CONSTRUCTION OF OPTIMAL SECOND - ORDER ROTATABLE CENTRAL COMPOSITE DESIGNS THROUGH RESOLUTIONS WITH APPLICATION TO WHITENESS OF COTTON

PhD. THESIS

BY

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A THESIS SUBMITTED IN FULFILMENT OF THE REQUIREMENTS FOR THE AWARD OF THE DEGREE OF DOCTOR OF PHILOSOPHY IN BIOSTATISTICS IN THE SCHOOL OF BIOLOGICAL AND PHYSICAL SCIENCES OF MOI UNIVERSITY, ELDORET, KENYA.

2017

DECLARATION BY THE CANDIDATE

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DEDICATION

This thesis is dedicated to my husband Lawrence Kinyua and son Solomon Mwangi.

ACKNOWLEDGEMENTS

Thanks to God for His grace and love.

I wish to express my sincere gratitude to my supervisor Prof. J. Koske for his professional guidance and availability for consultation throughout this research work.I will always be grateful for your patience, support and encouragement in every possible way..

My sincere thanks also go to my supervisor Prof. J. Kinyanjui for offering many valuable suggestions from time to time that led to the overall improvement of this work. Your advice that I dedicate more time to this study greatly motivated me to put more effort.

Many thanks go to Prof. Mutiso who contributed immensely in the initial stages of this study. Your comments and advice when I was writing my proposal assisted me greatly in laying the foundation for this study. Thank you.

To my classmates I appreciate the team work spirit and encouragement to push on and complete this work in time.

Most of all, I thank my husband Kinyua and my son Mwangi for their understanding and patience. Your unconditional love and unwavering support has been my anchor and encouragement from the beginning to the completion of my studies.

God bless you all.

ABSTRACT

Resolution of a design refers to the degree to which estimated main effects are confounded with estimated two or more than two-level interactions. Optimal designs reduce the costs of experimentation by allowing statistical models to be estimated with fewer experimental runs. The purpose of this study was to construct optimal rotatable designs through resolutions as well as explore and optimize response surfaces. Rotatable designs were constructed through resolutions III and IV for three and four factors based on the Central Composite Designs. Information matrices based on the parameter subsystem of interest on the second-degree Kronecker model were obtained. Optimal rotatable Weighted Central Composite Designs were derived and optimality was accomplished through application of D-, A- , E- and I-optimality criterion. A generalized form of the constructed D- and I-optimal rotatable WCCDs for m factors was derived together with the corresponding optimal values. The efficiency of the designs was also determined over the full CCD. A CCD with four factors was used to illustrate the practicability of the derived rotatable designs where optimal conditions for effects on whiteness of cotton using Peracetic Acid in the presence of a Bleaching Agent were obtained by locating the stationary points. Optimal whiteness index was obtained using full CCD and resolution IV CCD and the efficiency of the latter was found to be 0.9678. The derived rotatable designs were found to beD-, A-, E- and I- optimal as well as more efficient than uniformly weighted CCDs. It was concluded that rotatable designs constructed through resolution R and assigning different weights to the support points are better. The experimental runs are reduced hence economical and the resulting designs are improved in terms of optimality and estimation efficiency. The results also showed that the D-optimal resolution III design gives more weight to the cube portion while resolution IV design gives equal weight to both portions. But A- and I- optimal designs assign greater weight to the star portion than the cube portion.

ABBREVIATIONS

CCD - Central Composite Design

DOE - Design of Experiments

FDs - Factorial Designs

FFDs - Fractional Factorial Designs

GET - General Equivalence Theorem

RSM - Response Surface Methodology

WCCDs - Weighted Central Composite Designs

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CHAPTER ONE

INTRODUCTION

1.0 Background Information

Optimal designs refer to a class of experimental designs that are optimal ("best") with respect to some statistical criterion. In the Design of experiments (DOE) for estimating statistical models, optimal designs allow parameters to be estimated without bias and with minimum-variance. Such designs reduce the costs of experimentation byallowing statistical models to be estimated with fewer experimental runs. On the other hand, a non-optimal design requires a greater number of experimental runs to estimate the parameters with the same precision as an optimal design. Response Surface Designs are experimental designs used for fitting response surfaces. They are used for the study of response surface methodology (RSM) useful for modeling and analysis of problems where a response of interest is influenced by several variables and the objective is to optimize this response (Montgomery, 2005). The application of RSM to design optimization aims at reducing the cost of expensive analysis methods.

In many experimental situations, the relationship between the response and independent variables is a functional one. For example, the response Y may be represented as a suitable function f of the levels $x_{1u}, x_{2u}, \ldots, x_{mu}$ of the m factors and, θ the set of parameters. A typical model may be of the form:

$$y_u = f\left(x_{1u}, x_{2u}, \ldots, x_{mu}; \theta + e_u\right)^T \qquad (1.1)$$

where $u=1,2,\ldots,N$ represents the N observations with x_{iu} representing the level of the ith factor ($i=1,2,\ldots,m$) in the uth observation. The residual e_u measures the experimental error of the uth observation. The expected response $E(y_u)$ is called the response surface. In most RSM problems, the form of relationship between the response and the independent variables is unknown as well as the set of the parameters. Thus a suitable model approximation for the true functional relationship between the response variable and the set of independent variables should be developed (Montgomery, 2013). Attempts can be made to approximate the response surfaces by using derived polynomial equations, such that the objective of the study now becomes the estimated response surface whose statistical properties are determined by the moment matrix

$$M(\xi)=\int f(x)f(x)^T d\xi \quad . \tag{1.2}$$

The information that a design with moment matrix M contains for the model response surface $f(x)^T\theta$ is represented by the information surface given by

$$i_M(x)=\begin{cases} \dfrac{1}{f(x)^T M^{-1} f(x)}, for\, f(x)\in range\, M \\ 0, otherwise \end{cases} \tag{1.3}$$

And in terms of information matrices

$$i_M(x)=C_{f(x)}(M(\xi)). \tag{1.4}$$

Many experiments involve the study of the effects of two or more factors. Factorial designs (FDs) are most efficient for thesetype of experiments. A complete two-level factorial design 2^m is one in which each of the treatment combinations appears an equal number of times. Thus such a design assigns equal weight $\frac{1}{l}$ to each of the $l=2^m$ vertices of $[-1;1]^m$ (Pukelsheim, 1993). This design finds application in three areas as outlined by Myerset al.,(2009) among which is that a 2^m design is a basic building block used to create other response surface designs. For example, augmenting a 2^m design with axial runs and center points, a central composite designis obtained and it is one of the most important designs for fitting second-order response surface models.

The successful use of two-level fractional factorial designs (FFDs) is based on three ideas:

a) Main effects and low-order interactions dominate the system or process when there are many variables under consideration. For a large number of factors m, the total number of observations will be $N=2^{m-p}$, and this is kept relatively small as m gets large. The goal is to create designs that allow the experimenter to screen a large number of factors without having a very large experiment in which case the assumption is that only a few are very important. This is called sparsity of effects.

b) The projective property where fractional factorial designs can be projected into stronger designs in a subset of the significant factors.

c) Sequential experimentation referring to cases where it is possible to combine the runs from two or more FFDs to sequentially form a larger design to estimate the factor effects and interactions of interest. That is, one can add runs to a fractional factorial to resolve difficulties (or ambiguities) in interpretation.

Examples of response surface designs are the Central Composite designs (CCDs) and the Box-Behnken designs. The CCDs comprise of three portions: a 2^m factorial (or fractional factorial) design, center points (used for fitting first-order model) and $2m$ axial points at a distance α from the origin (added when the second-order terms are further incorporated). For rotatability, the value of α should be equal to $2^{m/4}$ (Box et al., 1957). But if a 2^{m-p} fractional factorial design is used in place of full 2^m factorial, then

$$\alpha = 2^{(m-p)/4} \quad . \tag{1.5}$$

Hence a CCD is useful and powerful in sequential experimentations. In a CCD, the cube portion may be a two-level FFD of resolution R. Resolution of a design refers to the degree to which estimated main effects are confounded with estimated two or more than two-level interactions. In other words, a resolution R design is a design in which no interaction of p factors is confounded to an interaction of less than R-p factors. Two-level fractional factorial designs are investigated in detail by Box and Hunter (1961).

The concept of design resolution is a useful way to categorize fractional factorial designs according to the class patterns they produce. A saturated design is one whose design's resolution is specified, number of runs is fixed and it accommodates only a certain maximum number of factors.

This thesis concentrates onmomentmatrixgiven in equation (1.2)on page 2,for the second-order Kroneckermodel. The Kronecker representation has several advantages such as offering attractive symmetry, more compact notations, more convenient invariance properties, and the homogeneity of the regression terms

(DraperandPukelsheim, 1998; Prescott et al.,2002). The benefits are that distinct terms are repeated appropriately, according to the number of times they can arise.

Examples of quadratic models include, the Scheffé model, the Kronecker model and the intercept (or slack variable) model. The three models are of the form:

The Full quadratic model: $Y_x = \theta_0 + \sum_{i=1}^{m} \theta_i x_i + \sum_{i=1}^{m} \theta_{ii} x_i^2 + \sum_{i,j=1}^{m} \theta_{ij} x_i x_j + \varepsilon_i$ (1.6)

The S-model: $Y_x = \theta_0 + \sum_{i=1}^{m} \theta_i x_i + \sum_{i,j=1}^{m} \theta_{ij} x_i x_j + \varepsilon_i$ (1.7)

For the Kronecker model, only the quadratic and interaction terms exist. This may be expressed as:

$$E(Y_x) = \theta_0 + \sum_{i=1}^{m} \theta_i x_i^2 + \sum_{i,j=1}^{m} \gamma_{ij} x_i x_j \quad (1.8)$$

These three reduced models are re-parameterizations of one another such that the parameters of the quadratic terms in the Kronecker model are equivalent to the parameters of the linear terms in the S-model whereas the parameters of the interaction terms can be obtained from the parameters of the S-model using the relation:

$$\gamma_{ij} = \beta_{ij} + \beta_i + \beta_j \quad (1.9)$$

As the number of factors in a second-order model increases, the number of terms also increases.Therefore, economic second-order designs with reasonable prediction variance are highly desirable.

1.1 Statement of the Problem

Several methods have been used to construct rotatable designs. The resulting designs have been shown to be D-, A- and E-optimal. Chigbu and Orisakwe (2011) constructed rotatable designs by varying cube and star points of CCD and obtained D-, A-and E-optimal values.ChigbuandUkaegbu(2014) investigated the small composite designsand the minimum-run resolution V designs using the *G*- and *I*-optimality criteria by replicating the star and cube portions.

While the central composite design (CCD) is widely applied in many fields to construct a second-order response surface model with quantitative factors to help increase the precision of the estimated model, attention has mainly been given to the designs where the cube portion is obtained from a full factorial design (Pukelsheim, (1993); Li (2006)). Construction of rotatable designs through resolutions has received minimal attention. Lavricet al., (2007) fitted a full quadratic model using a four factors CCD data on optimum conditions for effects on whiteness of cotton and obtained 85 as the predicted value of the whiteness index. This thesis therefore sought to construct rotatable designs through resolutions and to explore and optimize response surfaces with application to the data obtained by Lavric et al., (2007) about effects on whiteness of cotton using four factors CCD.

1.2 Objectives of the study

This thesis sought to achieve the following objectives.

1.2.1 The general objective of the study

The general objective of this study was to construct optimal rotatable Central Composite Design through resolutionsbased on the second order Kronecker model with application to optimization of whiteness of cotton.

1.2.2 Specific objectives

The specific objectives were to:

(a) Construct rotatable designs through resolutions III and IV for three and four factors based on the Central Composite Designs (CCDs).

(b) Derive the Optimal Rotatable Weighted Central Composite Designs (WCCDs).

(c) Determine the WCCDs D-, A-, E- and I- optimal values and their corresponding efficiencies.

(d) Illustrate the practicability of the derived optimal rotatable CCD using four factors experimental data about effects on whiteness of cotton.

1.3 Significance of the study

The factorial designs are widely used in experiments.In recent years more emphasis has beenplaced by the chemical and processing field on finding regions where there is animprovement in response instead of finding the optimum response (Myers et al, 1989). In practice, the experimenter aims at obtaining optimal designs with minimum cost. As the number of factors in a 2^m factorial design increases, the number of runs required for a complete replicate of the design exceed budget. When experimentation is expensive or time consuming, CCDs with cube portion obtained from fractional factorial designs are more appropriate.One of the aims ofdesign of experiment is to extract as much as possible information from a limited set of experimental study.

This study sought to address thisbyconstructingoptimal rotatable designs through resolution III andIVbased on the CCD which can be run sequentially, and are very efficient in providing much information on experiment variable effects and overall experimental error in a minimum number of required runs. Further a with resolution IV designall main effects can always be estimated unbiasedly and two-factor interactions can also be estimated.

1.4 Scope of the study

Considerations throughout this thesis were restricted to three and four factors CCD constructed through resolutions III and IV with no center points. Some experimental data with four factors about effects on whiteness of cotton was used to illustrate the practicability of the derived optimal rotatable CCD.

1.5 Thesis layout

In this thesis, Chapter one gives an introduction of experimental designs for optimization and second-degree Kronecker model. The statement of the problem, the objectives, the scope and the significance of the study are also given. Work previously done on two-level fractional factorial designs, response surface designs based on the CCD, optimality criteria as well as some background information on whiteness of cotton is reviewed in Chapter two.

An investigation of the methodology used in achieving the general objective of this study is done in Chapter three. Factors three and four basic 2^{m-p} ($for\ p=1$) designs are constructedthrough resolutions III and IV and a description of the CCD is given. Characterization of the coefficient matrix of the maximum parameter subsystem $K'\theta$ is done and the conditions for the existence of rotatable matrices are outlined. Theorems applied in this thesis as well as the various optimality criteriaused to derive optimal rotatable weighted central composite designs are stated.

Chapter fourdeals with the interpretation and explanation of the findings of this study with regard to the stated research objectives.Rotatable CCDs and their corresponding momentandinformation matrices are obtained.Optimal Rotatable WCCDs for three and four factors are obtainedusing the General Equivalence Theorem for D-, A-, E and I- optimality criteria. Numerical results foroptimal rotatable WCCD and uniformly weighted CCD are given and their efficiencies computed. Further, the practicability of the derived rotatable designs is illustrated using four factors CCD on effects of whiteness of cotton. An analysis of the same is done.In Chapter five, a summary is given and conclusions drawn.Recommendations for further research emanating from this work closethis research thesis. This is followed by references and an appendix section.

CHAPTER TWO

LITERATURE REVIEW

2.0 Introduction

This literature review discusses someresearched areas that relate to this study.Response Surface Designs, Two-level fractional factorialdesigns, and Second-order rotatable designs are discussed separately as well as optimality criteria and efficiency.

Further, a review is done on the Central Composite Designs and Whiteness of Bleached Cotton.

2.1 Response Surface Designs

In recent years, the use of optimal designs in industrial experimentation has grown rapidly, due to the fact that the methodology is now being introduced in standard DOE text books (Montgomery,2005) and also because facilities for constructing optimal designs have become readily available. Optimization process involves three major steps: performing the statistically designed experiments, estimating the coefficients in mathematical model and predicting the response as well as checking the adequacy of the model as explained by Sunitha, et al.,(2015). The aim of thisstudywas to evaluate the efficacy of the mathematical model CCDandRSM in optimizing parameters for enhancing plant growth of Pearl millet. The study revealed that RSM could be usedeffectively to optimize growth of Pearl milletand the CCD is simple, efficient, economical, timesaving and can be adopted for optimizing crop yields**.**

2.2 Two-Level Fractional Factorial Designs and Design Resolution

The regular fractional factorial designs were introduced by Box and Hunter (1961). These designs later became the standard tools for factor screening. Draper and Lin (1990) carried out a study on the maximum number of factors that can be accommodated in a specified resolution R design. Construction and analysis of half fraction factorial design is studied in details by Montgomery (2013).

2.3 Second-Order Rotatable Designs

Box and Hunter (1957) introduced rotatable designs for the exploration of response surfaces. The study of rotatable designs mainly emphasizes on the estimation of absolute response. Narasimham, et al., (1983)constructed Second Order Rotatable Designs (SORD) using a pair of incomplete block designs. Victorbabu and Rajyalakshmi (2012) studied a new method of construction of Robust Second Order Rotatable Designs using balanced incomplete block designs. Rajyalakshmi and Victorbabu (2014) suggested an empirical study of Second - Order Rotatable Designs under tridiagonal correlation structure of errors using central composite designs.

2.4 Second-Order Kronecker Model

Prescott and Draper (2009) examined three quadratic models, the Scheffé model, the Kronecker model and the intercept (or slack variable) model using data arising from mixture experiments thus the models did not contain the constant term (θ_0). The three models were of the form given in equations (1.6), (1.7) and (1.8) respectively. They concluded thatbecausethe estimates obtained are predicted responses at locations remote from the observed data, then the coefficients estimates do not seem to be representative of the data. The study proposed an alternative method of transformation where more design points within a larger region of the mixture space can be included. Coefficients estimates were now found to be more consistent.

2.5 Optimality Criteria and Efficiency

An optimality criterion is a criterion which summarizes how good a design is, and it is maximized or minimized by an optimal design. Most often, all the available criteria in literature may be classified into four types; information-based criteria, distance-based criteria, compound criteria and other types criteria. Information-based criteria are related to the information matrix $X^T X$. This matrix is important because it is proportional to the inverse of the variance-covariance matrix for the least-squares estimates of the linear parameters of the model of interest as investigated by El-Monsef, et al., (2009).The Information-based criteria considered include D-, A-and E-optimality criterion. The D-optimality criterion is estimation based and aims to minimize the variance of the factor-effect estimates. On the other hand an I-optimality criterion is prediction based and aims to minimize the average variance of prediction over the region of experimentation. For this reason, the I-optimality criterion would be a more appropriate one than the D-optimality criterion for generating response surface designs (Goos and Bradley, 2012). The General Equivalence Theorem for I-Optimality was used by GoosandSyafitri(2014) to investigate V-optimal mixture designs for the *q*th degree model using the simplex centroid design. In this study, optimal rotatable Weighted Central Composite Designs were derived and optimality was accomplished through the application of D-, A- , E- and I-optimality criteria which follows from the General Equivalence Theorem (Pukelsheim,1993; Goos and Bradley, 2012).

2.6 Central Composite Designs

The central composite designs comprise some of the most popular and commonly used classes of experimental designs for fitting the second order (Box and Wilson, 1951). These designs are mixtures of three building blocks: cubes, stars and center points where the cube portion may be obtained from a fractional factorial design of resolution down to resolution III. This allows smaller factorial fractions to be used.Several examples have been publishedwhere the recommended fractional design for the central composite differs dramatically from the fractional design standing alone (Hartley (1959), Draper and Lin, 1990)). Several authors have continued the quest for smaller designs. Lucas (1974) computes the D-criterion for saturated composite designs constructed using a subset of points from the saturated resolution V designs ofRechtschaffner (1967) whose study had used four different design generators to construct minimal point designs for estimating second - order surface. The study compares different CCDs using $\left|X^T X\right|$ criterion.

When a mass of α is placed on the cube-plus-star design and a mass of $(1-\alpha)$ is placed on the center point portion, the bottom line is that rotatability generates a complete class of designs with a single parameter α no matter how many factors m are being investigated (Pukelsheim, 1993)and the constructed design is an improvement of the standardized design. Oehlert (2002) constructed two-level equireplicated irregular fractions with resolution V. Chigbu and Orisakwe (2011) study On Optimal Partially Replicated Rotatable and Slope Rotatable CCDs investigated two, three and four factors central composite design using three rational variations: the one cube plus one star, the replicated cubes plus one star, and the one cube plus replicated stars.Each variation was considered for two to four factors where D-, A- and E-optimal values were obtained. The D-values for replicated cubes plus one star variation were found to be greater than those of one cube plus replicated stars and based on rotatability restriction the designs are A- and E-optimal. Li (2006)investigated split-plot second-order designs using the CCD by exploring the impact of a split-plot structure on traditional central composite designs and made concrete and practical recommendations on the choice of α for both wholeplot factors and subplot factors. The CCD was constructed by two sets of points plus n_c center runs that is a 2^k or a 2^{k-p} Resolution V fractional factorial design for all factors and the $2k$ axial runs for each factor with a distance of α from the center.

Yin-Jie (2007) constructed minimal-point designs for second-order response surface using a two-stage method to find the composite designs. The minimal-point designs were equal-weight designs and were formulated as:

$\xi = \frac{n_1+1}{p}\xi_1 + \left(1 - \frac{n_1+1}{p}\right)\xi_2$ where ξ_1 is the design of the first-order portion and one center point, n_1 is the number of the support points of the first-order design, and ξ_2 is the equal-weight design with the $(p - n_1 - 1)$ distinct added support points.A comparison was made with central composite designs, other small composite designs and minimal-point designs by relative efficiencies and the proposed composite designs performed well in general.

Ray-Bing et al., (2008) constructed small composite designs for a second-order response surface which they referred to as Conditionally Optimal Small Composite Designs. A two-stage method which reduces the number of runs for the first-order designs was used with only one center point and the proposed composite designs were found to be D-optimal and in cases where they are not, they have reasonably high D-efficiencies. The study proposed that this construction method can be easily extended to the composite designs with more than one center points and other optimal criteria can be adopted and were represented as $\xi = \frac{nc}{n}\xi_c + \frac{n_1}{n}\xi_1 + \frac{n_2}{n}\xi_2$ where ξ_c is the one-point design at center point, 0, with n_c replications. ξ_1 is the selected first-order design with n_1 number of supports points. ξ_2 is the equal-weight design for n_2 added points, and $n = n_1 + n_c + n_2$.

Chuan-Pin and Mong-Na (2011) investigated D-optimal designs for models where the qualitative factors interact with, respectively, the linear effects, or the linear effects and two-factor interactions or quadratic effects of the quantitative factors. The study showed that, at each qualitative level, the corresponding D-optimal design also consists of three portions as central composite design, i.e. the cube design, the axial design and center points, but with different weights. Rajyalakshmi and Victorbabu (2014) suggested an empirical study of second-order rotatable designs under tri-diagonal correlation structure of errors using central composite designs.

2.7 Whiteness of Bleached Cotton

Textile preparation of cotton typically includes scouring and bleaching at high temperature and high pH. Substantial amounts of wastewater are produced that must be treated prior to being released to receiving fresh water. Recent research in laboratories has focused on the development and application of compounds that enhance the bleaching process. Lavric et al.,(2007)studied the effects of temperature, pH and concentrations of activator and peracetic acid on the bleaching performance using a statistical design of experiment. A full CCD was used to determine the optimal conditions for bleaching cotton with Peracetic acid in the presence of a bleaching activator. The term pH refers to a scale which measures acidity or alkalinity: a pH of 0-6.9 isacid , a pHof 7.0 is neutral and a pH of 7.1-14.0 is alkaline. A quadratic design was developed and was shown to be statistically valid with $R^2=0.984$ with the results revealing that all the linear terms, the quadratic terms of temperature and Peracetic acid and the interaction term of temperature and pH were significant. According to a study on Optimization of

Parameters of Cotton Fabric Whiteness by Fijul, et al., (2014), whiteness index increases with the increase of time and after 80^0C it decreases. But at 80^0C optimum results are obtained. Theoretical results derived in this thesis were illustrated using the data generated by Lavric et al., (2007).

CHAPTER THREE

METHODOLOGY

3.0 Introduction

In this chapter,the second-degree Kronecker model (1.8) for three and four factors to be fitted is given and an explanation of how to construct correspondingbasic 2^{m-p} ($for\ p=1$) designs through resolutions III and IV is highlighted. These were then augmented with axial points to obtain rotatable CCDs (ξ). Conditions for rotatability of the second–order moment matrices are given as well as the form of the coefficient matrix for parameter subsystem of interest and the information matrices for the rotatable designs. Further, theorems which wereused to obtain the rotatable WCCDs based on the General Equivalent Thoerem for D-, A-, E- and I-optimality are stated and a procedure is givenon how the WCCDs were obtained. The formulae for computing D-, A-, E- and I-optimal values and their relative efficiencies are stated. The type of data that was used to illustrate the theoretical results and the method of presenting the results are outlined in this chapter.

3.1 Design of the studyand the Model

Information matrices (1.4) based on the parametersubsystem of interest and their corresponding rotatable CCDs for fitting second - degree Kronecker model wereinvestigated.

Definition 3.1.

In an $m-way$ second - degree model $m\geq 2$, the regression function is taken to be:

$$f(x)=\begin{pmatrix}1\\ x\\ x\otimes x\end{pmatrix}:T_{\sqrt{m}}\rightarrow R^{k} \qquad (3.1)$$

with $T_{\sqrt{m}}$ the ball of radius $\sqrt{m}$ in R^k and $k=1+m+m^2$. The moment matrix of a design $\tau\in T$ is given in (1.2). The portion $x\otimes x$ is an $m^2\times 1$ matrix and represents the mixed products for $i\neq j$ twice, as $x_i x_j$ and as $x_j x_i$. The experimental domain $T_{\sqrt{m}}$ is left invariant by arotation $R\in R=Orth(m)$, and commutes with the regression function f according to

$$f(Rx)=\begin{pmatrix}1\\ Rx\\ (R\otimes R)(x\otimes x)\end{pmatrix}=\begin{pmatrix}1&0&0\\ 0&R&0\\ 0&0&R\otimes R\end{pmatrix}f(x) \ . \qquad (3.2)$$

Therefore f is invariant relative to the $(1+m+m^2)\times(1+m+m^2)$ matrix group

$$Q_2=\left\{\begin{pmatrix}1&0&0\\ 0&R&0\\ 0&0&R\otimes R\end{pmatrix}:R\in Orth(m)\right\}\subseteq Orth(k) \ . \qquad (3.3)$$

Thus the second-degree Kronecker model is

$$E(Y_x)=f(x)'\theta=\theta_0+\sum_{i=1}^{m}\theta_i x_i+\sum_{i=1}^{m}\theta_{ii}x_i^2+\sum_{i,j=1}^{m}(\theta_{ij}+\theta_{ji})x_i x_j \qquad (3.4)$$

Where Y_x the observed response under the experimental conditions $x \in T$, is taken to be a scalar random variable and

$\Theta=(\theta_0,\theta_1,\ldots,\theta_{11},\theta_{22},\ldots,\theta_{mm})' \in R^{m^2}$ istheparameter vector.(3.5)

An $m-way$ second – degree Kronecker model (3.1) for $m \geq 2$ of the K-regression function f was fitted. This involves the Kronecker product whose powerful properties make f superior to any other form of parametrizing the second - degree model (Pulkelsheim, 1993). The model (3.4) has $(1+m+m^2)$ parameters and is expressed as:

(a) $m=3$

$$\eta(\theta,x)=\theta_0+\theta_1x_1+\theta_2x_2+\theta_3x_3+\theta_{11}x_1^2+\theta_{12}x_1x_2+\theta_{13}x_1x_3+\theta_{21}x_2x_1+\theta_{22}x_2^2+\theta_{23}x_2x_3+\theta_{31}x_3x_1+\theta_{32}x_3x_2+\theta_{33}$$

. (3.6)

(b) $m=4$

$$\eta(\theta,t)=\theta_0+\theta_1x_1+\theta_2x_2+\theta_3x_3+\theta_4x_4+\theta_{11}x_1^2+\theta_{12}x_1x_2+\theta_{13}x_1x_3+\theta_{14}x_1x_4+\theta_{21}x_2x_1+\theta_{22}x_2^2+\theta_{23}x_2x_3+\theta_{24}x_2x$$

. (3.7)

3.1.1 **Fractional Factorial Designs**

In this section, a method of constructing resolution R design of m -factors in n runs is explained.

Let X be the n by m design matrix, with high and low levels of a factor denoted by +1 and -1 respectively. To construct one-half fraction, a full 2^{m-1} factorial design is written down, then the mth factor is added by identifying its plus and minus levels with the signs of $ABC\ldots(M-1)$. $M=ABC\ldots(M-1)$ implying that

$I = ABC \ldots M$ where $A, B, C, \ldots, M = x_1, x_2, x_3, \ldots, x_m$ respectively. When additional factors are added to the interactions, generators are created. The set of distinct words formed by all possible products of any subset of the factors involving p generators gives the defining relation which contains 2^p terms including the identity term I. For a set of generators

$W = \{W_1, W_2, \ldots, W_p\}$, we have $IW = WI = W$ and $W^2 = I$.

Another way is to partition the runs into two blocks with the highest-order interaction $ABC \ldots M$ confounded.

3.1.2 **Fold-Over Designs**

Estimated main effects are confounded with two factor interactions in resolution III designs. To eliminate such a problem, the design is folded over. This means repeating the projected design with all signs reversed. This converts a resolution III design into a resolution IV design (Box et al., 1978) and doubles the size of the experiment.

Table 3.1. Resolution IV Design

Run	Original 2_{III}^{4-1} $x_1 x_2 x_1 x_2 x_4$	Factors		I
1	-1	-1	+1	+1
2	+1	-1	-1	+1
3	-1	+1	-1	+1
4	+1	+1	+1	+1
	Second 2_{III}^{4-1} with signs switched			
5	+1	+1	-1	-1
6	-1	+1	+1	-1
7	+1	-1	+1	-1
8	-1	-1	-1	-1

3.1.3 Resolutions III and IV designs

There is the maximum number of variables denoted by K_{max} that can be accommodated in a resolution R design of $N=2^m$ runs. Corollaries 3.1, 3.2 and 3.3 stated below are used in the construction of the resolution III and IV designs (Draper and Lin, 1990).

Corollary 3.1

Let m be the number of basic variables in a design and the number of experimental runs be N . The maximum number of variables K_{max} that can be accommodated in a Resolution III design is 2^m-1 .

Corollary 3.2

Let m be the number of basic variables in a design and the number of experimental runs be N . The maximum number of variables K_{max} that can be accommodated in a resolution IV design is 2^{m-1} .

Corollary 3.3

Let m be the number of basic variables in a design and the number of experimental runs be N . A saturated design of resolution $R=2l$ can be obtained by folding over a saturated design of resolution $(2l-1)$ plus an **I** column.

3.1.3.1 Resolution III Design

A Fractional Factorial Design in which the main effects are not aliased with each other, but main effects are aliased with two factor interactions is said to be of resolution III and is used in screening a large number of factors to find the most important factor(s). With reference to Corollary 3.1, to create Resolution III design, additional factors are assigned to the generators. For example in a 2^{7-4} design, we let $D=AB, E=AC, F=BC$ and $G=ABC$. These designs are called saturated designs

and with 2^{m-p} runs, one can estimate $(2^{m-p}-1)$ main effects assuming all two-way and higher effects are negligible. In case of fewer factors, we reduce p and m by equal amounts. That is 2^{6-3}, 2^{5-2}, 2^{4-1}. In each case, one fewer generator is needed allowing us more flexibility in selecting the confounding. Therefore for $m=3$ factors, a Resolution III design will be such that $x_3=x_1 x_2$ and hence the defining relation is given by $I=x_1 x_2 x_3$.

3.1.3.2 Resolution IV Design

A Fractional Factorial Design in which no main effects are aliased with two-factor interactions, but two-factor interactions are aliased with each other is said to be of resolution IV and is used in screening a large number of factors to find the most important factor. Using Corollary 3.2,for $m=4$ factors, a Resolution IV design will be such that $x_4=x_1 x_2 x_3$ and hence the defining relation is given by $I=x_1 x_2 x_3 x_4$ denoted as 2_{IV}^{4-1} design.

Further using Corollary 3.3, this may also be done by first creating a resolution III design as explained in section 3.1.2.

3.1.4 Resolutions *III* and *IV*RotatableCCDs

In this thesis, the CCD is a resolution R central composite design with the levels of each factor coded to the usual $-1,+1$, augmented by the following points:

$$(\pm\alpha,0,\ldots,0),(0,\pm\alpha,\ldots,0)\wedge(0,0,\ldots,\pm\alpha) \quad . \tag{3.8}$$

Generally, the design matrix for a CCD experiment involving m factors is derived from a matrix d , containing the following two different parts corresponding to the two types of experimental runs:

1. Matrix R isobtained from the fractional factorial (resolution R) experiment.
2. Matrix E corresponds to the axial points, with $2m$ rows.

Thus d is a vertical concatenation given by:

$$d=\begin{bmatrix} R \\ E \end{bmatrix} \quad . \tag{3.9}$$

The value of α is selected according to therotatabilityrestrictions(1.5). To fit the second-degree Kroneckermodel(3.4), the expanded design matrix X and the information matrix $X^T X$, for a general CCD were used. The design matrix X is the horizontal concatenation of a column of $1's$ (intercept) and all products of elements of a pair of columns of d (3.9) and takes the form:

$$X=\left[1\, d\, d(1)^2 d(1)\times d(2)\ldots d(1)\times d(m)\, d(2)\times d(1)\ldots d(m-1)\times d(m)\ldots d(m)\times d(m-1)\, d(m)^2\right]$$

(3.10)

3.1.5 **Rotatable Second-Degree Moment Matrices**

A definition by Pukelsheim(1993) outlining the characteristics of rotatable moment matrices of the constructed designs is given.

Definition 3.2

Let M be a symmetric $\left(1+m+m^2\right)\left(1+m+m^2\right)$ matrix. Then M is a rotatable second-degree moment matrix on the experimental domain $T_{\sqrt{m}}$ if and only if for some:

$$\mu_2 \in [0,1] \wedge \mu_{22} \in \left[\frac{m}{m+2}\mu_2^2; \frac{m}{m+2}\mu_2\right],$$

Then

$$M = \begin{pmatrix} 1 & 0 & \mu_2\left(\vec{I}_m\right)' \\ 0 & \mu_2 I_m & 0 \\ \mu_2 \vec{I}_m & 0 & \mu_{22} F_m \end{pmatrix} \tag{3.11}$$

Where $F_m = I_m \otimes I_m + I_{m,m} + (vec\, I_m)\left(\vec{I}_m\right)'$

The moment matrix in (3.11) is attained by a design $\tau \in T$ if and only if τ has all moments of

$$\int_{\tau_{\sqrt{m}}} (e_i' x)^2 d\tau = \mu_2 \quad for \;\; all \;\; i \le m$$

$$\int_{\tau_{\sqrt{m}}} (e_i' x)^2 (x' e_j)^2 d\tau = \mu_{22} \quad for \;\; all \;\; i \ne j \le m$$

$$\int_{\tau_{\sqrt{m}}} (e_i' x)^4 d\tau = 3\mu_{22} \quad for \;\; all \;\; i \le m$$

, while all other moments up to order 4 vanish.

3.1.6 The Central Composite Design

The following theorem holds for second - degree complete classes of designs (Pukelsheim, 1993).

Theorem 3.1

For $w \in [0;1]$, let $\tau_w = (1-\alpha)\tau_0 + \alpha\,\tilde{\tau}_{\sqrt{m}}$ be the central composite design which places mass α on the cube-plus-star design $\tilde{\tau}_{\sqrt{m}}$ while putting weight $(1-w)$ into 0 (on the center point portion) , then the following results hold:

a) (Kiefer completeness) For every design $\tau \in T$, there is some $w \in [0;1]$ such that the central composite τ_w improves upon τ in the Kiefer ordering $M_2(\tau_w) \gg M_2(\tau)$ relative to the group Q_2 defined in (3.3).

b) (Q_2 invariant ϕ) Let ϕ be an orthogonally invariant information function on

$NND(1+m+m^2)$. Then for some $w \in \left[\frac{2}{m+4};1\right]$, the central composite design τ_w is $\phi - optimal$ for θ in T .

For a central composite design, the following relations are true:

$\mu_4 = 2^{m-p} + 2\alpha^4$ and $\mu_{22} = 2^{m-p}$.

And forrotatability:

$$\mu_4 = 3\mu_{22} \text{ giving } \alpha = 2^{\frac{m-p}{4}} = \sqrt[4]{F} \quad \text{where} \quad F = 2^{m-p} . \qquad (3.12)$$

Rotatability also includes non-singularity condition:

$$\frac{\mu_4}{(\mu_{22})^2} > \frac{m}{m+2} \quad .$$

(3.13)

The rotatable CCD ξ was formed by combining a fractional factorial design (cube portion ξ_F replicated n_c times) obtained from resolution R (R equals III orIV) for sample size $2^{m-p} n_c$, a star portion (ξ_s replicated n_s times) for sample size $2 m n_s$ plus a center point portion (ξ_0 replicated n_0 times). Thus $\xi = n_c \xi_F + n_s \xi_s + n_0 \xi_0$ has sample size $n = 2^{m-p} n_c + 2 m n_s + n_0$ where $n_c = 1$, $n_s = 1$ and $n_0 = 0$. Therefore

$$\xi = \xi_F + \xi_s \qquad (3.14)$$

such that the sample size is $n = 2^{m-p} + 2m$ and $p = 1$.

3.1.6.1 Resolution III Rotatable CCD Moment Matrix

Definition 3.3:

FromDefinition3.2**,** let $X' X$ be a symmetric $(1+m+m^2) \times (1+m+m^2)$ matrix, and consider the Euclidean unit vectors in R^m denoted by $e_{1,} e_2, \ldots, e_m$, then for $Resolution\, III$ and $m=3$

(a) $$X^T X = \begin{bmatrix} N & 0_{m,1}^T & (F+2\alpha^2)(\vec{I}_m)^T \\ 0_{m,1} & (F+2\alpha^2) I_m & F(E_{ijk})^T \\ (F+2\alpha^2)\vec{I}_m & F\, E_{ijk} & H_m \end{bmatrix} \qquad (3.15)$$

where:

F is the number of experimental runs in the fractional factorial portion,

I_m is an $m \times m$ identity matrix,

$0_{m,1}$ is an $m \times 1$ matrix whose elements are all zeros

$H_m = (F + 2\alpha^4) V_1 + F V_2$,

with

$V_1 = \sum_{i=1}^{m} E_{ii}$ and define $E_{ii} = (e_i e_i') \otimes (e_i e_i')$,

$V_2 = \sum_{i \neq j = 1}^{m} (E_{ij} + E_{ij'} + E_{ji})$ where $E_{ij} = (e_i e_i') \otimes (e_j e_j')$,

$E_{ij'} = (e_i e_j') \otimes (e_i e_j')$ and $E_{ji} = (e_i e_j') \otimes (e_j ')$,

$E_{ijk} = \sum_{i \neq j \neq k = 1}^{m} (e_i \otimes e_j) e_k'$.

The moment matrix is then given by:

$$M = \frac{X^T X}{N} \quad . \tag{3.16}$$

The kronecker products were obtained using R- software.

(b) If the CCD is constructed from a full factorial design, the only nonvanishing moments are:

$$\mu_2(\tau) = \frac{n_c}{n} 2^{m-p} + \frac{n_s}{n} 2\alpha^2 \quad , \quad \mu_{22}(\tau) = \frac{n_c}{n} 2^{m-p} \quad , \quad \mu_4(\tau) = \frac{n_c}{n} 2^{m-p} + \frac{n_s}{n} 2\alpha^4 \tag{3.17}$$

where the cube and the star portion are replicated n_c and n_s times respectively (Pukelsheim, 1998). and the condition for rotatability is

$$\mu_4 = 3\mu_{22} \tag{3.18}$$

3.1.6.2 Resolution $R > III$ Rotatable CCD Moment Matrix

Definition 3.4

From Definition3.2,let $X^T X$ be a symmetric $(1+m+m^2)\times(1+m+m^2)$ matrix, and consider the Euclidean unit vectors in R^m denoted by $e_{1,}e_2,\dots,e_m$ thenfor $R>III\wedge m\geq 4$,

$$X^T X=\begin{pmatrix} N & 0_{m,1}^T & (F+2\alpha^2)(\vec{I}_m)^T \\ 0_{m,1} & (F+2\alpha^2)I_m & 0_{m^2,m}^T \\ (F+2\alpha^2)\vec{I}_m & 0_{m^2,m} & H_m \end{pmatrix} \tag{3.19}$$

Where

F is the number of experimental runs in the cube portion obtained through resolution R ,

I_m is an $m\times m$ identity matrix,

$0_{m,1}$ is an $m\times 1$ null vector while $0_{m^2,m}$ is an $m^2\times m$ null matrix

$H_m=(F+2\alpha^4)V_1+F V_2$,

$V_1=\sum_{i=1}^{m} E_{ii}$ and $V_2=\sum_{i\neq j=1}^{m}(E_{ij}+E_{ij}+E_{ji})+\sum_{i\neq j\neq k\neq l=1}^{m} E_{ijkl}$

Define

$E_{ii}=(e_i e_i^{'})\otimes(e_i e_i^{'})$, $E_{ij}=(e_i e_i^{'})\otimes(e_j e_j^{'})$, $E_l=(e_i e_j^{'})\otimes(e_l e_k^{'})$

$E_{ji}=(e_i e_j^{'})\otimes(e_j e_i^{'})$, $E_{ijkl}=(e_i e_j^{'})\otimes(e_k e_l^{'})$

Then the moment matrix is given by:

$$M=\frac{X^T X}{N} \quad .$$

The kronecker products were obtained using R- software.

3.1.7 **Subsystem of Interest of the Mean Parameters**

The parameter system of the Kronecker model contains a lot of repeated terms making it rank deficient hence not of all the parameters can be estimated efficiently. There are cases where the experimenter is only interested with a few parameters say s out of the total k components. Parameter subsystems could be linear functions or nonlinear functions of the full parameter vector.

Consider a subset s components out of the total k components, where $s \leq k$ and the linear parameter subsystem of the form $K^{'}\theta,$ where parameter vector $\theta \in R^{k}$ for some $k \times s$ matrix $K \in R^{k \times (m+1)}$ is assumed to have full column rank, K is called the coefficient matrix of the parameter subsystem $K^{'}\theta$.

Let the Euclidean unit vectors in R^{m} be denoted by $e_{1,}e_{2},\ldots,e_{m}$ and the sets $e_{ii}=e_i \otimes e_i, e_{ij}=e_i \otimes e_j, for i<j<k, i, j, k=\{1,2,\ldots,m\}.$

Then the $k \times s$ coefficient matrix:

$$\begin{matrix} m \\ (¿¿2+m+1) \times s \end{matrix}$$

$$K=\begin{pmatrix} 1 & 0^{T}_{m,1} & 0^{T}_{m^2,1} \\ 0_{m,1} & 0_{m,m} & 0_{m,s-(m+1)} \\ 0_{m^2,1} & K_1 & K_2 \end{pmatrix} \in R^{¿} \quad \text{for} \quad m \geq 3 \qquad (3.20)$$

such that

$0_{u,v}$ is a $u \times v$ matrix of zeros

$K_1=\sum_{i=1}^{m} e_{ii}e_{i}^{'}$, an $(m^2 \times m)$ matrix

and

$$e$$
$$(¿¿ij+e_{ji})E_r^{'}$$
$$\sum_{\substack{i,j=1\\ i<j}}^{m} ¿$$
$$¿$$
$$for\, m=3$$
$$¿$$
$$e$$
$$(¿¿ij+e_{ji}+e_{kl}+e_{lk})E_r^{'} \qquad (3.21)$$
$$\sum_{\substack{i,j=1\\ i<j\\ k<l}}^{m} ¿$$
$$¿$$
$$¿$$
$$¿$$
$$\frac{1}{2}¿$$
$$K_2=¿$$

where

K_2 is an $m^2 \times (s-(m+1))$ matrix.

and $r=1,\ldots,(s-(m+1))$, s number of parameters in the subsystem of interest.

Thus

$$\left\{\begin{matrix} \theta_0 \\ \theta_{ii}\, for\, 1 \le i \le m \\ \frac{1}{2}\{(\theta_{ij}+\theta_{ji})\}\, for i=1,\ldots,m \\ i<j\le m \end{matrix}\right\} for\, m=3\, factors$$
$$¿$$
$$¿$$
$$\theta_0 \qquad (3.22)$$
$$\theta_{ii}\, for\, 1 \le i \le m$$
$$\frac{1}{4}\{(\theta_{ij}+\theta_{ji}+\theta_{kl}+\theta_{lk})\}\, for i,j,k,l=1,\ldots,m\, for\, m=4\, factors$$
$$i \ne j \ne k \ne l$$
$$i<j,$$
$$¿$$
$$\{¿$$
$$K^T(\theta)=¿$$

Next is the definition of the information matrix as defined by Pukelsheim (1993) and cited by Cherutich et.al., (2012).

Definition 3.5

The information matrix for $K^T\theta$ with $k\times s$ coefficient matrix K of column rank s, is defined to be $C_k(M)$ when the mapping $C_k: NND(k)\rightarrow sym(s)$ is given by all $A\in NND(k)$ with minimum taken relative to the loewner ordering over all left inverses L of K where M is the moment matrix (3.4). The amount of information which the design ξ contains on the parameter subsystem $K^T\theta$ is captured by the information matrix (1.4) now defined as,

$$\begin{array}{c} m \\ S\times(¿¿2+m+1) \\ C_k(\xi)=min\{LM(\xi)L^T\}; L\in R^{¿} \end{array}$$

and this is the precision matrix of the best linear unbiased estimator for $K^T\theta$ under design τ (Pukelsheim, 1993). The information matrices for $K^T\theta$ are linear transformations of moment matrices and takes the following form:

$$C_k(M(\xi))=(K^TK)^{-1}K^TM(\xi)K(K^TK)^{-1}\in NND(s) \quad .$$

Further defining every left inverse L of K as

$$L=(K^TK)^{-1}K^T \qquad (3.23)$$

then

$$C_k(M(\xi))=LM(\xi)L^T \quad . \qquad (3.24)$$

3.2 Weighted Central Composite Designs

The derived basic 2^{m-p} designs and the corresponding rotatable CCDs (ξ) design matrices X for three and four factors were then used to obtain the respective moment and information matrices based on the parameter subsystem of interest on the second-degree Kronecker model.

The CCD was separated into a factorial (cube) block and an axial (star) point block. A convex combination:

$$\xi_{WCCD}(w)=\sum_{i=1}^{q} w_i \xi_i \quad \text{with} \quad w=(w_1, w_2, \ldots, w_q)^T \in T_q$$

is called a weighted central composite design with weight vector $\sum_{i=1}^{q} w_i = 1$.

From the linearity of the information matrix mapping C_K (definition 3.3), for every $w \in T_q$

$$C_K(M(\xi(w)))=\sum_{i=1}^{q} w_i C_K(M(\xi_i)) \, i=1,2 \quad . \qquad (3.25)$$

The information matrices $C_K(M(\xi_i))$ are obtained by using equation 3.24. The rotatable WCCD ($\alpha^4=2^{m-p}$¿ was expressed as:

$$\xi_{WCCD}=w_1 \xi_F + w_2 \xi_s \qquad (3.26)$$

where

a) $w_i, i=1,2$ satisfies the conditions $\sum_{i=1}^{2} w_i = 1$ and $w_1, w_2 \geq 0$ are different masses assigned to each of the two elementary designs ξ_F and ξ_s respectively.

b) ξ_F is the design with support points n_F determined by combining the first order design obtained from half- fraction factorial design (either Resolution III or IV) and ξ_s is the design with $2m$ distinct support points (the star portion) and thus the total support points is $n = n_F + 2m$.

From moment matrices to Designs, the General Equivalent Theorem (GET) concentrates on moment matrices and consequently the information matrices. However the statistical interest is in the designs themselves. The aim is at necessary conditions that aid in identifying the support points and the weights of optimal designs. The GETgiven in Pulkelsheim (1993) and as proved by Kinyanjui (2007)is adapted to in this studyto derive D-, A- and E-optimal rotatable Weighted Central Composite Designs (ξ_{WCCD}) for the three and four factors. The relations were used to compute the weights w_1 and w_2 using both the R and wxMaximasoftwares.

Theorem 3.2: Equivalence Theorem for D- and A- Optimality

Consider a matrix mean $\varphi❑_p$ with parameter p finite, $p \in ¿$. Let $w_i \in T_m$ be the weight vector of a weighted central composite design $\xi(w)$ which is feasible for $K^T\theta$. Further let $M(\xi) \in M(\Xi)$ be a competing moment matrix that is feasible for $K^T\theta$, with information matrix $C = C_K(M(\xi))$. Then $M(\xi)$ is $\varphi❑_p - ¿$ optimal for $K^T\theta$ in M and consequently $\xi(w)$ is $\varphi❑_p - ¿$ optimal for $K^T\theta$ in T if and only if

$$trace\, C_i C^{p-1} \begin{cases} ¿\, trace\, C^p\, for\, i = 1, 2 \\ ¿\, trace\, C^p\, otherwise \end{cases}$$

$$with\; p = 0, for\; D - optimality \wedge p = -1\, for\; A - optimality \qquad (3.27)$$

which results in

$$D-optimality, p=0 \quad \text{and} \quad trace\, C_i C^{-1} = trace\, C^0 = trace\, I_s \quad , \tag{3.28}$$

and

$$A-optimality, p=-1 \quad \text{and} \quad trace\, C_i C^{-2} = trace\, C^{-1} \qquad .(\quad i=1,2¿ \tag{3.29}$$

Theorem 3.3: Equivalence Theorem for E-Optimality

Let $M(\xi) \in M(\Xi)$ be a moment matrix that is feasible for $K^T \theta$, with information matrix $C = C_K(M(\xi))$. Then $M(\xi)$ is $\varphi \square_{-\infty} -¿$ optimal for $K^T \theta$ in M if and only if there exists a nonnegative definite $s \times s$ matrix E with trace equal to 1 and a generalized inverse G of M that satisfies the normality inequality

$$traceAGKCEC\, K^T G^T \leq \lambda_{min}(C)\, for\ all\ A \in M \quad .$$

The CCD $\xi(w)$ is E-optimal for $K^T \theta$ in T if and only if there is a matrix

$E \in sym(s, H) \cap NND(s)$ satisfying $traceE = 1$

and

$$trace\, C_i\, E \begin{cases} ¿\, \lambda_{min}(C)\, for\ all\ i \in \delta(\alpha) \\ ¿\, \lambda_{min}(C)\, otherwise \end{cases} \tag{3.30}$$

where $\lambda_{min}(C)$ is the smallest eigenvalue of C, the information matrix. If the smallest eigenvalue for C has multiplicity 1, then the only choice for matrix E is

$$E = \frac{z^T z}{\|z\|^2} \tag{3.31}$$

where $z \in R^s$ is the eigenvector corresponding to the smallest eigenvalue of the information matrix C.

Theorem 3.4: Equivalence Theorem for I- Optimality (GoosandSyafitri (2014))

Assuming that all runs of the experiment based on the simplex - centroid design with weights $w_1, w_2, \ldots, w_q$ are independent and that the responses have equal variance (which is assumed to be one, without loss of generality), the best linear unbiased estimator of β is the ordinary least squares estimator. The corresponding information matrix is:

$$C = X^T \wedge X \tag{3.32}$$

with $X = \left[f(x_1), f(x_2), \ldots, f(x_q) \right]^T$ the $q \times s$ model matrix (in this case comprising of regression vectors in the parameter subsystem of interest) corresponding to the *s* points of the second kronecker model central composite design and $\wedge$ is a diagonal matrix such that

$$\wedge = \begin{bmatrix} \frac{w_1}{F} I_F & 0 \\ 0 & \frac{w_2}{2m} I_{2m} \end{bmatrix}$$

(3.33)

where I_F is an $F \times F$ identity matrix, F is the number of experimental runs in the fractional factorial portion, I_{2m} is a $2m \times 2m$ identity matrix, $2m$ is the number of runs in the star portion and m is the number of factors.

Atkinson et al., (2007) explains that a continuous design with information matrix M is I- optimal if and only if

$$f^T(x)\,C^{-1}L\,C^{-1}f(x)\le tr\left(C^{-1}L\right) \qquad (3.34)$$

for each point x in the experimental region χ. The general equivalence theorem states that for a design to be $I-optimal$, the inequality (3.34) when evaluated at each of the design points becomes

$$f^T(x)\,C^{-1}L\,C^{-1}f(x)=tr\left(C^{-1}L\right) \qquad (3.35)$$

3.2.1 **Generalized WCCD**

A generalized form ofoptimalrotatableWCCDs for m factors was then obtained using the derived optimalrotatableresolution III and IV designs.

3.3 Optimality Criteria and Efficiency

Optimal designs are usually obtained by optimizing functions of the information matrix (3.24).

3.3.1 **Classical Optimality Criteria**

The purpose of any optimality criterion is to measure the largeness of a non-negative definite $s\times s$ information matrix. The optimality criteria used in this thesisis specified as those in the family of matrix means $\varnothing_p \, for\ p=-\infty,-1,0,1$. The D-optimality criterion maximizes the determinant of the information matrix or equivalently, minimizes the determinant of the inverse of the information matrix. A-optimality criterion seeks to minimize the average variance of the parameter estimates while the E-optimality criterion seeks to maximize the minimum eigenvalue of the information matrix.

This family is discussed in detail by Pukelsheim (1993) and cited by El-Monsef et.al.2009) and is defined as follows:

$$\varnothing_p(C) = ¿ \begin{cases} (\det C)^{\frac{1}{s}} \text{ for } p=0 \\ \left(\frac{1}{s} \operatorname{trace} C^{-1}\right)^{-1} \text{ for } p=-1 \\ \lambda_{min}(C) \text{ for } p=-\infty \end{cases} \quad (3.36)$$

for D-, A-, and E-optimality respectively.

For a CCD using a 2^{m-p} Resolution V fractional factorial design and n_c center runs, the determinant can be written as:

$$\left|X^T X\right| = \left(2^{m-p} + 2\alpha^2\right)^m \left(2\alpha^4\right)^{m-1} \left(2^{m-p}\right)^{\binom{m}{2}} \left[2^{m-p+1}\left(\alpha^2 - m\right)^2 + 2n_c\alpha^4 + mn_c 2^{m-p}\right] . \quad (3.37)$$

This is obtained by partitioning

$$X^T X = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

and then reducing $\left|X' X\right|$ by using the identity

$$\begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} = \left|A_{11}\right| . \left|A_{22} - A_{21} A_{11}^{-1} A_{12}\right| . \quad (3.38)$$

In a traditional CCD, A_{11} is of the form

$$\begin{pmatrix} A & B1' \\ B1 & (G-D)I + DJ \end{pmatrix}$$

Where

$$A = N = 2^{m-p} + 2m + n_c \; , \qquad B = 2^{m-p} + 2\alpha^2 \; ,$$

$$G = 2^{m-p} \; , \qquad D = 2^{m-p} + 2\alpha^4 . \quad (3.39)$$

3.3.2 I -optimality

$I-optimality$ seeks designs that minimize the averageprediction variance over the experimental region χ. According to Goos and Syafitri, (2014)by definition:

$$Average\ variance = \frac{\int_{\chi} f(x) M^{-1} f^{T}(x) dx}{\int_{\chi} dx} = \frac{\int f(x) \left(X^{T} X \right)^{-1} f^{T}(x) dx}{\int dx} \tag{3.40}$$

and can be calculated exactly for simplex shaped experimental regions as

$$\frac{1}{\Gamma q}\left[tr \left(X^{T} X \right)^{-1} \underbrace{\left[\int f(x) f^{T}(x) dx \right]}_{momentmatrix} \right]$$

. The numerator in (3.40) may be expressed as

$$\int_{\chi} f(x) M^{-1} f^{T}(x) dx = tr \left[M^{-1} \int_{\chi} f(x) f^{T}(x) dx \right]$$

Define $B=¿$

Then

$$I-optimality=¿ \frac{tr\left[M^{-1} B \right]}{\int_{\chi} dx}$$

(3.41)

Assuming that the experimental region χ is the full $m-1$ -dimensional simplex s_{q-1} , the elements of B can be obtained using the formula:

$$B = \int_{s_{q-1}} x_1^{p_1} x_2^{p2} \ldots x_m^{p_m} dx_1 dx_2 \ldots dx_m = \frac{\prod_{i=1}^{m} \Gamma(p_i + 1)}{\Gamma\left(m + \sum_{i=1}^{m} p_i\right)} = \frac{\prod_{i=1}^{m} p_i !}{\left(m - 1 + \sum_{i=1}^{m} p_i \right)!}$$

where p is the power of the factors and m is the number of factors.And

$$\int_{\chi} dx = \int_{S_{m-1}} dx = \frac{1}{\Gamma m}$$

Define

$L = \Gamma(m) \times B$ where $\Gamma(m) = (m-1)!$

(3.42)

Substituting (3.42) in (3.41) gives

$$I - optimality = tr[M^{-1}L] \tag{3.43}$$

3.3.3 **Efficiency**

Efficiency tests the goodness of a design. Let ξ and $\xi^{¿}$ be the full rotatable CCD and the derived optimal rotatable WCCD respectively. Further let ϕ_p be the optimality criteria(3.36) used to obtain the corresponding optimal values $\overset{\phi}{\underset{¿}{V(¿¿p(\xi^{¿}))}}$ and $\overset{\phi}{\underset{¿}{V(¿¿p(\xi))}}$ for D-, A- and E-optimum designs, then generally the ϕ -efficiency of design $\xi^{¿}$ relative to design ξ is given by

$$\phi \quad \phi \quad \frac{V(¿¿p(\xi))}{V(¿¿p(\xi^{¿}))} \quad ¿ \quad eff_{\phi_p}(\xi^{¿}) = ¿ \tag{3.44}$$

where $\overset{\phi}{\underset{\text{¿}}{V(\text{¿¿}\,p(\xi^{\text{¿}}))}}$ is the respective optimal value of the derived optimal rotatable WCCD and $\overset{\phi}{\underset{\text{¿}}{V(\text{¿¿}\,p(\xi))}}$ is the respective optimal value of the full rotatable CCD

Specifically

1) $\begin{array}{c}\phi\\ \phi\\ V(\text{¿¿}\,p(\xi^{\text{¿}}))\\ \underline{V(\text{¿¿}\,p(\xi))}\\ \text{¿}\\ D_{eff_{\phi_p}}(\xi^{\text{¿}})=\text{¿}\end{array}$ where $\xi^{\text{¿}}$ is $D-optimal$ design. (3.45)

A D-efficiency near one indicates that Design $\xi^{\text{¿}}$ is better than Design ξ in termsof the D-optimality criterion (Goos and Bradley, 2012).

2) $\begin{array}{c}\phi\\ \phi\\ V(\text{¿¿}\,p(\xi))\\ \underline{V(\text{¿¿}\,p(\xi^{\text{¿}}))}\\ \text{¿}\\ A_{eff_{\phi_p}}(\xi^{\text{¿}})=\text{¿}\end{array}$ where $\xi^{\text{¿}}$ is $A-optimal$. (3.46)

3) $\begin{array}{c}\phi\\ \phi\\ V(\text{¿¿}\,p(\xi^{\text{¿}}))\\ \underline{V(\text{¿¿}\,p(\xi))}\\ \text{¿}\\ E_{eff_{\phi_p}}(\xi^{\text{¿}})=\text{¿}\end{array}$ where $\xi^{\text{¿}}$ is $E-optimal$. (3.47)

Further using $I-optimality$ given in (3.43), $I-efficiency$ of a design ξ is defined as

4) $$I(\xi)=\frac{tr\left[M^{-1}L(\xi^{¿})\right]}{tr\left[M^{-1}L(\xi)\right]}$$

(3.48)

where $\xi^{¿}$ is $I-optimal$ (El-Monsef et.al., 2009).

AnI-efficiency which is less than one indicates that Design $\xi^{¿}$ is better than Design ξ in terms of the average prediction variance (Goos and Bradley, 2012).

Optimal values and weights for the weighted central composite designs were numerically obtained using both R and wxMaxima softwares.

3.4 Illustration

The theoretical results were illustrated using experimental data obtained from Journal of Statistical Education Data Archivethrough an application on optimization of a four factor CCD to determine effects on whiteness of cotton.

The following is a description of the data:

Source: P.K. Lavric, F. Kovac, P.F. Tavcer, P. Hauser, D. Hinks (2007).

"Enhanced PAA Bleaching of Cotton by Incorporating a Cationic Bleach Activator,"

Coloration Technology,**123** (4): 230-236.

Description: 4-Factor Design to determine effects on whiteness of cotton.

Factors: Temperature (40-80C)

Bleach Activator - TBBC (0-3 %owf)

pH (6.5-8.5)

Peracetic Acid - PAA (5-25ml/l)

Response: Whiteness Index

A full quadratic and a reduced quadratic model namely the second-order Kroneckermodelusing Resolution IV design were fitted and astationarityand matrix analysis was carried out to obtain a mathematical solution for the location of the Stationary Point. The efficiency of the designwas determined and basic diagnostic graphs and contour surface plots were plotted for this data.

CHAPTER FOUR

RESULTS AND DISCUSSION

4.0 Introduction

This chapter deals with the interpretation and explanation of the findings of this study with regard to the stated research objectives (1.2.2). These results are presented in four sections. In section 4.1, rotatable designs through resolutions III and IV for three and fourfactors based on the Central Composite Designsare constructed. Their moments and the corresponding information matrices for the parameter subsystem of interest are derived. These results are then used to derive optimal rotatable Weighted Central Composite Designsbased on the D-, A- , E- and I-optimality criteria for three and four factors in section 4.2. The moment, coefficient and information matrices for m -factors are also obtained. Further generalization of the D- optimal rotatable WCCD is given. In section 4.3, WCCDs D-, A-, E- and I- optimal values and their corresponding efficiencies are determined and a general form of D- and I- optimal values is given. Section 4.4 deals with data analysis where optimization of whiteness of cotton is done using four factor CCD.

4.1 Resolutions *III* and *IV* Rotatable CCDs

In this section, methods outlined in section 3.1were used to obtain the results.

4.1.1 Resolutions *III* Rotatable CCDs

For $m=3$, a full 2^{3-1} factorial design is written down, then the 3^{rd} factor is added by identifying its plus and minus levels with the signs of

$x_3 = x_1, \ldots, x_{3-1}$. Therefore a Resolution III design will be such that $x_3 = x_1 x_2$ and hence the defining relation is given by $I = x_1 x_2 x_3$. This results in:

Table 4.1. Resolution III Design

Run	Factors $x_1 x_2 x_3 = x_1 x_2$		
1	-1	-1	+1
2	+1	-1	-1
3	-1	+1	-1
4	+1	+1	+1

From 3.9 and using Table 4.1, matrix d for $m=3$ was given by:

$$d = \begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ -\alpha & 0 & 0 \\ \alpha & 0 & 0 \\ 0 & -\alpha & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & -\alpha \\ 0 & 0 & \alpha \end{bmatrix} \quad \text{where} \quad \alpha = 1.414$$

Then using (3.10), the design matrix is

$$X = \begin{bmatrix} 1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1.414 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1.414 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1.414 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1.414 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1.414 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 1 & 0 & 0 & 1.414 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} \qquad (4.1)$$

4.1.1.1 Three Factors Rotatable CCD Moment Matrix

Let $X^T X$ be a symmetric $(1+m+m^2)\times(1+m+m^2)$ for $m=3$ then equation 3.15 results in:

$$X^T X=\begin{pmatrix} 10 & 0_{3,1}^T & (4+2\alpha^2)(\vec{I}_3)^T \\ 0_{3,1} & (4+2\alpha^2) I_3 & 4 E_{ijk}^T \\ (4+2\alpha^2)\vec{I}_3 & 4 E_{ijk} & H_3 \end{pmatrix} \qquad (4.2)$$

Where

$H_3=(F+2\alpha^4)V_1+F V_2$,

and

$$E_{ijk}=\sum_{i\neq j\neq k=1}^{m}(e_i\otimes e_j)e_k' \quad . \qquad (4.3)$$

The matrix $0_{3,1}=\begin{bmatrix}0\\0\\0\end{bmatrix}$

F is the number of experimental runs in the fractional factorial portion and the value of α satisfies rotatability condition as stated in (3.12). Thus for $m=3$,

$\alpha=1.4142$,

$\vec{I}_3=[1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1]'$ and $I_3=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}$

Thus

$$(4+2\alpha^2)\vec{I}_3=[8 \quad 0 \quad 0 \quad 0 \quad 8 \quad 0 \quad 0 \quad 0 \quad 8]' \quad \text{and} \quad (4+2\alpha^2)I_3=\begin{bmatrix}8&0&0\\0&8&0\\0&0&8\end{bmatrix} \qquad (4.4)$$

Define E_i by considering the pairs of (i, j) as follows:

$$E_1 = e_1 e_1^{'} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \ , \ E_2 = e_2 e_2^{'} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \ ,$$

$$E_3 = e_3 e_3^{'} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} E_4 = e_1 e_2^{'} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \ , \ E_5 = e_1 e_3^{'} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \ ,$$

$$E_6 = e_2 e_1^{'} = (e_1 e_2^{'})' \ , \qquad E_8 = e_3 e_1^{'} = (e_1 e_3^{'})' \ , \quad E_9 = e_3 e_2^{'} = (e_2 e_3^{'})' \ ,$$

$$E_7 = e_2 e_3^{'} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \ , \quad E_{ii} = E_i \otimes E_i \quad \text{and} \quad E_{ij} = E_i \otimes E_j . \ , \text{ and } \ E_{ij} \ ,$$

$E_{ij^{'}}$ and E_{ji} are defined in definition 3.4.

Thus

$$V_1 = \sum_{i=1}^{3} E_{ii} = E_{11} + E_{22} + E_{33} = E_1 \otimes E_1 + E_2 \otimes E_2 + E_3 \otimes E_3$$

$$¿ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \qquad (4.5)$$

and

$$V_2=\sum_{i\neq j=1}^{3}\left(E_{ij}+E_{ij'}+E_{ji}\right)$$

$$¿\,E_1\otimes E_2+E_1\otimes E_3+E_2\otimes E_1+E_2\otimes E_3+E_3\otimes E_1+E_3\otimes E_2+E_4\otimes E_4+E_5\otimes E_5+E_6\otimes E_6+E_7\otimes E_7+E_8\otimes E_8$$

$$¿\begin{bmatrix}1&0&0&0&1&0&0&0&1\\0&1&0&1&0&0&0&0&0\\0&0&1&0&0&0&1&0&0\\0&1&0&1&0&0&0&0&0\\1&0&0&0&0&0&0&0&1\\0&0&0&0&0&1&0&1&0\\0&0&1&0&0&0&1&0&0\\0&0&0&0&0&1&0&1&0\\1&0&0&0&1&0&0&0&1\end{bmatrix} \quad (4.6)$$

Using results(4.5) and (4.6)in (4.3), the following are obtained

$$H_3=\begin{bmatrix}12&0&0&0&4&0&0&0&4\\0&4&0&4&0&0&0&0&0\\0&0&4&0&0&0&4&0&0\\0&4&0&4&0&0&0&0&0\\4&0&0&0&8&0&0&0&4\\0&0&0&0&0&4&0&4&0\\0&0&4&0&0&0&4&0&0\\0&0&0&0&0&4&0&4&0\\4&0&0&0&4&0&0&0&12\end{bmatrix}, \quad (4.7)$$

and

$$E_{ijk}=\begin{bmatrix}0&0&0\\0&0&1\\0&1&0\\0&0&1\\0&0&0\\1&0&0\\0&1&0\\1&0&0\\0&0&0\end{bmatrix}=E_{123} \quad \text{, for} \quad m=3 \quad (4.8)$$

Then by using (4.4), (4.7) and (4.8) in (4.2), the moment matrix corresponding to a CCD whose cube portion is constructed through Resolution III is obtained as;

$$\frac{X'X}{10}=\begin{bmatrix} 1 & 0'_{3,1} & 0.8\left(\vec{I}_3\right)' \\ 0_{3,1} & 0.8I_3 & 0.4\left(E_{123}\right)' \\ 0.8\vec{I}_3 & 0.4E_{123} & H_3 \end{bmatrix} \qquad (4.9)$$

In addition to the moments given in (3.17) which are nonvanishing, if a CCD is constructed through Resolution III, the other nonvanishing moment is $\mu_{111}(\tau)$ which is equal to $\mu_{22}(\tau)$.

Rotatability condition is satisfied since:

$\mu_4=3\mu_{22}=3\times 0.4=1.2$.

4.1.1.2 Three Factors Rotatable CCD Information Matrix

The following lemma is proved:

Lemma 4.1

The K -matrix for $m=3$ factors is given by

$$K=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

(4.10)

Proof:

From (3.21), for $m=3$

$$K_1 = e_{11} e_1^{'} + e_{22} e_2^{'} + e_{33} e_3^{'}$$

and

e
¿
e
e
$(¿¿23 + e_{32}) e_3^{'}$
$(¿¿13 + e_{31}) e_2^{'} + ¿$. (4.11)
$(¿12 + e_{21}¿) e_1^{'} + ¿$
¿
$K_2 = \frac{1}{2}$ ¿

Define

$$e_{ij} = e_i \otimes e_j \quad , \quad i, j = 1,2,3 \quad \text{where} \quad e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad , \quad e_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \text{and} \quad e_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Substituting these productsin(4.11), the following are obtained

$$K_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad K_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0.5 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0.5 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \\ 0 & 0 & 0 \end{bmatrix} .$$

Hence substituting this in (3.20),matrix K is obtained.

Then using (4.10) in (3.23) gives::

$$L=\begin{bmatrix}1&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&1&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&1&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&1\\0&0&0&0&0&1&0&1&0&0&0&0&0\\0&0&0&0&0&0&1&0&0&0&1&0&0\\0&0&0&0&0&0&0&0&0&1&0&1&0\end{bmatrix} \qquad (4.12)$$

Substituting (4.9) and (4.12) in(3.24), information matrix for three factors full CCD is obtained as:

$$C_K(M(\xi))=\begin{bmatrix}1 & 0.81_3 & 0_{3,1}^T\\ 0.81_3 & 1.2I_3+0.4\sum_{i\neq j=1}^{3}e_ie_j^{'} & 0_{3,3}\\ 0_{3,1} & 0_{3,3} & 1.6I_3\end{bmatrix} \qquad (4.13)$$

where $0_{3.1}$ is an 3×1 matrix and $0_{3,3}$ is an 3×3 matrix of zeros.

4.1.2 Resolutions IV Rotatable CCD

For $m=4$, a full 2^{4-1} factorial design is written down, then the 4^{th} factor is added by identifying its plus and minus levels with the signs of $x_4=x_1,\ldots,x_{4-1}$. Therefore a Resolution IV design will be such that $x_4=x_1x_2x_3$ and hence the defining relation is given by $I=x_1x_2x_3x_4$. This results in:

Table 4.2. Resolution IV Design

Run	Factors $x_1x_2x_3x_4=x_1x_2x_3$			
1	-1	-1	-1	-1
2	+1	-1	-1	+1
3	-1	+1	-1	+1
4	+1	+1	-1	-1
5	-1	-1	+1	+1
6	+1	-1	+1	-1
7	-1	+1	+1	-1
8	+1	+1	+1	+1

From 3.9 and using Table 4.2, matrix d for $m=4$ is obtained as

$$d=\begin{bmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ -\alpha & 0 & 0 & 0 \\ \alpha & 0 & 0 & 0 \\ 0 & -\alpha & 0 & 0 \\ 0 & \alpha & 0 & 0 \\ 0 & 0 & -\alpha & 0 \\ 0 & 0 & \alpha & 0 \\ 0 & 0 & 0 & -\alpha \\ 0 & 0 & 0 & \alpha \end{bmatrix},$$

Then using (3.10), the design matrix is

$$X=\left[\begin{array}{ccccccccccccccccccc}
1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 \\
1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 \\
1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 \\
1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\
1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -\alpha & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & \alpha & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 \\
1 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right.$$

Where $\alpha=1.6818$ (4.14)

4.1.2.1 Four Factors Rotatable CCD Moment Matrix

Let $X^T X$ be a symmetric $\left(1+m+m^2\right)\times\left(1+m+m^2\right)$ matrix. For $m=4$ equation (3.19) results in:

$$X^T X=\begin{pmatrix} N & 0_{4,1}^T & \left(F+2\alpha^2\right)\left(\vec{I}_4\right)^T \\ 0_{4,1} & \left(F+2\alpha^2\right)I_4 & 0_{16,4}^T \\ \left(F+2\alpha^2\right)\vec{I}_4 & 0_{16,4} & H_4 \end{pmatrix} \quad (4.15)$$

where

$N=16, F=8$, $\alpha=1.6818$,

$0_{4,1}$ is an 4×1 null vector and $0_{4^2,4}$ is an $4^2\times 4$ null matrix,

I_4 is an 4×4 identity matrix such that:

$$\left(F+2\alpha^2\right)I_4=\begin{bmatrix} 13.66 & 0 & 0 & 0 \\ 0 & 13.66 & 0 & 0 \\ 0 & 0 & 13.66 & 0 \\ 0 & 0 & 0 & 13.66 \end{bmatrix}$$

and

$\left(F+2\alpha^2\right)\left(\vec{I}_4\right)^T=13.66\left(\vec{I}_4\right)^T$ for

$$\vec{I}_4=\left[1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1\right]^T \quad (4.16)$$

$F+2\alpha^4=24$ such that

$$H_4=24V_1+8V_2 \quad (4.17)$$

Next define E_i by considering the pairs of (i, j) as follows

$E_1=e_1e_1^{'}$, $E_2=e_2e_2^{'}$, $E_3=e_3e_3^{'}$, $E_4=e_4e_4^{'}$, $E_5=e_1e_2^{'}$, $E_6=e_1e_3^{'}$,

$E_7=e_1e_4^{'}$, $E_8=e_2e_1^{'}$, $E_9=e_2e_3^{'}$, $E_{10}=e_2e_4^{'}$, $E_{11}=e_3e_1^{'}$,

$E_{12}=e_3 e_2^{'}$, $E_{13}=e_3 e_4^{'}$, $E_{14}=e_4 e_1^{'}$, $E_{15}=e_4 e_2^{'}$, $E_{16}=e_4 e_3^{'}$,

$E_{ii}=E_i \otimes E_i$, $E_{ij}=E_i \otimes E_j$

Thus

$$V_1=\sum_{i=1}^{4} E_{ii}=E_{11}+E_{22}+E_{33}+E_{44}=E_1 \otimes E_1+E_2 \otimes E_2+E_3 \otimes E_3+E_4 \otimes E_4$$

$$V_1=\begin{bmatrix}
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1
\end{bmatrix} \tag{4.18}$$

and

$$V_2=\sum_{i\neq j=1}^{4}\left(E_{ij}+E_{ij^{'}}+E_{ji}\right)+\sum_{i\neq j\neq k\neq l=1}^{4} E_{ijkl}$$

for $E_{ij}=\left(e_i e_i^{'}\right)\otimes\left(e_j e_j^{'}\right)$, $E_{lj^{'}}=\left(e_i e_j^{'}\right)\otimes\left(e_l e_j^{'}\right)$, $E_{ji}=\left(e_i e_j^{'}\right)\otimes\left(e_j e_i^{'}\right)$,

$E_{ijk}=\left(e_i e_j^{'}\right)\otimes\left(e_i e_k^{'}\right)$, $E_{ijkl}=\left(e_i e_j^{'}\right)\otimes\left(e_k e_l^{'}\right)$.

Thisresultsin

$$V_2 = \begin{bmatrix} 1&0&0&0&0&1&0&0&0&0&1&0&0&0&0&1 \\ 0&1&0&0&1&0&0&0&0&0&0&1&0&0&1&0 \\ 0&0&1&0&0&0&0&1&1&0&0&0&0&1&0&0 \\ 0&0&0&1&0&0&1&0&0&1&0&0&1&0&0&0 \\ 0&1&0&0&1&0&0&0&0&0&0&1&0&0&1&0 \\ 1&0&0&0&0&1&0&0&0&0&1&0&0&0&0&1 \\ 0&0&0&1&0&0&1&0&0&1&0&0&1&0&0&0 \\ 0&0&1&0&0&0&0&1&1&0&0&0&0&1&0&0 \\ 0&0&1&0&0&0&0&1&1&0&0&0&0&1&0&0 \\ 0&0&0&1&0&0&1&0&0&1&0&0&1&0&0&0 \\ 1&0&0&0&0&1&0&0&0&0&1&0&0&0&0&1 \\ 0&1&0&0&1&0&0&0&0&0&0&1&0&0&1&0 \\ 0&0&0&1&0&0&1&0&0&1&0&0&1&0&0&0 \\ 0&0&1&0&0&0&0&1&1&0&0&0&0&1&0&0 \\ 0&1&0&0&1&0&0&0&0&0&0&1&0&0&1&0 \\ 1&0&0&0&0&1&0&0&0&0&1&0&0&0&0&1 \end{bmatrix} \quad (4.19)$$

Substituting (4.18) and (4.19) in (4.17), the following is obtained

$$H_4 = \begin{bmatrix} 24&0&0&0&0&8&0&0&0&0&8&0&0&0&0&8 \\ 0&8&0&0&8&0&0&0&0&0&0&8&0&0&8&0 \\ 0&0&8&0&0&0&0&8&8&0&0&0&0&8&0&0 \\ 0&0&0&8&0&0&8&0&0&8&0&0&8&0&0&0 \\ 0&8&0&0&8&0&0&0&0&0&0&8&0&0&8&0 \\ 8&0&0&0&0&8&0&0&0&0&8&0&0&0&0&8 \\ 0&0&0&8&0&0&8&0&0&8&0&0&8&0&0&0 \\ 0&0&8&0&0&0&0&8&8&0&0&0&0&8&0&0 \\ 0&0&8&0&0&0&0&8&8&0&0&0&0&8&0&0 \\ 0&0&0&8&0&0&8&0&0&8&0&0&8&0&0&0 \\ 8&0&0&0&0&8&0&0&0&0&8&0&0&0&0&8 \\ 0&8&0&0&8&0&0&0&0&0&0&8&0&0&8&0 \\ 0&0&0&8&0&0&8&0&0&8&0&0&8&0&0&0 \\ 0&0&8&0&0&0&0&8&8&0&0&0&0&8&0&0 \\ 0&8&0&0&8&0&0&0&0&0&0&8&0&0&8&0 \\ 8&0&0&0&0&8&0&0&0&0&8&0&0&0&0&24 \end{bmatrix} \quad (4.20)$$

Thus using(4.16) and (4.20) in (4.15), the moment matrix corresponding to a CCD with cube portion constructed through resolution IV is obtained as;

$$M = \frac{X^T X}{16} = \begin{bmatrix} 1 & 0_{4,1}^T & 13.7\left(\vec{I}_4\right)^T \\ 0_{4,1} & 13.7\, I_4 & 0_{16,4}^T \\ 13.7\,\vec{I}_4 & 0_{16,4} & H_4 \end{bmatrix} \tag{4.21}$$

The only nonvanishing moments when the cube portion of the CCD is constructed through resolution $R \geq 4$ are:

$$\mu_2(\tau) = \frac{1}{n} 2^{m-p} + \frac{1}{n} 2\alpha^2 \quad , \quad \mu_{22}(\tau) = \frac{1}{n} 2^{m-p} \quad , \quad \mu_4(\tau) = \frac{1}{n} 2^{m-p} + \frac{1}{n} 2\alpha^4$$

4.1.2.2 Four Factors Rotatable CCD Information Matrix

The following lemma is proved:

Lemma 4.2

Let the parameter subsystem of interest be $K^T(\theta)$. Then for ¿4 ,

$$K=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.25 \\ 0 & 0 & 0 & 0 & 0 & 0.25 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.25 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.25 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.25 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \qquad (4.22)$$

Proof:

From equation (3.21),

$$K_1=e_{11}e_1^{'}+e_{22}e_2^{'}+e_{33}e_3^{'}+e_{44}e_4^{'} \quad , \text{ a } \left(4^2\times 4\right) \text{ matrix}$$

and

e
¿
e
e
¿
¿
$(¿¿13+e_{31}+e_{24}+e_{42})E_2^{'}+¿$
$(¿12+e_{21}+e_{34}+e_{43}¿)E_1^{'}+¿$
¿
$K_2=\frac{1}{4}¿$

$$+e_{32}¿E_3' \quad . \qquad (4.23)$$

Define

$$e_{ij}=e_i\otimes e_j \quad , \quad i,j=1,2,3 \quad ; \text{ where } \quad e_1=\begin{bmatrix}1\\0\\0\\0\end{bmatrix} \quad , \quad e_2=\begin{bmatrix}0\\1\\0\\0\end{bmatrix} \quad , \quad e_3=\begin{bmatrix}0\\0\\1\\0\end{bmatrix} \quad \text{and}$$

$$e_4=\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

$$E_1=\begin{bmatrix}1\\0\\0\end{bmatrix} \quad , \quad E_2=\begin{bmatrix}0\\1\\0\end{bmatrix} \quad , \quad E_3=\begin{bmatrix}0\\0\\1\end{bmatrix} \quad ,$$

Substituting these in (4.23), the following are obtained

$$K_1=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \text{ and } K_2=\begin{bmatrix} 0 & 0 & 0 \\ 0.25 & 0 & 0 \\ 0 & 0.25 & 0 \\ 0 & 0 & 0.25 \\ 0.25 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0.25 \\ 0 & 0.25 & 0 \\ 0 & 0.25 & 0 \\ 0 & 0 & 0.25 \\ 0 & 0 & 0 \\ 0.25 & 0 & 0 \\ 0 & 0 & 0.25 \\ 0 & 0.25 & 0 \\ 0.25 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad (4.24)$$

Using (3.20) and (4.24) gives the matrix K and hence the lemma.

Next substituting (4.22) in (3.23) results in:

$$L=\begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1 \\ 0&0&0&0&0&0&1&0&0&1&0&0&0&0&0&0&1&0&0&1&0 \\ 0&0&0&0&0&0&0&1&0&0&0&0&1&1&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&0&1&0&0&1&0&0&1&0&0&1&0&0&0 \end{bmatrix} \qquad (4.25)$$

Thus using (4.21) and (4.25) in (3.24), the information matrix for four factors full CCDis obtained as:

$$C_K\left(M(\xi)\right)=\begin{bmatrix} 1 & 0.851_4^T & 0_{3,1}^T \\ 0.851_4 & 1.5I_4+0.5\sum_{i\neq j=1}^{4} e_i e_j^{'} & 0_{3,4}^T \\ 0_{3,1} & 0_{3,4} & 8I_3 \end{bmatrix} \qquad (4.26)$$

where $0_{3,1}$ and $0_{3,4}$ are matrices of zeros of order 3×1 and 3×4 respectively,

4.1.3 Resolution *R* Rotatable CCD for m factors

In sections 4.1.1 and 4.1.2, resolutions III and IV rotatable CCDs for three and four factors have been derived and their corresponding information matrices obtained. In this section matrices for m factors namely momentmatrix $M(\xi)$,coefficient matrix K and information matrix $C_K(M(\xi))$ are presented.

4.1.3.1 Generalized Moment Matrix $M(\xi)$

Generally, for $m-¿$ factors and cube portion constructed through resolution R, the second – order kronecker model moment matrix of a rotatableCCD may be expressed as follows:

Let d be a vertical concatenation of the form $d=\begin{bmatrix} R \\ E \end{bmatrix}$ given in equation (3.9), then for $m-¿$ factors and N experimental runs, the design matrix X takes the form given in equation (3.10). By definition, the moment matrix (3.16) for a second-order kronecker model is given by:

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

$$¿\begin{cases} \frac{1}{N}\begin{bmatrix} N & 0'_{m,1} & \left(F+2\alpha^2\right)\left(\vec{I}_m\right)' \\ 0_{m,1} & \left(F+2\alpha^2\right)I_m & F\left(E_{ijk}\right)' \\ \left(F+2\alpha^2\right)\vec{I}_m & F\,E_{ijk} & H_m \end{bmatrix} \in R^{\left(1+m+m^2\right)\times\left(1+m+m^2\right)} for\, m\geq 3 \\ \qquad\qquad\qquad\qquad Resolution\ III \\ \frac{1}{N}\begin{bmatrix} N & 0'_{m,1} & \left(F+2\alpha^2\right)\left(\vec{I}_m\right)' \\ 0_{m,1} & \left(F+2\alpha^2\right)I_m & 0'_{m^2,m} \\ \left(F+2\alpha^2\right)\vec{I}_m & 0_{m^2,m} & H_m \end{bmatrix} \in R^{\left(1+m+m^2\right)\times\left(1+m+m^2\right)} for\, m\geq 4 \\ \qquad\qquad\qquad\qquad Resolution\, R\geq IV \end{cases} \tag{4.27}$$

where

N is the total number of experimental runs

$\alpha=2^{\frac{m-p}{4}}$ satisfying the condition for second-order rotatable designs,

m is the number of factors, F is the number of runs in the cube portion,

$I_m \in R^{m\times m}$ is an $m\times m$ identity matrix and $\vec{I}_m = I_m \otimes I_m$,

$0_{m,1}$ and $0_{m^2,m}$ are matrices of zeros of order $m\times 1$ and $m^2\times m$ respectively,

$E_{ijk}=\sum_{i\neq j\neq k=1}^{m}\left(e_i\otimes e_j\right)e'_k$, $e_i's$ are the Euclidean unit vectors in R^m denoted by $e_{1,}e_2,\ldots,e_m$

H_m is an $m^2\times m^2$ matrix whose entries are given by $\left(F+2\alpha^4\right)V_1+F\,V_2$

$$V_1 = \sum_{i=1}^{m} E_{ii} \quad \text{with} \quad E_{ii} = \left(e_i e_i^{'}\right) \otimes \left(e_i e_i^{'}\right)$$

$$V_2 = \begin{cases} \sum_{i \neq j=1}^{m} \left(E_{ij} + E_{i\,j^{'}} + E_{ji}\right) for\ m \geq 3\ Resolution\ III \\ \sum_{i \neq j=1}^{m} \left(E_{ij} + E_{i\,j^{'}} + E_{ji}\right) + \sum_{i \neq j \neq k \neq l=1}^{m} E_{ijkl} for\ m \geq 4\ Resolution\ R \geq IV \end{cases}$$

with $E_{ij} = \left(e_i e_i^{'}\right) \otimes \left(e_j e_j^{'}\right)$, $E_{i\,j^{'}} = \left(e_i e_j^{'}\right) \otimes \left(e_i e_j^{'}\right)$, $E_{ji} = \left(e_i e_j^{'}\right) \otimes \left(e_j e_i^{'}\right)$,

$E_{ijk} = \left(e_i e_j^{'}\right) \otimes \left(e_i e_k^{'}\right)$, $E_{ijkl} = \left(e_i e_j^{'}\right) \otimes \left(e_k e_l^{'}\right)$.

4.1.3.2 Coefficient Matrix K

For m factors and a parameter subsystem of interest,the coefficient matrix for the rotatable CCDis defined as:

$$K = \begin{pmatrix} 1 & 0_{m,1}^{T} & 0_{m^2,1}^{T} \\ 0_{m,1} & 0_{m,m} & 0_{m,s-(m+1)} \\ 0_{m^2,1} & K_1 & K_2 \end{pmatrix} \in R^{¿} \quad \text{for} \quad m \geq 3 \qquad (4.28)$$

(the superscript of R is printed as: m $(¿¿2+m+1) \times s$)

where

$$K_1 = \sum_{i=1}^{m} e_{ii} e_i^{'} \quad , \quad \left(m^2 \times m\right) \quad \text{matrix}$$

and

$$K_2=\frac{1}{r}¿\sum_{\substack{i,j=1\\ i\neq j}}^{m}¿(¿¿ij+e_{ji})e_l'\,e$$, an $m^2\times(s-(m+1))$ matrix

where r is the number of times each column corresponding to the interaction factors is repeated in the design matrix X of the respective CCD and $s<m$ is the number of parameters of interest.

4.1.3.3 Generalized Information Matrix

From definition (3.23), $L=(K'K)^{-1}K'$ such that $C_K(M(\xi))=LM(\xi)L'$. Usingresults (4.27) and (4.28), the Information matrix is obtained as

$$C_K(M(\xi))=\frac{1}{N}\begin{pmatrix} N & (F+2\alpha^2)(1_m)' & 0_{c,1}' \\ (F+2\alpha^2)1_m & G_m & 0_{c,m}' \\ 0_{c,1} & 0_{c,m} & 2(F+\alpha^4)I_c \end{pmatrix} \qquad (4.29)$$

where

$1_m=(1,\ldots,1)'\in R^m$ denotes the vector with all elements equal to 1,

G_m denotes an $m\times m$ circulant matrix with diagonal and off-diagonal elements a and b respectively and entries in a and b are given by $(F+2\alpha^4)$ and F . Thus

$$G_m=¿\,F+2\alpha^4¿I_m+F\sum_{i\neq j=1}^{m}e_ie_j'$$, where $e_i's$ and $e_j's$ are the Euclidean unit vectors in R^m denoted by $e_{1,}e_2,\ldots,e_m$ and $I_m\in R^{m\times m}$ denotes an identity matrix,

$I_c \in R^{c\times c}$ is an identity matrixwhere c is the number of parameters resulting from averaging the interaction factors,

$0_{c,1}$ is a $c\times 1$ vector with all elements zeros,

$0_{c,m}$ is a $c\times m$ matrix with all elements zeros,

Thus the information matrix $C_K(M(\xi))$ is of order $(1+m+c)\times(1+m+c)$.

4.2 Optimal Rotatable Weighted CCDs (WCCDs)

The methodology outlined in section 3.2 is applied to the results obtained in section 4.1 to derive Optimal Rotatable WCCDs for three and four factors.

4.2.1 Three Factors Optimal RotatableWCCD

The design matrix X given in (4.1) is separated into two blocks as explained in section 3.2. The cube portion obtained from resolution III (Table 4.1) formed one block denoted by ξ_F and star portion formed another block denoted by ξ_s . The relations (3.28), (3.29), (3.30) and (3.35) were then used to calculate the values of the weights assigned to the portions of the optimal rotatable WCCD (3.26).

4.2.1.1 Three Factors Rotatable WCCDInformation Matrix

Consider the design matrix X for $m=3$ given in (4.2) with $\alpha=\sqrt[4]{2^2}=1.4142$. The factorial portion is a fractional factorial design of resolution III. Axial points are added and no center point. Thus the two blocks representing the elementary designs are:

$$X_{\xi_F} = \begin{bmatrix} 1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad (4.30)$$

and

$$X_{\xi_s} = \begin{bmatrix} 1 & -\alpha & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \alpha & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 \\ 1 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 \\ 1 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 \end{bmatrix} \quad (4.31)$$

Thus the corresponding moment matrices are

$$M_{\xi_F} = \frac{(X_{\xi_F})^T (X_{\xi_F})}{4} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

(4.32)

and

$$M_{\xi_s} = \frac{\left(X_{\xi_s}\right)^T \left(X_{\xi_s}\right)}{6} = \begin{bmatrix} 1 & 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & 0 & \frac{2}{3} \\ 0 & \frac{2}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{2}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & 0 & 0 & \frac{4}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{4}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{4}{3} \end{bmatrix} \quad (4.33)$$

Then using (4.12), (4.32) and (4.33) in (3.24) the information matrices are obtained as

$$C_k\left(M_{\xi_F}\right) = L M_{\xi_F} L^T = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix} = C_F \quad (4.34)$$

and

$$C_k\left(M_{\xi_s}\right)=L M_{\xi_s} L^T=\begin{bmatrix} 1 & \frac{2}{3} & \frac{2}{3} & \frac{2}{3} & 0 & 0 & 0 \\ \frac{2}{3} & \frac{4}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & \frac{4}{3} & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & 0 & \frac{4}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}=C_s \qquad (4.35)$$

Using the corresponding information matrices (4.34) and (4.35), the information matrix for the WCCD is obtained as:

$$C_k\left(M(\xi)\right)=w_1 C_F+w_2 C_s$$

$$¿\, w_1\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix}+w_2\begin{bmatrix} 1 & \frac{2}{3} & \frac{2}{3} & \frac{2}{3} & 0 & 0 & 0 \\ \frac{2}{3} & \frac{4}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & \frac{4}{3} & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & 0 & \frac{4}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$¿\begin{bmatrix} w_1+w_2 & \frac{3w_1+2w_2}{3} & \frac{3w_1+2w_2}{3} & \frac{3w_1+2w_2}{3} & 0 & 0 & 0 \\ \frac{3w_1+2w_2}{3} & \frac{3w_1+4w_2}{3} & w_1 & w_1 & 0 & 0 & 0 \\ \frac{3w_1+2w_2}{3} & w_1 & \frac{3w_1+4w_2}{3} & w_1 & 0 & 0 & 0 \\ \frac{3w_1+2w_2}{3} & w_1 & w_1 & \frac{3w_1+4w_2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4w_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4w_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4w_1 \end{bmatrix}$$

(4.36)

4.2.1.2 D-Optimal Rotatable WCCD in three Factors

From (4.36),let $C_k(M(\xi))=C,$ so that C can be represented by:

$$C=\begin{bmatrix} C_{11} & (O_{3,4})^T \\ O_{3,4} & C_{22} \end{bmatrix}$$

where $O_{3,4}$ is a matrixof order 3×4 whose elements are zeros,

$$C_{11}=\begin{bmatrix} w_1+w_2 & \frac{3w_1+2w_2}{3} & \frac{3w_1+2w_2}{3} & \frac{3w_1+2w_2}{3} \\ \frac{3w_1+2w_2}{3} & \frac{3w_1+4w_2}{3} & w_1 & w_1 \\ \frac{3w_1+2w_2}{3} & w_1 & \frac{3w_1+4w_2}{3} & w_1 \\ \frac{3w_1+2w_2}{3} & w_1 & w_1 & \frac{3w_1+4w_2}{3} \end{bmatrix} \text{ and}$$

$$C_{22}=w_1\begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix}=4w_1 I_3 \quad .$$

(4.37)

Thus

$$c^{-1}=\begin{bmatrix} A & (O_{3,4})^T \\ O_{3,4} & B \end{bmatrix} \tag{4.38}$$

where

$$A=\begin{bmatrix} \frac{9w_1+4w_2}{w_1w_2} & \frac{-3w_1+2w_2}{w_1w_2} & \frac{-3w_1+2w_2}{w_1w_2} & \frac{-3w_1+2w_2}{w_1w_2} \\ \frac{-3w_1+2w_2}{w_1w_2} & \frac{3w_1+2w_2}{2w_1w_2} & \frac{3w_1+4w_2}{4w_1w_2} & \frac{3w_1+4w_2}{4w_1w_2} \\ \frac{-3w_1+2w_2}{w_1w_2} & \frac{3w_1+4w_2}{4w_1w_2} & \frac{3w_1+2w_2}{2w_1w_2} & \frac{3w_1+4w_2}{4w_1w_2} \\ \frac{-3w_1+2w_2}{w_1w_2} & \frac{3w_1+4w_2}{4w_1w_2} & \frac{3w_1+4w_2}{4w_1w_2} & \frac{3w_1+2w_2}{2w_1w_2} \end{bmatrix},$$

$$B=\begin{bmatrix} \frac{1}{4w_1} & 0 & 0 \\ 0 & \frac{1}{4w_1} & 0 \\ 0 & 0 & \frac{1}{4w_1} \end{bmatrix},$$

$O_{3,4}$ is a 3×4 matrix of zeros.

From (4.34), let $C_k(M_{\xi_F})=C_F$ so that

$$C_F=\begin{bmatrix} C_{F1} & (O_{3,4})^T \\ 0_{3,4} & C_{F2} \end{bmatrix}, \quad \text{where} \quad C_{F1}=\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad C_{F2}=\begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix} \tag{4.39}$$

Then

$$C_F C^{-1}=\begin{bmatrix} C_{F1}C_{11}^{-1} & (O_{3,4})^T \\ 0_{3,4} & C_{F2}C_{22}^{-1} \end{bmatrix}$$

such that

$$C_{F1}C_{11}^{-1}=\frac{1}{w_1}\begin{bmatrix}-2 & 1 & 1 & 1\\ -2 & 1 & 1 & 1\\ -2 & 1 & 1 & 1\\ -2 & 1 & 1 & 1\end{bmatrix} \tag{4.40}$$

and

$$C_{F2}C_{22}^{-1}=\frac{1}{w_1}I_4 \tag{4.41}$$

Therefore $$C_F C^{-1}=\frac{1}{w_1}\begin{bmatrix}-2 & 1 & 1 & 1 & 0 & 0 & 0\\ -2 & 1 & 1 & 1 & 0 & 0 & 0\\ -2 & 1 & 1 & 1 & 0 & 0 & 0\\ -2 & 1 & 1 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix} \tag{4.42}$$

From (3.28) the right hand side gives:

$$trace\, C^0=trace\, I_7=7 \quad ,$$

and the left-hand side results to

$$trace\, C_F C^{-1}=trace\, C_{F1}C_{11}^{-1}+trace\, C_{F2}C_{22}^{-1}=\frac{4}{w_1} \quad .$$

Thus

$$\frac{4}{w_1}=7\Rightarrow w_1=\frac{4}{7} \quad \text{and} \quad w_2=1-w_1=\frac{3}{7} \quad . \tag{4.43}$$

Next, (4.35) and (4.38) are used in (3.27) for $i=s$ to obtain

$$C_s C^{-1}=\frac{1}{w_2}\begin{bmatrix}3 & -1 & -1 & -1 & 0 & 0 & 0\\ 2 & 0 & -1 & -1 & 0 & 0 & 0\\ 2 & 1 & 0 & -1 & 0 & 0 & 0\\ 2 & -1 & -1 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0\end{bmatrix} \tag{4.44}$$

Thus, $trace\, C_s C^{-1} = \frac{3}{w_2}$

For $D-optimality$, the relation $trace\, C_i C^{-1} = trace\, C^0 = trace\, I_s = 7$ results to:

$\frac{3}{w_2} = 7 \Rightarrow w_2 = \frac{3}{7}$ and $w_1 = 1 - w_2 = \frac{4}{7}$

Hence the $D-$¿ optimal Rotatable WCCD for three factors is

$$\xi_{WCCD} = \frac{4}{7}\xi_F + \frac{3}{7}\xi_s = 0.57\,\xi_F + 0.43\,\xi_s \qquad (4.45)$$

4.2.1.3 A-Optimal Rotatable WCCD

Letting $\left(C_k\left(M(\xi)\right)\right)^{-1} = C^{-1} = \begin{bmatrix} A & \left(O_{3,4}\right)^T \\ O_{3,4} & B \end{bmatrix}$ in (4.37) we have

$$C^{-2} = \left(C^{-1}\right)^2 = \begin{bmatrix} A^2 & \left(O_{3,4}\right)^T \\ O_{3,4} & B^2 \end{bmatrix}$$

$$¿\begin{bmatrix}
\frac{108 w_1^2 + 108\,ab + 28 w_2^2}{w_1^2 w_2^2} & \frac{-36 w_1^2 + 45\,ab + 14 w_2^2}{w_1^2 w_2^2} & \frac{-36 w_1^2 + 45\,ab + 14 w_2^2}{w_1^2 w_2^2} & \frac{-36 w_1^2 + 45\,ab + 14 w_2^2}{w_1^2 w_2^2} \\
\frac{-36 w_1^2 + 45\,ab + 14 w_2^2}{w_1^2 w_2^2} & \frac{99 w_1^2 + 144\,ab + 56 w_2^2}{8 w_1^2 w_2^2} & \frac{189 w_1^2 + 288\,ab + 112 w_2^2}{16 w_1^2 w_2^2} & \frac{189 w_1^2 + 288\,ab + 112 w_2^2}{16 w_1^2 w_2^2} \\
\frac{-36 w_1^2 + 45\,ab + 14 w_2^2}{w_1^2 w_2^2} & \frac{189 w_1^2 + 288\,ab + 112 w_2^2}{16 w_1^2 w_2^2} & \frac{99 w_1^2 + 144\,ab + 56 w_2^2}{8 w_1^2 w_2^2} & \frac{189 w_1^2 + 288\,ab + 112 w_2^2}{16 w_1^2 w_2^2} \\
\frac{-36 w_1^2 + 45\,ab + 14 w_2^2}{w_1^2 w_2^2} & \frac{189 w_1^2 + 288\,ab + 112 w_2^2}{16 w_1^2 w_2^2} & \frac{189 w_1^2 + 288\,ab + 112 w_2^2}{16 w_1^2 w_2^2} & \frac{99 w_1^2 + 144\,ab + 56 w_2^2}{8 w_1^2 w_2^2} \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}$$

(4.46)

Thus using (4.33) in the left hand side of (3.29)for $i=F$, the following is obtained as

$$C_F C^{-2}=C_k\left(M_{\xi_F}\right)C^{-2}=\begin{bmatrix} \frac{-27w_1+14w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & 0 & 0 & 0 \\ \frac{-27w_1+14w_2}{w_1^2w_2^2} & \frac{9w_1+7w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & 0 & 0 & 0 \\ \frac{-27w_1+14w_2}{w_1^2w_2^2} & \frac{9w_1+7w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & 0 & 0 & 0 \\ \frac{-27w_1+14w_2}{w_1^2w_2^2} & \frac{9w_1+7w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & \frac{9w_1+7w_2}{w_1^2w_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{4w_1^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{4w_1^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{4w_1^2} \end{bmatrix}$$

(4.47)

Therefore

$$trace\, C_F C^{-2}=\frac{-27w_1+14w_2}{w_1^2w_2}+\left(\frac{9w_1+7w_2}{w_1^2w_2}\right)\times 3+\frac{1}{4w_1^2}\times 3=\frac{7w_2\times 4+3w_2}{4w_1^2w_2}=\frac{31}{4w_1^2}$$

(4.48)

Next using(4.37), the righthand side of (3.29) gives:

$$trace\, C^{-1}=\frac{9w_1+4w_2}{w_1w_2}+\left(\frac{3w_1+2w_2}{2w_1w_2}\right)\times 3+\frac{1}{4w_1}\times 3=\frac{54w_1+31w_2}{4w_1w_2}$$

(4.49)

Therefore equating (4.48) to (4.49) the following equation is obtained:

$$54w_1^2+31w_1w_2-31w_2=0 \qquad (4.50)$$

Using $w_1+w_2=1 \Rightarrow w_2=1-w_1$ in (4.71) gives $23w_1^2+62w_1-31=0$

which then gives

$w_1 = -3.13 \vee 0.43$. But $w_1 \geq 0$, hence

$$w_1 = 0.43 \Rightarrow w_2 = 1 - 0.43 = 0.57 \tag{4.51}$$

Similarly, using (4.35) in (3.29) for $i = s$, the following is obtained

$$C_s C^{-2} = \begin{bmatrix} \frac{36 w_1 + 18 w_2}{w_1 w_2^2} & \frac{-12 w_1 + 9 w_2}{w_1 w_2^2} & \frac{-12 w_1 + 9 w_2}{w_1 w_2^2} & \frac{-12 w_1 + 9 w_2}{4 w_1 w_2^2} & 0 & 0 & 0 \\ \frac{24 w_1 + 12 w_2}{w_1 w_2^2} & \frac{-15 w_1 + 12 w_2}{2 w_1 w_2^2} & \frac{-33 w_1 + 24 w_2}{4 w_1 w_2^2} & \frac{-33 w_1 + 24 w_2}{4 w_1 w_2^2} & 0 & 0 & 0 \\ \frac{24 w_1 + 12 w_2}{w_1 w_2^2} & \frac{-33 w_1 + 24 w_2}{4 w_1 w_2^2} & \frac{-15 w_1 + 12 w_2}{2 w_1 w_2^2} & \frac{-33 w_1 + 24 w_2}{4 w_1 w_2^2} & 0 & 0 & 0 \\ \frac{24 w_1 + 12 w_2}{w_1 w_2^2} & \frac{-33 w_1 + 24 w_2}{4 w_1 w_2^2} & \frac{-33 w_1 + 24 w_2}{4 w_1 w_2^2} & \frac{-15 w_1 + 12 w_2}{2 w_1 w_2^2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

(4.52)

Thus

$$trace\, C_s C^{-2} = \frac{27 w_1}{2 w_1 w_2^2} = \frac{27}{2 w_2^2}$$

(4.53)

Then using (4.49) and (4.53) yields

$$31 w_2^2 + 54 w_1 w_2 - 54 w_1 = 0 \tag{4.54}$$

Substituting $w_1 + w_2 = 1 \Rightarrow w_1 = 1 - w_2$ in (4.54) results in

$$-23 w_2^2 + 108 w_2 - 54 w_2 = 0$$

which then gives

$w_2 = 4.126719352 \vee 0.568932823$ but $0 \leq w_2 \leq 1$.

Therefore

$$w_2=0.57 \Rightarrow w_1=1-0.57=0.43 \quad (4.55)$$

Hence the $A-¿$ optimal rotatable WCCD for three factors is

$$\xi_{WCCD}=0.43\,\xi_F+0.57\,\xi_s \quad (4.56)$$

4.2.1.4 E-OptimalRotatableWCCD

From (3.31), $E=\frac{z_1 z_1^T}{\|z_1\|^2}$ and z is the iegenvector corresponding to the smallest eigenvalue.Let the elements of the information matrix (4.36) be represented as follows

$$w_1+w_2=e \quad , \quad \frac{3w_1+2w_2}{3}=b \quad , \quad \frac{3w_1+4w_2}{3}=a \quad , \quad w_1=c$$

(4.57)

Then define a variable d , the eigenvalues for the information matrix such that:

$$|C_k(M(\xi))-d\,I_7|=0$$

(4.58)

Then

$$|C_k(M(\xi))-d\,I_7|=\left\|\begin{bmatrix} e & b & b & b & 0 & 0 & 0 \\ b & a & c & c & 0 & 0 & 0 \\ b & c & a & c & 0 & 0 & 0 \\ b & c & c & a & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4c & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4c & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4c \end{bmatrix}-\begin{bmatrix} d & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & d & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & d & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & d & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & d & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & d & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & d \end{bmatrix}\right\|=0$$

$$\Rightarrow \left| \begin{bmatrix} e-d & b & b & b & 0 & 0 & 0 \\ b & a-d & c & c & 0 & 0 & 0 \\ b & c & a-d & c & 0 & 0 & 0 \\ b & c & c & a-d & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4c-d & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4c-d & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4c-d \end{bmatrix} \right| = 0$$

Equating the determinant to zero and solving for d gives:

$d = a - c$ or $d = 4c$, or

$$d = \frac{-\sqrt{e^2 + (-4c - 2a)e + 4c^2 + 4ac + 12b^2 + a^2} - e - 2c - a}{2} \quad \text{or}$$

$$d = \frac{\sqrt{e^2 + (-4c - 2a)e + 4c^2 + 4ac + 12b^2 + a^2} + e + 2c + a}{2}$$

(4.59)

Thus substituting (4.57) in (4.59) the eigenvalues are

$$d_1 = \frac{-\left(\sqrt{49w_2^2 + 156w_1w_2 + 144w_1^2}\right) - 7w_2 - 12w_1}{6},$$

$$d_2 = \frac{\left(\sqrt{49w_2^2 + 156w_1w_2 + 144w_1^2}\right) + 7w_2 + 12w_1}{6} \quad ,$$

$$d_3 = d_4 = \frac{4w_2}{3} \quad , \qquad d_5 = d_6 = d_7 = 4w_1 \quad , \tag{4.60}$$

while the corresponding eigenvectors are:

$$z_1=\begin{bmatrix} 1 \\ \dfrac{-\left(\sqrt{49\,w_2^2+156\,w_1\,w_2+144\,w_1^2}\right)-w_2-6\,w_1}{12\,w_2+18\,w_1} \\ \dfrac{-\left(\sqrt{49\,w_2^2+156\,w_1\,w_2+144\,w_1^2}\right)-w_2-6\,w_1}{12\,w_2+18\,w_1} \\ \dfrac{-\left(\sqrt{49\,w_2^2+156\,w_1\,w_2+144\,w_1^2}\right)-w_2-6\,w_1}{12\,w_2+18\,w_1} \\ 0 \\ 0 \\ 0 \end{bmatrix} .$$

$$z_2=\begin{bmatrix} 1 \\ \dfrac{\left(\sqrt{49\,w_2^2+156\,w_1\,w_2+144\,w_1^2}\right)+w_2+6\,w_1}{12\,w_2+18\,w_1} \\ \dfrac{\left(\sqrt{49\,w_2^2+156\,w_1\,w_2+144\,w_1^2}\right)+w_2+6\,w_1}{12\,w_2+18\,w_1} \\ \dfrac{\left(\sqrt{49\,w_2^2+156\,w_1\,w_2+144\,w_1^2}\right)+w_2+6\,w_1}{12\,w_2+18\,w_1} \\ 0 \\ 0 \\ 0 \end{bmatrix} ,$$

$$z_3=\begin{bmatrix}0\\1\\0\\-1\\0\\0\\0\end{bmatrix},\quad z_4=\begin{bmatrix}0\\0\\1\\-1\\0\\0\\0\end{bmatrix},\quad z_5=\begin{bmatrix}0\\0\\0\\0\\1\\0\\0\end{bmatrix},\quad z_6=\begin{bmatrix}0\\0\\0\\0\\0\\1\\0\end{bmatrix},\quad z_7=\begin{bmatrix}0\\0\\0\\0\\0\\0\\1\end{bmatrix}.$$

(4.61)

From theorem 3.3, if the smallest eigenvalue for C has multiplicity 1, then the only choice for matrix E will be obtained from either d_1 or d_2. Clearly $d_1<d_2$ and therefore d_1 is the smallest eigenvalue while the corresponding eigenvector is z_1. Hence

$$d_{min}(C)=\frac{-\left(\sqrt{49w_2^2+156w_1w_2+144w_1^2}\right)-7w_2-12w_1}{6}.$$

(4.62)

Therefore the matrix

$$E=\frac{z_1z_1^T}{\|z_1\|^2} \tag{4.63}$$

Taking $r=\frac{-\left(\sqrt{49w_2^2+156w_1w_2+144w_1^2}\right)+w_2+6w_1}{12w_2+18w_1}$, then

$$z_1=\begin{bmatrix}1\\r\\r\\r\\0\\0\\0\end{bmatrix} \text{ and thus } z_1z_1^T=\begin{bmatrix}1&r&r&r&0&0&0\\r&r^2&r^2&r^2&0&0&0\\r&r^2&r^2&r^2&0&0&0\\r&r^2&r^2&r^2&0&0&0\\0&0&0&0&0&0&0\\0&0&0&0&0&0&0\\0&0&0&0&0&0&0\end{bmatrix} \tag{4.64}$$

Next

$$\left\|z_1\right\|^2=\left(\sqrt{1+3r^2+0}\right)^2=1+3r^2 \tag{4.65}$$

Therefore (4.63) becomes

$$E=\begin{bmatrix} 1 & r & r & r & 0 & 0 & 0 \\ r & r^2 & r^2 & r^2 & 0 & 0 & 0 \\ r & r^2 & r^2 & r^2 & 0 & 0 & 0 \\ r & r^2 & r^2 & r^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}\times\frac{1}{1+3r^2} \tag{4.66}$$

Using (4.34) and (4.66) for $i=F$ gives

$$C_F E=\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix}\times\begin{bmatrix} 1 & r & r & r & 0 & 0 & 0 \\ r & r^2 & r^2 & r^2 & 0 & 0 & 0 \\ r & r^2 & r^2 & r^2 & 0 & 0 & 0 \\ r & r^2 & r^2 & r^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}\times\frac{1}{1+3r^2}$$

$$¿\begin{bmatrix} \frac{1+3r}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & 0 & 0 & 0 \\ \frac{1+3r}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & 0 & 0 & 0 \\ \frac{1+3r}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & 0 & 0 & 0 \\ \frac{1+3r}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & \frac{r+3r^2}{1+3r^2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

(4.67)

Thus

$$trace\, C_F E = \frac{1+3r}{1+3r^2} + 3 \times \frac{r+3r^2}{1+3r^2} \tag{4.68}$$

Using (4.62) and (4.68) in(3.30) yields

$$\Rightarrow \frac{(1+3r)^2}{1+3r^2} = \frac{-\left(\sqrt{49w_2^2+156w_1w_2+144w_1^2}\right)+7w_2+12w_1}{6} \tag{4.69}$$

Taking $b=1-a$ and $a=w_1$, and substituting r in (4.68) gives

$$w_1=\frac{16}{37} \Longrightarrow w_2=\frac{21}{37}$$

(4.70)

Similarly, using (4.35)and (4.66), the following is obtained

$$C_s E = \begin{bmatrix} 1+2r & r+2r^2 & r+2r^2 & r+2r^2 & 0 & 0 & 0 \\ \frac{2+4r}{3} & \frac{2r+4r^2}{3} & \frac{2r+4r^2}{3} & \frac{2r+4r^2}{3} & 0 & 0 & 0 \\ \frac{2+4r}{3} & \frac{2r+4r^2}{3} & \frac{2r+4r^2}{3} & \frac{2r+4r^2}{3} & 0 & 0 & 0 \\ \frac{2+4r}{3} & \frac{2r+4r^2}{3} & \frac{2r+4r^2}{3} & \frac{2r+4r^2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \times \frac{1}{1+3r^2}$$

(4.71)

Thus

$$trace\, C_s E = \lambda_{min}(C) = ¿$$

$$\frac{1+2r}{1+3r^2} + 3 \times \frac{2r+4r^2}{3+9r^2} = \frac{-\left(\sqrt{49w_2^2+156w_1w_2+144w_1^2}\right)+7w_2+12w_1}{6}$$

$$\Rightarrow \frac{(1+2r)^2}{1+3r^2} = \frac{-\left(\sqrt{49w_2^2+156w_1w_2+144w_1^2}\right)+7w_2+12w_1}{6} \tag{4.72}$$

Taking $a=1-b$, and $b=w_2$ and substituting r in (4.72) gives

$$w_2 = \frac{21}{37} \Longrightarrow w_1 = \frac{16}{37}$$

Hence for $i=F,s$, the $E-¿$ optimal rotatable WCCD for three factors is

$$\xi_{WCCD} = \frac{16}{37}\xi_F + \frac{21}{37}\xi_s = 0.43\xi_F + 0.57\xi_s \tag{4.73}$$

4.2.1.5 I-Optimal Rotatable WCCD

I-optimal rotatable WCCD for three factors based on the parameter subsystem of interest is derived in this section. From (3.22), the parameter subsystem of interest dealt

with in this thesis for $m=3$ is the vector $K'(\theta)=\begin{bmatrix}\theta_0\\ \theta_{11}\\ \theta_{22}\\ \theta_{33}\\ \frac{\theta_{12}+\theta_{21}}{2}\\ \frac{\theta_{13}+\theta_{31}}{2}\\ \frac{\theta_{23}+\theta_{32}}{2}\end{bmatrix}$ (4.74)

The corresponding regression vector of factors in the parameter subsystem of interest is

$$f(x)=\begin{bmatrix}1 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3\end{bmatrix}^T \quad (4.75)$$

This gives rise to the matrix X with the following entries;

$$X=\begin{bmatrix}1 & f(x_1) & f(x_2) & f(x_3) & f(x_4) & f(x_5) & f(x_6)\end{bmatrix}^T$$

Thus

$$X=\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 & 0 & 0 & 0 \end{bmatrix} \tag{4.76}$$

Let the design ξ_{WCCD} in (3.26) be represented by ξ_{IWCCD} such that

$$\xi_{IWCCD}=w_1\xi_F+w_2\xi_s \quad , \quad w_1+w_2=1 \quad \text{and} \quad w_1,w_2\geq 0 \tag{4.77}$$

Then each of the design points in the cube portion is assigned a mass of $\frac{1}{4}w_1$ while each of the design points in the star portion is assigned a mass of $\frac{1}{6}w_2$.

Then(3.33) becomes

$$\wedge=\begin{bmatrix} \frac{w_1}{4}I_4 & 0 \\ 0 & \frac{w_2}{6}I_6 \end{bmatrix} \tag{4.78}$$

Letting $w_2=1-w_1$ then

$$C = X^T \wedge X = \begin{bmatrix} 1 & \frac{w_1+2}{3} & \frac{w_1+2}{3} & \frac{w_1+2}{3} & 0 & 0 & 0 \\ \frac{w_1+2}{3} & \frac{-w_1-4}{3} & w_1 & w_1 & 0 & 0 & 0 \\ \frac{w_1+2}{3} & w_1 & \frac{-w_1-4}{3} & w_1 & 0 & 0 & 0 \\ \frac{w_1+2}{3} & w_1 & w_1 & \frac{-w_1-4}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & w_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & w_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & w_1 \end{bmatrix}$$

(4.79)

And

$$C^{-1} = \begin{bmatrix} \frac{-5w_1+4}{w_1^2-w_1} & \frac{w_1+2}{w_1^2-w_1} & \frac{w_1+2}{w_1^2-w_1} & \frac{w_1+2}{w_1^2-w_1} & 0 & 0 & 0 \\ \frac{w_1+2}{w_1^2-w_1} & \frac{-w_1+2}{2w_1^2-2w_1} & \frac{w_1-4}{4w_1^2-4w_1} & \frac{w_1-4}{4w_1^2-4w_1} & 0 & 0 & 0 \\ \frac{w_1+2}{w_1^2-w_1} & \frac{w_1-4}{4w_1^2-4w_1} & \frac{-w_1+2}{2w_1^2-2w_1} & \frac{w_1-4}{4w_1^2-4w_1} & 0 & 0 & 0 \\ \frac{w_1+2}{w_1^2-w_1} & \frac{w_1-4}{4w_1^2-4w_1} & \frac{w_1-4}{4w_1^2-4w_1} & \frac{-w_1+2}{2w_1^2-2w_1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{w_1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{w_1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{w_1} \end{bmatrix}$$

(4.80)

From (4.76), point x_1 in the cube portion is used such that

$$f(x_1) = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix}^T$$

Then the left-hand side of the relation (3.35)

$$f^T(x_1)C^{-1}L_3C^{-1}f(x_1)=\frac{211}{90\,w_1^2} \tag{4.81}$$

Further the right hand side results in

$$tr(C^{-1}L_3)=\frac{-81\,w_1+46}{20\,w_1^2-20\,w_1} \tag{4.82}$$

Equating (4.81) to (4.82) gives

$$\frac{211}{90\,w_1^2}=\frac{-81\,w_1+46}{20\,w_1^2-20\,w_1}$$

And this results in $w_1=0.379 \vee -1.526$ (4.83)

But $w_1>0$, therefore:

$$w_1=0.38 \text{ and hence } w_2=1-0.38=0.62 \tag{4.84}$$

Similarly, from (4.76), if point x_9 in thestar portion design is used, such that

$f(x_9)=[1 \quad 0 \quad 0 \quad 2 \quad 0 \quad 0 \quad 0]^T$,

samevalues of weights are obtained.

Thus design points in the factorial portion are assigned a mass equal to 0.38 and design points in the star portion are assigned a mass equal to 0.62 . Therefore the $I-optimal$ rotatable WCCD (ξ_{IWCCD}) for three factors is expressed as:

$$\xi_{IWCCD}=0.38\,\xi_F+0.62\,\xi_s \tag{4.85}$$

4.2.2 Four Factors Optimal Rotatable WCCD

The design matrix X given in (4.14) is separated into two blocks as explained in section 3.2. The cube portion obtained from resolutionIV(Table 4.2) formed one block denoted by ξ_F and star portion formed another block denoted by ξ_s . The relations

(3.28), (3.29), (3.30) and (3.35) were then used to calculate the values of the weightsassigned to the portions of the optimal rotatableWCCD (3.26).

4.2.2.1 Four Factors Rotatable WCCD Information Matrix

Consider the design matrix X for $m=4$ given in (4.14) with $\alpha=\sqrt[4]{2^3}=1.6818$

The factorial portion is a fractional factorial design of resolution IV. Axial points are added and no center point. Thus for the elementary designs, the two blocks are as follows:

$$X_{\xi_F}=\begin{bmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad (4.86)$$

$$X_{\xi_s}=\begin{bmatrix} 1 & -\alpha & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \alpha & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 \\ 1 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha^2 \end{bmatrix} \quad (4.87)$$

Thus the corresponding moment matrices are:

$$X$$

$$\left(X_{\xi_F}\right)^T \frac{(\text{¿¿}\,\xi_F)}{8} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}$$

$$M_{\xi_F} = \text{¿}$$

(4.88)

And

$$X$$

$$\left(X_{\xi_s}\right)^T \frac{(\text{¿¿}\,\xi_s)}{8} = \text{¿}$$

$$M_{\xi_s} = \text{¿}$$

$$\left[\begin{matrix}
1 & 0 & 0 & 0 & 0 & 0.7071 & 0 & 0 & 0 & 0 & 0.7071 & 0 & 0 & 0 & 0 & 0.7071 & 0 \\
0 & 0.7071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.7071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.7071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.7071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.7071 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.7071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.7071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & o & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.7071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{matrix}\right.$$

(4.89)

Then using (4.25), (4.88), (4.89) in (3.24), the corresponding matrices are obtained as

$$C_k\left(M_{\xi_F}\right)=\begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 16
\end{bmatrix} \qquad (4.90)$$

and

$$C_k\left(M_{\xi_s}\right)=\begin{bmatrix} 1 & 0.7071 & 0.7071 & 0.7071 & 0.7071 & 0 & 0 & 0 \\ 0.7071 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.7071 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0.7071 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0.7071 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad (4.91)$$

For $w\in[0;1]$, let $\xi_{WCCD}=w_1\xi_F+w_2\xi_s$ where $w_1+w_2=1\wedge w_1,w_2\geq 0$ are different masses assigned to each of the two designs ξ_F and ξ_s .Using the corresponding information matrices (4.90) and (4.91), the information matrix for the WCCD is obtained as

$$C_k(M(\xi))=w_1C_k\left(M_{\xi_F}\right)+w_2C_k\left(M_{\xi_s}\right)=¿$$

$$\begin{bmatrix} w_1+w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 & 0 & 0 & 0 \\ w_1+0.7071w_2 & w_1+2w_2 & w_1 & w_1 & w_1 & 0 & 0 & 0 \\ w_1+0.7071w_2 & w_1 & w_1+2w_2 & w_1 & w_1 & 0 & 0 & 0 \\ w_1+0.7071w_2 & w_1 & w_1 & w_1+2w_2 & w_1 & 0 & 0 & 0 \\ w_1+0.7071w_2 & w_1 & w_1 & w_1 & w_1+2w_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 16w_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 16w_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16w_1 \end{bmatrix}$$

(4.92)

4.2.2.2 D- Optimal Rotatable WCCD in Four Factors

From (4.36), let $C_k(M(\xi))=C_4$, so that C_4 can be represented by:

$$C=\begin{bmatrix} C_{11} & (O_{3,5})^T \\ O_{3,5} & C_{22} \end{bmatrix}$$

where $O_{3,5}$ is a 3×5 matrix whose elements are zeros,

$$C_{11}=\begin{bmatrix} w_1+w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 & w_1+0.7071w_2 \\ w_1+0.7071w_2 & w_1+2w_2 & w_1 & w_1 & w_1 \\ w_1+0.7071w_2 & w_1 & w_1+2w_2 & w_1 & w_1 \\ w_1+0.7071w_2 & w_1 & w_1 & w_1+2w_2 & w_1 \\ w_1+0.7071w_2 & w_1 & w_1 & w_1 & w_1+2w_2 \end{bmatrix}$$

(4.93)

And

$$C_{22}=w_1\begin{bmatrix} 16 & 0 & 0 \\ 0 & 16 & 0 \\ 0 & 0 & 16 \end{bmatrix}=16w_1I_3 \tag{4.94}$$

Thus

$$(¿¿4)^{-1}=\begin{bmatrix} e & a & a & a & a & 0 & 0 & 0 \\ a & c & d & d & d & 0 & 0 & 0 \\ a & d & c & d & d & 0 & 0 & 0 \\ a & d & d & c & d & 0 & 0 & 0 \\ a & d & d & d & c & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{16w_1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{16w_1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{16w_1} \end{bmatrix}$$

C ¿

(4.95)

with

$$e=\frac{5\times10^7w_2+10^8w_1}{959w_2^2+8.58\times10^6w_1w_2}$$

$$a=\frac{-1.77\times10^8w_2+2.5\times10^7w_1}{959w_2^2+8.58\times10^6w_1w_2}$$

$$c=\frac{\left(5\times 10^{8}w_{2}+7.57\times 10^{7}w_{1}\right)}{7672\,w_{2}^{2}+6.86\times 10^{7}w_{1}w_{2}}$$

$$d=\frac{5\times 10^{7}w_{2}+4.14\times 10^{7}w_{1}}{7672\,w_{2}^{2}+6.86\times 10^{7}w_{1}w_{2}}$$

From (4.90), let $C_{k}\left(M_{\xi_{F}}\right)=C_{F}$ so that

$$C\,(¿¿4)^{-1}=¿\,C_{F}¿$$

$$\begin{bmatrix} e+4a & a+c+3d & a+c+3d & a+c+3d & a+c+3d & 0 & 0 & 0 \\ e+4a & a+c+3d & a+c+3d & a+c+3d & a+c+3d & 0 & 0 & 0 \\ e+4a & a+c+3d & a+c+3d & a+c+3d & a+c+3d & 0 & 0 & 0 \\ e+4a & a+c+3d & a+c+3d & a+c+3d & a+c+3d & 0 & 0 & 0 \\ e+4a & a+c+3d & a+c+3d & a+c+3d & a+c+3d & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{w_{1}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{w_{1}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{w_{1}} \end{bmatrix} \quad (4.96)$$

With

$$e+4a=\frac{-2.07\times 10^{7}}{959\,w_{2}+8.58\times 10^{6}w_{1}}$$ and

$$a+c+3d=\frac{7.32\times 10^{6}}{959\,w_{2}+8.58\times 10^{6}w_{1}} \qquad (4.97)$$

Thus

$$C\,(¿¿4)^{-1}=e+4a+4(a+c+3d)+\frac{3}{w_{1}}\;trace\,C_{F}¿$$

$$¿-\frac{2.07\times10^7}{959w_2+8.58\times10^6w_1}+4\times\frac{7.32\times10^6}{959w_2+8.58\times10^6w_1}+\frac{3}{w_1}$$

(4.98)

And

$$trace\,C_4{}^0=trace\,I_8=8\quad. \tag{4.99}$$

Therefore using (4.98) and (4.99) in the relation (3.28) gives

$$\frac{-2.07\times10^7}{959w_2+8.58\times10^6w_1}+4\times\frac{7.32\times10^6}{959w_2+8.58\times10^6w_1}+\frac{3}{w_1}=8$$

$$\Longrightarrow 8.58\times10^6w_1+2877w_2+2.57\times10^7w_1=8w_1\left(959w_2+8.58\times10^6w_1\right) \tag{4.100}$$

Substituting $w_2=1-w_1$, in (4.100) gives

$$8.58\times10^6w_1+2877-2877w_1+2.57\times10^7w_1=7672w_1-7672w_1^2+6.86\times10^7w_1^2$$

$$\Longrightarrow 6.86\times10^7w_1^2-3.43\times10^7w_1-2877=0$$

$$\Longrightarrow w_1=-8.38\times10^{-5}\vee0.5$$

But $0\le w_1\le1$, therefore

$$w_1=0.5\Longrightarrow w_2=0.5 \tag{4.101}$$

Next from (4.91), let $C_k\left(M_{\xi_s}\right)=C_s$ so that

$$C_s=¿$$

$$\begin{bmatrix} e+2.8284a & a+0.7071(c+3d) & a+0.7071(c+3d) & a+0.7071(c+3d) & a+0.7071(c+3d) & 0 & 0 & 0 \\ 0.7071e+2a & 0.7071a+2c & 0.7071a+2d & 0.7071a+2d & 0.7071a+2d & 0 & 0 & 0 \\ 0.7071e+2a & 0.7071a+2d & 0.7071a+2c & 0.7071a+2d & 0.7071a+2d & 0 & 0 & 0 \\ 0.7071e+2a & 0.7071a+2d & 0.7071a+2d & 0.7071a+2c & 0.7071a+2d & 0 & 0 & 0 \\ 0.7071e+2a & 0.7071a+2d & 0.7071a+2d & 0.7071a+2d & 0.7071a+2c & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

(4.102)

where

$$e+2.8284a=\frac{959w_2+2.93\times10^7w_1}{959w_2^2+8.58\times10^6w_1w_2} \quad ,$$

$$a+0.7071(c+3d)=\frac{-7.32\times10^7w_1}{959w_2^2+8.58\times10^6w_1w_2} \quad ,$$

$$0.7071e+2a=\frac{2.07\times10^7w_1}{959w_2^2+8.58\times10^6w_1w_2} \quad ,$$

$$0.7071a+2d=\frac{-7.32\times10^6w_1}{959w_2^2+8.58\times10^6w_1w_2} \quad ,$$

$$0.7071a+2c=\frac{959w_2+1.26\times10^6w_1}{959w_2^2+8.58\times10^6w_1w_2} \quad .$$

Thus

$$C$$

$$(¿¿4)^{-1}=\frac{959w_2+2.93\times10^7w_1}{959w_2^2+8.58\times10^6w_1w_2}+4\times\frac{959w_2+1.26\times10^6w_1}{959w_2^2+8.58\times10^6w_1w_2}$$

$$trace\,C_s¿$$

(4.103)

and

$$trace\, C^0 = trace\, I_8 = 8 \quad . \qquad (4.104)$$

Therefore using (4.103) and (4.104) in relation (3.28) yields

$$\frac{959 w_2 + 2.93\times 10^7 w_1}{959 w_2^2 + 8.58\times 10^6 w_1 w_2} + 4\times \frac{959 w_2 + 1.26\times 10^6 w_1}{959 w_2^2 + 8.58\times 10^6 w_1 w_2} = 8 \quad .$$

(4.105)

But $w_1 = 1 - w_2$. thus (4.105) reduces to

$$\frac{3.43\times 10^7 w_2 - 3.43\times 10^7}{8.58\times 10^6 w_2^2 - 8.58\times 10^6 w_2} = 8$$

$$\Longrightarrow 6.86\times 10^7 w_2^2 - 1.03\times 10^8 w_2 + 3.43\times 10^7 = 0 \quad . \qquad (4.106)$$

Solving the quadratic equation (4.106) gives

$$w_2 = \frac{-5\sqrt{4.71\times 10^{13}} - 1.03\times 10^8}{1.37\times 10^8} = 1.00 \quad \text{or}$$

$$w_2 = \frac{-5\sqrt{4.71\times 10^{13}} + 1.03\times 10^8}{1.37\times 10^8} = 0.50 \quad .$$

But w_2 must be such that $0 \le w_2 \le 1$, then clearly:

$$w_2 = 0.50 \Longrightarrow w_1 = 1 - 0.50 = 0.50 \quad .$$

Hence the $D - optimal$ rotatable WCCD is

$$\xi_{WCCD} = 0.5\,\xi_F + 0.5\,\xi_s \quad . \qquad (4.107)$$

4.2.2.3 A-Optimal Rotatable WCCD in Four Factors

From (4.45), let $\left(C_k\left(M(\xi)\right)\right)^{-2}$ be represented by $(¿¿4)^{-2}$ C ¿ so that

Therefore $(¿¿4)^{-2} = ¿$ C ¿

$$\left[\begin{array}{cccccccc}
e^2+4a^2 & a(e+c+3d) & a(e+c+3d) & a(e+c+3d) & a(e+c+3d) & 0 & 0 & 0 \\
a(e+c+3d) & a^2+c^2+3d^2 & a^2+2cd+2d^2 & a^2+2cd+2d^2 & a^2+2cd+2d^2 & 0 & 0 & 0 \\
a(e+c+3d) & a^2+2cd+2d^2 & a^2+c^2+3d^2 & a^2+2cd+2d^2 & a^2+2cd+2d^2 & 0 & 0 & 0 \\
a(e+c+3d) & a^2+2cd+2d^2 & a^2+2cd+2d^2 & a^2+c^2+3d^2 & a^2+2cd+2d^2 & 0 & 0 & 0 \\
a(e+c+3d) & a^2+2cd+2d^2 & a^2+2cd+2d^2 & a^2+2cd+2d^2 & a^2+c^2+3d^2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{256w_1^2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{256w_1^2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{256w_1^2}
\end{array}\right.$$

(4.108)

where

$$e^2+4a^2=\frac{3.75\times10^{14}b^2+1.35\times10^{16}ab+1.25\times10^{16}a^2}{9.2\times10^5b^4+1.65\times10^{10}ab^3+7.36\times10^{13}a^2b^2}$$

$$a(e+c+3d)=\frac{-1.33\times10^{15}b^2+4.08\times10^{15}ab+3.13\times10^{15}a^2}{9.2\times10^5b^4+1.65\times10^{10}ab^3+7.36\times10^{13}a^2b^2}$$

$$a^2+c^2+3d^2=\frac{7.5\times10^{15}b^2+1.91\times10^{16}ab+1.27\times10^{16}a^2}{1.47\times10^7b^2+2.63\times10^{11}ab^3+1.18\times10^{15}a^2b^2}$$

$$a^2+2cd+2d^2=\frac{7.5\times10^{15}b^2+1.91\times10^{16}ab+1.24\times10^{16}a^2}{1.47\times10^7b^2+2.63\times10^{11}ab^3+1.18\times10^{15}a^2b^2} ,$$

(4.109)

Thus $for\, i=F$,using (4.90) and (4.108), the lefthand side of the relation (3.29) results in

C

$$\left(\text{¿¿}4\right)^{-2}=\begin{bmatrix} p & q & q & q & q & 0 & 0 & 0 \\ p & q & q & q & q & 0 & 0 & 0 \\ p & q & q & q & q & 0 & 0 & 0 \\ p & q & q & q & q & 0 & 0 & 0 \\ p & q & q & q & q & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{16\,w_1^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{16\,w_1^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{16\,w_1^2} \end{bmatrix} \qquad (4.110)$$

C_F ¿

where

$$p=\frac{1.55\times10^{15}w_2+2.80\times10^{15}w_1}{9.2\times10^5w_2^3+1.65\times10^{10}w_1w_2^2+7.36\times10^{15}w_1^2w_2} \qquad (4.111)$$

$$q=\frac{5.5\times10^{14}w_2+7.01\times10^{16}w_1}{9.2\times10^5w_2^3+1.65\times10^{10}w_1w_2^2+7.36\times10^{15}w_1^2w_2}\ .$$

(4.112)

Thus

C

$$\left(\text{¿¿}4\right)^{-2}=p+4q+\frac{3}{16\,w_1^2}\ . \qquad (4.113)$$

$trace\,C_F$ ¿

From equation (4.95),

$$trace\,c^{-1}=\frac{5\times10^7w_2+10^6w_1}{959\,w_2^2+8.58\times10^6w_1w_2}+4\times\left(\frac{\left(5\times10^7w_2+7.57\times10^7w_1\right)}{7672\,w_2^2+6.86\times10^7w_1w_2}\right)+\frac{3}{16\,w_1}\ .$$

(4.114)

Using (4.113) and (4.114) in (3.29)gives

$$w_1 = -2.93 \vee 0.43 \qquad (4.115)$$

But $w_1 > 0$, therefore $w_1 = 0.43 \Longrightarrow w_2 = 1 - w_1 = 0.57$ (4.116)

Similarly using(4.91.) and (4.108)for $i = s$ the following is obtained

$$\underset{C_s ¿}{\overset{C}{(¿¿4)^{-2}}} = \begin{bmatrix} v & u & u & u & u & 0 & 0 & 0 \\ g & x & x & x & x & 0 & 0 & 0 \\ g & x & x & x & x & 0 & 0 & 0 \\ g & x & x & x & x & 0 & 0 & 0 \\ g & x & x & x & x & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad (4.117)$$

$$v = \frac{4.8 \times 10^{10} w_2^2 + 2.0 \times 10^{15} w_1 w_2 + 3.66 \times 10^{15} w_1^2}{9.2 \times 10^5 w_2^4 + 1.65 \times 10^{10} w_1 w_2^3 + 7.36 \times 10^{13} w_1^2 w_2^2} .$$

(4.118)

$$u = \frac{-1.7 \times 10^{10} w_2^2 + 7 \times 10^{14} w_1 w_2 + 9.15 \times 10^{16} w_1^2}{9.2 \times 10^5 w_2^4 + 1.65 \times 10^{10} w_1 w_2^3 + 7.36 \times 10^{13} w_1^2 w_2^2} .$$

$$g = \frac{4.8 \times 10^{11} w_2^2 - 4 \times 10^{15} w_1 w_2 - 5 \times 10^{15} w_1^2}{7.36 \times 10^6 w_2^4 + 1.32 \times 10^{11} w_1 w_2^3 + 5.89 \times 10^{14} w_1^2 w_2^2} .$$

$$x = \frac{4.79 \times 10^{10} w_2^2 - 3.96 \times 10^{16} w_1 w_2 - 5.25 \times 10^{15} w_1^2}{7.36 \times 10^6 w_2^4 + 1.32 \times 10^{11} w_1 w_2^3 + 5.89 \times 10^{14} w_1^2 w_2^2} .$$

(4.119)

Thus

$$\underset{trace\, C_s ¿}{\overset{C}{(¿¿4)^{-2}}} = v + 4x$$

$$¿\frac{4.8\times 10^{10}w_2^2+2.0\times 10^{15}w_1w_2+3.66\times 10^{15}w_1^2}{9.2\times 10^5 w_2^4+1.65\times 10^{10}w_1w_2^3+7.36\times 10^{13}w_1^2w_2^2}+4\times\frac{4.79\times 10^{10}w_2^2-3.96\times 10^{16}w_1w_2-5.25\times 10^{15}w_1^2}{7.36\times 10^6 w_2^4+1.32\times 10^{11}w_1w_2^3+5.89\times 10^{14}w_1^2w}$$

.

(4.120)

Using(4.120) and (4.114) in (3.29) and substituting $w_1=1-w_2$ gives

$w_2=0.57\vee 3.93$.

But $w_2>0$, therefore $w_2=0.57\Longrightarrow w_1=1-w_2=0.43$. (4.121)

Hence the values obtained in (4.116) and (4.121) leads to the conclusion that for $i=F,s$, the $A-optimal$ rotatable WCCD is

$$\xi_{WCCD}=0.427\,\xi_F+0.573\,\xi_s \qquad (4.122)$$

4.2.2.4 E-Optimal Rotatable WCCD in Four Factors

From (3.31), $E=\frac{z_1z_1^T}{\|z_1\|^2}$ and z is the iegenvector corresponding to the smallest eigenvalue.

Let d be the eigenvalue for the information matrix (4.92). Then

$$\left|C_k\left(M\left(\xi\right)\right)-d\,I_8\right|=0 \quad .$$

(4.123)

Solving (4.123) gives

$$d_1=\frac{-\left(\sqrt{5.62\times 10^7 w_2^2+1.79\times 10^8 w_1w_2+1.56\times 10^8 w_1^2}\right)-7500\,w_2-12500\,w_1}{5000} \quad .$$

$$d_2=\frac{\left(\sqrt{5.62\times 10^7 w_2^2+1.79\times 10^8 w_1w_2+1.56\times 10^8 w_1^2}\right)+7500\,w_2+12500\,w_1}{5000} \quad .$$

$$d_3=d_4=d_5=2\,w_2 \quad , \quad d_6=d_7=d_8=16\,w_1 \quad , \qquad (4.124)$$

From theorem 3.3, if the smallest eigenvalue for C has multiplicity 1, then the only choice for matrix E is obtained from either d_1 or d_2 . Clearly $d_1<d_2$ and therefore d_1 is the smallest eigenvalue. Therefore:

$$\lambda_{min}(C)=d_1=\frac{-\left(\sqrt{5.62\times10^7 w_2^2+1.79\times10^8 w_1 w_2+1.56\times10^8 w_1^2}\right)-7500w_2-12500w_1}{5000} .$$

(4.125)

The eigenvectors are:

$z_1 \wedge z_2$ do not exist,

$$z_3=\begin{bmatrix}0\\1\\0\\0\\-1\\0\\0\\0\end{bmatrix},\quad z_4=\begin{bmatrix}0\\0\\1\\0\\-1\\0\\0\\0\end{bmatrix},\quad z_5=\begin{bmatrix}0\\0\\0\\1\\-1\\0\\0\\0\end{bmatrix},\quad z_6=\begin{bmatrix}0\\0\\0\\0\\0\\1\\0\\0\end{bmatrix},\quad z_7=\begin{bmatrix}0\\0\\0\\0\\0\\0\\1\\0\end{bmatrix},\quad z_8=\begin{bmatrix}0\\0\\0\\0\\0\\0\\0\\1\end{bmatrix}.$$

But eigenvector z_1 corresponding to the minimum eigenvalue λ_1 does not exist. This therefore means that an $E-optimal$ design for a CCD of $m=4$ factors where the fractional factorial portion is constructed through resolution IV does not exist.

Holger and Yuri (2014) suggested that designs with certain symmetry properties play a particular role for the construction of E-optimal designs. They called a design symmetric if for any $(q_1,\ldots,q_m)\in\{0,1,2\}^m$ with $\|q\|_1=|q_1|+\ldots+|q_m|\le 2$. The moments $\int_\chi x_1^{q_1},\ldots,x_m^{q_m}\xi(dx)$ are invariant with respect to all permutations of $q_1,\ldots,q_m$ and vanish if there is at least one oddindex among $q_1,\ldots q_m$.

4.2.2.5 I - Optimal Rotatable WCCD in Four Factors

$I-optimal$ WCCD for four factors based on the parameter subsystem of interest is derived in this section. From (3.22), the parameter subsystem of interest for $m=4$ is the vector:

$$K^T(\theta)=¿\begin{bmatrix} \theta_0 \\ \theta_{11} \\ \theta_{22} \\ \theta_{33} \\ \theta_{44} \\ \frac{\theta_{12}+\theta_{21}+\theta_{34}+\theta_{43}}{4} \\ \frac{\theta_{13}+\theta_{31}+\theta_{24}+\theta_{42}}{4} \\ \frac{\theta_{14}+\theta_{41}+\theta_{23}+\theta_{32}}{4} \end{bmatrix}.$$

The corresponding regression vector of factors in the parameter subsystem of interest is:

$$f(x)=\begin{bmatrix}1 & x_1^2 & x_2^2 & x_3^2 & x_4^2 & x_1x_2+x_3x_4 & x_1x_3+x_2x_4 & x_1x_4+x_2x_3\end{bmatrix}^T. \quad (4.126)$$

This gives rise to the matrix X with the following entries;

$$X=\begin{bmatrix}1 & f(x_1) & f(x_2) & f(x_3) & f(x_4) & f(x_5) & f(x_6) & f(x_7)\end{bmatrix}^T. \quad (4.127)$$

Thus

$$X = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 1 & 1 & 1 & 1 & -2 & -2 & 2 \\ 1 & 1 & 1 & 1 & 1 & -2 & 2 & -2 \\ 1 & 1 & 1 & 1 & 1 & 2 & -2 & -2 \\ 1 & 1 & 1 & 1 & 1 & 2 & -2 & -2 \\ 1 & 1 & 1 & 1 & 1 & -2 & 2 & -2 \\ 1 & 1 & 1 & 1 & 1 & -2 & -2 & 2 \\ 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 2.83 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2.83 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2.83 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2.83 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2.83 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2.83 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 2.83 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 2.83 & 0 & 0 & 0 \end{bmatrix} \quad (4.128)$$

Let the design ξ_{WCCD} in (3.26) be represented by ξ_{IWCCD} such that

$$\xi_{IWCCD} = w_1 \xi_F + w_2 \xi_s \quad , \quad w_1 + w_2 = 1 \quad \text{and} \quad w_1, w_2 \geq 0 \quad (4.129)$$

Then assuming that support points in the same portion are assigned equal weight, then each of the design points in the cube portion is assigned a mass of $\frac{1}{8}w_1$ while each of the design points in the star portion is assigned a mass of $\frac{1}{8}w_2$.

Then from (4.48)

$$\wedge = \begin{bmatrix} \frac{w_1}{8} I_8 & 0 \\ 0 & \frac{w_2}{8} I_8 \end{bmatrix}, \tag{4.130}$$

Letting $w_2 = 1 - w_1$ then

$$C_4 = X^T \wedge X$$

$$\text{¿} \left[\begin{matrix} 1 & \frac{117w_1+283}{400} & \frac{117w_1+283}{400} & \frac{117w_1+283}{400} & \frac{117w_1+283}{400} & 0 & 0 \\ \frac{117w_1+283}{400} & \frac{8089-4054w_1}{4045} & w_1 & w_1 & w_1 & 0 & 0 \\ \frac{117w_1+283}{400} & w_1 & \frac{8089-4054w_1}{4045} & w_1 & w_1 & 0 & 0 \\ \frac{117w_1+283}{400} & w_1 & w_1 & \frac{8089-4054w_1}{4045} & w_1 & 0 & 0 \\ \frac{117w_1+283}{400} & w_1 & w_1 & w_1 & \frac{8089-4054w_1}{4045} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4w_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4w_1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{matrix} \right. \tag{4.131}$$

From (4.128), point x_1 in the cube portion is used such that

$$f(x_1) = [1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 2 \quad 2 \quad 2]^T \ . \tag{4.132}$$

The left-hand side of the relation (3.35) results in

$$f^T(x_1)(C_4)^{-1}L_3(C_4)^{-1}f(x_1)=\frac{2.55\times10^{17}w_1^2+3.61\times10^9w_1+13}{6.87\times10^{16}w_1^4-1.24\times10^{10}w_1^3+560w_1^2}\quad.$$

(4.133)

Further the right hand side results in

$$tr\left((C_4)^{-1}L_4\right)=\frac{-5.2\times10^{13}w_1^2+4.35\times10^{13}w_1-8099}{1.005\times10^{13}w_1^3-1.005\times10^{13}w_1^2+9.07\times10^5w_1}\quad.$$

(4.134)

Equating (4.133) to (4.134) and solving the equation results in

$$w_1=-1.93\vee0.37 \tag{4.135}$$

But $w_1>0$, therefore:

$$w_1=0.3725\Longrightarrow w_2=1-0.3725=0.6275\quad. \tag{4.136}$$

On evaluating at other points in the factorial portion of the design, the following weights are obtained:

$$f(x_1)\wedge f(x_7)\quad \text{gives}\quad w_1=0.3725\quad,$$

$$f(x_2),f(x_3),f(x_4),f(x_5)\wedge f(x_6)\quad \text{gives}\quad w_1=0.4122\quad. \tag{4.137}$$

Similarly on working out the relation (3.35) using a point in the star portion design say

$$f(x_{13})=[1\quad 0\quad 2.83\quad 0\quad 0\quad 0\quad 0\quad 0]^T\quad,$$

then

$$w_2=0.5976\Longrightarrow w_1=1-0.5976=0.4024\quad. \tag{4.138}$$

But assuming that for optimalityuniform weight is assigned to each design point in the factorial portion, thentakingaverage of the different weights gives:

$$w_1=0.4023\quad.$$

Hence, the $I-optimal$ rotatableWCCD (ξ_{IWCCD}) for four factors is expressed as:

$$\xi_{IWCCD}=0.4024\,\xi_F+0.5976\,\xi_s \quad . \tag{4.139}$$

4.2.3 m - FactorsD-Optimal Rotatable WCCD

In this chapter D-, A-, E and I-optimal rotatable WCCDs for $m=3\wedge 4$ factors constructed through resolutions III and IV have been derived. Results obtained in sections (4.2.1.2) and (4.2.2.2) are usedto obtain a generalized form of D-optimal rotatable WCCD for m factors constructed through resolution R.

Let s be the number of parameters in the subsystem of interest vector $K^{'}(\theta)$. Further let a rotatable CCD of m factors comprise of elementary designs ξ_F and ξ_s i.e. the fractional factorial portion constructed through resolution R and the star portion respectively. Then $D-optimal$ Rotatable Weighted Central Composite Design(ξ_{WCCD})is given by:

$$\xi_{WCCD}=\frac{s-m}{s}\,\xi_F+\frac{m}{s}\,\xi_s \tag{4.140}$$

where $w_1=\frac{s-m}{s}$ and $w_2=\frac{m}{s}$ are the weights assigned to each of the design portions, factorial and starportions respectively.

4.3 Optimal Values and Efficiency

The D-, A-, E- and I-optimality criteria and efficiency explained in section 3.3 are used in this section.

4.3.1 Three Factors Central Composite Design

4.3.1.1 D-, A- and E-optimal Values

Optimal values for resolution III rotatable CCDbased on the D-, A and E-optimality criteria are computed in this section together with the optimal values for the derived optimal rotatable WCCD.

From equation (3.36) and using the information matrix

a) The $D-optimal$ value is

$$V(¿¿0)\left(C_K(M(\xi))\right)=(0.2097159)^{\frac{1}{7}}=0.8. \quad (4.141)$$

b) The $A-optimal$ value is

$$V¿ . \quad (4.142)$$

c) The $E-optimal$ value is

$$V¿ . \quad (4.143)$$

Next, the optimal values for the optimal rotatable WCCDderived in section 4.2.1 are obtained as follows:

a) From (3.36), the $D-optimal$ criterion for the optimal rotatable WCCD is given by

$$\varnothing_0(C)=(det\,C)^{\frac{1}{7}} .$$

Substituting the values of w_1 and w_2 (4.43) in (4.36), then

$$C_k(M(\xi))=\frac{4}{7}C_k(M_{\xi_F})+\frac{3}{7}C_k(M_{\xi_s}) . \quad (4.144)$$

Thus

$$det\left(C_k(M(\xi))\right)=\left|C_k(M(\xi))\right|=\frac{1024\,w_1^4 w_2^3}{27} .$$

Substituting the values of w_1 and w_2, this simplifies to

$$\left|C_k(M(\xi))\right| = ¿\ 0.318312462$$

Therefore D-optimal value is:

$$V(\varnothing_0) = (\det C)^{\frac{1}{7}} = 0.849139593 \tag{4.145}$$

b) From (3.36), the $A-optimal$ criterion for the optimal rotatable WCCD is given by

$$\varnothing_{-1}(C) = \left(\frac{1}{7} trace\, C^{-1}\right)^{-1}$$

Substituting the values of w_1 and w_2 (4.55) in (4.49)

$$trace\, C^{-1} = \frac{54 w_1 + 31 w_2}{4 w_1 w_2} = 41.71$$

Thus the $A-optimal$ value is

$$V(\varnothing_{-1}) = \left(\frac{41.71}{7}\right)^{-1} = 0.168 \tag{4.146}$$

c) From (3.36), the minimum eigenvalue criterion is

$$\varnothing_{-\infty}(C) = \lambda_{min}(C)$$

Thus substituting the values of w_1 and w_2 (4.69) in (4.61), the E $-optimal$ value is

$$V(¿¿-\infty) = \frac{\varnothing - \left(\sqrt{49\left(\frac{21}{37}\right)^2 + 156\left(\frac{16}{37}\right)\left(\frac{21}{37}\right) + 144\left(\frac{16}{37}\right)^2}\right) - 7\left(\frac{21}{37}\right) - 12\left(\frac{16}{37}\right)}{6}¿$$

$$¿\frac{1}{37} = 0.027$$

(4.147)

4.3.1.2 I-optimal Value

Optimal value for resolution III rotatable CCD based on the I-optimality criterion is computed in this section as well as the optimal value for the derived optimal rotatable WCCD.

a) For $m=3$

$$f(x)=\begin{bmatrix}1 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3\end{bmatrix}'$$

Thus

$$C_K(M(\xi))=f(x)f'(x)$$

gives

$$C_K(M(\xi))=\begin{bmatrix}
1 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3\\
x_1^2 & x_1^4 & x_1^2x_2^2 & x_1^2x_3^2 & x_1^3x_2 & x_1^3x_3 & x_1^2x_2x_3\\
x_2^2 & x_1^2x_2^2 & x_2^4 & x_2^2x_3^2 & x_1x_2^3 & x_1x_2^2x_3 & x_2^3x_3\\
x_3^2 & x_1^2x_3^2 & x_2^2x_3^2 & x_3^4 & x_1x_2x_3^2 & x_1x_3^2 & x_2x_3^3\\
x_1x_2 & x_1^3x_2 & x_1x_2^3 & x_1x_2x_3^2 & x_1^2x_2^2 & x_1^2x_2x_3 & x_1x_2^2x_3\\
x_1x_3 & x_1^3x_3 & x_1x_2^2x_3 & x_1x_3^2 & x_1^2x_2x_3 & x_1^2x_3^2 & x_1x_2x_3^2\\
x_2x_3 & x_1^2x_2x_3 & x_2^3x_3 & x_2x_3^3 & x_1x_2^2x_3 & x_1x_2x_3^2 & x_2^2x_3^2
\end{bmatrix} \quad (4.148)$$

From (3.42)

$$L_3=\Gamma 3\times B$$

where

$$B=\int_{S_{3-1}} x_1^{p_1}x_2^{p_2}x_2^{p_3}\,dx_1dx_2dx_3=\frac{\prod_{i=1}^{3}\Gamma(p_i+1)}{\Gamma(3+\sum_{i=1}^{m}p_i)}=\frac{\prod_{i=1}^{3}p_i!}{\left(3-1+\sum_{i=1}^{4}p_i\right)!}, \quad (4.149)$$

p is the power of the factors

and

$$\int_{\chi} dx = \frac{1}{\sqrt{3}}$$

Thus

$$L_3 = \begin{bmatrix} 1 & v & v & v & g & g & g \\ v & w & h & h & n & n & a \\ v & h & w & h & n & a & n \\ v & h & h & w & a & n & n \\ g & n & n & a & h & a & a \\ g & n & a & n & a & h & a \\ g & a & n & n & a & a & h \end{bmatrix} \quad (4.150)$$

with

$$v = \int x_i^2 dx, i = 1, 2, 3, h = \int x_1^2 x_2^2 dx, w = \int x_i^4 dx \quad , \quad a = \int x_i^2 x_j x_k dx \quad ,$$

$$g = \int x_i x_j dx \qquad n = \int x_i^3 x_j dx \quad \text{in each case} \quad i \neq j \neq k \quad (4.151)$$

From (4.13),

$$\left(C_K\left(M(\xi)\right)\right)^{-1} = \begin{bmatrix} 25 & -10 & -10 & -10 & 0 & 0 & 0 \\ -10 & 5 & \frac{15}{4} & \frac{15}{4} & 0 & 0 & 0 \\ -10 & \frac{15}{4} & 5 & \frac{15}{4} & 0 & 0 & 0 \\ -10 & \frac{15}{4} & \frac{15}{4} & 5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{5}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{5}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{8} \end{bmatrix} \quad (4.152)$$

Thus

$$\left(C_K(M(\xi))\right)^{-1}L_3=\begin{bmatrix} r & b & b & b & c & c & c \\ b & d & e & e & f & f & t \\ b & e & d & e & f & t & f \\ b & e & e & d & t & f & f \\ \frac{5g}{8} & \frac{5n}{8} & \frac{5n}{8} & \frac{5a}{8} & \frac{5h}{8} & \frac{5a}{8} & \frac{5a}{8} \\ \frac{5g}{8} & \frac{5n}{8} & \frac{5a}{8} & \frac{5n}{8} & \frac{5a}{8} & \frac{5h}{8} & \frac{5a}{8} \\ \frac{5g}{8} & \frac{5a}{8} & \frac{5n}{8} & \frac{5n}{8} & \frac{5a}{8} & \frac{5a}{8} & \frac{5h}{8} \end{bmatrix} \tag{4.153}$$

Where

$r=25-30v$, $b=-10w+25v-20h$, $c=-20n+25g-10a$

$d=\frac{10w-20v+15h}{2}$, $e=\frac{15w-40v+35h}{4}$, $t=\frac{15n-20g+10a}{2}$,

$f=\frac{35a-40g+15a}{4}$

From (3.43) $I-optimal$ value is equal to:

$$tr[\left(C_K(M(\xi))\right)^{-1}L_3]=r+3d+3\times\frac{5h}{8}$$

$$¿\frac{200-480v+120w+195h}{8}$$

(4.154)

where v , w and h are as defined in (4.154).

Then using (4.151) and (4.154)

$$tr[\left(C_K(M(\xi))\right)^{-1}L_3]$$

$$¿\frac{200}{8}-\frac{480}{8}\int x_1^2dx+\frac{120}{8}\int x_1^4dx+\frac{195}{8}\int x_1^2x_2^2dx \tag{4.155}$$

Using (4.149)

$$\int x_1^2 dx = \frac{\prod_{i=1}^{3} p_i!}{\left(3-1+\sum_{i=1}^{3} p_i\right)!} = 2! \times \frac{2!}{(3-1+2)!} = \frac{1}{6}$$

Similarly

$\lceil m \quad \int x_1 x_2 dx = \frac{1}{12}$, $\quad \lceil m \quad \int t_1^4 dx = \frac{1}{15}$, $\quad \lceil m \quad \int x_1^2 x_2^2 dx = \frac{1}{90}$

$\lceil m \quad \int x_1^3 x_2 dx = \frac{1}{60}$, $\quad \lceil m \quad \int x_1^2 x_2 x_3 dx = \frac{1}{180}$

Thus

$$L_3 = \begin{bmatrix} 1 & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{12} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{6} & \frac{1}{15} & \frac{1}{90} & \frac{1}{90} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} \\ \frac{1}{6} & \frac{1}{90} & \frac{1}{15} & \frac{1}{90} & \frac{1}{60} & \frac{1}{18} & \frac{1}{60} \\ \frac{1}{6} & \frac{1}{90} & \frac{1}{90} & \frac{1}{15} & \frac{1}{18} & \frac{1}{60} & \frac{1}{60} \\ \frac{1}{12} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} & \frac{1}{90} & \frac{1}{18} & \frac{1}{18} \\ \frac{1}{12} & \frac{1}{60} & \frac{1}{18} & \frac{1}{60} & \frac{1}{18} & \frac{1}{90} & \frac{1}{18} \\ \frac{1}{12} & \frac{1}{18} & \frac{1}{60} & \frac{1}{60} & \frac{1}{18} & \frac{1}{18} & \frac{1}{90} \end{bmatrix}$$

(4.156)

and

$$I-optimal\,value = 16.2708 \qquad (4.157)$$

b) Now on substituting the values of the weights in (4.79), the information matrix for a design that is $I-optimal$ becomes:

$$C=\begin{bmatrix} 1 & 0.79 & 0.79 & 0.79 & 0 & 0 & 0 \\ 0.79 & 1.21 & 0.38 & 0.38 & 0 & 0 & 0 \\ 0.79 & 0.38 & 1.21 & 0.38 & 0 & 0 & 0 \\ 0.79 & 0.38 & 0.38 & 1.21 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.38 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.38 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.38 \end{bmatrix}$$

(4.158)

Then from (3.43) the corresponding $I-optimal$ value is

$$tr\left(C^{-1}L_3\right)=16.2942 \qquad (4.159)$$

4.3.2 Four Factors Central Composite Design

4.3.2.1 D-, A- and E-optimal Values

Optimal values for resolution IV rotatable CCD and for the derived optimal rotatable WCCD based on the D-, A and E-optimality criteria are computed in this section.

From equation (3.36) and using matrix (4.26)

a) The $D-optimal$ value is:

$$\varnothing$$

$$V(¿¿0)\left(C_K\left(M(\xi)\right)\right)=(56.32)^{\frac{1}{8}}=1.655 \qquad (4.160)$$

¿

b) The $A-optimal$ value is:

∅
¿
V ¿
¿

(4.161)

c) The $E-optimal$ value is:

∅
¿
V ¿
¿

(4.162)

Next, the optimal values for the optimal rotatable WCCD derived in section 4.2.2 are computed.

a) From (3.36), the optimal criterion for the $D-optimal$ rotatable WCCD is given by

$$\varnothing_0(C)=(det\,C)^{\frac{1}{8}}$$

Substituting the values of w_1 and w_2 in (4.92)

$$C_k(M(\xi))=0.50\,C_k(M_{\xi_F})+0.50\,C_k(M_{\xi_s}) \quad (4.163)$$

The determinant is

$$det(C_k(M(\xi)))=|C_k(M(\xi))|=\frac{4.91\times10^5 w_1^3 w_2^5+4.39\times10^9 w_1^4 w_2^4}{390625}$$

And substituting the values of w_1 and w_2 this simplifies to

$$|C_k(M(\xi))|=43.93451$$

Therefore D-optimal value is

$$V(\varnothing_0)=(de\,t\,C)^{\frac{1}{8}}=43.93451^{\frac{1}{8}}=1.605 \quad (4.164)$$

b) From (3.36), the $A-optimal$ criterion for the optimal rotatable WCCD is given by

$$\varnothing_{-1}(C)=\left(\frac{1}{8}trace\,C^{-1}\right)^{-1}$$

Substituting the values of w_1 and w_2 in (4.114)gives

$$trace\,c^{-1}=\frac{5\times10^7 w_2+10^8 w_1}{959\,w_2^2+8.58\times10^6 w_1 w_2}+4\times\left(\frac{(5\times10^7 w_2+7.57\times10^7 w_1)}{7672\,w_2^2+6.86\times10^7 w_1 w_2}\right)+\frac{3}{16\,w_1} ¿48.95$$

(4.165)

Thus the $A-optimal$ value is

$$V(\varnothing_{-1})=\left(\frac{1}{8}trace\,C^{-1}\right)^{-1}=0.163 \quad (4.166)$$

4.3.2.2 I-optimal Value

Optimal value for resolution IV rotatable CCD and for the derived optimal rotatable WCCD based on the I-optimality criterion is computed in this section.

a) For $m=4$

$$f(x)=\left[1 \quad x_1^2 \quad x_2^2 \quad x_3^2 \quad x_4^2 \quad x_1x_2+x_3x_4 \quad x_1x_3+x_2x_4 \quad x_1x_4+x_2x_3\right]'$$

Let $x_1=a, x_2=b, x_3=c, x_4=d$

Therefore

$$1$$
$$a^2$$
$$b^2$$
$$c^2$$
$$d^2$$
$$cd+ab$$
$$bd+ac$$
$$ad+bc$$
$$a^2$$
$$a^4$$
$$a^2b^2$$
$$a^2c^2$$
$$a^2d^2$$
$$a^2(cd+ab)$$
$$a^2(bd+ac)$$
$$a^2(ad+bc)$$
$$b^2$$
$$a^2b^2$$
$$b^4$$
$$b^2c^2$$
$$b^2d^2$$
$$b^2(cd+ab)$$
$$b^2(bd+ac)$$
$$b^2(ad+bc)$$
$$c^2$$
$$a^2c^2$$
$$b^2c^2$$
$$c^4$$
$$c^2d^2$$
¿

$c^2(cd+ab)$	$c^2(bd+ac)$	$c^2(ad+bc)$	d^2	a^2d^2	b^2d^2	c^2d^2	d^4
$d^2(cd+ab)$	$d^2(bd+ac)$	$d^2(ad+bc)$	$cd+ab$	$cd+ab$	¿	$b^2(cd+ab)$	¿
$c^2(cd+ab)$	¿	$d^2(cd+ab)$	¿	$(cd+ab)^2$	¿	y	¿
y	¿	$bd+ac$	¿	$a^2(bd+ac)$	¿	$b^2(bd+ac)$	¿
$c^2(bd+ac)$	¿	$d^2(bd+ac)$	a^2¿	¿	¿	¿	¿
¿	¿	¿	¿	¿	¿	¿	¿

$C_K(M(\xi))=$¿

(4.167)

Where $y=(bd+ac)(cd+ab)$

From (3.42) $L_4 = \Gamma 4 \times B$ with

$$B = \int_{S_{4-1}} x_1^{p_1} x_2^{p_2} x_2^{p_3} x_4^{p_4} dx_1 dx_2 dx_3 dx_4 = \frac{\prod_{i=1}^{4} \Gamma(p_i+1)}{\Gamma(4+\sum_{i=1}^{m} p_i)} = \frac{\prod_{i=1}^{4} p_i!}{\left(4-1+\sum_{i=1}^{4} p_i\right)!} \quad (4.168)$$

where p is the power of the factors and

$$\int_{\chi} dx = \frac{1}{\Gamma 4}$$

Thus

$$L_4 = \begin{bmatrix} 1 & p & p & p & p & q & q & q \\ p & r & g & g & g & t & t & t \\ p & g & r & g & g & t & t & t \\ p & g & g & r & g & t & t & t \\ p & g & g & g & r & t & t & t \\ q & t & t & t & t & u & t & t \\ q & t & t & t & t & t & u & t \\ q & t & t & t & t & t & t & u \end{bmatrix} \quad (4.169)$$

where

$p = \int x_i^2 dx, i = 1, 2, 3, 4$, $\qquad g = \int x_1^2 x_2^2 dx, i \neq j$

$u = \int (x_i x_j + x_k x_l)^2 dx$, $\qquad r = \int x_i^4 dx$

$q = \int (x_i x_j + x_k x_l) dx$ (Sum of two-factor interactions)

$t = \int x_i^2 (x_i x_j + x_k x_l) dx$, $\qquad u = \int (x_i x_j + x_k x_l)^2 dx \quad$ (4.170)

And in each case $i \neq j \neq k \neq l$

And from (4.26)

$$\left(C_K\left(M\left(\xi\right)\right)\right)^{-1}=\begin{bmatrix} \frac{300}{11} & \frac{-85}{11} & \frac{-85}{11} & \frac{-85}{11} & \frac{-85}{11} & 0 & 0 & 0 \\ \frac{-85}{11} & \frac{133}{44} & \frac{89}{44} & \frac{89}{44} & \frac{89}{44} & 0 & 0 & 0 \\ \frac{-85}{11} & \frac{89}{44} & \frac{133}{44} & \frac{89}{44} & \frac{89}{44} & 0 & 0 & 0 \\ \frac{-85}{11} & \frac{89}{44} & \frac{89}{44} & \frac{133}{44} & \frac{89}{44} & 0 & 0 & 0 \\ \frac{-85}{11} & \frac{89}{44} & \frac{89}{44} & \frac{89}{44} & \frac{133}{44} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{8} \end{bmatrix} \tag{4.171}$$

Therefore

$$\left(C_K\left(M\left(\xi\right)\right)\right)^{-1}L_4=\begin{bmatrix} a & b & b & b & b & b & b & b \\ c & d & e & e & e & f & f & f \\ c & e & d & e & e & f & f & f \\ c & e & e & d & g & f & f & f \\ c & e & e & e & d & t & t & t \\ \frac{q}{8} & \frac{t}{8} & \frac{t}{6} & \frac{t}{8} & \frac{t}{8} & \frac{u}{8} & \frac{t}{8} & \frac{t}{8} \\ \frac{q}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{u}{8} & \frac{t}{8} \\ \frac{q}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{t}{8} & \frac{u}{8} \end{bmatrix} \tag{4.172}$$

where

$$a=\frac{-340p-300}{11}\;,\qquad b=\frac{-85r-300p+255g}{11}\;,\qquad c=\frac{100p-85}{11}$$

$$d=\frac{133r-340p+267g}{44}\;,\qquad e=\frac{89r-340p+311g}{44}\;,\qquad f=\frac{100t-85q}{11}$$

From (3.31) $I-optimal$ value is equal to:

$$tr[(C_K(M(\xi)))^{-1}L_4]=\frac{300-680p+133r+267g}{11}+\frac{3u}{8} \quad (4.173)$$

where p , r , g and u are as defined in (4.170).

Thus using (4.170) and (4.173)

$$tr[(C_K(M(\xi)))^{-1}L_4]$$

$$¿\frac{300}{11}-\frac{680}{11}\int x_1^2dx+\frac{133}{11}\int x_1^4dx+\frac{267}{11}\int x_1^2x_2^2dx+\frac{3}{8}\int(x_ix_j+x_kx_l)^2dx$$

for $i\neq j\neq k\neq l$ (4.174)

Using (4.160)

$$\lceil m \quad \int x_1^2dx=\frac{\prod_{i=1}^{4}p_i!}{(4-1+\sum_{i=1}^{4}p_i)!}3!\times\frac{2!}{(4-1+2)!}=\frac{1}{10}$$

Similarly

$$\lceil m \quad \int x_1x_2dx=\frac{1}{20}, \quad \lceil m \quad \int x_1^4dx=\frac{1}{35}, \quad \lceil m \quad \int x_1^2x_2^2dx=\frac{1}{210}$$

$$\lceil m \quad \int x_1^3x_2dx=\frac{1}{140}, \quad \lceil m \quad \int x_1^2x_2x_3dx=\frac{1}{420}, \quad \lceil m \quad \int x_1x_2x_3x_4dx=\frac{1}{840}$$

(4.175)

Thus substituting these values in (4.169) and (4.174) gives

$$L_4=\begin{bmatrix} 1 & \frac{1}{10} & \frac{1}{10} & \frac{1}{10} & \frac{1}{10} & \frac{1}{10} & \frac{1}{10} & \frac{1}{10} \\ \frac{1}{10} & \frac{1}{35} & \frac{1}{210} & \frac{1}{210} & \frac{1}{210} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{210} & \frac{1}{35} & \frac{1}{210} & \frac{1}{210} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{210} & \frac{1}{210} & \frac{1}{35} & \frac{1}{210} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{210} & \frac{1}{210} & \frac{1}{210} & \frac{1}{35} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{84} & \frac{1}{105} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{84} & \frac{1}{105} \\ \frac{1}{10} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{105} & \frac{1}{84} \end{bmatrix}$$

(4.176)

And

$$I-optimality=\frac{300}{11}-\frac{680}{11}\times\frac{1}{10}+\frac{133}{11}\times\frac{1}{35}+\frac{267}{11}\times\frac{1}{210}+\frac{3}{8}\times\frac{1}{84}$$

$$¿21.556 \qquad (4.177)$$

b) Now on substituting the values of the weights in (4.131), the information matrix for a design that is $I-optimal$ becomes:

$$C=X^T\wedge X=\begin{bmatrix} 1 & 0.825 & 0.825 & 0.825 & 0.825 & 0 & 0 & 0 \\ 0.825 & 1.596 & 0.402 & 0.402 & 0.402 & 0 & 0 & 0 \\ 0.825 & 0.402 & 1.596 & 0.402 & 0.402 & 0 & 0 & 0 \\ 0.825 & 0.402 & 0.402 & 1.596 & 0.402 & 0 & 0 & 0 \\ 0.825 & 0.402 & 0.402 & w_1 & 1.596 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.609 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.609 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.609 \end{bmatrix} \qquad (4.178)$$

Consequently, the optimal value for the $I-optimal$ weighted rotatable central composite design is:

$$tr\left(C^{-1}L_4\right)=26.78401 \tag{4.179}$$

4.3.3 m - Factors Design Optimal Values

In this section, results obtained in sections (4.2.1.1) and (4.2.2.1)are used to obtain a generalized form of D- and I- optimal values for m factors WCCD constructed through resolution R.

4.3.3.1 m - Factors D-Optimal Value

From (3.26) the D-optimal value is given by $\varnothing_0(C)=(det\,C)^{\frac{1}{s}}$ here s is the number of parameters in the subsystem of interest.The determinant of the information matrix is obtained by use of the formula for computing determinant of a partitioned symmetric matrix.

By definition, if $A=\begin{bmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{bmatrix}$, then the determinant of A is given by:

$$|A|=|A_{22}|\left|A_{11}-A_{12}A_{22}^{-1}A_{12}^T\right|=|A_{11}|\left|A_{22}-A_{12}^TA_{11}^{-1}A_{12}\right| .$$

Partition the general information matrix (4.41) such that

$$C_k(M(\xi))=\begin{bmatrix} U & \varnothing^T \\ \varnothing & V \end{bmatrix} \tag{4.180}$$

where $U=\begin{bmatrix} 1 & \frac{1}{N}\left(F+2\alpha^2\right)\left(1_m\right)^T \\ \frac{1}{N}\left(F+2\alpha^2\right)1_m & \frac{1}{N}G_m \end{bmatrix}$ and $V=\frac{2}{N}\left(F+\alpha^4\right)I_c$.

Then the determinant of (4.180) equal to

$$\left|C_k(M(\xi))\right|=|V|\left|U-\varnothing^TV\varnothing^T\right|=|V||U| \tag{4.181}$$

Now V is a $c\times c$ diagonal matrix (c is the number of parameters resulting from averaging the interaction factors)

Hence $|V| = \left(\frac{2}{N}\left(F+\alpha^4\right)\right)^c$ (4.182)

Next $|U| = |U_{11}|\left|U_{22} - U_{12}^T U_{11}^{-1} U_{12}\right|$

$$¿\left|\frac{1}{N}G_m - \frac{1}{N}\left(F+2\alpha^2\right)1_m \times \frac{1}{N}\left(F+2\alpha^2\right)\left(1_m\right)^T\right|$$

1
$¿$
$¿$
$\frac{1}{N}G_m - \frac{1}{N^2}\left(F+2\alpha^2\right)^2 ¿$ (4.183)
$¿¿$

Substituting G_m from(4.29)

$F+2\alpha^4 ¿ I_m + F\sum_{i\neq j=1}^{m} e_i e_j^T$
1
$¿$
$¿$
$¿ - \frac{1}{N^2}\left(F+2\alpha^2\right)^2 ¿$ (4.184)
$\frac{1}{N} ¿$
$|U| = ¿$

Thus (4.181) leads to

$F+2\alpha^4 ¿ I_m + F\sum_{i\neq j=1}^{m} e_i e_j^T$
1
$¿$
$¿$
$¿ - \frac{1}{N^2}\left(F+2\alpha^2\right)^2 ¿$
$\frac{1}{N} ¿$
$\left(\frac{2}{N}\left(F+\alpha^4\right)\right)^c \times ¿$

$$NF+2\alpha^4 ¿ I_m + NF \sum_{i \neq j=1}^{m} e_i e_j^T - \left(F+2\alpha^2\right)^2 J_m$$

$$\frac{1}{N^2} \left| ¿ \right| \qquad (4.185)$$

$$¿ \left(\frac{2}{N}\left(F+\alpha^4\right) \right)^c \times ¿$$

where I_m is an $m \times m$ identity matrix, J_m is an $m \times m$ matrix of ones and $e_i ' s$ are the Euclidean unit vectors in R^m denoted by $e_{1,} e_2 , \ldots , e_m$.

Consequently, D-optimal value is obtained using formula (3.36) as:

$$F+2\alpha^4 ¿ I_m + NF \sum_{i \neq j=1}^{m} e_i e_j^T - \left(F+2\alpha^2\right)^2 J_m$$

$$\left(\frac{2}{N}\left(F+\alpha^4\right) \right)^c \times \left| \frac{1}{N^2} \left| N ¿ \right| \right]$$

$$¿$$

$$¿ ¿$$

$$V\left(\varnothing_0\right) ¿$$

(4.186)

4.3.3.2 m - Factors I-Optimal Rotatable WCCD

In this section a general form of the $I-optimal$ value for $m-factors$ is given. In sections(4.3.1.2) and (4.3.2.2), $I-optimal$ values for the Rotatable CCD for three and fourfactors respectively are derived. Each of the values is a linear function of order four moments. Therefore generally for m factors

$$I-optimality = tr\left[\left(C_K\left(M\left(\xi\right)\right) \right)^{-1} L_m \right] \qquad (4.187)$$

where $C_K\left(M\left(\xi\right)\right)$ equal to the information matrix (4.29).

$L_m = \Gamma\left(m\right) \times B$,

$$B = \int_{s_{q-1}} x_1^{p_1} x_2^{p2} \ldots x_m^{p_m} dx_1 dx_2 \ldots dx_m = \frac{\prod_{i=1}^{m} p_i !}{\left(m - 1 + \sum_{i=1}^{m} p_i \right)!}$$

, p is the power of the factors and m is the number of factors.

Computing (4.187) results to

$I-optimality$

$$¿\beta_0 - \frac{\beta_1}{3m-1}\mu_2 + \frac{\beta_2}{3m-1}\mu_4 + \frac{\beta_3}{3m-1}\mu_{22} + \beta_4 \int (x_i x_j + x_k x_l)^2 dx$$

where β_i is a multiple of $\sqrt{m}$ and $i=1,2,\ldots,m$.

(4.188)

4.3.4 Numerical Results and Efficiency

In this section,theoretical results obtained insection 4.1, 4.2 and 4.3 are presented in table form. Tables 4.3, 4.4, 4.5 and 4.6presents the respective optimal values for the uniform weighted CCD and the optimal rotatable WCCD for three, four and five factors. Their corresponding relative efficiencies are computed using the ratios given in (3.45), (3.46), (3.47) and (3.48). The amount of mass assigned to each of the two portions (cube and star portions) of the optimal rotatable WCCDs are also given.

Table 4.3. D-optimal Rotatable Designs

m-Factors	Resolution R	Uniform weighted CCD	WCCD	Efficiency	Weights

3	*III*	0.8	0.84	0.9524	$w_1=\frac{4}{7}$	$w_2=\frac{3}{7}$
4	*IV*	1.66	1.60	1.0376	$w_1=\frac{1}{2}$	$w_2=\frac{1}{2}$
5	*V*	1.53	1.54	0.99	$w_1=\frac{11}{16}$	$w_2=\frac{5}{16}$

D-optimal WCCD for resolution *III* exists and the relative efficiency is 0.95. The amount of mass assigned to the cube portion in the resolution *III* design is greater than in the star portion as it is the case for resolution *V* design. Resolution *IV* WCCD also exists and the relative efficiency is slightly more than one. On the other hand, equal weight is assigned to both the cube and star portions.

Table 4.4. A-optimal Rotatable Designs

m-Factors	Resolution R	Uniform weighted CCD	WCCD	Efficiency	Weights	
3	*III*	0.1672	0.1678	1.004	$w_1=0.4311$	$w_2=0.5689$
4	*IV*	0.2013	0.1634	0.8119	$w_1=0.4270$	$w_2=0.5730$
5	*V*	1.53	1.54	1.0114	$w_1=0.4644$	$w_2=0.5356$

A-optimal WCCD for resolution *III* exists and the relative efficiency is greater than one. The same observation is made for resolution *V* design. Resolution *IV* WCCD also exists but it's relative efficiency is less than one. The amount of mass assigned to the cube portion in the three designs is less than in the star portion.

Table 4.5. E-optimal Rotatable Designs

m-Factors	Resolution R	Uniform weighted CCD	WCCD	Efficiency	Weights

3	*III*	0.0269	0.0270	0.996	$w_1=\frac{16}{37}$	$w_2=\frac{21}{37}$
4	*IV*	0.0277	$-¿$	$-¿$	$-¿$	$-¿$
5	*V*	0.0089	0.01	0.89	$w_1=\frac{46}{101}$	$w_2=\frac{55}{101}$

E-optimal WCCD for resolution III exists and the relative efficiency is near one. But for resolution V design the efficiency 0.89. The amount of mass assigned to the cube portion is less than the star portion in the two designs.From the theoretical results in section 4.2.2.4, an E-optimal resolution IV WCCD does not exist.

Table 4.6. I-optimal Rotatable Designs

m-Factors	Resolution R	Uniform weighted CCD	WCCD	Efficiency	Weights	
3	*III*	16.2708	16.294	1.001	$w_1=0.38$	$w_2=0.62$
4	*IV*	21.556	26.784	1.2425	$w_1=0.3725$	$w_2=0.6275$

I-optimal WCCD for both designs exist and the relative efficiency is one for Resolution III design but greater than 1 for resolution IV design. Further a greater weight is assigned to the star portion than the cube portion in both designs.

4.4 Data Analysis

Rotatable CCDs have been constructed through resolutions III and IV. Further, optimal rotatable WCCDs for three and four factors have been investigated under the $D-, A-, E-¿$ and $I-optimality$ criteria and the corresponding optimal values computed.Thissectionpresentsan application on optimization of a four factor CCD to determine effects on whiteness of cotton using the data described in section 3.4. A full quadratic model and a reduced quadratic model namely the second – order Kronecker model each with a constant termwere fitted. A mathematical solution for the location of the Stationary Point was obtained by carrying out astationarityand matrix analysis for the two models and design efficiency was determined. Contour and response surface plots were also plotted.

4.4.1 Optimization of Effects on Whiteness of Cotton using full CCD

The results in this section are based on the second-order Kronecker model given in (3.4)expressed as:

$$Y_x = f(x)'\theta + \varepsilon = \theta_0 + \sum_{i=1}^{m} \theta_i x_i + \sum_{i=1}^{m} \theta_{ii} x_i^2 + \sum_{i,j=1}^{m} (\theta_{ij} + \theta_{ji}) x_i x_j + \varepsilon_i \qquad (4.189)$$

The model errors ε_i are assumed to have constant variance, are uncorrelated and homoscedastic and are also independent normal.

The initial design has $(1+m+m^2)$ parameters while the information matrix for the subsystem parameters of interest is of order $(1+m+c)$ where m is the number of factors and c is the number of factors resulting from averaging the repeated interaction factors.

Most often in response surface methodology, the natural variables $\zeta_1, \zeta_2, \ldots, \zeta_m$ are transformed to coded variables $x_1, x_2, \ldots, x_m$ which are dimensionless with mean zero and equal variance. The variables Temperature (TEMP), Bleach Activator (BC), pH and Peracetic Acid (PAA) are natural variables expressed in the natural units of measurement. Codedvariables in the $(-1,1)$ interval were used. The natural variables are transformed to the coded variables T, B, H and P respectively using the formulae:

$$T=\frac{TEMP-60}{10}\quad,\qquad B=\frac{BC-1.5}{0.75}\quad,\qquad H=\frac{pH-7.5}{0.5}\quad,\quad P=\frac{PAA-15}{5}$$

(4.190)

The coded variables and the corresponding natural variablesare given as.

Coded Levels

Factors	$-\alpha$	-1	0	1	α
T	40	50	60	70	80
B	0	0.75	1.5	2.25	3
H	6.5	7	7.5	8	8.5
P	5	10	15	20	25

(4.191)

Table 4.7 presents the data set including the natural and coded variables as well as the response variable.

Table 4.7. Data Set for Full CCD

	Natural Variables				Coded Variables				Response Variable
Runs	TEMP	BC	pH	PAA	T	B	H	P	Index
1	50	0.75	7.0	10	-1	-1	-1	-1	68.0

2	70	0.75	7.0	10	1	-1	-1	-1	81.7
3	50	2.25	7.0	10	-1	1	-1	-1	68.9
4	70	2.25	7.0	10	1	1	-1	-1	83.5
5	50	0.75	8.0	10	-1	-1	1	-1	73.8
6	70	0.75	8.0	10	1	-1	1	-1	82.2
7	50	2.25	8.0	10	-1	1	1	-1	76.4
8	70	2.25	8.0	10	1	1	1	-1	84.2
9	50	0.75	7.0	20	-1	-1	-1	1	76.0
10	70	0.75	7.0	20	1	-1	-1	1	86.2
11	50	2.25	7.0	20	-1	1	-1	1	77.1
12	70	2.25	7.0	20	1	1	-1	1	86.6
13	50	0.75	8.0	20	-1	-1	1	1	78.8
14	70	0.75	8.0	20	1	-1	1	1	87.3
15	50	2.25	8.0	20	-1	1	1	1	78.8
16	70	2.25	8.0	20	1	1	1	1	87.3
17	40	1.50	7.5	15	-2	0	0	0	68.2
18	80	1.50	7.5	15	2	0	0	0	87.1
19	60	0.00	7.5	15	0	-2	0	0	79.0
20	60	3.00	7.5	15	0	2	0	0	81.7
21	60	1.50	6.5	15	0	0	-2	0	77.6
22	60	1.50	8.5	15	0	0	2	0	81.8
23	60	1.50	7.5	5	0	0	0	-2	71.9
24	60	1.50	7.5	25	0	0	0	2	83.2
25	60	1.50	7.5	15	0	0	0	0	81.1
26	60	1.50	7.5	15	0	0	0	0	81.5
27	60	1.50	7.5	15	0	0	0	0	81.8
28	60	1.50	7.5	15	0	0	0	0	81.3
29	60	1.50	7.5	15	0	0	0	0	81.7
30	60	1.50	7.5	15	0	0	0	0	81.7

Next, a scatter plot matrix for the above data is presented.

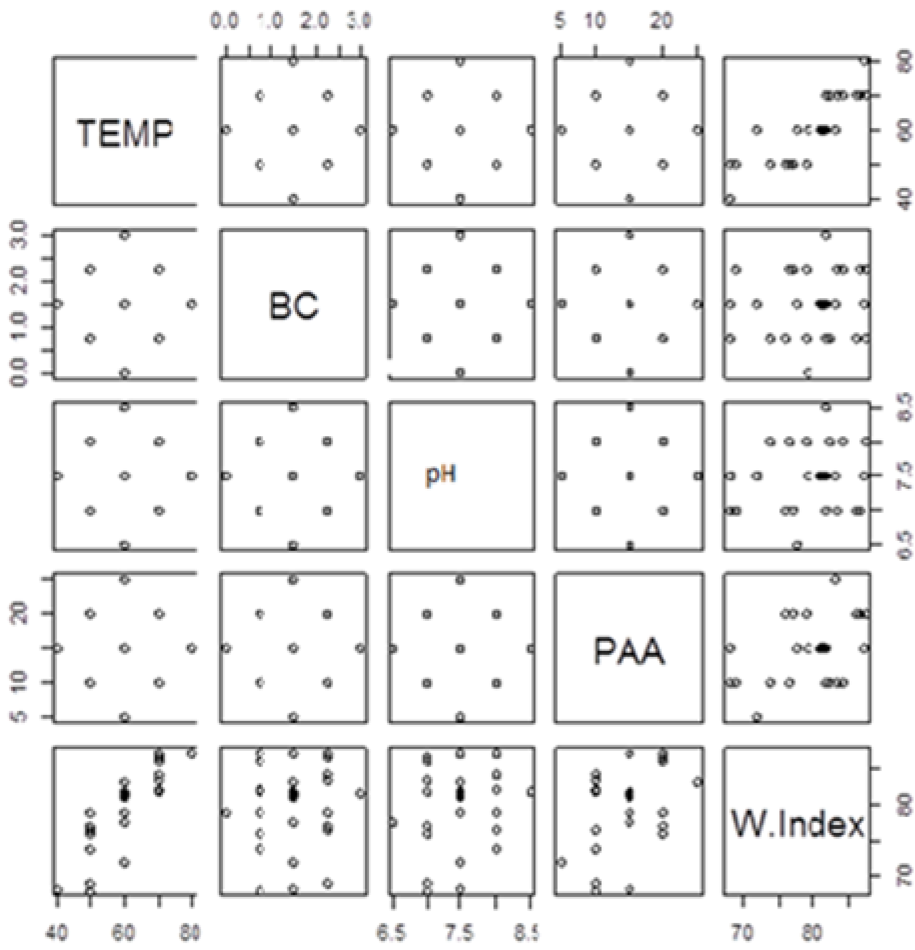

Figure 4.1. Scatter Plot Matrix

The squares in the fifth row presents the respective scatter plots of the whiteness Index against each of the explanatory variables TEMP, BC, Ph and PAA respectively. From the scatter matrix,as the temperature increases, the whiteness index increases thus showing a highpositivecorrelation between the response variable (whiteness index) and temperature. There is no linear correlation between the response variable and either bleach activator or pH (BC and Ph). But there is a very weak linear correlation betweenthe whiteness index and peraceticacid.The correlation generally is curved.

The response surface can also be visualized graphically using the graphs known as response surface plots that are helpful to see the shape of the response surface. An example of the plots arethe contour plots on which the shape of the response surface may be observed as hills, valleys or ridge lines. But for more than two independent variables, it is a bit difficult to interpret and thus a response surface model is essential to analyze the response surface function.

Thecontour plots and response surfaces are drawn for each two explanatory variables and the response variable while holding the other twoexplanatoryvariablesconstant. Observation of the plots and surfaces indicates that anoptimum point exists. The darker regions identify higher response values.

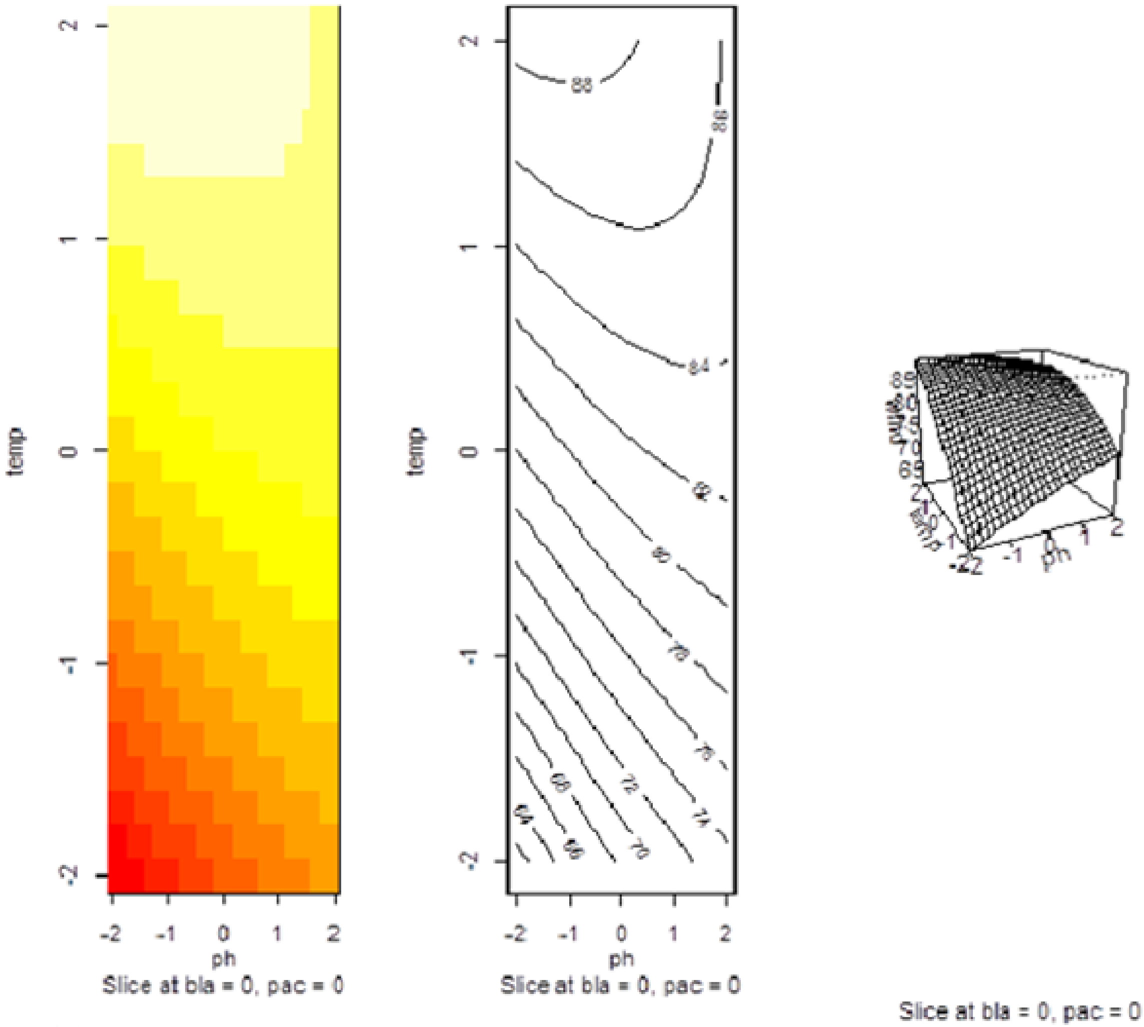

Figure 4.2. Temperature and pH

The contours shows a rising ridge pattern and that the response surface is at a maximum value of about 86 at the interaction of a pH of 7.75 and a temperature of 71℃ .

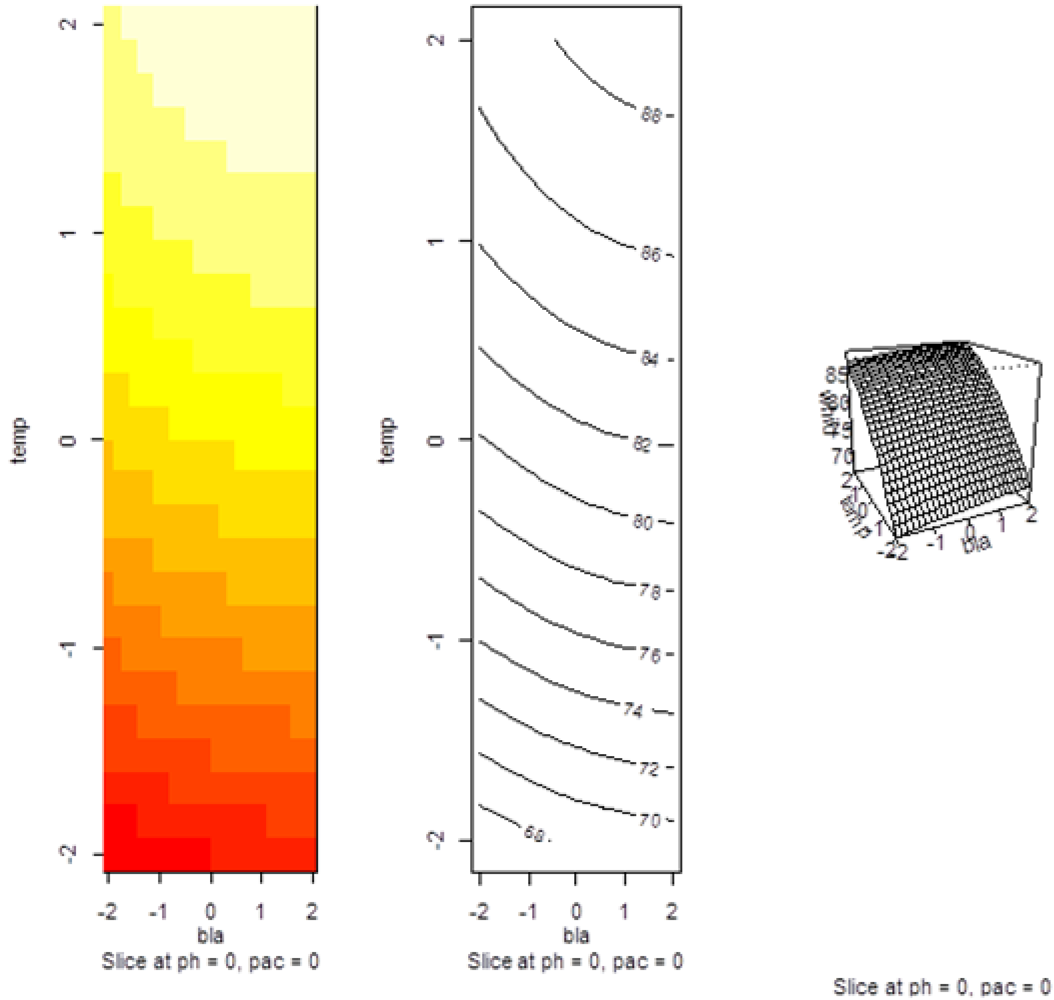

Figure 4.3. Temperature and Bleach A.

The contour plotshows an almost stationary ridge pattern indicating that the interaction between temperature and bleach activator had little or no effect on the whiteness index.

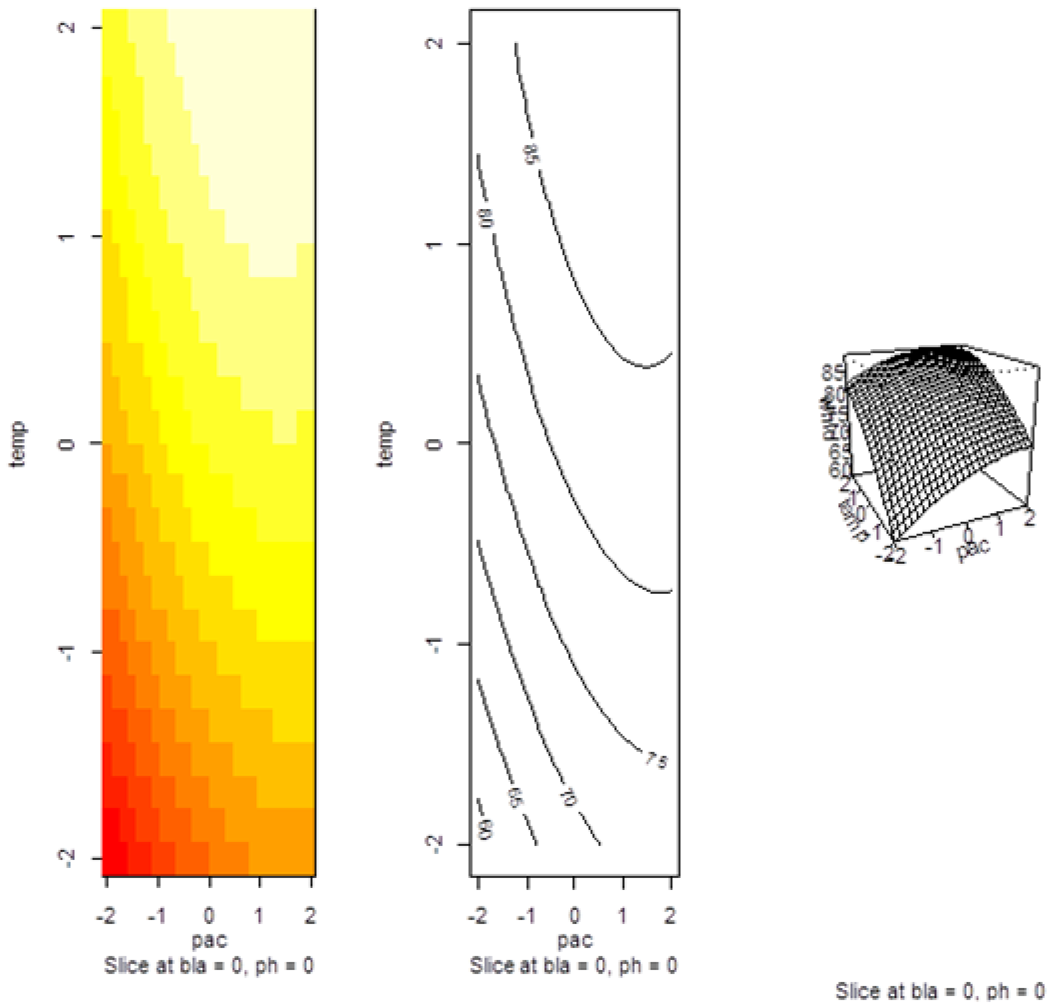

Figure 4.4. Temperature and P. Acid

The contour lines show a rising ridge pattern and the response surface plot indicates that a maximum point exists at the interaction of temperature and peracetic acid.

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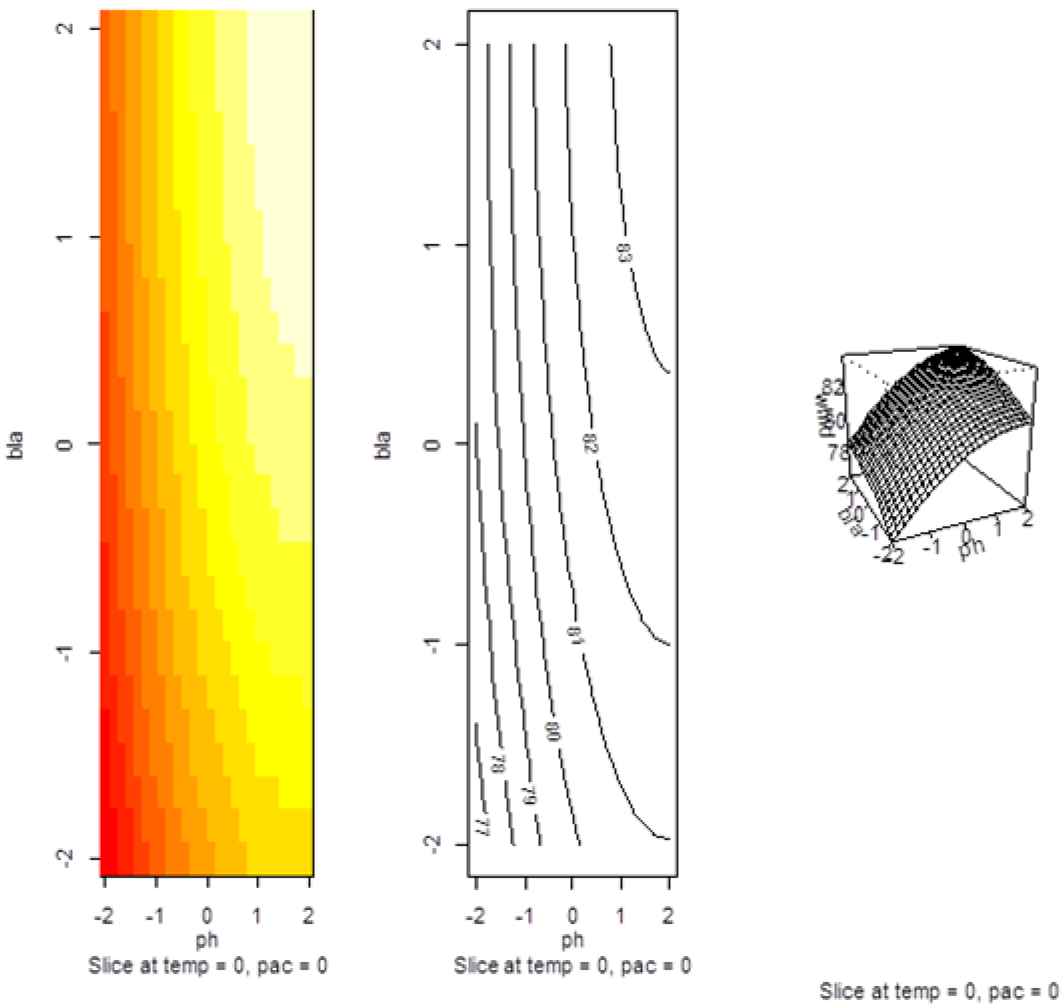


Figure 4.5. Bleach Activator and pH

From the response surface plot, it can be observed that the interaction of bleach activator and pH had effect on the whiteness index. The contour plot represents a rising ridge.

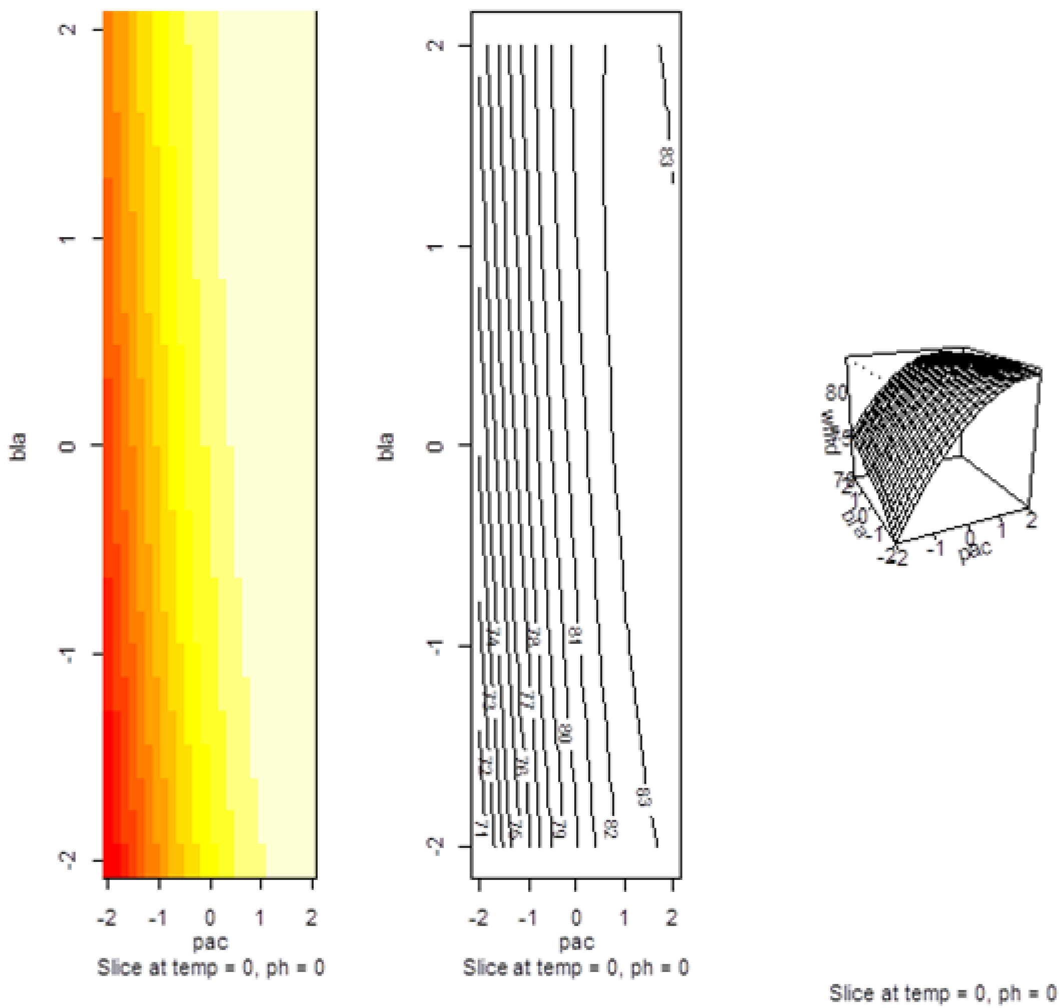


Figure 4.6.Bleach A. and Peracetic Acid

The response surface plot shows there is a maximum point at the interaction of bleach actvator and peracetic acid thus the two had some effect on the whiteness index.

A full parameter second –order model for the above data set is fitted using R-software.

The following is the R print out of the analysis:

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  81.5167     0.4005 203.533  < 2e-16 ***
T             4.9667     0.2003  24.802 1.37e-13 ***
B             0.5833     0.2003   2.913 0.010709 *
H             1.2083     0.2003   6.034 2.29e-05 ***
P             2.5750     0.2003  12.859 1.67e-09 ***
I(T * T)     -0.8000     0.1873  -4.271 0.000670 ***
I(B * B)     -0.1250     0.1873  -0.667 0.514713
I(H * H)     -0.2875     0.1873  -1.535 0.145654
I(P * P)     -0.8250     0.1873  -4.404 0.000513 ***
T:B          -0.0375     0.2453  -0.153 0.880516
T:H          -0.9375     0.2453  -3.822 0.001665 **
T:P          -0.5000     0.2453  -2.039 0.059515 .
B:H           0.0375     0.2453   0.153 0.880516
B:P          -0.3500     0.2453  -1.427 0.174049
H:P          -0.5000     0.2453  -2.039 0.059515 .
---
Signif.codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.981 on 15 degrees of freedom
Multiple R-squared:  0.9833,    Adjusted R-squared:  0.9677
F-statistic: 63.12 on 14 and 15 DF, p-value: 9.743e-11

Analysis of Variance Table

Response: WD
Df Sum Sq Mean Sq  F value    Pr(>F)
T          1 592.03  592.03 615.1281 1.368e-13 ***
B          1   8.17    8.17   8.4853 0.0107094 *
H1  35.04   35.04  36.4090 2.288e-05 ***
P          1 159.13  159.13 165.3446 1.672e-09 ***
I(T * T)   1  12.64   12.64  13.1337 0.0024993 **
I(B * B)   1   0.01    0.01   0.0058 0.9400720
I(H * H)   1   0.81    0.81   0.8372 0.3746608
I(P * P)   1  18.67   18.67  19.3970 0.0005126 ***
T:B        1   0.02    0.02   0.0234 0.8805161
T:H        1  14.06   14.06  14.6112 0.0016650 **
T:P        1   4.00    4.00   4.1561 0.0595148 .
B:H        1   0.02    0.02   0.0234 0.8805161
B:P        1   1.96    1.96   2.0365 0.1740492
H:P        1   4.00    4.00   4.1561 0.0595148 .
Residuals 15  14.44    0.96
Residual standard error: 0.9810425
```

The fitted model is:

$$Whiteness\,index = ¿$$
$$¿$$
$$\hat{y} = 81.52 + 5T + 0.58B + 1.2H + 2.58P - 0.8T^2 - 0.125B^2 - 0.2875H^2 - 0.825P^2 - 0.0375TB - 0.9375TH \quad (4.192)$$

The R outputcomprises of the computed coefficient estimates for the linear, quadratic and interaction terms in the second- order model. From the analysis,the*t*-tests reveal that the main effects T, B, H and P , the square terms T^2 and P^2 and the interaction term TH are significant at $\alpha = 0.05$ while the other factors are not. The small $p - ¿$ valuesalso suggests there is curvature in the response surface.

Refitting the model with the significant factors only yields the following results:

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  81.1042     0.3192 254.051  < 2e-16 ***
T             4.9667     0.2257  22.002< 2e-16 ***
B             0.5833     0.2257   2.584  0.01693 *
H             1.2083     0.2257   5.353 2.25e-05 ***
P             2.5750     0.2257  11.407 1.05e-10 ***
I(T * T)     -0.7484     0.2074  -3.609  0.00156 **
I(P * P)     -0.7734     0.2074  -3.730  0.00116 **
T:H          -0.9375     0.2765  -3.391  0.00263 **
---
Signif.codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.106 on 22 degrees of freedom
Multiple R-squared:  0.9689,    Adjusted R-squared:  0.959
F-statistic:  97.9 on 7 and 22 DF,  p-value: 4.271e-15

Analysis of Variance Table
Response: WD
Df Sum Sq Mean Sq  F value    Pr(>F)
T           1 592.03  592.03 484.0767 < 2.2e-16 ***
B           1   8.17    8.17   6.6776  0.016931 *
H1  35.04   35.04  28.6522 2.252e-05 ***
P           1 159.13  159.13 130.1184 1.046e-10 ***
I(T * T)    1  12.64   12.64  10.3356  0.003989 **
I(P * P)    1  17.02   17.02  13.9130  0.001162 **
T:P         1  14.06   14.06  11.4983  0.002628 **
Residuals 22  26.91    1.22
```

Clearly it can be concluded that the overall regression fit, with a *p*-value of 4.271×10^{-15} is highly significant. The refitted model has the value $R^2_{Adj} = 0.959$ which isless thanthe value $R^2_{Adj} = 0.9677$ of the first model.Denoting the response variable with a subscript reducedmodel (rm), the final fitted model for the response variable at $\alpha = 0.05$ significance level becomes:

$$Whiteness\,inde\,x_{reduceced\,model} = ¿$$

$$\hat{¿}$$

$$\widehat{y_{rm}} = 81.10 + 4.97\,T + 0.58\,B + 1.21\,H + 2.58\,P - 0.75\,T^2 - 0.77\,P^2 - 0.94\,TH \qquad (4.193)$$

To check the validity of the fitted model a residual analysiswas conducted and this is illustrated in figures 4.7 and 4.8.

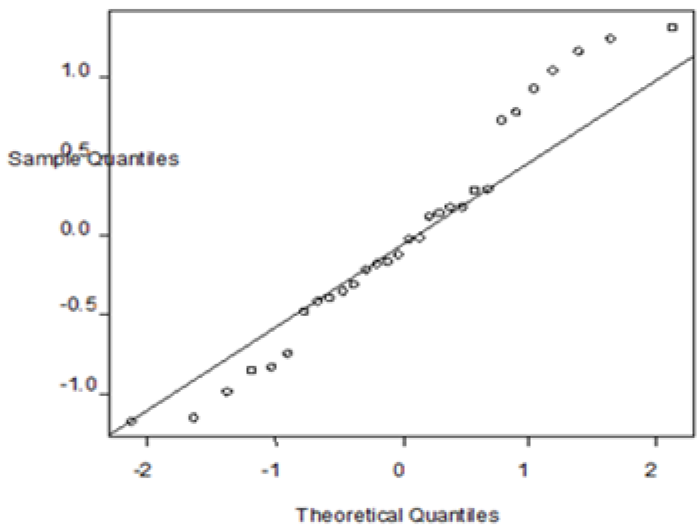


Figure 4.7. Normal Q-Q Plot

This reveals that the residuals are approximately normally distributed.

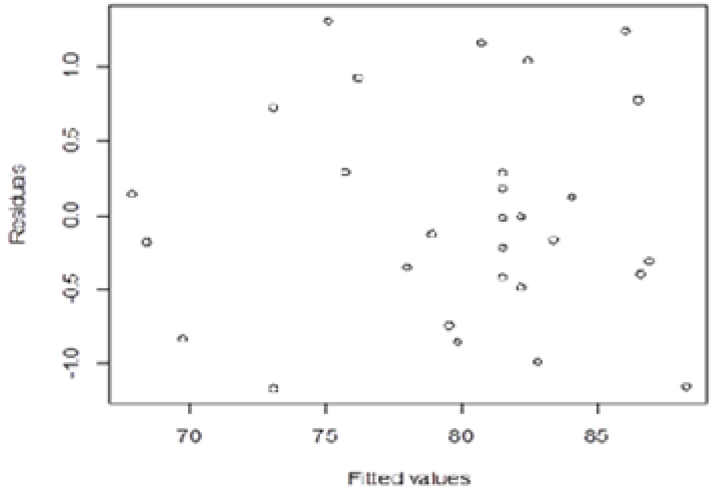


Figure 4.8. Residual vs Fitted Values

. The randomness of the plotted points indicates a good fit. The residuals are distributed randomly on the plot and this suggests that the variance of the original observation is constant for all values of Y.Fromfigures 4.7and 4.8, it can be concluded that the model is adequate to describe the whiteness index determined by the response surface. Later in this chapter, the study seeks to improve this design by using a resolution IV design and then make a comparison.

4.4.1.1 Location of the Stationary Point

The above analysis shows that the response surface is explained by the second order model.This suggests that an optimum point exists and should be located by finding the levels of the factors that optimize the predicted response.

The stationary point is the combination of design variables where the surface is at either a maximum or a minimum in all directions. A saddle point exists if the stationary point is a maximum in some direction or a minimum in another direction. A ridge system will be observed when the surface is curved in one direction but is fairly constant in another direction (Oehlert 2000).

A stationarityand matrix analysisis carried out to obtain a mathematical solution for the location of the stationary point.This point will be the set of T, B, H and P for which the partial derivatives:

$$\frac{d\hat{y}}{dT}=\frac{d\hat{y}}{dB}=\frac{d\hat{y}}{dP}=\frac{d\hat{y}}{dA}=0$$

Writing the second-ordermodelin matrix notation, we have

$$\hat{y}=\hat{\beta}_0+x'b+x'Bx \qquad (4.194)$$

where

$$x=\begin{bmatrix} T \\ B \\ H \\ P \end{bmatrix} b=\begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \\ \hat{\beta}_4 \end{bmatrix} \text{ and } B=\begin{bmatrix} \hat{\beta}_{11} & \frac{\hat{\beta}_{12}}{2} & \frac{\hat{\beta}_{13}}{2} & \frac{\hat{\beta}_{14}}{2} \\ \frac{\hat{\beta}_{12}}{2} & \hat{\beta}_{22} & \frac{\hat{\beta}_{23}}{2} & \frac{\hat{\beta}_{24}}{2} \\ \frac{\hat{\beta}_{12}}{2} & \frac{\hat{\beta}_{23}}{2} & \hat{\beta}_{33} & \frac{\hat{\beta}_{34}}{2} \\ \frac{\hat{\beta}_{12}}{2} & \frac{\hat{\beta}_{24}}{2} & \frac{\hat{\beta}_{24}}{2} & \hat{\beta}_{44} \end{bmatrix} \qquad (4.195)$$

b is a 4×1 vector of the first-order regression coefficients and B is a 4×4 symmetric matrix whose main diagonal elements are the pure quadratic coefficients $\hat{\beta}_{ii}$ and the off-diagonal elements are one-half the mixed quadratic coefficients $\hat{\beta}_{ij}, i\neq j$ (Montgomery 2005). The derivative of the response with respect to the elements of the vector x is equated to zero and the stationary point is the solution of this equation. This is outlined below.

$$\frac{dy}{dx}=b+2Bx=0 \Rightarrow x_s=\frac{-1}{2}B^{-1}b \qquad (4.196)$$

This then yields the predicted response at the stationary point as

$$\hat{y}=\hat{\beta}_0+\frac{1}{2}x_s^{'}b \tag{4.197}$$

Nextthelocation of the stationary point for whiteness index of cotton is now determined. Substituting the estimates of the coefficients in the matrices (4.195) the following is obtained:

$$B=\begin{bmatrix} -0.8 & -0.1875 & -0.46875 & -0.25 \\ -0.1875 & -0.125 & 0.1875 & -0.175 \\ -0.46875 & 0.1875 & -0.2875 & -0.25 \\ -0.25 & -0.175 & -0.25 & -0.825 \end{bmatrix}$$

$$b=\begin{bmatrix} 5 \\ 0.58 \\ 1.2 \\ 2.58 \end{bmatrix}$$

$$B^{-1}=\begin{bmatrix} -0.5509 & -1.7265 & -0.9387 & -0.81765 \\ -1.7265 & -0.0153 & 3.1868 & -0.4393 \\ -0.9387 & 3.1868 & 0.6395 & -0.5853 \\ -0.81765 & -0.4393 & -0.5853 & -1.1893 \end{bmatrix} \tag{4.198}$$

From (4.196), the stationary pointis

$$x_s=\begin{bmatrix} 1.3863 \\ 2.975 \\ 1.7939 \\ -0.0311 \end{bmatrix} \tag{4.199}$$

The stationary point is then obtained in terms of the natural variables Temperature, Bleach Activator, pH and Peracetic Acid using the equations in (4.190) and this resulted in:

$TEMP = 73.86^0 C$

$BC = 3.73\,\%owf$

$pH = 25.44$

$PAA = 14.84\,ml/l$ (4.200)

Thus the factors should be set at Temperature $73.86^0 C$, Bleach Activator $3.73\,\%owf$, pH 25.44 and Peracetic Acid $14.84\,ml/l$ to attain optimum effect onwhiteness of cotton. Using (4.197) the estimated optimum value of the whiteness index

$\hat{y}$ denoted by $V(¿¿p(\xi))$ is

$$V(¿¿p(\xi)) = 86.476 \quad (4.201)$$
$$optimum\,whiteness\,index = ¿$$

4.4.2 Illustration using Resolution IV CCD

From the above analysis, there is evidence that only two interactions are likely to exist. Thus a resolution IV design in the fractional factorial portion is appropriate. Theoretical results of this design have been derived in the previous chapters of this thesis. Therefore using the generator formed by the highest interaction $D = ABC$, the second-order model is fitted using the data values corresponding to half – fraction of the factorial portion. The data points corresponding to this design were obtained by putting the data in Table 4.7into two blocks with one block obtained from the generator $D = ABC$ and the second block from the generator $D = -ABC$.

For the purpose of analysis, the following assumptions were used:

1. The observed response variables are normally distributed with standard deviation 5.46.
2. The observed response variables for the second design whose cube portion is constructed through resolution IV differs from the original observed (y_i) with an error ε_i which is normally distributed with mean zero and standard deviation3.99. Thus the error term $\varepsilon_i \; N(0,3.99^2)$ is generated. Therefore the new response variable denoted by $new\, y_i$ is given by:

$$new\, y_i = y_i + \varepsilon_i$$

The new design points in terms of coded variables, the generated error term and the new response variable are given.

Table 4.8. Data Set for Half CCD

T	B	H	P	y	e	newy
-1	-1	-1	-1	68	-1.167	66.83
1	1	-1	-1	83.5	5.94	89.44
1	-1	1	-1	82.2	-0.747	81.45
-1	1	1	-1	76.4	1.427	77.83
1	-1	-1	1	86.2	0.0237	86.22
-1	1	-1	1	77.1	7.08	84.18
-1	-1	1	1	78.8	3.391	82.19
1	1	1	1	87.3	-1.949	85.35
-1.6818	0	0	0	68.2	-2.841	65.36
1.6818	0	0	0	87.1	-4.388	82.71
0	-1.6818	0	0	79	8.8761	87.88
0	1.6818	0	0	81.7	-0.206	81.49
0	0	-1.6818	0	77.6	5.836	83.44
0	0	1.6818	0	81.8	1.618	83.42
0	0	0	-1.6818	71.9	-7.132	64.77
0	0	0	1.6818	83.2	0.432	83.64
0	0	0	0	81.1	-5.984	75.12
0	0	0	0	81.8	0.141	81.94
0	0	0	0	81.3	-1.746	79.55

The following figure presents a scatter plot showing the effects of the explanatory variables on the response variable using this data set.

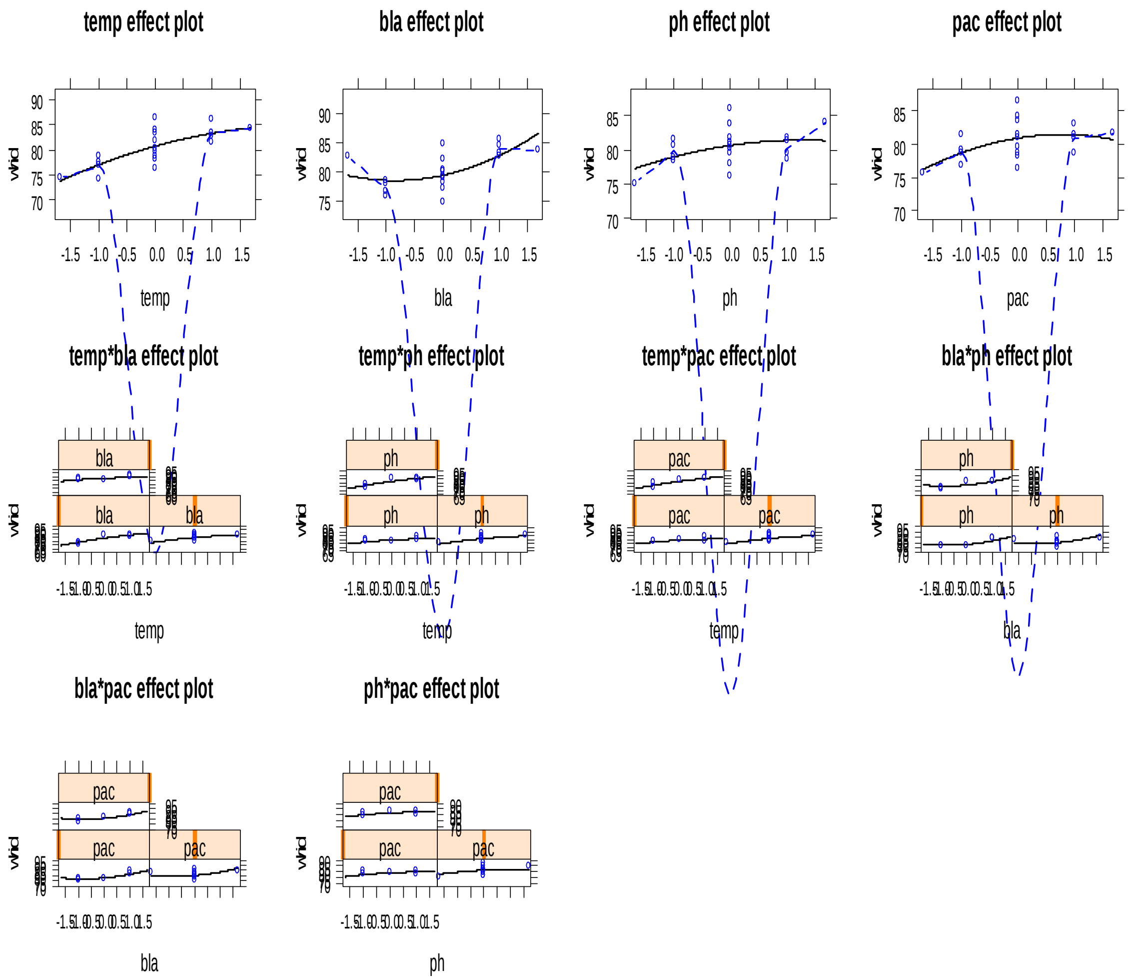


Figure 4.9. Effects Plots and Residuals

An observation of the curves reveals that while Temperature, pH and Peracetic Acid show a higher effect on the whiteness Index owing to the shape of the curves, Bleach Activator has a lower effect.

4.4.2.1 Effect on Whiteness of Cotton using Resolution IV CCD

In this section the objective was to determine the effect of the four factors on whiteness of cotton using half the number of experimental runs that were used in section 4.4.1. Asecond-order Kronecker model was fitted and an analysis done to find out the significant factors and the results were compared with the graphical observations.

Letting the variables b1, b2, b3 and b4 represent Temperature, Bleach Activator, pH andParacetic Acid respectively, the following is the R output for the fitted model:

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  78.0682     2.1256  36.727 2.88e-09 ***
I(b1 * b1)   -1.0627     1.0860  -0.979  0.36040
I(b2 * b2)    2.7025     1.0860   2.488  0.04169 *
I(b3 * b3)    2.2577     1.0860   2.079  0.07621 .
I(b4 * b4)   -1.0045     1.0860  -0.925  0.38575
b1            3.6086     1.0695   3.374  0.01186 *
b2           -0.7753     1.0695  -0.725  0.49203
b3            1.6375     1.0695   1.531  0.16962
b4            4.6249     1.0695   4.324  0.00346 **
b1:b2        -2.6287     1.3974  -1.881  0.10200
b1:b3        -2.2331     1.3974  -1.598  0.15407
b1:b4        -0.7336     1.3974  -0.525  0.61582
---
Signif.codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
Residual standard error: 3.952 on 7 degrees of freedom
Multiple R-squared:  0.8838,    Adjusted R-squared:  0.7012
F-statistic:  4.84 on 11 and 7 DF, p-value: 0.02323
```

Denoting the response variable with a subscript RIV(Resolution IV) the fitted model is of the form:

$$\widehat{New\ Whiteness\ index}_{RIV} = ¿$$

$$\hat{y}_{RIV} = 78.068 + 3.61\,T - 0.78\,B + 1.64\,P + 4.62\,A - 1.06\,T^2 + 2.70\,B^2 - 2.26\,P^2 - 1.0\,A^2 - 2.63\,TB - 2.23\,TP -$$

(4.202)

An observation of the coefficient estimates and the *t*-tests,shows that Peracetic Acid had the greatest effect on whiteness of cotton followed by temperature and the pH.The bleach Activator had nearly no effect on whiteness index and this is also evident from the contour plots figures 4.10, 4.11, 4.12, 4.13 and 4.14.

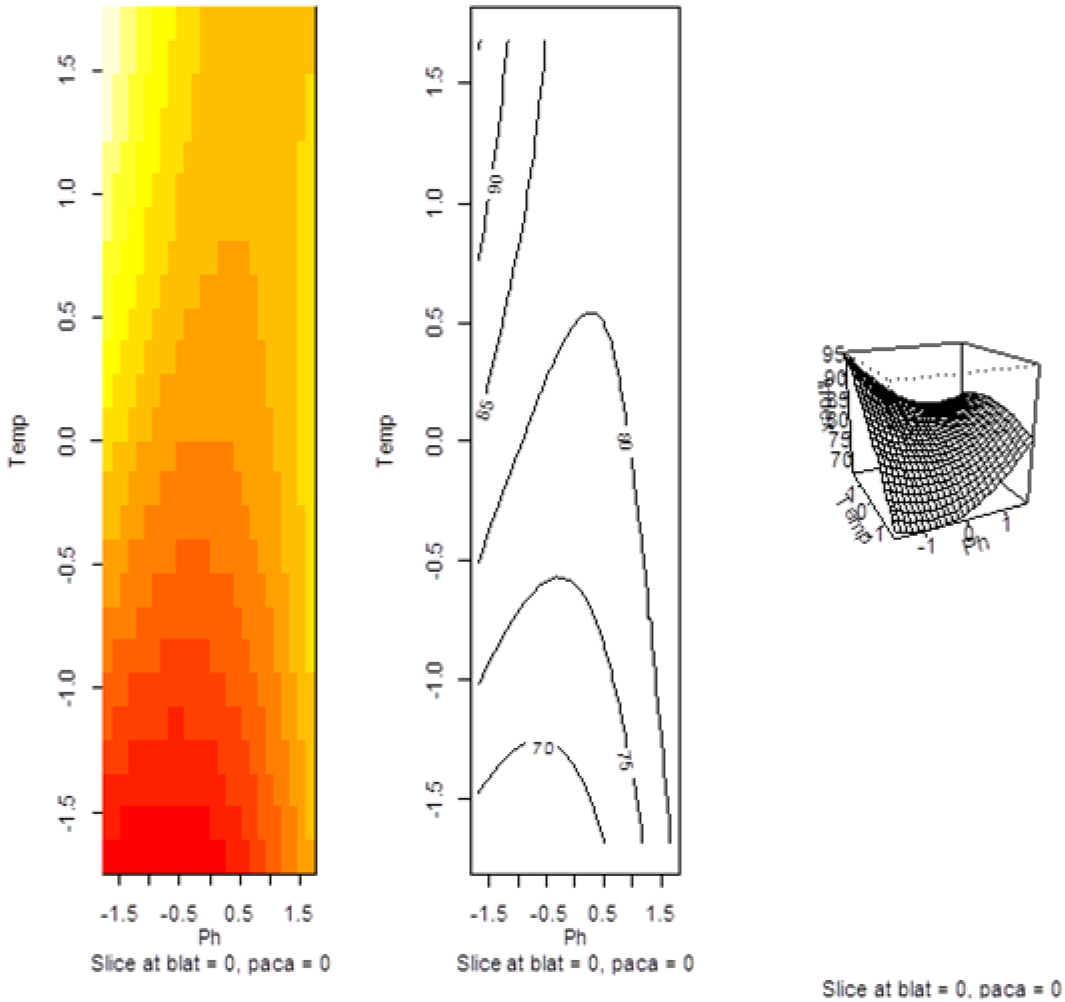


Figure 4.10. Temp and pH

The contours show a rising ridge indicating that temperature and Ph had effect on the whiteness index.

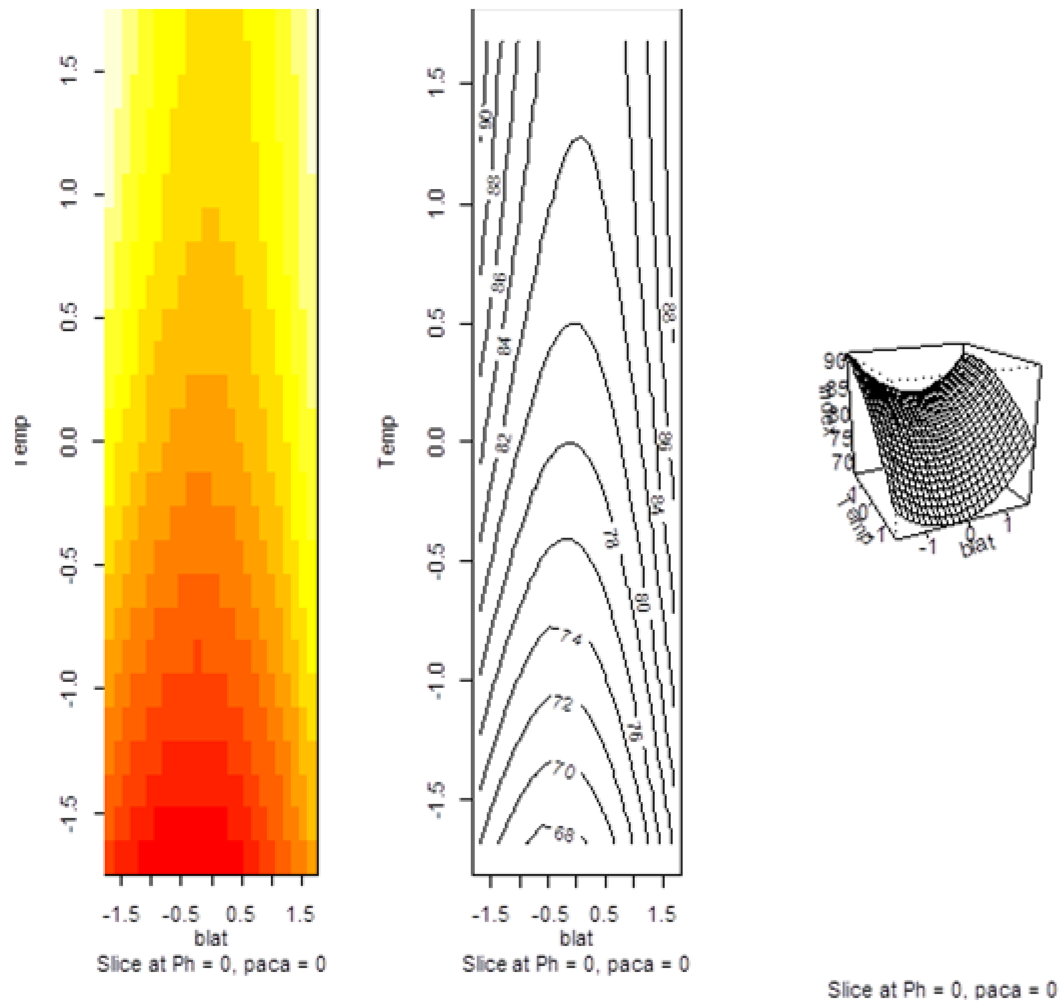
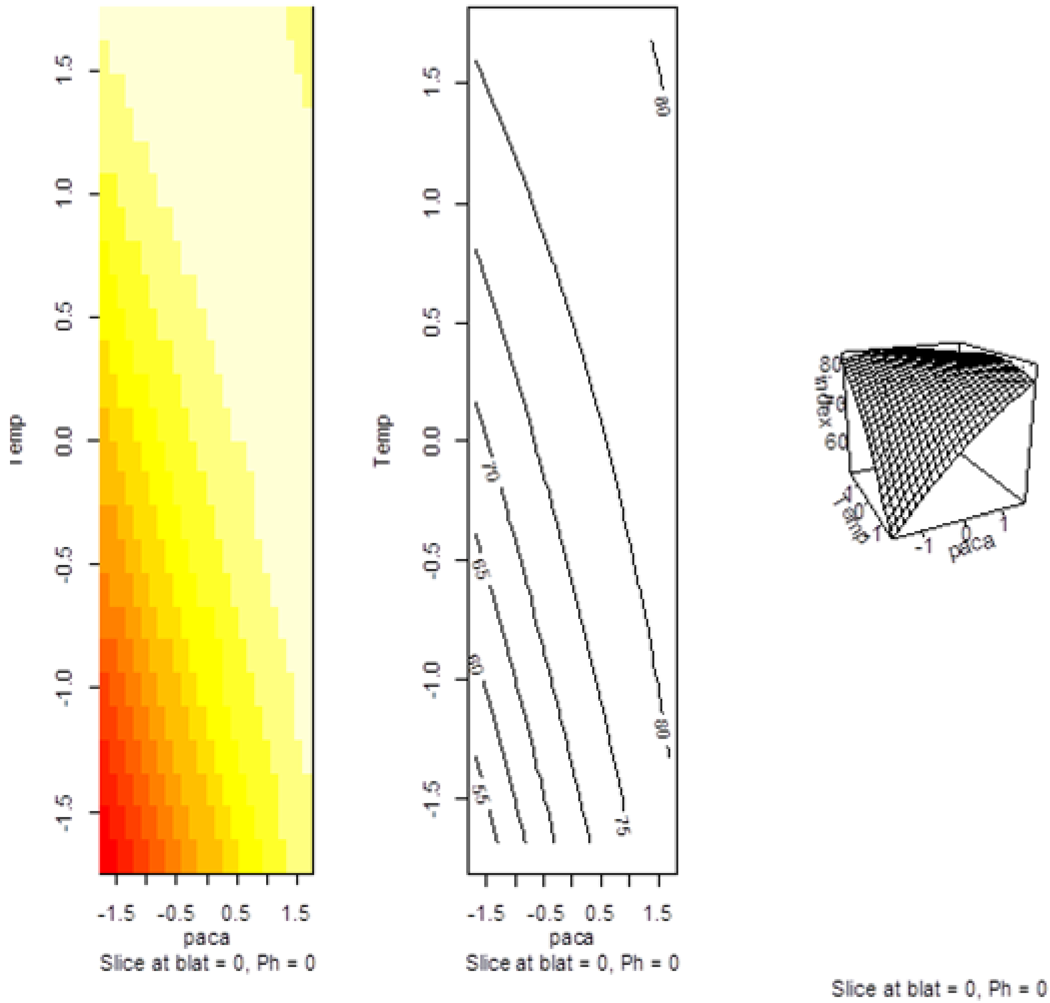


Figure 4.11. Temp and Bleach A.

The response surfaceplothas almost the same shape as the one between temperature and pH. This indicates that the interaction of temperature andpH as well as temperature and bleach activator had effect on the whiteness index.



Fgure 4.12. Temp and P. Acid

The response surface plot shows that the interaction of temperature and peracetic acid had effect on the whiteness index. The contour lines as well indicates a maximum point exists.

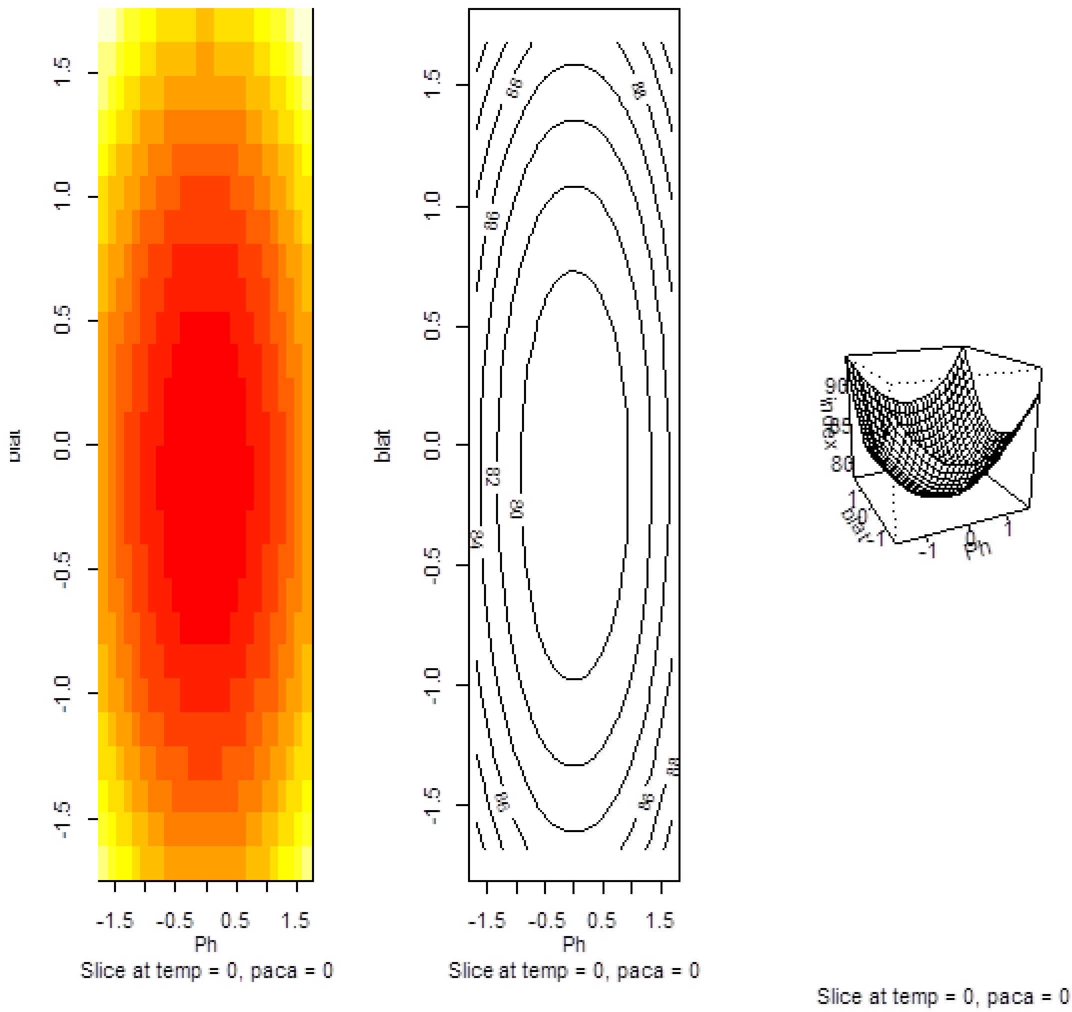


Figure 4.13.B.Activator and pH

The response surface plot and the contour lines shows that the interaction of bleach activator and pH had minimal effect on the whiteness index.

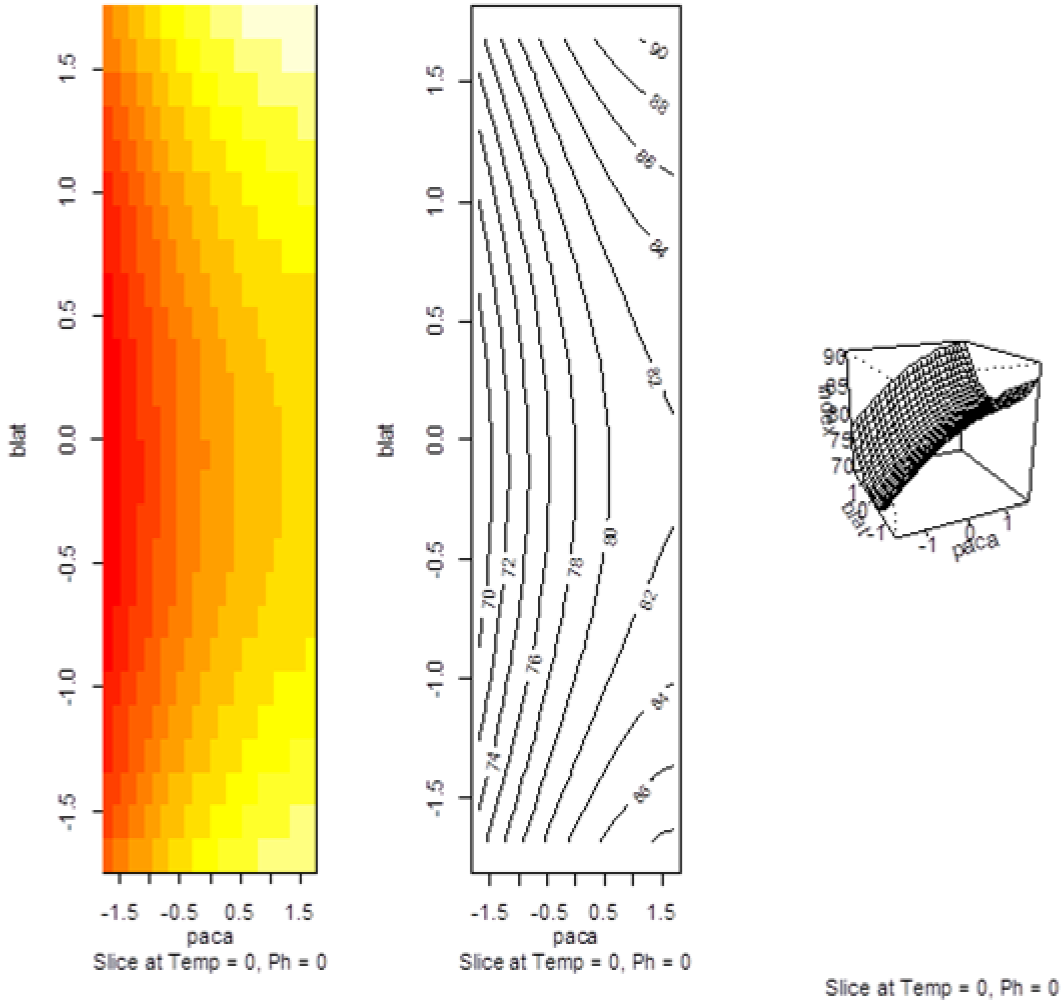


Figure 4.14. B. Activator. and P. Acid

The interaction of bleach activator and peracetic acid shows minimal effect on the whiteness index as evident from the contour plot and the response surface plot.

The analysis shows that two main effects Temperature and Peracetic Acid contribute significantly to the model at $\alpha = 0.05$ level. This is similar to the observation oftheEffects Plots (Figure 4.9). Further, this agrees with earlier findings where the main effectswere found to be significant.Comparing this model with the reduced model for the full CCD, it can be observed that this model has a value of

$R^2_{Adj}=0.7012$. This is less than $R^2_{Adj}=0.959$ for the full CCD. This indicates that reducing the number of experimental runs has resulted to a reduction in the value of R^2_{Adj} .

According toWuand Hamada (2000), in order for an interaction to be significant, at least one of its parent factors should be significant. This fundamental principle for factorial effects is called the effect heredity principle. Now since the two parent factors T and A are significant, then we may also conclude that the corresponding interaction is also significance as well as the corresponding quadratic terms:

$$\widehat{New\ Whiteness\ index}=80.8+3.2\,T+2.6\,A-0.59\,T^2-0.87\,A^2-1.73\,TA \qquad (4.203)$$

4.4.2.2 Location of the Stationary Point

A stationarity and matrix analysis is carried out to obtain a mathematical solution for the location of the Stationary Point and calculations were done using R. Substituting the estimates of the coefficients in the matrices (4.195), the following results are obtained:

$$B=\begin{bmatrix} -1.0627 & -1.3144 & -1.1167 & -0.3668 \\ -1.3144 & 2.7025 & 0 & 0 \\ -1.1167 & 0 & 2.2577 & 0 \\ -0.3668 & 0 & 0 & -1.0045 \end{bmatrix}$$

$$b=\begin{bmatrix} 3.6086 \\ -0.7753 \\ 1.6375 \\ 4.6249 \end{bmatrix}$$

$$B^{-1}=\begin{bmatrix} -04716 & -0.2294 & -0.2333 & 0.1722 \\ -0.2294 & 0.2585 & -0.1134 & 0.0837 \\ -0.2333 & -0.1134 & 0.3276 & 0.0852 \\ 0.1722 & 0.0837 & 0.0852 & -1.0584 \end{bmatrix} \qquad (4.204)$$

The stationary point is then determined using the equation (4.196) and this result to:

$$x_s = \begin{bmatrix} 0.5548 \\ 0.4133 \\ -0.0882 \\ 2.0995 \end{bmatrix} \quad (4.205)$$

Next using (4.190), the stationary point in terms of the natural variables: Temperature, Bleach Activator, pH and ParaceticAcid is obtained:

$TEMP = 65.55^{0}\,C$

$BC = 1.81\,\%owf$

$pH = 7.46$

$PAA = 25.5\,ml/l$ (4.206)

Thus the factors should be set at $65.55^{0}C$ Temperature, $1.81\%owf$ Bleach Activator, 7.46 pH and $25.5\,ml/l$ Peracetic Acid to attain optimum effect onwhiteness of cotton.

Using (4.197) the estimated optimum value of the whiteness index denoted by

$V(\text{¿¿}\,\overset{\phi}{\underset{\text{¿}}{p}}(\xi^{\text{¿}}))$ is obtained as:

$$V(\text{¿¿}\,\overset{\phi}{p}(\xi^{\text{¿}})) = 83.69125 \quad (4.207)$$

$optimum\ whiteness\ index = \text{¿}$

A comparison of the performance of the two designs in determining the effect of the four factors on the whiteness index of cotton was done by computing their efficiency using the formula given in (3.44):

$$\frac{\begin{matrix}\phi \\ \phi \\ V(¿¿p(\xi)) \\ V(¿¿p(\xi^{¿}))\end{matrix}}{\begin{matrix}¿ \\ eff_{\phi_p}(\xi^{¿}) = ¿\end{matrix}}$$

where the design ξ is the full CCD while $\xi^{¿}$ is the CCD obtained through resolution IV.

Thus using (4.201) and (4.207),

$$eff_{\phi_p}(\xi^{¿}) = \frac{83.69125}{86.47637} = 0.9678 \qquad (4.208)$$

The conclusion is that the second design performs better than the first design and it is 3.22% more efficient (anefficiencyof 96.78%).

CHAPTER FIVE

SUMMARY, CONCLUSION AND RECOMMENDATIONS

5.0 Introduction

In this chapter, a summary of the findings of this research is given, conclusions are drawn and recommendations for further research emanating from this work are outlined.

5.1 Summary

Response surface designs are important for the study of response surface methodology and an example of such designs is the Central Composite Design. In this thesis, two-level fractional factorial designs were investigated.RotatableCentral Composite Designsin the second-order Kronecker model were constructed through resolutions III and IV for three and four factors. Based onthe parameter subsystem $K'(\theta)$ of interest, moment matrices and corresponding information matrices were obtained. The moment matrices were found to satisfyrotatability conditions. Also, it was observed that the number of parameters resulting from averaging the interaction factors due to repetition of columns in the X design matrix play a role in determining the order of the information matrix.

Optimal rotatable WCCD for three and four factors were derived and optimality was accomplished through application of D-, A- , E- andI-optimality criteria which follows from the General Equivalence Theorem (Pukelsheim, 1993, Goosand Bradley, 2012).

D-, A- and I-optimal rotatable WCCD were found to exist for both resolution III and IV designs. An E- optimal rotatable WCCD exists for resolution III design but not for a resolution IV design. More weight is assigned to the cube portion in the resolution III and V D-optimal designs while resolution IV design assignsequal weight to both portions. On the other hand more weight is assigned to the star portion in the A-, E- and I-optimalresolution III and IV designs.

A general form of D- optimal rotatable WCCD and corresponding optimal value was derived as well as a general form of the I- optimal value. Optimal values were computed and efficiency of the constructed designs was computed relative to the corresponding uniformly weighted central composite designs. Resolution IV has a very high efficiency in terms of the I-optimality criterion.Resolution III D-, A-, E-and I-optimal rotatable Weighted Central Composite Designs (WCCDs) were found to exist. The D-, A- and E-efficiency for the Resolution III and IV designs are near one indicating that the optimal rotatable WCCDs perform better than the uniform weighted CCD in terms ofD-, A- and E-optimality criterion.

D- and A-optimalrotatableWCCDs exist for four factors. The D-efficiency is near one indicating that the WCCD is better in terms of the D-optimality criterion. But in terms of the A-optimality criterion, the efficiency is 0.81 and thus the full CCD is better than the WCCD.But an E- optimal rotatable WCCD for resolution IV does not exist.

I-optimal rotatableWCCDs exist for both resolution III and IV. The efficiency for resolution III is near one and thus the WCCD is better than the full CCD. The efficiency for resolution IV design is slightly more than one and thus in terms of I-optimality criterion, the optimal full CCD seems to perform better.Optimal values and weights for the weighted central composite designs were numerically obtained using both R and wxMaximasoftwares.

A resolution IV design was further investigated using data on whiteness of cotton. Scatter plot matrices and contour plots and the corresponding response surfaces were plotted for the secondary data. A second-order Kroneker model was fitted using the full CCD and a resolution IV design and a comparison was done. A stationarity and matrix analysis was carried out to obtain a mathematical solution for the location of the Stationary Point in both cases and the efficiency of the resolution IV design determined.

5.2 Conclusion

The generalobjective of this research thesis was to construct optimal second-order rotatable designs through resolutions with application to effects on whiteness of cotton using four factors Central Composite Design. The findings of this thesis are consistent with previous researches such asYin-Jie (2007)whoconstructed minimal-point designs for second-order response surface using a two-stage method to find the composite designs. The minimal-point designs were equal-weight designs and comparison was made between central composite designs, other small composite designs and minimal-point designs by relative efficiencies. Generally, the proposed composite designs performed well.Further,Lucas (1974) proposed that when $m \leq 5$, the D-efficiency of the optimal CCD is at least 0.9. This agrees with the results of this thesis.

Further, other than the resolution IV D-optimal rotatable WCCD that was found to assignamass of equal value to design points in both the cube and star portions, all the other designs assign different weights to the two portions of the CCD.But a resolution IV E-optimal rotatable WCCD does not exist. Observing the optimal values and efficiencies of these designs,the conclusion is that the resolution R WCCDs in general perform better than the uniform weighted CCD.

Thetheoretical results agree with the data analysis results. It was observed that the model that was fitted using Resolution IV design performed better than the one fitted using the full CCD.Peracetic acid is the most effective bleaching agent of cotton in the pH range of 6 to 7. The preferable bleaching temperature range is between 50℃ and 80℃ . The degree of brightness increases proportionately with the concentration of bleaching agent. A comparison of the optimum conditions for the whiteness of cotton showed that fitting the second model results in factor levels that satisfy the preferred conditions namely low temperatures and a high concentration of the peracetic acid. Further when bleaching is carried out at low temperature this means energy conservation with economic and environmental benefits.The second design performed better than the first design considering that it had an efficiency of 96.78%.

A comparison of the diagnostic graphs in the appendix (Figure A.1 and Figure B.1) shows that fitting the model using the resolution IV design does not distort the regression. An observation of the two plots showing Cook's distance shows that the red smoothed line is close to the horizontal gray dashed line and that no points have a large Cook's distance.

5.3 Further Research

Suggestions for further research that has emanated from the findings of this study are outlined in this section.

1. This thesis was restricted to CCD with no center points. It would be interesting to observe what happens if a similar study is carried out with center points added to both the cube and the star portions.
2. It is recommended that further research can be done on the practicability of the optimal rotatable Weighted Central Composite Designsand an investigation be carried out on the generalized form of A- and E-optimal rotatable WCCD constructed through resolution R.
3. An area for future research would be tofind out the optimum conditions and the corresponding optimum value of the whiteness index of cotton when Peracetic Acid is used in the presence of different bleach activators at different temperatures using the Resolution IV design based on the CCD.

REFERENCES

Atkinson A.C., Donev, A.N. and Tobias, R.D. (2007).*Optimum Experimental Designs, with SAS*.Oxford University Press.

Box, G. E. P. and Hunter, J. S. (1957).Multifactor Experimental Designs for Exploring Response Surfaces.*The Annals of Mathematical Statistics*,**28** (1), 195- 241.

Box, G.E.P. and Hunter, J. S. (1961). The 2^{k-p} Fractional factorial designs.*Technometrics*,**3**, 311-351.

Box, G.E.P., Hunter, W.G. and Hunter, J.S. (1978). *Statistics for Experimenter: An Introduction To Design, Data Analysis, and Model Building.* New York: Wiley. xviii, p. 653.

Box, G. E. P. and Wilson, K. B. (1951). On the Experimental Attainment of Optimum Conditions.*Journal of the Royal Statistical Society*, Series***B*13**, 1–45.

Cherutich M. R., Koske J. K., Kinyanjui J. K. andMutiso J. M. (2012). Information Matrices for Non-Maximal Parameter Subsystems for Second-Degree Mixture Experiments.*American Journal of Mathematics and Mathematical Sciences.* (Open Access Journal) **1**(2), 155-160.

Chigbu P. E. andOrisakwe N. C. (2011).Optimal Central Composite Designs Constrained by Rotatability and Slope Rotatability. *University of Nigeria, Nsukka, Nigeria*.

Chigbu P. E. andUkaegbu E. C. (2014). Prediction Variance Assessment of Variations of Two Second-Order Response Surface Designs. *Industrial Engineering Letters*, **4**, No.12.

Chuan-Pin L.andMong-Na L. H.(2011). D-Optimal Designs for Second-Order Response Surface Models with Qualitative Factors. *Journal of Data Science*,**9**, 139-153.

Draper, N.R. andPukelsheim, F. (1998b). Mixture models based on homogeneous polynomials.*J. Statist. Plann.Inference*,**71**,303-311.

Draper, N. R. and Lin, D. K. J. (1990).Capacity Considerations for Two-Level Fractional factorial designs.*Journal of Statistical Planning and Inference*, **24**, 25-35.

El-Monsef, M. M. E. A., Rady, E. A., andSeyam, M. M. (2009).Relationships among Several Optimality Criteria.*Interstat*, *European Scientific Journal*, **10**(36), 1857 – 7881.

Fijul K. S. M., Mohammad I. I.,Partha P. S., Mohammad M. R.andShabiha A. (2014).Optimization of Parameters of Cotton Fabric Whiteness.*European Scientific Journal(ESJ)*, **10**(36), 1857 - 7881.

Goos P. andBradleyJ. (2012).I-optimal versus D-optimal Split-Plot Response Surface Designs. .*Journal of Quality Technology*,**44**(2), 85-101.

GoosP.andSyafitri, U. (2014).V-optimal mixture designs for the *q*th degree model, *Chemometrics and Intelligent Laboratory Systems,***136**, 173–178.

Hartley H. O. (1959). Smallest Composite Designs for Quadratic Response Surfaces.*Biometrics*, **15**, 611-624.

Holger D.and Yuri G**.** (2014).*E*-optimal designs for second-order response surface models.*Annals of Statistics*, **42**(4), 1635-1656.

Koech E., Koech M., Koske J., Kerich G. and Argwings O. (2014).E-Optimal Designs For Maximal Parameter Subsystem Second- Degree Kronecker Model Mixture Experiments.*Mathematical Theory and Modeling*, **4**(5), 2224-5804.

Koske J. K., Kosgei M. K. and MutisoJ. M.(2011).A New Third Order Rotatable Design In Five DimensionsThrough Balanced Incomplete Block Designs. *Jomo Kenyatta University of Agriculture and Technology,***13**(1), 157-163.

Lavrič P.K., Franci K., Tavčer P.F., Peter H. and David H. (2007).Enhanced PAA Bleaching of Cotton by Incorporating a Cationic Bleach Activator.*Coloration Technology*, **123**, Issue 4, 230–236.

Li W. (2006).Recommendations for Design Parameters for Central Composite Designs with Restricted Randomization. *PHD ThesisVirginia Polytechnic Institute and State University, Blacksburg, Virginia.*

Lucas, J.M. (1974). Optimum Composite Designs.*Technometrics*,**16**, 561-567.

Montgomery, D.C. (2005). Design and analysis of experiments. (6th ed.). *Massachusetts: John Wiley.*

Montgomery, D.C. (2013). Design and analysis of experiments. (8th ed.). *Massachusetts: John Wiley.*

Myers, R.H., Montgomery, D.C. and Christine M. A. (2009).Response Surface Methodology: Process and Product Optimization Using Designed Experiments. (3rded*).John Wiley & Sons, Inc., Hoboken, New Jersey*.

Myers R. H., Khuri A. I. and Carter W. H., Jr. (1989).Response surface methodology.1966-1988. *Technometrics*, **31** (2), 137-153.

Narasimham, V. L.,Ramachandrarao P., and Rao K.N. (1983).Construction of second order rotatable designs through a pair of balanced incomplete block designs.*Journal of the Indian Society of Agricultural Statistics*, **35**, 36-40.

Oehlert G. W. (2002). Small,Efficient, EquireplicatedResolution V Fractions of Factorial designs and their Application to Central Composite Designs.*School of Statistics, University of Minnesota, Pat Whitcomb, Stat-Ease, Inc.*

Prescott, P., Dean, A. M., Draper, N. R., and Lewis, S. M. (2002).Mixture experiments: ill-conditioning and quadratic model specification.*Technometrics*, **44,** 260-268.

PrescottP. andDraperN. R. (2009).Modeling in Restricted Mixture Experiment Spaces forThree Mixture Components.*Quality Technology & Quantitative Management*, **6**(3), 207-217.

Pukelsheim, F. (1993).*Optimal Design of Experiments*.Wiley, New York.

Rajyalakshmi K. and Victorbabu B. R. (2014).Construction of Second Order Rotatable Designs under Tri-Diagonal Correlation Structure of Errors using Central Composite Designs.*Journal of Statistics: Advances in Theory and Applications*, **11** (2), 71-90.

Ray-Bing C., Yu-Jen T.and Lin D.K.J. (2008).Conditionally Optimal Small Composite Designs. *Statistics and Applications*, New Series **6** (1 & 2), 29-48.

Rechtschaffner,R.L. (1967). Saturated fractions of 2^n and 3^n factorial designs.*Technometrics*, **9**, 569-575.

Sunitha1. P., Aruna L. K. and Narayana S.K. V. (2015).Application of Response Surface Methodology forthe Optimization of Growth of Pearl Millet.*British Microbiology Research Journal*, **6**(3), 154-166.

Victorbabu, B. Re.andRajyalakshmi,K. (2012). A new method of construction of robust second order rotatable designs using balanced incomplete block designs. *Open Journal of Statistics*, **2**, 39-47.

Wu,C. F. J. and Hamada, M. (2000).*Experiments: Planning, Analysis, and Parameter Design Optimization***.** Wiley-Interscience; 1st Edition.

Yin-Jie Huang.(2007). A Study on Minimal-Point Composite Designs.*Institute of Statistics, National University of Kaohsiung, Kaohsiung, Taiwan 811 R.O.C.*

APPENDICES

AppendixA: Graphs for full CCD

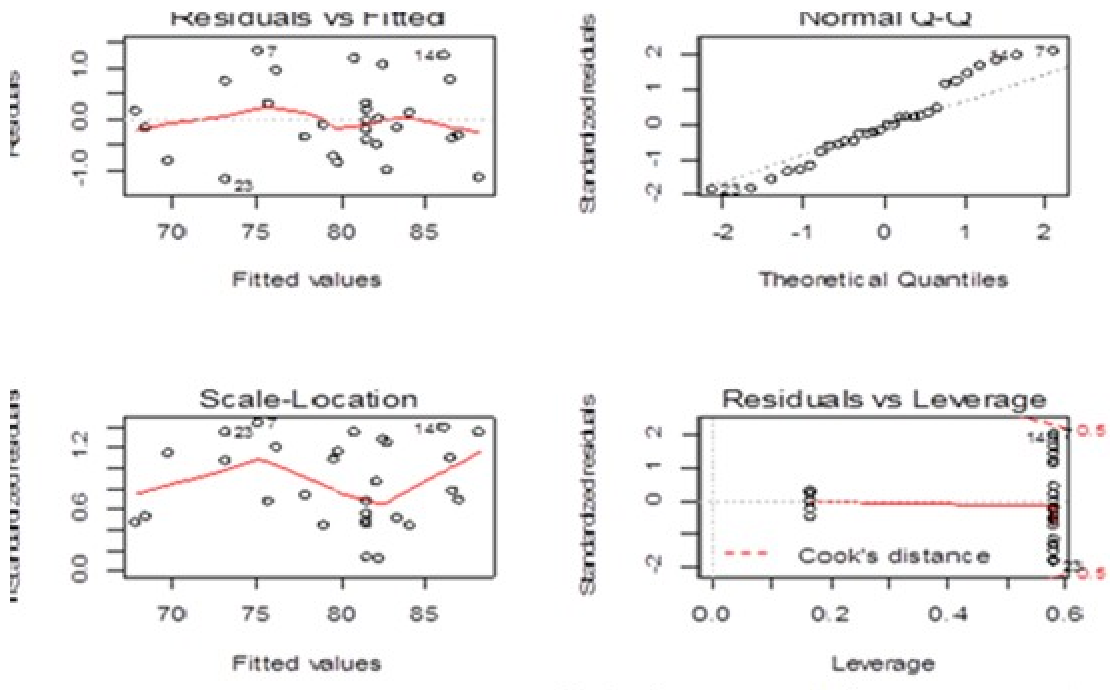


Figure A.1. Basic Diagnostic Graphs for the full CCD

Appendix B: Graphs forHalf CCD

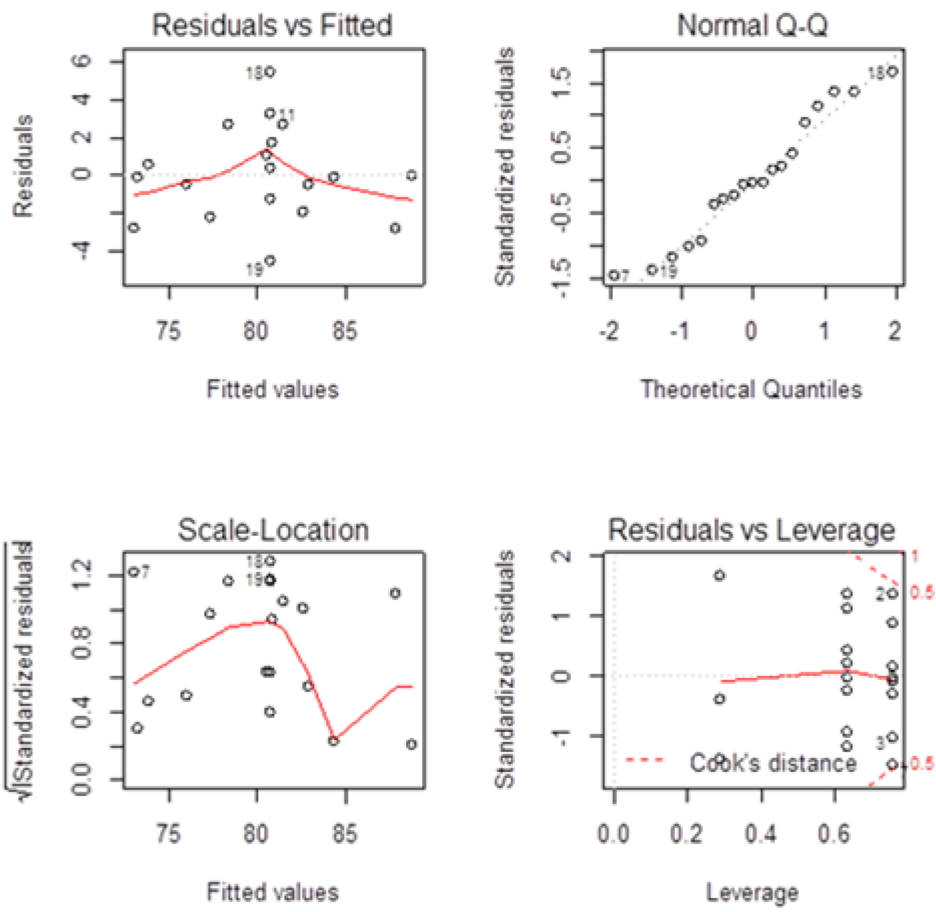


Figure B.1. Basic Diagnostic Graphs for Half CCD

Appendix C: R-codes

```
# for m=3
#input K matrix and L
w1=c(1,0,0)
w2=c(0,1,0)
w3=c(0,0,1)
#compute information matrix
Ck=L3%*%M3%*%t(L3)
Ck
#use data set for coded cotton data full
ccdcottonfull=read.csv("C:\\Users\\mwangi\\Desktop\\cottonfull.csv",sep=",",
header=TRUE)cottonfull

attach(cottonfull)

#fit the first model

fit23=lm(index~temp+bla+ph+pac+I(temp*temp)+I(bla*bla)+I(ph*ph)
+I(pac*pac)+I(temp*bla)+I(temp*ph)+I(temp*pac)+I(bla*ph)+I(bla*pac)
+I(ph*pac),data=cottonfull)

fit23

summary(fit23)

#plot the graphs

qqplot(fit23)

plot(aov(fit23))

plot(resid(fit23) ~ fitted(fit23))

abline(0,0)

#fit data for half ccd

cottonhalf=read.csv("C:\\Users\\mwangi\\Desktop\\cottonhalf.csv",sep=",",he
ader=TRUE)

cottonhalf

attach(cottonhalf)

fit26=lm(index~I(Temp*Temp)+I(blat*blat)+I(Ph*Ph)+I(paca*paca)
+Temp*blat+Temp*Ph+Temp*paca,data=cottonhalf)
```

```
fit26

#plot the graphs

qqnorm(residuals(fit26))

plot(Temp,index)

plot(blat,index)

plot(Ph,index)

plot(paca,index)

boxplot(index ~ temp)

boxplot(index~blat)

plot(cottonhalf) #plot pairs of scatter for whole data

#plot contour plots for half data temp and ph and response variable whid

library(rsm)

par(mfrow=c(1,3))

image(fit26, Temp ~ Ph)

contour(fit26, Temp ~ Ph)

persp(fit26, Temp ~ Ph, zlab = "index")

#plot contour plots for the data temp and bla and response variable whid

library(rsm)

par(mfrow=c(1,3))

image(fit26, Temp ~ blat)

contour(fit26, Temp ~ blat)

persp(fit26, Temp ~ blat, zlab = "index")
```