EVALUATION OF COMPOUND OPTIMALITY CRITERIA FOR SECOND ORDER ROTATABLE DESIGNS CONSTRUCTED USING BALANCED INCOMPLETE BLOCK DESIGN.

BY

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DECLARATIONS

Declaration by the student

This thesis is my original work and has not been presented for a Degree in any other University.

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DEDICATION

This thesis is dedicated to my lovely family; Mr. and Mrs. Matundura, future family; Zainab Mwan, cherished friends; Frank, James, Dickson, Robert and Dominic.

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ABSTRACT

The theory of optimal experimental designs is concerned with the construction of designs that are optimum with respect to some statistical criteria. These criteria include the alphabetic optimality criteria such as; D-, A-, E-, T-, G- and C- criterion. Compound optimality criteria are those that combine two or more alphabetic optimality criteria. Design optimality criteria have specific desired properties that are sufficient in one design and at the same time inadequate in another design. Thus, a compound optimality criterion gives a balance when any two or more alphabetic optimality criteria are combined. The purpose of this study was to obtain compound optimality criteria for second order rotatable designs constructed using Balanced Incomplete Block Designs (BIBDs). The objectives of the study were to determine C-optimality criteria for the designs with 32, 64 and 112 points in three, four and five dimensions respectively; to obtain compound optimality criteria and to evaluate the efficiencies for both the alphabetic and compound optimality criteria. The C- criterion was achieved through minimizing the variance of the information matrix, whereas the compound optimality criteria were obtained from the alphabetic criteria using the specified formulae. The efficiencies were determined by comparing the specific design optimality criteria to the optimal design Criterion. C-optimality criteria for designs with 32, 64 and 112 points were obtained with the optimal values as 7197.76, 36.63 and 75.33 respectively. The compound optimality criteria CD-, DT- and CDT-criterion and the respective efficiencies for the selected points were evaluated. In conclusion, the compound optimality criteria obtained provided better design characteristics in terms of minimizing variances for parameter estimates and model selection. Efficiencies for compound optimality criteria were found to be higher relative to the corresponding alphabetic optimality criteria counterparts. The study recommended that compound optimality to be used in the selection of designs that are used in performing experiments in order to achieve optimal response.

LIST OF ACRONYMS

BIBD: Balanced Incomplete Block Designs

RSM: Response Surface Methodology.

SORD: Second Order Rotatable Designs.

DOE: Design of Experiments.

D-: Determinant criterion**.**

T-: Trace criterion.

C-: C- Criterion

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CHAPTER ONE

INTRODUCTION

This chapter covers the background, the statement of the problem, the scope, the objectives and the justification of the study.

1.1Background of the study

In many life sciences, optimal designs are required in order to cut on the cost of experimentation. An experimenter is therefore advised to make the choice of a design to be used prior to carrying out any experiment. Response surface methodology (RSM) is a collection of statistical and mathematical techniques that are useful in analyzing, developing, improving and optimizing processes. According to Box and Draper (1959), RSM is either used to explore response surfaces or to estimate the parameters of a model. Bose and Draper (1959) point out that the technique of fitting a response surface is one widely used to help in the statistical analysis of experiments where the response of an output depends on some unknown level of a factor on one or more controllable variables. A specific selection of settings or factor levels at which observations are to be taken is called a design. Designs are usually chosen to satisfy some desirable criteria chosen by the experimenter.

The proper meaning of optimal designs depends on the situation and can include cost effective, minimum variance and minimum bias. The commonly used classical optimality criteria which were introduced and widely discussed by Pukelsheim (1993) includes; the Determinant criterion (D-), the average variance criterion (A-), the smallest Eigen value (E-) and the trace criterion (T-). Many results on optimal designs of experiments are derived under the assumption that the statistical model is known at the design stage. However, rarely it is known in advance which model is the most appropriate. Box and Hunter (1957) introduced rotatable designs in order to explore the response surfaces. They developed second order rotatable designs through Schlaflian vectors and matrices. According to Draper (1960), a second order rotatable design aids the fitting of a second order surface and provides spherical information contours and a third order rotatable design aids the fitting of a third order surface. Thus, the goal of an experiment should be dual: to choose an appropriate design and an adequate model.

Unfortunately, a design which is optimum for parameter estimation may be inappropriate for model discrimination and vice versa. Model adequacy has been a serious problem, thus, many authors have developed optimality criteria which are applicable to the dual problem of model discrimination and parameter estimation. Thus, this study evaluated the C-optimality criteria and further used it to combine with already evaluated classical alphabetic criteria to obtain compound optimality criteria and then checked their efficiency by determining their relative efficiencies. Relative efficiency shows how good a design is when compared with another (Kuhfeld *et al* 1994).

The study presents existing designs of order two in three, four and five dimensions constructed by Rambaei (2014). Here the alphabetic optimality of designs for the reduced parameter system of interest, with respect to the determinant criterion and the trace criterion but never considered C- criterion. The C- criterion provides a geometrical interpretation for finding C- optimal designs. This thesis introduces optimal characteristics for designs with selected points in 32, 64 and 112 points, in particular, the C- optimality criterion, the compound optimality criteria and their efficiencies.

1.2 Definitions

1. Optimal designs: These are designs that are constructed on the basis of certain optimality criterion that pertains to the closeness of the predicted response surface.

2. BIBD: A Balanced Incomplete Block Design (BIBD) may be defined as a pair (V, B) where V is a $v \geq 2$ element set and B is a family of $b > 0$ subsets of V, called blocks, such that each block is of order $k < v$, each element of V is contained in exactly $r > 0$ blocks, and each pair of elements in V is contained in exactly $\lambda > 0$ blocks. The values $\{v, b, k, r, \lambda\}$ are called the parameters of the design.

3. RSM: This is a collection of mathematical and statistical techniques useful for analyzing problems in which several independent variables influence a dependent variable and the goal is to optimize the dependent variable.

4. Rotatability: The design D is said to be rotatable if the prediction variance is constant at all points that are equidistant from the design center, where variance is only a function of $\rho^2 = x_1^2 + x_2^2 + \cdots + x_n^2$, where ρ^2 is the distance from the center of the design.

5. D- Optimal: This is a criterion that maximizes the determinant of the design matrix $X^/X$ or it minimizes the size of confidence region on the vector of parameters in the model.

6. T- Optimal: This is the criterion that maximizes the trace of a design matrix $X^/X$.

7. C- Optimal: This is a criterion that minimizes the variance of the best linear unbiased estimate for a given linear combination of the model parameters.

1.3 Statement of the Problem

Optimal designs are classified into three main groups depending on their uses. There are those designs useful either for parameter estimation, model discrimination or both. However, it is common that most experts who design experiments are interested with the optimality criteria for parameter estimation. The optimality criteria for parameter estimation include; D-, A- and E- optimality criteria whereas those for model discrimination include C- and T- optimality criteria. From the existing literature, it was evident that designs criteria for parameter estimation can be inadequate for model discrimination and at the same time criteria for model discrimination may be sufficient for parameter estimation. This has created a great need to design experts who are interested in designs in parameter estimation property and at the same time optimality criteria for model discrimination. This study, therefore, seeks to evaluate compound optimality criteria and their efficiencies for the existing second order rotatable designs constructed using Balanced Incomplete Block Designs.

1.4 Objectives of the Study

1.4.1 General Objective

The main objective of the study was to evaluate compound optimality criteria for second order rotatable designs constructed using Balanced Incomplete Block Design.

1.4.2 Specific Objectives

The specific objectives were to;

1. Determine C-optimality criteria for second order rotatable designs constructed using specific Balanced Incomplete Block Designs.

2. Obtain compound optimality criteria by combining two and three alphabetic optimality criteria for designs with 32, 64 and 112 points.
3. Examine the efficiencies for both the alphabetic and compound optimality criteria.

1.5 Significance of the Study

This study determined compound optimality criteria for designs with 32, 64 and 112 points. A Compound optimality criterion contains two statistical properties that are of great importance to any design expert interested in the dual properties. This study, therefore, was applicable to the dual problem of model discrimination and parameter estimation. The combinations of DT-, CD- and CDT- for designs become handy to researchers who are interested in designs with both desirable properties for optimal response.

CHAPTER TWO

LITERATURE REVIEW

2.1 Introduction

In this section, we trace the various streams of thought which have contributed to what is now call compound optimality criteria.

2.2 Optimal Designs

Different kinds of designs may be engaged in many life sciences such as in the military, the engineering field, the agricultural field, the marketing field, manufacturing industries and in medicine world. One needs some optimal information on the various designs that may be of interest to a particular field. Optimal design is an essential area that deserves special attention from researchers who are interested in data analysis that involve a statistical model with several parameters. By *"design"*, we mean the synthesis of a suitable experiment to test, estimate and develop a current conjectured model (Box and Draper, 1987).

Optimal designs are experimental designs that are generated based on a particular optimality criterion and are generally optimal only for a specific statistical model. Smith (1918) introduced the concept of how a criterion can be used to arrive on optimal designs for regression problems.

Fisher (1935) expounded on the development and applications of experimental designs in response surface methodology. Box and Wilson (1951) described the result of their study extending over few years concerning various experimental designs that they were investigating. Again in the same year, the two discussed experimental designs whose purpose is to find optimality using the smallest possible number of observations. They also introduced the concept of central composite designs (CCDs) to generalize the well-known factorial principle of experimental design making it applicable in the response surface methodology. Further, they discussed steepest ascent or descent in the search for the near stationary region around the optimum representing the models using Taylor series expansion and devised the coded level convention. Box (1952) wrote a paper on multifactor designs of First order; again Box (1954) explored response surfaces technique by considering general examples. Box and Youle (1955) illustrated the link between the fitted surface and the basic mechanism of the system. They gave remarks that the process of fitting the response surface can be complex and tedious if done haphazardly. Thus, Box and Hunter (1957) expanded the use of rotatable designs. They constructed rotatable designs through geometrical configurations and obtained several second order rotatable designs. They also examined that a second order rotatable design aids in the fitting of the second surface.

Box and Hunter (1957) denoted k coordinates as a set of points in the experimental space of a random vector $\underline{X} =(x_i\ i=1,2,\ldots,n)$. More so, they developed the moment and non-singularity conditions for the existence of first and second order rotatable designs. Kiefer (1959) developed useful computational procedures for finding optimum designs in regression problems of statistical inference. These designs ensure equal precision on the response estimates. Bose and Draper (1959) constructed second order rotatable designs in three dimensions. Gardner *et al* (1959) gave the moment and the non-singularity conditions for third order response surface designs.

Box and Draper (1963) managed to construct designs for second and third order response models. Draper and Beggs (1971) approximate the true relationship by a function, linear in some unknown parameters to be estimated and of some selected order in the independent variables. Draper and Beggs (1971) continued reiterating that under tentative assumption of the validity of this linear model(which can be justified on the basis of a Taylor expansion of the response function), this brought a sound pillar of performing experiments, fit the model using regression techniques and applied standard statistical procedures to determine whether this model appears adequate.

Extensive research opened up on how to ensure that the models constructed tend to be adequate and valid. Mead and Pike (1975) further stated that the theory of optimal design produced very strong reactions and the division between theoretical statisticians researching into the theory of optimal designs and practical statisticians designing experiments for applied research workers is still very wide because the assumptions in the theory of design have been restrictive as linear models are assumed almost exclusively and optimality criterion is based on the generalized variance of the parameter estimates. However, this restrictiveness undoubtedly explains some of the reluctance of practical statisticians to try to produce optimal designs for practical problems.

2.3 Optimality Criteria

An optimality criterion is that which summarizes how good a design is, and it is maximized or minimized to obtain an optimal design. There are many statistical properties issues to consider in the design of an empirical study. Among the problems are the control of unwanted variation and the internal validity of the study. How can we be sure that a study is internally valid? In other words, how can we be sure that the treatment effect is attributed to the variables that are manipulated and not mainly influenced by unwanted variation? (Cox,1958).

This led to the rise of optimal design theory which was initiated by Kiefer (1985). According to him, the experimental design is a discrete probability measure defined by the set of various experimental conditions and weight coefficients corresponding to them. The coefficients show how many experiments (with respect to their total amount) should be performed under the condition. Here, the optimality criteria are represented as various functions defined on the set of information matrices and possessing some statistical sense. A design at which such a functional attains its extreme is called the optimal one.

A Criterion is based on how well parameters or a response are estimated or researched. The research on how a design can attain its extreme led to the development of design optimality criteria. Design optimality criteria are primarily concerned with optimal properties of the *design* matrix for the model matrix *X*.

By studying the optimality criteria, the design expert can determine the adequacy of a proposed experimental design prior to running it. Although a design may be best among several designs properties by one optimality criteria again the same design may perform poorly when evaluated by a different optimality criterion. Hence, the choice of a design will itself depend upon the choice of the evaluation criteria.

Mutiso (1998) developed the theory for the optimum estimation of the free parameters in the rotatable design point sets, which were first considered by Draper (1960) for which Kosgei (2002) obtained alphabetic optimality criteria on the same. Monsef et al (1998) deduced in their paper that an optimality criterion showed how good a design is on either a set of statistical properties or on a particular property. Further, they classified various optimality criteria in the practical fields; alphabetical optimality criteria can be grouped into four major types; information-based criteria, distance-based criteria, compound design criteria and other criteria.

There are essentially two ways for the construction of design criteria in (DOE) which incorporate different purposes of the experiment. One approach is the construction of new optimality criteria by averaging several competitive design criteria. Alternatively one could try to maximize one primary optimality criteria subject to constraints for specific minimum efficiencies of other criteria, (Dette and Franke, 2000).

According to Pukelsheim (2006), real optimality criteria are functions with such properties as are appropriate to measure largeness of information matrices. The purpose of the experiment is to find out about the model and how adequate it is. Experiments can be designed to answer a variety of questions. Often, estimates of the parameters of interest together with the predictions of the response from the fitted model. The variances of the parameter estimates and predictions depend on the particular experimental design used and should be as small as possible. In most cases poorly designed experiments waste resources by yielding unnecessarily large variances and imprecise predictions (Atkinson *et al*, 2007).

2.4 Compound Optimality Criteria

An experimental design allows the allocation of individual units in experiments (Atkinson and Donev, 1992). Optimal design is a class of experimental designs which are oprimal with respect to some statistical criterion (Pukelsheim, 1993). Further studies on optimal design gave rise to optimality criteria. Keifer (1985) optimality criteria are simply taken to be the mean of order P of the positive Eigen values of moment matrix. Draper and Pukelsheim (1994) gave a mathematical approach to optimality criteria for various designs, where he derived the alphabetic optimality criteria. The information based criteria are used for parameter estimation and they include the D- criterion, A-criterion, and E-criterion while the distance based criteria that are used for model discrimination include C-criterion and T- criterion.

Research on optimality criteria for model discrimination began early where; C–optimality was defined by Elfving (1952) as criterion that minimizes the variance of the best linear unbiased estimate for a given linear combination of the model parameters. C-Criterion provides a geometrical interpretation for finding C-optimal designs and more development on this criterion was investigated by (Silvey and Titterington, 1973). The following year Fellman (1974) justified that at most linearly independent support points are needed for a C-optimal design and the same idea was furthered by (Titterington,1975). By using the technical knowledge of support points, Pukelsheim and Torsney (1991) gave a method for computing C-optimal weights given various support points. It is true that many authors have developed optimality criteria which are applicable to the dual problem of model discrimination and parameter estimation. Atkinson et al. (2007) discussed C-optimum designs for three features of a three-parameter compartmental model for the concentration of theophylline in the blood of a horse. C-optimum designs, for example, that for estimation of the area under a curve, all had either one or two points of support and so provided no information on the values of the parameters in the model. The optimum design theory provides designs of known properties with a specified balance between parameter estimation, discrimination and estimation of a parametric function such as the area under a curve.

Atkinson (2008) stated that the goal of an experiment should be dual: to obtain an adequate model and to estimate the parameters of the selected model efficiently. Unfortunately, this has never been the case a design which is optimum for parameter estimation may be inadequate for model discrimination and vice versa. A common strategy to solve this problem is through combining two alphabetic optimality criteria for model validation with another for parameter estimation in one design.

Dette (1993) proposed the use D1-criterion for model discrimination and the D-criterion for precise estimation of the parameters. The resulting compound criterion gave a weighted geometric mean of D1- and D-efficiencies) and it was called DD1-criterion. After various scrutiny of this criterion researchers like Zen and Tsai (2004) have generalized the DD1-criterion to the case of nested regression models which differ by more than one parameter by replacing the D1-criterion with the Ds-one (with s > 1). The criterion changed to be called the DDs-criterion. Atkinson $et\ al$(2007) defined compound criterion as a weighted product of the efficiencies that is to be maximized and they introduced DT- and CD-optimality criteria. A year later Atkinson (2008) considered the T-criterion as a measure of discrimination, hence combined it to yield the DT-criterion.

Many results on optimal designs of experiments are derived under the assumption that the statistical model is known at the design stage. However, rarely it is known a prior which model is the most appropriate. Thus in the quest of trying to fill this gap design experts are in the pursuit of ensuring we have a balance between the model validation criteria that can suit in parameter estimation. Tommasi (2009) proposed the DKL-optimality criterion, which is a compound criterion given by the weighted geometric mean of KL- and D-efficiencies. Considered the D-criterion as a measure of precision in parameter estimation and KL- as a measure of discrimination, however, (López-Fidalgo *et al*, 2007) stated that KL- is useful for model discrimination in a more general context than in nested regression models with Gaussian homoscedastic errors.

From the underlying historic literature nonlinear models are common in pharmacokinetics and pharmaco dynamics. Compound criterion is formed by maximizing a weighted product of efficiencies. Optimum designs for discrimination between models introduced by Fedorov (1975) and Atkinson (2008) they considered discrimination between two linear polynomial regression models. There is a long history of papers that seek to find a balance between model discrimination and parameter estimation, at least from Hill and Robatson (1968) to Biswas and Chaudhuri (2002) and Waterhouse *et al*. (2004). A specific and sequential rotatable design in three, four and five dimensions was constructed by (Mutiso, 1998) but did not identify their optimality criteria. Kosgei (2002) evaluated the optimality criteria for the second order rotatable designs in three dimensions for the sequential rotatable designs. Koske *et al* (2011) constructed a new third order rotatable design in five dimensions through Balanced Incomplete Block Designs. Mutai *et* al (2012) discussed optimal designs for mixture experiments and their application in agricultural research. Koske *et al* (2012) constructed a practical optimum second order rotatable design in three dimensions. Again Mutai *et al* (2013) gave a new method of constructing third order rotatable designs.

In the same year, Kosgei *et al* (2013) constructed a five level modified third order rotatable design using a pair of balanced incomplete block design and Eliud (2013) gave E-optimal designs for second-degree kronecker model mixture experiments. Kipkemoi *et al* (2014) constructed some new three associate class partially balanced incomplete block designs in two replicates. Rambaei (2014) gave a generalized optimality criterion for second order rotatable design in k dimensions where she utilized a reduced parameter system to obtain the information matrix. Cheruiyot (2015) gave the efficiencies for the second order rotatable designs in three dimensions, by efficiency we consider how effective or good a design is (Kuhfeld *et al*, 1994). Design are said to be good depending on the requirement of the experimenter or the researcher. D- Efficient designs are preferred in case the experimenter is interested in minimizing the content of the ellipsoidal confidence region for the parameter of the model. In case the researcher is interested in a design which minimizes the sum or the average of the variance of the parameter estimate A-optimal design is ideal.

Seyamet *et al* (1999) stipulated that some design experts may require the desirability of two or more properties in a single design. Such designs are obtained when the optimality criteria are combined and they include DT-, CD- and CDT-Criteria.

To date, most work in design in this area has concentrated on parameter estimation rather than in model discrimination. Here, the idea of optimization of both parameter estimation and model selection. However, experimental designs that provide powerful discrimination between a pair of competing model structures are rarely efficient in terms of estimating the parameters of each model. Conversely, designs which are efficient for parameter estimation may not provide suitable power to discriminate between the models (Waterhouse *et al*, 1994). This has posed a great challenge to a statistician who may want to utilize the two properties in one design.

Hence, the current study introduces the evaluation of the compound optimality criteria for the existing second order rotatable designs in three, four and five dimensions, specifically the study evaluated the DT-criterion, CD-criterion, and CDT-criterion using designs constructed by (Rambaei, 2014).

CHAPTER THREE

METHODOLOGY

3.1 Introduction

In this chapter; the method for determining C-optimality, obtaining the compound optimality and evaluating design efficiencies for designs with 32, 64 and 112 points were outlined. Existing second order rotatable designs constructed using BIBDs in three, four and five dimensions were considered.

3.2 Determining C- Optimality Criterion for Second Order Rotatable Designs Constructed Using BIBDs.

3.2.1 Second order model

The study focuses on the Balanced Incomplete Block Design for second order rotatable designs in three, four and five dimensions. Hence the second degree response model with k factors is represented as follows;

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum\sum_{i \angle j}^{k} \beta_{ij} x_i x_j + \varepsilon \tag{3.1}$$

where

β_o is the intercept

β_i is the linear coefficient for the i^{th} factor

β_{ii} is the quadratic coefficient for the i^{th} factors

β_{ij} is the cross product coefficient for the i^{th} and j^{th} factors

3.2.2 Evaluation of C-Criterion

The C-criterion for the second order rotatable design in k- dimensions was obtained through minimizing the variance of the linear unbiased estimator of the integral function $w^{/}(X^{/}X)^{-1}w$. Thus, the C- Criterion by Elfying (1952) was given as;

$$C\text{- Criterion} = \iint \dots \int w^{/}(X^{/}X)^{-1}\mathrm{w}\ d_{x1}d_{x2} \dots d_{xk}. \tag{3.2}$$

where

$$w^{/} = \left(1, \frac{1}{k}(x_1^2, x_2^2, x_3^2, \cdots, x_k^2\right), x_1, x_2, x_3, \dots, x_k, \frac{1}{\binom{k}{2}}(x_1x_2, x_1x_3, x_2x_3, \dots, x_{k-1}x_k) \tag{3.3}$$

3.2.2.1 Design Matrix

The generalized design matrix X for the second order rotatable design is given by

$$X = \begin{bmatrix} x_{o1} & x_{11}^2 \dots x_{k1}^2 & x_{11} \dots x_{k1} & x_{11}x_{21} \dots x_{(k-1)1}x_{k1} \\ x_{o2} & x_{12}^2 \dots x_{k2}^2 & x_{12} \dots x_{k2} & x_{12}x_{22} \dots x_{(k-2)2}x_{k2} \\ & & . & \\ & & . & \\ & & . & \\ x_{on} & x_{1n}^2 \dots x_{kn}^2 & x_{1n} \dots x_{kn} & x_{1n}x_{2n} \dots x_{(k-n)n}x_{kn} \end{bmatrix} \tag{3.4}$$

The vector in (3.3) was partitioned in the following order; the pure quadratic, the linear and the interaction effects by Rambaei, (2014). Consequently, the moment matrix was also partitioned as shown below.

$$M = \begin{bmatrix} B & 0 & 0 \\ 0 & A_1 & 0 \\ 0 & 0 & A_2 \end{bmatrix} \tag{3.5}$$

where

$$B=\begin{bmatrix} 1 & \lambda_2 & \lambda_2 & \lambda_2 & \cdots & \lambda_2 \\ \lambda_2 & 3\lambda_4 & \lambda_4 & \lambda_4 & \cdots & \lambda_4 \\ \lambda_2 & \lambda_4 & 3\lambda_4 & \lambda_4 & \cdots & \lambda_4 \\ \lambda_2 & \lambda_4 & \lambda_4 & 3\lambda_4 & \cdots & \lambda_4 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda_2 & \lambda_4 & \lambda_4 & \lambda_4 & \cdots & 3\lambda_4 \end{bmatrix}_{[k+1]\ \mathrm{x}\ [k+1]},$$

$$A_1=\begin{bmatrix} \lambda_2 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_2 \end{bmatrix}_{[k]\mathrm{x}[k]},$$

and

$$A_2=\begin{bmatrix} \lambda_4 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_4 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_4 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_4 \end{bmatrix} \left[\frac{K}{2}\right]\times\left[\frac{K}{2}\right],$$

The inverse of (3.5) is;

$$M^{-1}=\begin{bmatrix} \mathrm{B}^{-1} & 0 & 0 \\ 0 & \mathrm{A}_1^{-1} & 0 \\ 0 & 0 & \mathrm{A}_2^{-1} \end{bmatrix} \qquad (3.6)$$

where,

$$B^{-1}=\frac{1}{\Delta_1}\begin{bmatrix}\alpha & \beta & \beta & \cdots & \beta\\ \beta & \gamma & \mu & \cdots & \mu\\ \beta & \mu & \gamma & \cdots & \mu\\ & & \vdots & & \\ \beta & \mu & \mu & \cdots & \gamma\end{bmatrix}_{[k+1]\times[k+1]}. \tag{3.7}$$

In which;

$\propto = 2(\text{k}+2)\lambda_4^2$, $\beta = -2\lambda_2\lambda_4$, μ = - (λ_4-λ_2^2), γ = (k+1)λ_4 - (k-1)λ_2^2 and

Δ_1=2[(k+2)λ_4^2 –k$\lambda_2^2\lambda_4$];

$$A_1^{-1} = \frac{1}{\lambda_2}\begin{bmatrix}1 & 0 & 0 & \cdots & 0\\ 0 & 1 & 0 & \cdots & 0\\ 0 & 0 & 1 & \cdots & 0\\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & 1\end{bmatrix}_{[K]X[K]}, \tag{3.8}$$

and

$$A_2^{-1} = \frac{1}{\lambda_4}\begin{bmatrix}1 & 0 & 0 & \cdots & 0\\ 0 & 1 & 0 & \cdots & 0\\ 0 & 0 & 1 & \cdots & 0\\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & 1\end{bmatrix}_{\left[\frac{K}{2}\right]\times\left[\frac{K}{2}\right]}, \tag{3.9}$$

3.2.2.2 Coefficient Matrix

The coefficient matrix K' is determined from a reduced parameters system which was obtained by Rambaei (2014) where the reduced pure quadratic and the interaction effect is that;

$$K'\beta = \begin{bmatrix} \beta_0 \\ \dfrac{\sum_{i=1}^{k} \beta_{ii}}{k} \\ \beta_i \\ \dfrac{\sum_{i \langle j=1}^{k} \beta_{ij}}{\binom{k}{2}} \\ i = 1, 2, \ldots, k \end{bmatrix} \tag{3.10}$$

where

$$\beta = \left(\beta_0, \beta_{11}, \beta_{22}, \ldots, \beta_{kk}, \beta_1, \beta_2, \ldots, \beta_k, \beta_{12}, \ldots, \beta_{k-1,k}\right)^{/}$$

is the full parameter system and is the coefficient of the second order model $y = \beta_0 + \beta_{11}x_{1u}{}^2 + \beta_{22}x_{2u}{}^2 + \ldots + \beta_{kk}x_{ku}{}^2 + \beta_1 x_{1u} + \beta_2 x_{2u} + \ldots \beta_k x_{ku} + \beta_{12}x_{1u}x_{2u} + \ldots + \beta_{k-1,k}x_{k-1,u}, x_{ku}$ and $K^{/}$ defined as

$$K^{/} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{k} & \frac{1}{k} & \cdots & \frac{1}{k} & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \frac{1}{\begin{bmatrix} k \\ 2 \end{bmatrix}} & \frac{1}{\begin{bmatrix} k \\ 2 \end{bmatrix}} & \cdots & \frac{1}{\begin{bmatrix} k \\ 2 \end{bmatrix}} \end{bmatrix}. \tag{3.11}$$

is generalized coefficient matrix of the parameter system of interest.

The coefficients of $w^{/}$ in (3.3) are the diagonal elements of a k matrix in the parameter system of interest.

3.2.2.3 Information Matrix

Rambaei (2014) used the moment matrix for second order model to determine the information matrix for the parameter system of interest. Its information matrix C is determined by

$$C_k(M) = [K_k' M_k^{-1} K_k]^{-1}$$

where $M = \frac{1}{N} x'x$ and k is the number of factors and X is as defined in (3.4)

$$C_k(M) = \begin{bmatrix} 1 & k\lambda_2 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ k\lambda_2 & k[k+2]\lambda_4 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & \lambda_2 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 0 & \lambda_2 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 0 & 0 & \lambda_2 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \begin{bmatrix} k \\ 2 \end{bmatrix}\lambda_4 \end{bmatrix}_{[k+3][k+3]} .$$

Using the elements of the inverse of the moment matrix in (3.7), (3.8) and (3.9) respectively (3.3) was obtained.

The computation for the C- criterion was portioned into three parts; the linear effects the pure quadratic and the interaction effects which were denoted as β_{ij}. For the 32 points the parts are β_{11}, β_{12} and β_{13}, for the 64 points β_{21}, β_{22} and β_{23} and lastly the 112 points β_{31}, β_{32} and β_{33} with the help of matlab software.

The respective parameters the for designs with 32, 64 and 112 points evaluated by (Rambaei, 2014) were considered and were given as follows;

$$\lambda_2 = 0.034\rho^2 \quad \text{and} \quad \lambda_4 = 0.0008\rho^4 \tag{3.12}$$

$$\lambda_2 = 0.233258\rho^2 \quad \text{and} \quad \lambda_4 = 0.06251\rho^4 \tag{3.13}$$

$$\lambda_2 = 0.196433\rho^2 \quad \text{and} \quad \lambda_4 = 0.049111\rho^4 \tag{3.14}$$

3.3 Obtaining Compound Optimality Criteria for SORD

3.3.1 Compound Optimality Criteria for two combined Alphabetic Optimality Criteria

In this section, the DT- and CD- criteria were obtained by combining two alphabetic optimality criteria. The alphabetic optimality criteria D-and T- for the Balanced Incomplete Block Designs in three, four and five dimensions evaluated by Rambaei (2014) were considered and the C-criterion evaluated in this study was utilized for determining the compound optimality criteria CD- and CDT-.

3.3.1.1 DT- Optimality

This study combined two alphabetic optimality criteria D- and T- by using the concept that was introduced by Atkinson (2008), where DT optimality criterion is a combination of D-optimality criterion for parameter estimation with the T-optimality criterion for discriminating between models. D-optimality is essentially a parameter estimation criterion (Wald, 1943). Mandal (2000) considered the construction of D–optimal designs in a variety of examples. D–optimality is defined as:

$\phi(M) = \log\det M$, if M is non-singular

$= -\infty$, otherwise

The determinant criterion $\phi(C)$ differs from the determinant $\det(C)$ by taking the s^{th} root.

$$\phi(C) = \det(C)^{\frac{1}{s}} \qquad (3.15)$$

T–optimal design is a plan where the optimality is obtained by discriminating between two or more models, one of which is true. Atkinson and Fedorov (1975:1, 2) introduced experimental designs for discriminating between two models and also between several models.

The evaluation of the trace criterion is given by

$$\phi_{-\infty} = \frac{1}{s} trace(C) \qquad (3.16)$$

The DT- criterion provides a specified balance between model discrimination and parameter estimation.

The Generalized Determinant and Trace Criteria were given by Rambaei (2014) respectively as;

$$\phi_0 C_k(M) = \left[k \begin{bmatrix} k \\ 2 \end{bmatrix} \lambda_2{}^k \lambda_4 \left[[k+2]\lambda_4 - k\lambda_2{}^2 \right] \right]^{\frac{1}{k+3}} \qquad (3.17)$$

$$\phi_1 C_k(M) = \frac{1}{k+3}\left[1 + (k+2)k\lambda_4 + k\lambda_2 + \binom{k}{2}\lambda_4 \right] \qquad (3.18)$$

From (Rambaei, 2014), The alphabetic optimality criteria D- and T- for the design with 32, 64, and 112 points were considered and given as follows;

D- CRITERION:

$\emptyset_0 C_3(M)$= 0.02306464706 (3.19)

$\emptyset_0 C_4(M)$= 0.3541807443 (3.20)

$\emptyset_0 C_5(M) = 0.3194073098$ (3.21)

T-CRITERION:

$\emptyset_1 C_{3=}0.1860666667$ (3.22)

$\emptyset_1 C_4 = 0.5440474286$ (3.23)

$\emptyset_1 C_5(M) = 0.52402$ (3.24)

The DT- criterion was introduced by Atkinson (2008) as;

$\emptyset_2^{DT}(\varepsilon)$ = (1-k) log $\Delta_1(\varepsilon)$ + ($\frac{k}{p_1}$) log$|m_1(\varepsilon)|$. (3.25)

where $\emptyset_2^{DT}(\varepsilon)$ is a convex combination of two design criteria, the first criterion is log $\Delta_1(\varepsilon)$ which is the logarithm of T- optimality and the second log $|m_1(\varepsilon)|$ is also the logarithm of D- optimality.

Designs maximizing (3.25) are called DT-optimum. The quantities in (3.19) and (3.22) were substituted in (3.25) to obtain the DT-optimality criterion.

3.3.1.2 CD-Optimality

The CD-optimality that combines C-optimality for a model selection and D-optimality for parameter estimation which was introduced by Atkinson $et\ al$ (2007), provides a specified balance between model discrimination and parameter estimation. The criterion to be maximized was;

$$\emptyset_3^{CD}(\varepsilon) = (\frac{k}{p_1}) \log |m_1(\varepsilon)| - (1\text{-}k) \log w^T M^{-1}(\varepsilon) w \,. \qquad (3.26)$$

where $\emptyset_3^{CD}(\varepsilon)$ is a convex combination of two design criteria, the first criterion is log $|m_1(\varepsilon)|$ which is the logarithm of D- optimality and the second log $w^T M^{-1}(\varepsilon) w$ is the logarithm of C- optimality.

The designs maximizing (3.26) are called CD-optimality. The quantities in (3.19) and (3.2) were substituted in (3.26) to obtain the CD-optimality criterion.

3.3.2 Compound Optimality Criteria for Three Combined Alphabetic Optimality Criteria

3.3.2.1 CDT-Optimality

The CDT-optimality combines three alphabetic optimality criteria at once. These are T-criterion for model discrimination, D- criterion for parameter estimation and C- criterion for estimation of parametric function such as the area under the curve. Thus, the criterion to be maximized was introduced by El- Monsef et al (2011) and is given by;

$$\emptyset_4^{CDT}(\varepsilon) = \frac{(k-1)^2}{p} \log |m(\varepsilon)| - k\,(1\text{-}k) \log w^T M^{-1}(\varepsilon) w + k \log \Delta_1(\varepsilon). \qquad (3.27)$$

Where $\emptyset_4^{CDT}(\varepsilon)$ is a convex combination of three design criteria. The first criterion is log $|m_1(\varepsilon)|$ which is the logarithm of D- optimality, the second $\log w^T M^{-1}(\varepsilon) w$ is the logarithm for the C-optimality and the third log $\Delta_1(\varepsilon)$ is the logarithm for T- optimality. Designs maximizing (3.27) are called CDT-optimum. The quantities in (3.19), (3.22) and (3.2) were substituted to (3.27) to obtain the CDT-optimality criterion.

3.4 Examining Relative Efficiency of Designs

The relative efficiency for the alphabetic D-, T- and C- with their compound counterpart DT-, CD- and CDT- were evaluated for designs with 32, 64 and 112 points. Normally a design with the highest percentage of the ratio of the optimality criteria is considered to be of higher efficiency than the other.

3.4.1 Relative D-efficiency

The Relative D-efficiency of a design was defined by Burgess (2004) as;

$$\left|\frac{\mathrm{M}(\varepsilon)}{\mathrm{M}(\varepsilon^*)}\right|. \tag{3.28}$$

where

$\mathrm{M}(\varepsilon)$ is the value of particular D- criterion of designs and

$\mathrm{M}(\varepsilon^*)$ is the numerical value of D-optimal design.

3.4.2 Relative T-efficiency

The Relative T- efficiency of any designs was introduced by Cooke (1979) as;

$$\frac{\Delta_1(\varepsilon_T^*)}{\Delta_1(\varepsilon)}. \tag{3.29}$$

where

$\Delta_1(\varepsilon_T^*)$ is the value of the optimal design and $\Delta_1(\varepsilon)$ is the value of a specific T- design.

3.4.3 Relative C-efficiency

(Cook et al, 2012) defined the Relative C- efficiency of a design as;

$$\left[\frac{w^T M^{-1}(\varepsilon_C^*)w}{w^T M^{-1}(\varepsilon)w}\right]. \tag{3.30}$$

where

$w^T M^{-1}(\varepsilon_C^*)w$ is the value of the C-optimal design and $w^T M^{-1}(\varepsilon)w$ is the value of the C-design.

3.4.4 Relative DT-efficiency

The Relative DT-efficiency of any design introduced by Deb (1991) is given by;

$$\left[\frac{(1-\mathrm{k})\log\Delta_1(\varepsilon) + (\frac{k}{p_1})\log|m_1(\varepsilon)|.}{(1-\mathrm{k})\log\Delta_1(\varepsilon^*) + (\frac{k}{p_1})\log|m_1(\varepsilon^*)|.}\right]. \tag{3.31}$$

where

$(1-\mathrm{k})\log\Delta_1(\varepsilon) \ + \ (\frac{k}{p_1})\log|m_1(\varepsilon)|$ is the value of a specific DT- design and

$(1-\mathrm{k})\log\Delta_1(\varepsilon^*) \ + \ (\frac{k}{p_1})\log|m_1(\varepsilon^*)|$ is the value of the DT- optimal design.

3.4.5 Relative CD-efficiency

The Relative CD- efficiency of any design was defined by Atkinson et al (2008) as;

$$\left[\frac{(\frac{k}{p_1})\log|m_1(\varepsilon^*)| - (1-\mathrm{k})\log w^T M^{-1}(\varepsilon^*)w}{(\frac{k}{p_1})\log|m_1(\varepsilon)| - (1-\mathrm{k})\log w^T M^{-1}(\varepsilon)w}\right]. \tag{3.32}$$

where

$(\frac{k}{p_1})\log|m_1(\varepsilon^*)| - (1-\mathrm{k})\log w^T M^{-1}(\varepsilon^*)w$ is the value of the CD-optimal design and

$(\frac{k}{p_1})\log|m_1(\varepsilon)| - (1-\mathrm{k})\log w^T M^{-1}(\varepsilon)w$ is the value of a specific CD-design.

3.4.6 Relative CDT-efficiency

(El-Monsef et al, 2011) introduced the Relative CDT- efficiency of a design was as;

$$\left[\frac{\frac{(k-1)^2}{p}\log|m(\varepsilon^*)| - \mathrm{k}\,(1-\mathrm{k})\log w^T M^{-1}(\varepsilon^*)\mathrm{w} + \mathrm{k}\log\Delta_1(\varepsilon^*).}{\frac{(k-1)^2}{p}\log|m(\varepsilon)| - \mathrm{k}\,(1-\mathrm{k})\log w^T M^{-1}(\varepsilon)\mathrm{w} + \mathrm{k}\log\Delta_1(\varepsilon).}\right] \tag{3.33}$$

Where

$\frac{(k-1)^2}{p}\log|m(\varepsilon^*)| - \mathrm{k}\,(1-\mathrm{k})\log w^T M^{-1}(\varepsilon^*)\mathrm{w} + \mathrm{k}\log\Delta_1(\varepsilon^*)$ is the value of the CDT-optimal design and

$\frac{(k-1)^2}{p}\log|m(\varepsilon)| - \mathrm{k}\,(1-\mathrm{k})\log w^T M^{-1}(\varepsilon)\mathrm{w} + \mathrm{k}\log\Delta_1(\varepsilon)$ is the value of a specific CDT- design.

CHAPTER FOUR

RESULTS AND DISCUSSIONS

4.1The Optimality Criteria

In this chapter, the specific optimality criteria for optimal second order rotatable designs were evaluated. The result on the C-criterion, the two combined alphabetic optimality that yielded DT- and CD- criteria and the three combined alphabetic optimality that gave CDT- criterion were given. The relative efficiencies for both alphabetic and compound optimality criteria counterparts were evaluated and discussed.

4.2 C-Criterion for Second Order Rotatable Design in Three, Four and Five Dimension using BIBD

4.2.1 C- Criterion for the 32 Points in Three Dimensions

Using the C-criterion formula given in (3.2) and by substituting λ_2 and λ_4 given in (3.12) to (3.7) yielded the information matrix as;

$$B^{-1} = \begin{bmatrix} 7.500 & -63.900 & -63.900 & -63.900 \\ -63.900 & 1043.20 & 418.20 & 418.20 \\ -63.900 & 418.20 & 1043.20 & 418.20 \\ -63.900 & 418.20 & 418.20 & 1043.20 \end{bmatrix}$$

(4.1)

The vector w given in (3.10) was expanded to include all terms of a reduced second order rotatable design in three dimensions is given as;

$$w' = [1, \tfrac{1}{3}x_1^2, \tfrac{1}{3}x_2^2, \tfrac{1}{3}x_3^2, x_1, x_2, x_3, \tfrac{1}{3}x_1x_2, \tfrac{1}{3}x_1x_3, \tfrac{1}{3}x_2x_3] \qquad (4.2)$$

Taking only the pure quadratic terms from (4.2) then;

$$w' = [1, \tfrac{1}{3}x_1^2, \tfrac{1}{3}x_2^2, \tfrac{1}{3}x_3^2] \quad (4.3)$$

$$[1 \ \tfrac{1}{3}x_1^2 \ \tfrac{1}{3}x_2^2 \ \tfrac{1}{3}x_3^2 \ ]\begin{bmatrix} 7.500 & -63.900 & -63.900 & -63.900 \\ -63.900 & 1043.20 & 418.20 & 418.20 \\ -63.900 & 418.20 & 1043.20 & 418.20 \\ -63.900 & 418.20 & 418.20 & 1043.20 \end{bmatrix}\begin{bmatrix} 1 \\ \frac{1}{3}x_1^2 \\ \frac{1}{3}x_2^2 \\ \frac{1}{3}x_3^2 \end{bmatrix},$$

Substituting (4.1) and (4.3) to the integral function given in (3.2) where the limits were the maximum and minimum values from the experimental runs gave;

$$\beta_{11} = \iiint_{-1.316}^{1.316}[7.500 - 21.3x_1^2 - 21.3x_2^2 - 21.3x_3^2 - 21.3x_1^2 + 115.9111x_1^4 + 46.4667x_1^2x_2^2 + 46.4667x_1^2x_3^2 - 21.3x_2^2 + 46.4667x_1^2x_2^2 + 115.9111x_2^4 + 46.4667x_2^2x_3^2 - 21.3x_3^2 + 46.4667x_1^2x_3^2 + 46.4667x_2^2x_3^2 + 115.9111x_3^4]d_{x1}d_{x2}d_{x3}$$

$$= 1269.0568. \quad (4.4)$$

The value of λ_2 given in (3.12) is substituted to (3.8) to obtain;

$$A_1^{-1} = (x'x)^{-1} = \begin{bmatrix} 29.4118 & 0 & 0 \\ 0 & 29.4118 & 0 \\ 0 & 0 & 29.4118 \end{bmatrix}, \quad (4.5)$$

Taking only the linear terms in (4.2) as;

$$w' = [x_1, x_2, x_3] \quad (4.6)$$

Using (4.5) and (4.6) in (3.2) gave;

$$\beta_{22} = \iiint_{-1.316}^{1.316}[29.4118x_1^2 + 29.4118x_2^2 + 29.4118x_3^2] \ d_{x1}d_{x2}d_{x3}$$

$$= 232.18212. \quad (4.7)$$

The value of λ_4 given in (3.12) is substituted to (3.9) to obtain;

$$A_2^{-1} = (x'x)^{-1} = \begin{bmatrix} 1250 & 0 & 0 \\ 0 & 1250 & 0 \\ 0 & 0 & 1250 \end{bmatrix}, \tag{4.8}$$

Taking only the interactions terms of vector w in (4.2) we have;

$$w' = [\tfrac{1}{3}x_1x_2, \tfrac{1}{3}x_1x_3, \tfrac{1}{3}x_2x_3], \tag{4.9}$$

Using (4.8) and (4.9) in (3.2) gives;

$$\beta_{33} = \iiint_{-1.316}^{1.316} [\,1250x_1^2x_2^2 + 1250x_1^2x_3^2 + 1250x_2^2x_3^2] d_{x1} d_{x2} d_{x3}$$

$$= 5696.5246. \tag{4.10}$$

The C-criterion for a design with 32 points was obtained by summing the elements in (4.4), (4.7) and (4.10) to obtain;

$$= 7197.7633. \tag{4.11}$$

4.2.2 C- Criterion for the 64 Points in Four Dimension

Substituting λ_2 and λ_4 given in (3.13) to (3.7) yields the information matrix given as;

$$B^{-1} = \begin{bmatrix} 2.3825 & -1.4817 & -1.4817 & -1.4817 & -1.4817 \\ -1.4817 & 7.5871 & -0.4116 & -0.4116 & -0.4116 \\ -1.4817 & -0.4116 & 7.5871 & -0.4116 & -0.4116 \\ -1.4817 & -0.4116 & -0.4116 & 7.5871 & -0.4116 \\ -1.4817 & -0.4116 & -0.4116 & -0.4116 & 7.5871 \end{bmatrix} \tag{4.12}$$

The vector w given in (3.10) was expanded to include all terms of a second order rotatable design in four dimensions was given by,

w'=[1, $\frac{1}{4}x_1^2, \frac{1}{4}x_2^2, \frac{1}{4}x_3^2, \frac{1}{4}x_4^2, x_1, x_2, x_3, x_4, \frac{1}{6}x_1x_2, \frac{1}{6}x_1x_3, \frac{1}{6}x_1x_4, \frac{1}{6}x_2x_3, \frac{1}{6}x_2x_4, \frac{1}{6}x_3x_4$]

(4.13)

Taking only the pure quadratic terms from (4.13) then we have;

w'= [1, $\frac{1}{4}x_1^2, \frac{1}{4}x_2^2, \frac{1}{4}x_3^2, \frac{1}{4}x_4^2$] (4.14)

$$= [1\ \tfrac{1}{4}x_1^2\ \tfrac{1}{4}x_2^2\ \tfrac{1}{4}x_3^2\ \tfrac{1}{4}x_4^2] \begin{bmatrix} 2.3825 - 1.4817 - 1.4817 - 1.4817 - 1.4817 \\ -1.4817\ 7.5871 - 0.4116 - 0.4116 - 0.4116 \\ -1.4817\ - 0.4116\ 7.5871 - 0.4116 - 0.4116 \\ -1.4817\ - 0.4116 - 0.4116\ 7.5871\ - 0.4116 \\ -1.4817 - 0.4116 - 0.4116\ - 0.4116\ 7.5871 \end{bmatrix} \begin{bmatrix} 1 \\ \frac{1}{4}x_1^2 \\ \frac{1}{4}x_2^2 \\ \frac{1}{4}x_3^2 \\ \frac{1}{4}x_4^2 \end{bmatrix},$$

Substituting (4.12) and (4.14) to integral function in (3.2) gave

β_{21} $=\iint \iint_{-1}^{1}[2.3825 - 0.3704x_1^2 - 0.3704x_2^2 - 0.3704x_3^2 - 0.3704x_4^2 - 0.3704x_1^2 +$

$0.4742 - 0.02573x_1^2x_2^2 - 0.02573x_1^2x_3^2 - 0.02573x_1^2x_4^2 - 0.3704x_2^2 -$

$0.02573x_2^2x_1^2 + 0.4742x_2^4 - 0.02573x_2^2x_3^2 - 0.02573x_2^2x_4^2$-$0.3704x_3^2$-$0.02573x_1^2x_3^2 -$

$0.02573x_2^2x_3^2 + 0.4742x_3^4 - 0.02573x_3^2x_4^2 - 0.3704x_4^2 - 0.02573x_1^2x_4^2 -$

$0.02573x_2^2x_4^2 - 0.02573x_3^2x_4^2 + 0.4742x_4^4]d_{x1}d_{x2}d_{x3}d_{x4}$

=3.8586. (4.15)

The value of λ_2 given in (3.13) is substituted to (3.8) to obtain;

$$A_1^{-1} = \begin{bmatrix} 4.2871 & 0 & 0 & 0 \\ 0 & 4.2871 & 0 & 0 \\ 0 & 0 & 4.2871 & 0 \\ 0 & 0 & 0 & 4.2871 \end{bmatrix}, \quad (4.16)$$

Taking only the linear terms in (4.13) the outcome was;

w'= $[x_1, x_2, x_3, x_4]$. (4.17)

Using (4.16) and (4.17) in (3.2) gave;

β_{22}=$\int\iiint_{-1}^{1}$[$4.2871x_1^2$+$4.2871x_2^2$ +$4.2871x_3^2 + 4.2871x_4^2$] $d_{x1}d_{x2}d_{x3}d_{x4}$

= 11.43232. (4.18)

The value of λ_4 given in (3.13) was substituted to (3.9) to obtain;

$$A_2^{-1} = \begin{bmatrix} 15.9974 & 0 & 0 & 0 & 0 & 0 \\ 0 & 15.9974 & 0 & 0 & 0 & 0 \\ 0 & 0 & 15.9974 & 0 & 0 & 0 \\ 0 & 0 & 0 & 15.9974 & 0 & 0 \\ 0 & 0 & 0 & 0 & 15.9974 & 0 \\ 0 & 0 & 0 & 0 & 0 & 15.9974 \end{bmatrix}, \quad (4.19)$$

Taking only the interactions terms of vector C in (4.13) we have;

w'= [$\frac{1}{6}x_1x_2, \frac{1}{6}x_1x_3, \frac{1}{6}x_1x_4, \frac{1}{6}x_2x_3, \frac{1}{6}x_2x_4, \frac{1}{6}x_3x_4$] (4.20)

Substituting (4.19) and (4.20) to the integral function in (3.2) gave;

β_{23}=$\int\iiint_{-1}^{1}$[$15.9974x_1^2x_2^2 + 15.9974x_1^2x_3^2 + 15.9974x_1^2x_4^2 + 15.9974x_2^2x_3^2 +$

$15.9974x_2^2x_4^2 + 15.9974x_3^2x_4^2$] $d_{x1}d_{x2}d_{x3}d_{x4}$

= 21.33. (4.21)

The C-criterion for a design with 64 points was obtained by summing the elements in (4.15), (4.18) and (4.21) to obtain;

=36.62092 (4.22)

4.2.3 C- Criterion for the 112 Points in Five Dimensions

Substituting λ_2 and λ_4 given in (3.14) to (3.7) yielded the information matrix given by,

$$B^{-1} = \begin{bmatrix} 2.2790 & -1.3022 & -1.3022 & -1.3022 & -1.3022 & -1.3022 \\ -1.3022 & 9.4707 & -0.7104 & -0.7104 & -0.7104 & -0.7104 \\ -1.3022 & -0.7104 & 9.4707 & -0.7104 & -0.7104 & -0.7104 \\ -1.3022 & -0.7104 & -0.7104 & 9.4707 & -0.7104 & -0.7104 \\ -1.3022 & -0.7104 & -0.7104 & -0.7104 & 9.4707 & -0.7104 \\ -1.3022 & -0.7104 & -0.7104 & -0.7104 & -0.7104 & 9.4707 \end{bmatrix} \tag{4.23}$$

The vector w given in (3.10) was expanded to include all terms of a second order rotatable design in five dimensions is given by,

$$w' = (1, \tfrac{1}{5}x_1^2, \tfrac{1}{5}x_2^2, \tfrac{1}{5}x_3^2, \tfrac{1}{5}x_4^2, \tfrac{1}{5}x_5^2, x_1, x_2, x_3, x_4, x_5,$$

$$\tfrac{1}{10}x_1x_2, \tfrac{1}{10}x_1x_3, \tfrac{1}{10}x_1x_4, \tfrac{1}{10}x_1x_5, \tfrac{1}{10}x_2x_3, \tfrac{1}{10}x_2x_4, \tfrac{1}{10}x_2x_5, \tfrac{1}{10}x_3x_4, \tfrac{1}{10}x_3x_5, \tfrac{1}{10}x_4x_5) \quad (4.24)$$

Taking only the pure quadratic terms from (4.24) then we have;

$$w^{]}=[1, \tfrac{1}{5}x_1^2, \tfrac{1}{5}x_2^2, \tfrac{1}{5}x_3^2, \tfrac{1}{5}x_4^2, \tfrac{1}{5}x_5^2] \quad (4.25)$$

$[1, \frac{1}{5}x_1^2, \frac{1}{5}x_2^2\frac{1}{5}x_3^2\frac{1}{5}x_4^2\frac{1}{5}x_5^2]$

$$\begin{bmatrix} 2.2790 - 1.3022 - 1.3022 - 1.3022 - 1.3022 - 1.3022 \\ -1.3022\ 9.4707 - 0.7104 - 0.7104 - 0.7104 - 0.7104 \\ -1.3022 - 0.7104\ 9.4707 - 0.7104 - 0.7104 - 0.7104 \\ -1.3022 - 0.7104 - 0.7104\ 9.4707 - 0.7104 - 0.7104 \\ -1.3022 - 0.7104 - 0.7104 - 0.7104\ 9.4707 - 0.7104 \\ -1.3022 - 0.7104 - 0.7104 - 0.7104 - 0.7104\ 9.4707 \end{bmatrix} \begin{bmatrix} 1 \\ \frac{1}{5}x_1^2 \\ \frac{1}{5}x_2^2 \\ \frac{1}{5}x_3^2 \\ \frac{1}{5}x_4^2 \\ \frac{1}{5}x_5^2 \end{bmatrix}$$

Using (4.23) and (4.25) in (3.2) gave;

β_{31}=$\iint \iint_{-1}^{1} 2.279 - 1.3022x_1^2 - 1.3022x_2^2 - 1.3022x_3^2 - 1.3022x_4^2 - 1.3022x_5^2 -$

$-1.3022x_1^2 + 9.4707x_1^4 - 0.7104x_1^2x_2^2 - 0.7104x_1^2x_3^2 - 0.7104x_1^2x_4^2 -$

$0.7104x_1^2x_5^2 - 1.3022x_2^2 - 0.7104x_2^2x_1^2 + 9.4707x_2^4 - 0.7104x_2^2x_3^2 - 0.7104x_2^2x_4^2 -$

$0.7104x_2^2x_5^2 - 1.3022x_3^2$-$0.7104x_1^2x_3^2 - 0.7104x_2^2x_3^2 + 9.4707x_3^4 - 0.7104x_3^2x_4^2 -$

$0.7104x_3^2x_5^2 - 1.3022x_4^2 - 0.7104x_1^2x_4^2 - 0.7104x_2^2x_4^2 - 0.7104x_3^2x_4^2 + 9.4707x_4^4 -$

$0.7104x_4^2x_5^2 - 1.3022x_5^2 - 0.7104x_1^2x_5^2 - 0.7104x_2^2x_5^2 - 0.7104x_3^2x_5^2 -$

$0.7104x_4^2x_5^2 + 9.4707x_5^4]d_{x1}d_{x2}d_{x3}d_{x4}d_{x5}$

=12.7664. (4.26)

The value of λ_2 given in (3.14) is substituted to (3.8) to obtain;

$$A_1^{-1} = \begin{bmatrix} 5.0908 & 0 & 0 & 0 & 0 \\ 0 & 5.0908 & 0 & 0 & 0 \\ 0 & 0 & 5.0908 & 0 & 0 \\ 0 & 0 & 0 & 5.0908 & 0 \\ 0 & 0 & 0 & 0 & 5.0908 \end{bmatrix} \quad (4.27)$$

Taking only the linear terms in (4.24) we have;

w'= $[x_1, x_2, x_3, x_4, x_5]$ (4.28)

Using (4.27) and (4.28) in (3.2) gives;

$$\beta_{32}=\int\iiint_{-1.1}^{1.1}[\,5.0908x_1^2+5.0908x_2^2+5.0908x_3^2+5.0908x_4^2+5.0908x_5^2]d_{x1}d_{x2}d_{x3}d_{x4}d_{x5}$$

$$= 16.9691. \tag{4.29}$$

The value of λ_4 given in (3.14) was substituted to (3.9) to obtain;

$$A_2^{-1} =$$

$$\begin{bmatrix} 20.3620 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 20.3620 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 20.3620 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 20.3620 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 20.3620 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 20.362020 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 20.3620 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 20.3620 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 20.3620 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 20.3620 \end{bmatrix}$$

(4.30)

Taking only the interactions terms of vector w in (4.24) we have;

$$w'=$$

$$\left[\tfrac{1}{10}x_1x_2\ \tfrac{1}{10}x_1x_3\ \tfrac{1}{10}x_1x_4\ \tfrac{1}{10}x_1x_5\ \tfrac{1}{10}x_2x_3\ \tfrac{1}{10}x_2x_4\ \tfrac{1}{10}x_2x_5\ \tfrac{1}{10}x_3x_4\ \tfrac{1}{10}x_3x_5\ \tfrac{1}{10}x_4x_5\right] \tag{4.31}$$

Using (4.30) and (4.31) in (3.2) gives;

$$\beta_{33}==\int\iiint_{-1}^{1}[20.362x_1^2x_2^2+20.362x_1^2x_3^2+20.362x_1^2x_4^2+20.362x_1^2x_5^2+20.362x_2^2x_3^2+20.362x_2^2x_4^2+20.362x_2^2x_5^2+20.362x_3^2x_4^2+20.362x_3^2x_5^2+20.362x_4^2x_5^2]\,d_{x1}d_{x2}d_{x3}d_{x4}d_{x5}$$

$$= 45.5889. \tag{4.32}$$

The C-criterion for a design with 112 points was obtained by summing the elements in (4.26), (4.29) and (4.32) to obtain;

=75.3244. (4.33)

The C-optimal values obtained were found to be 7197.7633, 36.6261 and 75.3344 for a design with 32, 64, 112 points. The 32 points in three dimensions were found to be non-homogenous followed by the 112 points in five dimensions and the most homogenous were the 64 points in four dimensions. The smaller the optimality value the more desirable it was. The design with 64 points had the smallest value hence it was optimal.

4.3 Compound Optimality Criteria for Two and Three combined Alphabetic Optimality Criteria.

4.3.1 Compound Optimality Criteria for two combined Alphabetic Optimality Criteria

Two alphabetic optimality criteria are combined to give compound optimality criterion. The determinant criterion is combined with the trace criterion to give DT-Criterion; the C-Criterion is combined with the determinant criterion to give CD-criterion.

4.3.1.1 DT- criterion for 32 points in three dimension

The Determinant criterion was given in (3.19) and the trace criterion in (3.22) for k= 3 using the compound formula stated in (3.25) yielded the DT- compound optimality criteria as;

$\emptyset_1^{DT}(\varepsilon)$ = 0.6421362517. (4.34)

4.3.1.2 DT- criterion for 64 points in four dimension

For k=4, the determinant criterion was given in (3.20) and the trace criterion in (3.23) substituting it in the compound formula given in (3.25) results to the DT-compound optimality criteria given as;

$$\boldsymbol{\emptyset_2^{DT}(\varepsilon)} = 0.5355039691. \tag{4.35}$$

4.3.1.3 DT- criterion for 112 points in five dimension

.Substituting the determinant criterion given in (3.21) and the trace criterion given in (3.24) to the compound formula given in (3.25), for the design with $k = 5$, it gave;

$$\emptyset_1^{DT}(\varepsilon) = 0.8128240809. \tag{4.36}$$

The DT-optimal values were 0.6421362517, 0.5355039691 and 0.8128240809 for a design with 32, 64 and 112 points respectively. The 112 points in five dimensions were non-homogenous in terms of optimality value followed by the 32 points in three dimensions and the homogenous among them was the design with 64 points.

This implies that the smaller the value the more desirable a criteria were. The DT-optimal values for the four dimension lie between the D- optimal value and the T-optimal value in the 64 points for both cases. There was a balance between parameter estimation and model discrimination.

4.3.1.4 CD- criterion for 32 points in three dimension

The Determinant criterion was given in (3.19) and the C criterion in (4.11) for k= 3 using the compound formula stated in (3.26) yielded the CD- compound optimality criterion as;

$$\emptyset_1^{CD}(\varepsilon) = 6.8958868188. \tag{4.37}$$

4.3.1.5 CD- criterion for 64 points in four dimension

The Determinant criterion was given in (3.20) and the C criterion in (4.22) for k= 4 using the compound formula stated in (3.26) to yield the CD- compound optimality criterion as;

$$\emptyset_1^{CD}(\varepsilon) = 4.4336. \tag{4.38}$$

4.3.1.6 CD- criterion for 112 points in five dimension

The Determinant criterion was given in (3.21) and the C criterion in (4.33) for k= 5 using the compound formula stated in (3.26) yielded the CD- compound optimality criterion as;

$$\emptyset_1^{CD}(\varepsilon) = 7.197958256. \tag{4.39}$$

The CD-optimal values were found to be 6.8958868188, 4.4336 and 7.197958256 for the 32, 64 and 112 points respectively. The 112 points in five dimension were non-homogenous in terms of optimality followed by the 32 points in three dimensions and the preferred homogenous was the 64 points.

The CD-optimal values for the three, four and five dimensions lies between the C-optimal value and the D-optimal value for all points. There was a balance between parameter estimation and model discrimination.

4.3.2 Compound Optimality Criteria for Three Combined Alphabetic Optimality Criteria

4.3.2.1 CDT- criterion for 32 points in three dimension

The C criterion was given in (4.11), the determinant criterion given in (3.19) the trace criterion in (3.22) were combined using the compound formula stated in (3.27) to yield CDT criterion as;

$$\emptyset_1^{CDT}(\varepsilon) = 16.8608223. \quad (4.40)$$

4.3.2.2 CDT- criterion for 64 points in four dimension

The C criterion was given in (4.22), the determinant criterion given in (3.20) with the trace criterion in (3.23) were combined using the compound formula stated in (3.27) to obtain CDT criterion as;

$$\emptyset_1^{CDT}(\varepsilon) = 17.12773013. \quad (4.41)$$

4.3.2.3 CDT- criterion for 112 points in five dimension

The C criterion was given in (4.33), the determinant criterion was given in (3.21) and the trace criterion in (3.24) using the compound formula stated in (3.27) to give CDT criterion as;

$$\emptyset_1^{CDT}(\varepsilon) = 35.12951441. \quad (4.42)$$

The CDT-optimal values obtained were found to be 16.8608223, 17.12773013 and 35.12951441 for 32, 64 and 112 points respectively. The 112 points in five dimensions were the non-homogenous in terms of optimality followed by the 64 points in four dimensions and the homogenous among them was the 32 points.

This implies that the lesser the number of factors in a design the better the CDT-optimality criteria. The CDT-optimal values for the three, four and five dimensions lies between the C- optimal value, the D-optimal value and the T-optimal value for all points.

Table 4. 1 Summary of the optimality criteria for the BIB designs in thirty two, sixty-four and one hundred and twelve points

Number of points	D- criterion	T-criterion	C-criterion	DT-criterion	CD-criterion	CDT-criterion
32	0.02306465	0.1860666	7197.7633	0.6421363	6.8958868	16.860822
64	0.35418074	0.5440474	36.62092	0.5355039	4.4336	17.127730
112	0.31940731	0.52402	75.3244	0.8128241	7.1979582	35.129514

From Table 4.1, all the designs under consideration are D-optimal. Each of the C-, D-, T-, DT-, CD- and CDT- optimality criteria demands a specific statistical property. From the table above the smaller the criterion numerical value the more desirable it was. The alphabetic optimality criteria D- and T- for the 32 points design was the smallest, however, this was not the case for the C-optimality criterion. From the two combined optimality criteria DT- and CD- in both cases, the design with 64 points was the found to be the most homogenous. The three combined optimality criterion CDT- it was found that the lesser the number of factors the better the design.

4.4 Relative Efficiency

Relative efficiencies of any arbitrary designs show how good a design is in relation to another design. The higher the percentage output the better the design under consideration. Efficiencies for D-, T-, DT-, CD- and CDT- criteria were;

4.4.1 Relative D-efficiency for 32 points

From the formula given in (3.28), the D-efficiency for k=3 is stated as

$$\text{D-efficiency}=\frac{|M(\xi)|}{|M(\xi^*)|},$$

where $M(\varepsilon^*) = 0.02306464706$ is the value of the optimal to itself. Hence;

$$= \frac{0.02306464706}{0.02306464706} \times 100 = 100\% \tag{4.43}$$

4.4.2 Relative D-efficiency for 64 points

From the formula given in (3.28), the D-efficiency for k=4 is stated as

$$\text{D-efficiency}=\frac{|M(\xi)|}{|M(\xi^*)|},$$

where $M(\varepsilon^*) = 0.02306464706$ is the value of the optimal design and $M(\varepsilon)= 0.3541807443$ is the value of the specific design. Hence;

$$= \frac{0.3541807443}{0.02306464706} \times 100 = 15.356\% . \tag{4.45}$$

4.4.3 Relative D-efficiency for 112 points

Last using the formula given in (3.28) for k=5 is as follows

D-efficiency= $\frac{|M(\xi)|}{|M(\xi^*)|}$,

where M(ε^*) = 0.02306464706 is the value of the optimal design and M(ε) = 0.3194073098 is the value of the specific design. Hence;

$$= \frac{0.3194073098}{0.02306464706} \times 100 = 13.84835\% \quad (4.46)$$

The D- optimality for the 32 points was selected as the optimal value and was used to determine the D-efficiency for design with 64 and 112 points and was found to be 15.356%, and 13.84835%.

4.4.4 Relative T-efficiency for 32 points

From the formula given in (3.29), the T-efficiency for k=3 is stated as

$$\frac{\Delta_1(\varepsilon_T^*)}{\Delta_1(\varepsilon)}$$

where $\Delta_1(\varepsilon_T^*)$ = 0.18606667 is the value of the optimal design and by taking relative efficiency;

$$=\frac{0.18606667}{0.186066667} \times 100=100.00\% \quad (4.47)$$

4.4.5 Relative T-efficiency for 64 points

From the formula given in (3.29), the T-efficiency for k=4 is stated as

$$\frac{\Delta_1(\varepsilon_T^*)}{\Delta_1(\varepsilon)}$$

where $\Delta_1(\varepsilon_T^*)$ = 0.18606667 is the value of the optimal design and $\Delta_1(\varepsilon)$= 0.5440474286 is the value of the specific design. Hence;

$$=\frac{0.186066667}{0.5440474286} \times 100 = 34.20\% \qquad (4.48)$$

4.4.6 Relative T-efficiency for 112 points

Again, using the formula given in (3.29) for k=5 is as follows

$$\frac{\Delta_1(\varepsilon_T^*)}{\Delta_1(\varepsilon)}$$

where $\Delta_1(\varepsilon_T^*)$ = 0.18606667 is the value of the optimal design and $\Delta_1(\varepsilon)$= 0.52402 is the value of the specific design. Hence;

$$=\frac{0.186066667}{0.52402} \times 100 = 35.51\% \qquad (4.49)$$

The T- optimality for the 32 points was selected as the optimal value and was used to determine the T-efficiency for design with 64 and 112 points and was found to be 34.2%, and 35.51%.

4.4.7 Relative C-efficiency for 32 points

Using the formula given in (3.30), the relative efficiency for C- criterion for k=3 is as;

Relative T-efficiency = $\left[\frac{w^T M^{-1}(\varepsilon_i^*)w}{w^T M^{-1}(\varepsilon)w}\right]$

where numerator value = 36.62092 is the value of the optimal design and the denominator = 7193.76332 is the value of the specific design. Hence;

$$\frac{36.62092}{7193.76332} \times 100 = 0.51\ \% \tag{4.50}$$

4.4.8 Relative C-efficiency for 64 points

Using the formula given in (3.30), the relative efficiency for C- criterion for k=3 is as;

Relative T-efficiency = $\left[\frac{w^T M^{-1}(\varepsilon_i^*)w}{w^T M^{-1}(\varepsilon)w}\right]$

where numerator value = 36.62092 is the value of the optimal design and the denominator is the same value of the specific design. Hence;

$$\frac{36.62092}{36.62092} \times 100 = 100\ \% \tag{4.51}$$

4.4.9 Relative C-efficiency for 112 points

Again, using the formula given in (3.30) for k=5 is as follows

Relative T-efficiency = $\left[\frac{w^T M^{-1}(\varepsilon_i^*)w}{w^T M^{-1}(\varepsilon)w}\right]$

where numerator value = 36.62092 is the value of the optimal design and the denominator = 75.3244 is the value of the specific design. Hence;

$$\frac{\mathbf{36.62092}}{\mathbf{75.3244}} \times 100 = 48.62\ \% \tag{4.52}$$

The C- optimality for the 64 points was selected as the optimal value and was used to determine the C-efficiency for design with 32 and 112 points and was found to be 0.51%, and 48.62%.

4.4.10 Relative DT-efficiency for 32 points

Using the formula given in (3.31), the relative efficiency for DT- criterion for k=3 is as;

$$\text{Relative DT-efficiency} = \left[\frac{(1-\mathrm{k})\log\Delta_1(\varepsilon) + (\frac{k}{p_1})\log|m_1(\varepsilon)|.}{(1-\mathrm{k})\log\Delta_1(\varepsilon^*) + (\frac{k}{p_1})\log|m_1(\varepsilon^*)|.}\right]$$

where denominator value = 0.535503991 is the value of the optimal design and the numerator = 0.6421362517 is the value of the specific design. Hence;

$$= \frac{0.6421362517}{0.5355039691} \times 100 = 119.9125\% \qquad (4.53)$$

4.4.11 Relative DT-efficiency for 64 points

Using the formula given in (3.31), the relative efficiency for DT- criterion for k=4 is as;

$$\text{Relative DT-efficiency} = \left[\frac{(1-\mathrm{k})\log\Delta_1(\varepsilon) + (\frac{k}{p_1})\log|m_1(\varepsilon)|.}{(1-\mathrm{k})\log\Delta_1(\varepsilon^*) + (\frac{k}{p_1})\log|m_1(\varepsilon^*)|.}\right]$$

where denominator value = 0.535503991 is the value of the optimal design and the numerator is the same value of the specific design. Hence;

$$= \frac{0.5355039691}{0.5355039691} \times 100 = 100\% \qquad (4.54)$$

4.4.12 Relative DT-efficiency for 112 points

Again, using the formula given in (3.31) for k=5 is as follows

Relative DT-efficiency = $\left[\frac{(1-\mathrm{k})\log\Delta_1(\varepsilon) + (\frac{k}{p_1})\log|m_1(\varepsilon)|.}{(1-\mathrm{k})\log\Delta_1(\varepsilon^*) + (\frac{k}{p_1})\log|m_1(\varepsilon^*)|.}\right]$

where denominator value = 0.535503991 is the value of the optimal design and the numerator = 0.8128240809 is the value of the specific design. Hence;

$= \frac{0.8128240809}{0.5355039691} \times 100$ = 151.7867% (4.55)

The DT- optimality for the 64 points was selected as the optimal value and was used to determine the DT-efficiency for design with 32 and 112 points and was found to be 119.91%, and 151.79%.

4.4.13 Relative CD-efficiency for 32 points

Using the formula given in (3.32), the relative efficiency for CD- criterion for k=3 is as;

Relative CD-efficiency = $\left[\frac{(\frac{k}{p_1})\log|m_1(\varepsilon^*)| - (1-\mathrm{k})\log C^T M^{-1}(\varepsilon^*)C}{(\frac{k}{p_1})\log|m_1(\varepsilon)| - (1-\mathrm{k})\log C^T M^{-1}(\varepsilon)C}\right]$

where numerator value = 4.4336 is the value of the optimal design and the denominator = 6.8958868188 is the value of the specific design. Hence;

$= \frac{4.4336}{6.8958868188} \times 100$ = 64.29% (4.56)

4.4.14 Relative CD-efficiency for 64 points

Again, using the formula given in (3.32) for k=4 is as follows;

Relative CD-efficiency = $\left[\frac{(\frac{k}{p_1}) \log |m_1(\varepsilon^*)| - (1-\mathrm{k}) \log C^T M^{-1}(\varepsilon^*) C}{(\frac{k}{p_1}) \log |m_1(\varepsilon)| - (1-\mathrm{k}) \log C^T M^{-1}(\varepsilon) C}\right]$

where numerator value = 4.4336 is the value of the optimal design and the denominator is the same value of the specific design. Hence;

$$= \frac{4.4336}{4.4336} \times 100 = 100\% \qquad (4.57)$$

4.4.15 Relative CD-efficiency for 112 points

Again, using the formula given in (3.32) for k=5 is as follows;

Relative CD-efficiency = $\left[\frac{(\frac{k}{p_1}) \log |m_1(\varepsilon^*)| - (1-\mathrm{k}) \log C^T M^{-1}(\varepsilon^*) C}{(\frac{k}{p_1}) \log |m_1(\varepsilon)| - (1-\mathrm{k}) \log C^T M^{-1}(\varepsilon) C}\right]$

where numerator value = 4.4336 is the value of the optimal design and the denominator = 7.197958256 is the value of the specific design. Hence;

$$= \frac{4.4336}{7.197958256} \times 100 = 61.59\% \qquad (4.58)$$

The CD- optimality for the 64 points was selected as the optimal value and was used to determine the CD-efficiency for design with 32 and 112 points and was found to be 64.29%, and 61.59%.

4.4.16 Relative CDT-efficiency for 32 points

From the formula given in (3.33), the CDT-efficiency for k=3 is stated as;

$$\text{CDT-efficiency}=\left[\frac{\frac{(k-1)^2}{p}\log|m(\varepsilon^*)| - \mathrm{k}\,(1-\mathrm{k})\log C^T M^{-1}(\varepsilon^*)\mathrm{C} + \mathrm{k}\log\Delta_1(\varepsilon^*).}{\frac{(k-1)^2}{p}\log|m(\varepsilon)| - \mathrm{k}\,(1-\mathrm{k})\log C^T M^{-1}(\varepsilon)\mathrm{C} + \mathrm{k}\log\Delta_1(\varepsilon).}\right]$$

where numerator value = 16.8608223 is the value of the optimal design and the denominator is the same value of the specific design. Hence;

$$= \frac{16.8608223}{16.8608223} \times 100 = 100\% \tag{4.59}$$

4.4.17 Relative CDT-efficiency for 64 points

From the formula given in (3.33), the CDT-efficiency for k=4 is stated as;

$$\text{CDT-efficiency}=\left[\frac{\frac{(k-1)^2}{p}\log|m(\varepsilon^*)| - \mathrm{k}\,(1-\mathrm{k})\log C^T M^{-1}(\varepsilon^*)\mathrm{C} + \mathrm{k}\log\Delta_1(\varepsilon^*).}{\frac{(k-1)^2}{p}\log|m(\varepsilon)| - \mathrm{k}\,(1-\mathrm{k})\log C^T M^{-1}(\varepsilon)\mathrm{C} + \mathrm{k}\log\Delta_1(\varepsilon).}\right]$$

where numerator value = 16.8608223 is the value of the optimal design and the denominator = 17.1277013 is the value of the specific design. Hence;

$$= \frac{16.8608223}{17.1277013} \times 100 = 98.44\% \tag{4.60}$$

4.4.18 Relative CDT-efficiency for 112 points

Again, using the formula given in (3.33) for k=5 is as follows;

$$\text{CDT-efficiency}=\left[\frac{\frac{(k-1)^2}{p}\log|m(\varepsilon^*)| - \mathrm{k}\,(1-\mathrm{k})\log C^T M^{-1}(\varepsilon^*)\mathrm{C} + \mathrm{k}\log\Delta_1(\varepsilon^*).}{\frac{(k-1)^2}{p}\log|m(\varepsilon)| - \mathrm{k}\,(1-\mathrm{k})\log C^T M^{-1}(\varepsilon)\mathrm{C} + \mathrm{k}\log\Delta_1(\varepsilon).}\right]$$

where numerator value = 16.8608223 is the value of the optimal design and the denominator = 35.12951441 is the value of the specific design. Hence;

$$= \frac{16.8608223}{35.12951441} \times 100 = 47.99\% \tag{4.61}$$

The CDT- optimality for the 32 points was selected as the optimal value and was used to determine the CDT-efficiency for design with 64 and 112 points and was found to be 47.99%, and 98.44%.

Table 4.2 Summary of the relative efficiencies for the optimality criteria for the BIB designs with thirty-two, sixty-four and one hundred and twelve points.

Number of points	D-efficiency	T-efficiency	C-efficiency	DT-efficiency	CD-efficiency	CDT-efficiency	Average
32	100%	100%	0.5%	119.91%	64.29%	!00%	74.69%
64	15.4%	34.2%	100%	100%	100%	98.44%	73.2%
112	13.85%	35.51%	48.62%	151.79%	61.59%	47.99%	44.42%

From the above table 4.2, for the 32 point design, it was interesting to note that a design can show both the two statistical properties; parameter estimation and model discrimination from D-efficiencies and T- efficiencies but at the same time when the design is subjected to the C-Criterion it becomes inadequate.

In general, the design with 64 points performed better when it was subjected to the two combined alphabetic criteria. The three combined alphabetic optimality efficiency for 32 points was higher as compared to 64 and 112 points. The relationship of efficiencies in the three designs was linear indicating that the fewer the factor in a design the better.

4.4.19 Hypothetical Example

Suppose an experimenter considers utilizing a second order rotatable design points denoted by $s(1,1,1,1)+s(1.414,0,0,0)+s(0,0,0,0)$ to investigate the effects of four poultry feeds ingredients on production of eggs. The design factors for the experiment are fish meal (X_1), salt(X_2), crab meal (X_3) and cultured yeast (X_4). The response variable (Y) is production of white meat in grams.

Table 4. 3 Poultry feeds with coded variables

x1	x2	x3	x4	Y
1	1	1	1	27.6
-1	1	1	1	22.4
1	-1	1	1	18.6
1	1	-1	1	21.4
1	1	1	-1	24
-1	-1	1	1	16.6
-1	1	-1	1	17.4
-1	1	1	-1	19
-1	-1	-1	-1	12.6
1	-1	-1	-1	13
-1	1	-1	-1	14
-1	-1	1	-1	15.6
-1	-1	-1	1	14
1	1	-1	-1	17.4
1	-1	1	-1	17
1	-1	-1	1	15.4
1.414	0	0	0	23.4
-1.414	0	0	0	20.6
0	1.414	0	0	22.6
0	-1.414	0	0	13.4
0	0	1.414	0	20.6
0	0	-1.414	0	15.6
0	0	0	1.414	21
0	0	0	-1.414	17.6
0	0	0	0	22.6

This design contains 25 numbers of observations, 16 factorial points and 8 axial points with 1 center point.

The analysis of variance for fitting the data to the second-order and contour plots helped to characterize the response surface of interest.

Minitab version 17 was used to fit the data for the second-order model and carry out the analysis of variance for production of white meat.

4.4.19.1 Model fit for Poultry Feeds

Table 4.4 below gives the coefficients, standard errors, t values and p values of the Poultry Feeds model.

Table 4. 4 Model fit for poultry feeds

Term	Coef	SE Coef	T-Value	P-Value
Constant	21.463	0.434	49.48	0.000***
x1	1.892	229	8.27	0.000***
x2	3.776	0.229	16.52	0.000***
x3	3.017	0.229	13.2	0.000***
x4	1.811	0.229	7.92	0.000***
x1x1	0.821	0.511	1.61	0.139
x2x2	-3.179	0.511	-6.22	0.000***
x3x3	-3.079	0.511	-6.02	0.000***
x4x4	-1.879	0.511	-3.68	0.004**
x1x2	1.55	0.361	4.29	0.002**
x1x3	0.55	0.361	1.52	0.159
x1x4	0.3	0.361	0.83	0.426
x2x3	1.25	0.361	3.46	0.006**
x2x4	1	0.361	2.77	0.020*
x3x4	-0.2	0.361	-0.55	0.592

From table 4.4, the fitted model therefore was given as;

$$\hat{y} = 21.463 + 1.892x_1 + 3.776x_2 + 3.017x_3 + 1.811x_4 + 0.821x_1^2 - 3.179x_2^2 - 3.079x_3^2 - 1.879x_4^2 + 1.55x_1x_2 + 0.55x_1x_3 + 0.3x_1x_4 + 1.25x_2x_3 + 1x_2x_4 - 0.2x_3x_4$$

4.4.19.2 The analysis of variance for Poultry Feeds

Table 4.5 below gives the output of analysis of variance

Table 4. 5 Analysis of variance for poultry feeds

Source	DF	Adj SS	Adj MSS	F Value	P value
Model	14	371.469	26.533	50.74	0.000***
Linear	4	302.27	75.567	144.52	0.000***
Pure Quadratic	4	47.609	11.902	22.76	0.000***
Two way interactions	6	21.59	3.596	6.88	0.004**
Error	10	5.229	0.523		
Total	24	376.698			

The analysis of variance indicates that there are significant interactions between the factors. The small *p*-values for linear and square terms also point out that their contribution is significant to the model. Since, there are no replicated center points; the software could not obtain a lack-of- fit. But, small *p*-values for the interactions and the squared terms suggest there is curvature in the response surface. Moreover, the main effects can be referred to as significant at an individual .05 significant level. As a result, the final model for the response variable is concluded as follows:

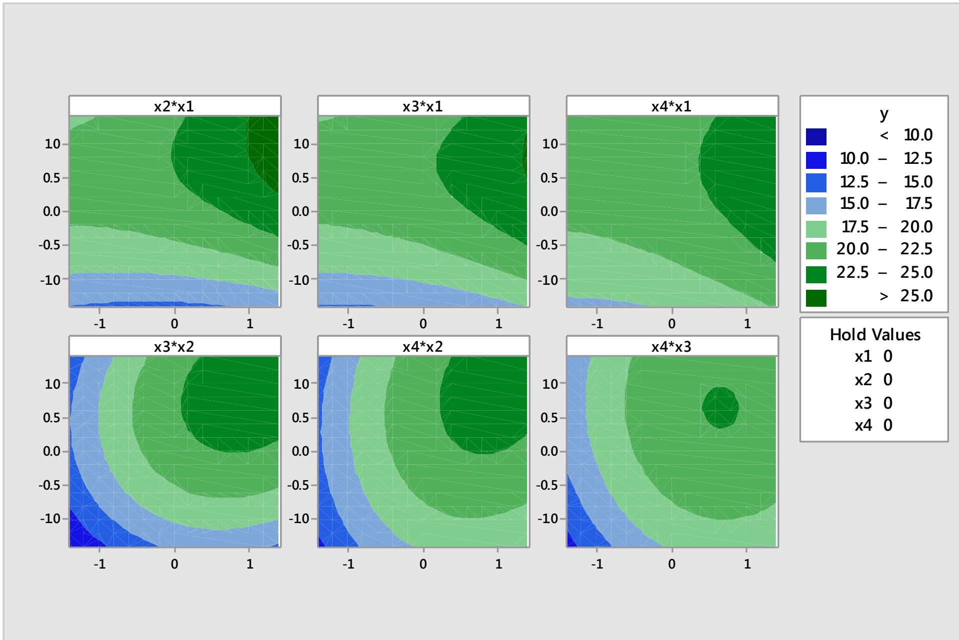
$$\hat{y} = 21.463 + 1.892x_1 + 3.776x_2 + 3.017x_3 + 1.811x_4 - 3.179x_2^2 - 3.079x_3^2 - 1.879x_4^2 + 1.55x_1x_2 + 1.25x_2x_3 + 1x_2x_4$$

Table 4. 6 Model summary for the production of white meat

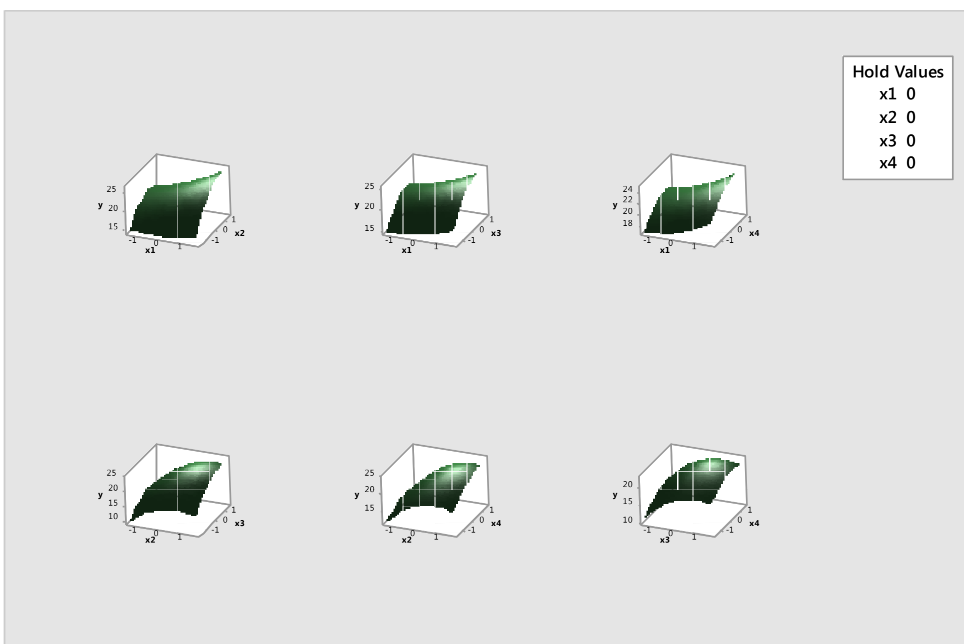
Model Summary		
S	R.sq	R.sq (adj)
0.723119	98.61%	96.67%

The results for the adjusted R^2 indicate that 96.67% (0.9667) of the variation in the response was explained by the model.

Since the response surface is explained by the second-order model, it was necessary to analyze the optimum setting. The graphical visualization is very helpful in understanding the second-order response surface. Specifically, contour plots helps to characterize the shape of the surface and locate the optimum response approximately. The graphed contour plot for production of white meat was shown in Figure 4.1 and 4.2.



4. 1 Figure Contour plots for expected white meat production



4. 2 Response surface plot for production of white meat

CHAPTER FIVE

CONCLUSION AND RECOMMENDATIONS

5.1 Introduction

This chapter outlines the conclusion and the recommendation derived from the result of the study. Besides, the conclusions and the recommendations for both the alphabetic and compound optimality are the implications of these findings as well as future projections based on the study.

5.2 Conclusion

The C- Criterion obtained exhibited large numerical values relative to the other alphabetic optimality criteria.

For the two combined alphabetic optimality criteria, the compound optimality value lies in between the specific alphabetic optimality values and it also applies to three combined alphabetic optimality criteria. This implies that a balance has been achieved between parameter estimation and model discrimination.

The compound optimality criteria obtained provides a better design characteristic in terms of minimizing variance for parameter estimates and model selection

The efficiencies for the compound optimality criteria were high as compared to the alphabetic counterparts.

5.3 Recommendation

The study recommends that compound optimality to be used in the selection of designs that are used in performing experiments in order to achieve optimal response.

This study also recommends the application of compound optimality criteria in designing of experiments for manufacturing products that involve more than one ingredient. For instance in the manufacture of a certain type of drug; here numerous kinds of factors are combined together in different amounts in order to obtain the most effective drug.

For further research, the study suggests that the U-criterion that can be obtained by combining the D-criterion, A-criterion and E-criterion to be also considered using Central Composite Designs.

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APPENDIX 1: Production of white meat Experimental data

Natural values fish meal	Salt	Crab meal	Culture yeast	Coded values x1	x2	x3	x4	Response white meat
15	10	98	25	1	1	1	1	27.6
5	5	98	25	-1	-1	1	1	16.6
15	5	92	25	1	-1	-1	1	15.4
5	10	92	25	-1	1	-1	1	17.4
15	5	98	15	1	-1	1	-1	17
5	10	98	15	-1	1	1	-1	19
15	10	92	15	1	1	-1	-1	17.4
5	5	92	15	-1	-1	-1	-1	12.6
15	5	98	25	1	-1	1	1	18.6
5	10	98	25	-1	1	1	1	22.4
15	10	92	25	1	1	-1	1	21.4
5	5	92	25	-1	-1	-1	1	14
15	10	98	15	1	1	1	-1	24
5	5	98	15	-1	-1	1	-1	15.6
15	5	92	15	1	-1	-1	-1	13
5	10	92	15	-1	1	-1	-1	14.4
17.07	7.5	95	20	1.414	0	0	0	23.4
2.93	7.5	95	20	-1.414	0	0	0	20.6
10	11.03	95	20	0	1.414	0	0	22.6
10	3.97	95	20	0	-1.414	0	0	13.4
10	7.5	99.24	20	0	0	1.414	0	20.6
10	7.5	90.76	20	0	0	-1.414	0	15.6
10	7.5	95	27.07	0	0	0	1.414	21
10	7.5	95	12.93	0	0	0	-1.414	17.6
10	7.5	95	20	0	0	0	0	22.6