{pmatrix} 193.9265 \\ -8.0625 \\ -26.2083 \\ 7.5833 \\ -8.2500 \\ 30.0000 \\ 3.4375 \\ -83.2059 \\ 1.1379 \\ -60.4871 \end{pmatrix}$$

The Design Matrix of Box-Behnken Design for Full Quadratic Model for 2 centre points is given as:

$$X=\begin{pmatrix}
1 & -1 & -1 & 0 & 1 & 0 & 0 & 1 & 1 & 0\\
1 & 1 & -1 & 0 & -1 & 0 & 0 & 1 & 1 & 0\\
1 & -1 & 1 & 0 & -1 & 0 & 0 & 1 & 1 & 0\\
1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0\\
1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1\\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1\\
1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1\\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1\\
1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\
1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\
1 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 1 & 1\\
1 & 0 & 1 & -1 & 0 & 0 & -1 & 0 & 1 & 1\\
1 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 1 & 1\\
1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1\\
1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0\\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0\\
1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0\\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0\\
1 & -1 & 0 & -1 & 0 & 1 & 0 & 1 & 0 & 1\\
1 & 1 & 0 & -1 & 0 & -1 & 0 & 1 & 0 & 1\\
1 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & 1\\
1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

The determinant was obtained as:

$$\left|\frac{x'x}{26}\right| = 4.4122\text{e}-006$$

The inverse of the normalized information matrix was obtained as:

$$\left(\frac{X'X}{26}\right)^{-1} = \begin{pmatrix} 5.9091 & 0 & 0 & 0 & 0 & 0 & 0 & -3.5455 & -3.5455 & -3.5455 \\ 0 & 2.1667 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.1667 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.1667 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6.5000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6.5000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6.5000 & 0 & 0 & 0 \\ -3.5455 & 0 & 0 & 0 & 0 & 0 & 0 & 4.7273 & 1.4773 & 1.4773 \\ -3.5455 & 0 & 0 & 0 & 0 & 0 & 0 & 1.4773 & 4.7273 & 1.4773 \\ -3.5455 & 0 & 0 & 0 & 0 & 0 & 0 & 1.4773 & 1.4773 & 4.7273 \end{pmatrix}$$

The parameters were obtained as shown below:

$$\underline{\hat{\beta}} = \begin{pmatrix} 155.4327 \\ -8.3850 \\ -27.2567 \\ 7.8867 \\ -8.5800 \\ 31.2000 \\ 3.5750 \\ -58.7836 \\ 28.9339 \\ -35.1561 \end{pmatrix}$$

3.2 Estimation of Sum of Square Errors of Three Factor Second-Order Designs for Full Model for increasing centre points

The Sum of square analysis for Box-Behnken Design for full model with 1centre point is obtained in the processes below:

Table 1: Sum of Square errors of Box-Behnken Design for full model

1	x2	x3	GDP	B	Ext GDP	Deviation	SquDeviat	extGDP/25
-1	-1	0	2.21	193.927	137.8793	-3.3052	10.92435	5.5152
1	-1	0	1.92	-8.0625	138.2543	-3.61017	13.03334	5.530172
-1	1	0	0.81	-26.208	102.9627	-3.30851	10.94623	4.118508
1	1	0	-1.62	7.5833	69.3377	-4.39351	19.30291	2.773508
0	0	-1	2.65	-8.25	125.8561	-2.38424	5.684619	5.034244
0	0	1	6.31	30	141.0227	0.669092	0.447684	5.640908

0	0	-1	6.61	3.4375	125.8561	1.575756	2.483007	5.034244
0	0	1	4.23	-83.206	141.0227	-1.41091	1.990661	5.640908
-1	0	0	5.31	1.1379	118.7831	0.558676	0.312119	4.751324
1	0	0	8.01	-60.487	102.6581	3.903676	15.23869	4.106324
-1	0	0	8.04		118.7831	3.288676	10.81539	4.751324
1	0	0	6.76		102.6581	2.653676	7.041996	4.106324
0	-1	-1	6.59		156.6398	0.324408	0.105241	6.265592
0	1	-1	6.06		97.3482	2.166072	4.691868	3.893928
0	-1	1	6.44		164.9314	-0.15726	0.024729	6.597256
0	1	1	9.25		119.3898	4.474408	20.02033	4.775592
0	-1	0	7.35		221.2727	-1.50091	2.252725	8.850908
0	1	0	15.33		168.8561	8.575756	73.54359	6.754244
0	-1	0	5.92		221.2727	-2.93091	8.590222	8.850908
0	1	0	5.02		168.8561	-1.73424	3.007602	6.754244
-1	0	-1	0.58		80.7127	-2.64851	7.014595	3.228508
1	0	-1	2.58		4.5877	2.396492	5.743174	0.183508
-1	0	1	2.94		35.8793	1.504828	2.264507	1.435172
1	0	1	4.2		79.7543	1.009828	1.019753	3.190172
0	0	0	-0.07		193.9265	-7.82706	61.26287	7.75706
							287.7622	

The Sum of Square Error $(SSE) = 287.7622$

The Sum of square analysis for Box-Behnken Design for Reduced model with 1 centre point is obtained in the processes below;

Table 2: Sum of Square errors of Box-Behnken Design for reduced model

x1	**x2**	**x3**	**GDP**	**B**	**Ext GDP**	**Deviation**	**squDeviat**	**extGDP/25**
-1	-1	0	2.21	193.927	144.9914	-3.3052	10.92435	5.5152
1	-1	0	1.92	-8.0625	295.2782	-9.89113	97.83441	11.81113
-1	1	0	0.81	-26.208	259.9866	-9.58946	91.95782	10.39946
1	1	0	-1.62	7.5833	76.4498	-4.67799	21.88361	3.057992
0	0	-1	2.65	-83.206	186.3432	-4.80373	23.0758	7.453728
0	0	1	6.31	1.1379	201.5098	-1.75039	3.063872	8.060392
0	0	-1	6.61	-60.487	186.3432	-0.84373	0.711877	7.453728
0	0	1	4.23		201.5098	-3.83039	14.6719	8.060392
-1	0	0	5.31		201.989	-2.76956	7.670463	8.07956
1	0	0	8.01		185.864	0.57544	0.331131	7.43456
-1	0	0	8.04		201.989	-0.03956	0.001565	8.07956
1	0	0	6.76		185.864	-0.67456	0.455031	7.43456
0	-1	-1	6.59		152.0644	0.507424	0.257479	6.082576
0	1	-1	6.06		220.622	-2.76488	7.644561	8.82488

0	-1	1	6.44	288.2052	-5.08821	25.88986	11.52821
0	1	1	9.25	114.8144	4.657424	21.6916	4.592576
0	-1	0	7.35	220.1348	-1.45539	2.118166	8.805392
0	1	0	15.33	167.7182	8.621272	74.32633	6.708728
0	-1	0	5.92	220.1348	-2.88539	8.325487	8.805392
0	1	0	5.02	167.7182	-1.68873	2.851802	6.708728
-1	0	-1	0.58	195.5436	-7.24174	52.44286	7.821744
1	0	-1	2.58	177.1428	-4.50571	20.30144	7.085712
-1	0	1	2.94	208.4344	-5.39738	29.13167	8.337376
1	0	1	4.2	194.5852	-3.58341	12.84081	7.783408
0	0	0	-0.07	193.9265	-7.82706	61.26287	7.75706
						591.6668	

The Sum of Square Error $(SSE) = 591.6668$

Table 3: Comparing the AIC and SBC of the Standard Designs

	BBD full		DD full		CCCD Full		ICCD Full	
C	**AIC**	**SBC**	**AIC**	**SBC**	**AIC**	**SBC**	**AIC**	**SBC**
1	81.08	93.27	70.64	76.29	66.49	73.57	68.98	76.06
2	82.57	95.15	73.29	79.68	68.75	76.48	70.70	78.42
3	85.29	98.25	75.78	82.87	69.65	77.98	71.80	80.13
4	88.51	101.83	78.33	86.06	71.10	80.00	73.28	82.18
5	89.94	101.61	81.25	89.58	71.74	81.18	73.77	83.22
1	93.10	101.63	59.84	63.80	60.91	65.87	62.59	67.55
2	85.41	94.21	61.84	66.31	62.79	68.20	64.79	70.20
3	83.96	93.03	64.11	69.06	65.53	71.36	67.07	72.91
4	88.20	97.53	66.35	71.75	67.93	74.17	69.64	75.88
5	88.95	98.52	68.90	74.74	75.01	81.63	74.10	80.71

Table 4: Comparison of D-Optimalities of the Three Factor Second-Order Designs for Centre Points 1-5

D-Optimality	**FULL MODEL**				
	C	**DD**	**BBD**	**CCCD**	**CCID**
	1	3.61e-9	5.05e-6	0.0033	1.30e-5
	2	3.22e-9	4.41e-6	0.0029	8.17e-6
	3	2.37e-9	3.71e-6	0.0022	5.19e-6
	4	1.64e-9	3.06e-6	0.0016	3.34e-6
	5	1.11e-9	2.49e-6	0.0011	2.20e-6

Table 5: Comparison

of the Sum of Square Errors of the three factor Second-Order Designs for Centre Points 1-5

Sum of Square errors	FULL MODEL C	DD	BBD	CCCD	CCID
	1	639.51	287.76	332.79	392.78
	2	629.84	288.43	336.86	380.33
	3	618.35	303.12	315.37	357.86
	4	612.89	323.44	307.73	347.37
	5	624.02	323.46	289.29	321.99

Table 6: Comparison of the Grand Means of the Three Factor Second-Order Designs for Centre Points 1-5

Grand Mean	FULL MODEL C	DD	BBD	CCCD	CCID
	1	86.55	193.93	133.40	105.86
	2	92.77	155.43	126.53	111.29
	3	96.71	122.47	140.97	123.76
	4	103.12	98.24	145.49	131.20
	5	118.83	106.14	178.65	155.32

Discussion of Results

Discussions Based on D-optimality Criterion for Full Model

It was observed that the determinant of the three factor Doehlert, Box-Behnken, and Central Composite Circumscribed and Inscribed designs decrease for increasing centre points. All the above-mentioned designs have maximum determinant at 1 centre point for full model. The D-optimality of these designs is maximized at 1 centre point, with central composite circumscribed design (CCCD) having the highest value. This shows that the CCCD is the best design on the basis of D-optimality criterion, followed by the central composite inscribed design (CCID), then the Box-Behnken design (BBD) and then the Doehlert design (DD). The DD design was found to be an inferior design among all the three factor designs considered on the basis of D-optimality. Generally, the D-optimality criterion decreases for increasing centre points. This simply indicates that addition of more centre points increases the power of the designs.

Discussion based on Sum of Square Errors

The study reveals that the Doehlert Design which produced the smallest determinants across all the studied centre points, produced the largest sum of square errors for all the centre points. Generally, it shows that a D-optimal design will give a smaller sum of square errors for full model, the Box-Behnken Design gives the smallest sum of square error for 1 to 3 centre points but for 4 and 5 centre points, the Central Composite Circumscribed Design gave better sum of square error. The sum of square error for Box-Behnken Design for 4 and 5 centre points are approximately equal. This shows that Box-Behnken Design is better than other studied designs for 1 to3 centre points for full model.

Discussion Based on the Grand Mean of the Designs

For full model, the Grand Mean of Doehlert Design increases as the centre points increases, this was also true for Central Composite Inscribed Design, while that of Box-Behnken Design decreases for increasing centre points from 1 to 4 but increases at 5 centre points. The Central Composite Circumscribed Design has its Grand Mean decreased from 1 centre point to 2 centre points, but increased from 3 to 5 centre points.

Discussion Based on the Akaike Information criterion (AIC) and Schwarz' Bayesian Criterion (SBC) criteria

The AIC and SBC generally increase for increasing centre points the CCCD proves to be the best design, followed by the CCID and then the DD. The BBD appears inferior for these criteria.

Conclusion

The study concludes that the design with minimized determinant gives a larger sum of square error for the full model and for all the three factor second-order designs studied, Central Composite Design was found to be the best for full model.

Recommendations

The study recommends that Central Composite Circumscribed design is the best second-order three factor design as revealed by the D-optimality, Sum of squares, AIC and SBC criteria.

Contribution to Knowledge

The study contributed the following:

1. Doehlert design was extremely inferior to the other three factor designs.
2. Doehlert design produced the smallest D-optimality across all designs studied, with the largest sum of square errors.
3. There is a strong relationship between D-optimality and Sum of square of a design.
4. All the above-mentioned designs have maximum determinant at 1 centre point for full model.

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