

Rotatability of Second-Order Response Surface Designs

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The concept of rotatability has been proposed in the literature as a desirable property of a good experimental design, with the intention of imposing stability on the scaled prediction variance of a design. Thus this allows the prediction variance to remain unchanged under any rotation of the coordinate axes. This study focuses on the rotatability of the Box-Behnken designs and the Circumscribed Central Composite Design in four and five variables. The statistical software MiniTab 16 was used to generate the design and analyses were carried out using RStudio software. The rotatability property of the Circumscribed Central Composite design was found to satisfy the two rotatability conditions for second-order designs perfectly. However, the Box-Behnken designs were either perfectly rotatable or near rotatable.

Keywords: Rotatability, Response surface, Scaled prediction variance, Design, Properties.

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INTRODUCTION

Rotatability is one desirable property of a good experimental design. It is particularly important in the construction of second-order response surface designs. For first-order response surface, an orthogonal, variance-optimal design is automatically rotatable as all first odd moments are zero and the second pure moments are equal. It was developed by Box and Hunter in 1957. Other desirable properties of the response surface designs include constant variance check, estimation of transformations, orthogonality and optimality, lack of fit detection, internal error estimation, suitability for blocking, construction of higher order designs and graphical analyses (Aanchal et al., 2016). These properties are very important in that they constitute the basis for which a design is chosen among other designs of its class.

Response Surface Designs and Models

Response surface designs are a major part of the concept of Response Surface Methodology (RSM) where it derives its name. These methodologies consist of statistical and mathematical techniques useful for empirical model building and model exploitation. RSM is an approximation of the response function

$$Y = f(\xi_1, \xi_2, \xi_3, \dots, \xi_k) + \varepsilon \quad (1)$$

Where

Y = response variable

$\xi_1, \xi_2, \xi_3, \dots, \xi_k$ = natural variables

ε is the experimental error

In most practical situations, the form of such a relationship is usually unknown, but can be approximated by a low-order polynomial such as the first-order (main effect or with interaction), the second-order and three-level fractional factorial models. These low-order polynomials are the major RSM approximating functions, which can be numerically as well as graphically applied in process optimization (Box and Hunter, 1957; Oyejola and Nwanya, 2015; Aanchal, et al., 2016).

The models when converted to the coded form (x) can be expressed as follows;

First-order main effect Model

$$\hat{y} = \beta_0 + \sum_{i=1}^k \beta_i x_i + \varepsilon \quad (2)$$

And first-order model with interaction

$$\hat{y} = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i < j=1}^k \beta_{ij} x_i x_j + \varepsilon \quad (3)$$

The second-order model

$$\hat{y} = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i < j=2}^k \beta_{ij} x_i x_j + \sum_{i=1}^k \beta_{ii} x_i^2 + \varepsilon \quad (4)$$

Where

\hat{y} = response variable

x_i = coded independent variables; $i = 1, 2, \dots, k$

β = unknown parameters

ε is the experimental error

Both first order models are used in approximating true response surface in a relatively small region of the independent space where there is little or no curvature in the function and with interaction among the variables [equation (3)]. However, when there is presence of substantial curvature, these models become inadequate and therefore a second-order model becomes necessary.

Rotatable Designs

Box and Hunter (1957) introduced rotatability as a natural and highly desirable property in response surface methodology for the exploration of response surfaces. They constructed these designs through geometrical configurations and obtained second-order rotatable designs (SORD). A rotatable design is one for which $\frac{NVar[\hat{y}(x)]}{\sigma^2}$ has the same value at any two locations from the center of the design.

Hence $\frac{NVar[\hat{y}(x)]}{\sigma^2}$ is constant on spheres.

Rotatable designs are mainly for the exploration of response surfaces. These designs provide the preferred property of constant prediction variance at all points that are equidistant from the design center, thus improving the quality of the prediction (Otieno-Roche, et al., 2017). Several researchers have considered varying aspects of the concept of rotatability in as many studies depending on their area of interest. Sulochana and Victorbabu (2021a) studied the

measure of slope rotatability for second order responses. In another study they also suggested the use of measure of slope rotatability for second order response surface designs using central composite designs under intra-class correlated structure of errors (Jyostna et al. 2021; Sulochana and Victorbabu, 2021b; Chiranjeevi and Victorbabu, 2021). Koech et al. (2017) applied Second-Order Rotatable Design to optimize potato tubers yield as a solution for cost effective farming methods.

This research is therefore aimed at studying the rotatability property of the second-order response surface designs with the following objectives in view.

1. To certify the necessary and sufficient conditions of rotatability for the Box-Behnken Designs (BBD) in $k = 4$ and 5 design variables.
2. To certify the necessary and sufficient conditions of rotatability for the Circumscribed Central Composite Designs (CCCD) in $k = 4$ and 5 design variables.
3. To establish design preference based on the rotatability principle.

CONCEPT OF SECOND-ORDER RESPONSE SURFACE

As stated in the earlier, the second-order model becomes imperative when there is strong evidence of curvature in response surface. In such a case, the first-order model is no longer adequate.

SECOND-ORDER MODEL

The second-order model is given by the function

$$\hat{y} = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i < j=2}^k \beta_{ij} x_i x_j + \sum_{i=1}^k \beta_{ii} x_i^2 + \varepsilon$$

with $1 + 2k + \frac{k(k-1)}{2}$ model parameters.

where

\hat{y} = response variable

x_i = coded independent variables; $i = 1, 2, \dots, k$

β = unknown parameters

ε is the experimental error

The model is assumed to be normally distributed $\varepsilon \sim N(\mu, \sigma^2)$.

The model can also be expressed in matrix form as $Y = X\beta + \varepsilon$

With

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix}; \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \\ \beta_{12} \\ \beta_{13} \\ \vdots \\ \beta_{jk} \\ \beta_{11} \\ \beta_{22} \\ \vdots \\ \beta_{kk} \end{bmatrix}; \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_k \end{bmatrix} \text{ and}$$

$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} & x_{11}x_{12} & x_{11}x_{13} & \cdots & x_{1(k-l)}x_{1k} & x_{11}^2 & x_{12}^2 & \cdots & x_{1k}^2 \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} & x_{21}x_{22} & x_{21}x_{23} & \cdots & x_{2(k-1)}x_{2k} & x_{21}^2 & x_{22}^2 & \cdots & x_{2k}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} & x_{n1}x_{n2} & x_{n1}x_{n3} & \cdots & x_{n(k-1)}x_{nk} & x_{n1}^2 & x_{n2}^2 & \cdots & x_{nk}^2 \end{bmatrix}$$

where

The vector Y is a $k \times 1$ vector of observations or responses

The vector β is a $k \times 1$ vector of unknown parameters which are estimated on the basis of n uncorrelated observations.

ε is the $k \times 1$ vector of random errors associated with Y .

X is the model matrix of dimension $n \times p$.

n is the number of experimental runs and p is the number of model parameters.

Second-Order Response Surface Designs (SORDS)

There are several second-order response surface designs. These include Central Composite designs (CCD), Box-Benken designs (BBD), Hooke designs, Small Composite designs (SCD), Minimum-run Resolution V designs (MinresV), Hybrid designs, etc (Box and Wilson, 1951; Myers and Montgomery, 2002; Zarhan, 2002). As studied by Myers and Montgomery (2002) and Montgomery (2005), a good response surface design possesses the following features: (a) provides a reasonable distribution of data points throughout the region of interest; (b) provides a good profile of the prediction variance in the experimental region; (c) does not require a large number of runs; etc. These attributes are typical of the second-order response surface designs (Chigbu et al., 2009).

Applicability of the Second-Order Response Surface Designs

Second-order response surface designs have applications in a wide variety of subject areas. These include mathematics, statistics, biological science, agricultural science, pharmacy etc. Aanchal et al. (2016) listed several authors who applied the SORS in optimization of cellulase produced by

microorganisms. Morshedi and Akbarian (2014) citing Mead and Pike (1975), Khuri and Cornell (1987) and Edmondson (1991) noted the application of second-order response surface designs in agriculture, production of snap bean yield and greenhouse experiments respectively. Peasura (2015) applied it to the modeling of postweld heat treatment process (under industrial technology). Khuri (2017) applied the second-order response surface designs in food sciences. Joshy and Balakrishna (2021) studied orthogonally blocked second order response surface designs under auto-correlated errors. Charankumar et al. (2020) combine the methods of modified second order response surface design and Taguchi design of experiments to determine optimum level of process parameters. Deepthi et al. (2021) proffered the best model for a second order response surface design in Bayesian approach. Bhatra Charyulu et al. (2022) suggested new series for the construction SORS using Binary Ternary Designs. Njoku and Otisi (2023) applied the CCD to optimize Biodiesel yield from transesterification of methanol and vegetable oil with a catalyst derived from eggshell. Czyski and Jarzębski (2020) considered various SORS as useful tools for evaluating the recovery of the fluoroquinolones from plasma. Their research applied the BBD, CCD and the Doehlert Design (DD). Usman et al. (2019) applied the CCD to optimize biosynthesized gold nanoparticles using sonochemical method. Maity (2023) described the applications of Box–Behnken, Central Composite, and mixture design in the field of textile engineering.

For the purpose of this study, the Circumscribed Central Composite designs (CCCD), Box-Benken designs (BBD) are compared for their rotatability. The choice of the two design type rests on the fact that they are mostly applied in real life experiments and have been the most standard designs in the literature.

CENTRAL COMPOSITE DESIGN (CCD)

The Central Composite designs (CCD) is the most popular class of the second-order designs developed by Box and Wilson (1951). It involves the use of a two-level factorial (or fraction) design of at least resolution V and above, combined with 2k axial (star) points and n_c center points. The factorial points [kept at (± 1) for the coded variable] represent a variance-optimal design for the first-order plus two-factorial interaction model. Center runs provide information about the existence of curvature in the system and the addition of axial (star) points allow for the efficient estimation of the pure quadratic terms (ie $x_1^2, x_2^2, \dots, x_k^2$). The number of experimental runs for the CCD is given by $N = 2^k + 2k + n_c$

For rotatability to be achieved in the CCD, the choice of α is most crucial. This is set as $\alpha = F^{\frac{1}{4}}$ where F is the number of factorial points or fraction of the factorial points up to resolution V or higher.

For example, the CCD in four variables has 2^4 factorial design points in its factorial portion.

$D = 2^4$

-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

The axial portion comprises of 2x4 design points as $[\pm\alpha, 0, 0, 0]$, $[0, \pm\alpha, 0, 0]$, $[0, 0, \pm\alpha, 0]$ and $[0, 0, 0, \pm\alpha]$ and the center runs comprises of $[0, 0, 0, 0]$ replicated 5 times.

BOX-BENKHEN DESIGNS (BBD)

The Box-Behnken designs (BBD) are a class of second-order designs that are based on three-level incomplete factorial designs. This design was developed by Box and Behnken (1960). The design requires only three levels to run an experiment $[+1, 0, -1]$. It is a special 3-level design because it does not contain any points at the vertices of the experiment region. For the BBD, each design can be thought of as a combination of a two-level (full or fractional) factorial design with an incomplete block design. In each block, a certain number of factors are put through all combinations for the

factorial design (± 1) , while the other factors are kept at the central values (0) with the addition of n_c centre points. The BBD in four variables with 5 replicated center runs is shown below.

D =

-1	-1	0	0
1	-1	0	0
-1	1	0	0
1	1	0	0
0	0	-1	-1
0	0	1	-1
0	0	-1	1
0	0	1	1
-1	0	0	-1
1	0	0	-1
-1	0	0	1
1	0	0	1
0	-1	-1	0
0	1	-1	0
0	-1	1	0
0	1	1	0
-1	0	-1	0
1	0	-1	0
-1	0	1	0
1	0	1	0
0	-1	0	-1
0	1	0	-1
0	-1	0	1
0	1	0	1
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0

PRINCIPLES OF ROTATABILITY

Scaled Prediction Variance (SPV)

One of the functions of the fitted response surface model, to an extent, the primary goal of many designed experiments, is to allow for good prediction of response values at various points of interest throughout the experimental region (Yakubu et al., 2014). In response surface methodology, interest is more on prediction than parameter estimation since the points on the fitted surface are predicted responses. Thus the prediction variance criteria are essential tools for selecting response surface designs as the researcher is provided with variance information regarding the worst prediction scenario. Box and Hunter (1957) noted that consideration of only the variances of the individual model coefficient estimates does not, for the case of second or higher-order models, lead to any unique class of "best" designs. Their argument is that the precision of the coefficient estimates should be studied simultaneously. Several measures of

prediction performance exist for comparing designs of which the most commonly considered is the scaled prediction variance (SPV).

For the second-order model, the scaled prediction variance of the expected response is given by

$$v(x) = \frac{NVar[\hat{y}(x)]}{\sigma^2} = Nf'(x)(X'X)^{-1}f(x)$$

where N is the design size, σ^2 is the observation error, and $f(x)$ is the general form of the $1 \times p$ model vector.

Desirable designs are those with the smallest maximum SPV, and with reasonably stable SPV (i.e. smallest range) in the design region. The SPV allows the experimenter to measure the precision of the predicted response on a per observation basis and it penalizes larger designs over small designs. It is this important property of the SPV that led to the concept of ROTABILITY of a design.

Important Properties of Rotatability

1. Rotatability imposes stability on the $v(x) = \frac{NVar[\hat{y}(x)]}{\sigma^2}$

$$\frac{1}{N}(X'X) = \begin{bmatrix} 1 & \frac{1}{N}\sum_{j=1}^N x_{1j} & \frac{1}{N}\sum_{j=1}^N x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}^2 & \frac{1}{N}\sum_{j=1}^N x_{2j}^2 \\ \frac{1}{N}\sum_{j=1}^N x_{1j} & \frac{1}{N}\sum_{j=1}^N x_{1j}^2 & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}^3 & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}^2 \\ \frac{1}{N}\sum_{j=1}^N x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{2j}^2 & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}^2 & \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{2j}^3 \\ \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}^2 & \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j}^2 & \frac{1}{N}\sum_{j=1}^N x_{1j}^3x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}^3 \\ \frac{1}{N}\sum_{j=1}^N x_{1j}^2 & \frac{1}{N}\sum_{j=1}^N x_{1j}^3 & \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}^3x_{2j} & \frac{1}{N}\sum_{j=1}^N x_{1j}^4 & \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j}^2 \\ \frac{1}{N}\sum_{j=1}^N x_{2j}^2 & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}^2 & \frac{1}{N}\sum_{j=1}^N x_{2j}^3 & \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}^3 & \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j}^2 & \frac{1}{N}\sum_{j=1}^N x_{2j}^4 \end{bmatrix}$$

The M matrix consists of the sample variances and covariance of the design model. The design matrix carries importance in characterizing variance properties and is clearly the function of the order of the model. Two notable components of the moment matrix are the 1) odd and 2) even moments.

Odd Moments: These are moments with at least one variable with an odd power. For the second-order, they are odd moments through order four (first pure moments, first mixed moments, second mixed moments, third pure moments and fourth mixed moments). The odd moments are analogous to the sample covariance. The odd moments in the above moment matrix are

$$\frac{1}{N}\sum_{j=1}^N x_{1j}, \frac{1}{N}\sum_{j=1}^N x_{1j}^2, \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}, \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j}, \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}^2, \frac{1}{N}\sum_{j=1}^N x_{1j}^3x_{2j} \text{ and } \frac{1}{N}\sum_{j=1}^N x_{1j}x_{2j}^3.$$

2. At any two location in the design space for which the distances from the origin are the same, the predicted values should be equally good (ie have equal variances).
3. It does not ensure stability or even near-stability throughout the design region.
4. It provides some guidelines for the choice of design parameters such as the choice of α and n_c in the central composite design.
5. Rotatability is easy to achieve without sacrifice of other important properties of the design.

Conditions For Rotatability

The conditions for rotatability are satisfied based on the characteristics of the moment matrix (M) given by

$$M = \frac{1}{N}(X'X)$$

For the second-order model in two variables the moment matrix is given by

Even Moments: These are moments with all variables with even powers. They are the second pure moments, fourth pure moments and fourth mixed moment. These moments characterize the variance of the design variables. The even moments in the above matrix are;

$$\left(\frac{1}{N}\sum_{j=1}^N x_{1j}^2, \frac{1}{N}\sum_{j=1}^N x_{2j}^2, \frac{1}{N}\sum_{j=1}^N x_{1j}^2x_{2j}^2, \frac{1}{N}\sum_{j=1}^N x_{1j}^4 \text{ and } \frac{1}{N}\sum_{j=1}^N x_{2j}^4\right).$$

Under the second-order model, the moments that affect rotatability are moments through order four.

The necessary and sufficient conditions for rotatability associated with the second-order response surface designs are

1. All odd moments through order four are zero

2. The ratio of moments $\frac{uuuu}{uuww} = 3 (u \neq w)$

Where

[uuuu] is the forth pure moments defined by

$$\frac{1}{N} \sum_{i=1}^N x_{iu}^4 ; u = 1, 2, \dots, k$$

[uuww] is the forth mixed moment defined by

$$\frac{1}{N} \sum_{i=1}^N x_{iu}^2 x_{iw}^2 ; (u \neq w)$$

If the above conditions are satisfied then the design is said to be rotatable.

$$\hat{y} = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i < j = 1}^k \beta_{ij} x_i x_j + \sum_{i=1}^k \beta_{ii} x_i^2 + \varepsilon$$

Where

\hat{y} = response variable

x_{ij} = coded independent variables; $i, j = 1, 2, \dots, k$

β = unknown parameters

ε is the experimental error

THE MOMENT MATRIX OF THE SECOND-ORDER RESPONSE SURFACE DESIGNS IN K VARIABLES

As stated earlier, the second-order model is given by the function

To obtain the moment matrix the X matrix is formulated using the model parameter and the number of experimental runs as can be seen below.

$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1k} & x_{11}x_{12} & x_{11}x_{13} & \dots & x_{1(k-1)}x_{1k} & x_{11}^2 & x_{12}^2 & \dots & x_{1k}^2 \\ 1 & x_{21} & x_{22} & \dots & x_{2k} & x_{21}x_{22} & x_{21}x_{23} & \dots & x_{2(k-1)}x_{2k} & x_{21}^2 & x_{22}^2 & \dots & x_{2k}^2 \\ 1 & x_{31} & x_{32} & \dots & x_{3k} & x_{31}x_{32} & x_{31}x_{33} & \dots & x_{3(k-1)}x_{3k} & x_{31}^2 & x_{32}^2 & \dots & x_{3k}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nk} & x_{n1}x_{n2} & x_{n1}x_{n3} & \dots & x_{n(k-1)}x_{nk} & x_{n1}^2 & x_{n2}^2 & \dots & x_{nk}^2 \end{bmatrix}$$

$$\begin{aligned}
 X'X &= \begin{bmatrix} N & \sum_{j=1}^N x_{1j} & \sum_{j=1}^N x_{2j} & \dots & \sum_{j=1}^N x_{kj} & \dots & \sum_{j=1}^N x_{kj}^2 \\ \sum_{i=1}^N x_{i1} & \sum_{i=1}^N x_{i1}^2 & \sum_{i=1}^N x_{1j} x_{2j} & \dots & \sum_{j=1}^N x_{kj} x_{j(k-1)} & \dots & \sum_{j=1}^N x_{1j}^2 x_{kj} \\ \sum_{j=1}^N x_{2j} & \sum_{i=1}^N x_{1j} x_{2j} & \sum_{i=1}^N x_{2j}^2 & \dots & x_{2(k-1)} x_{2k} & \dots & \sum_{j=1}^N x_{2j}^2 x_{n(k-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_{j=1}^N x_{kj}^2 & \sum_{j=1}^N x_{1j}^2 x_{n(k-1)} & \sum_{j=1}^N x_{2j}^2 x_{n(k-1)} & \dots & \dots & \dots & \sum_{i=1}^N x_{kj}^4 \end{bmatrix} \\
 \frac{1}{N} X'X &= \frac{1}{N} \begin{bmatrix} N & \sum_{j=1}^N x_{1j} & \sum_{j=1}^N x_{2j} & \dots & \sum_{j=1}^N x_{kj} & \dots & \sum_{j=1}^N x_{kj}^2 \\ \sum_{i=1}^N x_{i1} & \sum_{i=1}^N x_{i1}^2 & \sum_{i=1}^N x_{1j} x_{2j} & \dots & \sum_{j=1}^N x_{kj} x_{j(k-1)} & \dots & \sum_{j=1}^N x_{1j}^2 x_{kj} \\ \sum_{j=1}^N x_{2j} & \sum_{i=1}^N x_{1j} x_{2j} & \sum_{i=1}^N x_{2j}^2 & \dots & x_{2(k-1)} x_{2k} & \dots & \sum_{j=1}^N x_{2j}^2 x_{n(k-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_{j=1}^N x_{kj}^2 & \sum_{j=1}^N x_{1j}^2 x_{n(k-1)} & \sum_{j=1}^N x_{2j}^2 x_{n(k-1)} & \dots & \dots & \dots & \sum_{i=1}^N x_{kj}^4 \end{bmatrix}
 \end{aligned}$$

The moments associated with the second-order response surface designs are listed below

- i. The first moment defined by

$$\frac{1}{N} \sum_{i=1}^N x_{iu} ; u = 1, 2, \dots, k$$
- ii. The second pure moments defined by

$$\frac{1}{N} \sum_{i=1}^N x_{iu}^2 ; u = 1, 2, \dots, k$$

The second mixed moments defined by

$$\frac{1}{N} \sum_{i=1}^N x_{iu} x_{iw} ; u \neq w$$
- iii. The third pure moment defined by

$$\frac{1}{N} \sum_{i=1}^N x_{iu}^3 ; u = 1, 2, \dots, k$$

iv. The third mixed moments defined by

$$\frac{1}{N} \sum_{i=1}^N x_{iu}^2 x_{iw} \quad \text{and} \quad \frac{1}{N} \sum_{i=1}^N x_{iu} x_{iw}^2 ; u \neq w \quad \text{and} \quad \frac{1}{N} \sum_{i=1}^N x_{iu} x_{iw} x_{iv} ; u \neq w \neq v$$

v. The fourth pure moment defined by

$$\frac{1}{N} \sum_{i=1}^N x_{iu}^4 ; u = 1, 2, \dots, k$$

vi. The fourth mixed moments defined by

$$\begin{aligned} & \frac{1}{N} \sum_{i=1}^N x_{iu}^3 x_{iw} \quad \text{and} \quad \frac{1}{N} \sum_{i=1}^N x_{iu} x_{iw}^3 \quad \text{and} \quad \frac{1}{N} \sum_{i=1}^N x_{iu}^2 x_{iw}^2 \quad \text{and} \quad \frac{1}{N} \sum_{i=1}^N x_{iu}^2 x_{iw} x_{iv} \quad \text{and} \quad \frac{1}{N} \sum_{i=1}^N x_{iu} x_{iw}^2 x_{iv} \\ & \text{and} \quad \frac{1}{N} \sum_{i=1}^N x_{iu} x_{iw} x_{iv}^2 \quad \text{and} \quad \frac{1}{N} \sum_{i=1}^N x_{iu} x_{iw} x_{iv} x_{iz} ; u \neq w \neq v \neq z \end{aligned}$$

These are the moments used to satisfy the necessary and sufficient conditions for rotatability of second-order response surface designs.

COMPARATIVE ILLUSTRATIONS

For the purpose of this study, the BBD and CCD are compared for their rotatability using $k = 4$ and 5 and $n_c = 5$. The CCD axial points (α) were calculated based on $\alpha = \sqrt[4]{F}$ which is an axial distance for circumscribed central composite designs. The designs were generated using MiniTab 16 software and analyzed using RStudio software. Studies from available literature have shown the practical application of either of these second order designs with $k \geq 4$ to obtain acceptable results in different fields of human endeavor. Rohmatussolihat et al. (2021) applied a $k = 4$ design to optimize protease production by *Enterococcus faecalis* InaCC B745 in Biotechnology. The four variables at five-level combinations CCD were skim milk, yeast extract, glucose, and CaCO_3 . They further studied a BBD with up to 6 variables. Bhattacharya (2020) study showed the application of the CCD with various independent variables viz., entrapment efficacy percentage, zeta potential, particle size,

percentage of calmativ drug release of a polymeric nanoparticle formulation for evaluation and optimization purposes (Bhattacharya, 2021). Naseri et al. (2023) applied the Central Composite and Box–Behnken designs to optimize bioleaching methods using $k \geq 3$ independent variables. Other researches in Environmental Sciences, Food technology and Pharmaceutical studies (Lou et al. 2013; Hajji et al. 2018; Veli et al. 2018; Yakubu and Chukwu, 2018; Naseri et al. 2023)

BOX-BEHNKEN DESIGN (BBD), $k = 4$, $n_c = 5$

$$Y = \beta_0 + X_1 + X_2 + X_3 + X_4 + X_1X_2 + X_1X_3 + X_1X_4 + X_2X_3 + X_2X_4 + X_3X_4 + X_{11}^2 + X_{22}^2 + X_{33}^2 + X_{44}^2 + \varepsilon$$

The X matrix for the model is given as:

SUMMARY AND CONCLUSION

The concept of rotatability has been employed on two second-order designs to establish their preference. It is seen from all the comparative illustrations that the first condition of rotatability was satisfied. Precisely, all odd moments through order four were zero. However, the second condition for rotatability was not fully satisfied by all the second-order response surface designs studied. The ratio for each design is given below.

- i. The BBD with $k = 4$, $n_c = 5$ had its ratio as $\frac{0.4138}{0.1379} = 3.0007 \cong 3$
- ii. The CCCD with $k = 4$, $n_c = 5$ and $\alpha = 2.0$ had its ratio as $\frac{1.6552}{0.5517} = 3.0002 \cong 3$
- iii. The BBD with $k = 5$, $n_c = 5$ had its ratio as $\frac{0.7619}{0.1905} = 3.9995 \cong 4$
- iv. The CCCD with $k = 5$, $n_c = 5$ and $\alpha = 2.378$ had its ratio as $\frac{4.5693}{1.5238} = 2.9986 \cong 3$

Based on the above illustrations, it was obvious that CCCDs considered were perfectly rotatable for $k = 4$ and 5. However, the BBDs are rotatable or near rotatable. Specifically, BBD is rotatable for $k = 4$ but near rotatable for $k = 5$.

Conflict of Interests

The authors declare no conflict of interest.

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