A Proposed Inscribed-Doehlert Design for three-factor Spherical N-Point Design: Variation in Model Parameter Estimation

1 Inamete Emem Ndah H., ²Maxwell Azubuike Ijomah & ³Dele Joshua Osahogulu

¹Department of Mathematics and Statistics, School of Applied Sciences Federal Polytechnic of Oil and Gas, Bonny.

²Department of Mathematics and Statistics, Faculty of Science, University of Port Harcourt. ³Department of Mathematics and Statistics, Faculty of Natural and Applied Sciences, Ignatius Ajuru University of Education. P.M.B 5047, Rumuolumeni, Port Harcourt.

inameteemem@gmail.com [& maxwell.ijomah@uniport.edu.ng](mailto:maxwell.ijomah@uniport.edu.ng) Corresponding author: **inameteemem@gmail.com**

D.O.I[: 10.56201/ijasmt.v8.no3.2022.pg1](https://doi.org/10.56201/ijssmr.v8.no1.2022.pg32.40)6.37

ABSTRACT

This study considered and proposed three Factor Spherical N-point Design as applied to Variation in Model Parameter Estimation. Two quadratic models were considered: one contained all the parameters while the other model excluded the three interaction terms. The Box-Behnken, Central Composite Circumscribed, Central Composite Inscribed and Doehlert Designs were studied for these two quadratic models using the D-optimality criterion, Sum of Square Errors and Grand Means of the Designs. The study also proposed a 14-point Design from the Central Composite Inscribed and the Doehlert Designs. We found out that the determinant values of all the designs studied were higher for reduced model than for the full model and that the designs with smaller determinants usually produce larger Sum of Square Errors. We also ascertained that, as the centre points increase, the determinants of all the designs decrease for the full model, while the Box-Behnken Design has equal determinants for 1 and 2 centre points for the reduced model. The study found out that Box-Behnken Design was a better design for reduced model on the basis of Sum of Square Errors other than Central Composite Circumscribed design. Also, we found out that the reduced quadratic model was a better model for the three factor Spherical Second-Order Designs. The proposed design was found to be better than all the standard designs so far studied, because it gave smaller values of the sum of square errors and also better values of the AIC (Akaike Information Criterion) and SBC (Schwartz Bayesian Criterion) for both models and for all the 5 centre points added.

Key words: Inscribed-Doehlert design, Box Behnken design, Doehlert design and Central Composite design

1. Introduction

George Box and Donald Behnken proposed the Box and Behnken design in 1960. This design takes the midpoints of the edges of the process space and the centre point into consideration while constructing the design. The 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 hypersphere and are placed equidistant from the central point. Such designs have been used in optimisation studies involving enzyme assays, emulsion formation. The Box-Behnken design is a second class of experimental designs for modelling the quadratic response function which was introduced in 1960 by Box and Behnken. Assuming $k \ge 3$, 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, has 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.

Box and Hunter (1957) referred these types of experimental designs as rotatable designs and suggested that they can be utilized in experimentations. In such designs, the experimenters can use the optimality criteria to determine the adequacy of a proposed experimental design prior to running it.

Box and Wilson presented the Central Composite Design (CCD) in 1951. CCD consists of three types of designs-circumscribed, inscribed and face-centered. CCCD involves factorial points, centre points as well as star points. Star points represent the extreme values of the variables. The distance between the centre point and factorial point is ± 1 ; between centre point and star point is α. For CCD, α is greater than 1. For the Inscribed Central Composite design type, the star points take the specified limit values of the variables. The factorial points lie within the variable limits. The star points and factorial points are located at a distance of ± 1 from the centre point for the Face-centred Central Composite design (FCCD) and therefore, α is equal to 1. The number of experiments in CCD is calculated using the formula $N = k^2 + 2 + cp$ where k is the number of variables and cp is the number of replicates for the centre point. The α value is determined by using the equation $\alpha=2(k-p)/4$. The α value depends on the number of variables. It is 1.41, 1.68, and 2.00 for 2, 3 and 4 variables respectively. Another important aspect of CCD is that five factor levels are considered while constructing the design $-\alpha$, $-1,0,+1$ and $+\alpha$. Representations of two and three- factor optimizations carried out using central composite designs.

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 factor 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 center; 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 $n = k^2 + 2k + n0$. A CCD is obtained by augmenting the first-order design of a 2k factorial with additional experimental runs, the 2k axial points, and the *n*-centre point replications.

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.

A Statistician by name, Sir Ronald Fisher (1935) observed that experiments are only experience carefully planned in advance and designed to form a secure basis of new knowledge. Experiments are characterized by the following: (a) manipulation of one or more independent variables; (b) use of controls such as randomly assigning participants or experimental units to one or more independent variables; and (c) careful observation or measurement of one or more dependent variables.

There are several second-order model designs in the literature which include Central Composite designs (CCD), Box-Benkhen designs (BBD), Hooke designs, Small Composite designs (SCD), Minimum-run Resolution V de-signs (MinresV), Hybrid designs, etc, as propounded byBox and Wilson (1951); Myers and Montgomery (2002) and Zarhan, (2002). 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 were identified by Myers and Montgomery (2002) and Montgomery (2005) and are typical of the second-order response surface designs, some of whose performances in spherical regions will be investigated in this study. Several works have been done on response surface designs. Lucas (1976) compared the performances of several types of quadratic response surface designs in symmetric region. He compared the Central Composite designs (CCD), Box-Benkhen designs (BBD), Hooke designs, Pesotchinsky designs, etc, based on D- and G-optimality criteria. Myers et al. (1992) an extensive study of response variance properties of the following second-order designs: CCD, BBD, and Hybrid designs. These designs were studied using the variance dispersion graph. Borkowski (1995) studied the analytical properties of the Central Composite designs and Box-Benkhen designs in a spherical region. His studies yielded alternative approach to the computer-based algorithm approach for obtaining the minimum, maximum and average spherical prediction variances for the designs. Zarhan (2002) compared the prediction variances for the CCD, Box-Benkhen Designs, Small Composite designs (SCD) and Hybrid designs for 2, 3, 4, 5 and 6 factors in both spherical and cuboidal regions. These comparisons were made using the Variance Dispersion Graphs (VDG), Fraction of Design Space Criterion and the G- and Doptimality criteria. Park et al. (2005) evaluated the response variance properties of response surface designs on cuboidal region utilizing both the VDG and Fraction of Design Space Graph (FDSG). Borror et al (2006) compared the response variance performance for the variation of the CCD in both the spherical and cuboidal regions. Their interest is to know how these designs perform when axial distance of $4=k\alpha$ is employed. He used a fraction of design space as a criterion for comparison for 6 to 10 factors. However, in this study, we try to demonstrate that in

spherical regions with radius $=k\alpha$; none of the designs, CCD, SCD and MinResV is uniformly superior when evaluated under the G-and I-optimality criteria as well as the VDG. In this case, the method of Evolutionary operation (EVOP) is used. Evolutionary operation was proposed by Box (1957) as a procedure for the continuous monitoring and improvement of a full-scale process with the goal of moving the operating conditions towards the optimum. Here, response surface methodology is applied using the k^2 full factorial designs which form part of the three designs under consideration in this paper. In practice, EVOP can be applied to only two or three variables but in theory, it can be applied to k process variables. However, Montgomery (2005) gives the procedure for two process variables while Box and Draper (1969) discuss in detail the three-variable case and Myers and Montgomery (2002) investigate and discuss the computer implementation of EVOP. The second problem is confirming the exact location of the optimum in the region of interest. In this case, the class of CCD's is used to a large extent to tackle this situation.

Second-order designs like Central Composite, Box-Behnken as well as Doehlert designs estimate the curvature-interaction of the variables and present it in the form of a quadratic equation. Another set of design gives the user an option to choose the equation-linear, quadratic or cubic. Such designs are called optimal designs. This paper discusses two classic response surface Designs-Central Composite and Box-Behnken, and optimal designs like D-optimal and I-optimal ones.

Brandley, (2009), noted that the design of response surface models starts with the estimation of parameters, pure error, and lack of fit. Also, the experimenter needs to design a model that is efficient. Therefore, estimation of variances has to be taken into consideration. The orthogonal first-order designs minimize the variance of the regression coefficients kβ. A first-order design is orthogonal if the off-diagonal elements of the (X´X) matrix are all zero (Montgomery 2005). The orthogonal first-order designs include 2q factorial with center points and 2q-k fraction with resolution III or greater.

Anup and Saiket (2018), stated that Design of Experiment is an integral chemometric tool for process optimization. William and Alain (2018), said that Design of experiment is a method used for planning experiments and analyzing the information obtained.

Iwundu (2016b) stated that the N-point equiradial designs does correspondingly better for the reduced model than for the full model. Which implies that, the average variance of the estimates of the regression coefficients associated with the reduced model is better minimized using the equiradial designs than that observed for estimates of the regression coefficients associated with the full model. It was also posited that, when interest is in reducing the determinant of the information matrix of the design or equivalently reducing the determinant of the variancecovariance matrix, the N-point equiradial designs performed correspondingly better for the reduced model than for the full model.

Iwundu and Onu, (2017) observed that the determinant values of Central Composite Designs increase for increasing axial distance and decreases for increasing centre points.

Sergio et al. (2004) stated that, Doehlert matrix involved the optimization of a separation process. Onu et al. (2021) observed that the D-.Optimality of equiradial design is better for reduced model than for full model for all axial distance and centre points studied. This implies

IIARD – International Institute of Academic Research and Development Page 19

that equiradial design minimizes the variance of parameter estimates for reduced model than for full model.

2.1 Obtaining Parameters of Second-Order Spherical Designs for full and reduced Models

2.1.1 Obtaining parameters of Box-Behnken Design

 $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_{12} + \beta_{13} x_{13} + \beta_{23} x_{23} + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2$ (2.1) which is a Quadratic Model having all the variables present, while the reduced model will be given as:

$$
y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \varepsilon
$$
 (2.2)

Which is a Quadratic Model having all the interaction variables omitted, the models in (2.1 and 2.2) can be written in matrix form as:

$$
y = X\beta + \varepsilon \tag{2.3}
$$

Where X is an $N \times P$ matrix, y is an $N \times 1$ vector of observed responses, β 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) β is not known and represents real functional relationship between the response y and the explanatory variables (x_1, x_2, \ldots, x_n) .

The models in (2.1) and (2.2) 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.

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 full model in equation (2.1) , we obtain the design matrix, X, similarly, the design matrix for reduced model is also obtained from equation (2.2). The design matrices obtained from the two models 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, $\frac{x'}{x}$ $\frac{A}{N}$ which cancels out the effect of design sizes in a design for the reason of comparing two or more designs with different design size. The least square equation which will be used in the estimation of the parameters for both models is given as

$$
\underline{\hat{\beta}} = \left(\frac{X'X}{N}\right)^{-1}X'Y\tag{2.4}
$$

Where $\hat{\beta}$ is an N × 1 vector, given as $(\beta_0, \beta_1, \beta_2, \beta_{12} \dots, \beta_{11}, \beta_{22} \dots)'$ and $(\frac{x^{\gamma}}{x^{\gamma}})$ $\frac{X}{N}$)⁻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) and Iwundu and Onu (2017).

2.1.2 Obtaining parameters of Central Composite Designs

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 and reduced model of (2.1) and (2.2) respectively. 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

D-optimality:

The D-Optimality of any Design is given as

$$
D-Opt = Min \det(M^{-1}) \equiv Max \det(M) \tag{2.5}
$$

The design that has the highest determinant of the normalized information matrix is considered the best design under this criterion. Equation (2.5) 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)

From each of these designs with each centre point, the estimate of the regression sum of square errors were obtained.

Let the estimate of y be given as \hat{y} , then from the models in (2.1) and (2.2) which are the Full and Reduced Quadratic models respectively, the errors were obtained by making ε the subject in (2.1) and (2.2), 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.

$$
\varepsilon_i = (y_i - \hat{y}_i) \tag{2.6}
$$

Summing and squaring (2.6), we obtain the error sum of square for both the quadratic and cubic models and it is given as

$$
\sum \varepsilon_i^2 = \sum (y_i - \hat{y}_i)^2
$$
 (2.7)

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

was used.

2.3.2 Model Adequacy Criteria

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

Akaike Information Criterion (AIC)

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

$$
AIC = nInSSE - nInn + 2p
$$

(2.8)

The first term of (2.8) 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.

Schwarz' Bayesian Criterion (SBC)

This criterion is given as:

 $SBC_p = n \ln SSE - n \ln n + [\ln n]p$ (2.9)

Note that the smaller the SBC the better the model.

2.4 Proposed Three-Factor Second-Order Design (IDD)

The proposed design was obtained by the combination of the sets of points of the three-factor Inscribed Central Composite Design and the sets of points of the Doehlert Design. It was observed that the two designs have common radius of 1.0 and their sets of points are similar. The arithmetic mean of the sets of points of these designs was used to form the new design called Inscribed-Doehlert Design (IDD).

The Inscribed Design points are: (1 1 1 1 -1 -1 -1 -1 0.707 -0.707 0 0 0 0, 1 1 -1 -1 1 1 -1 -1 0 0 0.707 -0.707 0 0, 1 -1 1 -1 1 -1 1 -1 0 0 0 0 0.707 -0.707), while the Doehlert Design points are: (0 1 0 -1 -0.5 0.5 0.5 -0.5 0.5 0.5 0.5 -0.5 0 0, -1 0 1 1 -0.5 -0.5 0.5 0.5 -0.5 -0.5 0.5 0.5 0 -1, 0 0 0 0 0.707 0.707 0.707 0.707 -0.707 -0.707 -0.707 -0.707 0 0).

The proposed design is obtained as follows:

. . .

$$
X_1 \t X_2 \t X_3
$$
\n
$$
\frac{0+1}{2} = 0.5 \t \frac{-1+1}{2} = 0 \t \frac{0+1}{2} = 0.5
$$
\n
$$
\frac{1+1}{2} = 1 \t \frac{0+1}{2} = 0.5 \t \frac{0-1}{2} = -0.5
$$

$$
\frac{0+0}{2} = 0 \qquad \frac{-1+0}{2} = -0.5 \qquad \frac{0-0.707}{2} = -0.35
$$

. The simulation of the simulation of the simulation of the simulation \mathcal{L}_c . The simulation of the

The proposed design points (IDD) are: (0.5 1 0.5 0 -0.75 -0.25 -0.25 -0.75 0.60 -0.10 0.25 -0.25 0 0, 0 0.5 0 0 0.25 0.25 -0.25 -0.25 -0.25 -0.25 0.60 -0.10 0 -0.5, 0.5 -0.5 0.5 -0.5 0.85 -0.15 0.85 -0.15 -0.35 -0.35 -0.35 -0.35 0.35 -0.35).

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:

The determinant was obtained as:

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

The inverse of the normalized information matrix was obtained as:

$$
\left(\frac{X'X}{25}\right)^{-1} = \begin{pmatrix}\n7.3529 & 0 & 0 & 0 & 0 & 0 & 0 & -4.4118 & -4.4118 & -4.4118 \\
0 & 2.0833 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2.0833 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2.0833 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 6.2500 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 6.2500 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 6.2500 & 0 & 0 & 0 \\
-4.4118 & 0 & 0 & 0 & 0 & 0 & 0 & 5.1471 & 2.0221 \\
-4.4118 & 0 & 0 & 0 & 0 & 0 & 0 & 2.0221 & 5.1471 & 2.0221 \\
7.3529 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4.4118 & -4.4118 \\
0 & 2.0833 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\n\end{pmatrix}
$$

The parameters were obtained as shown below:

$$
\underline{\hat{\beta}} = \begin{pmatrix}\n193.9265 \\
-8.0625 \\
-26.2083 \\
7.5833 \\
-8.2500 \\
30.0000 \\
3.4375 \\
-83.2059 \\
1.1379\n\end{pmatrix}
$$

-60.4871

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

 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 X=

The determinant was obtained as:

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

The inverse of the normalized information matrix was obtained as:

$$
\left(\frac{X'X}{26}\right)^{-1} = \begin{pmatrix}\n5.9091 & 0 & 0 & 0 & 0 & 0 & 0 & 0.3.5455 & -3.5455 & -3.5455 \\
0 & 2.1667 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2.1667 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2.1667 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.5000 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.5000 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.55000 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.4.7273 & 1.4773 & 1.4773 \\
-3.5455 & 0 & 0 & 0 & 0 & 0 & 0.14773 & 4.7273 & 1.4773 \\
-3.5455 & 0 & 0 & 0 & 0 & 0 & 0 & 1.4773 & 4.7273 & 1.4773 \\
-3.5455 & 0 & 0 & 0 & 0 & 0 & 0 & 1.4773 & 1.4773 & 4.7273\n\end{pmatrix}
$$

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:

IIARD – International Institute of Academic Research and Development Page 27

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;

x1	x2	x3	GDP	B	Ext GDP	Deviation	squDeviat	extGDP/25
-1	-1	$\overline{0}$	2.21	193.927	144.9914	-3.3052	10.92435	5.5152
1	-1	$\boldsymbol{0}$	1.92	-8.0625	295.2782	-9.89113	97.83441	11.81113
-1		$\overline{0}$	0.81	-26.208	259.9866	-9.58946	91.95782	10.39946
		$\overline{0}$	-1.62	7.5833	76.4498	-4.67799	21.88361	3.057992
$\overline{0}$	$\overline{0}$	-1	2.65	-83.206	186.3432	-4.80373	23.0758	7.453728
θ	$\overline{0}$		6.31	1.1379	201.5098	-1.75039	3.063872	8.060392
$\overline{0}$	$\overline{0}$	-1	6.61	-60.487	186.3432	-0.84373	0.711877	7.453728
θ	$\overline{0}$		4.23		201.5098	-3.83039	14.6719	8.060392
-1	$\overline{0}$	$\overline{0}$	5.31		201.989	-2.76956	7.670463	8.07956
	$\overline{0}$	$\overline{0}$	8.01		185.864	0.57544	0.331131	7.43456
-1	$\overline{0}$	θ	8.04		201.989	-0.03956	0.001565	8.07956
	$\overline{0}$	$\overline{0}$	6.76		185.864	-0.67456	0.455031	7.43456
θ	-1	-1	6.59		152.0644	0.507424	0.257479	6.082576
θ	1	-1	6.06		220.622	-2.76488	7.644561	8.82488
Ω	-1		6.44		288.2052	-5.08821	25.88986	11.52821

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

IIARD – International Institute of Academic Research and Development Page 28

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	
$\mathbf C$	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
$\overline{2}$	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
$\overline{4}$	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
$\mathbf{1}$	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
$\overline{4}$	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

D-Optimality	FULL MODEL						
		DD.	BBD	CCCD	CCID		
			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 4: Comparison of D-Optimalities of the Three Factor Second-Order Designs for Centre Points 1-5

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

Sum		of FULL MODEL						
Square		C	DD	BBD	CCCD	CCID		
errors								
			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

Table 7: Comparing IDD with REDUCED BBD for full and reduced models

	Design size	IDD	$\mathbf C$	AIC	SBC	Red BBD	AIC	SBC
Full	15	27.0698	1	28.856	35.936			
model	16	27.07009	2	28.413	36.139			
	17	28.49175	3	28.779	37.111			
	18	31.63094	$\overline{4}$	30.148	39.051			
	19	88.7411	5	49.284	58.729			
Reduced	15	54.18286	$\mathbf 1$	33.265	38.221	101.9091	42.741	47.697
model	16	54.36612	$\overline{2}$	33.570	38.979	101.9452	43.630	49.038
	17	66.76614	3	37.256	43.088	107.9813	45.429	51.261
	18	86.44645	$\overline{4}$	42.245	48.477	107.9888	46.250	52.482
	19	234.1652	5	61.720	68.331	159.8952	54.472	61.083

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.

Discussions Based on D-optimality Criterion for Reduced Model

The study reveals that for reduced model, the determinant of the Doehlert Design is maximum at 2 centre points, but decreases as the centre points increases, these processes continues until the 5 centre points studied.

The Box-Behnken design for reduced model produced equal determinant value for 1 and 2 centre

points, but decreases as the centre points increases.

The Central Composite Design Circumscribed has its maximum determinant at 2 centre points, just like the Doehlert Design.

The Central Composite Design Inscribed has its determinant steadily decreasing for increasing centre points for a reduced model.

Comparison of Full and Reduced Model on the Basis of D-optimality

For full model, Central Composite Design Circumscribed has the highest determinant value for all the added centre points. This design is optimal for 1 centre point on the basis of D-optimality criterion. The second-best design was found to be the Central Composite Design Inscribed which was also optimal for 1 centre point, followed by the Box-Behnken Design that is also optimal at 1 centre point, but for 5 centre points, the determinant value of the Box-Behnken Design is greater than the Central Composite Inscribed Design. This suggests that, from 5 centre points and above, the Box-Behnken Design may be better than the Central Composite Design Inscribed on the basis of D-optimality criterion for full model.

For reduced model, Central Composite Circumscribed Design produces the highest determinant, but it is optimal at 2 centre points, followed by the Box-Behnken Design that is optimal at 1 and 2 centre points, and then followed by the Central Composite Inscribed Design that is optimal at 1 Centre point. This shows that Box-Behnken Design is better for reduced model than for full model. Generally, the study reveals that the determinant values of all the three factor Spherical Second-Order Design studied are higher for reduced model than for full model.

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.

For reduced model, the Central Composite Circumscribed Design proved to be better than other designs for 1 to 4 centre points on the basis of sum of square errors but for 5 centre points all the other designs became better than Central Composite Circumscribed Design. This reveals that the estimation strength of Central Composite Circumscribed Design decreases with increasing centre points, which is so visible at 5 centre points. The Box-Behnken Design becomes better as the centre points increases on the basis of sum of square errors for reduced model. The Central Composite Inscribed Design performs better than Box-Behnken Design and Doehlert Design for 1 and 2 centre points, but for 3 centre points, Box-Behnken Design became better than Central Composite Inscribed Design and Doehlert Design, while for 4 centre points, the Box-Behnken Design increased and became equal to the value of Central Composite Inscribed Design on the

basis of sum of square error. At exactly 5 centre points, the Box-Behnken Design became generally better than all the other designs studied and this was followed by the Doehlert Design and then the Central Composite Inscribed Design. This shows that the inferior designs become stronger for increasing centre points while the superior designs loss strength as the centre points increases for reduced 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.

For the reduced model, a similar result was also observed and the Box-Behnken Design for the full model has equal or approximately equal Grand Mean, likewise the Central Composite Circumscribed Design and Central Composite Inscribed Design, but the Doehlert Design shows a significant difference in Grand Mean for both models.

Discussion Based on the Proposed Design

It was observed that the new design, Inscribed Doehlert Design (IDD) was better than all the designs studied– Central Composite Design, Box Behnken Design, and Doehlert Design, as revealed by the sum of square error analysis, AIC and SBC criteria.

When the new design (IDD) was compared with Box Behnken Design, whose points were reduced to the 14 point design to be equal in number with this new design, it was observed that for the full model case, the Box Behnken design gave a similar matrix, but for the reduced model is 1 centre point.

4.1 Conclusion

This work was able to propose a spherical second-order design which was found to be more efficient than the studied standard designs; it also concluded that, for three second-order designs, the determinant of the reduced quadratic model was better than the determinant of the full quadratic model. Also, the design with minimised determinant gives a larger sum of square error for the two models and for all the three factor second-order designs studied. The Box-Behnken model was proposed as the better design for the reduced quadratic model while the Central Composite Design was better for the full model.

The proposed design was found to be better than all the standard designs so far studied because it gave smaller values of the sum of squuare errors and better values of the AIC and SBC for both models and for all the five centre points added.

4.2 Recommendations

The following recommendations are made from this research:

1. The Box-Behnken Design is the best Design for Reduced models for three factor Second-Order Designs

- 2. The Reduced quadratic model is the best model for studying the three factor Second-Order Designs.
- 3. The Inscribed-Doehlert Design (IDD) is generally the best for analysis in three factor settings.

4.3 Contribution to Knowledge

We were able to propose a spherical second-order design called Inscribed Doehlert Design which was found to be more efficient than the studied standard designs. The proposed design was obtained by the combination of the sets of points of the three-factor Inscribed Central Composite Design and the sets of points of the Doehlert Design. It was observed that the two designs have common radius of 1.0 and their sets of points are similar. The arithmetic mean of the sets of points of these designs was used to form the new design called Inscribed-Doehlert Design (IDD).

In this research, using three factor Second-Order designs, we found out that the reduced model was the best model for such analysis, because, it gives smaller sum of square errors and larger determinant values than the full model counterpart.

REFERENCES

- Anup, K. D., &Saikat, D*.* (2018). Optimization of Extraction using Mathematical Models and Computation.10(3), 75-106. DOI: 10.1016/B978-0-12-812364-5.00003-1
- Atkinson, A.C. & Donev, A.N. (1992).*Optimum experimental designs*, Oxford. Clarendon.
- Box, G.E.P.& Draper, N.R. (1963). The choice of a second order rotatable design, *Biometrika*, *50*, 335–352.
- Box, G.E.P. & Draper, N.R. (1975). Robust designs, *Biometrika62*, 347–352.
- Box, G.E.P.& Draper, N.R. (1987).*Empirical model-building and response* surfaces, Wiley.
- Box, G.E.P.& Hunter, J.S. (1957). Multifactor experimental designs for exploring response surfaces, *Annals of Mathematical Statistics*, *28*, 195–241. Cochran, W. and Cox, D.R. (1957).*Experimentaldesigns*, John Wiley.
- Chigbu, P.E., Ukaegbu, E.C. & Nwanya, J. C. (2009). On comparing the prediction variances of some Central Composite Designs in Spherical regions: *A Review. STATISTICA, anno LXIX,4*.
- Dette, H. & Grigoriev, Y. (2014). Construction of efficient and optimal experiment design for response surface models. *The annals of statistics*. V. *42*,(4), 1635-1656. DOI: 10.1214/14-AOS1241.
- Draper, N.R. (1982). Center points in second-order response surface designs.*Technometrics24*(2), 127–133.
- Draper, N.R. & John, J.A. (1998). Response surface designs where levels of some factors are difficult to change.*Australian and New Zealand Journal of Statistics*,*40*(4), 487–495.
- Draper, N.R. & Lin, D.K.J. (1990). Small response-surface designs.*Technometrics32*, 187–194.
- Frits, B. S., & David, C. M. (2018) . $13th$ International Symposium on process systems Engineering. *44*(3), 1-28
- Giovannitti-Jensen, A. & Myers, R.H. (1989). Graphical Assessment of the Prediction Capability of Response Surface Designs, *Technometrics*, *31*, 2, 159-171.
- Iwundu, M. P. & Albert-Udochukwuka, E. B. (2014). On the behaviour of D-optimal exact designs under changing regression polynomials. *International Journal of Statistics andProbability*, 3(4), 67-85. doi:10.5539/ijsp.v3n4p67 URL: http://dx.doi.org/10.5539/ijsp.v3n4p67.
- Iwundu, M. P. (2015) Optimal partially replicated cube, star and center runs in face-centered central composite designs. *International Journal of Statistics and Probability*; *4*(4), doi:10.5539/ijsp.v4n4p1 URL: http://dx.doi.org/10.5539/ijsp.v4n4p1.
- Iwundu, M. P. (2016a). Alternative Second-Order N-Point Spherical Response Surface methodology designs and their efficiencies. *International Journal of Statistics and Probability*; 5(4),22-30. doi:10.5539/ijsp.v5n4p22 URL:http:// $dx.doi.org/10.5539/ijsp.v5n4p22$.
- Iwundu, M. P. (2016a). Alternative second-order n-point spherical response surface methodology designs and their efficiencies. *International Journal of Statistics and Probability; 5(4), 22-30*.
- Iwundu, M.P. & Onu, O.H. (2017). Preferences of equiradial designs with changing axial distances, design sizes and increase center points and their relationship to the N-point central composite design*: International Journal of Advanced Statistics and Probability,* 5 (2), 77-82.
- Khuri, A. I. & Cornel, J. A. (1996). *Response Surface: Design and Analysis.* Second Edition. Marcel Dekker, Inc.
- Khuri, A.I. (1988). A measure of rotatability for response-surface designs, *Technometrics,30*, 95– 104.
- Lucas, J. M. (1976) response surface design is the best: A performance comparison of several types of quadratic response surface designs in symmetric regions. *Technometrics*, 18, 411-417.
- Lucas, J.M. (1976). Which response surface design is best: a performance comparison of several types of quadratic response surface designs in symmetric regions.*Technometrics* 18(4), 411–417.
- Magangi O. J. (2018). Construction of modified optimal second order rotatable designs. *20*(8), 2467-2478.
- Montgomery, D.C. (1991).*Design and analysis of experiments*. John Wiley.
- Myers, R.H. (1971).*Responsesurfacemethodology*. Edwards Brothers.
- Myers, R. H., Montgomery, D. C. & Anderson-Cook, C. M. (2009). *Response surface methodology: Process and product optimization using designed experiments*. 3rd Edition. John Wiley & Sons, Inc.
- Myers, R. H., Montgomery, D. C., & Anderson-Cook, C. M. (2007).*Response surface methodology: Process and product optimization using designed experiments. 3rd* Edition.John Wiley & Sons, Inc.
- Myers, R. H., Vinning, G. G., Giovannitti-Jensen, A. & Myers, S. L. (1992). Variance Dispersion properties of Second-order response surface designs. *Journal of quality technology*, 24, 1-11.
- Nalimov, V.V., Golikova, T.I. & Mikeshina, N.G. (1970). On practical use of the concept of Doptimality,*Technometrics12*(4), 799–812.
- Nitin, V. &Vivek, K. (2019).Application of Box-Behnken design for the optimization of cellulase production under solid-state fermentation. *SpringerLink*.1(1733).
- Nwobi, F.N., Okoroafor, A.C. & Onukogu, I.B. (2001). Restricted second-order designs on one and two concentric balls, *Statistica,LXI*(1), 103–112.
- Onukogu, I. B. & Iwundu, M. P. (2007).A Combinatorial Procedure for constructing D-optimal designs.*Statistica*, 67 (4), 415-423.
- Oyejola, B. A. & Nwanya, J. C. (2015).Selecting the right central composite design.*Journal of Statistics and Applications*, 5(1), 21-30.
- Oyejola, B. A., &Nwanya, J. C. (2015). Selecting the right central composite design.*Journal of Statistics and Applications, 5*(1), 21-30.
- Pazman, A. (1986).*Foundations of optimal experimental designs*,D. Reidel Publishing Company.
- Rady, E. A., Abd El-Monsef, M. M. E. & Seyam, M. M. (2009). *Relationship among several optimality criteria*. interstat.statjournals.net>YEAR>articles.
- Robert, W. M., (2009). *New Box-Behnken Design.*Knoxville, TN 37996-0532, U.S.A.
- Satriani, A. P., Rusli, D., Mohamad, Y. M. & Osman H. (2013).Application of Box-Behnken design in optimization of glucose production from oil palm empty fruit bunch cellulose.

International Journal of Polymer Science.5(4), 29-33.

- Sergio, L. C., Walter, N. L., Cristina, M. Q., Benicio, B. N, & Juan, M. B. (2004). Doehlert matrix: Achemometric tool for analytical chemistry –review. *Talanta,63*(4),1061-1067.
- Shruti, S. R., & Padma, T., (2017).*Selection of a design for response surface School of Biosciences and Technology*. Vellore Institute of Technology.*263*(2), 638-646.
- Suliman, R. (2017). Response surface methodology and its application in optimizing the efficiency of organic solar cells*, university Open PRAIRIE: Open Public Research Access Institutional Repository and Information Exchange. 7*(2). 2232-2241
- Ukaegbu, E.C. & Chigbu, P.E. (2015). Graphical evaluation of the prediction capabilities of partially replicated orthogonal central composite designs.*Quality and Reliability Engineering International,31*, 707 – 717.
- Verdooren, (2017).Use of Doehlert Designs for Second-order Polynomial Models. *Springer Nature, 5*(2), 62-67.
- Wagna, P. C., Diogenes, R. G., Alete, P. T., Antonio, C. S., &Coata, M. G. (2008). Use of Doehlert design for optimizing the digestion of beans formulti-element determination by inductively coupled plasma optical emission spectrometry. *Journal of the Brazilian chemical society, 19*(1)*.*
- Wardrop, D. M. (1985). Optimality criteria applied to certain responses suface designs. *86*(1), 1- 20
- William, G. W. & Alain, G. (2018). Cell Culture media in Bio processing. *24*(5), 116-121.