OPTIMAL DESIGNS FOR THIRD DEGREE KRONECKER MODEL MIXTURE EXPERIMENTS WITH APPLICATION IN BLENDING OF CHEMICALS FOR CONTROL OF MITES IN STRAWBERRIES

PhD. THESIS

By

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DECLARATION

Declaration by the student

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

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DEDICATION

This thesis is dedicated to my mother Kong'ato Tabasei and late father Silisil Chepkeitany.

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ABSTRACT

Mixture experiments are special type of response surface designs where the factors under study are proportions of the ingredients of a mixture. In response surface designs the main interest of the experimenter may not always be in the response at individual locations, but the differences between the responses at various locations is of great interest. Most of the studies on estimation of slope (rate of change) have concentrated in Central Composite Designs (CCD) yet mixture experiments are intended to show the response for all possible formulations of the mixture and to identify optimal proportions for each of the ingredients at different locations. Slope optimal mixture designs for third degree Kronecker model were studied in order to obtained optimal formulations for all possible ingredients in simplex centroid. Weighted Simplex Centroid Designs (WSCD) and Uniformly Weighted Simplex Centroid Designs (UWSCD) mixture experiments were obtained in order to identify optimal proportions for each of the ingredients formulation. Derivatives of the Kronecker model mixture experiment were used to obtain Slope Information Matrices (SIM) for four ingredients. Maximal parameters of interest for third degree Kronecker model were considered. D-, E-, A-, and T- optimal criteria and their efficiencies for both WSCD and UWSCD were obtained. Although mixtures experiments are usually intended to predict the response for all possible formulations of the mixture and to identify optimal proportions for each of the ingredients, little research has been done on I-optimal third degree Kronecker designs. I-optimal designs were also studied in order to predict the optimal response(s) for all possible formulations or ingredients in the simplex centroid. The general equivalence theorem for I-optimality was used to test optimality of different mixture formulations. UWSCD was found to perform better than WSCD in terms of slope and average prediction variance with most formulations satisfying general equivalent theorem for I-optimality. The pure blend (1,0,0,0) for Vendex (V) and four mixture pesticides (¼, ¼, ¼, ¼) for Vendex (V), Omite (O), Kelthane (K) and Dibrom (D) for UWSC designs yielded more optimal results therefore recommended for use in mites eradication in straw berries plants. R-program was used in the analysis of data. This work could also be extended to cover mixture-process experiment Kronecker model and graphical methods for evaluating mixture designs with respect to slope such as slope along Cox direction.

TABLE OF CONTENTS

LIST OF TABL

ABBREVIATIONS AND ACRONYMS

ANOVA Analysis of Variance

APV	Average Prediction Variance
AV	Average Variance
MSS	Mean Sum of Squares
MSSE	Mean Sum of Squares due to Error
MSSR	Mean Sum of Squares due to Regression
RSM	Response Surface Methodology
SIM	Slope Information Matrices
SSE	Error Sum of Squares
SSR	Regression Sum of Squares
SST	Total Sum of Squares
UWSC	Uniform Weighted Simplex Centroid
UWSCD	Uniformly Weighted Simplex Centroid Design
VIF	Variance Inflation Factor
WSC	Weighted Simplex Centroid
WSCD	Weighted Simplex Centroid Design

CHAPTER ONE

INTRODUCTION

1.1 BACKGROUND OF THE STUDY

Response surface methodology (RSM) is a collection of mathematical and statistical tools or techniques that are useful for modeling and analysis of problems in which a response of interest is influenced by several factors or variables and the objective is to optimize this response, Montgomery (2001). Response Surface Methodology is an important subject in the statistical design and analysis of experiments. It is widely used in many disciplines such as Manufacturing Industry, Biological, Clinical, Social, Food processing, Engineering, Agricultural sciences, amongst others. It is a tool in statistical analysis of experiments where the yield is believed to be influenced or determined by one or more controllable factors. The main goal of RSM is to use a sequence of designed experiments to obtain an optimal response as introduced by Box and Wilson (1951). Their idea was motivated by the need to run experiments efficiently through a proper choice of design, and to determine operating conditions on a set of controllable variables that give rise to an optimal response.

Response surface methodology focus on approximating the functional relationship between a given response and the factors or variables involved as well as permitting a variety of experimental designs which allows one to achieve the estimate as efficiently and as economical as possible. For instance when the production yield y is affected by both the temperature t_1 and pressure t_2, the true relationship between response and explanatory variables can be expressed mathematically as

$$y = f(t_1, t_2) + e \tag{1.1}$$

where e in equation (1.1) is the experimental error which represents any measurement error on the response as well as other types of variations not explained by the variation in the explanatory variables. This implies that there are cases in which variation in the response variable Y is not fully explained by the explanatory variables.

Mixture experiments are special type of response surface designs where the factors under study are proportions of the ingredients of a mixture. Mixture experiments are common problems in many disciplines, such as the chemical technology, food, pharmaceutical, and the process industries. Cornell (2002) defines that in mixture experiments, the response is assumed to depend only on the relative proportions of the mixture components and not on the amount of the mixture. A mixture experiment involves mixing various proportions of two or more components to make different compositions of an end product.

In recent years, prediction-based optimality criteria have gained substantial popularity for generating response surface designs in industry. The best known prediction-based optimality criteria are the G-criterion, which seeks designs that minimize the maximum prediction variance over the experimental region, and the I-optimality criterion, which seeks designs that minimize the average prediction variance over the experimental region.

Mixture components proportions t_i are subject to the constraints

$$0 \le t_i \le 1, \text{ i=1, 2, ..., q and } \sum_{i=1}^{q} t_i = 1 \tag{1.2}$$

where q is the number of components. Therefore, the factor space reduces to regular $(q-1)$ dimensional simplex. The components proportions are often subjected to single or multiple-components constraints. The constraints in equation (1.2) yield a simplex experimental region, while single or multiple-component constraints generally yield a polyhedral constrained region. Cornell (2002) discussed experimental design methods for simplex and constrained region mixture experiments. The mixture constraint in (1.2) has a substantial impact on the fitted model. The first major consequence of the mixture constraint is that the linear model cannot contain an intercept. Otherwise, the model's parameters cannot be estimated uniquely. Another consequence of mixture constraints is that all cross products of proportions $t_i t_j$ and the squares t_i^2 should not be included simultaneously as this leads to perfect collinearity. For every proportion t_i

$$t_i^2 = t_i\left(1 - \sum_{i \neq j}^{q} t_j\right) = t_i - \sum_{i \neq j}^{q} t_i t_j. \tag{1.3}$$

Thus, the square of a proportion is a linear combination of its cross products. Scheffé (1958) proposed the Scheffé mixture model for first order as

$$E(Y) = \sum_{i=1}^{q} \beta_i t_i. \tag{1.4}$$

whereas the second order Scheffé model is given by

$$E(Y) = \sum_{i=1}^{q} \beta_i t_i + \sum_{i=1}^{q-1} \sum_{j=1}^{q} \beta_{ij} t_i t_j. \tag{1.5}$$

The special cubic Scheffé model is written as

$$E(\mathrm{Y}) = \sum_{i=1}^{q} \beta_i t_i + \sum_{i=1}^{q-1} \sum_{j=1+1}^{q} \beta_{ij} t_i t_j + \sum_{i}^{q-2} \sum_{j=i+1}^{q-1} \sum_{k=j+1}^{q} \beta_{ijk} t_i t_j t_k . \tag{1.6}$$

The full cubic Scheffé model is

$$E(\mathrm{Y}) = \sum_{i=1}^{q} \beta_i t_i + \sum_{i=1}^{q-1} \sum_{j=1+1}^{q} \beta_{ij} t_i t_j + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} \gamma_{ij} t_i t_j (\mathrm{t}_i - \mathrm{t}_j) + \sum_{i}^{q-2} \sum_{j=i+1}^{q-1} \sum_{k=j+1}^{q} \beta_{ijk} t_i t_j t_k . \tag{1.7}$$

When there is curvature arising from non-linear blending between component pairs, the parameters represent either synergistic or antagonistic effect. Higher order terms are frequently necessary in mixture models because, the phenomena studied may be complex hence cannot be well studied by lower order terms or the experimental region is frequently the entire operability region and is therefore large, requiring an elaborate model.

There are standard mixture designs for fitting standard models, such as simplex-lattice designs and simplex centroid designs. When mixture components are subject to additional constraints, such as a maximum or minimum value of component designs other than the standard mixture designs, referred to as constrained mixture designs or extreme vertices designs are appropriate.

1.2 SIMPLEX-LATTICE DESIGNS

To accommodate a polynomial equation to represent the response surface over the entire simplex region, a natural choice for a design would be one whose points are spread evenly over the whole simplex factor space, Cornell (2003). An ordered arrangement consisting of a uniformly spaced distribution of points on a simplex is known as a lattice. The name lattice is used to make reference to an array of points.

Scheffé (1958, 1963) introduced the $\{q, m\}$ simplex lattice designs and simplex-centroid designs. A $\{q, m\}$ simplex-lattice design for q ingredients involves all possible formulations, the q individual ingredient proportions belonging to the set $\left\{0, \frac{1}{m}, \frac{2}{m}, \frac{3}{m}, \ldots, 1\right\}$.

In total, there are $\binom{m+q-1}{m}$ points in a $\{q, m\}$ simplex-lattice design.

For $\{3, 2\}$ simplex-lattice design involves six design points, the pure components $(1, 0, 0)$, $(0,1,0)$, $(0,0,1)$ and binary mixture $\left(\frac{1}{2}, \frac{1}{2}, 0\right)$, $\left(\frac{1}{2}, 0, \frac{1}{2}\right)$ and $\left(0, \frac{1}{2}, \frac{1}{2}\right)$. In general, there are

q pure components and $\binom{q}{m} = m\left(\frac{m-1}{2}\right)$ binary mixtures.

1.3 SIMPLEX-CENTROID DESIGNS

Simplex centroid designs, introduced in Scheff´e (1963), are mixture designs in which coordinates are zero or equal to each other. The q-component simplex-centroid design

involves $2^q - 1 = q + \binom{q}{2} + \ldots + \binom{q}{r} + \ldots + 1$ distinct design points in total: the q pure components, the $\binom{q}{2}$ binary mixtures, the $\binom{q}{3}$ permutations of four component mixture $\left(\frac{1}{3},\frac{1}{3},\frac{1}{3},0,...,0\right)$, the $\binom{q}{4}$ permutation of four component mixture $\left(\frac{1}{4},\frac{1}{4},\frac{1}{4},\frac{1}{4},0,...,0\right)$ and so on up to mixtures involving $\left(\frac{1}{q},\frac{1}{q},\frac{1}{q},...,\frac{1}{q}\right)$ of equal proportion of all q components or q-nary mixtures.

1.4 EXTREME VERTICES DESIGNS

When both minimum and maximum component restrictions exist for at least one mixture component, the extreme vertices designs introduced by McLean and Anderson (1966) can be used. In many mixture problems, the experimenter will have information on lower and upper bounds of each component that they wish to examine before the experiment is designed. The extreme vertices design contains mixtures that satisfy the lower and upper bound constraints on every component. Consider the situation where lower and upper bounds (L_i and U_i) are to be placed on each of the i-components in a q-component mixture. We determine the lower (L_i) bounds and upper (U_i) bounds for each proportion $t_1,\ t_2,\ ...\ ,\ t_q$ in the mixture:

$$0 \le L_1 \le t_1 \le U_1 \le 1$$
$$0 \le L_2 \le t_2 \le U_2 \le 1$$
$$\vdots$$
$$0 \le L_q \le t_q \le U_q \le 1.$$

1.5 MIXTURE-AMOUNT DESIGNS

Mixture-amount experiment is a mixture experiment that is performed at two or more levels of total amount. Mixture experiment methodology has been extended to cater for situations where the response factors depend on the proportions of ingredient and the amount of the mixture. A common example of the application on mixture-amount designs is the formulation of organic fertilizers composed of different proportions of nitrogen, phosphate and potassium. The experimenter wishes to investigate how much fertilizer to apply, as well as to find the best relative proportions of the main components. For this kind of mixture-amount experiments, several levels of total amount are needed. The amount can vary between some minimum and maximum value so that:

$$0 \le B_{i(\min)} \le B_i \le B_{i(\max)}$$

where $B_{i(\min)}$ is the lower limit and $B_{i(\max)}$ is the upper limit of the amount in the in mixtures in terms of grams.

1.6 MIXTURE-PROCESS VARIABLE DESIGNS

Process variables are factors in an experiment that do not form any part or portion of the mixture but whose levels, when changed or altered, could affect the blending properties of ingredients. While introducing process variables, Scheffé (1963) defined complete simplex centroid with factorial experiment as one in which at each of $2^q - 1$ points of the simplex centroid designs, a complete s^k factorial experiment is conducted with k process variables each at ‘s’ levels.

In general, a mixture-process variable model is the reduced model resulting from the product of a Scheffé mixture model in q components and a response surface design with k process variables. According to Cornell (2003), in order to include process variables in the design and analysis of mixture experiments, there are two different approaches that can be taken in working with the mixture component. The first approach deals directly with the mixture components $t_1, t_2, ..., t_q$ while the second approach deals with k mathematically independently variables $w_1, w_2, ..., w_k$.

1.7 KRONECKER MODELS

Draper and Pukelshiem (1998) proposed a set of mixture experiments models referred to as K-models or Kronecker models. K-models are alternative representation of mixture models. The models are based on Kronecker algebra of vectors and matrices. K-models offer attractive symmetries, compact notations and homogeneous model functions. The expected response to any mixture experiment, when studied using K-models, is homogeneous in ingredients. The mixture ingredients, t_i, can conveniently be written as a $q \times 1$ vector $t = (t_1, t_2, ..., t_q)$. The Kronecker square is a vector of q^2 cross products $t_i t_j$ arranged lexicographically as

$t \otimes t = (t_1t_1,\ t_1t_2,\ \ldots,t_1t_q,\ t_2t_1,\ \ldots,t_2t_q,\ldots,t_qt_1,\ldots,t_qt_q\ ),$ where symmetry is attained along with duplication of terms. The Kronecker cube $t \otimes t \otimes t$ is a $q^3 \times 1$ vector of all the terms of the form $t_it_jt_k$ arranged lexicographically such that,

$t \otimes t \otimes t = (t_1t_1t_1,\ t_1t_1t_2,\ \ldots,t_1t_1t_q,\ t_1t_2t_2,\ \ldots,t_1t_2t_q,\ldots,t_qt_qt_1,\ldots,t_qt_qt_q\ ).$

1.8 AXIAL DESIGNS

The (q,m) simplex-lattice and q-component simplex-centroid designs are boundary designs in that, with the exception of the overall centroid, the points of these designs are positioned on the boundaries (vertices, edges, faces, etc.) of the simplex factor spaced. Axial designs on the other hand, are designed consisting mainly of complete mixture or q-component blends where most of the points are positioned inside the simplex. Axial designs have been recommended for use when component effects are to be measured and in screening experiments, particularly when first-degree models are to be fitted. Designs with points lying on the axis of components that is imaginary line extending the base points $t_i = 0,\ t_j = \frac{1}{q-1}$ for all i≠j to the vertex where t_i=1, t_j=0 ∀ i≠j are called axial designs.

1.9 STATEMENT OF THE PROBLEM

Goos et al (2016), studied the I-optimal mixture experiments on second order, special cubic and q^{th} degree Scheff`e models, also Goos and Syafitri (2014) studied the problem of finding continuous V-optimal mixture designs for the qth degree model but little has been done in the literature on I-optimal design third degree Kronecker model mixture experiments. Yet I-optimal designs minimize the average variance of prediction and, therefore more appropriate for mixture experiments than the commonly used optimal designs, which focus on a precise model estimation rather than precise predictions. Prediction variance provides a measure of the precision of the estimated response at any point in the design space. It is desirable that the distribution of the prediction variance throughout the design space should be reasonable small and stable. The aim of I-optimality is to minimize the average of the scale prediction variance throughout the whole region of interest. In this study, we obtained the I-optimal designs for two, three and four mixture components for both Weighted Simplex Centroid Design (WSCD) and Uniform Weighted Simplex Centroid Designs (UWSCD) for third degree Kronecker model for mixture experiments.

In response surface designs, the main interest of the experimenter may not necessarily be in the response at individual locations but, the differences between the responses at various locations may be of greater interest, Box and Draper (1980). Mixture experiments are special type of response where the factors under study are ingredients. When interest is in difference between responses at points close together in the factor space, the estimation of local slopes of the response surface becomes very important. Sung et al (2009), considered a class of multifactor designs for estimating the slope of a second order response surface regression model with correlated error. Second order slope-rotatability over all directions and also with equal maximum directional variance in the case of two factors was derived for a general correlated error structure.

Marquardt and Snee (1974) discussed test statistics for mixture models. They noted that some portions of standard analysis of variance (ANOVA) table and related statistics for no-intercept models are incorrect for mixture experiment models and presented the proper formulas. Unfortunately, some publications still appear containing incorrect results.

From these literature, it is a clear indication that most of the work has been done on central composite designs and other rotatable designs hence there was a need to extend the concept of slope to mixture experiments third degree Kronecker, this method was therefore used for proper identification of the ingredients ratio that leads to an optimal response.

1.10 GENERAL OBJECTIVE

To determine optimal designs for third degree Kronecker model mixture experiments with application in blending of chemicals for control of mites in strawberries.

1.10.1 Specific Objectives

The specific objectives for this study was to,

(i) Derive slope information designs using Weighted Simplex Centroid (WSC) and Uniformly Weighted Simplex Centroid (UWSC) designs for third degree Kronecker model mixture experiments.

(ii) Determine D-, E-, A- and T-optimal values for both Weighted Simplex Centroid (WSC) and Uniform Weighted Simplex Centroid (UWSC) designs mixtures experiments.

(iii) Obtain I-optimality for parameter sub-system Weighted Simplex Centroid (WSC) and their Uniform Weighted Simplex Centroid (UWSC) designs counterparts.

(iv) Determine the optimal model for simplex centroid designs using four ingredients mixture experiments for blending of chemical pesticides.

1.11 JUSTIFICATION OF THE STUDY

In mixture experiments, the factors under study are proportions of the ingredients of mixture. There are many problems that deal with investigation of mixtures of m factors or ingredients which influence the response through the ratios or proportions which are mixed together. For any mixture experiment to be successful, it must focus on a precise response predictions prior experimentation. The I-optimality criterion seeks to minimize the average prediction variance over the experimental region. It was also important to study optimal slope designs at different points of the simplex centroid for proper identification of ingredients ratio leading to an optimal response.

1.12 SCOPE OF THE STUDY

The study was restricted to simplex centroid designs, with Kronecker model as put forward by Draper and Pukelsheim (1998). We obtained a set of weighted centroid and uniformly weighted designs for the maximal parameter sub-system for two, three and four ingredients mixture experiments. The information matrices for the feasible weighted centroid designs were obtained based on the parameter of interest. The I-optimal values were calculated and the slope information matrices were used to obtain D-, A-, E- and T-optimal values for both Weighted Simplex Centroid (WSC) and Uniform Weighted Simplex Centroid (UWSC) designs.

CHAPTER TWO

LITERATURE REVIEW

2.1 INTRODUCTION

In this chapter, literature on response surfaces methodology, slope mixture designs and optimality of mixture experiments were reviewed. The research gaps on slope and I-optimality designs were identified for study.

2.2 RESPONSE SURFACE METHODOLOGY

Early seminal work done by Scheffé' (1958, 1963) suggested and analyzed canonical model forms when the regression function for the expected response is a polynomial of degree one, two or three for the expected response otherwise referred to as the S-models or S-polynomials. The main experimental domain is a probability simplex given by;

$$T_m = \left\{ t = (t_1, ..., t_m)' \in [0,1]^n : \sum_{i=1}^{m} t_i = 1 \right\}.$$

Under the experimental condition $t \in T_m$ where the response Y_t is taken to be the real valued random variable. In a polynomial regression model the expected value $E(Y_t)$ is a polynomial function of t.

Draper and Pukelsheim (1998) suggested the second degree Kronecker model as;

$$E(\mathrm{y}_t) = \mathrm{f(t)}'\theta = \sum_{i,j=1}^{m} \theta_{ij} t_i^2 + \sum_{i,j=1}^{m} (\theta_i + \theta_{ij})\ t_i t_j.$$

where y_t, the observed response under the experimental conditions $t \in T$, is taken to be scalar random variable and $\Theta = (\theta_{11}, \theta_{12}, ..., \theta_{mm})^t \in \Re^{m^2}$ is unknown parameter.

The Kronecker models are best-studied using permutationally invariant or exchangeable designs. Draper and Pukelshiem (1999) showed that for first degree Kronecker model vertex point designs are unique optimal designs under the Kiefer Ordering. Kiefer ordering comprises of two steps; the first step is the majorization ordering to improve balancedness of a design. The second step is an improvement relative to the Loewner matrix ordering within the class of exchangeable moment matrices. Many design problems enjoy symmetry properties, in that they remain invariant under a group of linear transformation. Thus use of invariant design for homogenous symmetric K-models helps to obtain the prime attributes of good experimental designs, that is, symmetry and balancedness. Draper and Pukelshiem (1999) and Draper *et al* (2000) showed that for the second-degree mixture model, the set of weighted simplex centroid designs constitutes the convex complete class for Kiefer ordering. The Kronecker representation has several advantages, this include; more compact notation, more convenient invariance properties, and the homogeneity of the regression terms, Draper and Pukelsheim (1998) and Prescott, *et al* (2002). The moment matrix $m(\eta) = \int f(t) f(t)^T \, d\eta$ for the third degree Kronecker model has all entries homogeneous in degree six and reflects the statistical properties of a design τ . Prescott and Drapper (2004) also proposed several models for fitting data from the mixture amounts experiment. Smith (1918) was the first to develop optimal designs for regression problems, many years later, Kiefer (1959) developed useful computational procedures for finding optimum designs in regression problems of statistical inference.

Box and Hunter (1957) suggested that the basic requirement for any response surface design was that it could be used in blocks. Piepel and Cornell (1994) used a five-component waste grout example to compare five approaches to analyze a mixture experiment: component proportions, mixture-amount, mixture-process variable, mathematically independent variables and the slack variable. Using a six- factor fish-patty example, Gorman and Cornell (1982) proposed a reparametrized model form which allows the process variables to be estimated distinctly from the effects of the mixture components. Montgomery and Voth (1994) discussed the impact of multicollinearity in mixture experiments. Cornell and Gorman (2003) introduced two model forms to encounter the problem of collinearity that arises when the mixture region is highly constrained.

Snee (1981) discussed the construction of gasoline blending models to illustrate some of the practical problems met in mixture experimentation. The attention was focused on the use of simplex and extreme vertices designs in the development of blending models. It was noted that the interaction (quadratic) model provided an accurate account of gasoline blending characteristics over the total composition range. Kowalski *et al* (2000) proposed a new class of designs for mixture experiments with process variables which is based on central composite designs in the process variables. They presented a new model type to accommodate these new designs.

Pukelsheim (1993) gives a review of the general design of experiment. As a consequence, the search for optimal designs may be restricted to weighted centroid designs for most criteria. For particular criteria applied to mixture experiments Kiefer (1959, 1975 and 1978) and Galil and Kiefer (1977). Many of these studies have concentrated on second degree Kronecker model. Korir (2008) extended the work to third degree Kronecker model by use of equivalent theorem in calculation of weights; also Kerich *et al* (2014) studied the D-optimal designs for third degree Kronecker model mixture experiments with application in artificial sweetener experiment.

Marquardt (1970) suggested a rule of thumb that Variance Inflation Factor (VIF) greater than 5 indicates harmful multicollinearity in mixture experiments. Marquardt and Snee (1974) discussed test statistics for mixture models. They noted that some portions of standard analysis of variance (ANOVA) table and related statistics for no-intercept models are incorrect for mixture experiment models and presented the proper formulas. Therefore, it is important to note that, in canonical polynomials ANOVA, the regression sum of squares (SSR) and total sum of squares (SST) are always uncorrected.

2.3 SLOPE DESIGNS

Draper (1963) suggested simple derivations of the technique and proofs of ridge analysis for unrestricted mixture variables. Estimation of slopes is particularly relevant in situations where the experimenter wishes to determine optimal settings of the factors in order to produce the maximum (minimum) value of the response. In response surface designs the main interest of the experimenter may not always be in the response at individual locations but, the differences between the responses at various locations may be of greater interest, Herzberg (1967), Box and Draper (1980), Huda and Mukerjee (1984) and Huda (2006a). They suggested that when interest is in the difference between responses at points close together in the factor space, the estimation of local slopes (rate of change) of the response surface becomes very important. Atkinson (1970) initiated research on designs for estimating slopes. Subsequently, Ott and Mendenhall (1972), Murty and Studden (1972), Myers and Lahoda (1975), Mukerjee and Huda (1985) also contributed towards optimal design of experiments for estimating slopes. A review of the previous work in this area is provided in Huda (2006b). Huda and Al-Shiha (1999) extended the concepts of D-, E- and A-optimality criteria to designs for estimating the slopes of a response surface and consider the problem of deriving optimal designs under the D-optimality criterion. Sung et al (2009), considered a class of multifactor designs for estimating the slope of a second order response surface regression model with correlated error. Second order slope-rotatability over all directions and also with equal maximum directional variance in the case of two factors was derived for a general correlated error structure.

Draper and John (1977) suggested the designs for the models with inverse terms, using three and four mixture components. For such models, having both polynomial and inverse terms, near D-optimal designs and n-point exact designs were proposed. Also efficient exact designs were obtained when the set of candidate points were restricted to the points of support of the D-optimal design. Hader and Park (1978) proposed similar rotatable properties for slope rotatable designs as given by Box and Hunter (1957). It was pointed out that for central composite design this property could be achieved by adjusting the axial distance α.

2.4 OPTIMALITY CRITERIA

Design optimality criteria are often called the alphabetical optimality criteria because they are named by some of the letters of the alphabet. Kiefer and Wolfowitz (1959) were among the first authors who developed these optimality criteria. These are single number criteria where each one is intended to capture a different aspect of the 'goodness' of a design. However a best design is typically more complicated than can be summarized by single numbers. These are just simplifications of the whole process of rating a design. Box and Hunter (1957), Box and Draper (1959, 1963, 1975), and Myers and Montgomery (2002) discussed some of the properties for comparing designs.

2.5 I-OPTIMALITY

I-optimal designs minimize the average variance of prediction and therefore more appropriate for mixture experiments for precise predictions of responses. Average prediction variance provides a measure of the precision of the estimated response at any point in the design space. The I-optimal designs criterion is often called the V-optimality criterion, Atkinson *et al* (2007), but the names IV- or Q-optimality have been used as well, Borskowski (2003). The generation of I-optimal completely randomized designs is discussed in Haines (1987), Meyer and Nachtsheim (1988, 1995), Hardin and Sloane (1993) and Borkowski (2003a). Hardin and Sloane (1993) demonstrated that D-optimal response surface designs perform poorly in terms of the I-optimal criterion, while I-optimal designs perform reasonably well with respect to the D-optimality criterion. This phenomenon is more pronounced when the experimental region is cuboidal than when it is spherical. Laake (1975) analytically derived the I-optimal weights for the design points in the case $q \geq 3$, assuming that the design points are the points of the $(q, 2)$. In experiments with mixtures, Liu and Neudecker (1995) applied Weighted Simplex Centroid (WSC) to obtain V-optimal allocation of observations which was shown to be an optimal design over the entire simplex on Scheffé's polynomial model using the equivalence theorem.

According to Borkowski (2003b), an experimenter using the IV-criterion or some Average Prediction Variance (APV) measure as a design evaluation criterion needs to be aware of specific methods used by statistical software packages. If the estimate of IV is the average taken over a relatively large random set of evaluation points, the Monte Carlo method will be reliable. Monte Carlo method would also be appropriate if the design space was the hyper sphere or irregularly-shaped design region rather than the hypercube. Goos et al (2016) studied I-optimal designs of mixture experiments for second order, special cubic and q^{th} degree models. Goos and Syafitri (2014) studied the problem of finding continuous V-optimal mixture designs for the qth degree model. They provided a critical look at the results published in Liu and Neudecker (1995) and found out that their designs were not V-optimal. In this study, the work work of Goos and Syafitri (2014) was extended to cover an average prediction variance third degree Kronecker model mixture experiment which is more appropriate for mixture experiments than the commonly used optimal designs that focus on a precise model estimation rather than precise predictions. Also from the work of Hader and Park (1978), Huda and Al-Shiha (1999) and Huda (2006a), most of the work has been done on central composite designs hence there was a need to extend the concept of slope to mixture experiments third degree Kronecker, this method was therefore used for proper identification of the ingredients ratio that leads to an optimal response.

CHAPTER THREE

METHODOLOGY

3.1 INTRODUCTION

Mixture experiments are associated with the investigation of the m factors, assumed to influence the response only through proportions in which they are blended together. The mixture ingredients t_1, t_2 ,…, t_m are such that $t_i \geq 0$ and further restricted by $\sum t_i = 1$. Thus the experimental domain is the probability simplex

$$T_m = \left\{ t = (t_1 \ ,\ldots, \ t_m ,)' \in [0,1]^m : \sum_{i=1}^{m} t_i = 1 \right\}.$$

Under experimental condition $t \in T_m$, the response Y_t is taken to be a real-valued random variable. In a polynomial regression model the expected value $E(Y_t)$ is a polynomial function of t.

The work done by Draper and Pukelsheim (1998) is being extended to polynomial regression model for third degree mixture model, where by the S-polynomial and expected response takes the form

$$E(Y_t) = f(t)'\theta = \sum_{i=1}^{m} \theta_i t_i + \sum_{\substack{i,j=1 \\ i<j}}^{m} \theta_{ij} t_i t_j + \sum \sum \sum_{i<j<k}^{m} \theta_{ijk} t_i t_j t_k \tag{3.1}$$

and when the regression function is the homogeneous third-degree K-polynomial, the expected response takes the form

$$E(Y_t) = f(t)'\theta = (t \otimes t \otimes t)'\theta = \sum_{i=1}^{m} \sum_{j=1}^{m} \sum_{k=1}^{m} \theta_{ijk} t_i t_j t_k . \tag{3.2}$$

The Kronecker powers $t^{\otimes 3} = (t \otimes t \otimes t),\ (\mathrm{m}^3+1)$ vectors, consists of pure cubic and three-way interactions of components of t in lexicographic order of the sub scripts with evident that third-degree restrictions are $\theta_{ijk} = \theta_{ikl} = \theta_{jik} = \theta_{jki} = \theta_{kij} = \theta_{kji}$ for all i, j and k. All observations taken in an experiment are assumed to be of equal unknown variance and uncorrelated.

3.2 MOMENT MATRIX

The moment matrix $M(\eta) = \sum_{j=1}^{t} w_j f(t_j) f(t_j)^t = \int_{\eta} f(t) f(t)^t d\eta$ for the third degree Kronecker model has all entries homogeneous in degree six and reflects the statistical properties of a design η.

The simplex restriction has an immediate effect on moment matrices,

$1_m^{'} M(\eta) 1_m = \int_\eta 1_m^{'} t t^{'} 1_m \, d\eta = 1$ that is, the entries of any third degree Kronecker moment matrix sum to one. The moment matrix can be partition into sub moments according to the number of ingredients in a simplex centroid design as follows

$$M(\eta) = \alpha_1 M(\eta_1) + \alpha_2 M(\eta_2) + ... + \alpha_m M(\eta_m). \qquad (3.3)$$

In Uniformly Weighted Simplex Centroid Designs (UWSCD), the weights are assumed to be distributed uniformly in the sub moments matrices hence $\alpha_1 = \alpha_2 = ... = \alpha_m = \frac{1}{m}$ and their moment matrix is given by

$$M(\eta) = \tfrac{1}{m} M(\eta_1) + \tfrac{1}{m} M(\eta_2) + ... + \tfrac{1}{m} M(\eta_m). \qquad (3.4)$$

3.3 INFORMATION MATRIX

Consider the Euclidean unit vectors in $\Re^m$ denoted by $e_1, e_2, ..., e_m$ and the set for

$$e_{iij} = e_i \otimes e_i \otimes e_j, \; e_{ijk} = e_i \otimes e_j \otimes e_k \text{ for i<j<k, i,j,k=\{1,2,...,m\}}. \qquad (3.5)$$

Let K be a $k \times s$ coefficient matrix such that

$$K = (K_1; K_2; K_3) \in \Re^{m^3 \times (m+1)} \qquad (3.6)$$

where

$$K_1 = \sum_{i=1}^{m} e_{iii} e_i^{'} \;, \qquad K_2 = \frac{1}{3(m-1)} [\sum_{\substack{i,j=1 \\ i<j}}^{m} (e_{iij} + e_{iji} + e_{jii}) \, e_i^{'}] \quad \text{and} \quad K_3 = \frac{1}{m(m-1)(m-2)} \sum_{\substack{i,j,k=1 \\ i \neq j \neq k}}^{m} (e_{ijk}).$$

The Kronecker model of the full parameter vector $\theta \in \Re^{m^3}$ is not estimable. When fitting this model, the parameter subsystem considered in this study can be written as

$$K'\theta = \begin{Bmatrix} (\theta_{iii})_{1 \le i \le m} \\ \frac{1}{3(m-1)} \left\{ \sum_{i,j=1}^{m} (\theta_{iij} + \theta_{iji} + \theta_{jii}) \right\} \\ \frac{1}{m(m-1)(m-2)} \sum_{\substack{i,j,k=1 \\ i \ne j \ne k}}^{m} (\theta_{ijk}) \end{Bmatrix} \in \Re^{(m+1)} \quad \text{for all } \theta \in \Re^{m^3} \tag{3.7}$$

where $K \in \Re^{m^3 \times (m+1)}$.

The parameter subsystem $K'\theta$ of interest is a maximal parameter system in the full parameter model. The information matrix for the parameter subsystem is given by

$$C_k(M(\eta)) = LM(\eta)L' \in NND(s) \tag{3.8}$$

where L is the left inverse of coefficient matrix K and is defined by

$$L`=(K'K)^{-1}K'. \tag{3.9}$$

Thus the information matrices for $K`\theta$ are linear transformation of moment matrices.

3.4 SLOPE OPTIMALITY

In many applications of response surface methodology, good estimation of the derivatives of the response function is as important as estimation of the mean response. In order to maximize the response, the movement of the design center must be in the direction of the directional derivatives of the response function, that is, $\frac{\partial Y_t}{\partial t}$. The computation of a stationary point analysis and steepest ascent of ridge analysis employ gradient techniques. The steepest ascent of ridge analysis depends heavily on the partial derivatives of the estimated response function with respect to the design variables. Since the designs that attain certain properties in Y (estimated response) do not enjoy the same properties for the estimated derivatives (slopes), we considered the use of derivatives in constructions of such experimental designs in order to achieve the specified property.

In practice, it is often of interest to investigate the slope of the response surface at a point t not only over the axial directions, but also over any specified direction. We develop the concept of robust slope over all directions. Let H be a matrix arising from the differentiation of $f(t)'\theta$ with respect to each of the m independent factors, Sung. et al (2009). That is;

$$H = \left(\frac{\partial f'(t)}{\partial t_1}, \frac{\partial f'(t)}{\partial t_2}, ..., \frac{\partial f'(t)}{\partial t_m} \right)', \tag{3.10}$$

where, $f(t) = t \otimes t \otimes t.$

Therefore, slope information matrix D_c is given by

$$D_c = HC_k(M(\eta))H'. \tag{3.11}$$

3.5 OPTIMAL WEIGHTED CENTROID DESIGNS

A convex combination $\eta(\alpha) = \sum_{i=1}^{m} \alpha_i \eta_i$ with $\alpha = (\alpha_1, \alpha_2, ..., \alpha_m)' \in \mathrm{T}_m$ is called a weighted centroid design with weight vector, where the weights satisfy

$$\sum_{i=1}^{m} \alpha_i = 1. \tag{3.12}$$

For m ingredients, there are m elementary centroid designs, n_i , placing equal weights $\frac{1}{\binom{m}{i}}$

on the points having i out of their m components equal to $\frac{1}{i}$ and zero elsewhere. The lower order moments are expressed in form of sixth order moments. The optimal weights $\alpha_1,\ \alpha_2,...,\alpha_m$ were obtained using simplex restrictions for $i = 1,\ 2,\ 3,\ ...\ ,m$.

3.6 OPTIMALITY CRITERIA AND THEIR EFFICIENCIES

Optimal designs are experimental designs that are generated based on a particular optimality criterion and are generally optimal only for a specific statistical model.

3.6.1 D-Optimality

The most commonly optimality criterion to select designs is the D-optimality criterion which seeks designs that maximize the determinant of the information matrix. The aim of D-optimality is essentially a parameter estimation criterion.

Let C be a parameter subsystem information matrix of S dimension, then D-optimality is given by

$$\phi_0(C) = (\det C)^{\frac{1}{s}}. \tag{3.13}$$

Maximization of the determinant of the information matrices is the same as minimizing

the determinant of the dispersion matrices that is $(\det C)^{-1} = \det(C^{-1})$.

We derive optimal weighted centroid designs for the determinant criterion, ϕ_0 that is, D-optimality criteria. The D-criterion has an important property in optimal designs because it minimizes the variances and the covariance of the parameters estimates. D-efficiency of a design η over the design η^* is given by

$$D(\tau) = \left\{ \frac{|M(\eta)|}{|M(\eta^*)|} \right\}^{\frac{1}{s}} \tag{3.14}$$

where $M(\eta)$ and $M(\eta^*)$ are moments of WSC and UWSC designs respectively.

3.6.2 E-Optimality

It is the minimization of the largest Eigen value of the dispersion matrix. It is given by

$$\frac{1}{\phi_{-\infty(C_k(A))}} = \lambda_{\max}\left(C_k(A)^{-1}\right). \tag{3.15}$$

The Eigen value criterion $\phi_{-\infty}$ is one extreme member of the matrix means ϕ_p corresponding to the parameter $p = -\infty$. It is one of the four particular members of the one dimensional family of matrix means ϕ_p that submit itself to the principles that a reasonable criteria must meet as presented in Pukelsheim (1993), therefore expressed it in the form

$$\phi_{-\infty}(C) = \lambda_{\min}(C). \tag{3.16}$$

The E- efficiency for two optimal designs $\phi_{-\infty}(C_1) = \lambda_{\min}(C_1)$ and $\phi_{-\infty}(C_2) = \lambda_{\min}(C_2)$ are given as

$$\frac{\phi_{-\infty}(C_1)}{\phi_{-\infty}(C_2)} = \frac{\lambda_{\min}(C_1)}{\lambda_{\min}(C_2)}. \tag{3.17}$$

3.6.3 A-Optimality

Invariance under reparameterization loses its appeal if the parameters of interest have a definite physical meaning. The average variance criterion saves the situation by providing a reasonable alternative. If the coefficients matrix is partitioned into its columns, $K = (c_1, c_2, ..., c_s)$ then the inverse $\frac{1}{\phi_{-1}}$ can be represented as $\frac{1}{\phi_{-1(C_k(A))}} = \frac{1}{s} trace\, C_k(A)^{-1}$.

This corresponds to the average of the standardized variances of the optimal estimates of the scalar parameter systems $c_1'\theta, ..., c_s'\theta$ formed from the columns of K, Pukelsheim (1993). Therefore the average variance criterion is given by

$$\phi_{-1}(C) = \left(\frac{1}{s} traceC^{-1}\right)^{-1}. \tag{3.18}$$

The A-efficiency for two A-optimal designs $\phi_{-1}(C_1)$ and $\phi_{-1}(C_2)$ is given by

$$\frac{\phi_{-1}(C_1)}{\phi_{-1}(C_2)} = \frac{\left(\frac{1}{s} traceC_1^{-1}\right)^{-1}}{\left(\frac{1}{s} traceC_2^{-1}\right)^{-1}}. \tag{3.19}$$

3.6.4 T-Optimality

To discriminate between competing models, Atkinson and Fedorov (1975) introduced T-optimality design criterion in the context of optimal design theory. The T-criterion is given by

$$\phi_{-1}(C) = \frac{1}{s} traceC. \tag{3.20}$$

The T-efficiency for two T-optimal designs C_1 and C_2 is given as

$$\frac{\phi(C_1)}{\phi(C_2)} = \frac{\left(\frac{1}{s} traceC_1\right)}{\left(\frac{1}{s} traceC_2\right)}. \tag{3.21}$$

The optimality properties of designs are determined by their moment matrices, Pukelsheim (1993). The class of φ_p -criteria, that is T-, D-, A- and E- corresponding to parameter values 1, 0, -1 and -∞ respectively are summarized in equation (3.22) as given in Pukelsheim (1993).The amount of information inherent to $C_k(M(\eta))$ is provided by φ_p -criteria with $C_k(M(\eta))$ ¿ PD(m), defined by:

$$\varphi_p(C) = \begin{cases} \lambda_{\min}(C), & if \quad p = -\infty \\ \det(C)^{\frac{1}{s}}, & if \quad p = 0 \\ \left[\frac{1}{s} traceC^p\right]^p, & if \quad p \neq 0, \pm\infty \end{cases}$$

(3.22)

for all C in PD(m). By definition φ_p (C) is a scalar measure which is a function of the eigen values, determinant, trace and average variance of C for all p ¿ [- ∞ ;1].

3.7 I-OPTIMALITY FOR THIRD DEGREE KRONECKER MODEL

I-optimal design minimizes average or integrated prediction variance over the experimental region of interest given as;

$$AV = \frac{1}{\int_{\tau} dt} tr[(t't)^{-1} M].$$

The matrix M is the moment matrix because its elements are proportional to moments of uniform distribution on the design region τ . In the calculation of average prediction variance (APV), we exploit the following formula

$$AV = \int_{\tau} f'(t) M^{-1} f(t) dt = tr[M^{-1} \int_{\tau} f(t) f(t)' dt]. \tag{3.23}$$

This expression can be simplified as

$$= \frac{1}{\int_{\tau} dt} tr[M^{-1} \int_{\tau} f(t) f'(t) dt]. \tag{3.24}$$

Letting $R = \int_{\tau} f(t) f'(t) dt$, the AV is expressed as

$$AV = \frac{1}{\int_{\tau} dt} tr[M^{-1} R]. \tag{3.25}$$

In this case, we assumed all the runs of mixture experiment based on the simplex-centroid design with weights $r_1, r_2, \ldots, r_q$ are independent and that the responses have an equal variance. The information matrix (M) for the parameter system is given as

$$M = T' \wedge T \tag{3.26}$$

where

$$T = [f(t_1),\ f(t_2),\ \ldots,\ f(t_p)]' \tag{3.27}$$

the $p \times p$ model matrix corresponding to p points of the simplex centroid design and the diagonal

$$\wedge = diag(r_1 I_{11}, r_2 I_{22},\ \ldots, \mathrm{r}_q I_{qq}) \tag{3.28}$$

where I_{ii} is the identity matrix of dimension $\begin{pmatrix} q \\ i \end{pmatrix} \times \begin{pmatrix} q \\ i \end{pmatrix}$. The variance-covariance matrix of the ordinary least squares estimator is M^{-1} and the variance of prediction at a given point of t is $f'(t)M^{-1}f(t)$. For parameter sub system of interest, inverse of information matrix (3.8) was used instead of matrix (3.26) as given by

$$C_k^{-1} = (LM(\eta)L` \in NND(s)\ )^{-1}. \tag{3.29}$$

Assuming that the experimental region η is the full $(q-1)$ dimensional simplex S_{q-1}, the elements of R can be obtained using the formula,

$$R = \int_{S_{q-1}} t_1^{p_1},\ t_2^{p_2}, t_3^{p_3}, \ldots, t_q^{p_q} dt_1, dt_2, dt_3, \ldots, dt_q = \frac{\prod_{i=1}^{q} \Gamma(p_i + 1)}{\Gamma(q + \sum_{i=1}^{q} p_i)} = \frac{\prod_{i=1}^{q} (p_i\,!)}{(\sum_{i=1}^{q} p_i + q - 1)!}. \tag{3.30}$$

When the experimental region η is the full $(q-1)$ dimensional simplex S_{q-1}, then its volume is given by

$$volume = \int_{\mathcal{X}} dt = \int_{S_{q-1}} dt = \frac{1}{\Gamma(q)} = \frac{1}{(q-1)!}. \tag{3.31}$$

Therefore average prediction variance is obtained by

$$\text{AV} = (q-1)!\,tr[C_k^{-1}R]. \tag{3.32}$$

I-efficiency of a design η and the design η^* is defined as

$$I(\xi) = \frac{tr\left[C_k^{-1}(\eta^*)R\right]}{tr\left[C_k^{-1}(\eta)R\right]}. \tag{3.33}$$

3.7.1 Equivalence Theorem

The general equivalence theorem provides a methodology to check the optimality of a given continuous design, for any convex and differentiable design optimality criterion. Atkinson *et al* (2007) explain that a continuous design with information matrix C is I-optimal if and only if

$$f^{'}(t)C^{-1}LC^{-1}f(t) \leq tr(C^{-1}L) \tag{3.34}$$

for each point t in the experimental region η according to the general equivalence theorem. The equivalence theorem designs is not constructive, but it can be used to check optimality of a given designs.

3.8 MODEL VALIDITY

The model validity provides important examination to the fitted model whether it offers an adequate approximation of the true response surface. Analysis of variance (ANOVA) and Coefficient of variations were used to examine the fitted Kronecker model.

3.8.1 The Analysis of Variance

The Analysis of Variance for fitted Kronecker model was obtained. The total sum of squares (SST), regression sum of squares (SSR) and error sum of squares (SSE) were calculated. The total sum of squares (SST) for fitted model is given as

$$SST = \sum_{u=1}^{N} (y_u - \bar{y})^2 = y'y - (1'y)^2 / N. \tag{3.35}$$

The regression sum of squares for the fitted model is obtained as

$$SSR = \sum_{u}^{N} (\hat{y}_u - \bar{y})^2 = \hat{\theta}T'y - (1'y)^2 / N. \tag{3.36}$$

The sum of squares due to error is given as

$$SSE = \sum_{u}^{N} (\bar{y}_u - \hat{y})^2 = y'y - \hat{\theta}X'y. \tag{3.37}$$

The analysis of variance table is summarized in Table 3.1 below

Table 3.1: Analysis of Variance

Sources of Variations	**Degrees of Freedom**	**Sum of Squares**	**MSS**	**F**
Regression	$p-1$	$SSR = \sum_{u}^{N} (\hat{y}_u - \bar{y})^2$	$SSR / P-1$	$MSSR / MSSE$
Error	$N-p$	$SSE = \sum_{u}^{N} (\bar{y}_u - \hat{y})^2$	$SSE / N-p$	
Total	$N-1$	$SST = \sum_{u=1}^{N} (y_u - \bar{y})^2$		

3.8.2 Coefficient of Variation

In order to determine how well the estimated model fits the data, R^2 value can be used. The R^2 lies in the interval [0, 1], when R^2 is closer to the 1, the better the estimated model fits the sample data. In general, the R^2 measures percentage of the variation of y around $\bar{y}$ that is explained by the regression model. However, adding a variable to the model always increased R^2, regardless of whether or not the variable is statistically significant. Thus, some experimenter would rather use adjusted R_A^2. When variables are added to the model, the R_A^2 will not necessarily increase.

Therefore R^2 and R_A^2 are given respectively as,

$$R^2 = \frac{SSR}{SST} \tag{3.38}$$

and

$$R_A^2 = 1 - \frac{MSSE}{MSST}. \tag{3.39}$$

3.8.3 Testing the Adequacy of Parameters

To test the adequacy of each parameter in the model, we employed student t test to check the validity of the cubic, two and three interactions in a model. The parameter with the smallest standard error was considered better than the other. The R statistical software was used in the analysis of secondary data.

CHAPTER FOUR

RESULTS AND DISCUSSIONS

4.1 INTRODUCTION

In this chapter, weighted simplex centroids designs and their corresponding uniform designs were discussed. The slope information matrices for third degree Kronecker model were used to obtain D-, A-, E- and T-optimal values and their efficiencies. I-optimal values for the parameter subsystem Kronecker model were obtained for two, three and four ingredients for both weighted and uniformly weighted simplex centroid designs and their corresponding I-optimal efficiencies.

4.2 DESIGNS FOR TWO FACTORS MIXTURE EXPERIMENTS

4.2.1 Simplex Centroid Designs

In two ingredients mixture experiments, there are two elementary centroid designs, η_1 and η_2, placing optimal weights α_1 and α_2 on the two designs respectively as

$$\begin{Bmatrix} 1 & 0 \\ 0 & 1 \end{Bmatrix} \eta_1$$
$$\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \eta_2. \tag{4.1}$$

The two elementary designs, η_1 and η_2, represent moments for pure and binary blends respectively.

4.2.2 Weighted Simplex Centroid Designs

A convex combination $\eta(\alpha)=\sum_{i=1}^{m}\alpha_i\eta_i$ with $\alpha=(\alpha_1,\alpha_2,...,\alpha_m)' \in \mathrm{T}_m$ is called a weighted centroid design with weight vector, where the weights satisfy equation (3.12). The optimal weights α_1 and α_2 are obtained using simplex restrictions. The simplex restriction has an immediate effect on moment matrices, $1_m' M(\eta)1_m = \int_\eta 1_m' tt' 1_m \, d\eta = 1$ that is, the entries of any third degree Kronecker moment matrix sum to one. For two ingredients model, let η be an arbitrary exchangeable design, then its sixth order moments μ_{ij}, were calculated from design (4.1) as given by,

$$
\begin{aligned}
(i)\quad & \mu_6 = \int t_1^6 d\tau = \tfrac{1}{3}[(1)^6 + (\tfrac{1}{2})^6] = \tfrac{65}{192} = 0.3385416\\
(ii)\quad & \mu_{51} = \int t_1^5 t_2^1 d\tau = \tfrac{1}{3}[0 + (\tfrac{1}{2})^5(\tfrac{1}{2})] = \tfrac{1}{192} = 0.00520833\\
(iii)\quad & \mu_{42} = \int t_1^4 t_2^2 d\tau = \tfrac{1}{3}[0+(\tfrac{1}{2})^4(\tfrac{1}{2})^2] = \tfrac{1}{192} = 0.00520833\\
(iv)\quad & \mu_{33} = \int t_1^3 t_2^3 d\tau = \tfrac{1}{3}[0 + (\tfrac{1}{2})^3(\tfrac{1}{2})^3] = \tfrac{1}{192} = 0.00520833.
\end{aligned}
\tag{4.2}
$$

The set of moments of order six determines all the lower order moments. They are expressed in the form of sixth order moments as

$$(i) \quad \mu_5 = \int_t t_1^5 (t_1 + t_2) dt = \int (t_1^6 + t_1^5 t_2) dt = \mu_6 + \mu_{51}$$

$$(ii) \quad \mu_{41} = \int_t t_1^4 t_2^1 (t_1 + t_2) dt = \mu_{51} + \mu_{42}$$

$$(iii) \quad \mu_4 = \int_t t_1^4 (t_1 + t_2) dt = \mu_5 + \mu_{41} = \mu_6 + \mu_{42} + 2\mu_{51}$$

$$(iv) \quad \mu_{32} = \int_t t_1^3 t_2^2 (t_1 + t_2) dt = \mu_{42} + \mu_{33}$$

$$(v) \quad \mu_{31} = \int_t t_1^3 t_2^1 (t_1 + t_2) dt = \mu_{41} + \mu_{32} = 2\mu_{42} + \mu_{33} + \mu_{51}$$

(4.3)

$$(vi) \quad \mu_3 = \int_t t_1^3 (t_1 + t_2) dt = \mu_4 + \mu_{31} = \mu_6 + 3\mu_{42} + 3\mu_{51} + \mu_{33}$$

$$(vii) \quad \mu_{22} = \int_t t_1^2 t_2^2 (t_1 + t_2) dt = \mu_{32} + \mu_{32} = 2(\mu_{42} + \mu_{33})$$

$$(viii) \quad \mu_{21} = \int_t t_1^2 t_2^1 (t_1 + t_2) dt = \mu_{31} + \mu_{22} = 4\mu_{42} + 3\mu_{33} + \mu_{51}$$

$$(ix) \quad \mu_2 = \int_t t_1^2 (t_1 + t_2) dt = \mu_3 + \mu_{21} = \mu_6 + 7\mu_{42} + 4\mu_{51} + 4\mu_{33}$$

$$(x) \quad \mu_{11} = \int_t t_1^1 t_2^1 (t_1 + t_2) dt = \mu_{21} + \mu_{21} = 2(4\mu_{42} + 3\mu_{33} + \mu_{51})$$

$$(xi) \quad \mu_1 = \int_t t_1^1 (t_1 + t_2) dt = \mu_2 + \mu_{11} = \mu_6 + 15\mu_{42} + 6\mu_{51} + 10\mu_{33}.$$

Therefore the weights α_1 and α_2 were calculated using (4.2) and (4.3) relationship. From equation (4.1), μ_{11}, is given by

$$\mu_{11}(\eta) = \tfrac{1}{2}\alpha_1 \mu_{11}(\eta_1) + \alpha_2 \mu_{11}(\eta_2)$$
$$\mu_{11} = \tfrac{1}{2}\alpha_1(0) + \alpha_2(\tfrac{1}{4}) \tag{4.4}$$

where

$$\alpha_2 = 4\mu_{11}. \tag{4.5}$$

Using (x), (4.3), we have $\mu_{11} = \frac{1}{12}$, therefore equation (4.5) becomes

$$\alpha_2 = \tfrac{1}{3}. \tag{4.6}$$

From equation (3.12), we have

$$\alpha_1 = 1 - \alpha_2 = \tfrac{2}{3}. \tag{4.7}$$

Therefore the weights α_1 and α_2 were obtained as 2/3 and 1/3 in equations (4.7) and (4.6) respectively.

4.2.3 Uniformly Weighted Simplex Centroid Designs (UWSCD)

The Uniformly Weighted Simplex Centriod Designs (UWSCD) for two ingredients were assumed to assign uniform weights to the two elementary centroid designs, n_1 and n_2, as given in equation (3.4), where all weights are equal, that is,

$$\alpha_1 = \alpha_2 = 0.5. \tag{4.8}$$

4.2.4 Moment Matrix for Weighted Simplex Centroid Design

The full parameter system, third degree Kronecker model for the two ingredients mixture experiments is given as

$$E(\mathrm{y}) = \theta_{111}t_1t_1t_1 + \theta_{112}t_1t_1t_2 + \theta_{121}t_1t_2t_1 + \theta_{211}t_2t_1t_1 + \theta_{122}t_1t_2t_2 + \theta_{212}t_2t_1t_2 + \theta_{221}t_2t_2t_1 + \theta_{222}t_2t_2t_2 \tag{4.9}$$

The moment matrix $M(\eta) = \sum_{j=1}^{t} w_j f(t_j) f(t_j)^t = \int_\eta f(t) f(t)^t d\eta$ for the third degree Kronecker model has all entries given in (4.2), and reflects the statistical properties of a design η .Hence

$$m(\eta)=\begin{pmatrix} \mu_6 & \mu_{51} & \mu_{51} & \mu_{42} & \mu_{51} & \mu_{42} & \mu_{42} & \mu_{33} \\ \mu_{51} & \mu_{42} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} \\ \mu_{51} & \mu_{42} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} \\ \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{42} & \mu_{51} \\ \mu_{51} & \mu_{42} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} \\ \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{42} & \mu_{51} \\ \mu_{42} & \mu_{33} & \mu_{33} & \mu_{42} & \mu_{33} & \mu_{42} & \mu_{42} & \mu_{51} \\ \mu_{33} & \mu_{42} & \mu_{42} & \mu_{51} & \mu_{42} & \mu_{51} & \mu_{51} & \mu_6 \end{pmatrix}. \tag{4.10}$$

The moment matrix is given by equation (3.3) where weights α_1 and α_2 were given in (4.7) and (4.6) respectively. Hence,

$$M(\eta)=\tfrac{2}{3}M(\eta_1)+\tfrac{1}{3}M(\eta_2). \tag{4.11}$$

where

$$M(\eta_1)=0.5(e_8e_8^{'}+e_1e_1^{'}). \tag{4.12}$$

$$M(\eta_2)=0.015625(J_8). \tag{4.13}$$

Therefore equation (4.11) becomes,

$$M(\eta)=\tfrac{1}{192}J_8+\tfrac{1}{3}(e_8e_8{}'+e_1e_1{}')$$

(4.14)

where, J_8 is a eight by eight matrix of ones and, e_1 and e_8 are unit vectors of size eight.

An experimenter may find it expensive, cumbersome and unnecessary to work with the full parameter system θ, and therefore may wish to study s out of the k , $s \leq k$ components. This is achieved by studying the linear parameter subsystem of interest $K'\theta$ for some $k \times s$ matrix K. K is referred to as the coefficient matrix of the parameter subsystem $K'\theta$. Let the choice of the model be given in equation (3.7) as

$$E(\mathrm{y}) = \theta_{111}t_1t_1t_1 + \theta_{222}t_2t_2t_2 + \frac{\theta_{112}t_1t_1t_2 + \theta_{121}t_1t_2t_1 + \theta_{211}t_2t_1t_1}{3} + \frac{\theta_{122}t_1t_2t_2 + +\theta_{212}t_2t_1t_2 + \theta_{221}t_2t_2t_1}{3} \quad (4.15)$$

so that the parameter of interest $K'\theta$ satisfy equation (3.7) given by

$$K'\theta = \begin{pmatrix} \theta_{111} \\ \theta_{222} \\ \dfrac{\theta_{112} + \theta_{121} + \theta_{211}}{3} \\ \dfrac{\theta_{122} + \theta_{212} + \theta_{221}}{3} \end{pmatrix} \quad (4.16)$$

with the coefficient matrix K. From equation (3.6), K is given as

$$K = (\mathrm{K}_1, K_2) \quad (4.17)$$

where

$$K_1 = \sum_{i=1}^{2} e_{iii}e_i' = e_{111}e_1' + e_{222}e_2' \quad ,$$

$$K_2 = \tfrac{1}{3}\left\{\sum_{ij=1}^{2}(e_{iij} + e_{iji} + e_{jii})e_i\,'\right\}$$
$$= \tfrac{1}{3}\left\{ (e_{112} + e_{121} + e_{211})e_1\,' + (e_{122} + e_{212} + e_{221})e_2\,'\right\}$$

and $e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

4.2.5 Slopes for Two Ingredients Mixture Experiments

In mixture experimental designs, the slope or the gradient of mixture ingredients is calculated through differentiation of the parameter subsystem with respect to every parameter; the slope information matrix was first obtained by utilizing equation (3.11). The derivative matrix H was obtained by differentiating the parameter subsystem of interest model with respect to t_1 and t_2 given as

$$H = \frac{\partial y_i}{\partial t_i}\{t_1t_1t_1 + t_2t_2t_2 + \frac{t_1t_1t_2 + t_1t_2t_1 + t_2t_1t_1}{3} + \frac{t_1t_2t_2 + t_2t_1t_2 + t_2t_2t_1}{3}\},\ \ \text{i=1,2} \tag{4.18}$$

leading to the derivative matrix H given as

$$H = \begin{pmatrix} 3t_1^2 & 0 & 2t_1t_2 & t_2^2 \\ 0 & 3t_2^2 & t_1^2 & 2t_1t_2 \end{pmatrix}. \tag{4.19}$$

The Information matrix C given in (3.8) was obtained, where L is expressed in unit vectors defined in (3.9) as,

$$L' = (\mathrm{K}_1, 3K_2\ ). \tag{4.20}$$

The information matrix becomes

$$C_k(M_1) = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} \qquad (4.21)$$

where,

$$c_{11} = x_{11} I_2 + y_{11} J_2 \ ; \ \ x_{11} = 3333.33 \times 10^{-4}, \ \ y_{11} = 156.25 \times 10^{-4}$$
$$c_{12} = c_{21} = x_{12} J_2 \ ; \ \ x_{12} = 156.25 \times 10^{-4}$$
$$c_{22} = x_{22} J_2 \ ; \ \ x_{22} = 468.75 \times 10^{-4}$$

From (4.21) and (4.19), the slope information information matrix D_c , was obtained as,

$$D_c = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad (4.22)$$

$$a = \frac{15625023t_2^4 + 62500092t_1t_2^3 + 93750138t_1^2t_2^2 + 62500092t_1^3t_2 + 1015626496t_1^4}{333333824}$$

$$b = \frac{421875003t_2^4 + 1687500012t_1t_2^3 + 2531249991t_1^2t_2^2 + 1687500012t_1^3t_2 + 421875003t_1^4}{9000000064}$$

$$c = \frac{421875003t_2^4 + 1687500012t_1t_2^3 + 2531249991t_1^2t_2^2 + 1687500012t_1^3t_2 + 421875003t_1^4}{9000000064}$$

$$d = \frac{1015626496t_2^4 + 62500092t_1t_2^3 + 93750138t_1^2t_2^2 + 62500092t_1^3t_2 + 15625023t_1^4}{333333824}$$

4.2.6 The Slope Information Matrices (SIM)

The slope information matrices were obtained from equation (4.22) for pure and binary blends mixture experiments. We substitute the values of t_i in matrix D_c at different points of the simplex centroid.

For pure blends at a point (1, 0), we have Slope Information Matrix (SIM) as,

$$SIM_1 = \tfrac{3}{64}\left(J_2 + 64 e_1 e_1 '\right). \tag{4.23}$$

For the binary mixtures at the center point (½, ½), we have the slope information matrix as

$$SIM_2 = \tfrac{3}{65}(J_2 + 4I_2) \tag{4.24}$$

where, J_2 is a two by two matrix of ones.

4.2.7 Moment Matrices for Uniform Weighted Simplex Centroids Designs (UWSCD)

The moment matrix for uniformly weighted simplex centriod designs for two ingredients is given by $M(\eta) = \alpha_1 M(\eta_1) + \alpha_2 M(\eta_2)$, where weights are all equal, that is $\alpha_1 = \alpha_2 = 1/2$ as given in equation (3.4). Hence,

$$M(\eta) = \tfrac{1}{2} M(\eta_1) + \tfrac{1}{2} M(\eta_2) \tag{4.25}$$

where $M(\eta_1)$ and $M(\eta_2)$ are given in equations (4.12) and (4.13) respectively. Thus, the moment matrix $M(\eta)$ becomes,

$$M(\eta) = a_1 J_8 + a_2 (e_8 e_8' + e_1 e_1')$$

(4.26)

where, J_8 is a eight by eight matrix of ones, e_1 and e_8 are unit vectors each of size eight, $a_1 = 0.0078125$ and $a_2 = 0.25$.

Using equations (4.20) and (4.26), we obtained the information matrix for uniform weighted simplex centroid designs as

$$C_u(M_u) = \begin{pmatrix} x_{11} I_2 + y_{11} J_2 & x_{12} J_2 \\ x_{12} J_2 & x_{22} J_2 \end{pmatrix} \quad (4.27)$$

where

$x_{11} = 2500 \times 10^{-4}$, $y_{11} = 78.125 \times 10^{-4}$, $x_{12} = 234.375 \times 10^{-4}$, $x_{22} = 703.125 \times 10^{-4}$,
J_2 is a two by two matrix of ones.

The information matrix (4.27) together with (4.19) were used to obtain slope information matrix D_c as,

$$D_c = \begin{bmatrix} \frac{9t_2^4 + 36t_1t_2^3 + 54t_1^2t_2^2 + 36t_1^3t_2 + 297t_1^4}{128} & \frac{9t_2^4 + 36t_1t_2^3 + 54t_1^2t_2^2 + 36t_1^3t_2 + 9t_1^4}{128} \\ \frac{9t_2^4 + 36t_1t_2^3 + 54t_1^2t_2^2 + 36t_1^3t_2 + 9t_1^4}{128} & \frac{297t_2^4 + 36t_1t_2^3 + 54t_1^2t_2^2 + 36t_1^3t_2 + 9t_1^4}{128} \end{bmatrix} \quad (4.28)$$

4.2.8 Slope Information Matrices (SIM) for Uniform Weighted Centroid Designs

The slope information matrices at different points of the simplex centroid were obtained from equation (4.28) for mixture experiments.

Slope information matrix for pure blends at a point (1, 0) is given as

$$SIM_{1u} = 0.0703125(J_2) + 2.25(e_1 e_1'). \qquad (4.29)$$

Slope information matrix for binary blends at a central point (1/2, 1/2) is given by

$$SIM_{2u} = 0.140625(I_2) + 0.0703125(J_2). \qquad (4.30)$$

The slope information matrices (4.29) and (4.30) were compared through D-, E-, A- and T-optimal criteria so as to determine the optimal design.

4.2.9 Optimal Values for Slope Designs

We obtained the optimal values for both Weighted Simplx Centroid (WSC) designs and Uniform Weighted Simplex Centroid (UWSC) designs for two ingredients mixture experiments. In this case, we consider the D-, E-, A- and T-optimal criteria based on the equations (3.13), (3.16), (3.18) and (3.20) respectively. The optimal values for pure and binary blends in Weighted Simplex Centroid (WSC) designs and Uniformly Weighted Simplex Centroid (UWSC) designs were calculated based on their slope information matrices (4.23), (4.24), (4.29) and (4.30) respectively. The optimal values are summarized in Table 4.1.

Table 4. 1: Optimal Values for Two Ingredients

	WEIGHTED SIMPLEX CENTROID (WSC)				**UNIFORM WEIGHTED SIMPLEX CENTROID (UWSC)**			
BLENDS	**D-**	**E-**	**A-**	**T-**	**D-**	**E-**	**A-**	**T-**
1, 0	0.3750	0.0461	0.0909	1.5469	0.3977	0.06812	0.1325	1.1953
½, ½	0.2290	0.1875	0.2250	0.2344	0.1989	0.1406	0.1875	0.2109

From Table 4.1, comparing each blend of the simplex centroid for the two designs, binary blend (½, ½) was found to be more D- and T-optimal than pure blends. Pure blends (1, 0), Weighted Simplex Centroid (WSC) designs were observed to yield better results than Uniform Weighted Simplex Centroid (UWSC) counter parts except T-criterion. In binary (½, ½) blend mixtures, Uniform Weighted Simplex Centroid performed better than Weighted Simplex Centroids due its smaller optimal values.

4.2.10 Efficiencies for Two Ingredients

The performance of the WSCD in comparison to the UWSCD was measured by the D-, E-, A- and T-efficiencies defined in (3.14), (3.17), (3.19) and (3.21) respectively. Using the optimal values in Table 4.1, their efficiencies at different point of the simplex centroid designs were obtained as given in Table 4.2.

Table 4. 2: Efficiency for Two Ingredients

	Efficiencies (%)			
BLENDS	**D-**	**E-**	**A-**	**T-**
1, 0	94.2	67.67	68.6	129.41
½, ½	115.13	133.35	120	111.14

It is noted from Table 4.2 that is, at (1, 0), WSCD was more efficient than UWSCD for all optimal criteria except T-criterion. It was also found that, in binary blends (½, ½) mixtures, UWSCD was more efficient than WSCD for all the optimal criteria.

4.2.11 I-Optimality for Weighted Simplex Centroid Designs

In third degree Kronecker model for two ingredients mixture designs, let the parameter sub-system of interest be given in equation (4.8), using information matrix (3.29), the generalized inverse was given as,

$$C^{-1} = \begin{pmatrix} 3\mathrm{I}_2 & -0.5\mathrm{J}_2 \\ -0.5\mathrm{J}_2 & 5.5\mathrm{J}_2 \end{pmatrix}. \tag{4.31}$$

The moment matrix L from the parameter subsystem of interest obtained as

$$L = k\int f(t)f(t)'dt = k\int \begin{pmatrix} t_1^6 & t_1^3t_2^3 & t_1^5t_2 & t_1^4t_1^2 \\ t_2^3t_1^3 & t_2^6 & t_1^2t_2^4 & t_1t_2^5 \\ t_1^5t_2 & t_1^2t_2^4 & t_1^4t_2^2 & t_1^3t_2^3 \\ t_1^4t_2^2 & t_1t_2^5 & t_1^3t_2^3 & t_1^2t_2^4 \end{pmatrix} dt \tag{4.32}$$

where $k = (q-1)! = (2-1)! = 1.$

The values of each of the integrals of t_i in (4.32) were calculated using equation (3.30). Therefore,

$$\int_\tau t_1^6 dt_1 = \int_\tau t_2^6 dt_2 = \frac{\prod_{i=1}^{2}(p_i!)}{(q+\sum_1^2 p_i - 1)!} = \frac{6!}{7!} = \frac{1}{7}$$

$$\int_\tau t_1^5 t_2 dt_1 dt_2 = \int_\tau t_1 t_2^5 dt_1 dt_2 = \frac{\prod_{i=1}^{2}(p_i!)}{(q+\sum_{i=1}^2 p_i - 1)!} = \frac{1}{42}$$

$$\int_\tau t_1^3 t_2^3 dt_1 dt_2 = \frac{\prod_{i=1}^{2}(p_i!)}{(q+\sum_1^2 p_i - 1)!} = \frac{1}{140}$$

$$\int_\tau t_1^4 t_2^2 dt_1 dt_2 = \int_\tau t_1^2 t_2^4 dt_1 dt_2 = \frac{\prod_{i=1}^{2}(p_i!)}{(q+\sum_{i=1}^2 p_i - 1)!} = \frac{1}{105} \tag{4.33}$$

Hence, the moment matrix L in (4.32) becomes

$$L = \begin{pmatrix} x_{11}I_2 + y_{11}J_2 & x_{12}I_2 + y_{12}J_2 \\ x_{12}I_2 + y_{12}J_2 & x_{22}I_2 + y_{22}J_2 \end{pmatrix} \tag{4.34}$$

where

$x_{11} = 1357.14286 \times 10^{-4}$, $y_{11} = 71.42857 \times 10^{-4}$, $x_{12} = 142.8571 \times 10^{-4}$, $y_{12} = 95.2381 \times 10^{-4}$, $x_{22} = 23.8095 \times 10^{-4}$, $y_{22} = 71.42857 \times 10^{-4}$.

Now using matrices (4.31) and (4.34), $C^{-1}L$ becomes,

$$C^{-1}L = \begin{pmatrix} v_1 & v_2 \\ v_3 & v_4 \end{pmatrix} \tag{4.35}$$

where

$$\begin{aligned} v_1 &= x_{11}I_2 + y_{11}J_2; \;\; x_{11} = 4071.4285 \times 10^{-4}, \;\; y_{11} = 47.61905 \times 10^{-4} \\ v_2 &= x_{12}I_2 + y_{11}J_2 \; ; \; x_{12} = 428.5714 \times 10^{-4}, \; y_{12} = 202.381 \times 10^{-4} \\ v_3 &= x_{21}J_2 \; ; x_{21} = 1083.33 \times 10^{-4} \\ v_4 &= x_{22}J_2 \; ; x_{22} = 750 \times 10^{-4}. \end{aligned}$$

By taking the trace of matrix (4.35), we obtained the Average Prediction Variance (APV) as

$$APV = tr[C^{-1}L] = 0.9738095. \tag{4.36}$$

4.2.12 I-Optimality for Uniform Weight Simplex Centroid Designs

Information matrix (4.27) had no direct inverse; we therefore use generalized inverse given as,

$$C_u^{-1} = \begin{pmatrix} 4I_2 & -0.6666667J_2 \\ -0.6666667J_2 & 3.7777778J_2 \end{pmatrix}. \tag{4.37}$$

Now using matrices (4.34) and (4.37), we obtained $C_u^{-1}L$ as

$$C_u^{-1}L = \begin{pmatrix} x_{11}I_2 + y_{11}J_2 & x_{12}I_2 + y_{12}J_2 \\ x_{21}J_2 & x_{22}J_2 \end{pmatrix} \tag{4.38}$$

where

$x_{11} = 5428.57143 \times 10^{-4}$, $y_{11} = 63.49206 \times 10^{-4}$, $x_{12} = 571.4285 \times 10^{-4}$,
$y_{12} = 269.8413 \times 10^{-4}$, $x_{21} = 259.25926 \times 10^{-4}$, $x_{22} = 407.4074 \times 10^{-4}$.

The average prediction variance was obtained from the trace of $C_u^{-1}L$ in (4.38) as

$$APV = tr[C_u^{-1}L] = 1.179894. \tag{4.39}$$

Comparing APV's in (4.36) and (4.39), we conclude that, the WSCD performed better than UWSCD since it had smaller average prediction variance.

4.2.13 Equivalence Theorem for Weighted Simplex Centroid

Using the equivalence theorem given in equation (3.34), the design is I-optimal if and only if

$$f^{'}(t)C^{-1}LC^{-1}f(t) \leq 0.9738095 \tag{4.40}$$

at a given design point of the simplex centroid designs. The equivalence theorem for WSCD was summarized in Table 4.3.

Table 4. 3: Equivalence Theorem for Two Ingredients (WSCD)

Average Prediction Variances				
BLENDS	$f^{'}(t)C^{-1}LC^{-1}f(t)$		$tr[C^{-1}L]$	**Optimality**
1, 0	1.194048	>	0.9738095	Not I Optimal
½, ½	0.1125	<	0.9738095	I-Optimal

It was observed that the pure blend did not satisfy the general equivalence theorem for I-optimality whereas the binary blends satisfied the general equivalence theorem, therefore, I-optimal.

4.2.14 Equivalence Theorem for Uniform Weighted Simplex Centroid

Similarly as above, the design is I-optimal if and only if

$$f^{'}(t)C_u^{-1}LC_u^{-1}f(t) \leq 1.179894 \tag{4.41}$$

at a given design point. These were summarized in Table 4.4.

Table 4. 4: Equivalence Theorem for Two Ingredients (UWSCD)

Average Prediction Variances				
BLENDS	$f^{'}(t)C_u^{-1}LC_u^{-1}f(t)$		$tr[C_u^{-1}L]$	**Optimality**
1, 0	2.12275	>	1.179894	Not I Optimal
½, ½	0.08806584	<	1.179894	I-Optimal

It was observed that the pure blends did not satisfy the general equivalence theorem for I-optimality but the binary blends were found to satisfy the general equivalence theorem, therefore, I-optimal.

4.3 DESIGNS FOR THREE FACTORS MIXTURE EXPERIMENTS

4.3.1 Simplex Centroid Designs

In the three ingredients mixture experiments, there are three elementary centroid designs: n_1 is supported on the vertices, n_2 is supported on the edge midpoints, and n_3 on the overall centroid point, placing equal weights α_1, α_2 and α_3 on the points respectively. The optimal weights α_1, α_2 and α_3 were obtained using simplex restrictions for $j = 1, 2, 3$. The simplex centroid design for three ingredients is given as

$$\left.\begin{Bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Bmatrix}\right\} \eta_1$$
$$\left.\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{Bmatrix}\right\} \eta_2$$
$$\left.\begin{Bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{Bmatrix}\right\} \eta_3 \qquad (4.42)$$

4.3.2 Weighted Simplex Centroid Designs (WSCD)

The weights for simplex centroid designs for three ingredients were obtained through lower order moments of the simplex centroids Kronecker designs. Let η be an arbitrary exchangeable design, then its sixth order moments were obtained from (4.42) as

$$(i)\ \ \mu_6 = \int t_1^6 d\tau = \int t_2^6 d\tau = \int t_3^6 d\tau = \tfrac{1}{7}[(1)^6 + (\tfrac{1}{2})^6 + (\tfrac{1}{2})^6 + (\tfrac{1}{3})^6] = 0.1475$$

$$(ii)\ \ \mu_{51} = \int t_1^5 t_2^1 d\tau = \int t_1^5 t_3^1 d\tau = \int t_2^5 t_3^1 d\tau = \tfrac{1}{7}[(\tfrac{1}{2})^5(\tfrac{1}{2}) + (\tfrac{1}{3})^5(\tfrac{1}{3})] = 0.002428$$

$$(iii)\ \ \mu_{42} = \int t_1^4 t_2^2 d\tau = \int t_1^4 t_3^2 d\tau = \int t_2^4 t_3^2 d\tau = \tfrac{1}{7}[(\tfrac{1}{2})^4(\tfrac{1}{2})^2 + (\tfrac{1}{3})^4(\tfrac{1}{3})^2] = 0.002428$$

$$(iv)\ \ \mu_{33} = \int t_1^3 t_2^3 d\tau = \int t_1^3 t_3^3 d\tau = \int t_2^3 t_3^3 d\tau = \tfrac{1}{7}[(\tfrac{1}{2})^3(\tfrac{1}{2})^3 + (\tfrac{1}{3})^3(\tfrac{1}{3})^3] = 0.002428 \qquad (4.43)$$

$$(v)\ \ \mu_{411} = \int t_1^4 t_2^1 t_3^1 d\tau = \int t_1^1 t_2^4 t_3^1 d\tau = \int t_1^1 t_2^1 t_3^4 d\tau = \tfrac{1}{7}[(\tfrac{1}{3})^4(\tfrac{1}{3})(\tfrac{1}{3})] = 0.0001959$$

$$(vi)\ \ \mu_{321} = \int t_1^3 t_2^2 t_3^1 d\tau = \int t_1^2 t_2^3 t_3^1 d\tau = \int t_1^1 t_2^2 t_3^3 d\tau = \tfrac{1}{7}[(\tfrac{1}{3})^3(\tfrac{1}{3})^2(\tfrac{1}{3})] = 0.0001959$$

$$(vii)\ \ \mu_{222} = \int t_1^2 t_2^2 t_3^2 d\tau = \tfrac{1}{7}[(\tfrac{1}{3})^2(\tfrac{1}{3})^2(\tfrac{1}{3})^2] = 0.0001959$$

The lower order moments for three ingredients were expressed in form of sixth order moments given as

$$(i)\quad \mu_5 = \int_t t_1^5(t_1+t_2+t_3)dt = \int(t_1^6+t_1^5t_2+t_1^5t_3)dt = \mu_6 + 2\mu_{51}$$

$$(ii)\quad \mu_{41} = \int_t t_1^4t_2(t_1+t_2+t_3)dt = \int(t_1^5t_2+t_1^4t_2^2+t_1^4t_2t_3)dt = \mu_{51}+\mu_{42}+\mu_{411}$$

$$(iii)\quad \mu_{32} = \int_t t_1^3t_2^2(t_1+t_2+t_3)dt = \mu_{42}+\mu_{33}+\mu_{321}$$

$$(iv)\quad \mu_{221} = \int_t t_1^3t_2^2t_3(t_1+t_2+t_3)dt = 2\mu_{321}+\mu_{222}$$

$$(v)\quad \mu_4 = \int_t t_1^5(t_1+t_2+t_3)dt = \mu_6+4\mu_{51}+2\mu_{42}+2\mu_{411}$$

$$(vi)\quad \mu_{311} = \int_t t_1^3t_2t_3(t_1+t_2+t_3)dt = \mu_{411}+2\mu_{321}$$

$$(vii)\quad \mu_{211} = \int_t t_1^2t_2t_3(t_1+t_2+t_3)dt = \mu_{411}+6\mu_{321}+2\mu_{222}$$

$$(viii)\quad \mu_{41} = \int_t t_1^4t_2(t_1+t_2+t_3)dt = \int(t_1^5t_2+t_1^4t_2^2+t_1^4t_2t_3)dt = \mu_{51}+2\mu_{42}+2\mu_{411}+3\mu_{321}+\mu_{33}$$

$$(ix)\quad \mu_3 = \int_t t_1^3(t_1+t_2+t_3)dt = \mu_6+6(\mu_{51}+\mu_{42}+\mu_{411}+\mu_{321})+2\mu_{33}$$

$$(x)\quad \mu_{21} = \int_t t_1^2t_2(t_1+t_2+t_3)dt = \mu_{51}+4\mu_{42}+3\mu_{411}+12\mu_{321}+3\mu_{33}+3\mu_{222}$$

$$(xi)\quad \mu_{22} = \int_t t_1^2t_2^2(t_1+t_2+t_3)dt = 2\mu_{42}+4\mu_{321}+2\mu_{33}+\mu_{222}$$

$$(xii)\quad \mu_2 = \int_t t_1^2(t_1+t_2+t_3)dt = \mu_6+8\mu_{51}+14\mu_{42}+12\mu_{411}+30\mu_{321}+8\mu_{33}+6\mu_{222} \tag{4.44}$$

$$(xiii)\quad \mu_1 = \int_t t_1(t_1+t_2+t_3)dt = \mu_6+8\mu_{51}+22\mu_{42}+21\mu_{411}+72\mu_{321}+14\mu_{33}+18\mu_{222}$$

$$(xiv)\quad \mu_{111} = \int_t t_1t_2t_3(t_1+t_2+t_3)dt = 3\mu_{411}+18\mu_{321}+6\mu_{222}$$

$$(xv)\quad \mu_{11} = \int_t t_1t_2(t_1+t_2+t_3)dt = 2\mu_{51}+8\mu_{42}+9\mu_{411}+44\mu_{321}+6\mu_{33}+12\mu_{222}$$

Using the lower order moments, we obtained the optimal weights for Weighted Simplex Centroid Designs (WSCD) from (4.42) as

$$\mu_{111} = \tfrac{1}{27}\alpha_3, \quad (4.45)$$

$$\alpha_3 = 27\mu_{111}. \quad (4.46)$$

From equation (xiv), (4.44), μ_{111} is given as

$$\alpha_3 = 81[\mu_{411} + 6\mu_{321} + 2\mu_{222}]. \quad (4.47)$$

Also from moment equations (4.43), μ_{411}, μ_{321} and μ_{222} are given as

$$\mu_{411} = \mu_{321} = \mu_{222} = \tfrac{1}{5103}. \quad (4.48)$$

Substituting (4.48) in (4.47), we have

$$\alpha_3 = \tfrac{1}{7}. \quad (4.49)$$

Next, we obtained α_2 using μ_{11} from (4.42) given as

$$\mu_{11}(\eta) = \alpha_1(0) + \tfrac{1}{3}\alpha_2(\tfrac{1}{4}) + \tfrac{1}{9}\alpha_3 = \mu_{11} = \tfrac{1}{12}\alpha_2 + \tfrac{1}{9}\alpha_3. \quad (4.50)$$

Since $\alpha_3 = \tfrac{1}{7}$, we substitute it in (4.50) to obtain α_2 as

$$\alpha_2 = 12(\mu_{11} - \tfrac{1}{63}). \quad (4.51)$$

From equation (xv),(4.44), we substitute μ_{11} in (4.51) so that,

$$\alpha_2 = 12(2\mu_{51} + 8\mu_{42} + 9\mu_{411} + 44\mu_{321} + 6\mu_{33} + 12\mu_{222} - \tfrac{1}{63}). \qquad (4.52)$$

But from (4.43), we have

$$\mu_{51} = \mu_{42} = \mu_{33} = 0.002428 \qquad (4.53)$$

and

$$\mu_{411} = \mu_{321} = \mu_{222} = 0.0001959. \qquad (4.54)$$

Using (4.53) and (4.54) in (4.52), we obtained the value of α_2 as

$$\alpha_2 = \tfrac{3}{7}. \qquad (4.55)$$

From equation (3.12), we use (4.49) and (4.55) to obtained the value of α_1 as

$$\alpha_1 = 1 - \alpha_2 - \alpha_3 = \tfrac{3}{7}. \qquad (4.56)$$

Hence the optimal weights α_1, α_2 and α_3 were obtained as 3/7, 3/7 and 1/7 respectively.

4.3.3 Uniformly Weighted Simplex Centroid Designs (UWSCD)

The Uniformly Weighted Simplex Centriod Designs (UWSCD) for three ingredients assigns uniform weights to the three elementary centroid designs, n_1, n_2 and n_3, as given in equation (3.4), where weights are all equal, that is,

$$\alpha_1 = \alpha_2 = \alpha_3 = 1/3. \qquad (4.57)$$

4.3.4 Moment Matrix for Weighted Simplex Centroid Designs (WSCD)

The full parameter system, third degree Kronecker model for the three ingredients mixture experiments is given as;

$$\begin{aligned}E(\mathrm{y}) =&\theta_{111}t_1t_1t_1+\theta_{112}t_1t_1t_2+\theta_{113}t_1t_1t_3+\theta_{121}t_1t_2t_1+\theta_{122}t_1t_2t_2+\theta_{123}t_1t_2t_3+\theta_{131}t_1t_3t_1+\theta_{132}t_1t_3t_2\\&+\theta_{133}t_1t_3t_3+\theta_{211}t_2t_1t_1+\theta_{212}t_2t_1t_2+\theta_{213}t_2t_1t_3+\theta_{221}t_2t_2t_1+\theta_{222}t_2t_2t_2+\theta_{223}t_2t_2t_3+\theta_{231}t_2t_3t_1\\&+\theta_{232}t_2t_3t_2+\theta_{233}t_2t_3t_3+\theta_{311}t_3t_1t_1+\theta_{312}t_3t_1t_2+\theta_{313}t_3t_1t_3+\theta_{321}t_3t_2t_1+\theta_{322}t_3t_2t_2+\theta_{323}t_3t_2t_3\\&+\theta_{331}t_3t_3t_1+\theta_{332}t_3t_3t_2+\theta_{333}t_3t_3t_3.\end{aligned} \quad (4.58)$$

The moment matrix for the third degree Kronecker model has all entries given in (4.43), and reflects the statistical properties of a design η. Therefore, the moment matrix as given in equation (3.3), where weights α_1, α_2 and α_3 were given in (4.56), (4.55) and (4.49) respectively, yields

$$M(\eta)=\tfrac{3}{7}M(\eta_1)+\tfrac{3}{7}M(\eta_2)+\tfrac{1}{7}M(\eta_3) \quad (4.59)$$

where

$$M(\eta_1)=\tfrac{1}{3}[e_{111}(e_{111})'+e_{222}(e_{222})'+e_{333}(e_{333})'] \quad (4.60)$$

$$\begin{aligned}M(\eta_2)=\tfrac{1}{192}[&(c_1\otimes c_1\otimes c_1)(c_1\otimes c_1\otimes c_1)'+(c_2\otimes c_2\otimes c_2)(c_2\otimes c_2\otimes c_2)'\\&+(c_3\otimes c_3\otimes c_3)(c_3\otimes c_3\otimes c_3)']\end{aligned}$$

(4.61)

$$M(\eta_3)=0.001371742112J_{27} \quad (4.62)$$

also, $c_1=(1_3-e_3),\ \ c_2=(1_3-e_2),\ \ c_3=(1_3-e_1)$ and

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } \quad e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Let the choice of the Kronecker model as given in equation (3.7) be represented as

$$\begin{aligned} E(\mathrm{y}) &= \theta_{111}t_1t_1t_1 + \theta_{222}t_2t_2t_2 + \theta_{333}t_3t_3t_3 \\ &+ \frac{\theta_{112}t_1t_1t_2 + \theta_{121}t_1t_2t_1 + \theta_{211}t_2t_1t_1 + \theta_{113}t_1t_1t_3 + \theta_{131}t_1t_3t_1 + \theta_{311}t_3t_1t_1}{6} + \\ &\frac{\theta_{122}t_1t_2t_2 + \theta_{212}t_2t_1t_2 + \theta_{221}t_2t_2t_1 + \theta_{223}t_2t_2t_3 + \theta_{232}t_2t_3t_2 + \theta_{322}t_3t_2t_2}{6} + \\ &\frac{\theta_{233}t_2t_3t_3 + \theta_{323}t_3t_2t_3 + \theta_{332}t_3t_3t_2 + \theta_{133}t_1t_3t_3 + \theta_{313}t_3t_1t_3 + \theta_{331}t_3t_3t_1}{6} + \\ &\frac{\theta_{123}t_1t_2t_3 + \theta_{132}t_1t_3t_2 + \theta_{213}t_2t_1t_3 + \theta_{231}t_2t_3t_1 + \theta_{312}t_3t_1t_2 + \theta_{321}t_3t_2t_1}{6} \end{aligned}$$

(4.63)

such that the coefficient matrix K for the three ingredients parameters of interest as given in (3.7) was obtained as,

$$K'\theta = \begin{pmatrix} \theta_{111} \\ \theta_{222} \\ \theta_{333} \\ \dfrac{\theta_{112} + \theta_{121} + \theta_{211} + \theta_{113} + \theta_{131} + \theta_{311}}{6} \\ \dfrac{\theta_{122} + \theta_{212} + \theta_{221} + \theta_{223} + \theta_{232} + \theta_{322}}{6} \\ \dfrac{\theta_{233} + \theta_{323} + \theta_{332} + \theta_{133} + \theta_{313} + \theta_{331}}{6} \\ \dfrac{\theta_{123} + \theta_{132} + \theta_{213} + \theta_{231} + \theta_{312} + \theta_{321}}{6} \end{pmatrix}.$$

(4.64)

Therefore, K is given as

$$K = (K_1, K_2, K_3) \tag{4.65}$$

where

$$K_1 = \sum_{i=1}^{3} e_{iii} e_i' = e_{111} e_1' + e_{222} e_2' + e_{333} e_3'$$

$$K_2 = \tfrac{1}{6}\left\{ \sum_{\substack{ij=1 \\ i \neq j}}^{3} (e_{iij} + e_{iji} + e_{jii}) e_i' \right\}$$

$$= \tfrac{1}{6}\left\{ (e_{112} + e_{121} + e_{211}) e_1' + (e_{122} + e_{212} + e_{221}) e_2' + (e_{133} + e_{313} + e_{331}) e_3' \right\}$$

and

$$K_3 = \tfrac{1}{6}\left\{ \sum_{\substack{ijk=1 \\ i \neq j \neq k}}^{3} e_{ijk} \right\} = \tfrac{1}{6}\left\{ e_{123} + e_{132} + e_{231} + e_{213} + e_{312} + e_{321} \right\}.$$

The left inverse L in equation (3.9) for three ingredients is given as,

$$L' = (K_1, 6K_2, 6K_3). \tag{4.66}$$

4.3.5 Slope information Matrix

The H_1 matrix is obtained by differentiating the parameter sub-system of interest model in (4.63) with respect to t_1, t_2 and t_3 as given in (3.10). Hence,

$$H_1 = \frac{\partial y_i}{\partial t_i}\left\{\begin{array}{l} t_1t_1t_1 + t_2t_2t_2 + t_3t_3t_3 + \\ \frac{t_1t_1t_2 + t_1t_2t_1 + t_2t_1t_1 + t_1t_1t_3 + t_1t_3t_1 + t_3t_1t_1}{6} + \\ \frac{t_1t_2t_2 + t_2t_1t_2 + t_2t_2t_1 + t_2t_2t_3 + t_2t_3t_2 + t_3t_2t_2}{6} + \\ \frac{t_2t_3t_3 + t_3t_2t_3 + t_3t_3t_2 + t_1t_3t_3 + t_3t_1t_3 + t_3t_3t_1}{6} + \\ \frac{t_1t_2t_3 + t_1t_3t_2 + t_2t_1t_3 + t_2t_3t_1 + t_3t_1t_2 + t_3t_2t_1}{6} \end{array}\right\}, \text{ i=1,2,3} \quad (4.67)$$

which led to the following derivative matrix in form of parameters t_1, t_2 and t_3

$$H_1 = \begin{pmatrix} 3t_1^2 & 0 & 0 & (t_1t_2 + t_1t_3) & \frac{1}{2}t_2^2 & \frac{1}{2}t_3^2 & t_2t_3 \\ 0 & 3t_2^2 & 0 & \frac{1}{2}t_1^2 & (t_1t_2 + t_2t_3) & \frac{1}{2}t_3^2 & t_1t_3 \\ 0 & 0 & 3t_3^2 & \frac{1}{2}t_1^2 & \frac{1}{2}t_2^2 & (t_2t_3 + t_1t_3) & t_1t_2 \end{pmatrix}$$

(4.68)

Using (4.59) and (4.66), we obtained the information matrix for weighted simplex centroid designs as

$$C_1 = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{12} & c_{22} & c_{23} \\ c'_{13} & c'_{23} & c_{33} \end{pmatrix} \quad (4.69)$$

where

$$c_{11} = x_{11}I_3 + y_{11}J_3 \; ; \quad x_{11} = 1450.89286\times10^{-4} \; , \quad y_{11} = 24.28106\times10^{-4}$$
$$c_{12} = x_{12}I_3 + y_{11}J_3 \; ; \; x_{12} = 66.96429\times10^{-4}, \quad y_{12} = 145.68636\times10^{-4}$$
$$c_{22} = x_{22}I_3 + y_{22}J_3 \; ; \; x_{22} = 200.89287\times10^{-4}, \quad y_{22} = 271.43955\times10^{-4}$$

$$c_{13} = x_{13} 1_3 \; ; \; x_{13} = 11.75778 \times 10^{-4}$$
$$c_{23} = x_{23} 1_3 \; ; \; x_{23} = 70.54668 \times 10^{-4}$$
$$c_{33} = 70.54668 \times 10^{-4}.$$

The information matrix (4.69) together with (4.68) were used to obtain slope information matrix D_{cc}, as

$$D_{cc} = \begin{pmatrix} A & B & C \\ B' & E & G \\ C' & G' & I \end{pmatrix} \tag{4.70}$$

where,

$$\begin{aligned} A = {} & 0.5t_3^2(0.023616621t_3^2 + 0.027143955(t_1t_3 + t_1t_2) + 0.007054668t_2t_3 \\ & + 0.0135719775t_2^2 + 0.023616621t_1^2) + (t_1t_3 + t_1t_2)(0.0135719775t_3^2 \\ & + 0.047233242(t_1t_3 + t_1t_2) + 0.007054668t_2t_3 + 0.0135719775t_2^2 \\ & + 0.043705908t_1^2) + 0.5t_2^2(0.0135719575t_1^2 + 0.023616621t_1^2) \\ & + 3t_1^2(0.0039361035t_3^2 + 0.014568636(t_1t_3 + t_1t_2) + 0.001175778t_2t_3 \\ & + 0.0039361035t_2^2 + 0.442552176t_1^2) + t_2t_3(0.003527334t_3^2 \\ & + 0.007054668(t_1t_3 + t_1t_2) + 0.007054668t_2t_3 \\ & + 0.003527334t_2^2 + 0.003527334t_1^2) \end{aligned}$$

$$\begin{aligned} B = {} & 0.5t_3^2(0.023616621t_3^2 + 0.027143955(t_2t_3 + t_1t_2) + 0.007054668t_1t_3 + 0.023616621t_2^2 \\ & + 0.0135719775t_1^2) + 0.5t_2^2(0.0135719775t_3^2 + 0.047233242(t_2t_3 + t_1t_2) + 0.007054668t_1t_3 \\ & + 0.043705908t_2^2 + 0.0135719775t_1^2) + (t_1t_3 + t_1t_2)(0.0135719775t_3^2 \\ & + 0.027143955(t_2t_3 + t_1t_2) + 0.007054668t_1t_3 + 0.023616621t_2^2 + 0.023616621t_1^2) \\ & + 3t_1^2(0.0039361035t_3^2 + 0.007872207(t_2t_3 + t_1t_2) + 0.001175778t_2t_3 + 0.007284318t_2^2 \\ & + 0.007284318t_1^2) + t_2t_3(0.003527334t_3^2 + 0.007054668(t_2t_3 + t_1t_2) \\ & + 0.007054668t_1t_3 + 0.003527334t_2^2 + 0.003527334t_1^2) \end{aligned}$$

$$C = 0.5t_3^2(0.043705908t_3^2 + 0.047233242(t_2t_3 + t_1t_3) + 0.0135719775t_2^2 + 0.007o54668t_1t_2$$
$$+0.0135719775t_1^2) + 0.5t_2^2(0.023616621t_3^2 + 0.027143955(t_2t_3 + t_1t_3) + 0,023616621t_2^2$$
$$+0.007054668t_1t_2 + 0.0135719775t_1^2) + (t_2t_3 + t_1t_3)(0.023616621t_3^2 + 0.027143955(t_2t_3 + t_1t_3)$$
$$+0.0135719775t_2^2 + 0.007054668t_1t_2 + 0.023616621t_1^2) + 3t_1^2(0.007284318t_3^2$$
$$+0.007872207(t_2t_3 + t_1t_3) + 0.0039361035t_2^2 + 0.001175778t_1t_2 + 0.007284318t_1^2)$$
$$+t_2t_3(0.003527334t_3^2 + 0.007054668(t_2t_3 + t_1t_3) + 0.003527334t_2^2 + 0.007054668t_1t_2$$
$$+0.003527334t_1^2)$$

$$E = 0.5t_3^2(0.023616621t_3^2 + 0.027143955(t_2t_3 + t_1t_2) + 0.007054668t_1t_3 + 0.023616621t_2^2$$
$$+0.0135719775t_1^2) + (t_2t_3 + t_1t_2)(0.0135719775t_3^2 + 0.047233242(t_2t_3 + t_1t_2)$$
$$+0.007054668t_1t_3 + 0.043705908t_2^2 + 0.0135719775t_1^2) + 0.5t_1^2(0.0135719775t_3^2$$
$$+0.027143955(t_2t_3 + t_1t_2) + 0.007054668t_1t_3 + 0.023616621t_2^2 + 0.023616621t_1^2)$$
$$+3t_2^2(0.007284318t_3^2 + 0.007872207(t_2t_3 + t_1t_3) + 0.0039361035t_2^2 + 0.001175778t_1t_2$$
$$+0.0039361035t_1^2) + t_1t_3(0.003527334t_3^2 + 0.007054668(t_2t_3 + t_1t_2)$$
$$+0.007054668t_1t_3 + 0.003527334t_2^2 + 0.003527334t_1^2$$

$$G = 0.5t_3^2(0.043705908t_3^2 + 0.047233242(t_2t_3 + t_1t_3) + 0.0135719775t_2^2 + 0.007054668t_1t_2$$
$$+0.0135719775t_1^2) + (t_2t_3 + t_1t_3)(0.023616621t_3^2 + 0.027143955(t_2t_3 + t_1t_3) + 0.023616621t_2^2$$
$$+0.007054668t_1t_2 + 0.0135719775t_1^2) + 0.5t_1^2(0.023616621t_3^2 + 0.027143955(t_2t_3 + t_1t_3)$$
$$+0.0135719775t_2^2 + 0.007054668t_1t_2 + 0.023616621t_1^2) + 3t_2^2(0.007284318t_3^2$$
$$+0.007872207(t_2t_3 + t_1t_3) + 0.007284318t_2^2 + 0.001175778t_1t_2 + 0.0039361035t_1^2)$$
$$+t_1t_3(0.003527334t_3^2 + 0.007054668(t_2t_3 + t_1t_3) + 0.003527334t_2^2$$
$$+0.007054668t_1t_2 + 0.003527334t_1^2)$$

$$I = 3t_3^2(0,442552176t_3^2 + 0.014568636(t_2t_3 + t_1t_3) + 0.0039361035t_2^2 + 0.001175778t_1t_2$$
$$+0.0039361035t_1^2) + (t_2t_3 + t_1t_3)(0.043705908t_3^2 + 0.047233242(t_2t_3 + t_1t_3)$$
$$+0.0135719775t_2^2 + 0.007054668t_1t_2 + 0.01357719775t_1^2) + 0.5t_2^2(0.023616621t_3^2$$
$$+0.027143955(t_2t_3 + t_1t_3) + 0.023616621t_2^2 + 0.007054668t_1t_2 + 0.0135719775t_1^2)$$
$$+0,5t_1^2(0.023616621t_3^2 + 0.027143955(t_2t_3 + t_1t_3) + 0.0135719775t_2^2$$
$$+0.007054668t_1t_2 + 0.023616621t_1^2) + t_1t_2(0.003527334t_3^2 + 0.007054668(t_2t_3 + t_1t_3)$$
$$+0.003527334t_2^2 + 0.007054668t_1t_2 + 0.003527334t_1^2)$$

4.3.6 Slope Information Matrices for Weighted Simplex Centroid Designs

The slope information matrices (4.70) for the three ingredients mixture experiment Kronecker model was used to obtained other slope information matrices for different ingredients formulations as follows.

At the point, $(1,\ 0,\ 0)$, the slope information matrix

$$SIM_{31} = \frac{1}{72576}\begin{pmatrix} a & b \\ b & c \end{pmatrix} \tag{4.71}$$

where

$$\begin{aligned} a &= x_{11} = 96356 \\ b &= x_{12}1'_2 \ ; \ \ x_{12} = 1586, \\ c &= x_{22}J_2 \ ; \ x_{22} = 857. \end{aligned}$$

At the point $(1/2,\ 1/2,\ 0)$, the slope information matrix is of the form,

$$SIM_{32} = \begin{pmatrix} a & b \\ b' & c \end{pmatrix} \tag{4.72}$$

where

$$\begin{aligned} a &= x_{11}I_2 + y_{11}J_2; \ \ x_{11} = 831.82198 \times 10^{-4}, \ \ y_{11} = 121.222 \times 10^{-4} \\ b &= x_{12}1_2 \ ; \ \ x_{12} = 64.7209 \times 10^{-4} \\ c &= x_{22} \ ; \ x_{22} = 36.4704 \times 10^{-4}. \end{aligned}$$

At the centroid point, $(1/3,\ 1/3,\ 1/3)$, the slope information matrix is of the form

$$SIM_{33} = x_{11}I_3 + y_{11}J_3 \tag{4.73}$$

where

$$x_{11} = 174.23115 \times 10^{-4}, \; y_{11} = 65.3797 \times 10^{-4}.$$

4.3.7 Moment Matrix for Uniformly Weighted Simplex Centroids Designs

The moment matrix for uniformly weighted simplex centriod designs for three ingredients is given by $M(\eta) = \alpha_1 M(\eta_1) + \alpha_2 M(\eta_2) + \alpha_3 M(\eta_3)$, where weights are all equal, that is $\alpha_1 = \alpha_2 = \alpha_3 = 1/3$ as given in (3.4). Hence

$$M(\eta) = \tfrac{1}{3} M(\eta_1) + \tfrac{1}{3} M(\eta_2) + \tfrac{1}{3} M(\eta_3) \qquad (4.74)$$

where $M(\eta_1)$, $M(\eta_2)$ and $M(\eta_3)$ are given in (4.60), (4.61) and (4.62) respectively.

Using equations (4.66) and (4.74), we obtained uniform information matrix as

$$C_u = \begin{pmatrix} x_{11} I_3 + y_{11} J_3 & x_{12} I_3 + y_{12} J_3 & x_{13} 1_3 \\ x_{12} I_3 + y_{12} J_3 & x_{22} I_3 + y_{22} J_3 & x_{23} 1_3 \\ x_{13} 1'_3 & x_{23} 1'_3 & x_{33} \end{pmatrix} \qquad (4.75)$$

where

$x_{11} = 1128.4722 \times 10^{-4}$, $y_{11} = 21.93358 \times 10^{-4}$, $x_{12} = 52.0833 \times 10^{-4}$, $y_{12} = 79.51818 \times 10^{-4}$, $x_{13} = 27.43484 \times 10^{-4}$, $x_{22} = 156.25 \times 10^{-4}$, $y_{22} = 320.85905 \times 10^{-4}$, $x_{23} = 164.60905 \times 10^{-4}$, $x_{33} = 164.60905 \times 10^{-4}$.

The information matrix (4.75) together with (4.68) were used to obtain slope information matrix D_{ccu}, as

$$D_{ccu} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{12}' & A_{22} & A_{23} \\ A_{13}' & A_{23}' & A_{33} \end{pmatrix} \tag{4.76}$$

where

$$A_{11} = 0.5t_3^2(0.0238554525t_3^2 + 0.032085905(t_1t_3 + t_1t_2) + 0.016460905t_2t_3 + 0.0160429525t_2^2 + 0.023855454t_1^2) + (t_1t_3 + t_1t_2)(0.0160429525t_3^2 + 0.047710905(t_1t_3 + t_1t_2) + 0.016460905t_2t_3 + 0.0160429525t_2^2 + 0.039480453t_1^2) + 0.5t_2^2(0.0160429525t_3^2 + 0.032085905(t_1t_3 + t_1t_2) + 0.016460905t_2t_3 + 0.0160429525t_2^2 + 0.023855454t_1^2) + t_2t_3(0.0160429525t_3^2 + 0.016460905(t_1t_3 + t_1t_2) + 0.016460905t_2t_3 + 0.0082304525t_2^2 + 0.0082304525t_1^2) + 3t_1^2(0.003975909t_3^2 + 0.013160151(t_1t_3 + t_1t_2) + 0.002743484t_2t_3 + 0.003975909t_2^2 + 0.345121743t_1^2).$$

$$A_{12} = 0.5t_3^2(0.0238554525t_3^2 + 0.032085905(t_1t_3 + t_1t_2) + 0.016460905t_2t_3 + 0.0160429525t_2^2 + 0.023855454t_1^2) + 0.5t_1^2(0.0160429525t_3^2 + 0.047710905(t_1t_3 + t_1t_2) + 0.016460905t_2t_3 + 0.0160429525t_2^2 + 0.039480453t_1^2) + (t_2t_3 + t_1t_2)(0.0160429525t_3^2 + 0.032085905(t_1t_3 + t_1t_2) + 0.016460905t_2t_3 + 0.0238554525t_2^2 + 0.023855454t_1^2)t_2^2 + 0.008230452t_1^2) + 3t_2^2(0.003975909t_3^2 + 0.007951818(t_1t_3 + t_1t_2) + 0.002743484t_2t_3 + 0.0065800755t_2^2 + 0.006580074t_1^2).$$

$$A_{13} = 0.5t_3^2(0.039480453t_3^2 + 0.047710905(t_2t_3 + t_1t_3) + 0.0160429525t_2^2 + 0.016460905t_1t_2 \; 0.0160429525t_1^2) + 0.5t_2^2(0.023855454t_3^2 + 0.032085905(t_2t_3 + t_1t_3) + 0.0238554525t_2^2 + 0.016460905t_1t_2 + 0.0160429525t_1^2) + (t_1t_3 + t_1t_2)(0.023855454t_3^2 + 0.032085905(t_2t_3 + t_1t_3) + 0.0160429525t_1^2 + 0.016460905t_1t_2 + 0.0238554525t_1^2)t_2^2 + 0.0082304525t_1^2) + 3t_1^2(0.006580074t_3^2 + 0.007951818(t_2t_3 + t_1t_3) + 0.003975909t_2t_3 + 0.0065800755t_2^2 + 0.002743484t_1t_2 + 0.0065800755t_1^2).$$

$$A_{22} = 0.5t_3^2(0.0238554525t_3^2 + 0.032085905(t_2t_3 + t_1t_2) + 0.0160429525t_1^2 + 0.016460905t_1t_3$$
$$+ 0.023855454t_2^2) + (t_2t_3 + t_1t_2)(0.0160429525t_3^2 + 0.047710905(t_2t_3 + t_1t_2)$$
$$+0.016460905t_1t_3 + 0.039480453t_2^2 + 0.0160429525t_1^2) + 0.5t_1^2(0.0160429525t_3^2$$
$$+0.032085905(t_2t_3 + t_1t_3) + 0.016460905t_1t_3 + 0.023855454t_2^2 + 0.0238554525t_1^2)$$
$$+t_1t_3(0.0082304525t_3^2 + 0.016460905(t_2t_3 + t_1t_2) + 0.016460905t_1t_3 + 0.008230452t_2^2$$
$$+0.0082304525t_1^2) + 3t_2^2(0.003975909t_3^2 + 0.013160151(t_2t_3 + t_1t_2) + 0.002743484t_1t_3$$
$$+0.345121743t_2^2 + 0.003975909t_1^2).$$

$$A_{23} = 0.5t_3^2(0.039480453t_3^2 + 0.047710905(t_2t_3 + t_1t_2) + 0.0160429525t_2^2 + 0.016460905t_1t_3$$
$$+ 0.016049525t_1^2) + (t_2t_3 + t_1t_2)(0.023855454t_3^2 + 0.032085905(t_2t_3 + t_1t_2)$$
$$+0.0238554525t_2^2 + 0.016460905t_1t_2 + 0.0160429525t_1^2) + 0.5t_1^2(0.023855454t_3^2$$
$$+0.032085905(t_2t_3 + t_1t_3) + 0.0160429525t_2^2 + 0.016460905t_1t_2 + 0.0238554525t_1^2)$$
$$+t_1t_3(0.008230452t_3^2 + 0.016460905(t_2t_3 + t_1t_3) + 0.016460905t_1t_2 + 0.008230452t_2^2$$
$$+0.0082304525t_1^2) + 3t_2^2(0.006580074t_3^2 + 0.007951818(t_2t_3 + t_1t_3) + 0.002743484t_1t_2$$
$$+0.0065800755t_2^2 + 0.003975909t_1^2).$$

$$A_{33} = 0.3t_3^2(0.345121743t_3^2 + 0.013160151(t_2t_3 + t_1t_3) + 0.003975909t_2^2 + 0.002743484t_1t_2$$
$$+0.003975909t_1^2) + (t_2t_3 + t_1t_2)(0.039480453t_3^2 + 0.047710905(t_2t_3 + t_1t_3) + 0.0160429525t_2^2 +$$
$$+0.016460905t_1t_2 + 0.0160429525t_1^2) + 0.5t_2^2(0.023855454t_3^2 + 0.032085905(t_2t_3 + t_1t_3)$$
$$+0.0160429525t_1^2 + 0.016460905t_1t_2 + 0.0238554525t_2^2) + 0.5t_1^2(0.023855454t_3^2$$
$$+0.032085905(t_2t_3 + t_1t_3) + 0.0160429525t_2^2 + 0.016460905t_1t_2 + 0.0082304525t_1^2)$$
$$+t_1t_2(0.008230452t_3^2 + 0.016460905(t_2t_3 + t_1t_3) + 0.008230452t_2^2$$
$$+ 0.016460905t_1t_2 + 0.0082304525t_1^2).$$

4.3.8 Slope Information Matrices (SIM) for Uniform Weighted Centroid Designs

Using matrix (4.76), we obtained other slope information matrices corresponding to pure, binary and centroid components for the three mixture experiments. At a point (1, 0, 0), we have,

$$SIM_{31u} = \begin{pmatrix} xJ_2 & y1_2 \\ y1'_2 & z \end{pmatrix} \tag{4.77}$$

where $x = 119.2773 \times 10^{-4}$, $y = 197.4023 \times 10^{-4}$, $z = 10353.6523 \times 10^{-4}$.

At point (½, ½, 0), we obtained the information matrix as given by

$$SIM_{32u} = \begin{pmatrix} xI_2 + yJ_2 & z1_2 \\ z1'_2 & q \end{pmatrix} \tag{4.78}$$

where

$x = 646.97266 \times 10^{-4}$, $y = 121.71867 \times 10^{-4}$, $z = 77.77336 \times 10^{-4}$, $q = 55.8007 \times 10^{-4}$.

The information matrix for ternary mixture experiments at the central point of the simplex centroid design is given as

$$SIM_{33u} = x_{11} I_3 + y_{11} J_3 \tag{4.79}$$

where

$x_{11} = 135.51312 \times 10^{-4}$, $y_{11} = 78.28575 \times 10^{-4}$.

4.3.9 Optimal Values for Slope Designs

We obtained the optimal values for both Weighted Simplx Centroid (WSC) designs and Uniform Weighted Simplex Centroid Designs (UWSCD) for three ingredients mixture experiments. In this case, we considered the D-, E-, A- and T-optimality criteria based on the formulas (3.13), (3.16), (3.18) and (3.20) respectively.

The optimal values for pure, binary and ternary blends were calculated from matrices (4.71), (4.72) and (4.73) for Weighted Simplex Centroid Designs and (4.77), (4.78) and (4.79) for Uniformly Weighted Simplex Centroid Designs respectively. The optimal values were summarized in Table 4.5 below.

Table 4. 5: Optimal Values for Three Ingredients

	WEIGHTED SIMPLEX CENTROID (WSC)				**UNIFORM WEIGHTED SIMPLEX CENTROID (UWSC)**			
BLENDS	**D-**	**E-**	**A-**	**T-**	**D-**	**E-**	**A-**	**T-**
1, 0, 0	0.0000	0.0000	0.0000	0.4504	0.0000	0.0000	0.0000	0.3531
½, ½, 0	0.0294	0.0028	0.0081	0.0648	0.0289	0.0042	0.0112	0.0531
1/3, 1/3, 1/3	0.0224	0.0174	0.0212	0.0239	0.0189	0.0136	0.0172	0.0214

From Table 4.5, it was observed that the D- and T- optimality yield better results in Uniformly Weighted Simplex Centroids (UWSC) than Weighted Simplex Centroid (WSC) designs. In Weighted Simplex Centroid (WSC), only binary mixtures (½, ½, 0) were found to be E- and A-optimal due to their smaller optimal values.

4.3.10 Efficiencies for Three Ingredients

The performance of the WSCD in comparison to the UWSCD was measured by the D-, E-, A- and T-efficiencies defined in (3.14), (3.17), (3.19) and (3.21) respectively. Their efficiencies at different point of the simplex centroid designs were obtained for three ingredients in Table 4.6.

Table 4. 6: Efficiencies for Three Mixture Experiments

	Efficiencies (%)			
BLENDS	**D-**	**E-**	**A-**	**T-**
1, 0, 0	100	100	100	127.55
½, ½, 0	101.73	66.66	72.32	122.03
1/3, 1/3, 1/3	118.52	127.94	123.25	111.68

For pure blends, there was no difference between the performance of WSCD and UWSCD in terms of D-, E- and A- optimal criteria, except for T-efficiency where UWSCD was 27.55% more efficient than WSCD. At the centre point, UWSCD was found to be more efficient than WSCD by 18.52%, 27.94%, 23.25% and 11.68% for D-, E-, A- and T-optimal criteria respectively. This clearly indicates that Uniformly Weighted Simplex Centroids (UWSC) performed better than the usual Weighted Simplex Centroid designs.

4.3.11 I-Optimal for Weighted Simplex Centroid Designs

In the three ingredients designs, we obtained the inverse of the information matrix (4.69) for parameter subsystem of interest as,

$$C_1^{-1} = \begin{pmatrix} 7(I_3) & -2.3333(I_3) & 1.6667(1_3) \\ -2.3333(I_3) & 50.555(I_3) - 12.444(J_3) & -12.8333(1_3) \\ 1.6667(1'_3) & -12.8333(1'_3) & 179.6667 \end{pmatrix}. \tag{4.80}$$

Next, we obtained the matrix L through integration of the parameter subsystem of interest of the Kronecker model as given in (3.30). Thus, L becomes,

$$L = k\int f(t)\,f(t)'dt =$$

$$k\int \begin{pmatrix} t_1^6 & t_1^3t_2^3 & t_1^3t_3^3 & \frac{(t_1^5t_2+t_1^5t_3)}{2} & \frac{(t_1^4t_2^2+t_1^3t_2^2t_3)}{2} & \frac{(t_1^4t_2^2+t_1^3t_2t_3^2)}{2} & t_1^4t_2t_3 \\ t_1^3t_2^3 & t_2^6 & t_2^3t_3^3 & \frac{(t_1^2t_2^4+t_1^2t_2^3t_3)}{2} & \frac{(t_1t_2^5+t_2^5t_3)}{2} & \frac{(t_1t_2^3t_3^2+t_2^4t_3^2)}{2} & t_1t_2^4t_3 \\ t_1^3t_3^3 & t_2^3t_3^3 & t_3^6 & \frac{(t_1^4t_2^2+t_1^3t_2^2t_3)}{2} & \frac{(t_1t_2^2t_3^3+t_2^2t_3^4)}{2} & \frac{(t_1t_3^5+t_2t_3^5)}{2} & t_1t_2t_3^4 \\ \frac{(t_1^5t_2+t_1^5t_3)}{2} & \frac{(t_1^2t_2^4+t_1^2t_2^3t_3)}{2} & \frac{(t_1^2t_2t_3^3+t_1^2t_3^4)}{2} & \frac{(t_1^2t_2+t_1^2t_3)^2}{4} & \frac{(t_1^2t_2+t_1^2t_3)(t_1t_2^2+t_2^2t_3)}{4} & \frac{(t_1^2t_2+t_1^2t_3)(t_1t_3^2+t_2t_3^2)}{4} & \frac{(t_1^3t_2^2t_3+t_1^3t_2t_3^2)}{2} \\ \frac{(t_1^4t_2^2+t_1^3t_2^2t_3)}{2} & \frac{(t_1t_2^5+t_2^5t_3)}{2} & \frac{(t_1t_2^2t_3^3+t_2^2t_3^4)}{2} & \frac{(t_1^2t_2+t_1^2t_3)(t_1t_2^2+t_2^2t_3)}{4} & \frac{(t_1t_2^2+t_2^2t_3)^2}{4} & \frac{(t_1t_3^2+t_2t_3^2)(t_1t_2^2+t_2^2t_3)}{4} & \frac{(t_1^2t_2^3t_3+t_1t_2^3t_3^2)}{2} \\ \frac{(t_1^4t_2^2+t_1^3t_2t_3^2)}{2} & \frac{(t_1t_2^3t_3^2+t_2^4t_3^2)}{2} & \frac{(t_1t_3^5+t_2t_3^5)}{2} & \frac{(t_1^2t_2+t_1^2t_3)(t_1t_3^2+t_2t_3^2)}{4} & \frac{(t_1t_3^2+t_2t_3^2)(t_1t_2^2+t_2^2t_3)}{4} & \frac{(t_1t_3^2+t_2t_3^2)^2}{4} & \frac{(t_1^2t_2t_3^3+t_1t_2^2t_3^3)}{2} \\ t_1^4t_2t_3 & t_1t_2^4t_3 & t_1t_2t_3^4 & \frac{(t_1^3t_2^2t_3+t_1^3t_2t_3^2)}{2} & \frac{(t_1^2t_2^3t_3+t_1t_2^3t_3^2)}{2} & \frac{(t_1^2t_2t_3^3+t_1t_2^2t_3^3)}{2} & t_1^2t_2^2t_3^2 \end{pmatrix} dt \tag{4.81}$$

The integrals of L matrix are calculated as

$$(q-1)!\int_\tau t_1^6 dt_1 = \int_\tau t_2^6 dt_2 = \int_\tau t_3^6 dt_3 = \frac{(q-1)!\prod_{i=1}^{3}(p_i!)}{(q+\sum_1^3 p_i - 1)!} = \frac{2!6!}{8!} = \frac{1}{28}$$

$$(q-1)!\int_\tau t_1^2 t_2^2 t_3^2 dt_1 dt_2 dt_3 = \frac{(q-1)!\prod_{i=1}^{3}(p_i!)}{(q+\sum_1^3 p_i - 1)!} = \frac{2!2!2!2!}{8!} = \frac{1}{2520}$$

$$(q-1)!\int_\tau t_1^5 t_2 dt_1 dt_2 = \int_\tau t_1 t_2^5 dt_1 dt_2 = \int_\tau t_1 t_3^5 dt_1 dt_3 = \frac{(q-1)!\prod_{i=1}^{3}(p_i!)}{(q+\sum_{i=1}^3 p_i - 1)!} = \frac{1}{168} \tag{4.82}$$

$$(q-1)!\int_\tau t_1^4 t_2 t_3 dt_1 dt_2 dt_3 = \int_\tau t_1 t_2^4 t_3 dt_1 dt_2 dt_3 = \int_\tau t_1 t_2 t_3^4 dt_1 dt_2 dt_3 = \frac{(q-1)!\prod_{i=1}^{3}(p_i!)}{(q+\sum_{i=1}^3 p_i - 1)!} = \frac{1}{840}$$

$$(q-1)!\int_\tau t_1^3 t_2^2 t_3 dt_1 dt_2 dt_3 = \int_\tau t_1^2 t_2 t_3^3 dt_1 dt_2 dt_3 = \int_\tau t_1 t_2^3 t_3^2 dt_1 dt_2 dt_3 \frac{(q-1)!\prod_{i=1}^{3}(p_i!)}{(q+\sum_1^3 p_i - 1)!} = \frac{1}{1680}$$

$$(q-1)!\int_\tau t_1^3 t_2^3 dt_1 dt_2 = \int_\tau t_1^3 t_3^3 dt_1 dt_3 = \int_\tau t_2^3 t_3^3 dt_2 dt_3 \frac{(q-1)!\prod_{i=1}^{3}(p_i!)}{(q+\sum_1^3 p_i - 1)!} = \frac{1}{560}$$

$$(q-1)!\int_\tau t_1^4 t_2^2 dt_1 dt_2 = \int_\tau t_1^2 t_2^4 dt_1 dt_2 = \int_\tau t_2^2 t_3^4 dt_2 dt_3 = \int_\tau t_1^2 t_3^4 dt_1 dt_3 = \int_\tau t_1^4 t_3^2 dt_1 dt_3$$

$$= \int_\tau t_2^4 t_3^2 dt_1 dt_3 = \frac{(q-1)!\prod_{i=1}^{3}(p_i!)}{(q+\sum_{i=1}^3 p_i - 1)!} = \frac{1}{420}.$$

Hence L matrix becomes,

$$L = \begin{pmatrix} m_1 & m_2 & m_3 \\ m_2 & m_4 & m_5 \\ m'_3 & m'_5 & m_6 \end{pmatrix} \tag{4.83}$$

where

$$m_1 = x_{11} I_3 + y_{11} J_3; \;\; x_{11} = 339.28572 \times 10^{-4}, \;\; y_{11} = 17.85714 \times 10^{-4}$$
$$m_2 = x_{12} I_3 + y_{11} J_3 \; ; \; x_{12} = 44642.2858 \times 10^{-4}, \; y_{12} = 14.88095 \times 10^{-4}$$

$$m_3 = x_{13} 1_3 \;;\; x_{13} = 11.904762 \times 10^{-4}$$
$$m_5 = x_{23} I_3 \;;\; x_{23} = 5.952381 \times 10^{-4}$$
$$m_6 = x_{22} \;;\; x_{22} = 3.968254 \times 10^{-4}$$

$$m_4 = \begin{pmatrix} 5.9523 \times 10^{-4} (I_2) + 11.90476 \times 10^{-4} (J_2) & 8.43254 \times 10^{-4} (1_2) \\ 8.43254 \times 10^{-4} (1'_2) & 17.857143 \times 10^{-4} \end{pmatrix}.$$

Using matrices (4.80) and (4.83), we obtained (4.84) matrix as

$$C_1^{-1} L = \begin{pmatrix} 0.23750000 & 0.01041667 & 0.01041667 & 0.038194444 & 0.008333333 & 0.009143519 & 0.007407 \\ 0.01041667 & 0.23750000 & 0.01041667 & 0.008333333 & 0.038194444 & 0.009143519 & 0.007407 \\ 0.01041667 & 0.01041667 & 0.23750000 & 0.009143519 & 0.009143519 & 0.038194444 & 0.007407 \\ 0.09120370 & -0.05532407 & -0.05532407 & 0.021219136 & 0.001543210 & -0.011689815 & 0.000000 \\ -0.05532407 & 0.09120370 & -0.05532407 & 0.001543210 & 0.021219136 & -0.011689815 & 0.000000 \\ -0.05532407 & -0.05532407 & 0.09120370 & -0.016010802 & -0.016010802 & 0.025540123 & 0.000000 \\ 0.14513889 & 0.14513889 & 0.14513889 & 0.068344907 & 0.068344907 & 0.072800926 & 0.0525463 \end{pmatrix}.$$

(4.84)

Therefore, the average prediction variance is given by the trace of the I-optimal information matrix (4.84) as

$$APV = tr[C_1^{-1} L] = 0.8330247. \qquad (4.85)$$

4.3.12 I-Optimal for Uniform Weight Simplex Centroid Designs

Similarly, we obtained the inverse of (4.75) for Uniformly Weighted Simplex Centroid Designs as

$$C_{1u}^{-1} = \begin{pmatrix} 9(I_3) & -3(I_3) & 1.5(1_3) \\ -3(I_3) & 65(I_3)-16(J_3) & -16.5(1_3) \\ 1.5(1'_3) & -16.5(1'_3) & 109.5 \end{pmatrix}.$$

(4.86)

Using the integral matrix (4.83) and inverse of information matrix (4.86), we obtained matrix $C_{1u}^{-1}L$ given as

$$C_{1u}^{-1}L = \begin{pmatrix} 0.30535714 & 0.01339286 & 0.01339286 & 0.049107143 & 0.010714286 & 0.01175595 & 0.009523810 \\ 0.01339286 & 0.30535714 & 0.01339286 & 0.010714286 & 0.049107143 & 0.01175595 & 0.009523810 \\ 0.01339286 & 0.01339286 & 0.30535714 & 0.011755952 & 0.011755952 & 0.04910714 & 0.009523810 \\ 0.11726190 & -0.07113095 & -0.07113095 & 0.027281746 & 0.001984127 & -0.01502976 & 0.000000000 \\ -0.07113095 & 0.11726190 & -0.07113095 & 0.001984127 & 0.027281746 & -0.01502976 & 0.00000000 \\ -0.07113095 & -0.07113095 & 0.11726190 & -0.020585317 & -0.020585317 & 0.03283730 & 0.000000000 \\ 0.04196429 & 0.04196429 & 0.04196429 & 0.015550595 & 0.015550595 & 0.02127976 & 0.01934524 \end{pmatrix}.$$

(4.87)

Therefore, from matrix (4.87), the Average Prediction Variance becomes

$$APV = tr[C_{1u}^{-1}L] = 1.022817. \tag{4.88}$$

From APV's in (4.85) and (4.88), we conclude that WSCD performance were better than that of UWSCD in terms of prediction variance. That is, prediction of the responses is more accurate when Weighted Simplex Centroid Designs are used.

4.3.13 Equivalence Theorem for Weighted Simplex Centroid Kronecker

Using the equivalence theorem given in (3.34), the design is I-optimal if and only if,

$$f^{'}(t)C_1^{-1}LC_1^{-1}f(t) \leq 0.8330247 \tag{4.89}$$

at all the design points in the simplex centroid designs.

Table 4. 7: Equivalence Theorem for Three Ingredients (WSCD)

Average Prediction Variances				
BLENDS	$f^{'}(t)C_1^{-1}LC_1^{-1}f(t)$		$tr[C_1^{-1}L]$	**Optimality**
1, 0, 0	1.582022	>	0.8330247	Not I Optimal
½, ½, 0	0.06375145	<	0.8330247	I-Optimal
1/3, 1/3, 1/3	0.0230086	<	0.8330247	I-Optimal

In Table 4.7, it was observed that the pure blends for WSCD did not satisfy the general equivalence theorem for I-optimality. The binary and ternary blends were found to satisfy the general equivalence theorem, therefore, I-optimal.

4.3.14 Equivalence Theorem for Uniform Weighted Simplex Centroid Kronecker

For three ingredients, the design is said to be I-optimal if and only if it satisfy,

$$f^{'}(t)C_{1u}^{-1}LC_{1u}^{-1}f(t) \leq 1.022817 \tag{4.90}$$

at all the design points.

Table 4. 8: Equivalence Theorem for Three Ingredients (UWSCD)

Average Prediction Variances

BLENDS	$f^{'}(t)C_1^{-1}LC_1^{-1}f(t)$		$tr[C_{1u}^{-1}L]$	Optimality
1, 0, 0	2.615179	>	1.022817	Not I Optimal
½, ½, 0	0.105385	<	1.022817	I-Optimal
1/3, 1/3, 1/3	0.01402579	<	1.022817	I-Optimal

It was observed Table 4.8 that the pure blends for UWSCD did not satisfy the general equivalence theorem for I-optimality. The binary and ternary blends were found to satisfy the general equivalence theorem, therefore, I-optimal. However, the ternary mixtures were better than the binary due to their small prediction variance, therefore, it was more accurate to predict responses at (0.33, 0.33, 0.33) point of the simplex centroid designs.

4.4 DESIGNS FOR FOUR FACTORS MIXTURE EXPERIMENTS

4.4.1 Simplex Centroid Designs

In four ingredients mixture designs, there are four designs, η_1, η_2, η_3 and η_4 placing equal weights α_1, α_2, α_3 and α_4 on each design respectively.

$$\left.\begin{Bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{Bmatrix}\right\}\eta_1$$

$$\left.\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{Bmatrix}\right\}\eta_2$$

$$\left.\begin{Bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \end{Bmatrix}\right\}\eta_3$$

$$\begin{Bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{Bmatrix} \eta_4. \qquad (4.91)$$

The design (4.91) was used to obtain optimal weights for each design.

4.4.2 Weighted Simplex Centroid Designs

The weights for simplex centroid designs for four ingredients were obtained through lower order moments of the simplex centroids Kronecker designs. Let η be an arbitrary exchangeable design, then its sixth order moments were obtained from design (4.91) as

$$(i)\quad \mu_6 = \int t_1^6 d\tau = \int t_2^6 d\tau = \int t_3^6 d\tau = \int t_3^6 d\tau = \tfrac{1}{15}[(1)^6 + 3(\tfrac{1}{2})^6 + 3(\tfrac{1}{3})^6 + (\tfrac{1}{4})^6] = 0.07008$$

$$(ii)\quad \mu_{51} = \int t_1^5 t_2^1 d\tau = \int t_1^5 t_3^1 d\tau = \int t_1^5 t_4^1 d\tau = \int t_2^5 t_3^1 d\tau = \int t_2^5 t_4^1 d\tau = \int t_3^5 t_4^1 d\tau = 0.001149392182$$

$$(iii)\quad \mu_{42} = \int t_1^4 t_2^2 d\tau = \int t_1^4 t_3^2 d\tau = \int t_1^4 t_4^2 d\tau = \int t_2^4 t_3^2 d\tau = \int t_2^4 t_4^2 d\tau = \int t_3^4 t_4^2 d\tau = 0.001149392182$$

$$(iv)\quad \mu_{33} = \int t_1^3 t_2^3 d\tau = \int t_1^3 t_3^3 d\tau = \int t_1^3 t_4^3 d\tau + \int t_2^3 t_3^3 d\tau + \int t_2^3 t_4^3 d\tau = \int t_3^3 t_4^3 d\tau = 0.001149392182 \qquad (4.92)$$

$$(v)\quad \mu_{411} = \int t_1^4 t_2^1 t_3^1 d\tau = \int t_1^1 t_2^4 t_3^1 d\tau = \int t_1^1 t_2^1 t_3^4 d\tau = \int t_1^1 t_2^1 t_4^4 d\tau = \int t_1^1 t_2^4 t_4^1 d\tau = \int t_2^1 t_3^1 t_4^4 d\tau = 0.000107725$$

$$(vi)\quad \mu_{321} = \int t_1^3 t_2^2 t_3^1 d\tau = \int t_1^2 t_2^3 t_3^1 d\tau = \int t_1^1 t_2^2 t_3^3 d\tau = \int t_1^1 t_2^3 t_4^2 d\tau = \int t_1^1 t_2^2 t_4^3 d\tau = \int t_2^1 t_3^2 t_4^3 d\tau = 0.000107725$$

$$(vii)\quad \mu_{222} = \int t_1^2 t_2^2 t_3^2 d\tau = \int t_1^2 t_2^2 t_4^2 d\tau = \int t_2^2 t_3^2 t_4^2 d\tau = 0.000107725$$

$$(viii)\quad \mu_{2211} = \int t_1^2 t_2^2 t_3^1 t_4^1 d\tau = \int t_1^2 t_2^1 t_3^2 t_4^1 d\tau = \int t_1^2 t_2^1 t_3^1 t_4^2 d\tau = \int t_1^1 t_2^2 t_3^2 t_4^1 d\tau = \int t_1^1 t_2^1 t_3^2 t_4^2 d\tau = 0.000016276$$

$$(ix)\quad \mu_{3111} = \int t_1^3 t_2^1 t_3^1 t_4^1 d\tau = \int t_1^1 t_2^3 t_3^1 t_4^1 d\tau = \int t_1^1 t_2^1 t_3^3 t_4^1 d\tau = \int t_1^1 t_2^1 t_3^1 t_4^3 d\tau = 0.000016276.$$

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he lower order moments for four ingredients are expressed in form of sixth order moments as

$$(i)\quad \mu_5 = \int_t t_1^5(t_1+t_2+t_3+t_4)dt = \int(t_1^6+t_1^5t_2+t_1^5t_3+t_1^5t_4)dt = \mu_6 + 3\mu_{51}$$

$$(ii)\quad \mu_{41} = \int_t t_1^4 t_2(t_1+t_2+t_3+t_4)dt = \int(t_1^5t_2+t_1^4t_2^2+t_1^4t_2t_3+t_1^4t_2t_4)dt = \mu_{51} + \mu_{42} + 2\mu_{411}$$

$$(iii)\quad \mu_{32} = \int_t t_1^3t_2^2(t_1+t_2+t_3+t_4)dt = \mu_{42} + \mu_{33} + 2\mu_{321}$$

$$(iv)\quad \mu_{221} = \int_t t_1^3t_2^2t_3(t_1+t_2+t_3+t_4)dt = 2\mu_{321} + \mu_{222} + \mu_{2211}$$

$$(v)\quad \mu_4 = \int_t t_1^5(t_1+t_2+t_3+t_4)dt = \mu_6 + 6\mu_{51} + 3\mu_{42} + 6\mu_{411}$$

$$(vi)\quad \mu_{311} = \int_t t_1^3t_2t_3(t_1+t_2+t_3+t_4)dt = \mu_{411} + 2\mu_{321} + \mu_{3111}$$

$$(vii)\quad \mu_{211} = \int_t t_1^2t_2t_3(t_1+t_2+t_3+t_4)dt = \mu_{411} + 6\mu_{321} + 2\mu_{3111} + 2\mu_{222} + 5\mu_{2211}$$

$$(vii) \quad \mu_{31} = \int_t t_1^3 t_2 (t_1 + t_2 + t_3 + t_4) dt = \int (t_1^5 t_2 + t_1^4 t_2^2 + t_1^4 t_2 t_3) dt = \mu_{51} + 2\mu_{42} + 4\mu_{411}$$
$$+ 6\mu_{321} + \mu_{33} + 2\mu_{3111}$$

$$(viii) \quad \mu_3 = \int_t t_1^3 (t_1 + t_2 + t_3 + t_4) dt = \mu_6 + 9\mu_{51} + 9\mu_{42} + 18\mu_{411} + 18\mu_{321}) + 3\mu_{33} + 6\mu_{3111}$$

$$(ix) \quad \mu_{21} = \int_t t_1^2 t_2 (t_1 + t_2 + t_3 + t_4) dt = \mu_{51} + 4\mu_{42} + 5\mu_{411} + 20\mu_{321} + 3\mu_{33}$$
$$+ 4\mu_{222} + 4\mu_{3111} + 7\mu_{2211}$$

$$(x) \quad \mu_{22} = \int_t t_1^2 t_2^2 (t_1 + t_2 + t_3 + t_4) dt = 2\mu_{42} + 8\mu_{321} + 2\mu_{33} + 2\mu_{222} + 2\mu_{2211}$$

$$(xi) \quad \mu_2 = \int_t t_1^2 (t_1 + t_2 + t_3 + t_4) dt = \mu_6 + 10\mu_{51} + 13\mu_{42} + 23\mu_{411} + 38\mu_{321} + 6\mu_{33}$$
$$+ 10\mu_{3111} + 4\mu_{222} + 7\mu_{2211}$$

(4.94)

$$(xii) \quad \mu_1 = \int_t t_1 (t_1 + t_2 + t_3 + t_4) dt = \mu_6 + 16\mu_{51} + 37\mu_{42} + 65\mu_{411} + 230\mu_{321} + 24\mu_{33} + 52\mu_{222}$$
$$+ 58\mu_{3111} + 109\mu_{2211}$$

$$(xiii) \quad \mu_{111} = \int_t t_1 t_2 t_3 (t_1 + t_2 + t_3 + t_4) dt = 27\mu_{321} + 37\mu_{3111}$$

$$(xiv) \quad \mu_{11} = \int_t t_1 t_2 (t_1 + t_2 + t_3 + t_4) dt = 16\mu_{42} + 130\mu_{321} + 110\mu_{2211}$$

$$(xv) \quad \mu_{1111} = \int_t t_1 t_2 t_3 t_4 (t_1 + t_2 + t_3 + t_4) dt = 4\mu_{3111} + 12\mu_{2211}.$$

The optimal weights $\alpha_1, \alpha_2, \alpha_3$ and α_4 were obtained from (4.92) and (4.93) such that,

$$\mu_{1111}(\eta) = \alpha_1(\eta_1) + \alpha_2(\eta_2) + \alpha_3(\eta_3) + \alpha_4(\eta_4)$$

$$\alpha_4 = 256\mu_{1111}. \tag{4.94}$$

Using (xv)(4.93), the moment μ_{1111} is substituted in (4.94) so that,

$$\alpha_4 = 256\,[4(\mu_{3111} + 3\mu_{2211})]. \tag{4.95}$$

But from equations (4.92), we have,

$$\mu_{3111} = \mu_{2211} = 0.000016276. \tag{4.96}$$

Substituting equation (4.96) in equation (4.95), we have,

$$\alpha_4 = \tfrac{1}{15}. \tag{4.97}$$

We use (4.93) to obtain α_3, where moment μ_{111} in (4.91) is given as

$$\mu_{111}(\eta) = \alpha_1(\eta_1) + \alpha_2(\eta_2) + \alpha_3(\eta_3) + \alpha_4(\eta_4)$$

$$\mu_{111} = \alpha_1(0) + \alpha_2(0) + \alpha_3(\tfrac{1}{108}) + \alpha_4(\tfrac{1}{64})$$

$$\alpha_3 = 108\mu_{111} - (\tfrac{108}{64})\alpha_4. \tag{4.98}$$

By substituting the value of α_4 in equation (4.97), we have α_3 as

$$\alpha_3 = 108\mu_{111} - (\tfrac{9}{80}). \tag{4.99}$$

From equation $(xiii)$,(4.93), we have,

$$\mu_{111} = 27\mu_{321} + 37\mu_{3111}. \tag{4.100}$$

Therefore,

$$\alpha_3 = 108(27\mu_{321} + 37\mu_{3111}) - (\tfrac{9}{80}). \qquad (4.101)$$

From equation (4.92), we substitute the values of μ_{321} and μ_{3111} into (4.101), so that

$$\alpha_3 = \tfrac{4}{15}. \qquad (4.102)$$

Next we obtained the weight α_2 from (4.91), using μ_{11} as given by

$$\mu_{11}(\eta) = \alpha_1(0) + \alpha_2(\eta_2) + \alpha_3(\eta_3) + \alpha_4(\eta_4)$$

$$\mu_{11} = (\tfrac{1}{6})(\tfrac{1}{2})^2\alpha_2 + \tfrac{1}{4}[(\tfrac{1}{3})^2 + (\tfrac{1}{3})^2]\alpha_3 + (\tfrac{1}{4})^2\alpha_4. \qquad (4.103)$$

By substituting equations (4.97) and (4.102) in to equation (4.103), we have,

$$\mu_{11} = \tfrac{1}{24}\alpha_2 + \tfrac{41}{2160}. \qquad (4.104)$$

From (xiv) ,(4.93), we have μ_{11} as

$$\mu_{11} = 16\mu_{42} + 130\mu_{321} + 110\mu_{2211} = \tfrac{77}{2160}. \qquad (4.105)$$

By substituting (4.105) in (4.104), we have,

$$\alpha_2 = \tfrac{2}{5}. \qquad (4.106)$$

Since the weights of the simplex centroid designs satisfy (3.12), we have,

$$\alpha_1 = 1 - \alpha_2 - \alpha_3 - \alpha_4 = \tfrac{4}{15}. \qquad (4.107)$$

4.4.3 Uniformly Weighted Simplex Centroid Designs (UWSCD)

The Uniformly Weighted Simplex Centriod Designs (UWSCD) for four ingredients were assumed to assign uniform weights to the four elementary centroid designs, $\eta_1, \eta_2, \ \eta_3$ and η_4, as given in (3.4), such that all weights are equal. That is,

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1/4. \qquad (4.108)$$

4.4.4 Moment Matrix

The full parameter for the third degree Kronecker model four ingredients is given as;

$$\begin{aligned} E(\mathrm{y}) =\; & \theta_{111}t_1t_1t_1 + \theta_{112}t_1t_1t_2 + \theta_{113}t_1t_1t_3 + \theta_{114}t_1t_1t_4 + \theta_{121}t_1t_2t_1 + \theta_{122}t_1t_2t_2 \\ & + \theta_{123}t_1t_2t_3 + \theta_{124}t_1t_2t_4 + \theta_{131}t_1t_3t_1 + \theta_{132}t_1t_3t_2 + \theta_{133}t_1t_3t_3 + \theta_{134}t_1t_3t_4 + \theta_{141}t_1t_4t_1 \\ & + \theta_{142}t_1t_4t_2 + \theta_{143}t_1t_4t_3 + \theta_{144}t_1t_4t_4 + \theta_{211}t_2t_1t_1 + \theta_{212}t_2t_1t_2 + \theta_{213}t_2t_1t_3 + \theta_{214}t_2t_1t_4 \\ & + \theta_{221}t_2t_2t_1 + \theta_{222}t_2t_2t_2 + \theta_{223}t_2t_2t_3 + \theta_{224}t_2t_2t_4 + \theta_{231}t_2t_3t_1 + \theta_{232}t_2t_3t_2 + \theta_{233}t_2t_3t_3 \\ & + \theta_{234}t_2t_3t_4 + \theta_{241}t_2t_4t_1 + \theta_{242}t_2t_4t_2 + \theta_{243}t_2t_4t_3 + \theta_{244}t_2t_4t_4 + \theta_{311}t_3t_1t_1 + \theta_{312}t_3t_1t_2 \\ & + \theta_{313}t_3t_1t_3 + \theta_{314}t_3t_1t_4 + \theta_{321}t_3t_2t_1 + \theta_{322}t_3t_2t_2 + \theta_{323}t_3t_2t_3 + \theta_{324}t_3t_2t_4 + \theta_{331}t_3t_3t_1 \\ & + \theta_{332}t_3t_3t_2 + \theta_{333}t_3t_3t_3 + \theta_{334}t_3t_3t_4 + \theta_{341}t_3t_4t_1 + \theta_{342}t_3t_4t_2 + \theta_{343}t_3t_4t_3 + \theta_{344}t_3t_4t_4 \\ & + \theta_{411}t_4t_1t_1 + \theta_{412}t_4t_1t_2 + \theta_{413}t_4t_1t_3 + \theta_{414}t_4t_1t_4 + \theta_{421}t_4t_2t_1 + \theta_{422}t_4t_2t_2 + \theta_{423}t_4t_2t_3 \\ & + \theta_{424}t_4t_2t_4 + \theta_{431}t_4t_3t_1 + \theta_{432}t_4t_3t_2 + \theta_{433}t_4t_3t_3 + \theta_{434}t_4t_3t_4 + \theta_{441}t_4t_4t_1 + \theta_{442}t_4t_4t_2 \\ & + \theta_{443}t_4t_4t_3 + \theta_{444}t_4t_4t_4. \end{aligned}$$

(4.109)

Let the parameter system of interest model obtained from equation (3.7) be given as

$$E(\text{y}) = \theta_{111}t_1t_1t_1 + \theta_{222}t_2t_2t_2 + \theta_{333}t_3t_3t_3 + \theta_{444}t_4t_4t_4 +$$

$$\frac{\theta_{112}t_1t_1t_2 + \theta_{121}t_1t_2t_1 + \theta_{211}t_2t_1t_1 + \theta_{113}t_1t_1t_3 + \theta_{131}t_1t_3t_1 + \theta_{311}t_3t_1t_1 + \theta_{114}t_1t_1t_4}{9}$$

$$+\frac{\theta_{141}t_1t_4t_1 + \theta_{411}t_4t_1t_1}{9} +$$

$$\frac{\theta_{122}t_1t_2t_2 + \theta_{212}t_2t_1t_2 + \theta_{221}t_2t_2t_1 + \theta_{223}t_2t_2t_3 + \theta_{232}t_2t_3t_2 + \theta_{322}t_3t_2t_2}{9} +$$

$$\frac{\theta_{224}t_2t_2t_4 + \theta_{242}t_2t_4t_2 + \theta_{422}t_4t_2t_2}{9} +$$

$$\frac{\theta_{233}t_2t_3t_3 + \theta_{323}t_3t_2t_3 + \theta_{332}t_3t_3t_2 + \theta_{133}t_1t_3t_3 + \theta_{313}t_3t_1t_3 + \theta_{331}t_3t_3t_1}{9} +$$

$$\frac{\theta_{334}t_3t_3t_4 + \theta_{343}t_3t_4t_3 + \theta_{433}t_4t_3t_3}{9} + \frac{\theta_{144}t_1t_4t_4 + \theta_{244}t_2t_4t_4 + \theta_{344}t_3t_4t_4}{9} +$$

$$\frac{\theta_{414}t_4t_1t_4 + \theta_{424}t_4t_2t_4 + \theta_{434}t_4t_3t_4 + \theta_{442}t_4t_4t_2 + \theta_{443}t_4t_4t_3 + \theta_{441}t_4t_4t_1}{9}$$

$$+\tfrac{1}{24}\left\{\begin{array}{l} \theta_{123}t_1t_2t_3 + \theta_{132}t_1t_3t_2 + \theta_{213}t_2t_1t_3 + \theta_{231}t_2t_3t_1 + \theta_{312}t_3t_1t_2 + \theta_{321}t_3t_2t_1 \\ +\theta_{124}t_1t_2t_4 + \theta_{134}t_1t_3t_4 + \theta_{142}t_1t_4t_2 + \theta_{143}t_1t_4t_3 + \theta_{214}t_2t_1t_4 + \theta_{234}t_2t_3t_4 + \theta_{241}t_2t_4t_1 \\ +\theta_{243}t_2t_4t_3 + \theta_{314}t_3t_1t_4 + \theta_{324}t_3t_2t_4 + \theta_{341}t_3t_4t_1 + \theta_{342}t_3t_4t_2 + \theta_{412}t_4t_1t_2 + \theta_{413}t_4t_1t_3 \\ +\theta_{421}t_4t_2t_1 + \theta_{423}t_4t_2t_3 + \theta_{431}t_4t_3t_1 + \theta_{432}t_4t_3t_2 \end{array}\right\}$$

(4.110)

The moment matrix is given by $M(\eta) = \alpha_1 M(\eta_1) + \alpha_2 M(\eta_2) + \alpha_3 M(\eta_3) + \alpha_4 M(\eta_4)$, where the weights α_1, α_2, α_3 and α_4 were given in equations (4.107), (4.106) (4.102) and (4.97) respectively. Hence,

$$M(\eta) = \tfrac{4}{15}M(\eta_1) + \tfrac{6}{15}M(\eta_2) + \tfrac{4}{15}M(\eta_3) + \tfrac{1}{15}M(\eta_4) \qquad (4.111)$$

where,

$$M(\eta_1) = \tfrac{1}{4}[e_{111}(e_{111})' + e_{222}(e_{222})' + e_{333}(e_{333})' + e_{444}(e_{444})']$$

(4.112)

$$\begin{aligned} M(\eta_2) = \tfrac{1}{384}[&(d_1 \otimes d_1 \otimes d_1)(d_1 \otimes d_1 \otimes d_1)' + (d_2 \otimes d_2 \otimes d_2)(d_2 \otimes d_2 \otimes d_2)' \\ &+ (d_3 \otimes d_3 \otimes d_3)(d_3 \otimes d_3 \otimes d_3)' + (d_4 \otimes d_4 \otimes d_4)(d_4 \otimes d_4 \otimes d_4)' \\ &+ (d_5 \otimes d_5 \otimes d_5)(d_5 \otimes d_5 \otimes d_5)' + (d_6 \otimes d_6 \otimes d_6)(d_6 \otimes d_6 \otimes d_6)'] \end{aligned}$$

(4.113)

$$\begin{aligned} M(\eta_3) = \tfrac{1}{2916}[&(f_1 \otimes f_1 \otimes f_1)(f_1 \otimes f_1 \otimes f_1)' + (f_2 \otimes f_2 \otimes f_2)(f_2 \otimes f_2 \otimes f_2)' \\ &+ (f_3 \otimes f_3 \otimes f_3)(f_3 \otimes f_3 \otimes f_3)' + (f_4 \otimes f_4 \otimes f_4)(f_4 \otimes f_4 \otimes f_4)'] \end{aligned}$$

(4.114)

$$M(\eta_4) = \tfrac{1}{4096} J_{64}$$

(4.115)

also,

$$d_1 = (1_4 - e_4 - e_3),\ d_2 = (1_4 - e_2 - e_4),\ d_3 = (1_4 - e_1 - e_4),\ d_4 = (1_4 - e_1 - e_3),$$
$$d_4 = (1_4 - e_1 - e_3),\ d_5 = (1_4 - e_1 - e_2),\ d_6 = (1_4 - e_2 - e_3)$$

$$f_1 = (1_4 - e_4),\ f_2 = (1_4 - e_2),\ f_3 = (1_4 - e_3),\ f_4 = (1_4 - e_1),$$

$$e_1 = \begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad e_2 = \begin{pmatrix}0\\1\\0\\0\end{pmatrix},\quad e_3 = \begin{pmatrix}0\\0\\1\\0\end{pmatrix} \text{ and } \quad e_4 = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

The coefficient matrix K for the four ingredients parameter subsystems of interest in (3.6) and (3.7) is given as

$$K^{'}\theta = \begin{pmatrix} \theta_{111} \\ \theta_{222} \\ \theta_{333} \\ \theta_{444} \\ \dfrac{\theta_{112}+\theta_{121}+\theta_{211}+\theta_{113}+\theta_{131}+\theta_{311}+\theta_{114}+\theta_{141}+\theta_{411}}{9} \\ \dfrac{\theta_{122}+\theta_{212}+\theta_{221}+\theta_{223}+\theta_{232}+\theta_{322}+\theta_{224}+\theta_{242}+\theta_{422}}{9} \\ \dfrac{\theta_{233}+\theta_{323}+\theta_{332}+\theta_{133}+\theta_{313}+\theta_{331}+\theta_{334}+\theta_{343}+\theta_{433}}{9} \\ \dfrac{\theta_{144}+\theta_{244}+\theta_{344}+\theta_{414}+\theta_{424}+\theta_{434}+\theta_{442}+\theta_{443}+\theta_{441}}{9} \\ \dfrac{1}{24}\begin{Bmatrix} \theta_{123}+\theta_{132}+\theta_{213}+\theta_{231}+\theta_{312}+\theta_{321}+\theta_{124}+\theta_{134}+\theta_{142}+\theta_{143}+\theta_{214}+\theta_{234} \\ +\theta_{241}+\theta_{243}+\theta_{314}+\theta_{324}+\theta_{341}+\theta_{342}+\theta_{412}+\theta_{413}+\theta_{421}+\theta_{423}+\theta_{431}+\theta_{432} \end{Bmatrix} \end{pmatrix}$$

(4.116)

therefore K is given as

$$K = (\mathrm{K}_1, K_2, K_3) \tag{4.117}$$

where

$$K_1 = \sum_{i=1}^{4} e_{iii}e_i' = e_{111}e_1' + e_{222}e_2' + e_{333}e_3' + +e_{444}e_4'$$

$$K_2 = \tfrac{1}{9}\left\{\sum_{\substack{ij=1\\ i\neq j}}^{3}(e_{iij}+e_{iji}+e_{jii})e_i'\right\}$$

$$=\tfrac{1}{9}\left\{(e_{112}+e_{121}+e_{211})e_1'+(e_{122}+e_{212}+e_{221})e_2'+(e_{133}+e_{313}+e_{331})e_3'+(e_{144}+e_{414}+e_{441})e_4'\right\}$$

and

$$K_3 = \tfrac{1}{24}\left\{\sum_{\substack{ijk=1\\ i\neq j\neq k}}^{4} e_{ijk}\right\}$$

$$=\tfrac{1}{24}(e_{123}+e_{132}+e_{231}+e_{213}+e_{312}+e_{321}+e_{124}+e_{134}+e_{142}+e_{143}+e_{214}+e_{234}$$
$$+e_{241}+e_{243}+e_{314}+e_{324}+e_{341}+e_{342}+e_{412}+e_{413}+e_{421}+e_{423}+e_{431}+e_{432}).$$

The left inverse L in equation (3.9) for three ingredients is given as,

$$L' = (\mathrm{K}_1, 6K_2, 24K_3). \tag{4.118}$$

4.4.5 Slope for Weighted Simplex Centroid Designs (WSCD)

The H_4 matrix was obtained by differentiating the parameter subsystem model (3.7) with respect to t_1, t_2, t_3 and t_4 as given in equation (3.10). Hence,

$$H_4 = \frac{\partial y_i}{\partial t_i}\left\{\begin{array}{l} t_1t_1t_1 + t_2t_2t_2 + t_3t_3t_3 + t_4t_4t_4 + \\ \frac{t_1t_1t_2 + t_1t_2t_1 + t_2t_1t_1 + t_1t_1t_3 + t_1t_3t_1 + t_3t_1t_1 + t_1t_1t_4 + t_1t_4t_1 + t_4t_1t_1}{9} + \\ \frac{t_1t_2t_2 + t_2t_1t_2 + t_2t_2t_1 + t_2t_2t_3 + t_2t_3t_2 + t_3t_2t_2 + t_2t_2t_4 + t_2t_4t_2 + t_4t_2t_2}{9} + \\ \frac{t_2t_3t_3 + t_3t_2t_3 + t_3t_3t_2 + t_1t_3t_3 + t_3t_1t_3 + t_3t_3t_1 + t_3t_3t_4 + t_3t_4t_3 + t_4t_3t_3}{9} \\ + \frac{t_1t_4t_4 + t_2t_4t_4 + t_3t_4t_4 + t_4t_1t_4 + t_4t_2t_4 + t_4t_3t_4 + t_4t_4t_2 + t_4t_4t_3 + t_4t_4t_1}{9} \\ + \frac{1}{24}\left\{\begin{array}{l} t_1t_2t_3 + t_1t_3t_2 + t_2t_1t_3 + t_2t_3t_1 + t_3t_1t_2 + t_3t_2t_1 + t_1t_2t_4 + t_1t_3t_4 \\ + t_1t_4t_2 + t_1t_4t_3 + t_2t_1t_4 + t_2t_3t_4 + t_2t_4t_1 + t_2t_4t_3 + t_3t_1t_4 + t_3t_2t_4 \\ + t_3t_4t_1 + t_3t_4t_2 + t_4t_1t_2 + t_4t_1t_3 + t_4t_2t_1 + t_4t_2t_3 + t_4t_3t_1 + t_4t_3t_2 \end{array}\right\} \end{array}\right\}; i=1,2,3,4. \quad (4.119)$$

By differentiating with respect to each parameter in the model, the derivative matrix was obtained as,

$$H_4 = \begin{pmatrix} 3t_1^2 & 0 & 0 & 0 & \frac{2}{3}(t_1t_2 + t_1t_3 + t_1t_4) & \frac{1}{3}(t_2^2) & \frac{1}{3}(t_3^2) & \frac{1}{3}(t_4^2) & \frac{1}{4}(t_2t_3 + t_2t_4 + t_3t_4) \\ 0 & 3t_2^2 & 0 & 0 & \frac{1}{3}(t_1^2) & \frac{2}{3}(t_1t_2 + t_2t_3 + t_2t_4) & \frac{1}{3}(t_3^2) & \frac{1}{3}(t_4^2) & \frac{1}{4}(t_1t_3 + t_1t_4 + t_3t_4) \\ 0 & 0 & 3t_3^2 & 0 & \frac{1}{3}(t_1^2) & \frac{1}{3}(t_2^2) & \frac{2}{3}(t_1t_3 + t_2t_3 + t_3t_4) & \frac{1}{3}(t_4^2) & \frac{1}{4}(t_1t_2 + t_1t_4 + t_2t_4) \\ 0 & 0 & 0 & 3t_4^2 & \frac{1}{3}(t_1^2) & \frac{1}{3}(t_2^2) & \frac{1}{3}(t_3^2) & \frac{2}{3}(t_1t_4 + t_2t_4 + t_3t_4) & \frac{1}{4}(t_1t_2 + t_1t_3 + t_2t_3) \end{pmatrix}.$$

(4.120)

Using the moment matrix (4.111) and (4.118), we obtained the information matrix for weighted simplex centroid designs as

$$C_2 = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c'_{12} & c_{22} & c_{23} \\ c'_{13} & c'_{23} & c_{33} \end{pmatrix} \quad (4.121)$$

where,

$$c_{11} = x_{11} I_4 + y_{11} J_4 \ ; \quad x_{11} = 688.4 \times 10^{-4} \ , \quad y_{11} = 12.40842 \times 10^{-4}$$
$$c_{12} = x_{12} I_4 + y_{11} J_4 \ ; \ x_{12} = 67.98697 \times 10^{-4}, \quad y_{12} = 43.68878 \times 10^{-4}$$
$$c_{22} = x_{22} I_4 + y_{22} J_4 \ ; \ x_{22} = 220.42181 \times 10^{-4}, \quad y_{22} = 172.77722 \times 10^{-4}$$

$$c_{13} = x_{13} 1_4 \ ; \ x_{13} = 20.36716 \times 10^{-4}$$
$$c_{23} = x_{23} I_4 \ ; \ x_{23} = 133.92168 \times 10^{-4}$$
$$c_{33} = x_{22} \ ; \ x_{22} = 225.43724 \times 10^{-4}.$$

From the formula (3.11), the derivative matrix (4.120) together with information matrix

(4.121) were used to obtain slope information matrix D_{cu}

$$D_{cu} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{pmatrix}. \qquad (4.122)$$

where,

$$C_{11} = 0.6309 t_1^4 + 0.0044\left(t_2^4 + t_3^4 + t_4^4\right) + 0.0077\left(t_1 t_2^3 + t_1 t_3^3 + t_1 t_4^3\right) + 0.0263\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_1^2 t_4^2\right)$$
$$+ 0.0448\left(t_1^3 t_2 + t_1^3 t_3 + t_1^3 t_4\right) + 0.0022\left(t_2 t_3^3 + t_2^3 t_3 + t_2 t_4^3 + t_2^3 t_4 + t_3^3 t_4 + t_3 t_4^3\right)$$
$$+ 0.0053\left(t_2^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right) + 0.0122\left(t_1 t_2 t_3^2 + t_1 t_2^2 t_3 + t_1 t_2 t_4^2 + t_1 t_3 t_4^2 + t_1 t_2^2 t_4 + t_1 t_3^2 t_4\right)$$
$$+ 0.0379\left(t_1^2 t_2 t_3 + t_1^2 t_2 t_4 + t_1^2 t_3 t_4\right) + 0.0050\left(t_2 t_3 t_4^2 + t_2 t_3^2 t_4 + t_2^2 t_3 t_4\right) + 0.0134\left(t_1 t_2 t_3 t_4\right)$$

$$C_{12} = 0.0112\left(t_1^4 + t_2^4\right) + 0.0044\left(t_3^4 + t_4^4\right) + 0.0175\left(t_1 t_2^3 + t_1^3 t_2\right) + 0.0204\left(t_1^2 t_2^2\right)$$
$$+0.0050\left(t_1 t_3^3 + t_2 t_3^3 + t_1 t_4^3 + t_2 t_4^3\right) + 0.0086\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right)$$
$$+0.0168\left(t_1 t_2 t_3^2 + t_1 t_2 t_4^2\right) + 0.0102\left(t_1^3 t_3 + t_2^3 t_3 + t_1^3 t_4 + t_2^3 t_4\right)$$
$$+0.0198\left(t_1 t_2^2 t_3 + t_1^2 t_2 t_3 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right) + 0.0022\left(t_3 t_4^3 + t_3^3 t_4\right)$$
$$+0.0053\left(t_3^2 t_4^2\right) + 0.0086\left(t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_1 t_3^2 t_4 + t_2 t_3^2 t_4\right)$$
$$+0.0071\left(t_1^2 t_3 t_4 + t_2^2 t_3 t_4\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{13} = 0.0112\left(t_1^4 + t_3^4\right) + 0.0044\left(t_2^4 + t_4^4\right) + 0.0050\left(t_1 t_2^3 + t_3 t_2^3 + t_1 t_4^3 + t_3 t_4^3\right)$$
$$+0.0086\left(t_1^2 t_2^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_3^2 t_4^2\right) + 0.0102\left(t_1^3 t_2 + t_3^3 t_2 + t_1^3 t_4 + t_3^3 t_4\right) + 0.0204\left(t_1^2 t_3^2\right)$$
$$+0.0175\left(t_1 t_3^3 + t_1^3 t_3\right) + 0.0198\left(t_1 t_2 t_3^2 + t_1^2 t_2 t_3 + t_1 t_3^2 t_4 + t_1^2 t_3 t_4\right) + 0.0168\left(t_1 t_2^2 t_3 + t_1 t_3 t_4^2\right)$$
$$+0.0022\left(t_2 t_4^3 + t_2^3 t_4\right) + 0.0053\left(t_2^2 t_4^2\right) + 0.0086\left(t_2 t_3 t_4^2 + t_1 t_2^2 t_4 + t_2^2 t_3 t_4 + t_1 t_2 t_4^2\right)$$
$$+0.0071\left(t_1^2 t_2 t_4 + t_2 t_3^2 t_4\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{14} = 0.0112\left(t_1^4 + t_4^4\right) + 0.0044\left(t_2^4 + t_3^4\right) + 0.0050\left(t_1 t_2^3 + t_2^3 t_4 + t_3^3 t_4 + t_1 t_3^3\right) + 0.0086\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right)$$
$$+0.0102\left(t_1^3 t_2 + t_1^3 t_3 + t_2 t_4^3 + t_3 t_4^3\right) + 0.0204\left(t_1^2 t_4^2\right) + 0.0175\left(t_1 t_4^3 + t_1^3 t_4\right) + 0.0198\left(t_1 t_2 t_4^2 + t_4^2 t_1 t_3 + t_2 t_1^2 t_4 + t_1^2 t_3 t_4\right)$$
$$+0.0168\left(t_1 t_2^2 t_4 + t_1 t_4 t_3^2\right) + 0.0022\left(t_2 t_3^3 + t_2^3 t_3\right) + 0.0053\left(t_2^2 t_3^2\right) + 0.0086\left(t_1 t_2 t_3^2 + t_1 t_2^2 t_3 + t_3^2 t_2 t_4 + t_3 t_4 t_2^2\right)$$
$$+0.0071\left(t_1^2 t_2 t_3 + t_2 t_4^2 t_3\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{21} = 0.0112\left(t_1^4 + t_2^4\right) + 0.0044\left(t_3^4 + t_4^4\right) + 0.0175\left(t_1 t_2^3 + t_1^3 t_2\right) + 0.0204\left(t_1^2 t_2^2\right) + 0.0050\left(t_1 t_3^3 + t_2 t_3^3 + t_1 t_4^3 + t_2 t_4^3\right)$$
$$+0.0086\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right) + 0.0168\left(t_1 t_2 t_3^2 + t_1 t_2 t_4^2\right) + 0.0102\left(t_1^3 t_3 + t_2^3 t_3 + t_1^3 t_4 + t_2^3 t_4\right)$$
$$+0.0198\left(t_1 t_2^2 t_3 + t_1^2 t_2 t_3 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right) + 0.0022\left(t_3 t_4^3 + t_3^3 t_4\right) + 0.0053\left(t_3^2 t_4^2\right)$$
$$+0.0086\left(t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_1 t_3^2 t_4 + t_2 t_3^2 t_4\right) + 0.0071\left(t_1^2 t_3 t_4 + t_2^2 t_3 t_4\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{22} = 0.6309 t_2^4 + 0.0044\left(t_1^4 + t_3^4 + t_4^4\right) + 0.0077\left(t_2 t_3^3 + t_2 t_1^3 + t_2 t_4^3\right) + 0.0263\left(t_1^2 t_2^2 + t_2^2 t_3^2 + t_2^2 t_4^2\right)$$
$$+0.0448\left(t_2^3 t_1 + t_2^3 t_3 + t_2^3 t_4\right) + 0.0022\left(t_1 t_3^3 + t_1^3 t_3 + t_1 t_4^3 + t_1^3 t_4 + t_3^3 t_4 + t_3 t_4^3\right) + 0.0053\left(t_1^2 t_3^2 + t_1^2 t_4^2 + t_3^2 t_4^2\right)$$
$$+0.0123\left(t_1 t_2 t_3^2 + t_2 t_1^2 t_3 + t_1 t_2 t_4^2 + t_2 t_3 t_4^2 + t_2 t_1^2 t_4 + t_2 t_3^2 t_4\right) + 0.0379\left(t_2^2 t_1 t_3 + t_2^2 t_1 t_4 + t_2^2 t_3 t_4\right)$$
$$+0.0050\left(t_1 t_3 t_4^2 + t_1 t_3^2 t_4 + t_1^2 t_3 t_4\right) + 0.0134\left(t_1 t_2 t_3 t_4\right)$$

$$C_{23} = 0.0044\left(t_1^4 + t_4^4\right) + 0.0112\left(t_2^4 + t_3^4\right) + 0.0102\left(t_1 t_2^3 + t_2^3 t_4 + t_3^3 t_4 + t_1 t_3^3\right)$$
$$+0.0086\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right) + 0.0050\left(t_1^3 t_2 + t_1^3 t_3 + t_2 t_4^3 + t_3 t_4^3\right) + 0.0204\left(t_2^2 t_3^2\right) +$$
$$0.0175\left(t_2 t_3^3 + t_2^3 t_3\right) + 0.0198\left(t_1 t_2 t_3^2 + t_2^2 t_1 t_3 + t_2 t_3^2 t_4 + t_2^2 t_3 t_4\right) + 0.0168\left(t_2 t_1^2 t_3 + t_2 t_3 t_4^2\right)$$
$$+0.0022\left(t_1 t_4^3 + t_3^3 t_4\right) + 0.0053\left(t_1^2 t_4^2\right) + 0.0086\left(t_1 t_2 t_4^2 + t_1 t_4^2 t_3 + t_1^2 t_2 t_4 + t_3 t_4 t_1^2\right)$$
$$+0.0071\left(t_2^2 t_1 t_4 + t_1 t_3^2 t_4\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{24} = 0.0044\left(t_1^4 + t_3^4\right) + 0.0112\left(t_2^4 + t_4^4\right) + 0.0050\left(t_2 t_1^3 + t_2 t_3^3 + t_4 t_1^3 + t_4 t_3^3\right) + 0.0086\left(t_1^2 t_2^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_3^2 t_4^2\right)$$
$$+0.0102\left(t_2^3 t_1 + t_2^3 t_2 + t_1^3 t_4 + t_3^3 t_4\right) + 0.0204\left(t_2^2 t_4^2\right) + 0.0175\left(t_2 t_4^3 + t_2^3 t_4\right) + 0.0198\left(t_1 t_2 t_4^2 + t_4^2 t_2 t_3 + t_1 t_2^2 t_4 + t_2^2 t_3 t_4\right)$$
$$+0.0168\left(t_2 t_1^2 t_4 + t_2 t_4 t_3^2\right) + 0.0022\left(t_1 t_3^3 + t_1^3 t_3\right) + 0.0053\left(t_1^2 t_3^2\right) + 0.0086\left(t_4 t_3 t_1^2 + t_1 t_3^2 t_4 + t_1^2 t_3 t_2 + t_1 t_2 t_3^2\right)$$
$$0.0071\left(t_2^2 t_1 t_3 + t_1 t_4^2 t_3\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{31} = 0.0112\left(t_1^4 + t_3^4\right) + 0.0044\left(t_2^4 + t_4^4\right) + 0.0050\left(t_1 t_2^3 + t_3 t_2^3 + t_1 t_4^3 + t_3 t_4^3\right) + 0.0086\left(t_1^2 t_2^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_3^2 t_4^2\right)$$
$$+0.0102\left(t_1^3 t_2 + t_3^3 t_2 + t_1^3 t_4 + t_3^3 t_4\right) + 0.0204\left(t_1^2 t_3^2\right) + 0.0175\left(t_1 t_3^3 + t_1^3 t_3\right) + 0.0198\left(t_1 t_2 t_3^2 + t_1^2 t_2 t_3 + t_1 t_3^2 t_4 + t_1^2 t_3 t_4\right)$$
$$+0.0168\left(t_1 t_2^2 t_3 + t_1 t_3 t_4^2\right) + 0.0022\left(t_2 t_4^3 + t_2^3 t_4\right) + 0.0053\left(t_2^2 t_4^2\right) + 0.0086\left(t_2 t_3 t_4^2 + t_1 t_2^2 t_4 + t_2^2 t_3 t_4 + t_1 t_2 t_4^2\right)$$
$$0.0071\left(t_1^2 t_2 t_4 + t_2 t_3^2 t_4\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{32} = 0.0044\left(t_1^4 + t_4^4\right) + 0.0112\left(t_2^4 + t_3^4\right) + 0.0102\left(t_1 t_2^3 + t_2^3 t_4 + t_3^3 t_4 + t_1 t_3^3\right) + 0.0086\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right)$$
$$+0.0050\left(t_1^3 t_2 + t_1^3 t_3 + t_2 t_4^3 + t_3 t_4^3\right) + 0.0204\left(t_2^2 t_3^2\right) + 0.0175\left(t_2 t_3^3 + t_2^3 t_3\right) + 0.0198\left(t_1 t_2 t_3^2 + t_2^2 t_1 t_3 + t_2 t_3^2 t_4 + t_2^2 t_3 t_4\right)$$
$$+0.0168\left(t_2 t_1^2 t_3 + t_2 t_3 t_4^2\right) + 0.0022\left(t_1 t_4^3 + t_3^3 t_4\right) + 0.0053\left(t_1^2 t_4^2\right) + 0.0086\left(t_1 t_2 t_4^2 + t_1 t_4^2 t_3 + t_1^2 t_2 t_4 + t_3 t_4 t_1^2\right)$$
$$0.0071\left(t_2^2 t_1 t_4 + t_1 t_3^2 t_4\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{33} = 0.6309 t_3^4 + 0.0044\left(t_1^4 + t_2^4 + t_4^4\right) + 0.0077\left(t_3 t_2^3 + t_3 t_1^3 + t_3 t_4^3\right) + 0.0263\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_3^2 t_4^2\right) +$$
$$0.0448\left(t_3^3 t_2 + t_3^3 t_1 + t_3^3 t_4\right) + 0.0022\left(t_1 t_2^3 + t_1^3 t_2 + t_1 t_4^3 + t_4^3 t_2 + t_1^3 t_4 + t_4 t_2^3\right) + 0.0053\left(t_1^2 t_2^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right)$$
$$+0.0122\left(t_1 t_3 t_2^2 + t_2 t_1^2 t_3 + t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_3 t_1^2 t_4 + t_3 t_2^2 t_4\right) + 0.0379\left(t_3^2 t_2 t_1 + t_2^2 t_1 t_4 + t_3^2 t_2 t_4\right)$$
$$+0.0050\left(t_1 t_2 t_4^2 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right) + 0.0134\left(t_1 t_2 t_3 t_4\right)$$

$$C_{34} = 0.0044\left(t_1^4 + t_2^4\right) + 0.0112\left(t_3^4 + t_4^4\right) + 0.0022\left(t_1 t_2^3 + t_1^3 t_2\right) + 0.0053\left(t_1^2 t_2^2\right)$$
$$+0.0102\left(t_1 t_3^3 + t_2 t_3^3 + t_1 t_4^3 + t_2 t_4^3\right) + 0.0086\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right) + 0.0071\left(t_1 t_2 t_3^2 + t_1 t_2 t_4^2\right)$$
$$+0.0050\left(t_1^3 t_3 + t_2^3 t_3 + t_1^3 t_4 + t_2^3 t_4\right) + 0.0086\left(t_1 t_2^2 t_3 + t_1^2 t_2 t_3 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right) + 0.0175\left(t_3 t_4^3 + t_3^3 t_4\right)$$
$$+0.0204\left(t_3^2 t_4^2\right) + 0.0198\left(t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_1 t_3^2 t_4 + t_2 t_3^2 t_4\right) + 0.0168\left(t_1^2 t_3 t_4 + t_2^2 t_3 t_4\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{41} = 0.0112\left(t_1^4 + t_4^4\right) + 0.0044\left(t_2^4 + t_3^4\right) + 0.0050\left(t_1 t_2^3 + t_2^3 t_4 + t_3^3 t_4 + t_1 t_3^3\right) +$$
$$0.0086\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right) + 0.0102\left(t_1^3 t_2 + t_1^3 t_3 + t_2 t_4^3 + t_3 t_4^3\right) + 0.0204\left(t_1^2 t_4^2\right)$$
$$+0.0175\left(t_1 t_4^3 + t_1^3 t_4\right) + 0.0198\left(t_1 t_2 t_4^2 + t_4^2 t_1 t_3 + t_2 t_1^2 t_4 + t_1^2 t_3 t_4\right) + 0.0168\left(t_1 t_2^2 t_4 + t_1 t_4 t_3^2\right)$$
$$+0.0022\left(t_2 t_3^3 + t_2^3 t_3\right) + 0.0053\left(t_2^2 t_3^2\right) + 0.0086\left(t_1 t_2 t_3^2 + t_1 t_2^2 t_3 + t_3^2 t_2 t_4 + t_3 t_4 t_2^2\right)$$
$$+0.0071\left(t_1^2 t_2 t_3 + t_2 t_4^2 t_3\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{42} = 0.0044\left(t_1^4 + t_3^4\right) + 0.0112\left(t_2^4 + t_4^4\right) + 0.0050\left(t_2 t_1^3 + t_2 t_3^3 + t_4 t_1^3 + t_4 t_3^3\right) + 0.0086\left(t_1^2 t_2^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_3^2 t_4^2\right)$$
$$+0.0102\left(t_2^3 t_1 + t_2^3 t_2 + t_1^3 t_4 + t_3^3 t_4\right) + 0.0204\left(t_2^2 t_4^2\right) + 0.0175\left(t_2 t_4^3 + t_2^3 t_4\right) + 0.0198\left(t_1 t_2 t_4^2 + t_4^2 t_2 t_3 + t_1 t_2^2 t_4 + t_2^2 t_3 t_4\right)$$
$$+0.0168\left(t_2 t_1^2 t_4 + t_2 t_4 t_3^2\right) + 0.0022\left(t_1 t_3^3 + t_1^3 t_3\right) + 0.0053\left(t_1^2 t_3^2\right) + 0.0086\left(t_4 t_3 t_1^2 + t_1 t_3^2 t_4 + t_1^2 t_3 t_2 + t_1 t_2 t_3^2\right)$$
$$+0.0071\left(t_2^2 t_1 t_3 + t_1 t_4^2 t_3\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{43} = 0.0044\left(t_1^4 + t_2^4\right) + 0.0112\left(t_3^4 + t_4^4\right) + 0.0022\left(t_1 t_2^3 + t_1^3 t_2\right) + 0.0053\left(t_1^2 t_2^2\right) + 0.0102\left(t_1 t_3^3 + t_2 t_3^3 + t_1 t_4^3 + t_2 t_4^3\right)$$
$$+0.0086\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right) + 0.0071\left(t_1 t_2 t_3^2 + t_1 t_2 t_4^2\right) + 0.0050\left(t_1^3 t_3 + t_2^3 t_3 + t_1^3 t_4 + t_2^3 t_4\right)$$
$$+0.0086\left(t_1 t_2^2 t_3 + t_1^2 t_2 t_3 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right) + 0.0175\left(t_3 t_4^3 + t_3^3 t_4\right) + 0.0204\left(t_3^2 t_4^2\right)$$
$$+0.0198\left(t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_1 t_3^2 t_4 + t_2 t_3^2 t_4\right) + 0.0168\left(t_1^2 t_3 t_4 + t_2^2 t_3 t_4\right) + 0.0227\left(t_1 t_2 t_3 t_4\right)$$

$$C_{44} = 0.6309 t_4^4 + 0.0044\left(t_1^4 + t_2^4 + t_3^4\right) + 0.0077\left(t_4 t_2^3 + t_4 t_3^3 + t_4 t_1^3\right) + 0.0263\left(t_1^2 t_4^2 + t_4^2 t_3^2 + t_2^2 t_4^2\right) +$$
$$0.0448\left(t_4^3 t_1 + t_4^3 t_2 + t_4^3 t_3\right) + 0.0022\left(t_1 t_2^3 + t_1^3 t_2 + t_1 t_3^3 + t_1^3 t_3 + t_2^3 t_3 + t_2 t_3^3\right) + 0.0053\left(t_2^2 t_1^2 + t_2^2 t_3^2 + t_3^2 t_1^2\right)$$
$$+0.0122\left(t_1 t_4 t_2^2 + t_2 t_1^2 t_4 + t_1 t_4 t_3^2 + t_2 t_4 t_3^2 + t_3 t_1^2 t_4 + t_3 t_2^2 t_4\right) + 0.0379\left(t_4^2 t_2 t_1 + t_4^2 t_2 t_3 + t_4^2 t_3 t_1\right)$$
$$+0.0050\left(t_1 t_2 t_3^2 + t_1 t_2^2 t_3 + t_1^2 t_3 t_2\right) + 0.0134\left(t_1 t_2 t_3 t_4\right).$$

4.4.6 Slope Information Matrices (SIM)

Using the slope information matrix (4.122), we obtained other slope information matrices for different points; pure, binary, ternary and quaternary mixture experiments for weighted simplex centroid designs.

At (1, 0, 0, 0), the slope information matrix is given as

$$SIM_{41} = \begin{pmatrix} a & b1_3 \\ b1_3 & cJ_3 \end{pmatrix} \tag{4.123}$$

where $a = 6307.40393 \times 10^{-4}$, $b = 111.67574 \times 10^{-4}$, $c = 43.6887 \times 10^{-4}$.

At the binary blend point (1/2, 1/2, 0, 0) the slope information matrix is of the form

$$SIM_{42} = \begin{pmatrix} aI_2 + bJ_2 & cJ_2 \\ cJ_2 & dJ_2 \end{pmatrix} \tag{4.124}$$

where

$a = 399.23626 \times 10^{-4}$, b $= 48.7828 \times 10^{-4}$, c $= 25.5644 \times 10^{-4}$, $d = 13.14636 \times 10^{-4}$.

At the point (1/3, 1/3, 1/3, 0) the slope information matrix is

$$SIM_{43} = \begin{pmatrix} aI_3 + bJ_3 & c1_3 \\ c1'_3 & d \end{pmatrix} \tag{4.125}$$

where

$a = 84.2478 \times 10^{-4}$, b $= 22.98775 \times 10^{-4}$, c $= 12.51869 \times 10^{-4}$, $d = 7.0857 \times 10^{-4}$.

At the point (¼, ¼, ¼, ¼), the slope information matrix is given as

$$SIM_{44} = \begin{pmatrix} 549/125029 & 61156/30546869 & 4185/2854654 & 4185/2854654 \\ 61156/30546869 & 3764/639087 & 5241/2207668 & 61156/30546869 \\ 4185/2854654 & 5241/2207668 & 549/125029 & 4185/2854654 \\ 4185/2854654 & 61156/30546869 & 4185/2854654 & 549/125029 \end{pmatrix}. \tag{4.126}$$

4.4.7 Uniform Weighted Simplex Centroids Mixture Experiments

The moment matrix for uniformly weighted simplex centroid designs for four ingredients is given by $M(\eta) = \alpha_1 M(\eta_1) + \alpha_2 M(\eta_2) + \alpha_3 M(\eta_3) + \alpha_4 M(\eta_4)$, where all weights are equal in elementary centroid designs, $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1/4$ as given in (3.4). Hence

$$M(\eta) = \tfrac{1}{4} M(\eta_1) + \tfrac{1}{4} M(\eta_2) + \tfrac{1}{4} M(\eta_3) + \tfrac{1}{4} M(\eta_4) \tag{4.127}$$

where $M(\eta_1)$, $M(\eta_2)$, $M(\eta_3)$ and $M(\eta_4)$ are given in (4.112), (4.113), (4.114) and (4.115) respectively.

Using (4.118) and (4.127), we obtained the information matrix for uniform weighted simplex centroid designs as,

$$C_{2u} = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c'_{13} & c'_{23} & c_{33} \end{pmatrix} \tag{4.128}$$

where $c_{11}, c_{12}, c_{13}, c_{22}, c_{23}$ and c_{33} are given as

$$c_{11} = x_{11} I_4 + y_{11} J_4; \;\; x_{11} = 638.8782 \times 10^{-4}, \;\; y_{11} = 8.8354 \times 10^{-4}$$
$$c_{12} = c'_{21} = x_{12} I_4 + y_{11} J_4 \; ; \; x_{12} = 44.2062 \times 10^{-4}, \; y_{12} = 35.3124 \times 10^{-4}$$
$$c_{22} = x_{22} I_4 + y_{22} J_4 \; ; x_{22} = 148.05 \times 10^{-4}, \; y_{22} = 169.7616 \times 10^{-4}$$

$$c_{13} = c'_{31} = x_{13} 1_4 \; ; \; x_{13} = 30.0810 \times 10^{-4}$$
$$c_{23} = c'_{32} = x_{23} 1_4 \; ; \; x_{23} = 224.4348 \times 10^{-4}$$
$$c_{33} = x_{22} \; ; \; x_{22} = 475.0416 \times 10^{-4}.$$

The derivative matrix (4.120) together with information matrix (4.128) were used in (3.11) to obtain slope information matrix D_{cu} as,

$$D_{cu} = \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} \\ d_{21} & d_{22} & d_{23} & d_{24} \\ d_{31} & d_{32} & d_{33} & d_{34} \\ d_{41} & d_{42} & d_{43} & d_{44} \end{pmatrix} \tag{4.129}$$

where,

$$d_{11} = 0.5832 t_1^4 + 0.0035\left(t_2^4 + t_3^4 + t_4^4\right) + 0.0076\left(t_1 t_2^3 + t_1 t_3^3 + t_1 t_4^3\right) + 0.0211\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_1^2 t_4^2\right) +$$
$$0.0320\left(t_1^3 t_2 + t_1^3 t_3 + t_1^3 t_4\right) + 0.0037\left(t_2 t_3^3 + t_2^3 t_3 + t_2 t_4^3 + t_2^3 t_4 + t_3^3 t_4 + t_3 t_4^3\right) + 0.0067\left(t_2^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right)$$
$$+0.0150\left(t_1 t_2 t_3^2 + t_1 t_2^2 t_3 + t_1 t_2 t_4^2 + t_1 t_3 t_4^2 + t_1 t_2^2 t_4 + t_1 t_3^2 t_4\right) + 0.0328\left(t_1^2 t_2 t_3 + t_1^2 t_2 t_4 + t_1^2 t_3 t_4\right)$$
$$+0.0097\left(t_2 t_3 t_4^2 + t_2 t_3^2 t_4 + t_2^2 t_3 t_4\right) + 0.0224\left(t_1 t_2 t_3 t_4\right)$$

$$d_{12} = 0.0080\left(t_1^4 + t_2^4\right) + 0.0035\left(t_3^4 + t_4^4\right) + 0.0141\left(t_1 t_2^3 + t_1^3 t_2\right) + 0.0175\left(t_1^2 t_2^2\right)$$
$$+0.0056\left(t_1 t_3^3 + t_2 t_3^3 + t_1 t_4^3 + t_2 t_4^3\right) + 0.0091\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right)$$
$$+0.0181\left(t_1 t_2 t_3^2 + t_1 t_2 t_4^2\right) + 0.0093\left(t_1^3 t_3 + t_2^3 t_3 + t_1^3 t_4 + t_2^3 t_4\right)$$
$$+0.0202\left(t_1 t_2^2 t_3 + t_1^2 t_2 t_3 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right) + 0.0037\left(t_3 t_4^3 + t_3^3 t_4\right)$$
$$+0.0067\left(t_3^2 t_4^2\right) + 0.0123\left(t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_1 t_3^2 t_4 + t_2 t_3^2 t_4\right)$$
$$+0.0116\left(t_1^2 t_3 t_4 + t_2^2 t_3 t_4\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{13} = 0.0080\left(t_1^4 + t_3^4\right) + 0.0035\left(t_2^4 + t_4^4\right) + 0.0056\left(t_1 t_2^3 + t_3 t_2^3 + t_1 t_4^3 + t_3 t_4^3\right)$$
$$+0.0091\left(t_1^2 t_2^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_3^2 t_4^2\right) + 0.0093\left(t_1^3 t_2 + t_3^3 t_2 + t_1^3 t_4 + t_3^3 t_4\right) + 0.0175\left(t_1^2 t_3^2\right)$$
$$+0.0141\left(t_1 t_3^3 + t_1^3 t_3\right) + 0.0202\left(t_1 t_2 t_3^2 + t_1^2 t_2 t_3 + t_1 t_3^2 t_4 + t_1^2 t_3 t_4\right) + 0.0181\left(t_1 t_2^2 t_3 + t_1 t_3 t_4^2\right)$$
$$+0.0037\left(t_2 t_4^3 + t_2^3 t_4\right) + 0.0067\left(t_2^2 t_4^2\right) + 0.0123\left(t_2 t_3 t_4^2 + t_1 t_2^2 t_4 + t_2^2 t_3 t_4 + t_1 t_2 t_4^2\right)$$
$$+0.0116\left(t_1^2 t_2 t_4 + t_2 t_3^2 t_4\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{14} = 0.0080\left(t_1^4 + t_4^4\right) + 0.0035\left(t_2^4 + t_3^4\right) + 0.0056\left(t_1 t_2^3 + t_2^3 t_4 + t_3^3 t_4 + t_1 t_3^3\right) + 0.0091\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right)$$
$$+0.0093\left(t_1^3 t_2 + t_1^3 t_3 + t_2 t_4^3 + t_3 t_4^3\right) + 0.0175\left(t_1^2 t_4^2\right) + 0.0141\left(t_1 t_4^3 + t_1^3 t_4\right) + 0.0202\left(t_1 t_2 t_4^2 + t_4^2 t_1 t_3 + t_2 t_1^2 t_4 + t_1^2 t_3 t_4\right)$$
$$+0.0181\left(t_1 t_2^2 t_4 + t_1 t_4 t_3^2\right) + 0.0037\left(t_2 t_3^3 + t_2^3 t_3\right) + 0.0067\left(t_2^2 t_3^2\right) + 0.0123\left(t_1 t_2 t_3^2 + t_1 t_2^2 t_3 + t_3^2 t_2 t_4 + t_3 t_4 t_2^2\right)$$
$$+0.0116\left(t_1^2 t_2 t_3 + t_2 t_4^2 t_3\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{21} = 0.0080\left(t_1^4 + t_2^4\right) + 0.0035\left(t_3^4 + t_4^4\right) + 0.0141\left(t_1 t_2^3 + t_1^3 t_2\right) + 0.0175\left(t_1^2 t_2^2\right) + 0.0056\left(t_1 t_3^3 + t_2 t_3^3 + t_1 t_4^3 + t_2 t_4^3\right)$$
$$+0.0091\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right) + 0.0181\left(t_1 t_2 t_3^2 + t_1 t_2 t_4^2\right) + 0.0093\left(t_1^3 t_3 + t_2^3 t_3 + t_1^3 t_4 + t_2^3 t_4\right)$$
$$+0.0202\left(t_1 t_2^2 t_3 + t_1^2 t_2 t_3 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right) + 0.0037\left(t_3 t_4^3 + t_3^3 t_4\right) + 0.0067\left(t_3^2 t_4^2\right)$$
$$+0.0123\left(t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_1 t_3^2 t_4 + t_2 t_3^2 t_4\right) + 0.0116\left(t_1^2 t_3 t_4 + t_2^2 t_3 t_4\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{22} = 0.5832t_2^4 + 0.0035\left(t_1^4 + t_3^4 + t_4^4\right) + 0.0076\left(t_2t_3^3 + t_2t_1^3 + t_2t_4^3\right) + 0.0211\left(t_1^2t_2^2 + t_2^2t_3^2 + t_2^2t_4^2\right)$$
$$+0.0320\left(t_2^3t_1 + t_2^3t_3 + t_2^3t_4\right)$$
$$+0.0037\left(t_1t_3^3 + t_1^3t_3 + t_1t_4^3 + t_1^3t_4 + t_3^3t_4 + t_3t_4^3\right) + 0.0067\left(t_1^2t_3^2 + t_1^2t_4^2 + t_3^2t_4^2\right)$$
$$+0.0150\left(t_1t_2t_3^2 + t_2t_1^2t_3 + t_1t_2t_4^2 + t_2t_3t_4^2 + t_2t_1^2t_4 + t_2t_3^2t_4\right) + 0.0328\left(t_2^2t_1t_3 + t_2^2t_1t_4 + t_2^2t_3t_4\right)$$
$$+0.0097\left(t_1t_3t_4^2 + t_1t_3^2t_4 + t_1^2t_3t_4\right) + 0.0224\left(t_1t_2t_3t_4\right)$$

$$d_{23} = 0.0035\left(t_1^4 + t_4^4\right) + 0.0080\left(t_2^4 + t_3^4\right) + 0.0093\left(t_1t_2^3 + t_2^3t_4 + t_3^3t_4 + t_1t_3^3\right) + 0.0091\left(t_1^2t_2^2 + t_1^2t_3^2 + t_2^2t_4^2 + t_3^2t_4^2\right)$$
$$+0.0056\left(t_1^3t_2 + t_1^3t_3 + t_2t_4^3 + t_3t_4^3\right) + 0.0175\left(t_2^2t_3^2\right) + 0.0141\left(t_2t_3^3 + t_2^3t_3\right)$$
$$+0.0202\left(t_1t_2t_3^2 + t_2^2t_1t_3 + t_2t_3^2t_4 + t_2^2t_3t_4\right) + 0.0181\left(t_2t_1^2t_3 + t_2t_3t_4^2\right)$$
$$+0.0037\left(t_1t_4^3 + t_3^3t_4\right) + 0.0067\left(t_1^2t_4^2\right) + 0.0123\left(t_1t_2t_4^2 + t_1t_4^2t_3 + t_1^2t_2t_4 + t_3t_4t_1^2\right)$$
$$+0.0116\left(t_2^2t_1t_4 + t_1t_3^2t_4\right) + 0.0285\left(t_1t_2t_3t_4\right)$$

$$d_{24} = 0.0035\left(t_1^4 + t_3^4\right) + 0.0080\left(t_2^4 + t_4^4\right) + 0.0056\left(t_2t_1^3 + t_2t_3^3 + t_4t_1^3 + t_4t_3^3\right) + 0.0091\left(t_1^2t_2^2 + t_2^2t_3^2 + t_1^2t_4^2 + t_3^2t_4^2\right)$$
$$+0.0093\left(t_2^3t_1 + t_2^3t_2 + t_1^3t_4 + t_3^3t_4\right) + 0.0175\left(t_2^2t_4^2\right) + 0.0141\left(t_2t_4^3 + t_2^3t_4\right) + 0.0202\left(t_1t_2t_4^2 + t_4^2t_2t_3 + t_1t_2^2t_4 + t_2^2t_3t_4\right)$$
$$+0.0181\left(t_2t_1^2t_4 + t_2t_4t_3^2\right) + 0.0037\left(t_1t_3^3 + t_1^3t_3\right) + 0.0067\left(t_1^2t_3^2\right) + 0.0123\left(t_4t_3t_1^2 + t_1t_3^2t_4 + t_1^2t_3t_2 + t_1t_2t_3^2\right)$$
$$+0.0116\left(t_2^2t_1t_3 + t_1t_4^2t_3\right) + 0.0285\left(t_1t_2t_3t_4\right)$$

$$d_{31} = 0.0080\left(t_1^4 + t_3^4\right) + 0.0035\left(t_2^4 + t_4^4\right) + 0.0056\left(t_1 t_2^3 + t_3 t_2^3 + t_1 t_4^3 + t_3 t_4^3\right)$$
$$+0.0091\left(t_1^2 t_2^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_3^2 t_4^2\right) + 0.0093\left(t_1^3 t_2 + t_3^3 t_2 + t_1^3 t_4 + t_3^3 t_4\right) + 0.0175\left(t_1^2 t_3^2\right)$$
$$+0.0141\left(t_1 t_3^3 + t_1^3 t_3\right) + 0.0202\left(t_1 t_2 t_3^2 + t_1^2 t_2 t_3 + t_1 t_3^2 t_4 + t_1^2 t_3 t_4\right) + 0.0181\left(t_1 t_2^2 t_3 + t_1 t_3 t_4^2\right)$$
$$+0.0037\left(t_2 t_4^3 + t_2^3 t_4\right) + 0.0067\left(t_2^2 t_4^2\right) + 0.0123\left(t_2 t_3 t_4^2 + t_1 t_2^2 t_4 + t_2^2 t_3 t_4 + t_1 t_2 t_4^2\right)$$
$$+0.0116\left(t_1^2 t_2 t_4 + t_2 t_3^2 t_4\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{32} = 0.0035\left(t_1^4 + t_4^4\right) + 0.0080\left(t_2^4 + t_3^4\right) + 0.0093\left(t_1 t_2^3 + t_2^3 t_4 + t_3^3 t_4 + t_1 t_3^3\right)$$
$$+0.0091\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right) + 0.0056\left(t_1^3 t_2 + t_1^3 t_3 + t_2 t_4^3 + t_3 t_4^3\right)$$
$$+0.0175\left(t_2^2 t_3^2\right) + 0.0141\left(t_2 t_3^3 + t_2^3 t_3\right) + 0.0202\left(t_1 t_2 t_3^2 + t_2^2 t_1 t_3 + t_2 t_3^2 t_4 + t_2^2 t_3 t_4\right)$$
$$+0.0181\left(t_2 t_1^2 t_3 + t_2 t_3 t_4^2\right) + 0.0037\left(t_1 t_4^3 + t_3^3 t_4\right) + 0.0067\left(t_1^2 t_4^2\right)$$
$$+0.0123\left(t_1 t_2 t_4^2 + t_1 t_4^2 t_3 + t_1^2 t_2 t_4 + t_3 t_4 t_1^2\right) + 0.0116\left(t_2^2 t_1 t_4 + t_1 t_3^2 t_4\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{33} = 0.5832 t_3^4 + 0.0035\left(t_1^4 + t_2^4 + t_4^4\right) + 0.0076\left(t_3 t_2^3 + t_3 t_1^3 + t_3 t_4^3\right) + 0.0211\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_3^2 t_4^2\right)$$
$$+0.0320\left(t_3^3 t_2 + t_3^3 t_1 + t_3^3 t_4\right) + 0.0037\left(t_1 t_2^3 + t_1^3 t_2 + t_1 t_4^3 + t_4^3 t_2 + t_1^3 t_4 + t_4 t_2^3\right)$$
$$+0.0067\left(t_1^2 t_2^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right) + 0.0150\left(t_1 t_3 t_2^2 + t_2 t_1^2 t_3 + t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_3 t_1^2 t_4 + t_3 t_2^2 t_4\right)$$
$$+0.0328\left(t_3^2 t_2 t_1 + t_2^2 t_1 t_4 + t_3^2 t_2 t_4\right) + 0.0097\left(t_1 t_2 t_4^2 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right) + 0.0224\left(t_1 t_2 t_3 t_4\right)$$

$$d_{34} = 0.0035\left(t_1^4 + t_2^4\right) + 0.0080\left(t_3^4 + t_4^4\right) + 0.0037\left(t_1 t_2^3 + t_1^3 t_2\right) + 0.0067\left(t_1^2 t_2^2\right)$$
$$+0.0093\left(t_1 t_3^3 + t_2 t_3^3 + t_1 t_4^3 + t_2 t_4^3\right) + 0.0091\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right) + 0.0116\left(t_1 t_2 t_3^2 + t_1 t_2 t_4^2\right)$$
$$+0.0056\left(t_1^3 t_3 + t_2^3 t_3 + t_1^3 t_4 + t_2^3 t_4\right) + 0.0123\left(t_1 t_2^2 t_3 + t_1^2 t_2 t_3 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right)$$
$$+0.0141\left(t_3 t_4^3 + t_3^3 t_4\right) + 0.0175\left(t_3^2 t_4^2\right) + 0.0202\left(t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_1 t_3^2 t_4 + t_2 t_3^2 t_4\right)$$
$$+0.0181\left(t_1^2 t_3 t_4 + t_2^2 t_3 t_4\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{41} = 0.0080\left(t_1^4 + t_4^4\right) + 0.0035\left(t_2^4 + t_3^4\right) + 0.0056\left(t_1 t_2^3 + t_2^3 t_4 + t_3^3 t_4 + t_1 t_3^3\right)$$
$$+0.0091\left(t_1^2 t_2^2 + t_1^2 t_3^2 + t_2^2 t_4^2 + t_3^2 t_4^2\right) + 0.0093\left(t_1^3 t_2 + t_1^3 t_3 + t_2 t_4^3 + t_3 t_4^3\right) + 0.0175\left(t_1^2 t_4^2\right)$$
$$+0.0141\left(t_1 t_4^3 + t_1^3 t_4\right) + 0.0202\left(t_1 t_2 t_4^2 + t_4^2 t_1 t_3 + t_2 t_1^2 t_4 + t_1^2 t_3 t_4\right) + 0.0181\left(t_1 t_2^2 t_4 + t_1 t_4 t_3^2\right)$$
$$+0.0037\left(t_2 t_3^3 + t_2^3 t_3\right) + 0.0067\left(t_2^2 t_3^2\right) + 0.0123\left(t_1 t_2 t_3^2 + t_1 t_2^2 t_3 + t_3^2 t_2 t_4 + t_3 t_4 t_2^2\right)$$
$$+0.0116\left(t_1^2 t_2 t_3 + t_2 t_4^2 t_3\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{42} = 0.0035\left(t_1^4 + t_3^4\right) + 0.0080\left(t_2^4 + t_4^4\right) + 0.0056\left(t_2 t_1^3 + t_2 t_3^3 + t_4 t_1^3 + t_4 t_3^3\right)$$

$$+0.0091\left(t_1^2 t_2^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_3^2 t_4^2\right) + 0.0093\left(t_2^3 t_1 + t_2^3 t_2 + t_1^3 t_4 + t_3^3 t_4\right) + 0.0175\left(t_2^2 t_4^2\right)$$

$$+0.0141\left(t_2 t_4^3 + t_2^3 t_4\right) + 0.0202\left(t_1 t_2 t_4^2 + t_4^2 t_2 t_3 + t_1 t_2^2 t_4 + t_2^2 t_3 t_4\right) + 0.0181\left(t_2 t_1^2 t_4 + t_2 t_4 t_3^2\right)$$

$$+0.0037\left(t_1 t_3^3 + t_1^3 t_3\right) + 0.0067\left(t_1^2 t_3^2\right) + 0.0123\left(t_4 t_3 t_1^2 + t_1 t_3^2 t_4 + t_1^2 t_3 t_2 + t_1 t_2 t_3^2\right)$$

$$+0.0116\left(t_2^2 t_1 t_3 + t_1 t_4^2 t_3\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{43} = 0.0035\left(t_1^4 + t_2^4\right) + 0.0080\left(t_3^4 + t_4^4\right) + 0.0037\left(t_1 t_2^3 + t_1^3 t_2\right) + 0.0067\left(t_1^2 t_2^2\right)$$

$$+0.0093\left(t_1 t_3^3 + t_2 t_3^3 + t_1 t_4^3 + t_2 t_4^3\right) + 0.0091\left(t_1^2 t_3^2 + t_2^2 t_3^2 + t_1^2 t_4^2 + t_2^2 t_4^2\right) + 0.0116\left(t_1 t_2 t_3^2 + t_1 t_2 t_4^2\right)$$

$$+0.0056\left(t_1^3 t_3 + t_2^3 t_3 + t_1^3 t_4 + t_2^3 t_4\right) + 0.0123\left(t_1 t_2^2 t_3 + t_1^2 t_2 t_3 + t_1 t_2^2 t_4 + t_1^2 t_2 t_4\right)$$

$$+0.0141\left(t_3 t_4^3 + t_3^3 t_4\right) + 0.0175\left(t_3^2 t_4^2\right) + 0.0202\left(t_1 t_3 t_4^2 + t_2 t_3 t_4^2 + t_1 t_3^2 t_4 + t_2 t_3^2 t_4\right)$$

$$+0.0181\left(t_1^2 t_3 t_4 + t_2^2 t_3 t_4\right) + 0.0285\left(t_1 t_2 t_3 t_4\right)$$

$$d_{44} = 0.5832 t_4^4 + 0.0035\left(t_1^4 + t_2^4 + t_3^4\right) + 0.0076\left(t_4 t_2^3 + t_4 t_3^3 + t_4 t_1^3\right) + 0.0211\left(t_1^2 t_4^2 + t_4^2 t_3^2 + t_2^2 t_4^2\right)$$

$$+0.0320\left(t_4^3 t_1 + t_4^3 t_2 + t_4^3 t_3\right) + 0.0037\left(t_1 t_2^3 + t_1^3 t_2 + t_1 t_3^3 + t_1^3 t_3 + t_2^3 t_3 + t_2 t_3^3\right) + 0.0067\left(t_2^2 t_1^2 + t_2^2 t_3^2 + t_3^2 t_1^2\right)$$

$$+0.0150\left(t_1 t_4 t_2^2 + t_2 t_1^2 t_4 + t_1 t_4 t_3^2 + t_2 t_4 t_3^2 + t_3 t_1^2 t_4 + t_3 t_2^2 t_4\right) + 0.0328\left(t_4^2 t_2 t_1 + t_4^2 t_2 t_3 + t_4^2 t_3 t_1\right)$$

$$+0.0097\left(t_1 t_2 t_3^2 + t_1 t_2^2 t_3 + t_1^2 t_3 t_2\right) + 0.0224\left(t_1 t_2 t_3 t_4\right).$$

4.4.8 Slope Information Matrices (SIM) for Uniform Weighted Centroid Designs

Using (4.129), the slope information matrices were obtained at different points of the simplex centroids designs. At point (1, 0, 0, 0), the slope information matrix is given by,

$$SIM_{41u} = \begin{pmatrix} x & y1'_3 \\ y1_3 & zJ_3 \end{pmatrix} \qquad (4.130)$$

where $x = 5829.4224 \times 10^{-4}$, $y = 79.5186 \times 10^{-4}$, $z = 35.3124 \times 10^{-4}$.

For binary blends at points (½, ½, 0, 0), we have information matrix as,

$$SIM_{42u} = \begin{pmatrix} xI_2 + yJ_2 & zJ_2 \\ zJ'_2 & qJ_2 \end{pmatrix} \qquad (4.131)$$

where

$x = 365.92289 \times 10^{-4}$, $y = 38.46044 \times 10^{-4}$, $z = 22.25155 \times 10^{-4}, q = 13.30321 \times 10^{-4}$.

At the ternary point (1/3, 1/3, 1/3, 0), we have slope information matrix as,

$$SIM_{43u} = \begin{pmatrix} xI_3 + yJ_3 & z1_3 \\ z1'_3 & q \end{pmatrix} \qquad (4.132)$$

where

$x = 76.08877 \times 10^{-4}$, $y = 21.21016 \times 10^{-4}$, $z = 14.0479 \times 10^{-4}, q = 10.16018 \times 10^{-4}$.

At the central point (¼, ¼, ¼, ¼) of the simplex centroid design, we have the slope information matrix given as,

$$SIM_{44u} = \begin{pmatrix} 0.004131819 & 0.002094689 & 0.001552438 & 0.001552438 \\ 0.002094689 & 0.005561169 & 0.002341674 & 0.002094689 \\ 0.001552438 & 0.002341674 & 0.004131819 & 0.001552438 \\ 0.001552438 & 0.002094689 & 0.001552438 & 0.004131819 \end{pmatrix}.$$

(4.133)

4.4.9 Optimal Values for Slope Designs

We obtained the optimal values for both Weighted Simplx Centroid (WSC) designs and Uniform Weighted Simplex Centroid Designs (UWSCD) for four ingredients mixture experiments. We considered the D-, E-, A- and T-optimality criteria based on the formulas (3.13), (3.16), (3.18) and (3.20) respectively.

The optimal values for pure, binary, ternary and quaternary blends were calculated from matrices (4.123), (4.124), (4.125) and (4.126) for Weighted Simplex Centroid Designs and (4.130), (4.131), (4.132) and (4.133) for Uniformly Weighted Simplex Centroid Designs. The optimal values are summarized in Table 4.9 below.

Table 4. 9: Optimal Values for Four Ingredients

	WEIGHTED SIMPLEX CENTROID (WSC)				**UNIFORM WEIGHTED SIMPLEX CENTROID (UWSC)**			
BLENDS	**D-**	**E-**	**A-**	**T-**	**D-**	**E-**	**A-**	**T-**
1, 0, 0, 0	0.0000	0.0000	0.0000	0.1609	0.0000	0.0000	0.0000	0.1484
½, ½, 0, 0	0.0000	0.0000	0.0000	0.0229	0.0000	0.0000	0.0000	0.0208
1/3, 1/3, 1/3, 0	0.0046	0.0004	0.0014	0.0082	0.0047	0.0005	0.0019	0.0075
¼, ¼, ¼, ¼	0.0039	0.0027	0.0035	0.0048	0.0036	0.0024	0.0031	0.0045

Uniformly Weighted Simplex Centroids Design (UWSCD) was observed to yield more optimal values than Weighted Simplex Centroid Designs (WSCD) at all points of the simplex centroids mixture experiments except point (1/3, 1/3, 1/3, 0).

4.4.10 Efficiencies for Four Ingredients

The performance of the WSCD in comparison to the UWSCD was measured by the D-, E-, A- and T-efficiencies defined in (3.14), (3.17), (3.19) and (3.21) respectively. Their efficiencies at different point of the simplex centroid designs were summarized as given in Table 4.10 below.

Table 4. 10: Efficiencies for Four Ingredients

	Efficiencies (%)			
BLENDS	**D-**	**E-**	**A-**	**T-**
1, 0, 0, 0	100	100	100	108.42
½, ½, 0, 0	100	100	100	110.09
1/3, 1/3, 1/3, 0	97.87	80	73.68	109.33
¼, ¼, ¼, ¼	108.33	112.5	112.90	106.66

From Table 4.10, at points (1, 0, 0, 0) and (½, ½, 0, 0), there was no difference between the two designs in their D-, E- and A- efficiency. However, UWSCD was 8.42% and 10.09% more T- efficient than WSCD at respective points. For ternary mixture (1/3, 1/3, 1/3, 0), WSCD was 2.13%, 20% and 26.32% more D-, E- and A- efficient than UWSCD respectively. It was also observed that WSCD was 9.33% less T-efficient than UWSCD. At point (¼, ¼, ¼, ¼), UWSCD was 8.33%, 12.5%, 12.9% and 6.66% more D-, E-, A- and T- efficient respectively than WSCD. Generally, the D-, E-, A- and T-optimal values for Uniformly Weighted Simplex Centroid (UWSC) designs were better than those of Weighted Simplex Centroid (WSC) designs for two, three and four ingredients.

4.4.11 I-Optimal for Four Ingredients

In the four ingredients designs, we obtained the inverse of the information matrix (4.121) for parameter subsystem of interest as,

$$C_2^{-1} = \begin{pmatrix} 14.9825(I_4) + 0.0023(J_4) & -4.6212(I_4) - 0.72399(J_4) & 1.5628(1_4) \\ -4.6212(I_4) - 0.72399(J_4) & 46.79292(I_4) - 7.08239148(J_4) & -10.52455(1_4) \\ 1.5628(1'_4) & -10.52455(1'_4) & 39629.9676 \end{pmatrix}. \tag{4.134}$$

The matrix L was obtained through integration of the parameter subsystem of interest of the Kronecker model as given in (3.30). Thus, L becomes,

$$L = k\int \begin{pmatrix} R_1 & R_2 & R_3 \\ R_2^{'} & R_4 & R_5 \\ R_3^{'} & R_5^{'} & R_6 \end{pmatrix} dt \tag{4.135}$$

where,

$$R_1 = \begin{pmatrix} t_1^6 & t_1^3 t_2^3 & t_1^3 t_3^3 & t_1^3 t_4^3 \\ t_1^3 t_2^3 & t_2^6 & t_2^3 t_3^3 & t_1^3 t_2^3 \\ t_1^3 t_3^3 & t_2^3 t_3^3 & t_3^6 & t_3^3 t_4^3 \\ t_1^3 t_4^3 & t_2^3 t_4^3 & t_3^3 t_4^3 & t_4^6 \end{pmatrix}$$

$$R_2 = \begin{pmatrix} \frac{t_1^3(t_1^2 t_4 + t_1^2 t_3 + t_1^2 t_2)}{3} & \frac{t_1^3(t_2^2 t_4 + t_2^2 t_3 + t_1 t_2^3)}{3} & \frac{t_1^3(t_3^2 t_4 + t_2 t_3^2 + t_1 t_3^2)}{3} & \frac{t_1^3(t_3 t_4^2 + t_2 t_4^2 + t_1 t_4^2)}{3} \\ \frac{t_2^3(t_1^2 t_4 + t_1^2 t_3 + t_1^2 t_2)}{3} & \frac{t_2^3(t_2^2 t_4 + t_2^2 t_3 + t_1 t_2^3)}{3} & \frac{t_2^3(t_3^2 t_4 + t_2 t_3^2 + t_1 t_3^2)}{3} & \frac{t_2^3(t_3 t_4^2 + t_2 t_4^2 + t_1 t_4^2)}{3} \\ \frac{t_3^3(t_1^2 t_4 + t_1^2 t_3 + t_1^2 t_2)}{3} & \frac{t_3^3(t_2^2 t_4 + t_2^2 t_3 + t_1 t_2^3)}{3} & \frac{t_3^3(t_3^2 t_4 + t_2 t_3^2 + t_1 t_3^2)}{3} & \frac{t_3^3(t_3 t_4^2 + t_2 t_4^2 + t_1 t_4^2)}{3} \\ \frac{t_4^3(t_1^2 t_4 + t_1^2 t_3 + t_1^2 t_2)}{3} & \frac{t_4^3(t_2^2 t_4 + t_2^2 t_3 + t_1 t_2^3)}{3} & \frac{t_4^3(t_3^2 t_4 + t_2 t_3^2 + t_1 t_3^2)}{3} & \frac{t_4^3(t_3 t_4^2 + t_2 t_4^2 + t_1 t_4^2)}{3} \end{pmatrix}$$

$$R_3 = \begin{pmatrix} \dfrac{t_1^3(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)}{4} \\ \dfrac{t_2^3(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)}{4} \\ \dfrac{t_3^3(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)}{4} \\ \dfrac{t_4^3(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)}{4} \end{pmatrix}$$

$$R_4 =$$

$$\begin{pmatrix} \frac{(t_1^2t_4 + t_1^2t_3 + t_1^2t_2)^2}{9} & \frac{(t_1^2t_4 + t_1^2t_3 + t_1^2t_2)(t_2^2t_4 + t_2^2t_3 + t_1t_2^2)}{9} & \frac{(t_1^2t_4 + t_1^2t_3 + t_1^2t_2)(t_3^2t_4 + t_2t_3^2 + t_1t_3^2)}{9} & \frac{(t_1^2t_4 + t_1^2t_3 + t_1^2t_2)(t_3t_4^2 + t_2t_4^2 + t_1t_4^2)}{9} \\ \frac{(t_1^2t_4 + t_1^2t_3 + t_1^2t_2)(t_2^2t_4 + t_2^2t_3 + t_1t_2^2)}{9} & \frac{(t_2^2t_4 + t_2^2t_3 + t_1t_2^2)^2}{9} & \frac{(t_2^2t_4 + t_2^2t_3 + t_1t_2^2)(t_3^2t_4 + t_2t_3^2 + t_1t_3^2)}{9} & \frac{(t_2^2t_4 + t_2^2t_3 + t_1t_2^2)(t_3t_4^2 + t_2t_4^2 + t_1t_4^2)}{9} \\ \frac{(t_1^2t_4 + t_1^2t_3 + t_1^2t_2)(t_3^2t_4 + t_2t_3^2 + t_1t_3^2)}{9} & \frac{(t_2^2t_4 + t_2^2t_3 + t_1t_2^2)(t_3^2t_4 + t_2t_3^2 + t_1t_3^2)}{9} & \frac{(t_3^2t_4 + t_2t_3^2 + t_1t_3^2)^2}{9} & \frac{t_3^3(t_3t_4^2 + t_2t_4^2 + t_1t_4^2)(t_3^2t_4 + t_2t_3^2 + t_1t_3^2)}{9} \\ \frac{(t_1^2t_4 + t_1^2t_3 + t_1^2t_2)(t_3t_4^2 + t_2t_4^2 + t_1t_4^2)}{9} & \frac{(t_2^2t_4 + t_2^2t_3 + t_1t_2^3)(t_3t_4^2 + t_2t_4^2 + t_1t_4^2)}{9} & \frac{(t_3^2t_4 + t_2t_3^2 + t_1t_3^2)(t_3t_4^2 + t_2t_4^2 + t_1t_4^2)}{9} & \frac{(t_3t_4^2 + t_2t_4^2 + t_1t_4^2)^2}{9} \end{pmatrix}$$

$$R_5 = \begin{pmatrix} \frac{(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)(t_1^2t_4 + t_1^2t_3 + t_1^2t_2)}{12} \\ \frac{(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)(t_2^2t_4 + t_2^2t_3 + t_1t_2^3)}{12} \\ \frac{(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)(t_3^2t_4 + t_2t_3^2 + t_1t_3^2)}{12} \\ \frac{(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)(t_3t_4^2 + t_2t_4^2 + t_1t_4^2)}{12} \end{pmatrix}$$

$$R_6 = \left(\frac{(t_2t_3t_4 + t_1t_3t_4 + t_1t_2t_4 + t_1t_2t_3)^2}{16} \right)$$

Next, we integrate each component in (4.135) as,

$$(q-1)!\int_\tau t_1^6 dt_1 = \int_\tau t_2^6 dt_2 = \int_\tau t_3^6 dt_3 = \int_\tau t_4^6 dt_4 = \frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{1}^{4} p_i - 1)!} = \frac{3!6!}{9!} = \frac{1}{84}$$

$$(q-1)!\int_\tau t_1^5 t_2 dt_1 dt_2 = \int_\tau t_1 t_2^5 dt_1 dt_2 = \int_\tau t_1 t_3^5 dt_1 dt_3 = \frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{i=1}^{4} p_i - 1)!} = \frac{1}{504}$$

$$(q-1)!\int_\tau t_1^4 t_2 t_3 dt_1 dt_2 dt_3 = \int_\tau t_1 t_2^4 t_3 dt_1 dt_2 dt_3 = \int_\tau t_1 t_2 t_3^4 dt_1 dt_2 dt_3 = \frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{i=1}^{4} p_i - 1)!} = \frac{1}{2520}$$

$$(q-1)!\int_\tau t_1^3 t_2^2 t_3 dt_1 dt_2 dt_3 = \int_\tau t_1^2 t_2 t_3^3 dt_1 dt_2 dt_3 = \int_\tau t_1 t_2^3 t_3^2 dt_1 dt_2 dt_3 \frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{1}^{4} p_i - 1)!} = \frac{1}{5040}$$

$$(q-1)!\int_\tau t_1^3 t_2^3 dt_1 dt_2 = \int_\tau t_1^3 t_3^3 dt_1 dt_3 = \int_\tau t_2^3 t_3^3 dt_2 dt_3 \frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{1}^{4} p_i - 1)!} = \frac{1}{1680}$$

(4.136)

$$(q-1)!\int_\tau t_1^4t_2^2dt_1dt_2=\int_\tau t_1^2t_2^4dt_1dt_2=\int_\tau t_2^2t_3^4dt_2dt_3=\int_\tau t_1^2t_3^4dt_1dt_3=\int_\tau t_1^4t_3^2dt_1dt_3=\int_\tau t_2^4t_3^2dt_1dt_3=\frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{i=1}^{4}p_i-1)!}=\frac{1}{1260}$$

$$(q-1)!\int_\tau t_1^2t_2^2t_3^2dt_1dt_2dt_3=\int_\tau t_1^2t_2^2t_4^2dt_1dt_2dt_4=\int_\tau t_1^2t_3^2t_4^2dt_1dt_3dt_4=\int_\tau t_2^2t_3^2t_4^2dt_2dt_3dt_4=\frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{i=1}^{4}p_i-1)!}=\frac{1}{7560}$$

$$(q-1)!\int_\tau t_1^3t_2t_3t_4dt_1dt_2dt_3dt_4=\int_\tau t_1t_2^3t_3t_4dt_1dt_2dt_3dt_4=\int_\tau t_1t_2t_3^3t_4dt_1dt_2dt_3dt_4=\int_\tau t_1t_2t_3t_4^3dt_1dt_2dt_3dt_4$$
$$=\frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{i=1}^{4}p_i-1)!}=\frac{1}{10080}$$

$$(q-1)!\int_\tau t_1^2t_2^2t_3t_4dt_1dt_2dt_3dt_4=\int_\tau t_1^2t_2t_3^2t_4dt_1dt_2dt_3dt_4=\int_\tau t_1t_2^2t_3^2t_4dt_1dt_2dt_3dt_4=\int_\tau t_1^2t_2t_3t_4^2dt_1dt_2dt_3dt_4$$
$$=\frac{(q-1)!\prod_{i=1}^{4}(p_i!)}{(q+\sum_{i=1}^{4}p_i-1)!}=\frac{1}{15120}$$

Therefore the integral matrix L is becomes,

$$L=\begin{pmatrix} 0.0113(I_4)+0.0006(J_4) & 0.00158(I_4)+0.0004(J_4) & 0.00032(1_4) \\ 0.00158(I_4)+0.0004(J_4) & 0.00033(I_4)+0.0002(J_4) & 0.00014(1_4) \\ 0.00032(1'_4) & 0.00014(1'_4) & 0.00008 \end{pmatrix}. \tag{4.137}$$

Now using (4.134) and (4.137), we obtained $C_2^{-1}L$ as,

$$C_2^{-1}L=\begin{pmatrix} 0.1621098(I_4)+0.007390487(J_4) & 0.0222535(I_4)+0.005174219(J_4) & 0.004272272(1_4) \\ 0.0222535(I_4)+0.005174219(J_4) & 0.008138595(I_4)-0.002221494(J_4) & 0.0001414522(1_4) \\ 0.004272272(1'_4) & 0.0001414522(1'_4) & 0.0017869842 \end{pmatrix}. \tag{4.138}$$

Therefore, the average prediction variance is given by the trace of (4.138). Hence,

$$APV=tr[C_2^{-1}L]=0.7034569. \tag{4.139}$$

4.4.12 I-Optimal for Uniform Weight Simplex Centroid Designs

Similarly, we obtained the inverse of the information matrix (4.128) for the parameter subsystem of interest (4.110) as,

$$C_{2u}^{-1} = \begin{pmatrix} 15.982644(I_4) + 0.0007984(J_4) & -4.77225248(I_4) - 0.08245342(J_4) & 1.398217(1_4) \\ -4.77225248(I_4) - 0.08245342(J_4) & 68.96969(I_4) - 10.63118966(J_4) & -12.17091(1_4) \\ 1.398217(1'_4) & -12.17091(1'_4) & 43.69736 \end{pmatrix}.$$

(4.140)

Using (4.134) and (4.140), we obtained the matrix $C_{2u}^{-1}L$, for the I-optimal design, such that,

$$C_{2u}^{-1}L = \begin{pmatrix} 0.11731810951_4 + 0.007819716J_4 & 0.0237911151I_4 + 0.005501782J_4 & 0.004552701(1_4) \\ 0.0555038I_4 - 0.014274488J_4 & 0.01523243I_4 - 0.002134630J_4 & 0.001065428(1_4) \\ -0.005406623(1'_4) & -0.003104111(1'_4) & -0.001426310 \end{pmatrix}.$$

(4.141)

Thus, the average prediction variance becomes,

$$tr[C_{2u}^{-1}L] = 0.7749682. \qquad (4.142)$$

Comparing (4.139) and (4.142), Weighted Simplex Centroid Designs performed better than Uniform Weighted Simplex Centroid due to its smaller average prediction variance leading to more accurate prediction of responses in mixture experiments.

4.4.13 Equivalence Theorem for Weighted Simplex Centroid Designs

For four ingredients, the design is said to be I-optimal, if it satisfy the following inequality

$$f^{'}(t)C_2^{-1}LC_2^{-1}f(t) \leq 0.7034569. \qquad (4.143)$$

at a given design points of the simplex centroid.

Table 4. 11: Equivalence Theorem for Four Ingredients (WSCD).

	Average Prediction Variances			
BLENDS	$f^{'}(t)C_1^{-1}LC_1^{-1}f(t)$		$tr[C_1^{-1}L]$	**Optimality**
1, 0, 0, 0	2.41681	>	0.7034569	Not I Optimal
½, ½, 0, 0	0.07862874	<	0.7034569	I-Optimal
1/3, 1/3, 1/3, 0	0.01026738	<	0.7034569	I-Optimal
¼, ¼, ¼, ¼	0.002332298	<	0.7034569	I-Optimal

It was observed in Table 4.11 that the pure blends in WSCD did not satisfy the general equivalence theorem for I-optimality in inequality (4.143). The binary, ternary and quaternary blends were found to satisfy the general equivalence theorem, therefore, I-optimal. However, the centre point mixtures (¼, ¼, ¼, ¼) were better than the binary and ternary mixtures due to smaller prediction variance.

4.4.14 Equivalence Theorem for Uniform Weighted Simplex Centroid Kronecker

For three ingredients, the design is said to be I-optimal if and only if it satisfy,

$$f^{'}(t)C_{2u}^{-1}LC_{2u}^{-1}f(t) \leq 0.7749682. \qquad (4.144)$$

at a given design points of the simplex centroid designs.

Table 4. 12: Equivalence Theorem for Four Ingredients (UWSCD)

	Average Prediction Variances			
BLENDS	$f^{'}(t)C_2^{-1}LC_2^{-1}f(t)$		$tr[C_2^{-1}L]$	**Optimality**

1, 0, 0, 0	2.755831	>	0.7749682	Not I Optimal
½, ½, 0, 0	0.09881055	<	0.7749682	I-Optimal
1/3, 1/3, 1/3, 0	0.01341913	<	0.7749682	I-Optimal
¼, ¼, ¼, ¼	0.002813837	<	0.7749682	I-Optimal

In Table 4.12, it was observed that the pure blends for UWSCD did not satisfy the general equivalence theorem for I-optimality in inequality (4.144). The binary, ternary and quaternary blends were found to satisfy the general equivalence theorem, therefore, I-optimal. However, the centre point mixtures (¼, ¼, ¼, ¼) were better than all the binary and ternary mixtures due to their smaller prediction variance. Prediction of responses at this point was accurately achieved than any other point in the simplex centroid designs.

Generally, Weighted Simplex Centroid Designs (WSCD) performed better than Uniformly Weighted Simplex Centroid Designs (UWSC) for two, three and four ingredients mixture experiments. This was due to their smaller average prediction variances exhibited in all the three mixture experiments as given in Table 4.11.

The general equivalence theorem for I-optimality was satisfied in all the mixtures combination except pure blends for two, three and four mixture ingredients.

The centroid points (0.5, 0.5), (0.33, 0.33, 0.33), and (0.25, 0.25, 0.25, 0.25) mixtures for two, three and four ingredients respectively were found to be more optimal than the other mixture combinations.

4.5 BLENDING OF FOUR CHEMICAL PESTICIDES FOR CONTROL OF MITES

Research and development in the chemical and chemical engineering disciplines rely heavily on the development of accurate empirical and theoretical equations that express mixture properties in terms of compositions and pure components attributes or ingredients. Mixture experiments models are applied in chemical engineering to assist with the design of process plants and the optimization of product formulations.

Four chemical pesticides Vendex (V), Omite (O), Kelthane (K) and Dibrom (D) were sprayed on strawberry plants in an attempt to control the mite population, Cornel (2003). Each chemical was applied individually and in combination with each of the others to comprise the four pure component blends, six binary blends, four ternary blends, and four chemicals together. Each of the 15 chemical treatments was sprayed on three plants in each of four m blocks of 45 plants. Seven days after spraying, the total number of mites on 10 leaves sampled from each plant was recorded. This number was divided by the total number of mites recorded from 10 leaves of the same plant just prior to spraying and then multiplied by 100 percent to approximate the mites mean percentage survival per plant.

4.5.1 Initial Statistical Inference

In this experiment, the response was the average percentage of mites on the plants seven days after treatment relative to the number on the plants just prior to spraying, treatments with average response less or equal to ten were considered more effective than those greater than twenty.

Vendex (V) was the most effective pure or single chemical; its estimate was 1.8 which was significantly lower than the other three single chemicals. The VO, VK, and OK were the most effective binary component with 4.9, 3.1 and 3.4 averages respectively, which were smaller than other binary mixtures. For ternary mixtures, VOD and VKD with averages of 2.6 and 2.4 respectively appear to be more effective than VOK and OKD. VOKD was the most effective blend of all the chemicals, with average response of 0.8 which was significantly smaller than all other responses. The initial analysis took into consideration the special cubic model in the form of equation (1.6), the Design Expert software, was used to compute analysis of variance for special cubic model.

4.5.2 Estimated Model

The estimates for the coefficients of the Kronecker model were obtained through the R statistical software. Therefore the estimated third degree Kronecker model is given as

$$E(\hat{y}) = 0.98209\ t1\_ + 0.74609\ t2\_ + 0.71409\ t3\_ + 0.61509\ t4\_ + 5.8742\ t1\_2t2 + 6.0502\ t1\_2t3 + 4.1012\ t1\_2t4 + 6.2622\ t2\_2t3 + 3.6412\ t2\_2t4 + 5.8092\ t3\_2t4 + 1.144\ t1\_t2\_t3 + 11.212\ t1\_t2\_t4 + 8.955\ t1\_t3\_t4 + 7.019\ t2\_t3\_t4. \quad (4.145)$$

4.5.3 Model Validity

In this case, the analysis of the model validity was performed. It is important to examine the fitted model if it provides an adequate approximation of the true response surface. Normality probability plot and Analysis of variance (ANOVA) was used to examine the Kronecker model.

4.5.3.1 Normal Probability Plot

In normal probability plot of residuals, the error term e_i must be normally and independently distributed with mean zero and variance s^2. The error term e_i is the difference between the observed value y_i and the corresponding fitted value $\hat{y}_i$, that is $e_i = y_i - \hat{y}_i$. To check this assumption, the normal probability of residuals was plotted as given in Figure (4.1).

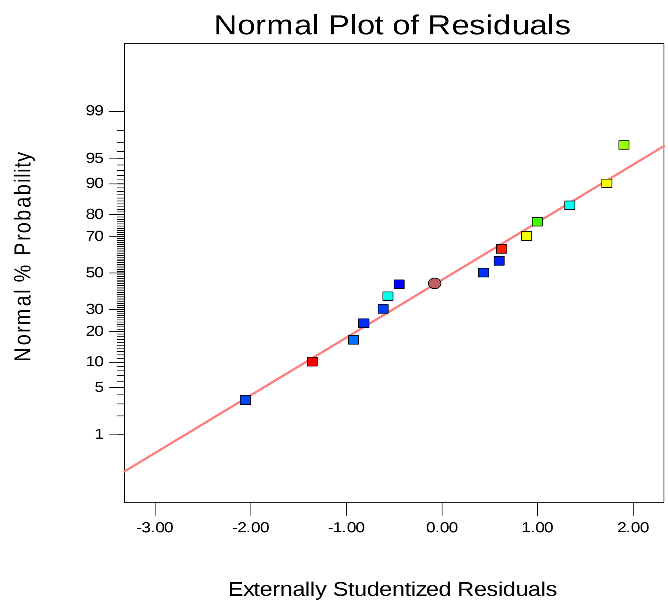

Figure 4.1: Normal Probability Plot of Residual

In figure (4.1), the residuals plot were approximately along a straight line, hence the normality assumption was satisfied.

4.5.3.2 The Analysis of Variance

The Analysis of Variance for fitted Kronecker model was obtained. It is important to note that, in polynomials ANOVA, the regression sum of squares (SSR) and total sum of squares (SST) are always uncorrected, see Marquardt and Snee (1974). Therefore using (3.5), (3.6) and (3.37), the calculated sums of squares becomes, $SST = 5951.1$, $SSR = 5930.238$ and $SSE = 20.86$ respectively as given in Table 4.13.

Table 4. 13: Analysis of Variance

Sources of Variations	Degrees of Freedom	Sum of Squares	MSS	F
Regression	13	5930.238	456.172	21.86
Error	1	20.86	20.86	
Total	14	5951.1		

The statistical hypotheses tested are

$$H_0 : \beta_i = \beta_j \quad \forall ij$$
$$H_1 : \beta_i \neq \beta_j$$

Therefore the observed statistic F is given as $F = \frac{MSSR}{MSSE} = 21.86$ as shown in the ANOVA Table 4.13, since the calculated F value (21.86) is greater than the F tabulated (4.61) at 5% level of significance, we reject the null hypothesis and conclude that the estimates were different from zero hence significant.

4.5.3.3 Coefficient of Variation

In order to determine how well the estimated model fits the data, R^2 and R_A^2 values were used as given in equation (3.38) and (3.39). Since both the values of R^2 and R_A^2 exceeds 0.90, this means that the error variance estimate obtained from the analysis of the fitted model is less than 10% of the error variance estimate obtained with the model hence confident in using the fitted model in predicting the response values of the chemicals.

4.5.3.4 Testing the Adequacy of Parameters

To test the adequacy of each parameter in the model, we employ student t test as given in the Table 4.14 below

Table 4. 14: T-Test

Term	Coef	SE Coef	T-Value	P-Value	VIF
t111	0.98209	0.00771	127.45	0.005	1.05
t222	0.74609	0.00771	96.82	0.007	1.05
t333	0.71409	0.00771	92.67	0.007	1.05
t444	0.61509	0.00771	79.82	0.008	1.05
t11t2	5.8742	0.0623	94.24	0.007	1.21
t11t3	6.0502	0.0623	97.06	0.007	1.21
t11t4	4.1012	0.0623	65.79	0.010	1.21
t22t3	6.2622	0.0623	100.46	0.006	1.21
t22t4	3.6412	0.0623	58.41	0.011	1.21
t32t4	5.8092	0.0623	93.20	0.007	1.21
t1t2t3	1.144	0.224	5.11	0.123	1.30
t1t2t4	11.212	0.224	50.04	0.013	1.30
t1t3t4	8.955	0.224	39.97	0.016	1.30
t2t3t4	7.019	0.224	31.32	0.020	1.30

From Table 4.14, all the parameters in the model were significant at 5% level of significant except $t_1t_2t_3$ with p-value of 0.123 greater than 0.05. The model was chosen on the basis of smallest value of standard error of estimates of y, that is, smallest mean square error. The pure blends, two interactions and three interactions had standard errors of 0.00771, 0.0623 and 0.224 respectively. The variance inflation factors (VIF) of 1.05, 1.21, and 1.30 for pure, two interactions and three interactions were also reasonably small and good since they were less than five.

4.6 SLOPE FOR THIRD DEGREE KRONECKER MODEL

The third degree Kronecker model for the pesticides used in mite eradication experiments is given as

$$E(\hat{y}) = 0.9821t_1^3 + 0.7461t_2^3 + 0.714t_3^3 + 0.6151t_4^3 + 5.8742t_1^2t_2 + 6.0502t_1^2t_3$$
$$+ 4.1012t_1^2t_4 + 6.2622t_2^2t_3 + 3.6412t_2^2t_4 + 5.8092t_3^2t_4 + 1.1444t_1t_2t_3$$
$$+ 11.2118t_1t_2t_4 + 8.9554t_1t_3t_4 + 7.0185t_2t_3t_4.$$

(4.146)

The required estimated model corresponding to the parameter subsystem of interest given in (3.7) is

$$E(\hat{y}) = 0.9821t_1^3 + .7461t_2^3 + 0.714t_3^3 + 0.6151t_4^3 + \frac{5.8742t_1^2t_2 + 6.0502t_1^2t_3 + 4.1012t_1^2t_4}{3}$$
$$+ \frac{5.8742t_1t_2^2 + 6.2622t_2^2t_3 + 3.6412t_2^2t_4}{3} + \frac{5.8092t_3^2t_4 + 6.0502t_3^2t_1 + 6.2622t_3^2t_2}{3}$$
$$+ \frac{4.1012t_4^2t_1 + 3.6412t_4^2t_2 + 5.8092t_4^2t_3}{3}$$
$$+ \frac{1.1444t_1t_2t_3 + 11.2118t_1t_2t_4 + 8.9554t_1t_3t_4 + 7.0185t_2t_3t_4}{4}.$$

(4.147)

We obtain the slope of the Kronecker model by differentiating the parameter subsystem of interest model in (4.147) with respect to each parameter t_1, t_2, t_3 and t_4 as given in (3.10), so that the resulting H_d matrix is,

$$H_d =$$
$$\begin{pmatrix} \frac{4499t_1^2}{1527} & 0 & 0 & 0 & \frac{11.7484t_1t_2 + 12.1004t_1t_3 + 8.2024t_1t_4}{3} & \frac{5.874t_2^2}{3} & \frac{6.0502t_3^2}{3} & \frac{4.1012t_4^2}{3} & a \\ 0 & \frac{22383t_2^2}{10000} & 0 & 0 & \frac{5.874t_1^2}{3} & \frac{11.7484t_1t_2 + 12.5244t_2t_3 + 7.2824t_2t_4}{3} & \frac{6.2622t_3^2}{3} & \frac{3.6412t_4^2}{3} & b \\ 0 & 0 & \frac{1071t_3^2}{500} & 0 & \frac{6.0502t_1^2}{3} & \frac{6.2622t_2^2}{3} & \frac{11.6184t_3t_4 + 12.1004t_1t_3 + 12.5244t_2t_3}{3} & \frac{5.8092t_4^2}{3} & c \\ 0 & 0 & 0 & \frac{18453t_1^2}{10000} & \frac{4.1012t_1^2}{3} & \frac{3.6412t_2^2}{3} & \frac{5.8092t_3^2}{3} & \frac{11.6184t_3t_4 + 7.2824t_2t_4 + 8.2024t_1t_4}{3} & d \end{pmatrix}$$

(4.148)

where

$a = \frac{1.1444 t_2 t_3 + 11.2118 t_2 t_4 + 8.9554 t_3 t_4}{4}$, b= $\frac{1.1444 t_1 t_3 + 11.2118 t_1 t_4 + 7.0185 t_3 t_4}{4}$, c= $\frac{1.1444 t_1 t_2 + 8.9554 t_1 t_4 + 7.0185 t_2 t_4}{4}$,
d= $\frac{11.2118 t_1 t_2 + 8.9554 t_1 t_3 + 7.0185 t_2 t_3}{4}$.

The information matrix (4.121) together with H_d matrix (4.148) were used to obtain slope information matrix given as,

$$D_c = \begin{pmatrix} f_{11} & f_{12} & f_{13} & f_{14} \\ f'_{12} & f_{22} & f_{23} & f_{24} \\ f'_{13} & f'_{23} & f_{33} & f_{34} \\ f'_{14} & f'_{24} & f'_{34} & f_{44} \end{pmatrix} \quad (4.149)$$

where,

$$
\begin{aligned}
f_{11} =\ & 0.6085t_1^4 + 0.1507t_2^4 + 0.2653t_1t_2^3 + 0.6535t_1^2t_2^2 + 0.2585t_1^3t_2 + 0.1598t_3^4 + 0.2815t_1t_3^3 \\
& + 0.0155t_2t_3^3 + 0.6917t_1^2t_3^2 + 0.1385t_2^2t_3^2 + 0.3042t_1t_2t_3^2 + 0.2662t_1^3t_3 + 0.0150t_2^3t_3 + 0.3033t_1t_2^2t_3 \\
& + 1.2449t_1^2t_2t_3 + 0.0734t_4^4 + 0.1293t_1t_4^3 + 0.0103t_2t_4^3 + 0.0820t_3t_4^3 + 0.3292t_1^2t_4^2 + 0.2694t_2^2t_4^2 \\
& + 0.3906t_1t_2t_4^2 + 0.2082t_3^2t_4^2 + 0.3548t_1t_3t_4^2 + 0.2929t_2t_3t_4^2 + 0.1804t_1^3t_4 + 0.1471t_2^3t_4 \\
& + 0.4794t_1t_2^2t_4 + 0.8746t_1^2t_2t_4 + 0.1210t_3^2t_4 + 0.4328t_1t_3^2t_4 + 0.1803t_2t_3^2t_4 \\
& + 0.8932t_1^2t_3t_4 + 0.1536t_2^2t_3t_4 + 0.5589t_1t_2t_3t_4
\end{aligned}
$$

$$
\begin{aligned}
f_{12} =\ & 0.0646t_1^4 + 0.0491t_2^4 + 0.3399t_1t_2^3 + 0.3396t_1^2t_2^2 + 0.3521t_1^3t_2 + 0.1654t_3^4 + 0.1534t_1t_3^3 \\
& + 0.1537t_2t_3^3 + 0.1108t_1^2t_3^2 + 0.1066t_2^2t_3^2 + 0.5712t_1t_2t_3^2 + 0.3121t_1^3t_3 + 0.3225t_2^3t_3 \\
& + 0.3451t_1t_2^2t_3 + 0.3499t_1^2t_2t_3 + 0.0652t_4^4 + 0.1088t_1t_4^3 + 0.1030t_2t_4^3 + 0.0686t_3t_4^3 \\
& + 0.1647t_1^2t_4^2 + 0.1458t_2^2t_4^2 + 0.4664t_1t_2t_4^2 + 0.1801t_3^2t_4^2 + 0.2954t_1t_3t_4^2 \\
& + 0.2869t_2t_3t_4^2 + 0.2269t_1^3t_4 + 0.1993t_2^3t_4 + 0.4120t_1t_2^2t_4 + 0.4373t_1^2t_2t_4 + 0.1100t_3^2t_4 \\
& + 0.2837t_1t_3^2t_4 + 0.2996t_2t_3^2t_4 + 0.2311t_1^2t_3t_4 + 0.2222t_2^2t_3t_4 + 0.6125t_1t_2t_3t_4
\end{aligned}
$$

$$f_{13} = 0.0665t_1^4 + 0.1606t_2^4 + 0.1489t_1t_2^3 + 0.1104t_1^2t_2^2 + 0.3121t_1^3t_2 + 0.0484t_3^4 + 0.3577t_1t_3^3$$
$$+0.3321t_2t_3^3 + 0.3594t_1^2t_3^2 + 0.1073t_2^2t_3^2 + 0.3514t_1t_2t_3^2 + 0.3720t_1^3t_3 + 0.1494t_2^3t_3 + 0.5670t_1t_2^2t_3$$
$$+0.3506t_1^2t_2t_3 + 0.1040t_4^4 + 0.1326t_1t_4^3 + 0.1049t_2t_4^3 + 0.1497t_3t_4^3 + 0.1548t_1^2t_4^2 + 0.2256t_2^2t_4^2$$
$$+0.3419t_1t_2t_4^2 + 0.1966t_3^2t_4^2 + 0.5365t_1t_3t_4^2 + 0.3400t_2t_3t_4^2 + 0.2299t_1^3t_4 + 0.1244t_2^3t_4 + 0.2676t_1t_2^2t_4$$
$$+0.2141t_1^2t_2t_4 + 0.3165t_3^2t_4 + 0.4775t_1t_3^2t_4 + 0.1995t_2t_3^2t_4 + 0.4225t_1^2t_3t_4$$
$$+0.3619t_2^2t_3t_4 + 0.7350t_1t_2t_3t_4$$

$$f_{14} = 0.0451t_1^4 + 0.0934t_2^4 + 0.1558t_1t_2^3 + 0.2091t_1^2t_2^2 + 0.2669t_1^3t_2 + 0.1535t_3^4 + 0.1956t_1t_3^3$$
$$+0.0548t_2t_3^3 + 0.1938t_1^2t_3^2 + 0.1192t_2^2t_3^2 + 0.3162t_1t_2t_3^2 + 0.2299t_1^3t_3 + 0.0507t_2^3t_3 + 0.2536t_1t_2^2t_3$$
$$+0.2846t_1^2t_2t_3 + 0.0283t_4^4 + 0.1691t_1t_4^3 + 0.1408t_2t_4^3 + 0.2163t_3t_4^3 + 0.1682t_1^2t_4^2 + 0.1358t_2^2t_4^2$$
$$+0.3007t_1t_2t_4^2 + 0.1784t_3^2t_4^2 + 0.3390t_1t_3t_4^2 + 0.2515t_2t_3t_4^2 + 0.1823t_1^3t_4 + 0.1278t_2^3t_4$$
$$+0.4913t_1t_2^2t_4 + 0.3707t_1^2t_2t_4 + 0.1932t_3^2t_4 + 0.5700t_1t_3^2t_4 + 0.2607t_2t_3^2t_4 + 0.3640t_1^2t_3t_4$$
$$+0.2876t_2^2t_3t_4 + 0.7889t_1t_2t_3t_4$$

$$f_{22} = 0.1507t_1^4 + 0.3512t_2^4 + 0.1963t_1t_2^3 + 0.6413t_1^2t_2^2 + 0.2653t_1^3t_2 + 0.1712t_3^4 + 0.0160t_1t_3^3$$
$$+0.3015t_2t_3^3 + 0.1433t_1^2t_3^2 + 0.7261t_2^2t_3^2 + 0.3148t_1t_2t_3^2 + 0.0150t_1^3t_3 + 0.2093t_2^3t_3 + 1.2876t_1t_2^2t_3$$
$$+0.3129t_1^2t_2t_3 + 0.0579t_4^4 + 0.0912t_1t_4^3 + 0.1019t_2t_4^3 + 0.0571t_3t_4^3 + 0.2590t_1^2t_4^2 + 0.2555t_2^2t_4^2$$
$$+0.3468t_1t_2t_4^2 + 0.1569t_3^2t_4^2 + 0.2306t_1t_3t_4^2 + 0.2895t_2t_3t_4^2 + 0.1471t_1^3t_4 + 0.1217t_2^3t_4$$
$$+0.7723t_1t_2^2t_4 + 0.4586t_1^2t_2t_4 + 0.0982t_3^2t_4 + 0.1794t_1t_3^2t_4 + 0.3716t_2t_3^2t_4 + 0.1282t_1^2t_3t_4$$
$$+0.1823t_2^2t_3t_4 + 0.5164t_1t_2t_3t_4$$

$$f_{23} = 0.1552t_1^4 + 0.0523t_2^4 + 0.3225t_1t_2^3 + 0.1056t_1^2t_2^2 + 0.1441t_1^3t_2 + 0.0501t_3^4 + 0.3321t_1t_3^3$$
$$+0.3818t_2t_3^3 + 0.1067t_1^2t_3^2 + 0.3827t_2^2t_3^2 + 0.3522t_1t_2t_3^2 + 0.1444t_1^3t_3 + 0.3836t_2^3t_3$$
$$+0.3466t_1t_2^2t_3 + 0.5622t_1^2t_2t_3 + 0.0924t_4^4 + 0.1091t_1t_4^3 + 0.1099t_2t_4^3 + 0.1268t_3t_4^3$$
$$+0.2491t_1^2t_4^2 + 0.1200t_2^2t_4^2 + 0.3193t_1t_2t_4^2 + 0.1724t_3^2t_4^2 + 0.3260t_1t_3t_4^2$$
$$+0.4594t_2t_3t_4^2 + 0.1345t_1^3t_4 + 0.2070t_2^3t_4 + 0.1898t_1t_2^2t_4 + 0.2663t_1^2t_2t_4$$
$$+0.3252t_3^2t_4 + 0.1843t_1t_3^2t_4 + 0.4498t_2t_3^2t_4 + 0.3445t_1^2t_3t_4$$
$$+0.3607t_2^2t_3t_4 + 0.7364t_1t_2t_3t_4$$

$$f_{24} = 0.1052t_1^4 + 0.0304t_2^4 + 0.1993t_1t_2^3 + 0.2017t_1^2t_2^2 + 1.6616t_1^3t_2 + 0.1589t_3^4 + 0.0700t_1t_3^3$$
$$+0.1889t_2t_3^3 + 0.1294t_1^2t_3^2 + 0.1611t_2^2t_3^2 + 0.3461t_1t_2t_3^2 + 0.0640t_1^3t_3 + 0.2070t_2^3t_3$$
$$+0.2636t_1t_2^2t_3 + 0.2803t_1^2t_2t_3 + 0.0251t_4^4 + 0.1408t_1t_4^3 + 0.1355t_2t_4^3 + 0.1912t_3t_4^3$$
$$+0.1473t_1^2t_4^2 + 0.1324t_2^2t_4^2 + 0.2834t_1t_2t_4^2 + 0.1487t_3^2t_4^2 + 0.2472t_1t_3t_4^2 + 0.2821t_2t_3t_4^2$$
$$+0.1440t_1^3t_4 + 0.1397t_2^3t_4 + 0.3281t_1t_2^2t_4 + 0.5016t_1^2t_2t_4 + 0.1854t_3^2t_4 + 0.2747t_1t_3^2t_4$$
$$+0.5180t_2t_3^2t_4 + 0.3150t_1^2t_3t_4 + 0.2991t_2^2t_3t_4 + 0.7633t_1t_2t_3t_4$$

$$f_{33} = 0.1598t_1^4 + 0.1712t_2^4 + 0.0160t_1t_2^3 + 0.1475t_1^2t_2^2 + 0.0155t_1^3t_2 + 0.3216t_3^4 + 0.1935t_1t_3^3$$
$$+0.2003t_2t_3^3 + 0.6774t_1^2t_3^2 + 0.7243t_2^2t_3^2 + 1.3260t_1t_2t_3^2 + 0.2815t_1^3t_3 + 0.3015t_2^3t_3 + 0.3233t_1t_2^2t_3$$
$$+0.3222t_1^2t_2t_3 + 0.0147t_4^4 + 0.1162t_1t_4^3 + 0.0911t_2t_4^3 + 0.2595t_3t_4^3 + 0.2479t_1^2t_4^2 + 0.2091t_2^2t_4^2$$
$$+0.1916t_1t_2t_4^2 + 0.6259t_3^2t_4^2 + 0.5026t_1t_3t_4^2 + 0.4618t_2t_3t_4^2 + 0.1210t_1^3t_4 + 0.0982t_2^3t_4$$
$$+0.1478t_1t_2^2t_4 + 0.1237t_1^2t_2t_4 + 0.1858t_3^2t_4 + 1.2470t_1t_3^2t_4 + 1.2859t_2t_3^2t_4$$
$$+0.5123t_1^2t_3t_4 + 0.4760t_2^2t_3t_4 + 0.4699t_1t_2t_3t_4$$

$$f_{34} = 0.1084t_1^4 + 0.0996t_2^4 + 0.0831t_1t_2^3 + 0.1098t_1^2t_2^2 + 0.0810t_1^3t_2 + 0.0465t_3^4 + 0.31655t_1t_3^3$$
$$+0.3252t_2t_3^3 + 0.2015t_1^2t_3^2 + 0.1795t_2^2t_3^2 + 0.2395t_1t_2t_3^2 + 0.1559t_1^3t_3 + 0.1367t_2^3t_3 + 0.3154t_1t_2^2t_3$$
$$+0.3121t_1^2t_2t_3 + 0.0400t_4^4 + 0.2163t_1t_4^3 + 0.1912t_2t_4^3 + 0.3262t_3t_4^3 + 0.1442t_1^2t_4^2 + 0.1147t_2^2t_4^2$$
$$+0.2109t_1t_2t_4^2 + 0.3291t_3^2t_4^2 + 0.3902t_1t_3t_4^2 + 0.3331t_2t_3t_4^2 + 0.1364t_1^3t_4 + 0.11622t_2^3t_4$$
$$+0.25511t_1t_2^2t_4 + 0.2685t_1^2t_2t_4 + 0.3312t_3^2t_4 + 0.4703t_1t_3^2t_4 + 0.4392t_2t_3^2t_4$$
$$+0.5303t_1^2t_3t_4 + 0.4658t_2^2t_3t_4 + 0.7039t_1t_2t_3t_4$$

$$
\begin{aligned}
f_{44} = {} & 0.4699t_1^4 + 0.0579t_2^4 + 0.0912t_1t_2^3 + 0.2342t_1^2t_2^2 + 0.1027t_1^3t_2 + 0.1474t_3^4 + 0.1162t_1t_3^3 \\
& + 0.0911t_2t_3^3 + 0.2044t_1^2t_3^2 + 0.1506t_2^2t_3^2 + 0.3222t_1t_2t_3^2 + 0.0820t_1^3t_3 + 0.0571t_2^3t_3 + 0.2941t_1t_2^2t_3 \\
& + 0.3467t_1^2t_2t_3 + 0.2387t_4^4 + 0.1130t_1t_4^3 + 0.1003t_2t_4^3 + 0.1601t_3t_4^3 + 0.3160t_1^2t_4^2 + 0.2513t_2^2t_4^2 \\
& + 0.5424t_1t_2t_4^2 + 0.6209t_3^2t_4^2 + 0.8488t_1t_3t_4^2 + 0.7519t_2t_3t_4^2 + 0.1293t_1^3t_4 + 0.1019t_2^3t_4 \\
& + 0.2972t_1t_2^2t_4 + 0.3202t_1^2t_2t_4 + 0.2595t_3^2t_4 + 0.4156t_1t_3^2t_4 + 0.3448t_2t_3^2t_4 + 0.3472t_1^2t_3t_4 \\
& + 0.2768t_2^2t_3t_4 + 0.5651t_1t_2t_3t_4.
\end{aligned}
$$

4.6.1 Slope Information Matrices (SIM) for Weighted Simplex Centroid Designs

Using (4.149), we obtained other slope information matrices at different points of the weighted simplex centroid designs, namely, pure (1, 0, 0, 0), binary (½, ½, 0, 0), ternary (1/3, 1/3, 1/3, 0) and quaternary (¼, ¼, ¼, ¼) blends as shown in Table 4.16 below.

Table 4. 15: Slope Information Matrices (SIM) for Mites Experiments for WSCD

BLENDS	Slope Information Matrices
(1, 0, 0, 0)	$\begin{pmatrix} 0.60836220 & 0.06442412 & 0.06635663 & 0.04498063 \\ 0.06442412 & 0.15074323 & 0.15526501 & 0.10524823 \\ 0.06635663 & 0.15526501 & 0.15992243 & 0.10840532 \\ 0.04498063 & 0.10524823 & 0.10840532 & 0.07348384 \end{pmatrix}$
(½, ½, 0, 0)	$\begin{pmatrix} 0.12094927 & 0.07152661 & 0.04988450 & 0.04521866 \\ 0.07152661 & 0.10024311 & 0.04871613 & 0.04362167 \\ 0.04988450 & 0.04871613 & 0.03187603 & 0.02987508 \\ 0.04521866 & 0.04362167 & 0.02987508 & 0.03454864 \end{pmatrix}$
(1/3, 1/3, 1/3, 0)	$\begin{pmatrix} 0.06611028 & 0.04600234 & 0.04679692 & 0.02814543 \\ 0.04600234 & 0.06235590 & 0.04706020 & 0.02794125 \\ 0.04679692 & 0.04706020 & 0.06394457 & 0.02965144 \\ 0.02814543 & 0.02794125 & 0.02965144 & 0.02089163 \end{pmatrix}$

(¼, ¼, ¼, ¼)	$\begin{pmatrix} 0.04533734 & 0.03379086 & 0.03676478 & 0.03180408 \\ 0.03379086 & 0.04122442 & 0.03554552 & 0.03035651 \\ 0.03676478 & 0.03554552 & 0.04960163 & 0.03405616 \\ 0.03180408 & 0.03035651 & 0.03405616 & 0.03660972 \end{pmatrix}$

4.6.2 Slope Information Matrices (SIM) for Uniformly Weighted Simplex Centroid Design

The information matrix (4.128) together with H matrix (4.148) were used to obtained slope information matrix given as,

$$D_{cu} = \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b'_{12} & b_{22} & b_{23} & b_{24} \\ b'_{13} & b'_{23} & b_{33} & b_{34} \\ b'_{14} & b'_{24} & b'_{34} & b_{44} \end{pmatrix} \tag{4.150}$$

where,

$$b_{11} = 0.5625t_1^4 + 0.1219t_2^4 + 0.2607t_1t_2^3 + 0.5281t_1^2t_2^2 + 0.1846t_1^3t_2 + 0.1293t_3^4 + 0.2766t_1t_3^3$$
$$+0.0258t_2t_3^3 + 0.5589t_1^2t_3^2 + 0.1381t_2^2t_3^2 + 0.3202t_1t_2t_3^2 + 0.1901t_1^3t_3 + 0.0251t_2^3t_3 + 0.3187t_1t_2^2t_3$$
$$+1.0097t_1^2t_2t_3 + 0.0594t_4^4 + 0.1271t_1t_4^3 + 0.1717t_2t_4^3 + 0.1371t_3t_4^3 + 0.2659t_1^2t_4^2 + 0.4642t_2^2t_4^2$$
$$+0.5254t_1t_2t_4^2 + 0.3318t_3^2t_4^2 + 0.4617t_1t_3t_4^2 + 0.6137t_2t_3t_4^2 + 0.1289t_1^3t_4 + 0.2459t_2^3t_4$$
$$+0.6738t_1t_2^2t_4 + 0.7305t_1^2t_2t_4 + 0.2023t_3^2t_4 + 0.5920t_1t_3^2t_4 + 0.3141t_2t_3^2t_4 + 0.7410t_1^2t_3t_4$$
$$+0.2726t_2^2t_3t_4 + 0.9343t_1t_2t_3t_4$$

$$b_{12} = 0.0462t_1^4 + 0.0351t_2^4 + 0.2745t_1t_2^3 + 0.3318t_1^2t_2^2 + 0.2842t_1^3t_2 + 0.1339t_3^4 + 0.1561t_1t_3^3$$
$$+0.1565t_2t_3^3 + 0.1145t_1^2t_3^2 + 0.1120t_2^2t_3^2 + 0.5634t_1t_2t_3^2 + 0.2537t_1^3t_3 + 0.2619t_2^3t_3$$
$$+0.3472t_1t_2^2t_3 + 0.3492t_1^2t_2t_3 + 0.0528t_4^4 + 0.1422t_1t_4^3 + 0.1326t_2t_4^3 + 0.1146t_3t_4^3$$
$$+0.2297t_1^2t_4^2 + 0.2035t_2^2t_4^2 + 0.6578t_1t_2t_4^2 + 0.2767t_3^2t_4^2 + 0.4975t_1t_3t_4^2 + 0.4602t_2t_3t_4^2$$
$$+0.1950t_1^3t_4 + 0.1700t_2^3t_4 + 0.5518t_1t_2^2t_4 + 0.5759t_1^2t_2t_4 + 0.1839t_3^2t_4$$
$$+0.4126t_1t_3^2t_4 + 0.4475t_2t_3^2t_4 + 0.3845t_1^2t_3t_4 + 0.3697t_2^2t_3t_4 + 0.7900t_1t_2t_3t_4$$

$$b_{13} = 0.0475t_1^4 + 0.1300t_2^4 + 0.1515t_1t_2^3 + 0.1138t_1^2t_2^2 + 0.2537t_1^3t_2 + 0.0346t_3^4 + 0.2889t_1t_3^3$$
$$+0.2696t_2t_3^3 + 0.3514t_1^2t_3^2 + 0.1130t_2^2t_3^2 + 0.3544t_1t_2t_3^2 + 0.3003t_1^3t_3 + 0.1523t_2^3t_3$$
$$+0.5592t_1t_2^2t_3 + 0.3503t_1^2t_2t_3 + 0.0842t_4^4 + 0.1586t_1t_4^3 + 0.1753t_2t_4^3 + 0.1871t_3t_4^3 + 0.2040t_1^2t_4^2$$
$$+0.3466t_2^2t_4^2 + 0.5432t_1t_2t_4^2 + 0.2709t_3^2t_4^2 + 0.6446t_1t_3t_4^2 + 0.5392t_2t_3t_4^2 + 0.1951t_1^3t_4$$
$$+0.2080t_2^3t_4 + 0.3872t_1t_2^2t_4 + 0.3560t_1^2t_2t_4 + 0.2628t_3^2t_4 + 0.5895t_1t_3^2t_4 + 0.3315t_2t_3^2t_4$$
$$+0.5308t_1^2t_3t_4 + 0.5196t_2^2t_3t_4 + 0.9245t_1t_2t_3t_4$$

$$b_{14} = 0.3222t_1^4 + 0.7557t_2^4 + 0.2037t_1t_2^3 + 0.3039t_1^2t_2^2 + 0.1950t_1^3t_2 + 0.1242t_3^4 + 0.2339t_1t_3^3$$
$$+0.0917t_2t_3^3 + 0.2691t_1^2t_3^2 + 0.1299t_2^2t_3^2 + 0.4445t_1t_2t_3^2 + 0.1951t_1^3t_3 + 0.0847t_2^3t_3$$
$$+0.3734t_1t_2^2t_3 + 0.4739t_1^2t_2t_3 + 0.0202t_4^4 + 0.1365t_1t_4^3 + 0.1210t_2t_4^3 + 0.1812t_3t_4^3$$
$$+0.1637t_1^2t_4^2 + 0.1933t_2^2t_4^2 + 0.3956t_1t_2t_4^2 + 0.2522t_3^2t_4^2 + 0.4117t_1t_3t_4^2$$
$$+0.4202t_2t_3t_4^2 + 0.1471t_1^3t_4 + 0.1570t_2^3t_4 + 0.6822t_1t_2^2t_4 + 0.4646t_1^2t_2t_4$$
$$+0.2299t_3^2t_4 + 0.6874t_1t_3^2t_4 + 0.4162t_2t_3^2t_4 + 0.4331t_1^2t_3t_4$$
$$+0.4389t_2^2t_3t_4 + 1.1454t_1t_2t_3t_4$$

$$b_{22} = 0.1219t_1^4 + 0.3246t_2^4 + 0.1402t_1t_2^3 + 0.5184t_1^2t_2^2 + 0.2607t_1^3t_2 + 0.1386t_3^4 + 0.0268t_1t_3^3$$
$$+0.2963t_2t_3^3 + 0.1429t_1^2t_3^2 + 0.5869t_2^2t_3^2 + 0.3314t_1t_2t_3^2 + 0.0251t_1^3t_3 + 0.1495t_2^3t_3$$
$$+1.0436t_1t_2^2t_3 + 0.3281t_1^2t_2t_3 + 0.0468t_4^4 + 0.1524t_1t_4^3 + 0.1002t_2t_4^3 + 0.0954t_3t_4^3$$
$$+0.4540t_1^2t_4^2 + 0.2004t_2^2t_4^2 + 0.4664t_1t_2t_4^2 + 0.2324t_3^2t_4^2 + 0.4828t_1t_3t_4^2$$
$$+0.3631t_2t_3t_4^2 + 0.2459t_1^3t_4 + 0.0869t_2^3t_4 + 0.6422t_1t_2^2t_4 + 0.6534t_1^2t_2t_4$$
$$+0.1641t_3^2t_4 + 0.3098t_1t_3^2t_4 + 0.5005t_2t_3^2t_4$$
$$+0.2301t_1^2t_3t_4 + 0.6681t_2^2t_3t_4 + 0.8632t_1t_2t_3t_4$$

$$b_{23} = 0.1256t_1^4 + 0.0374t_2^4 + 0.2619t_1t_2^3 + 0.1104t_1^2t_2^2 + 0.1468t_1^3t_2 + 0.0358t_3^4 + 0.2696t_1t_3^3$$
$$+0.3084t_2t_3^3 + 0.1121t_1^2t_3^2 + 0.3747t_2^2t_3^2 + 0.3558t_1t_2t_3^2 + 0.1472t_1^3t_3 + 0.3098t_2^3t_3$$
$$+0.3497t_1t_2^2t_3 + 0.5545t_1^2t_2t_3 + 0.0747t_4^4 + 0.1824t_1t_4^3 + 0.1276t_2t_4^3 + 0.1560t_3t_4^3$$
$$+0.4041t_1^2t_4^2 + 0.1536t_2^2t_4^2 + 0.4920t_1t_2t_4^2 + 0.2300t_3^2t_4^2 + 0.5254t_1t_3t_4^2$$
$$+0.5296t_2t_3t_4^2 + 0.2248t_1^3t_4 + 0.1729t_2^3t_4 + 0.3156t_1t_2^2t_4 + 0.3947t_1^2t_2t_4$$
$$+0.2683t_3^2t_4 + 0.3060t_1t_3^2t_4 + 0.5392t_2t_3^2t_4 + 0.4918t_1^2t_3t_4$$
$$+0.4487t_2^2t_3t_4 + 0.9435t_1t_2t_3t_4$$

$$b_{24} = 0.0851t_1^4 + 0.0217t_2^4 + 0.1700t_1t_2^3 + 0.2970t_1^2t_2^2 + 0.2139t_1^3t_2 + 0.1285t_3^4 + 0.1171t_1t_3^3$$
$$+0.2195t_2t_3^3 + 0.1434t_1^2t_3^2 + 0.2223t_2^2t_3^2 + 0.4932t_1t_2t_3^2 + 0.1070t_1^3t_3 + 0.1729t_2^3t_3$$
$$+0.4388t_1t_2^2t_3 + 0.4085t_1^2t_2t_3 + 0.0179t_4^4 + 0.1210t_1t_4^3 + 0.1094t_2t_4^3$$
$$+0.1592t_3t_4^3 + 0.2125t_1^2t_4^2 + 0.1289t_2^2t_4^2 + 0.3667t_1t_2t_4^2 + 0.2057t_3^2t_4^2$$
$$+0.4131t_1t_3t_4^2 + 0.3299t_2t_3t_4^2 + 0.1768t_1^3t_4 + 0.1127t_2^3t_4 + 0.4116t_1t_2^2t_4$$
$$+0.6924t_1^2t_2t_4 + 0.2135t_3^2t_4 + 0.4300t_1t_3^2t_4 + 0.5871t_2t_3^2t_4$$
$$+0.4982t_1^2t_3t_4 + 0.3457t_2^2t_3t_4 + 1.0564t_1t_2t_3t_4$$

$$b_{33} = 0.1293t_1^4 + 0.1386t_2^4 + 0.0268t_1t_2^3 + 0.1470t_1^2t_2^2 + 0.0258t_1^3t_2 + 0.2793t_3^4 + 0.1382t_1t_3^3$$
$$+0.1431t_2t_3^3 + 0.5476t_1^2t_3^2 + 0.5855t_2^2t_3^2 + 1.0746t_1t_2t_3^2 + 0.2766t_1^3t_3 + 0.2963t_2^3t_3$$
$$+0.3398t_1t_2^2t_3 + 0.3380t_1^2t_2t_3 + 0.1192t_4^4 + 0.1942t_1t_4^3 + 0.1522t_2t_4^3 + 0.2550t_3t_4^3$$
$$+0.3709t_1^2t_4^2 + 0.2837t_2^2t_4^2 + 0.3980t_1t_2t_4^2 + 0.5060t_3^2t_4^2 + 0.6540t_1t_3t_4^2$$
$$+0.5793t_2t_3t_4^2 + 0.2023t_1^3t_4 + 0.1641t_2^3t_4 + 0.2571t_1t_2^2t_4 + 0.2194t_1^2t_2t_4$$
$$+0.1327t_3^2t_4 + 1.0222t_1t_3^2t_4 + 1.0508t_2t_3^2t_4 + 0.6701t_1^2t_3t_4$$
$$+0.6030t_2^2t_3t_4 + 0.7854t_1t_2t_3t_4$$

$$b_{34} = 0.0877t_1^4 + 0.0806t_2^4 + 0.1388t_1t_2^3 + 0.1282t_1^2t_2^2 + 0.1354t_1^3t_2 + 0.0332t_3^4 + 0.2628t_1t_3^3$$
$$+0.2683t_2t_3^3 + 0.2789t_1^2t_3^2 + 0.2419t_2^2t_3^2 + 0.3983t_1t_2t_3^2 + 0.1949t_1^3t_3 + 0.1682t_2^3t_3$$
$$+0.4739t_1t_2^2t_3 + 0.4600t_1^2t_2t_3 + 0.0286t_4^4 + 0.1808t_1t_4^3 + 0.1592t_2t_4^3 + 0.2635t_3t_4^3$$
$$+0.1951t_1^2t_4^2 + 0.1488t_2^2t_4^2 + 0.3524t_1t_2t_4^2 + 0.3223t_3^2t_4^2 + 0.4974t_1t_3t_4^2$$
$$+0.4151t_2t_3t_4^2 + 0.1623t_1^3t_4 + 0.1338t_2^3t_4 + 0.4071t_1t_2^2t_4 + 0.4526t_1^2t_2t_4$$
$$+0.2675t_3^2t_4 + 0.5774t_1t_3^2t_4 + 0.5214t_2t_3^2t_4 + 0.6483t_1^2t_3t_4$$
$$+0.5359t_2^2t_3t_4 + 1.0017t_1t_2t_3t_4$$

$$b_{44} = 0.0594t_1^4 + 0.0468t_2^4 + 0.1524t_1t_2^3 + 0.4296t_1^2t_2^2 + 0.1717t_1^3t_2 + 0.1192t_3^4 + 0.1942t_1t_3^3$$
$$+0.1522t_2t_3^3 + 0.3281t_1^2t_3^2 + 0.2261t_2^2t_3^2 + 0.6164t_1t_2t_3^2 + 0.1371t_1^3t_3 + 0.0954t_2^3t_3$$
$$+0.5890t_1t_2^2t_3 + 0.7036t_1^2t_2t_3 + 0.2207t_4^4 + 0.0807t_1t_4^3 + 0.0717t_2t_4^3 + 0.1143t_3t_4^3$$
$$+0.2554t_1^2t_4^2 + 0.2031t_2^2t_4^2 + 0.4531t_1t_2t_4^2 + 0.5020t_3^2t_4^2 + 0.6982t_1t_3t_4^2$$
$$+0.6173t_2t_3t_4^2 + 0.1271t_1^3t_4 + 0.1002t_2^3t_4 + 0.4177t_1t_2^2t_4 + 0.4562t_1^2t_2t_4$$
$$+0.2550t_3^2t_4 + 0.5685t_1t_3^2t_4 + 0.4642t_2t_3^2t_4 + 0.4542t_1^2t_3t_4 + 0.3506t_2^2t_3t_4$$
$$+0.9447t_1t_2t_3t_4.$$

Using (4.150), we also obtained other slope information matrices at different points of the uniformly weighted simplex centroid designs, that is pure, binary, ternary and quaternary blends as shown in Table 4.16 below.

Table 4. 16: Slope Information Matrices (SIM) for Mites Experiments used in UWSCD

Blends	Slope Information Matrices (SIM)
(1, 0, 0, 0)	$\begin{pmatrix} 0.56225969 & 0.04587313 & 0.04724917 & 0.03202841 \\ 0.04587313 & 0.12184147 & 0.12549630 & 0.08506916 \\ 0.04724917 & 0.12549630 & 0.12926076 & 0.08762094 \\ 0.03202841 & 0.08506916 & 0.08762094 & 0.05939490 \end{pmatrix}$
(½, ½, 0, 0)	$\begin{pmatrix} 0.10350488 & 0.06068932 & 0.04349430 & 0.05032995 \\ 0.06068932 & 0.08527681 & 0.04259198 & 0.04899768 \\ 0.04349430 & 0.04259198 & 0.02920351 & 0.03548313 \\ 0.05032995 & 0.04899768 & 0.03548313 & 0.05329411 \end{pmatrix}$
(1/3, 1/3, 1/3, 0)	$\begin{pmatrix} 0.05736488 & 0.04213816 & 0.04282277 & 0.03364219 \\ 0.04213816 & 0.05418541 & 0.04310879 & 0.03363844 \\ 0.04282277 & 0.04310879 & 0.05555690 & 0.03498448 \\ 0.03364219 & 0.03363844 & 0.03498448 & 0.03310580 \end{pmatrix}$
(¼, ¼, ¼, ¼)	$\begin{pmatrix} 0.04938289 & 0.04011214 & 0.04269684 & 0.04036110 \\ 0.04011214 & 0.04453090 & 0.04094920 & 0.03841084 \\ 0.04269684 & 0.04094920 & 0.05125504 & 0.04150688 \\ 0.04036110 & 0.03841084 & 0.04150688 & 0.04445404 \end{pmatrix}$

4.6.3 The Optimal Values

The D-, A-, E- and T- optimal values for the Weighted Simplex Centroid Designs (WSCD) and Uniform Weighted Simplex Centroid Designs (UWSCD) were obtained from slope information matrices at different points of simplex centroid as shown in Table 4.15 and 4.16 respectively.

The optimal values for Weighted Simplex Centroid Designs (WSCD) and Uniform Weighted Simplex Centroid Designs (UWSCD) were summarized in the Table 4.17, given as

Table 4. 17: Optimal Values for Chemical Experiments

	WEIGHTED SIMPLEX CENTROID (WSC)				UNIFORM WEIGHTED SIMPLEX CENTROID (UWSC)			
BLENDS	**D-**	**E-**	**A-**	**T-**	**D-**	**E-**	**A-**	**T-**
(1, 0, 0, 0)	0.0000	0.0000	0.0000	0.2481	0.0000	0.0000	0.0000	0.2181
(½, ½, 0, 0)	0.0216	0.0019	0.0063	0.0719	0.0223	0.0019	0.0065	0.0678
(1/3,1/3,1/3, 0)	0.0223	0.00471	0.01203	0.0533	0.0210	0.0069	0.0131	0.0500
(¼, ¼, ¼, ¼)	0.0183	0.0080	0.0119	0.0431	0.0149	0.0058	0.0086	0.0474

Table 4.17 indicates that the pure blend (1, 0, 0, 0) of Vendex pesticide had smaller optimal values hence yielding better results than any other mixture. This is followed by quaternary mixtures of Vendex, Omite, Kelthane and Dibrom ingredients in equal proportion of (¼, ¼, ¼, ¼) and binary mixtures (½, ½, 0, 0) of Vendex and Omite for both Weighted Simplex Centroid and Uniformly Weighted Simplex Centroid (UWSC) designs.

In terms of optimality criterion, the D-, E- and A-optimality for pure blends performed better than all other mixture blends in both simplex centroids designs. T-optimality criterion also yielded good results in a mixture of four chemicals (¼, ¼, ¼, ¼) as compared to other points of the simplex centroid while pure blends (1, 0, 0, 0) performed poorly.

4.6.4 I-Optimality for Chemical Experiment

We now obtained the matrix L_2 through integration of the parameter subsystem of interest in (4.147) of the Kronecker model as given in (3.30). Therefore, L_2 becomes,

$$L_2 = k\int \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{12}' & R_{22} & R_{23} \\ R_{13}' & R_{23}' & R_{33} \end{pmatrix} dt \tag{4.151}$$

where

$$R_{11} = \begin{pmatrix} 0.96452041t_1^6 & 0.73274481t_1^3t_2^3 & 0.7012194t_1^3t_3^3 & 0.60408971t_1^3t_4^3 \\ 0.73274481t_1^3t_2^3 & 0.55666521t_2^6 & 0.5327154t_2^3t_3^3 & 0.45892611t_2^3t_4^3 \\ 0.7012194t_1^3t_3^3 & 0.5327154t_2^3t_3^3 & 0.509796t_3^6 & 0.4391814t_3^3t_4^3 \\ 0.60408971t_1^3t_4^3 & 0.45892611t_2^3t_4^3 & 0.4391814t_3^3t_4^3 & 0.37834801t_4^6 \end{pmatrix}$$

$$R_{12} = \begin{pmatrix} w_{11} & w_{12} & w_{13} & w_{14} \\ w_{21} & w_{22} & w_{23} & w_{24} \\ w_{31} & w_{32} & w_{33} & w_{34} \\ w_{41} & w_{42} & w_{43} & w_{44} \end{pmatrix}$$

where,

$$w_{11} = \left(\frac{201389426t_1^5t_4 + 297095071t_1^5t_3 + 288452591t_1^5t_2}{150000000} \right)$$

$$w_{12} = \left(\frac{178801126t_1^3t_2^2t_4 + 307505331t_1^3t_2^2t_3 + 288452591t_1^4t_2^2}{150000000} \right)$$

$$w_{13} = \left(\frac{285260766t_1^3t_3^2t_4 + (307505331t_1^3t_2 + 297095071t_1^4)t_3^2}{150000000} \right)$$

$$w_{14} = \left(\frac{(142630383t_1^3t_3 + 89400563t_1^3t_2 + 100694713t_1^4)t_4^2}{75000000} \right)$$

$$w_{21} = \left(\frac{50998422t_1^2t_3^2t_4 + 75234237t_1^2t_2^3t_3 + 73045677t_1^2t_2^4}{50000000} \right)$$

$$w_{22} = \left(\frac{45278322t_2^5t_4 + 77870457t_2^5t_3 + 73045677t_2^5t_1}{50000000} \right)$$

$$w_{23} = \left(\frac{72237402t_2^3t_3^2t_4 + (77870457t_2^4 + 75234237t_1t_2^3)t_3^2}{50000000} \right)$$

$$w_{24} = \left(\frac{(36118701t_2^3t_3 + 22639161t_2^4 + 25499211t_1t_2^3)t_4^2}{25000000} \right)$$

$$w_{31} = \left(\frac{2440214t_1^2t_3^3t_4 + 3599869t_1^2t_3^4 + 297095071t_1^2t_2t_3^3}{25000000} \right)$$

$$w_{32} = \left(\frac{2166514t_2^2t_3^3t_4 + 3726009t_2^2t_3^4 + 3495149t_1t_2^2t_3^3}{25000000} \right)$$

$$w_{33} = \left(\frac{3456474t_3^5t_4 + (3726009t_2 + 3599869t_1)t_3^5}{2500000} \right)$$

$$w_{34} = \left(\frac{(1728237t_3^4 + (1083257t_2 + 1220107t_1)t_3^3)t_4^2}{1250000} \right)$$

$$w_{41} = \left(\frac{126132406t_2^2t_4^4 + (186073901t_1^2t_3 + 180661021t_1^2t_2)t_4^3}{150000000} \right)$$

$$w_{42} = \left(\frac{111985106t_2^2t_4^4 + (192593961t_2^2t_3 + 180661021t_1t_2^2)t_4^3}{150000000} \right)$$

$$w_{43} = \left(\frac{178661946t_3^2t_4^4 + (192593961t_2 + 180661021t_1)t_3^2t_4^3}{150000000} \right)$$

$$w_{44} = \left(\frac{(89330973t_3 + 55992553t_2 + 63066203t_1)t_4^5}{75000000} \right)$$

$$R_{13} = \begin{pmatrix} 0.245525t_1^3(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3) \\ 0.186525t_2^3(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3) \\ 0.1785t_3^3(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3) \\ 0.153775t_4^3(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3) \end{pmatrix}$$

$$R_{14} = \begin{pmatrix} \dfrac{(4.1012t_1^2t_4 + 6.0502t_1^2t_3 + 5.8742t_1^2t_2)(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3)}{12} \\ \dfrac{(3.6412t_2^2t_4 + 6.2622t_2^2t_3 + 5.8742t_1t_2^2)(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3)}{12} \\ \dfrac{(6.0502t_3^2t_1 + 6.2622t_3^2t_2 + 5.8092t_3^2t_4)(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3)}{12} \\ \dfrac{(4.1012t_1t_4^2 + 3.6412t_2t_4^2 + 5.8092t_3t_4^2)(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3)}{12} \end{pmatrix}$$

$$R_{33} = \left(\frac{(7.0185t_2t_3t_4 + 8.955t_1t_3t_4 + 11.2118t_1t_2t_4 + 1.1444t_1t_3t_3)}{16} \right)$$

and

$$R22 = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{12}' & a_{22} & a_{23} & a_{24} \\ a_{13}' & a_{23}' & a_{33} & a_{34} \\ a_{14}' & a_{24}' & a_{34}' & a_{44} \end{pmatrix}$$

where

$$a_{32} = \left(\frac{420496036t_2^4t_4^2 + (1240654012t_1^4t_3 + 1204563452t_1^4t_2)t_4}{225000000} + \frac{915123001t_1^4t_3^2 + 1777004242t_1^4t_2t_3 + 862655641t_1^4t_2^2}{225000000} \right)$$

$$a_{12} = \left(\frac{373332236t_1^2t_2^2t_4^2 + (1192813072t_1^2t_2^2t_3 + 534728426t_1^2t_2^3 + 602261726t_1^3t_2^2)t_4}{225000000} + \frac{947189061t_1^2t_2^2t_3^2 + (919635381t_1^2t_2^3 + 888502121t_1^3t_2^2)t_3 + 862655641t_1^3t_2^3}{225000000} \right)$$

$$a_{13} = \left(\frac{595617276t_1^2t_3^2t_4^2 + (878670546t_1^2t_3^3 + (1495173432t_1^2t_2 + 620327006t_1^3)t_3^2)t_4}{225000000} + \frac{(947189061t_1^2t_2 + 9151230011t_1^3)t_3^3 + (919635381t_1^2t_2^2 + 888502121t_1^3t_2)t_3^2}{225000000} \right)$$

$$a_{14} = \left(\frac{(297808638t_1^2t_3 + 186666118t_1^2t_2 + 210248018t_1^3)t_4^3}{112500000} + \frac{(439335273t_1^2t_3^2 + (701929886t_1^2t_2 + 310163503t_1^3)t_3 + 267364213t_1^2t_2^2 + 301140863t_1^3t_2)t_4^2}{112500000} \right)$$

$$a_{22} = \left(\frac{(331458436t_2^4t_4^2 + (1140096132t_2^4t_3 + 1069456852t_1t_2^4)t_4}{2250000000} + \frac{980378721t_2^4t_3^2 + 1839270762t_1t_2^4t_3 + 862655641t_1^2t_1^4}{2250000000} \right)$$

$$a_{23} = \left(\frac{(528811476t_2^2t_3^2t_4^2 + (909459306t_2^2t_3^3 + (570048066t_2^3 + 1403859772t_1t_2^2)t_3^2)t_4}{225000000} + \frac{(980378721t_2^3 + 947189061t_2^2t_1)t_3^3 + (919635381t_1t_2^3 + 888502121t_1^2t_2^2)t_3^2}{225000000} \right)$$

$$a_{24} = \left(\frac{(264405738t_2^2t_3 + 165729218t_2^3 + 186666118t_1t_2^2)t_4^3 + (454729653t_2^2t_3^2}{112500000} + \frac{(285024033t_2^3 + 747586716t_1t_2^2)t_3 + 267364213t_1t_2^3 + 301140863t_1^2t_2^2)t_4^2}{112500000} \right)$$

$$a_{33} = \left(\begin{array}{l} \dfrac{(843670116t_3^4t_4^2 + (1818918612t_2 + 1757341092t_1)t_3^4t_4}{225000000} + \\ \dfrac{(980378721t_2^2 + 1894378122t_1t_2 + 915123001t_1^2)t_3^4}{225000000} \end{array} \right)$$

$$a_{34} = \left(\begin{array}{l} \dfrac{(421835058t_3^2 + (264405738t_2 + 297808638t_1)t_3^2)t_4^3}{112500000} + \\ \dfrac{((454729653t_2 + 439335273t_1)t_3^3 + (285024033t_2^2 + 596406536t_1t_2 + 310163503t_1^3)t_3^2)t_4^2}{112500000} \end{array} \right)$$

$$a_{44} = \left(\dfrac{(210917529t_3^2 + (264405738t_2 + 297808638t_1)t_3 + 82864609t_2^2 + 186666118t_1t_2 + 105124009t_1^2)t_4^4}{56250000} \right)$$

The integral of each parameter in (4.151) were obtained in (4.134), therefore L_2 becomes,

$$L_2 = \begin{pmatrix} 0.0114820 & 0.0004360 & 0.0004170 & 0.0003595 & 0.0104092 & 0.0021695 & 0.0023560 & 0.0016794 & 0.0022473 \\ 0.0004360 & 0.0066260 & 0.0003170 & 0.0002730 & 0.0016604 & 0.0077855 & 0.0018212 & 0.0012077 & 0.0015998 \\ 0.0004170 & 0.0003170 & 0.0060690 & 0.0002614 & 0.0016139 & 0.0016322 & 0.0085574 & 0.0014629 & 0.0014111 \\ 0.0003595 & 0.0002730 & 0.0002614 & 0.0045040 & 0.0011525 & 0.0010862 & 0.0014462 & 0.0055130 & 0.0016764 \\ 0.0104092 & 0.0021695 & 0.0023560 & 0.0016794 & 0.0152007 & 0.0134528 & 0.0066919 & 0.0042889 & 0.0052323 \\ 0.0016604 & 0.0077855 & 0.0018212 & 0.0012077 & 0.0134528 & 0.0014811 & 0.0067904 & 0.0039749 & 0.0048773 \\ 0.0016139 & 0.0016322 & 0.0085574 & 0.0014629 & 0.0066919 & 0.0067904 & 0.0193104 & 0.0058508 & 0.0060533 \\ 0.0011525 & 0.0010862 & 0.0014462 & 0.0055130 & 0.0042886 & 0.0039749 & 0.0058508 & 0.0109114 & 0.0051308 \\ 0.0022473 & 0.0015998 & 0.0014111 & 0.0016764 & 0.0052323 & 0.0048773 & 0.0060533 & 0.0051308 & 0.0043776 \end{pmatrix}. \quad (4.152)$$

Using the inverse of the information matrix (4.134) for parameter subsystem of interest together with (4.152), we obtain $C_2^{-1}L_2$ as,

$$C_2^{-1}L_2 = \begin{pmatrix} 0.1263939 & -0.0018927 & -0.0034447 & -0.0004561 & 0.0910529 & -0.0238722 & 0.0110699 & 0.0115716 & 0.0148067 \\ 0.0013271 & 0.0648963 & -0.0024715 & 0.0004277 & -0.0319488 & 0.1155934 & 0.0026021 & 0.0059554 & 0.0067461 \\ 0.0012573 & -0.0011927 & 0.0525785 & -0.0009254 & -0.0014019 & -0.0011339 & 0.0456697 & 0.0011100 & -0.0015157 \\ 0.0025281 & 0.0006713 & -0.0015716 & 0.0439230 & 0.0027913 & 0.0036967 & 0.0013257 & 0.0384046 & 0.0067223 \\ 0.3043709 & -0.0076467 & -0.0074795 & -0.0109651 & 0.3263369 & 0.3852095 & -0.0361773 & -0.0390280 & 0.0370647 \\ -0.0539651 & 0.2265370 & -0.0320423 & -0.0326376 & 0.2849776 & -0.2009342 & -0.0290968 & -0.0515412 & 0.0234455 \\ -0.0560532 & -0.0322387 & 0.2565830 & -0.0206424 & -0.0311698 & 0.0759392 & 0.5256213 & 0.0350583 & 0.0793460 \\ -0.0773777 & -0.0575843 & -0.0493327 & 0.1492677 & -0.1414950 & -0.0532831 & -0.0713305 & 0.2531423 & 0.0349535 \\ 0.0183160 & -0.0113535 & -0.0411195 & 0.0199721 & -0.0339509 & 0.0849021 & 0.0319362 & 0.1050363 & 0.0879188 \end{pmatrix}. \quad (4.153)$$

Therefore, the average prediction variance is given by the trace of (4.153). Hence,

$$APV = tr[C_2^{-1}L_2] = 1.279877.$$

(4.154)

Similarly, using the inverse of the information matrix in (4.140) for parameter subsystem

of interest together with integral matrix (4.148), we obtained $C_{2u}^{-1}L_2$ as,

$$C_{2u}^{-1}L_2 = \begin{pmatrix} 0.1357665 & -0.0021870 & -0.0037693 & -0.0007337 & 0.0978847 & -0.0248152 & 0.0110085 & 0.0114919 & 0.0153186 \\ 0.0009737 & 0.0699446 & -0.0028153 & 0.0001349 & -0.0336028 & 0.1220754 & 0.0019909 & 0.0054514 & 0.0066640 \\ 0.0008919 & -0.0015248 & 0.0569700 & -0.0012684 & -0.0020813 & -0.0016080 & 0.0499046 & 0.0005779 & -0.0019641 \\ 0.0021748 & 0.0003777 & -0.0019144 & 0.0472114 & 0.0020135 & 0.0031018 & 0.0004815 & 0.0411587 & 0.0066785 \\ 0.4770016 & -0.0072862 & -0.0080131 & -0.0115917 & 0.5124506 & 0.5838629 & -0.0353749 & -0.0415263 & 0.0699169 \\ -0.0736861 & 0.3505073 & -0.0444208 & -0.0437119 & 0.4336499 & -0.2686226 & -0.0260292 & -0.0609317 & 0.0485227 \\ -0.0768026 & -0.0437757 & 0.3927228 & -0.0260555 & -0.0324253 & 0.1269233 & 0.8053245 & 0.0672307 & 0.1305316 \\ -0.1083508 & -0.0812232 & -0.0700191 & 0.2330319 & -0.1959783 & -0.0646552 & -0.0890435 & 0.3969306 & 0.0656410 \\ -0.0646169 & -0.0736406 & -0.1010543 & -0.0392400 & -0.2330002 & -0.0819373 & -0.1859855 & -0.0665962 & -0.0581781 \end{pmatrix}.$$

(4.155)

Therefore, the average prediction variance is given by the trace of (4.155). Hence,

$$APV = tr[C_{2u}^{-1} L_2] = 1.697798.$$

(4.156)

Comparing APV's in (4.154) and (4.156), Weighted Simplex Centroid Designs performed better than Uniform Weighted Simplex Centroid due to its smaller average prediction variance leading to more accurate prediction of responses in chemical mixture experiments.

4.6.5 Equivalence Theorem for I-Optimality

For Weighted Simplex Centroid Design (WSCD) for four ingredients, the design is said to be I-optimal if and only if it satisfies,

$$f^{'}(t) C_2^{-1} L_2 C_2^{-1} f(t) \leq 1.279877. \quad (4.157)$$

at a given design points of the simplex centroid designs as given in Table 4.18.

Table 4. 18: Equivalence Theorem for Four Ingredients (WSCD)

	Average Prediction Variances			
BLENDS	$f^{'}(t) C_2^{-1} L_2 C_2^{-1} f(t)$		$tr[C_2^{-1} L]$	**Optimality**
1, 0, 0, 0	1.436986	>	1.279877	Not I Optimal
½, ½, 0, 0	1.671055	>	1.279877	Not I Optimal
1/3, 1/3, 1/3, 0	0.5835306	<	1.279877	I-Optimal
¼, ¼, ¼, ¼	0.1532235	<	1.279877	I-Optimal

For Uniformly Weighted Simplex Centroid Design (UWSCD) for four ingredients, the design is said to be I-optimal if and only if it satisfies,

$$f^{'}(t)C_{2u}^{-1}LC_{2u}^{-1}f(t) \leq 1.697798. \qquad (4.158)$$

at a given design points of the simplex centroid designs as given in Table 4.19.

Table 4. 19: Equivalence Theorem for Four Ingredients (UWSCD)

	Average Prediction Variances			
BLENDS	$f^{'}(t)C_{2u}^{-1}L_2C_{2u}^{-1}f(t)$		$tr[C_{2u}^{-1}L_2]$	**Optimality**
1, 0, 0, 0	1.65552	<	1.697798	I- Optimal
½, ½, 0, 0	3.747908	>	1.697798	Not I-Optimal
1/3, 1/3, 1/3, 0	1.350695	<	1.697798	I-Optimal
¼, ¼, ¼, ¼	0.1341891	<	1.697798	I-Optimal

In Table 4.18, two design points (1, 0, 0, 0) and (½, ½, 0, 0) did not satisfy the general equivalence theorem for I-optimality whereas in Table 4.19, only one point (½, ½, 0, 0) did not. This clearly indicates that the UWSC designs were better than WSC designs in terms of predictions of optimal chemical responses.

CHAPTER FIVE

CONCLUSION AND RECOMMENDATION

5.1 INTRODUCTION

This chapter outlines the concluding remarks and also suggests areas for further research which have emerged during the course of study.

5.2 CONCLUSION

It was noted that Uniformly Weighted Simplex Centroid (UWSC) designs performed better than Weighted Simplex Centroid (WSC) designs in terms of D-, A-, E- and T-optimal criteria in most of the points in two, three and four mixture designs of the simplex centroid.

The T-optimal criterion appeared to be the most consistent among the four optimal criteria, where all its values in WSC designs were larger than that of UWSC designs for all the mixture components.

Two ingredients mixture experiments were observed to yield poor D-, A-, E- and T-optimal values compared to three and four ingredients mixture experiments for both SWC and UWSC designs.

The average prediction variances for WSC designs were slightly lower than those of UWSC designs for two, three and four ingredients mixture experiments. All mixtures formulations except pure blend satisfied the general equivalence theorem for I-optimality at different points of the simplex centroid designs.

Two ingredients mixture experiments were observed to yield poor average predictions variances compared to three and four ingredients mixture experiments for both SWC and UWSC designs.

The third degree mixture Kronecker model was considered adequate and reliable since the coefficient of determination exceeded 90% and its standard errors were small.

In pesticides experiment for control of mites, it was noted that WSC had smaller average prediction variance than UWSC designs. However, pure and binary blends did not satisfy the general equivalence theorem for I-optimality whereas in UWSC, all the points were satisfied except binary mixtures (0.5, 0.5, 0, 0). Despite their smaller average prediction variances, we conclude that UWSC designs yields better results since most of its points satisfied the general equivalent theorem.

The most optimal blend was the pure blend of Vendex (V) pesticide for both WSC and UWSC designs. This is followed closely by a mixture of the four ingredients Vendex (V), Omite (O), Kelthane (K) and Dibrom (D) in equal proportion of (¼, ¼, ¼, ¼) respectively.

5.3 RECOMMENDATION

Uniformly Weighted Simplex Centroid (UWS) were recommended for use in third degree Kronecker mixture experiments with three and four ingredients over Weighted Simplex Centroid (WSC) designs due to its efficiency.

T-optimality was also recommended to be used in measuring the performance of both SWC and USWC designs due to its consistency in both three and four factors mixture experiments.

Two ingredients mixture experiments were observed to yield poor D-, A-, E- and T-optimal values compared to three and four ingredients mixture experiments for both SWC and UWSC designs therefore not recommended for use.

The average prediction variances for WSC designs were slightly lower than those of UWSC designs for two, three and four factor mixture experiments hence recommended for use in accurate prediction of response in mixture experiments.

The third degree mixture Kronecker model was considered adequate and reliable and therefore recommended for use in estimation and prediction of pesticides required in eradication of mites in strawberries.

The pure blend of Vendex (V) pesticide for both WSC and UWSC designs was recommended for use in mites eradication in straw berries plants. This is followed closely by a mixture of the four ingredients Vendex (V), Omite (O), Kelthane (K) and Dibrom (D) in equal proportion of (¼, ¼, ¼, ¼) respectively.

5.4 FURTHER RESEARCH

In this study, we considered mixture experiments for a weighted simplex centroid and uniform weighted simplex centroid designs Kronecker model. The mixture experiments could be extended to cover mixture-process experiment Kronecker model where other factors apart from mixture proportion could affect the yield or response of an experiment.

Secondly, the graphical method could be used to evaluate a given design's support for the fitted model in terms of slope variance. Graphical methods for evaluating mixture designs with respect to slope such as slope along Cox direction could be studied. The Fraction of Design Space (FDS) plots, introduced by Zahran, *et al* (2003) could be used to examine a design's prediction variance properties through a graphical approach. This is because the various optimality criteria studied summarizes important information for each design to a single number. This may be too simplistic a summary for understanding the inherent properties of the design. Hence, graphical methods based on the scaled prediction variance can provide a more detailed way of comparing competing designs, for experiments where prediction of future observations is a priority.

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APPENDIX 1
Table A. 1: Optimal Values

	WEIGHTED SIMPLEX CENTROID (WSC)				UNIFORM WEIGHTED SIMPLEX CENTROID (UWSC)			
BLENDS	**D-**	**E-**	**A-**	**T-**	**D-**	**E-**	**A-**	**T-**
1, 0	0.3750	0.0461	0.0909	1.5469	0.3977	0.06812	0.1325	1.1953
½, ½	0.2290	0.1875	0.2250	0.2344	0.1989	0.1406	0.1875	0.2109
1, 0, 0	0.0000	0.0000	0.0000	0.4504	0.0000	0.0000	0.0000	0.3531
½, ½, 0	0.0294	0.0028	0.0081	0.0648	0.0289	0.0042	0.0112	0.0531
1/3, 1/3, 1/3	0.0224	0.0174	0.0212	0.0239	0.0189	0.0136	0.0172	0.0214
1, 0, 0, 0	0.0000	0.0000	0.0000	0.1609	0.0000	0.0000	0.0000	0.1484
½, ½, 0, 0	0.0000	0.0000	0.0000	0.0229	0.0000	0.0000	0.0000	0.0208
1/3, 1/3, 1/3, 0	0.0046	0.0004	0.0014	0.0082	0.0047	0.0005	0.0019	0.0075
¼, ¼, ¼, ¼	0.0039	0.0027	0.0035	0.0048	0.0036	0.0024	0.0031	0.0045

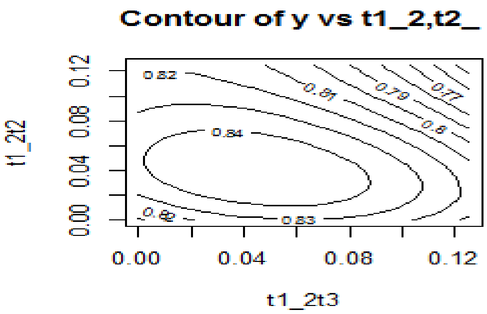
Table A. 2: Average Prediction Variance

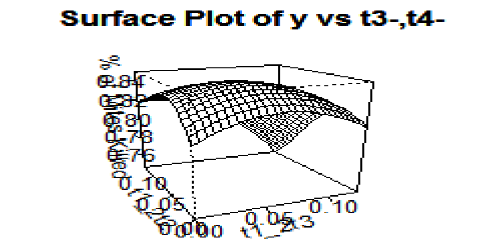
AVERAGE VARIANCE		
Ingredients	Weighted Simplex Centroid Design (WSC D)	Uniform Weighted Simplex Centroid Design (UWSCD)
Two	0.9738095	1.179894
Three	0.8330247	1.022817
Four	0.7034569	0.7749682

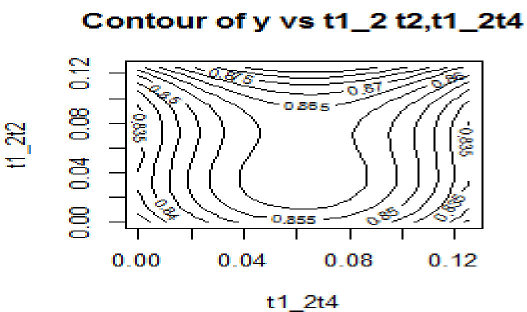
Table A. 3: Average Percentage of Mites Per Plant Relative to Initial Numbers 7 Days After Spraying The Chemical Treatment

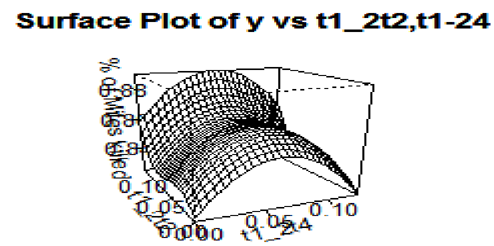
Chemicals Proportions				Blend	Average	
					Percentage	Percentage
t_1	t_2	t_3	t_4	Designation	Survival	Killed
1	0	0	0	V	1.8	98.2
0	1	0	0	O	25.4	74.6
0	0	1	0	K	28.6	71.4
0	0	0	1	D	38.5	61.5
0.5	0.5	0	0	VO	4.9	95.1
0.5	0	0.5	0	VK	3.1	96.9
0.5	0	0	0.5	VD	28.7	71.3
0	0.5	0.5	0	OK	3.4	96.7
0	0.5	0	0.5	OD	37.4	62.6
0	0	0.5	0.5	KD	10.7	89.3
0.33	0.33.	0.33	0	VOK	22.0	78.0
0.33	0.33	0	0.33	VOD	2.6	97.4
0.33	0	0.33	0.33	VKD	2.4	97.6
0	0.33	0.33	0.33	OKD	11.1	88.9
0.25	0.25	0.25	0.25	VOKD	0.8	99.2

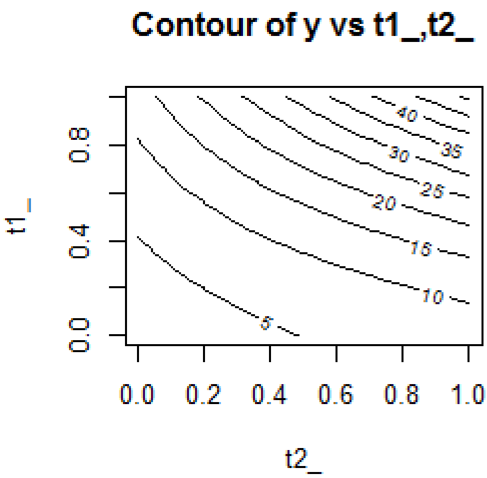
Contour Plots

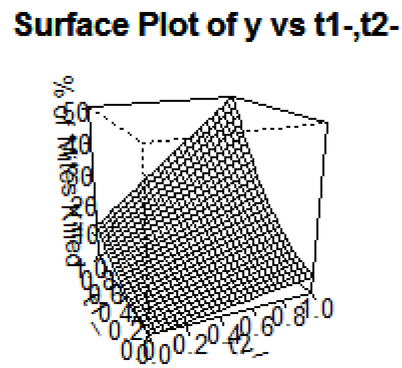


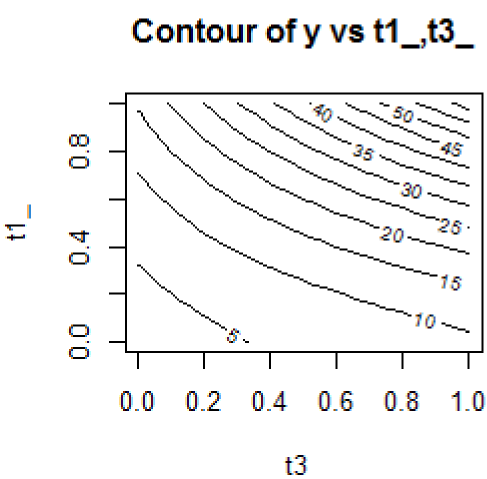


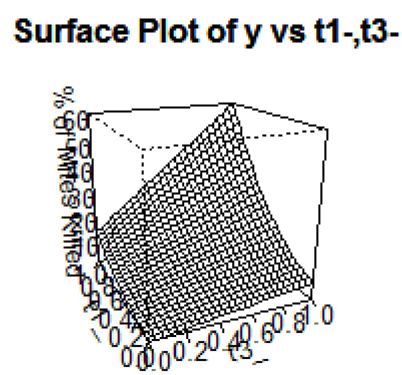





Contour of y vs t1_,t2_
t1_
t2_
0.0 0.2 0.4 0.6 0.8 1.0
0.0 0.4 0.8
5 10 15 20 25 30 35 40


Surface Plot of y vs t1-,t2-
t2_


Contour of y vs t1_,t3_
t1_
t3_
0.0 0.2 0.4 0.6 0.8 1.0
0.0 0.4 0.8
5 10 15 20 25 30 35 40 45 50


Surface Plot of y vs t1-,t3-
t3_

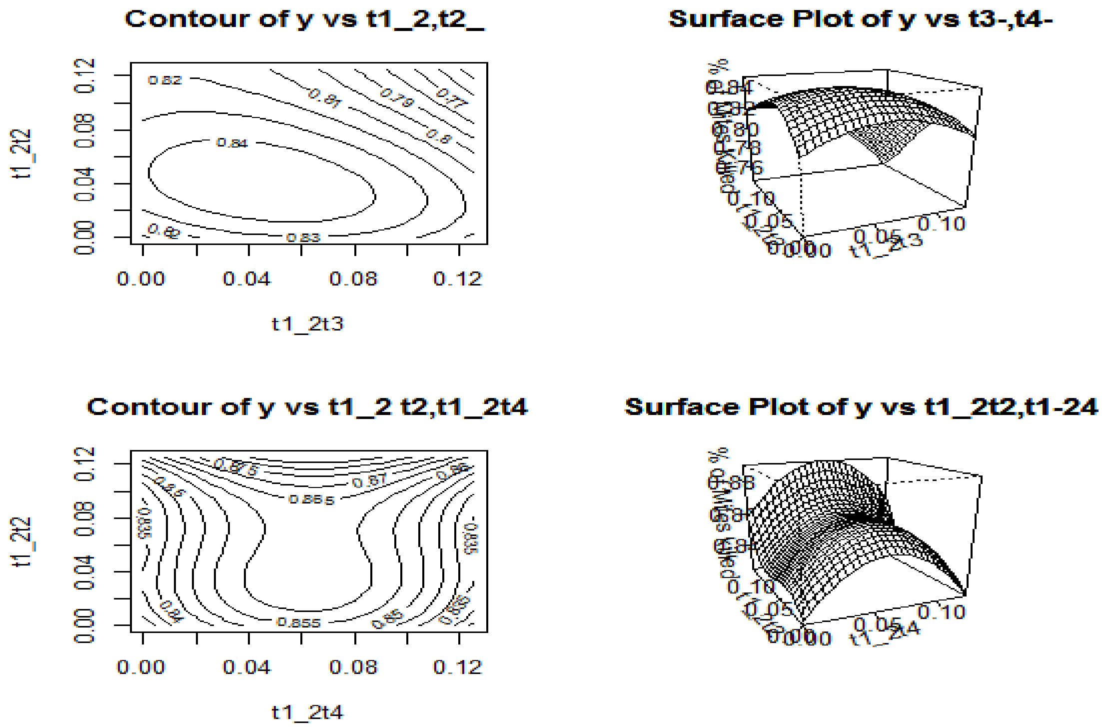


Figure A . 1: Contours for Response Surfaces

APPENDIX 2

R- PROGRAM

```
t11a=rbind(1,0)####pure blends for two ingredients

t12a=rbind(0,1)

t13a=rbind(1/2,1/2)

t11akt11a=(t11a%x%t11a%x%t11a)

k11a=t11akt11a%*%t(t11akt11a)

k11a

mnn1=(1/2*k11a)

mnn1##############################moment for mn1

t12akt12a=(t12a%x%t12a%x%t12a)

k12a=t12akt12a%*%t(t12akt12a)

k12a

mnn2=(1/2*k12a)

mnn2

mnnn1=mnn1+mnn2
```

```
mnnn1

t13akt13a=(t13a%x%t13a%x%t13a)

mnn3=t13akt13a%*%t(t13akt13a)

mnn3

Mnnn=(2/3*mnnn1+1/3*mnn3)

Mnnn###############MOMENT MATRIX for two ingredients

library(MASS)

Mnnnfrac=as.fractions(Mnnn)

Mnnnfrac

########################################################

KT=c(1,rep(0,14),1,0,1/3,1/3,0,1/3,rep(0,6),1/3,0,1/3,1/3,0)

KT

KTT=matrix(KT,nrow=4,ncol=8,byrow=T)##coefficient matrix

KTT

CKK=solve(KTT%*%t(KTT))%*%KTT%*%Mnnn%*%t(KTT)%*%solve(KTT%*
%t(KTT))###information matrix

CKK

library(MASS)

CKKfrac=as.fractions(CKK)

CKKfrac

LKK=t(KTT)%*%solve(KTT%*%t(KTT))####transpose of left inverse

LKK

#####################################################I-Optimal

#####################points 1,0

H1H=c(3,0,0,0,0,0,1,0)

H1H

H11H=matrix(H1H,nrow=2,ncol=4,byrow=T)

H11H

Dc111=H11H%*%CKKfrac%*%t(H11H)

Dc111

library(MASS)
```

```
Dc111frac=as.fractions(Dc111)
Dc111frac
det(Dc111)
##########OPTIMAL VALUE
det(Dc111)^(1/2)################### D optimal
AA10=solve(1/2*sum(diag(solve(Dc111))))
AA10############################ A optimal
EE10=min(eigen(Dc111)$values)
EE10############################ E optimal
T11=0.5*sum(diag(Dc111))
T11
#############Points 1/2, 1/2
HFH=c(3/4,0,1/2,1/4,0,3/4,1/4,1/2)
HFH
HF1H=matrix(HFH,nrow=2,ncol=4,byrow=T)
HF1H
DcF111=HF1H%*%CKKfrac%*%t(HF1H)
DcF111
library(MASS)
DcF111frac=as.fractions(DcF111)
DcF111frac
det(DcF111)
##########OPTIMAL VALUE
det(DcF111)^(1/2)################### D optimal
AA11=solve(1/2*sum(diag(solve(DcF111))))
AA11############################ A optimal
EE11=min(eigen(DcF111)$values)
EE11############################ E optimal
T12=0.5*sum(diag(DcF111))
T12
```

```
##################################################THREE INGREDIENTS

KT3=c(1,rep(0,39),1,rep(0,39),1,0,1/6,1/6,1/6,0,0,1/6,0,0,1/6,rep(0,8),1/6,rep(0,12),1/6,rep(0,5),1/6,0,1/6,0,1/6,0,1/6,rep(0,5),1/6,rep(0,12),1/6,rep(0,8),1/6,0,0,1/6,0,0,1/6,1/6,1/6,rep(0,6),1/6,0,1/6,rep(0,3),1/6,rep(0,3),1/6,rep(0,3),1/6,0,1/6,rep(0,5))

KT3

KTT3=matrix(KT3,nrow=7,ncol=27,byrow=T)##transpose of coefficient matrix K for three ingredients

KTT3

LKK3=solve(KTT3%*%t(KTT3))%*%KTT3#######Left inverse

LKK3

MX3=read.csv("D:\\three33.csv",header=F)####moment matrix for three ingredients

MX3

MX33=as.matrix(MX3)

MX33

####################################################################

t1a=rbind(1,0,0)####pure blends for three ingredients

t2a=rbind(0,1,0)

t3a=rbind(0,0,1)

t1akt1a=(t1a%x%t1a%x%t1a)

k1a=t1akt1a%*%t(t1akt1a)

k1a

t2akt2a=(t2a%x%t2a%x%t2a)

k2a=t2akt2a%*%t(t2akt2a)

k2a

t3akt3a=(t3a%x%t3a%x%t3a)

k3a=t3akt3a%*%t(t3akt3a)

k3a

n1=k1a+k2a+k3a

n1

Mn1=(1/3*n1)

Mn1

t1b=rbind(1/2,1/2,0)
```

```
t2b=rbind(1/2,0,1/2)

t3b=rbind(0,1/2,1/2)

t1c=rbind(1/3,1/3,1/3)

t1bkt1b=(t1b%x%t1b%x%t1b)#######binary blend

k1b=t1bkt1b%*%t(t1bkt1b)

k1b

k1b*64

t2bkt2b=(t2b%x%t2b%x%t2b)

k2b=t2bkt2b%*%t(t2bkt2b)

k2b

t3bkt3b=(t3b%x%t3b%x%t3b)

k3b=t3bkt3b%*%t(t3bkt3b)

k3b

n2=k1b+k2b+k3b

n2

Mn2=(1/3*n2)

Mn2

library(MASS)

Mn2frac=as.fractions(192*(Mn2))

Mn2frac


t1ckt1c=(t1c%x%t1c%x%t1c)

Mn3=t1ckt1c%*%t(t1ckt1c)

Mn3

###########Moment Matrix for three ingredients

Mn11=(3/7*Mn1+3/7*Mn2+1/7*Mn3)

Mn11

CKK3=solve(KTT3%*%t(KTT3))%*%KTT3%*%Mn11%*%t(KTT3)%*%solve(KTT3%*
%t(KTT3))####information matrix

CKK3

library(MASS)
```

```
CKK3frac=as.fractions(CKK3)
CKK3frac
############################pure ingredients
Ht2=c(0,0,0,0,0,1/2,0,0,0,0,0,0,1/2,0,0,0,3,0,0,0,0)
Ht2
HHt2=matrix(Ht2,nrow=3,ncol=7,byrow=T)
HHt2
DDDc11=HHt2%*%CKK3frac%*%t(HHt2)
DDDc11
library(MASS)
DDDc11frac=as.fractions(DDDc11)
DDDc11frac
det(DDDc11)
#######OPTIMAL VALUES
det(DDDc11)^(1/3)################### D optimal
A11=solve(1/3*sum(diag(solve(DDDc11))))
A11############################# A optimal
E11=min(eigen(DDDc11)$values)
E11############################# E optimal
T31=1/3*sum(diag(DDDc11))
T31
##############t1=1/2, t2=1/2,and t3=0
Ht3=c(3/4,0,0,1/4,1/8,0,0,0,3/4,0,1/8,1/4,0,0,0,0,0,1/8,1/8,0,1/4)
Ht3
HHt3=matrix(Ht3,nrow=3,ncol=7,byrow=T)
HHt3
DDDc=HHt3%*%CKK3frac%*%t(HHt3)
DDDc
library(MASS)
DDDcfrac=as.fractions(DDDc)
```

```
DDDcfrac

det(DDDc)

det(DDDc)^(1/3)################### D optimal

A311=solve(1/3*sum(diag(solve(DDDc))))

A311############################ A optimal

E311=min(eigen(DDDc)$values)

E311############################# E optimal

T32=1/3*sum(diag(DDDc))

T32

#################t1=1/2 t2=0 and t3=1/2

Ht33=c(3/4,0,0,1/4,0,1/8,0,0,0,0,1/8,0,1/8,1/4,0,0,3/4,1/8,0,1/4,0)

Ht33

HHt33=matrix(Ht33,nrow=3,ncol=7,byrow=T)

HHt33

DDDc2=HHt33%*%CKK3frac%*%t(HHt33)

DDDc2

library(MASS)

DDDc2frac=as.fractions(DDDc2)

DDDc2frac

det(DDDc2)

###########OPTIMAL VALUES

det(DDDc2)^(1/3)################### D optimal

A31=solve(1/3*sum(diag(solve(DDDc2))))

A31############################ A optimal

E31=min(eigen(DDDc2)$values)

E31############################# E optimal

T321=1/3*sum(diag(DDDc2))

T321

###############t1=0,t2=1/2,t3=1/2

Htt3=c(0,0,0,0,1/8,1/8,1/4,0,3/4,0,0,1/4,1/8,0,0,0,3/4,0,1/8,1/4,0)
```

```
Htt3
Htt33=matrix(Htt3,nrow=3,ncol=7,byrow=T)
Htt33
DDDc3=Htt33%*%CKK3frac%*%t(Htt33)
DDDc3
library(MASS)
DDDc3frac=as.fractions(DDDc3)
DDDc3frac
det(DDDc3)
######OPTIMAL VALUES
det(DDDc3)^(1/3)################## D optimal
A32=solve(1/3*sum(diag(solve(DDDc3))))
A32############################ A optimal
E32=min(eigen(DDDc3)$values)
E32############################ E optimal
T322=1/3*sum(diag(DDDc3))
T322
##################t1=1/3,t2=1/3 and t3=1/3
HHtt3=c(1/3,0,0,2/9,1/18,1/18,1/9,0,1/3,0,1/18,2/9,1/18,1/9,0,0,1/3,1/18,1/18,2/9,1/9)
HHtt3
HHtt33=matrix(HHtt3,nrow=3,ncol=7,byrow=T)
HHtt33
DDDc33=HHtt33%*%CKK3frac%*%t(HHtt33)
DDDc33
library(MASS)
DDDc33frac=as.fractions(DDDc33)
DDDc33frac
det(DDDc33)
################OPTIMAL VALUES
det(DDDc33)^(1/3)################## D optimal
```

```
A33=solve(1/3*sum(diag(solve(DDDc33))))

A33############################ A optimal

E33=min(eigen(DDDc33)$values)

E33############################ E optimal

T33=1/3*sum(diag(DDDc33))

T33

#########FOUR INGREDIENTS############################four ingredients

############################################

t41a=rbind(1,0,0,0)####pure blends for four ingredients

t42a=rbind(0,1,0,0)

t43a=rbind(0,0,1,0)

t44a=rbind(0,0,0,1)

t41akt41a=(t41a%x%t41a%x%t41a)

k41a=t41akt41a%*%t(t41akt41a)

k41a

t42akt42a=(t42a%x%t42a%x%t42a)

k42a=t42akt42a%*%t(t42akt42a)

k42a

t43akt43a=(t43a%x%t43a%x%t43a)

k43a=t43akt43a%*%t(t43akt43a)

k43a

t44akt44a=(t44a%x%t44a%x%t44a)

k44a=t44akt44a%*%t(t44akt44a)

k44a

n4=(k41a+k42a+k43a+k44a)

n4

Mn41=(1/4*n4)

Mn41############################moment for pure blends four ingredients

t51a=rbind(1/2,1/2,0,0)#####binary blends

t52a=rbind(1/2,0,1/2,0)
```

```
t53a=rbind(1/2,0,0,1/2)

t54a=rbind(0,1/2,1/2,0)

t55a=rbind(0,1/2,0,1/2)

t56a=rbind(0,0,1/2,1/2)

t51akt51a=(t51a%x%t51a%x%t51a)

k51a=t51akt51a%*%t(t51akt51a)

k51a

t52akt52a=(t52a%x%t52a%x%t52a)

k52a=t52akt52a%*%t(t52akt52a)

k52a

t53akt53a=(t53a%x%t53a%x%t53a)

k53a=t53akt53a%*%t(t53akt53a)

k53a

t54akt54a=(t54a%x%t54a%x%t54a)

k54a=t54akt54a%*%t(t54akt54a)

k54a

t55akt55a=(t55a%x%t55a%x%t55a)

k55a=t55akt55a%*%t(t55akt55a)

k55a

t56akt56a=(t56a%x%t56a%x%t56a)

k56a=t56akt56a%*%t(t56akt56a)

k56a

n5=(k51a+k52a+k53a+k54a+k55a+k56a)

n5

Mn51=(1/6*n5)

Mn51###############################moment for binary blends, four ingredients

t61a=rbind(1/3,1/3,1/3,0)####ternary blends

t62a=rbind(1/3,1/3,0,1/3)

t63a=rbind(1/3,0,1/3,1/3)

t64a=rbind(0,1/3,1/3,1/3)
```

```
t61akt61a=(t61a%x%t61a%x%t61a)

k61a=t61akt61a%*%t(t61akt61a)

k61a

t62akt62a=(t62a%x%t62a%x%t62a)

k62a=t62akt62a%*%t(t62akt62a)

k62a

t63akt63a=(t63a%x%t63a%x%t63a)

k63a=t63akt63a%*%t(t63akt63a)

k63a

t64akt64a=(t64a%x%t64a%x%t64a)

k64a=t64akt64a%*%t(t64akt64a)

k64a

n6=(k61a+k62a+k63a+k64a)

n6

Mn61=(1/4*n6)

Mn61 ###################moment for ternary

t71a=rbind(1/4,1/4,1/4,1/4)#####Quarternary blends

t71akt71a=(t71a%x%t71a%x%t71a)

Mn71=t71akt71a%*%t(t71akt71a)

Mn71###############quartenary blends

W=c(4/15,6/15,4/15,1/15)####weights for 4 ingredients

W

###################################Overall moment matrix

Mnn4=((4/15*Mn41+6/15*Mn51+4/15*Mn61+1/15*Mn71),rond='5')

Mnn4

round(Mnn4,5)

##############Coefficient matrix K for four igredients

K81=c(1,rep(0,63))

K81

K82=c(rep(0,21),1,rep(0,42))
```

```
K82

K83=c(rep(0,42),1,rep(0,21))

K83

K84=c(rep(0,63),1)

K84

K85=c(0,rep(1/9,4),rep(0,3),1/9,rep(0,3),1/9,rep(0,3),1/9,rep(0,15),1/9,rep(0,15),1/9,rep(0,15))

K85

K86=c(rep(0,5),1/9,rep(0,11),1/9,0,0,1/9,0,1/9,1/9,0,1/9,rep(0,3),1/9,rep(0,7),1/9,rep(0,15),1/9,rep(0,10))

K86

K87=c(rep(0,10),1/9,rep(0,15),1/9,rep(0,7),1/9,rep(0,3),1/9,0,1/9,1/9,0,1/9,0,0,1/9,rep(0,11),1/9,rep(0,5))

K87

K88=c(rep(0,15),1/9,rep(0,15),1/9,rep(0,15),1/9,rep(0,3),1/9,rep(0,3),1/9,rep(0,3),rep(1/9,4),0)

K88

K89=c(rep(0,6),1/24,1/24,0,1/24,0,1/24,0,1/24,1/24,rep(0,3),1/24,1/24,rep(0,4),1/24,0,0,1/24,1/24,0,1/24,0,
0,1/24,0,1/24,1/24,0,0,1/24,rep(0,4),1/24,1/24,rep(0,3),1/24,1/24,0,1/24,0,1/24,0,1/24,1/24,rep(0,6))

K89

K800=c(K81,K82,K83,K84,K85,K86,K87,K88,K89)

K800

K900=matrix((K800),9,64,byrow=T)

K900

K901=t(K900)#######coefficient matrix K for four ingredients

K901

##############information matrix

Ck4=solve(t(K901)%*%K901)%*%t(K901)%*%Mnn4%*%K901%*%solve(t(K901)%*%K901)

Ck4

L4=solve(t(K901)%*%K901)%*%t(K901)

L4

t(L4)

library(MASS)

Ck4frac=as.fractions(Ck4)

Ck4frac
```

```
##############at point (1, 0, 0, 0)
HS4=c(3,rep(0,12),1/3,rep(0,8),1/3,rep(0,8),1/3,rep(0,4))
HS4
HSS4=matrix(HS4,nrow=4,ncol=9,byrow=T)
HSS4
HSS41=HSS4%*%Ck4%*%t(HSS4)
HSS41
library(MASS)
HSS41frac=as.fractions(HSS41)
HSS41frac
det(HSS41frac)
det(HSS41)^0.25################## D optimal
A001=solve(0.25*sum(diag(solve(HSS41))))
A001############################ A optimal
E001=min(eigen(HSS41)$values)
E001############################ E optimal
T41=1/4*sum(diag(HSS41))
T41
################points(0, 1, 0, 0)
HS41=c(rep(0,5),1/3,rep(0,4),3,rep(0,12),1/3,rep(0,8),1/3,rep(0,3))
HS41
HS41=matrix(HS41,nrow=4,ncol=9,byrow=T)
HS41
HS411=HS41%*%Ck4%*%t(HS41)
HS411
library(MASS)
HS411frac=as.fractions(HS411)
HS411frac
det(HS411)
det(HS411)^0.25################## D optimal
```

```
A04=solve(0.25*sum(diag(solve(HS411))))
A04############################ A optimal
E04=min(eigen(HS411)$values)
E04############################# E optimal
T411=1/4*sum(diag(HS411))
T411
############################points (0,0,1,0)
HS42=c(rep(0,6),1/3,rep(0,8),1/3,rep(0,4),3,rep(0,12),1/3,rep(0,2))
HS42
HSS42=matrix(HS42,nrow=4,ncol=9,byrow=T)
HSS42
HSS422=HSS42%*%Ck4%*%t(HSS42)
HSS422
library(MASS)
HSS422frac=as.fractions(HSS422)
HSS422frac
det(HSS422)^0.25################### D optimal
A400=solve(0.25*sum(diag(solve(HSS422))))
A400############################ A optimal
E400=min(eigen(HSS422)$values)
E400############################# E optimal
###############points (0,0,0,1)
HS43=c(rep(0,7),1/3,rep(0,8),1/3,rep(0,8),1/3,rep(0,4),3,rep(0,5))
HS43
HSS43=matrix(HS43,nrow=4,ncol=9,byrow=T)
HSS43
HSS433=HSS43%*%Ck4%*%t(HSS43)
HSS433
library(MASS)
HSS433frac=as.fractions(HSS433)
```

```
HSS433frac

det(HSS433)

det(HSS433)^0.25################### D optimal

A40=solve(0.25*sum(diag(solve(HSS433))))

A40############################# A optimal

E40=min(eigen(HSS433)$values)

E40############################# E optimal

####################points 1/2, 1/2, 0,0

HB=c(3/4,rep(0,3),1/6,1/12,rep(0,4),3/4,rep(0,2),1/12,1/6,rep(0,7),1/12,1/12,rep(0,2),1/16,rep(0,4),1/12,1/12,0,0,1/16)

HB

HB1=matrix(HB,nrow=4,ncol=9,byrow=T)

HB1

HB11=HB1%*%Ck4%*%t(HB1)

HB11

det(HB11)

library(MASS)

HB11frac=as.fractions(HB11)

HB11frac

det(HB11frac)

det(HB11)^0.25################### D optimal

A41=solve(0.25*sum(diag(solve(HB11))))

A41############################# A optimal

E41=min(eigen(HB11)$values)

E41############################# E optimal

T42=1/4*sum(diag(HB11))

T42

##############################points 1/2,0,1/2,0

HBB=c(3/4,rep(0,3),1/6,0,1/12,rep(0,6),1/12,0,1/12,0,1/16,rep(0,2),3/4,0,1/12,0,1/6,rep(0,6),1/12,0,1/12,0,1/16)

HBB
```

```
HBB1=matrix(HBB,nrow=4,ncol=9,byrow=T)

HBB1

HBB11=HBB1%*%Ck4%*%t(HBB1)

HBB11

det(HBB11)

library(MASS)

HBB11frac=as.fractions(HBB11)

HBB11frac

det(HBB11)^0.25################### D optimal

A42=solve(0.25*sum(diag(solve(HBB11))))

A42############################# A optimal

E42=min(eigen(HBB11)$values)

E42############################# E optimal

T421=1/4*sum(diag(HBB11))

T421

##############points 1/3, 1/3, 1/3, 0

HT=c(1/3,rep(0,3),4/27,1/27,1/27,0,1/36,0,1/3,0,0,1/27,4/27,1/27,0,1/36,0,0,1/3,0,1/27,1/27,4/27,0,1/36,rep
(0,4),1/27,1/27,1/27,0,1/12)

HT

HT1=matrix(HT,nrow=4,ncol=9,byrow=T)

HT1

HT11=HT1%*%Ck4%*%t(HT1)

HT11

library(MASS)

HT11frac=as.fractions(HT11)

HT11frac

det(HT11)^0.25################### D optimal

A43=solve(0.25*sum(diag(solve(HT11))))

A43############################# A optimal

E43=min(eigen(HT11)$values)

E43############################# E optimal
```

```
T43=1/4*sum(diag(HT11))

T43

######################## point 1/4, 1/4, 1/4, 1/4

HF=c(3/16,0,0,0,1/8,rep(1/48,3),3/64,0,3/16,0,0,1/48,1/8,1/8,1/48,3/64,0,0,3/16,0,1/48,1/48,1/8,1/48,3/64,0
,0,0,3/16,rep(1/48,3),1/8,3/64)

HF

HF1=matrix(HF,nrow=4,ncol=9,byrow=T)

HF1

HF11=HF1%*%Ck4%*%t(HF1)

HF11

library(MASS)

HF11frac=as.fractions(HF11)

HF11frac

det(HF11)^0.25###################D

A44=solve(0.25*sum(diag(solve(HF11))))

A44############################ A optimal

E44=min(eigen(HF11)$values)

E44

T44=1/4*sum(diag(HF11))

T44

#################UNIFORM WEIGHTED SIMPLEX CENTROID DESIGNS

########################################################################

Mnuniform1=(1/2*mnnn1+1/2*mnn3)

Mnuniform1################Uniform moment matrix for two ingredients

CKKuniform=solve(KTT%*%t(KTT))%*%KTT%*%Mnuniform1%*%t(KTT)%*%solve(KTT%*
%t(KTT))###information matrix

CKKuniform

###########UNIFORM Moment Matrix for three ingredients

Mnuniform2=(1/3*Mn1+1/3*Mn2+1/3*Mn3)

Mnuniform2

CKKK3=solve(KTT3%*%t(KTT3))%*%KTT3%*%Mnuniform2%*%t(KTT3)%*%solve(KTT3%*
%t(KTT3))####information matrix
```

```
CKKK3

##################################Overall moment matrix for uniform four igredients

Mnuniform4=round((1/4*Mn41+1/4*Mn51+1/4*Mn61+1/4*Mn71),8)

Mnuniform4

Ck4uniform=solve(t(K901)%*%K901)%*%t(K901)%*%Mnuniform4%*%K901%*%solve(t(K901)%*
%K901)

Ck4uniform###information matrix for uniform

###########################################################

############### UNIFORM TWO INGREDIENTS

S1=H11H%*%CKKuniform%*%t(H11H)#######At point (1,0)

S1

det(S1)

##########OPTIMAL VALUE

det(S1)^(1/2)################### D optimal

Au1=solve(1/2*sum(diag(solve(S1))))

Au1############################ A optimal

Eu1=min(eigen(S1)$values)

Eu1############################ E optimal

Tu11=0.5*sum(diag(S1))

Tu11

S11=HF1H%*%CKKuniform%*%t(HF1H)#######At point (1/2,1/2)

S11

det(S11)

##########OPTIMAL VALUE

det(S11)^(1/2)################### D optimal

Au11=solve(1/2*sum(diag(solve(S11))))

Au11############################ A optimal

Eu11=min(eigen(S11)$values)

Eu11############################ E optimal

Tu12=0.5*sum(diag(S11))

Tu12
```

```
###########THREE INGREDIENTS UNIFORM
##########(1,0,0)
S21=HHt2%*%CKK3%*%t(HHt2)
S21
det(S21)
##########OPTIMAL VALUE
det(S21)^(1/3)################### D optimal
Au31=solve(1/3*sum(diag(solve(S21))))
Au31############################ A optimal
Eu31=min(eigen(S21)$values)
Eu31############################ E optimal
Tu21=1/3*sum(diag(S21))
Tu21
######1/2,1/2,0
S2=HHt3%*%CKK3%*%t(HHt3)
S2
det(S2)
##########OPTIMAL VALUE
det(S2)^(1/3)################### D optimal
Au32=solve(1/3*sum(diag(solve(S2))))
Au32############################ A optimal
Eu32=min(eigen(S2)$values)
Eu32############################ E optimal
Tu31=1/3*sum(diag(S2))
Tu31
#############1/3, 1/3, 1/3
S3=HHtt33%*%CKK3%*%t(HHtt33)
S3
det(S3)
##########OPTIMAL VALUE
```

```
det(S3)^(1/3)################### D optimal

Au33=solve(1/3*sum(diag(solve(S3))))

Au33############################ A optimal

Eu33=min(eigen(S3)$values)

Eu33############################ E optimal

Tu33=1/3*sum(diag(S3))

Tu33

#######UNIFORM FOUR INGREDIENTS

########Uniform for Four ingredients

######### 1, 0, 0, 0

S41=HSS4%*%Ck4uniform%*%t(HSS4)

S41

det(S41)

solve(S41)

##########OPTIMAL VALUE

det(S41)^(1/4)################### D optimal

Au441=solve(1/4*sum(diag(solve(S41))))

Au441############################ A optimal

Eu441=min(eigen(S41)$values)

Eu441############################ E optimal

Tu41=0.25*sum(diag(S41))

Tu41

########1/2, 1/2, 0, 0

S42=HB1%*%Ck4uniform%*%t(HB1)

S42

det(S42)

##########OPTIMAL VALUE

det(S42)^(1/4)################### D optimal

Au442=solve(1/4*sum(diag(solve(S42))))

Au442############################ A optimal
```

```
Eu442=min(eigen(S42)$values)

Eu442############################ E optimal

Tu42=0.25*sum(diag(S42))

Tu42

########1/3, 1/3, 1/3, 0

S43=HT1%*%Ck4uniform%*%t(HT1)

S43

det(S43)

##########OPTIMAL VALUE

det(S43)^(1/4)################### D optimal

Au443=solve(1/4*sum(diag(solve(S43))))

Au443############################ A optimal

Eu443=min(eigen(S43)$values)

Eu443############################ E optimal

Tu41=0.25*sum(diag(S43))

Tu41

######## 1/4, 1/4, 1/4, 1/4

S44=HF1%*%Ck4uniform%*%t(HF1)

S44

det(S44)

##########OPTIMAL VALUE

det(S44)^(1/4)################### D optimal

Au444=solve(1/4*sum(diag(solve(S44))))

Au444############################ A optimal

Eu444=min(eigen(S44)$values)

Eu444############################ E optimal

Tu44=0.25*sum(diag(S44))

Tu44

###############MITES MODEL##########################

###1,0,0,0H1000=matrix(c(2.9463,rep(0,12),5.874/3,rep(0,8),6.0502/3,rep(0,8),4.1012/3,0,0,0,0),4,9,byro
w=T)
```

```
H1000

slop1000=H1000%*%Ck4%*%t(H1000)

slop1000

#####Optimal values

det(slop1000)^(1/4)################## D optimal

Aslop1000=solve(1/4*sum(diag(solve(slop1000))))

Aslop1000########################### A optimal

Eslop1000=min(eigen(slop1000)$values)

Eslop1000########################### E optimal

Tslop1000=0.25*sum(diag(slop1000))###T optimal

Tslop1000

#####1/2,1/2,0,0

H2000=matrix(c(0.7366,0,0,0,0.979,0.4895,rep(0,4),0.5596,0,0,0.4895,0.979,rep(0,7),0.5042,0.52185,0,0,0
.0715,rep(0,4),0.33418,0.3034,0,0,0.7007),4,9,byrow=T)

H2000

slop2000=H2000%*%Ck4%*%t(H2000)

slop2000

#####Optimal values

det(slop2000)^(1/4)################## D optimal

Aslop2000=solve(1/4*sum(diag(solve(slop2000))))

Aslop2000########################### A optimal

Eslop2000=min(eigen(slop2000)$values)

Eslop2000########################### E optimal

Tslop2000=0.25*sum(diag(slop2000))###T optimal

Tslop2000

######1/3,1/3,1/3,0

H3000=matrix(c(0.3274,rep(0,3),0.8833,0.2176,0.2241,0,0.0318,0,0.2383,0,0,0.2176,0.8989,0.2319,0,0.03
18,0,0,0.238,0,0.2241,0.2319,0.912,0,0.0318,rep(0,4),0.1519,0.1349,0.2152,0,0.5602),4,9,byrow=T)

H3000

slop3000=H3000%*%Ck4%*%t(H3000)

slop3000
```

```
#####Optimal values
det(slop3000)^(1/4)################## D optimal
Aslop3000=solve(1/4*sum(diag(solve(slop3000))))
Aslop3000########################### A optimal
Eslop3000=min(eigen(slop3000)$values)
Eslop3000########################### E optimal
Tslop3000=0.25*sum(diag(slop3000))###T optimal
Tslop3000
######1/4,1/4,1/4,1/4
H4000=matrix(c(0.1841,0,0,0,0.6677,0.1224,0.126,0.0854,0.333,0,0.1399,0,0,0.1224,0.6574,0.1305,0.0759,0.3027,0,0,0.1339,0,0.126,0.1305,0.755,0.121,0.2675,0,0,0,0.1153,0.0854,0.0759,0.121,0.5647,0.4248),4,9,byrow=T)
H4000
slop4000=H4000%*%Ck4%*%t(H4000)
slop4000
#####Optimal values
det(slop4000)^(1/4)################## D optimal
Aslop4000=solve(1/4*sum(diag(solve(slop4000))))
Aslop4000########################### A optimal
Eslop4000=min(eigen(slop4000)$values)
Eslop4000########################### E optimal
Tslop4000=0.25*sum(diag(slop4000))###T optimal
Tslop4000
##############################################################
####UNIFORM SCD SLOPE
###at point 1,0,0,0
slop1111=H1000%*%Ck4uniform%*%t(H1000)
slop1111
#####Optimal values
det(slop1111)^(1/4)################## D optimal
Aslop1111=solve(1/4*sum(diag(solve(slop1111))))
```

```
Aslop1111############################ A optimal
Eslop1111=min(eigen(slop1111)$values)
Eslop1111############################ E optimal
Tslop1111=0.25*sum(diag(slop1111))###T optimal
Tslop1111
###at point 1/2,1/2,0,0
slop2222=H2000%*%Ck4uniform%*%t(H2000)
slop2222
#####Optimal values
det(slop2222)^(1/4)################### D optimal
Aslop2222=solve(1/4*sum(diag(solve(slop2222))))
Aslop2222############################ A optimal
Eslop2222=min(eigen(slop2222)$values)
Eslop2222############################ E optimal
Tslop2222=0.25*sum(diag(slop2222))###T optimal
Tslop2222
####at point 1/3,1/3,1/3,0
slop3333=H3000%*%Ck4uniform%*%t(H3000)
slop3333
#####Optimal values
det(slop3333)^(1/4)################### D optimal
Aslop3333=solve(1/4*sum(diag(solve(slop3333))))
Aslop3333############################ A optimal
Eslop3333=min(eigen(slop3333)$values)
Eslop3333############################ E optimal
Tslop3333=0.25*sum(diag(slop3333))###T optimal
Tslop3333
#####at point 1/4,1/4,1/4,1/4
slop4444=H4000%*%Ck4uniform%*%t(H4000)
slop4444
```

```
#####Optimal values

det(slop4444)^(1/4)################## D optimal

Aslop4444=solve(1/4*sum(diag(solve(slop4444))))

Aslop4444############################ A optimal

Eslop4444=min(eigen(slop4444)$values)

Eslop4444############################ E optimal

Tslop4444=0.25*sum(diag(slop4444))###T optimal

Tslop4444

####################################################################

L2=matrix(c(1/7,1/140,1/42,1/105,1/140,1/7,1/105,1/42,1/42,1/105,1/105,1/140,1/105,1/42,1/140,1/105),4,
4,byrow=T)

L2

library(MASS)

R=ginv(CKK)

R

L2fr=as.fractions(L2)

L2fr

AV=R%*%L2

AV

APV=sum(diag(AV))

APV

#######Equivalence Theorem

##at point 1,0

f2=matrix(c(1,0,0,0),1,4,byrow=T)

f2

q=f2%*%R%*%L2%*%R%*%t(f2)

q

####at point 0, 1

f20=matrix(c(0,1,0,0),1,4,byrow=T)

f20

q20=f20%*%R%*%L2%*%R%*%t(f20)
```

```
q20

####at point 1/2,1/2

f21=matrix(c(1/8,1/8,1/8,1/8),1,4,byrow=T)

f21

q21=f21%*%R%*%L2%*%R%*%t(f21)

q21

############THREE INGR

R1=solve(CKK3)

R1

L3=matrix(c(1/28,1/560,1/560,1/168,1/672,1/672,1/840,1/560,1/28,1/560,1/672,1/168,1/672,1/840,1/560,1/560,1/28,1/672,1/672,1/168,1/840,1/168,1/672,1/672,1/560,1/840,17/20160,1/1680,1/672,1/168,1/672,1/840,1/560,17/20160,1/1680,1/672,1/672,1/168,17/20160,17/20160,1/560,1/1680,1/840,1/840,1/840,1/1680,1/1680,1/1680,1/2520),7,7,byrow=T)

L3

L3fra=as.fractions(L3)

L3fra

AVV=R1%*%L3

AVV

APPV=sum(diag(AVV))

APPV

###########EQUIVALENCE THEOREM

#####At point 1,0,0

f31=matrix(c(1,0,0,0,0,0,0),1,7,byrow=T)

f31

q31=f31%*%R1%*%L3%*%R1%*%t(f31)

q31

####at point 1/2,1/2,0,

f32=matrix(c(1/8,1/8,0,1/16,1/16,0,0),1,7,byrow=T)

f32

q32=f32%*%R1%*%L3%*%R1%*%t(f32)

q32

####at point 1/3,1/3,1/3
```

```
f33=matrix(c(1/27,1/27,1/27,1/27,1/27,1/27,1/27),1,7,byrow=T)

f33

q33=f33%*%R1%*%L3%*%R1%*%t(f33)

q33

###################FOUR INGRED

R2=solve(Ck4)

R2

LL5=c(1/84,rep(1/1680,3),1/504,rep(1/2520,3),13/40320,1/1680,1/84,rep(1/1680,2),1/2520,1/504,1/2520,1/2520,13/40320,rep(1/1680,2),1/84,1/1680,1/2520,1/2520,1/504,1/2520,13/40320,rep(1/1680,3),1/84,rep(1/2520,3),1/504,13/40320,1/504,rep(1/2520,3),1/1890,rep(1/5040,3),17/120960,1/2520,1/504,rep(1/2520,2),1/5040,1/1890,1/5040,1/5040,17/120960,rep(1/2520,2),1/504,1/2520,rep(1/5040,2),1/1890,1/5040,17/120960,rep(1/2520,3),1/504,rep(1/5040,3),1/1890,17/120960,rep(13/40320,4),rep(17/120960,4),1/12096)

LL5

LL6=matrix((LL5),9,9,byrow=T)

LL6

LLL6=round(LL6,5)

LLL6

AVVV=R2%*%LL6

AVVV

APPPV=sum(diag(AVVV))

APPPV

#######EQUIVALENCE THEOREM

###at point 1,0,0,0

f41=matrix(c(1,0,0,0,0,0,0,0,0),1,9,byrow=T)

f41

q41=f41%*%R2%*%LL6%*%R2%*%t(f41)

q41

#####at point 1/2,1/2,0,0

f42=matrix(c(1/8,1/8,0,0,1/24,1/24,0,0,0),1,9,byrow=T)

f42

q42=f42%*%R2%*%LL6%*%R2%*%t(f42)

q42
```

```
#####at point 1/3,1/3,1/3,0

f43=matrix(c(1/27,1/27,1/27,0,2/81,2/81,2/81,0,1/108),1,9,byrow=T)

f43

q43=f43%*%R2%*%LL6%*%R2%*%t(f43)

q43

#######at point 1/4,1/4,1/4,1/4

f44=matrix(c(rep(1/64,9)),1,9,byrow=T)

f44

q44=f44%*%R2%*%LL6%*%R2%*%t(f44)

q44

#############Uniform APV SIMPLEX CENTROID DESIGNS

##########################

library(MASS)

CU1=ginv(CKKuniform)

CU1

LL2=matrix(c(1/7,1/140,1/42,1/105,1/140,1/7,1/105,1/42,1/42,1/105,1/105,1/140,1/105,1/42,1/140,1/105),
4,4,byrow=T)

LL2

LL2fr=as.fractions(LL2)

LL2fr

AVU=CU1%*%LL2

AVU

APVU=(sum(diag(AVU)))

APVU

########################################

#######Equivalence Theorem

##at point 1,0

ff2=matrix(c(1,0,0,0),1,4,byrow=T)

ff2

qq=ff2%*%CU1%*%LL2%*%CU1%*%t(ff2)

qq
```

```
####at point 0, 1

f200=matrix(c(0,1,0,0),1,4,byrow=T)

f200

q200=f200%*%CU1%*%LL2%*%CU1%*%t(f200)

q200

####at point 1/2,1/2

f211=matrix(c(1/8,1/8,1/8,1/8),1,4,byrow=T)

f211

q211=f211%*%CU1%*%LL2%*%CU1%*%t(f211)

q211

###########THREE UNIFORM

CU2=solve(CKKK3)

CU2

L33=matrix(c(1/28,1/560,1/560,1/168,1/672,1/672,1/840,1/560,1/28,1/560,1/672,1/168,1/672,1/840,1/560,
1/560,1/28,1/672,1/672,1/168,1/840,1/168,1/672,1/672,1/560,1/840,17/20160,1/1680,1/672,1/168,1/672,1/
840,1/560,17/20160,1/1680,1/672,1/672,1/168,17/20160,17/20160,1/560,1/1680,1/840,1/840,1/840,1/1680,
1/1680,1/1680,1/2520),7,7,byrow=T)

L33

L33fra=as.fractions(L33)

L33fra

AVVU=CU2%*%L33

AVVU

APPVU=sum(diag(AVVU))

APPVU

###########EQUIVALENCE THEOREM

#####At point 1,0,0

f311=matrix(c(1,0,0,0,0,0,0),1,7,byrow=T)

f311

q311=f311%*%CU2%*%L33%*%CU2%*%t(f311)

q311

####at point 1/2,1/2,0,

f322=matrix(c(1/8,1/8,0,1/16,1/16,0,0),1,7,byrow=T)
```

```
f322

q322=f322%*%CU2%*%L33%*%CU2%*%t(f322)

q322

####at point 1/3,1/3,1/3

f333=matrix(c(1/27,1/27,1/27,1/27,1/27,1/27,1/27),1,7,byrow=T)

f333

q333=f333%*%CU2%*%L33%*%CU2%*%t(f333)

q333

###########FOUR UNIFORM

CU3=solve(Ck4uniform)

CU3

LL55=c(1/84,rep(1/1680,3),1/504,rep(1/2520,3),13/40320,1/1680,1/84,rep(1/1680,2),1/2520,1/504,1/2520,
1/2520,13/40320,rep(1/1680,2),1/84,1/1680,1/2520,1/2520,1/504,1/2520,13/40320,rep(1/1680,3),1/84,rep(
1/2520,3),1/504,13/40320,1/504,rep(1/2520,3),1/1890,rep(1/5040,3),17/120960,1/2520,1/504,rep(1/2520,2
),1/5040,1/1890,1/5040,1/5040,17/120960,rep(1/2520,2),1/504,1/2520,rep(1/5040,2),1/1890,1/5040,17/120
960,rep(1/2520,3),1/504,rep(1/5040,3),1/1890,17/120960,rep(13/40320,4),rep(17/120960,4),1/12096)

LL55

LL66=matrix((LL55),9,9,byrow=T)

LL66

LLL66=round(LL66,5)

LLL66

AVVV6=CU3%*%LL66

AVVV6

APPPV5=sum(diag(AVVV6))

APPPV5

#######EQUIVALENCE THEOREM

###at point 1,0,0,0

f411=matrix(c(1,0,0,0,0,0,0,0,0),1,9,byrow=T)

f411

q411=f411%*%CU3%*%LL66%*%CU3%*%t(f411)

q411

#####at point 1/2,1/2,0,0
```

```
f422=matrix(c(1/8,1/8,0,0,1/24,1/24,0,0,0),1,9,byrow=T)

f422

q422=f422%*%CU3%*%LL66%*%CU3%*%t(f422)

q422

#####at point 1/3,1/3,1/3,0

f433=matrix(c(1/27,1/27,1/27,0,2/81,2/81,2/81,0,1/108),1,9,byrow=T)

f433

q433=f433%*%CU3%*%LL66%*%CU3%*%t(f433)

q433

#######at point 1/4,1/4,1/4,1/4

f444=matrix(c(rep(1/64,9)),1,9,byrow=T)

f444

q444=f444%*%CU3%*%LL66%*%CU3%*%t(f444)

q444

##############################I-OPTIMUM FOR MITES EXPERIMENTS

Rm1=c(0.011482,0.000436,0.000417,0.0003595,0.01040922,0.00216946,0.00235601,0.00167939,0.00224
7316)

Rm1

Rm2=c(0.000436,0.006626,0.000317,0.000273,0.001660378,0.00778549,0.0018212439,0.001207734,0.00
15997812)

Rm2

Rm3=c(0.000417,0.000317,0.006069,0.0002614,0.001613876,0.0016321983,0.00855742,0.001462906,0.0
014110602)

Rm3

Rm4=c(0.0003595,0.000273,0.0002614,0.004504,0.001152466,0.001086237,0.00144618,0.00551295,0.00
16763549)

Rm4

Rm5=c(0.01040922,0.00216946,0.00235601,0.00167939,0.015200654,0.01345283,0.006691902,0.004288
859,0.00523233)

Rm5

Rm6=c(0.001660378,0.00778549,0.0018212439,0.001207734,0.0134528,0.001481095,0.006790385,0.003
97488,0.004877308)

Rm6
```

```
Rm7=c(0.001613876,0.001632198,0.00855742,0.001462906,0.006691902,0.006790385,0.019310373,0.005850755,0.00605334)

Rm7

Rm8=c(0.001152466,0.001086237,0.00144618,0.00551295,0.0042885939,0.00397488,0.005850755,0.010911412,0.0051308209)

Rm8

Rm9=c(0.002247316,0.0015997812,0.0014110602,0.0016763549,0.00523233,0.004877308,0.00605334,0.0051308209,0.0043776)

Rm9

RMM=matrix(c(Rm1,Rm2,Rm3,Rm4,Rm5,Rm6,Rm7,Rm8,Rm9),9,9,byrow=T)

RMM

RM=round(RMM,7)

RM

AVRMM=R2%*%RM

AVRMM

AVRM=round(AVRMM,7)

AVRM

APVRM=sum(diag(AVRM))

APVRM

#######################################Uniform Weights

AVRMMU=CU3%*%RM

AVRMMU

AVVRMMU=round(AVRMMU,7)

AVVRMMU

APPRMU=sum(diag(AVVRMMU))

APPRMU

#########Equivalence

###at point 1,0,0,0

F411=matrix(c(0.9821,0,0,0,0,0,0,0,0),1,9,byrow=T)

F411

QQ411=F411%*%R2%*%RM%*%R2%*%t(F411)

QQ411
```

```
#####at point 1/2,1/2,0,0

F422=matrix(c(0.12276,0.09326,0,0,0.24475,0.24475,0,0,0),1,9,byrow=T)

F422

QQ422=F422%*%R2%*%RM%*%R2%*%t(F422)

QQ422

#####at point 1/3,1/3,1/3,0

F433=matrix(c(0.03637,0.02762,0.02644,0,0.147214,0.10148,0.152004,0,0.01059),1,9,byrow=T)

F433

QQ433=F433%*%R2%*%RM%*%R2%*%t(F433)

QQ433

#######at point 1/4,1/4,1/4,1/4

F444=matrix(c(0.01534,0.01165,0.01115,0.00961,0.08346,0.082175,0.09438,0.07058,0.11066),1,9,byrow=
T)

F444

QQ444=F444%*%R2%*%RM%*%R2%*%t(F444)

QQ444

######################UNIFORM

###at point 1,0,0,0

F411=matrix(c(0.9821,0,0,0,0,0,0,0,0),1,9,byrow=T)

F411

Q411=F411%*%CU3%*%RM%*%CU3%*%t(F411)

Q411

#####at point 1/2,1/2,0,0

F422=matrix(c(0.12276,0.09326,0,0,0.24475,0.24475,0,0,0),1,9,byrow=T)

F422

Q422=F422%*%CU3%*%RM%*%CU3%*%t(F422)

Q422

#####at point 1/3,1/3,1/3,0

F433=matrix(c(0.03637,0.02762,0.02644,0,0.147214,0.10148,0.152004,0,0.01059),1,9,byrow=T)

F433

Q433=F433%*%CU3%*%RM%*%CU3%*%t(F433)
```

```
Q433

#######at point 1/4,1/4,1/4,1/4

F444=matrix(c(0.01534,0.01165,0.01115,0.00961,0.08346,0.082175,0.09438,0.07058,0.11066),1,9,byrow=
T)

F444

Q444=F444%*%CU3%*%RM%*%CU3%*%t(F444)

Q444

CKK3=solve(KTT3%*%t(KTT3))%*%KTT3%*%Mn11%*%t(KTT3)%*%solve(KTT3%*
%t(KTT3))####information matrix

CKK3

CKKK3=solve(KTT3%*%t(KTT3))%*%KTT3%*%Mnuniform2%*%t(KTT3)%*%solve(KTT3%*
%t(KTT3))####information matrix

CKKK3
```