OPTIMAL SLOPE DESIGNS FOR SECOND DEGREE KRONECKER MODEL MIXTURE EXPERIMENTS WITH APPLICATION IN BLENDING OF SELECTED FRUITS

By

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DECLARATION

Declaration by Candidate

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To my ambitious daughters: Stellah Nyagûthiî, Abigael Njeri, Agnes Wanjirû and Ashley Nyambura.

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ABSTRACT

Response surface methodology is a set of techniques that includes setting up a series of experiments that yields adequate and reliable measurements of the response of interest, determine a model that best fits the data collected from the experimental design chosen and determine the optimal settings of the experimental factors that produce the maximum (or minimum) value of response. The aim of the study was to investigate D- and A- optimal slope designs in the second degree Kronecker model for mixture experiments with assumptions that the errors are independent and with constant variance. The objectives of study were to obtain: equivalence relation that serve as the necessary and sufficient condition for the existence of optimal slope designs; optimal slope designs for the D- and A-optimality criteria and numerical optimal weighted centroid designs and to demonstrate the practical use of generated design in analysis of data obtained from a designed experiment on fruit blending. The equivalence relation was proved using matrix algebra. Support points, elementary centroid designs, coefficient, moment, information and slope matrices, were used to derive optimal designs. D- and A-optimal designs were employed to generate numerical optimal designs. The data collected from the designed experiment were analyzed using SAS (Version 8) software. As a result, the study was able to obtain generalized optimal slope design for a mixture experiment with at least two ingredients. The Kronecker models fitted to the data from the experiment on fruit blending explained the variation adequately well with coefficients of determination 98.2, 96.3 and 96.67 percent for the blend of two, three and four ingredients respectively. Kronecker model with the weighted centroid design is very economical considering the few support points that are necessary for a particular number of ingredients experiment. In conclusion, the findings of this study strongly supports the use of the form of the Kronecker model discussed to analyze the response surfaces for mixture experiments. The study therefore highly recommends use of these models to describe juice qualities that depend on variations in mixture amounts.

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CHAPTER ONE

1.0 Introduction

This study deals with the exploration and optimization of response surface. This is a problem faced by experimenters in many technical fields, where in general the response of interest is affected by a set of predictor variables. Experiments are performed by investigators in virtually all fields of inquiry, usually to discover something about a particular process or system.

An experiment is a test or a series of tests in which purposeful changes are made to the input variables of a process so that we may observe and identify the reasons for changes that may be observed in the output response. The objectives of the experiment may include determining:

i. Which variables are most influential on the response
ii. Where to set the independent variables so that the response is almost near the desired nominal value
iii. Where to set the influential factors so that variability in response is small
iv. Where to set the controllable factors so that the effects of uncontrollable factors are minimized.

1.1 Response Surface Methodology

Response Surface Methodology (RSM) is a collection of mathematical and statistical techniques that are useful for modeling and analyzing a problem in which a response of interest is influenced by several variables with the objective of optimizing this response, Montgomery (2001). The optimum value may be a maximum or minimum value depending on the problem at hand. In most RSM problems, the form of the relationship between the response and the independent variables is unknown. Thus the first step is to find a suitable approximation for the true functional relationship between the response and the set of independent factors. Usually, a low-order polynomial in some region of the independent factors is employed. To fit polynomials to the response surfaces the researcher employs response surface designs.

RSM is a sequential procedure. Often the exodus is a point on the response surface that is remote from the optimum. The objective is to lead the experimenter rapidly and efficiently along the path of improvement toward the general vicinity of the optimum. Once the region of the optimum has been found, a second-order model may be employed. Then an analysis is performed to locate the optimum. (Montgomery (2001)).

The eventual objective of the RSM is to determine the optimum operating conditions for the system or to determine the region of the factor space in which operating requirements are satisfied.

1.2 Mixture Experiments

A mixture experiment is a special type of response surface experiments in which the factors are the ingredients or components of a mixture and the response is a function of the proportions of each ingredient. These proportional amounts of each ingredient are typically measured by weight, volume, mole ratio and so forth, Montgomery (2001).

In general, suppose that the mixture consist of m ingredients and let x_i represent the proportion of the *ith* ingredient in the mixture. Then, we must require that $x_i \geq 0,\ i = 1, 2, ..., m$ and $\sum_{i=1}^{m} x_i = 1$. The latter constraint makes the levels of the factors x_i interdependent as opposed to the usual response surface experiments where the factors are purely independent. The experimental region for a mixture problem is a simplex, which is a regularly sided figure with m vertices in $m-1$ dimensions. Scheffe'

(1958) laid the foundation for the development of mixture tools (design and models) by introducing the simplex lattice designs and their associated canonical polynomials.

1.3 Simplex Designs

Simplex designs or mixture designs are used to study the effects of mixture components on the response variable. A $\{p, m\}$ simplex lattice design for p components consists of points designed by the following coordinate settings; the proportions assumed by each component take the (m+1) equally spaced values from 0 to 1, $x_i = 0, \frac{1}{m}, \frac{2}{m}, ..., 1, \ i = 1, 2, ..., p$ and all possible combinations (mixtures) of these proportions are used, Montgomery (2015).

In general the number of points in a $\{p, m\}$ simplex lattice design is $\binom{p+m-1}{m}$. In a simplex centroid design there are $2^p - 1$ points corresponding to the p permutations of (1, 0, 0, …, 0) pure blends, the $\binom{p}{2}$ permutations of $\left(\frac{1}{2}, \frac{1}{2}, 0, 0, ..., 0\right)$ binary blends, $\binom{p}{3}$ permutations of $\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0, ..., 0\right)$ ternary blends, …. and the overall centroid $\left(\frac{1}{p}, \frac{1}{p}, \frac{1}{p}, ..., \frac{1}{p}\right)$. See Scheffe’ (1963) for more details.

The simplex factor space is a straight line for two factors. For three factors, the simplex factor space is an equilateral triangle. The coordinate system used for the values $x_i \geq 0, \ i = 1, 2, ..., m$ is called simplex coordinate system. The geometric description of the factor space containing the m-components consists of all points on or inside the boundaries (vertices, edges, faces, etc.) of a regular (m - 1) dimensional simplex

After considering Scheffe's designs, Murty and Das (1968) developed symmetric-simplex designs. Saxena and Nigam (1973) came up with symmetric-simplex block designs for experiments with mixtures. Cornell (1975) proposed the use of axial designs. Axial designs comprise mainly of complete mixture or q - component blends where most of the points are positioned inside the simplex. An axial design's points are positioned only on the components axes. The designs are useful when an inquest involves measuring component effects.

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, Cornell (2002). Cornell (2002) lists a number of the products where two or more ingredients are combined by ratio in order to obtain an end product.

1.4 Weighted Centroid Designs

An alternative to simplex-lattice designs are simplex centroid designs which were introduced by Scheffe` (1963). The j[th] elementary centroid design $\eta_j, \quad j \in \{1,...,m\}, \quad m \geq 2$ is the uniform distribution on all points taking the form, $\frac{1}{j}\sum_{i=1}^{j} e_k \in T_m$ with $1 \leq k_1 < k_2 < \cdots < k_j \leq m$.

A convex combination, $\eta(\alpha) = \sum_{j=1}^{m} \alpha_j \eta_j$ with $\alpha = (\alpha_1,..., \alpha_m)' \in T_m$ is called a weighted centroid design with weight vector α restricted by $\sum_{i=1}^{m} \alpha_i = 1$. Weighted centroid designs are exchangeable, that is, they are invariant under permutations, see Klein (2004). The weighted centroid designs are a fundamental concept for this study.

1.5 Models for Mixture Experiments

Mixture models contrast with the regular polynomials employed in response surface methodology because of the restriction, $\sum_{i=1}^{m} x_i = 1$ for a mixture of m ingredients. A major impact of this constraint being that the linear models do not have an intercept. Otherwise the regression coefficients cannot be estimated uniquely. Scheffé (1958) came up with acknowledged polynomials for simplex-lattice designs by altering the usual models in x_i by employing the ingredients condition, to have models without an intercept. It has to be appreciated that Scheffés polynomial models are sufficient for good systems.

Draper and Pukelsheim (1998) came up with a set of regression functions for mixture experiments called Kronecker or K-models. These models are based on Kronecker algebra. Let $\underset{\sim}{t} = (t_1,...,t_m)'$ be an $m \times 1$ vector representing the ingredients in a mixture. The Kronecker square is an $m^2 \times 1$ vector of cross products $t_i t_j$ arranged lexicographically as;

$$\underset{\sim}{t} \otimes \underset{\sim}{t} = (t_1 t_1 \;\; t_1 t_2 \cdots t_1 t_m \;\; t_2 t_1 \;\; t_2 t_2 \;\cdots t_2 t_m \cdots t_m t_1 \;\; t_m t_2 \cdots \; t_m t_m)' \; .$$

The symmetry is attained along with the replication of terms.

K-models have outstanding symmetries and compacted representation and are consistent model functions. Draper and Pukelshiem (1999) and Prescott *et al.* (2002) lists numerous merits of the Kronecker model, in particular the similarity of regression terms and reduced ill-conditioning of information matrices. Any mixture experiment with projected response, when analyzed by means of K-models is homogeneous in ingredients.

1.6 Statement of the Problem

Blend experiment strategy procedures are presented by Cornell (2002) for simplex and polyhedral regions. Subsequent to selecting appropriate design and performing mixture experiments, is fitting models used to screen the components, predict response(s), determine ingredients effects on the response(s), or optimize the response(s) over the experimental region.

Scheffé (1958) came up with linear mixture model in which the coefficient estimate for a component is the predicted value of the response for that pure component. Darroch and Waller (1985) presented D-optimal axial designs for quadratic and cubic additive mixture models. Snee and Marquardt (1974) and Chan *et al.* (1998) compared the saturated D-optimal axial design and D-optimal design for the quadratic model on the basis of their efficiency and uniformity. Cox (1971) suggested a linear mixture model in which the coefficient estimate for an ingredient is the projected difference in the response at the pure ingredient and a pre-specified reference mixture. Component Slope Linear Mixture (CSLM) regression function was postulated by Greg (2007). In the CSLM model, the coefficient parameter for an ingredient is the estimated gradient of the response surface in the Cox effect direction for the ingredient. Wambua et. al. (2017), presented optimal values for the Slope Optimal Design for Second Degree Kronecker Model Mixture Experiment with three factors for a maximal parameter subsystem with the interaction parameter is scaled by two. From the reviewed literature there lacks information on optimal slope designs for the second degree Kronecker model mixture experiments for maximal parameter subsystem where the interaction coefficient is scaled by the number of ingredients in the model. This study sought to fill this knowledge gap. Thus the concept of slope was extended to second degree polynomial regression and choice of optimal designs. The information matrices are directly linked to slope matrices to derive the slope optimal information for the weighted centroid designs.

1.7 General Objective

The overall objective of the study was to determine optimal slope designs for second degree Kronecker model mixture experiments with application in juice blending using selected fruits.

1.8 Specific Objectives

The specific objectives of the study were to:

(i) Derive equivalence theorem for existence of $\phi_p -$ optimal slope mixture designs.

(ii) Derive optimal slope weighted centroid designs for second degree Kronecker model for mixture experiments for the D- and A-optimality criteria.

(iii) Obtain numerically $\phi_p -$ optimal slope weighted centroid designs for the maximal parameter subsystem.

(iv) Demonstrate the practical use of optimal slope weighted centroid design to analyze data from a designed experiment on fruit blending.

1.9 Research Questions

The study was guided by the following research questions:

i) What is the equivalence condition for the existence of optimal slope mixture designs?

ii) Are there D- and A- optimal slope weighted centroid designs for the second degree Kronecker model mixture experiments?

iii) Can the proposed Kronecker model adequately describe blended juice quality data?

1.10 Research Hypotheses

The study demonstrates the application of the Kronecker model in describing the response (attributes of interest) describing juice quality based on personal preference. The data must be assessed for compliance to model requirements and the model be tested on whether it adequately describe the response. The following null hypotheses were thus tested:

i) The juice blending data are not normally distributed

ii) The Kronecker model does not adequately describe the response in the juice blending data

iii) The Kronecker model regression parameters that describe the response in the juice blending data are not significant

1.11 Scope of the Study

In recognition of the strong property that the class of weighted centroid designs is essentially complete (Klein (2004)), the study was restricted to weighted centroid designs, with the second degree Kronecker model as put forward by Draper and Pukelsheim (1998). We present a group of weighted centroid designs and characterize the feasible weighted centroid designs for the maximal parameter subsystem for the mixture regression equation with two or more ingredients. After obtaining the feasible weighted centroid designs, the slope information matrices of the designs are obtained. D- and A-optimal slope weighted centroid designs are then derived from the information matrices with the help of the equivalence condition. The study also demonstrates the use of the Kronecker model in describing the sensory attributes of blended juice from selected fruits.

1.12 Significance of the Study

Many blends are mixtures of different ingredients. In these mixtures the response is dependent on the ratio of the ingredient in the blend. Mixture experiments are often conducted to come up with product formulations with desirable or optimum responses. A *mixture experiment* involves mixing the ingredients in various proportions within a composition region of interest and recording the response(s) for each mixture. The ingredients are presumed to affect the response only through the proportions in which they are mixed. Competing designs arise. This study puts forward optimal slope designs for use in describing dependent factor(s) in mixture experiments.

CHAPTER TWO

LITERATURE REVIEW

2.0 Introduction

This chapter reviews the relevant theoretical and empirical literature applicable to the study

2.1 Response Surface Designs

Response Surface Methodology (RSM) was established by Box and Wilson (1951) to help in the enhancement of manufacturing procedures in the chemical industry. In RSM mathematical and statistical tools are used formulate models and analyze data from experiments with intensions of gaining optimal the response, Montgomery (2015). A mixture of factors impacts the response through the ratios in which they are blended together. The response is a measurable quality or property of interest on the product. In this study it is assumed that, the experimenter can measure quantities of the ingredients in the mixture accurately. It is further assumed that, the responses are functionally related to the blend composition and that, by varying the composition through the changing of ingredients amounts, the responses will also vary. The experimenter's motives to studying regression equations linking the response and the controllable factors are to;

i. determine whether some combination of the factors can be considered best in some sense
ii. gain a better understanding of the overall system by studying the roles the different factors in the system.

Classical experimental designs deal with comparative experiments where effects of various treatments are compared and estimation of treatment contrasts done. On the contrary, for response surface designs, treatments are various combinations of different levels of the factors that are quantitative. Here the main objective of the experimenter is to estimate the absolute response or the parameters of a functional relationship between the response and the ingredients.

Rotatable designs (like weighted centroid designs) have the good characteristic that the variance of the estimated response is constant at points equidistant from the centre of the factor space after transformation when required. Rotatable designs generate data from the response surface that are equally spaced in all directions and are therefore useful when no or little knowledge is available about the nature of the response surface. The class of rotatable designs is also very rich in the sense that under many normally employed criteria, the optimal designs for polynomial regression functions over hyperspherical regions may be found within this class, Kiefer (1960).

Draper and Pukelshiem (1999) studied the Kiefer design ordering of simplex designs for first and second degree mixture models by discussing the improvement of a given design in terms of increasing symmetry as well as finding a larger moment matrix in the Loewner ordering of matrices. The two criteria collectively explain the Kiefer design ordering. Draper and Pukelshiem (1999) prove that for the second-degree mixture model, the set of weighted centroid designs form a convex complete class for the Kiefer ordering. For four ingredients, the class is minimal complete and for at least five ingredients, the set of weighted centroid design is complete. Klein (2004) presented optimal weighted centroid designs for second degree Kronecker model mixture experiments.

Chan (2000) presented analytical and numerical results of optimal designs for various regression equations for experiments with mixtures. Cornell (2002) availed a remarkable result on study of designs and alternative model forms. Prescott (2008) demonstrated the use of nearly uniform designs to model mixture experiments.

In many designed experiments, resources constraints often force certain factors to be much harder to change than others. A good method to this constrains randomization thereby forming a split-plot structure. Geoffrey, *et al.* (2018) showed how the common central composite design can be modified to accommodate the split-plot structure. They also established conditions to make ordinary least squares and weighted least squares estimates similar. The consequence is that standard experimental design software can be used to analyze second-order response surfaces.

In response surface experiments, the principal interest is on prediction compared with parameter estimation since the points on the fitted surface are predicted responses. In choosing optimal designs, it's important to concentrate on predictive competence of the designs, Bradley J. and Peter Goos (2017). Lee *et al.* (2006) utilized response surface methodology to optimize the enzymatic interpretation process of banana juice.

Mukesh, *et al.* (2016) employed RSM involving Box-Behnken Design to optimize process coefficients in production of an extracellular acidic pectin methylesterase on dried papaya peel under solid state fermentation. Rahul, C. *et al.* (2018) employed RSM to investigate parameters in transesterification experiment. Olusola, *et al.* (2019) demonstrated use of RSM in optimizing coagulation process of surface water using *Moringa Oleifera* seed. Mert Gülüm *et al.* (2019) relied on concepts in RSM in determining optimum reaction parameters to model biodiesel production process mathematically.

2.2 Optimal Designs

The exodus of development of optimal designs for regression problems can be traced to Smith (1918). Kiefer (1959) formulated computational steps necessary for selecting optimum designs in regression problems of statistical inference. Cornell (1975) introduced the concept of axial designs which are very useful when measuring the effects of the components. Snee and Marquardt (1974), discussed the usefulness of extreme vertices designs in experimentation with mixtures when the response surface is well captured by a linear model. Chan *et al*. (1998) considered D-optimal axial designs for quadratic and cubic additive mixture functions which were invented by Darroch and Waller (1985) and compared the saturated D-optimal axial design and D-optimal design for the quadratic model in relation to their efficiency and uniformity.

Prescott and Draper (1998) deliberated the case when the researcher is not able to explore the entire simplex due to the additional upper and lower bound constraints imposed on factors in the mixture for Scheffé's quadratic equation. Prescott and Draper (1998) remedied the predicament by proposing D-optimal orthogonal block designs and demonstrated how to simplify the restricted region using pseudo components by developing designs for the specifics scenario where the lower bound is located at the origin for all but one ingredients. Aggarwal and Singh (2006) found D-optimal designs in two orthogonal blocks for Darroch and Waller's (1985) quadratic model in constrained mixture blends.

Hilgers (2000), Cornell (2002) and Hilgers and Heiligers (2003) described various situations where Becker (1968) three mixture models were employed and emerged a better fit than the polynomial models. Aggarwal *et al.* (2013) present D-, A- and E-optimal orthogonal block designs for four mixture components in two experimental conditions for Becker's models and K-model.

Chan et. al. (1998a) introduced A-optimal weighted simplex-centroid designs for Darroch and Waller"s (1985) quadratic polynomial model. Chan *et al.* (1998b) obtained D-optimal saturated axial designs for quadratic and cubic additive mixture models. Aggarwal et. al. (2008) studied orthogonal blocking of blends for Darroch and Waller's quadratic model using F-squares in some components which assume equal volume fraction. Aggarwal et. al. (2008) have also given the D-, A- and E-optimalities of the different designs with four ingredients.

Yuanzhi, *et al.* (2019), advanced original multistage optimization procedure to construct D-optimal designs. This involved a two phased protocol. First was to device conventional point and co-ordinate exchange algorithm. Second, to develop a unique multistage optimization process to construct D-optimal designs. They also applied their designs to experiments with non-linear regression models.

2.3 Optimal Slope Designs

It is imperative to recognize that in response surface designs the main interest of the experimenter may not be limited to the response at distinct points. Sometimes, the differences between the responses at various locations may be the key interest (Herzberg (1967), Box and Draper (1980), Mukerjee and Huda (1985) and Huda (2006a).

If focus is in the difference between responses at points close together in the factor space, the estimation of instantaneous slopes of the response surface becomes crucial. Estimation of slopes is particularly pertinent when the researcher intends to establish optimal settings of the factors so as to realize the optimal value of the response.

Atkinson (1970) introduced research into designs for estimating slopes. Subsequently, Ott and Mendenhall (1972), Murty and Studden (1972), Myers and Lahoda (1975), Mukerjee and Huda (1985) later contributed concepts geared towards realization of optimal design of experiments for estimating slopes. A detailed appraisal of the past studies in this field is provided in Huda (2006b).

Alam, *et al.* (2014) developed two methods of constructing multifactor mixture experiments. First, they developed an algorithm for constructing efficient designs with few support points using Kronecker product of single factor mixture designs. Secondly, they constructed multifactor designs using Kronecker sum of matrices for designs where all the factors have equal number of ingredients. They demonstrated how the developed designs can be utilized to fit second order model.

Rabinda N. Das, *et al.* (2015) gives an elaborate discussion and analysis of robust slope-rotatable designs. Huda and Benkherouf (2016) utilized the D-minimax criterion to derive optimal designs of experiments focusing on estimation of slope of a response surface. Huda and Fatemah (2019) employed the minimax criterion to maximize variance of slope at a point over all design points to estimate slope of response surface. Huda and Fatemah (2019) explored the efficiencies of exact optimal designs under the minimax criterion.

Mitra, *et al.* (2020) utilized RSM simulations with bed slopes, attack angle and drift angle as key factors to analyze the hydrodynamic performance of autonomous underwater vehicles. Rajyalakshmi and Victorbabu (2018), constructed a second order slope rotatable design tri-diagonal correlated errors by means of symmetrical unequal block arrangements with two unequal block sizes.

Many practical problems relate to investigation of a mixture of m ingredients, presumed to impact on the response only through the amounts in which they are blended together. The m factors, t_1, t_2, …, t_m are such that $t_i \geq 0$ and subject to the simplex constriction $\sum_{i=1}^{m} t_i = 1$. The conclusive text by Cornell (1990) provides plentiful examples and give a thorough discussion of both theory and practice. Earlier study by Scheffe' (1958, 1963) recommended and analyzed recognized model forms when the regression equation for the predictable response is a polynomial of degree one, two or three.

Scheffé (1958) devised undisputed polynomials for simplex-lattice designs by adjusting the normal models in x_i with the help of the simplex limitation $\sum_{i=1}^{m} x_i = 1$. For instance, a linear model for three factors whose quantities are symbolized by x_1, x_2 and x_3. The expected linear response is,

$$E(y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 . \quad \text{(2.1)}$$

With the simplex restriction, the intercept can be written as,

$$\beta_0 = \beta_0 (x_1 + x_2 + x_3) . \quad \text{(2.2)}$$

This then implies that (2.1) becomes;

$$E(y) = (\beta_0 + \beta_1) x_1 + (\beta_0 + \beta_2) x_2 + (\beta_0 + \beta_3) x_3 = \beta'_1 x_1 + \beta'_2 x_2 + \beta'_3 x_3 , \quad \text{(2.3)}$$

so that the intercept is removed from the model.

Scheffe' (1958) proposed a second order model;

$$E(y) = \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m-1} \sum_{j=1}^{m} \beta_{ij} x_i x_j \quad \text{(2.4)}$$

It has to be appreciated that Scheffé's polynomial models are satisfactory for good systems.

Let $1_m=(1, \ldots, 1)' \in \Re^m$ be the unity vector. Thus the experimental conditions $t=(t_1, t_2, \ldots, t_m)$ with $t_i \geq 0$ of a mixture experiments are points in the probability simplex,

$$T_m = \{t = (t_1, \quad t_2, \quad \ldots, \quad t_m)' \in [0, \quad 1]^m : 1_m' t = 1\} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2.5)$$

Under experimental conditions, $t \in T_m$, the response Y_t is taken to be a scalar randomvariable. Replications under similar conditions and responses from separate experimental settings are taken to be of equal (unknown) variance and independent.

An experimental design τ on the experimental domain T_m is a probability measure with a finite number of support points. If τ assigns weights $w_1, w_2, \ldots$ to its points of support in T_m , then the experimenter is instructed to draw proportions $w_1, w_2, \ldots$ of all observations under the respective experimental settings.

Draper and Pukelsheim (1998) suggested the second-degree Kronecker model as an adequate polynomial regression model for mixture experiments. Its regression equation is,

$$f : T_m \to \Re^{m^2}; t = (t_1, \quad t_2, \quad \ldots, \quad t_m)' \to t \otimes t = t_i t_j, \text{ i,j=1, …, m, } \ldots\ldots\ldots\ldots\ldots\ldots(2.6)$$

with the index pairs (i, j), $1 \leq i < j \leq m$ ordered lexicographically. The equation is a smooth functional relationship:

$$E(Y_t) = f(t)'\theta = \sum_{i=1}^{m} \theta_{ii} t_i^2 + \sum_{\substack{i,j=1 \\ i<j}}^{m} (\theta_{ij} + \theta_{ji}) t_i t_j \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2.7)$$

where Y_t, the response under experimental condition $t \in T_m$, is taken to be a real-valued random variable and $\theta = (\theta_{11}, \quad \theta_{12}, \quad \ldots, \quad \theta_{mm}) \in \Re^{m^2}$ an unknown parameter. All observations taken in an experiment are assumed to be independent and to have constant variance $\sigma^2 \in (0, \infty)$.

Draper and Pukelsheim (1998) put laid down merits of the Kronecker model. Particularly that it has a more compact notation, more convenient invariance properties and the homogeneity of regression terms. The Kronecker model also has reduced ill-conditioning of information matrices as revealed by Draper and Pukelshiem (1999) and Prescott *et al.* (2002). The moment matrix $M(\tau) = \int_{\tau} f(t) f(t)' d\tau$ for the Kronecker model of degree two has all entries homogeneous of degree four. This matrix reflects the statistical properties of a design τ.

Pukelsheim (1993) examines the general design environment. Klein (2004) asserts that the class of weighted centroid designs is fundamentally complete for a design with at least two factors for the kiefer ordering. Cheng, S. C. (1995) presented results for moment matrices of designs over permutation invariant groups that showing the group is a complete set. Consequently, the search for optimal designs may be limited to weighted centroid designs for most criteria. For specific criteria applied to mixture experiments see Kiefer (1959, 1975, 1978). Galil and Kiefer (1977) compared simplex designs for second degree mixture models.

Weighted centroid designs were presented by Scheffe’ (1963). These designs are exchangeable and hence invariant under permutations as proven by Klein (2004).

Klein (2004) abridged the work by Draper and Pukelsheim (1999) and Draper, Heiligers and Pukelsheim (2000) by a concept that asserts the importance of weighted centroid design for the Kronecker model. The researcher demonstrated that, in the second degree Kronecker model for mixture experiments with at least two factors, the class of weighted centroid designs is a fundamentally complete class. That is, for every p $\in$ [-∞ ;1] and for every design $\tau \in$ T there exists a weighted centroid design η with $(\phi_p \circ C_k \circ M)(\eta) \geq (\phi_p \circ C_k \circ M)(\tau)$.

Thus for every design $\tau \in$ T there is a weighted centroid design η with a moment matrix M(η) improved upon M(τ) in the kiefer ordering. See also Draper, Heiligers and Pukelsheim (1998).

Under the kiefer ordering, a moment matrix M is said to be more informative than a moment matrix N if M is greater than or equal to some intermediate matrix F under the loewner ordering, and F is majorized by N under the group that leaves the problem invariant:

$$M >> N \Leftrightarrow M >> F \prec N \text{ for some matrix F.}$$

Two moment matrices M and N are said to be kiefer equivalent when M>>N and N>>M. We call M kiefer better than N when M>>N without M and N being equivalent. A design τ is kiefer better than a design ξ if and only if M(τ) is kiefer better than M(ξ).

For the information matrix obtained, the matrix is an improvement of a given design in terms of increasing symmetry and that it is a larger moment matrix under the loewner ordering. These two criteria demonstarte that the information matrix realized is kiefer optimal for $K'\theta$, the parameter subsystem of interest.

2.4 General Design Problem

The problem of discovering a design with maximum information on the parameter subsystem $K'\theta$ can be expressed as;

Maximize $\varphi_p(C_k(M(\tau)))$ with $\tau \in T$

Subject to $C_k(M(\tau)) \in PD(s)$ $\tau \in T$

where T denotes the set of all designs T_m and $PD(s)$ denotes the set of $s \times s$ positive definite matrices. The side condition $C_k(M(\tau)) \in PD(s)$ is equal to the existence of an unbiased linear estimator for $K'\theta$ under τ, Pukelsheim (1993). In which case, the design τ is said to be feasible for $K'\theta$. Any design solving the problem above for a fixed p∈ (-∞, 1] is called $\phi_p - optimal$ for $K'\theta$ in T. For all p∈ (-∞, 1], the existence of $\phi_p - optimal$ design for $K'\theta$ is guaranteed by Theorem 7.13 in Pukelsheim (1993). The formulation allows for estimation of the maximal parameter subsystem that is unbiased. It also then points to the existence of optimal slope designs with the necessary adjustments to the information matrices to include the slope aspect.

CHAPTER THREE

METHODOLOGY

3.0 Introduction

Mixture experiments are allied with the examination of the m factors, assumed to influence the response only through quantities 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 region is the probability simplex,

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

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 of the response $E(Y_t)$ is a polynomial equation in t.

3.1 Equivalence Theorem

The equivalence theorem provides the necessary and sufficient conditions for the existence of $\phi_p -$ optimal slope mixture designs. The assertion of the theorem statement is that a weighted design $\eta(\alpha)$ is $\phi_p - slope\, optimal$ for $K'\theta$ in T if and only if;

$$trace H_0 C_j C^{p-1} H_0' \begin{cases} = trace H_0 C^p H_0' & for\ all\ j \in \partial(\alpha) \\ \leq trace H_0 C^p H_0' & otherwise \end{cases} \quad , \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.1)$$

with proper definition of information matrices C and adjusted slope matrix H_0 was proven by employing the properties of symmetric matrices. The information matrices involved are a linear mapping, therefore taking trace as the information function, the theorem was algebraically demonstrated.

To prove the equivalence theorem, sufficient conditions available from the following two theorems are applied.

Theorem 3.1

Let $\alpha \in T_m$ be the weight vector of a weighted centroid design $\eta(\alpha)$ which is feasible for $K'\theta$ and let $\partial(\alpha) = \{j = (1,2,\cdots,m : \alpha_j > 0)\}$, be a set of active indices. Furthermore, let $C = C_k(M(\eta(\alpha)))$ and $p \in (-\infty,1]$. Then $\eta(\alpha)$ is $\phi_p - optimal$ for $K'\theta$ in T if and only if;

$$traceC_j C^{p-1}\begin{cases} = traceC^p & for\ all\ j \in \partial(\alpha) \\ < traceC^p & otherwise \end{cases}$$

Proof

Kinyanjui (2007), gives the elaborate proof ▪

Theorem 3.2

Let $p \in (-\infty,1)$ and $\eta(\alpha)$ with $\alpha \in T_m$ be a weighted centroid design that is $\phi_p - optimal$ for $K'\theta$ in T. Then the following assertions hold:

i. If $\partial(\alpha) = \{1,2\}$, then there is no further design $\tau \in T$ that is $\phi_p - optimal$ for $K'\theta$ in T, that is, $\eta(\alpha)$ is the unique.

ii. If $\partial(\alpha) = \{1,2,3\}$, then there is no further exchangeable design $\bar{\tau} \in T$ that is $\phi_p - optimal$ for $K'\theta$ in T.

iii. If there is a non-exchangeable design which is $\phi_p - optimal$ for $K'\theta$, then all its support points are centroids of depths 1, 2 or 3.

Proof

Klein (2004) postulated and proved the theorem▪

A consequence of this theorem to this study is that we restricted the work to the first two centroids η_1 and η_2, hence derived weighted optimal slope designs that are unique.

3.2 Optimal Slope Weighted Centroid designs

This section presents the tools and methods that were engaged to derive optimal slope weighted centroid designs for the A- and D-optimality criteria.

3.2.1 Slope Information matrices

The basic model for this study is the second degree Kronecker regression model. For this model the full parameter vector is not estimable, basically due to the redundancies introduced by repetition of terms. A coefficient matrix was employed to select a maximal parameter sub vector. The coefficient matrix was derived by employing unique relations of vectors formed from Kronecker products of canonical vectors. Hence a need to demonstrate how the Kronecker products are performed.

The statistical properties of the designs are captured in moment matrices. Finally, the slope information matrices are formed from liner combinations of the moment matrices and adjusted slope matrices. The tools employed to come up with these matrices are as follows:

3.2.2 Support Points of a Simplex Centroid Design

In a simplex centroid design with m ingredients, there are $2^m - 1$ points of support. The points corresponds to the m permutations of (1, 0, 0, …, 0) pure blends, the $\binom{m}{2}$

permutations of $\left(\frac{1}{2},\frac{1}{2},0,0,...,0\right)$ binary blends, $\binom{m}{3}$ permutations of $\left(\frac{1}{3},\frac{1}{3},\frac{1}{3},0,...,0\right)$ ternary blends, …. and the overall centroid $\left(\frac{1}{m},\frac{1}{m},\frac{1}{m},...,\frac{1}{m}\right)$, Scheffe' (1963)….. (3.2)

The j[th] elementary centroid design η_j, j$\in$ {1, …, m}, m≥2 is the uniform distribution on all points taking the form

$\frac{1}{j}\sum_{i=1}^{j} e_{k_i} \in T_m$ with $1 \le k_1 < k_2 < \ldots < k_j \le m$. ………………………………………..…….(3.3)

A convex combination, $\eta(\alpha)=\sum_{j=1}^{m}\alpha_j\eta_j$, with $\alpha=(\alpha_1,...,\alpha_m)' \in T_m$, is called a weighted centroid design with weight vector α restricted by $\sum_{i=1}^{m}\alpha_i = 1$.

3.2.3 Kronecker products

The Kronecker product of a vector $s \in \Re^m$ and another vector $t \in \Re^n$ is a vector of order mn,

$$s \otimes t = \begin{pmatrix} s_1 t \\ \vdots \\ s_m t \end{pmatrix} = (s_i t_j)_{\substack{i=1,\ldots,m,\, j=1,\ldots,n \in \Re^{mn} \\ in \quad lexicographic \quad order}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(3.4)}$$

This study utilized the canonical unit vectors in $\Re^m$ denoted by $e_1,...,e_m$. The vector e_{ij} is taken as the Kronecker product of the vectors e_i and e_j, for $i, j \subseteq \{1,2,...,m\}$. The canonical vectors in $\Re^{\binom{m}{2}}$ are denoted by E_{ij}, ordered lexicographically according to their indices $(i, j) \in \{1,2,...,m\}^2$ with i<j.

The model around which the study revolves is the second degree Kronecker model with expected response:

$$E(Y_t) = f(t)'\theta = (t \otimes t)'\theta = \sum_{i=1}^{m} \theta_{ii} t_i^{\,2} + \sum_{\substack{i,j=1 \\ i<j}}^{m} (\theta_{ij} + \theta_{ji}) t_i t_j \ \ldots\ldots\ldots\ldots(3.5)$$

where $f(t) = t \otimes t$ and unknown parameter vector,

$\theta = (\theta_{11}, \quad \theta_{12}, \quad ..., \quad \theta_{mm}) \in \Re^{m^2}$.

The whole parameter vector for the model is not estimable. This necessitates the estimation of selected parameters from the whole vector. The study selected the maximal parameter subsystem of interest with the use of coefficient matrix.

3.2.4 Coefficient Matrix

Let $e_1,..., e_m$ denote the unit vectors in $\Re^m$ and E_{ij} denote the canonical vectors in $\Re^{\binom{m}{2}}$ that are ordered lexicographically according to their indices $(i, j) \in \{1,2,..., m\}^2$ with i<j. The unit vector e_{ij} is for this study the Kronecker product of the unit vectors e_i and e_j, for $i, j \subseteq \{1,2,..., m\}$.

The coefficient matrix K that aided in selecting a maximal parameter subsystem for the Kronecker regression function with a fixed number of ingredients, was defined as;

$$K = (K_1, K_2) \in \Re^{m^2 \times \binom{m+1}{2}}, \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.6)$$

where;

$$K_1 = \sum_{i=1}^{m} e_{ii} e_i' \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.7)$$

and

$$K_2 = \frac{1}{m}\sum_{\substack{i,j=1\\i<j}}^{m}(e_{ij}+e_{ji})E'_{ij} \quad \text{…………………..………………………………(3.8)}$$

The matrix K is of full column rank. The parameter subsystem $K'\theta$ of the model (3.5) considered in this study can be written as;

$$K'\theta = \begin{Bmatrix} (\theta_{ii})_{1\le i\le m} \\ \frac{1}{m}(\theta_{ij}+\theta_{ji}),_{1\le i<j\le m} \end{Bmatrix} \in \Re^{\binom{m+1}{2}} \text{ for all } \theta \in \Re^{m^2} \text{ and } m \ge 2. \quad \text{………………(3.9)}$$

3.2.5 Moment Matrix

An experimental design τ is a probability measure on the experimental domain with a finite number of support points. Each support point s $\in$ supp(τ) directs the experimenter to take a proportion T({t}) of all observations under experimental condition T. The statistical properties of a design are reflected by its moment matrix:

$$M(\tau) = \int_\tau f(t)f(t)'d\tau \in NND(m^2), \quad \text{………………………(3.10)}$$

where, NND(m^2) denotes the cone of nonnegative definite $m^2 \times m^2$ matrices. The entries of M(τ) are fourth moments of τ, since the regression function f(t) is purely quadratic. The unique moments of order four are, for j=1, 2, …, m:

$$\mu_4(\eta_j) = \frac{1}{j^3 m}, \quad \mu_{31}(\eta_j) = \mu_{22}(\eta_j) = \frac{j-1}{j^3 m(m-1)} \text{ and } \mu_{211}(\eta_j) = \frac{(j-1)(j-2)}{j^3 m(m-1)(m-2)} \quad \text{…..(3.11)}$$

3.2.6 Information matrix

In many applications of response surface methodology, good estimation of derivatives of the response function may be as important or perhaps more important than estimation of the mean response. We know that 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, $\frac{\partial Y_t}{\partial t}$. Certainly the computation of a stationary point in a second-order analysis or the use of gradient techniques for example, the steepest ascent of ridge analysis relies on the partial derivatives of the estimated response function with respect to the design factors. Since the designs that achieve certain properties in Y (estimated response) do not enjoy the similar properties for the estimated derivatives (slopes), we reflect on experimental designs that are constructed with derivatives in mind.

In practice, frequently we are concerned with investigation the slope of the response surface at a point t, not only over the axial directions, but also over any indicated path. We established the concept of robust slope over all directions. Define D, a matrix derived by differentiating the function $f(t)'\theta$ with respect to each of the m independent factors, (see Sung. et al (2009)). That is;

$$D = \left(\frac{\partial f'(t)}{\partial t_1}, \frac{\partial f'(t)}{\partial t_2}, ..., \frac{\partial f'(t)}{\partial t_m} \right)', \quad \text{where, } f(t) = t \otimes t \text{.} \quad \ldots\ldots\ldots\ldots\ldots(3.12)$$

Define also an $m \times \binom{m+1}{2}$, adjusted slope matrix

$$H_0 = DK \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(3.13)$$

The amount of information a design t contains on K’θ is contained in the information matrix:

$$C_k(M(\tau)) = \min\{LM(\tau)L' \mid L \in \Re^{\binom{m+1}{2} \times m^2}; \ LK = I_{\binom{m+1}{2}}\} \quad \ldots\ldots\ldots\ldots\ldots\ldots(3.14)$$

Where $I_{\binom{m+1}{2}}$ denotes the $\binom{m+1}{2} \times \binom{m+1}{2}$ identity matrix and L is the left inverse of K defined as,

$$L = (K'K)^{-1}K' \;. \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(3.15)$$

The above minimum is interpreted relative to the Loewner ordering on the space $sym\left(\binom{m+1}{2}\right)$ of symmetric $\binom{m+1}{2} \times \binom{m+1}{2}$ matrices, defined by $A \le B$ if and only if $B - A$ is nonnegative definite.

The information matrix $C_k(M(\tau))$ is the precision matrix of the best linear unbiased estimator for K'θ under design τ, see Pukelsheim (1993, chapter 3). The information matrices for K'θ takes the form:

$$c_0 = LM(\tau)L' \in NND\left(\binom{m+1}{2}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.16)$$

where $L = (K'K)^{-1}K'$.

To get the information matrix for the design $\eta(\alpha)$ we used the linear function;

$$C_0 = C_k(M(\eta(\alpha))) = \alpha_1 C_k(M(\eta_1)) + \alpha_2 C_k(M(\eta_2)) \ldots\ldots\ldots\ldots\ldots\ldots..\ldots\ldots\ldots(3.17)$$

where

$$C_k(M(\eta_j)) = LM(\eta_j)L' \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.18)$$

is the information matrix for the jth centroid.

Thus the information matrices for K'θ are linear transformations of the moment matrices.

Then, we consider optimizing for a particular criterion the slope information matrices for K'θ of the form:

$$C = H_0 C_0 H_0' \in NND(m) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.19)$$

3.2.7 Optimal Slope Weighted Centroid Designs

The problem of discovering a design carrying maximum information on the parameter subsystem $K'\theta$ can be formulated as;

$$\text{Maximize } \phi_p (C_k(M(\tau))) \text{ with } \tau \in T$$

$$\text{Subject to } C_k(M(\tau)) \in PD(m) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.20)$$

where T denotes the set of all designs T_m. The side condition $C_k(M(\tau)) \in PD(m)$ is equal to the existence of an unbiased linear estimator for $K'\theta$ under τ, Pukelsheim (1993). In which case, the design τ is called feasible for $K'\theta$. Any design solving problem (3.20) above for a fixed $p \in (-\infty,1]$ is called $\phi_p - optimal$ for $K'\theta$ in T. For all $p \in (-\infty,1]$, the existence of $\phi_p - optimal$ design for $K'\theta$ is guaranteed by Theorem 7.13 in Pukelsheim (1993).

The formulation allows for estimation of the maximal parameter subsystem that is unbiased. It also then points to the existence of optimal slope designs with the necessary adjustments to the information matrices to include the slope aspect.

Suppose $\eta(\alpha)$ satisfies the side condition $C_k(M(\tau)) \in PD(m)$ and write $C_j=C_k(M(\eta_j))$ for j=(1, 2, …, m). For all $p \in (-\infty,1]$, $\eta(\alpha)$ solves problem (3.23) if and only if;

$$trace H_0 C_j C^{p-1} H_0' \begin{cases} = trace H_0 C^p H_0' & for\ all\ j \in \partial(\alpha) \\ \leq trace H_0 C^p H_0' & otherwise \end{cases} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.21)$$

Weighted centroid designs are exchangeable, that is, they are invariant under permutations of ingredients. This fact considerably simplifies the solving of optimality condition (3.20). The set of weighted centroid designs is a convex complete class relative to Kiefer ordering.

3.2.8 Optimality Criteria

The most prominent optimality criteria in the design of experiments are the determinant criterion ϕ_0, the average-variance criterion ϕ_{-1}, the smallest eigenvalue criterion $\phi_{-\infty}$ and the trace criterion ϕ_1. These are a particular cases of the matrix means ϕ_p with parameter $p \in [-\infty;1]$.

The optimality properties of designs are determined by their moment matrices (Pukelsheim 1993, chapter 5). We computed optimal design for the polynomial fit model, the second degree Kronecker model. This involved searching for the optimum in a set of competing moment matrices. The matrix mean ϕ_p which is an information function (Pukelsheim (1993)) was exploited in this study.

The amount of information innate to C(M(τ)) is provided by kiefers ϕ_p-criteria with

C(M(τ)) $\in$ PD(m). These are defined by:

$$\phi_p(C) = \begin{cases} \lambda_{\min}(C) & if \quad p = -\infty \\ (\det C)^{\frac{1}{m}} & if \quad p = 0 \\ \left[\frac{1}{m} traceC^p\right]^p & if \quad p \in [-\infty;1] \setminus \{0\} \end{cases} \quad \ldots\ldots\ldots\ldots\ldots\ldots(3.22)$$

for all C in PD(m), the set of positive definite $m \times m$ matrices, where $\lambda_{\min}$(C) refers to the smallest eigenvalue of C. By definition ϕ_p(C) is a scalar measure which is a function of the eigenvalues of C for all $p \in [-\infty;1]$. (See, Pukelsheim 1993, chapter 6). For optimal slope designs we considered optimizing the information matrices of the form $C = H_0 C_0 H_0'$. The class of ϕ_p-criteria includes the prominently used T-, D-, A- and E-criteria corresponding to parameter values 1, 0, -1 and -∞ respectively.

Defining the group

$$H = \left\{ H = \begin{pmatrix} R_\pi & 0 \\ 0 & S_\pi \end{pmatrix}, \quad \pi \in \vartheta_m \right\} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.23)$$

With $R_\pi = \sum_{i=1}^{m} e_{\pi_i} e'_i$ and $S_\pi = \sum_{\substack{i,j=1 \\ i<j}}^{m} E_{(\pi(i),\pi(j))\uparrow} E'_{ij} \in perm\left(\binom{m}{2}\right)$ for all $\pi \in \vartheta_m$ where $(\pi_{(i)}, \pi_{(j)})\uparrow$ denotes the pair of indices $\pi_{(i)}, \pi_{(j)}$ in ascending order, and ϑ_m denotes the symmetric group of degree m. The set H is a subgroup of perm$\left(\binom{m+1}{2}\right)$, the set of $\binom{m+1}{2} \times \binom{m+1}{2}$ permutation matrices and is isomorphic to ϑ_m. This group acts on the space $sym\left(\binom{m+1}{2}\right)$ through congruence transformation. The group perm(m) of $m \times m$ permutation matrices acts on the set T of designs through $(R, \tau) \mapsto \tau^R = \tau \circ R^{-1}$. The direct implication of exchangeability of weighted designs is that, for any design $\tau \in T$ then $\tau = \tau^R$ for all $R \in perm(m)$. The equivalence property:

$$C_k(M(\tau^{R_\pi})) = C_k(R_\pi \otimes R_\pi)M(\tau)(R_\pi \otimes R_\pi)' = H_\pi C_k M(\tau) H_\pi' \ldots\ldots\ldots\ldots\ldots(3.24)$$

for all $\pi \in \vartheta_m$ and $\tau \in$ T links the action of H on $C_k(M(\tau))$ to the action of perm(m) on T (see Klein 2002). This now means that the information matrices involved in this study lie in the quadratic subspace $sym(m, H)$ of H-invariant symmetric matrices defined as:

$$sym(m,H) = \{C_0 \in sym(m) : HC_0H' = C_0 \quad for \quad all \quad H \in H\}$$

This group is closed under formation of matrix powers C^n with $n \in \mathrm{N}$. A particular case of the quadratic subspace of $sym\left(\binom{m+1}{2}, H\right)$ is analyzed in Koske and Kinyanjui (2007).

It is possible to obtain a characterization of feasible weighted centroid designs for the parameter subsystem $K'\theta$ of interest since the set of weighted centroid designs is a convex complete class relative to Kiefer ordering.

3.3 Numerical Optimal Slope Weighted Centroid Designs

We generated numerical ϕ_p – optimal slope weighted centroid designs for the A- and D- criteria for $m \subseteq [5, 20]$. These were based on the general expressions for the weight vectors and optimal values for each case of a design with m ingredients. The information matrices were explored in the context of the properties of the feasibility cone in which they are contained.

3.3.1 The Quadratic Subspace $\mathbf{sym(s, H)}$

Since H is a subgroup of the permutation matrix group, H-invariance of a matrix $C \in sym(s)$ means that certain entries of C coincide. The following lemma describing the linear structure of $sym(s, H)$, ($s = \binom{m+1}{2}$), shows that an H-invariant symmetric matrix has at most seven distinct elements.

Lemma

We define the identity matrices $U_1 = I_m$ and $W_1 = I_{\binom{m}{2}}$, and write $1_m = (1,1,\cdots,1)' \in \Re^m$. Furthermore, we define

$$U_2 = 1_m 1_m' - I_m \in sym(m),\ V_1 = \sum_{\substack{i,j=1 \\ i<j}}^{m} E_{ij}(e_i + e_j)' \in \Re^{\binom{m}{2}\times m},\ V_2 = \sum_{\substack{i,j=1 \\ i<j}}^{m} \sum_{\substack{k=1 \\ k\notin\{i,j\}}}^{m} E_{ij} e_k' \in \Re^{\binom{m}{2}\times m}$$

,

$$W_2 = \sum_{\substack{i,j=1 \\ i<j}}^{m} \sum_{\substack{k,l=1 \\ k<l}}^{m} E_{ij} E'_{kl} \in sym\left(\binom{m}{2}\right) \text{ and } W_3 = \sum_{\substack{i,j=1 \\ i<j}}^{m} \sum_{\substack{k,l=1 \\ k<l}}^{m} E_{ij} E'_{kl} \in sym\left(\binom{m}{2}\right).$$
$$\left|\{i,j\} \cap \{k,l\}\right| = 1 \qquad\qquad \{i,j\} \cap \{k,l\} = \phi$$

Then any matrix $A \in sym(s, H)$ can distinctively be represented in the form

$$A = \begin{pmatrix} aI_m + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \text{..................................(3.25)}$$

With coefficients $a, \cdots, g \in \Re$. The terms containing V_2, W_2 and W_3 only occur for $m \geq 3$ and $m \geq 4$ respectively, Klein (2004).

In particular, $\dim sym(s, H) = \begin{cases} 4 & for \quad m = 2 \\ 6 & for \quad m = 3 \\ 7 & for \quad m \geq 4 \end{cases}$.

The information matrices for the designs studied definitely belongs to this space.

The matrix (3.25) can be partitioned according to the block structure,

$$A = \begin{pmatrix} A_{11} & A'_{21} \\ A_{21} & A_{22} \end{pmatrix} \text{..(3.25a)}$$

with $A_{11} \in sym(m)$, $A_{21} \in \Re^{\binom{m}{2} \times m}$ and $A_{22} \in sym\left(\binom{m}{2}\right)$. From the linearity of the information mapping A, we have, for every $\alpha \in T_m$,

$$A_k(M(\eta(\alpha))) = \sum_{j \in \partial(\alpha)} \alpha_j A_k(M(\eta_j)) \text{,..(3.25b)}$$

with $\partial(\alpha) = \{j = 1,2,...,m : \alpha_j > 0\}$.

Since the information matrices $A_j = A_k M(\eta_j)$ are non-negative definite, this implies;

$$\Re(A_k(M(\eta(\alpha)))) = \sum_{j \in \partial(\alpha)} \Re(A_j) \,.$$

The above equation suggests studying the ranges of the information matrices; A_1, A_2, …, A_m of the elementary centroid designs. These matrices can be calculated by invoking the linear transformation to moment matrices $M(\eta_j)$ given by Draper, Heiligers and Pukelsheim (2000).

For j=1,2, …, m, we obtain

$$A_j = \begin{pmatrix} A_{11,j} & A'_{21,j} \\ A_{21,j} & A_{22,j} \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.25c)$$

with blocks

$$A_{11,j} = \frac{1}{j^3 m} I_m + \frac{1}{j^3 m}\frac{j-1}{m-1} U_2 \,, \; A_{21,j} = \frac{2}{j^3 m}\frac{j-1}{m-1} V_1 + \frac{2}{j^3 m}\frac{j-1}{m-1}\frac{j-2}{m-2} V_2 \text{ and}$$

$$A_{22,j} = \frac{4}{j^3 m}\frac{j-1}{m-1} I_{\binom{m}{2}} + \frac{4}{j^3 m}\frac{j-2}{m-1}\frac{j-2}{m-2} W_2 + \frac{4}{j^3 m}\frac{j-1}{m-1}\frac{j-2}{m-2}\frac{j-3}{m-1} W_3 \,, \ldots\ldots\ldots(3.25d)$$

3.3.2 Multiplication Identities for Information Matrices

Multiplication identities of the matrices in Quadratic Subspace $\mathbf{sym}(\mathbf{s}, \mathbf{H})$ are as follows:

(i) Products in $span\{U_1, U_2\}$

$$V_1'V_1 = (m-1)U_1 + U_2 \,, \quad V_2'V_2 = \binom{m-1}{2} U_1 + \binom{m-2}{2} U_2 \,, \quad \ldots\ldots\ldots(3.26)$$
$$V_1'V_2 = V_2'V_1 = (m-2)U_2 \,, \quad U_2^2 = (m-1)U_1 + (m-2)U_2 \,.$$

(ii) Products in $span\{V_1, V_2\}$

$$V_1'U_2 = V_1 + 2V_2, \qquad V_2U_2 = (m-2)V_1 + (m-3)V_2,$$
$$W_2V_1 = (m-2)V_1 + 2V_2, \quad W_2V_2 = (m-2)V_1 + 2(m-3)V_2, \quad \ldots\ldots\ldots\ldots(3.27)$$
$$W_3V_1 = (m-3)V_2, \qquad W_3V_2 = \binom{m-2}{2}V_1 + \binom{m-3}{2}V_2.$$

(iii) Products in $span\{W_1, W_2, W_3\}$

$$V_1V_1' = 2W_1 + W_2, \; V_2V_2' = (m-2)W_1 + (m-3)W_2 + (m-4)W_3,$$

$$V_1V_2' = V_2V_1' = W_2 + 2W_3, \;\; W_2^2 = 2(m-2)W_1 + (m-2)W_2 + 4W_3, \ldots\ldots(3.28)$$

$$W_3^2 = \binom{m-2}{2}W_1 + \binom{m-3}{2}W_2 + \binom{m-4}{2}W_3,$$

$$W_2W_3 = W_3W_2 = (m-3)W_2 + 2(m-4)W_3 \;.$$

(Results available from Klein (2004)).

3.4 Sensory Evaluation Experiment

The designs developed were employed in assessing the sensory attributes of various mixtures of juices. The mixtures were formulated using two, three and four ingredients. The ingredients actually refer to the different selected fruits making the mixture. The attributes focused on were texture, colour, taste and smell. The rating of the attributes was based on a 15-point scale.

The candidates involved were first taken through a training on how to taste and assign distinct scores on the various attributes. This was done to prepare them for the task and guide them on how to objectively assign scores on the various samples (juice blends) one tasted. In between samples the candidates rinsed the mouth using distilled water.

This basically was to clean the mouth, so that the attributes of one sample do not influence the ratings of the subsequent sample.

After training, a pilot experiment was conducted to ascertain the effectiveness of the procedure for mixture preparations and efficiency of the data collection tool, the questionnaire, as well as to ensure that it was sufficient. After the pilot experiment, necessary adjustments were made on the preparation procedure and the construct of the questions on the questionnaire. The participants were required to sign a consent validating their willingness to voluntarily take part in the study.

Then the experiment was conducted as follows: Pure blends of juices were prepared for the fruits involved. Then variations were then made on the blend formulations using the ratios as directed by the appropriate support points for the design. The amounts to be tasted, ‘samples’ were put in clear containers since colour was one of the attributes scored. The designs involved have finite support points, a decision was made on the eventual sample size. Each formulation was replicated four times. This was done to allow for the estimation of error and improve on the precision of estimates. Then the participants were availed samples to taste that bore labels that they noted on the questionnaires. The labels represented specific formulations only known to the technical assistants and the lead researcher who supervised the conduct of the experiment.

Randomization was actualized at the point of entry of the participants and in placing the samples on the benches. This was done to ensure that the observations were independent within and between formulations (mixtures/juice blends/samples). The participants were not made aware of the composition of the mixtures.

3.4.1 Model Validity

The model validity provides necessary examination to the fitted model to guarantee that it offers a good approximation of the true response surface. The process begins with tests to confirm whether the data agree to the assumptions of the model. Then, testing for the significance of individual factors to testing the validity of the overall fitted response. The requisite test statistics and probability values (p-values) were generated from the SAS (version 8) software.

3.4.1.1 Testing for Model Assumptions

Data that are fitted the Kronecker model need to be independent with a constant variance. The error terms are independent and normally distributed. Scatter plot would show if the data are distributed with a constant variance. A normal probability plot for the residuals shows whether the errors are normally distributed or not.

3.4.1.2 Testing for the Overall Model Fit

Analysis of variance (ANOVA) and Coefficient of variations were used to examine the fitted Kronecker model. From the ANOVA table (generated from the SAS software), the p-values were compared with the level of significance (α) to make a decision on whether the model fit was adequate of not.

3.4.1.3 Testing for the Adequacy of Parameters

To test the adequacy of each parameter (the significance of a factor or interaction) in the model, we employed student t-test based on the p-values from the analysis output from the SAS software. The parameter with the smallest standard error was considered better than the others.

CHAPTER FOUR

RESULTS AND DISCUSSIONS

4.0 Introduction

This chapter presents the findings and analysis of the study as set out in the research methodology. The requisite equivalence relation is presented as well as derivations of optimal slope weighted designs for particular criteria.

4.1 Equivalence Theorem

The theorem provides the necessary conditions for the existence of $\phi_p -$ optimal slope mixture designs. This theorem provides a necessary and sufficient condition applicable to the specific problem of this study. The object here is to solve the design problem;

Maximize ϕ_p ($C_k(M(\tau))$) with $\tau \in T$

Subject to $C_k(M(\tau)) \in$ PD(m) …..………………………………………….. (4.0)

Suppose $\eta(\alpha)$ satisfies the side condition $C_k(M(\tau)) \in$ PD(m) and write $C_j=C_k(M(\eta_j))$ for j=(1, 2, …, m).

Theorem

Let $\alpha \in T_m$ be the weight vector of a weighted centroid design $\eta(\alpha)$ which is feasible for $K'\theta$ and let $\partial(\alpha) = \{j = (1, 2, \cdots, m : \alpha_j > 0)\}$, be a set of active indices. Furthermore, let $C = C_k(M(\eta(\alpha)))$ and $p \in (-\infty, 1]$. Then $\eta(\alpha)$ is $\phi_p - slope\,optimal$ for $K'\theta$ in T if and only if;

$$trace H_0 C_j C^{p-1} H_0' \begin{cases} = trace H_0 C^p H_0' & for\ all\ j \in \partial(\alpha) \\ \leq trace H_0 C^p H_0' & otherwise \end{cases} \quad \text{……………………......(4.1)}$$

where, $H_0 = DK$ is an adjusted slope matrix with for a slope matrix defined as

$D = \left(\frac{\partial f'(t)}{\partial t_1}, \frac{\partial f'(t)}{\partial t_2}, ..., \frac{\partial f'(t)}{\partial t_m} \right)'$ for a regression vector, $f(t) = t \otimes t$.

Proof

We begin by adopting the following theorems (3.1) and (3,2), that provides a sufficient condition for existence of $\phi_p - optimal$ designs for $K'\theta$ and their uniqueness.

The two major arguments of the proof are the linearity of the information matrix mapping as depicted by equation (3.10) and the fact that $\eta(T_m)$ is the convex hull of the elementary centroid designs $\eta_1, \eta_2, \cdots, \eta_m$.

From the equivalence theorem 7.19 in Pukelsheim (1993), that $\eta(\alpha)$ is $\phi_p - optimal$ for $K'\theta$ in T if and only if there exists a generalized inverse G of $M = M(\eta(\alpha))$ satisfying

$$traceM(\eta(\beta))GKC^{p+1}K'G' \leq traceC^p \text{ for all } \beta \in T_m \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.1.1)$$

with

$C = (K'K)^{-1}K'MK(K'K)^{-1}$, $M = K(K'K)^{-1}K'M$ and $M(\eta(\beta)) = KC_k(M(\eta(\alpha)))K'$,

To incorporate the slope concept, we rewrite (4.1.1) as;

$$traceH_0M(\eta(\beta))GKC^{p+1}K'G'H_0' \leq traceH_0C^pH_0' \text{ for all } \beta \in T_m \ldots\ldots\ldots\ldots\ldots\ldots(4.1.2)$$

where $H_0 = DK$.

The left-hand side may be written as,

$$traceH_0 M(\eta(\beta))GKC^{p+1}K'G'H' = traceH_0(K'GMK(K'K)^{-1})'C_k(M(\eta(\beta)))(K'GMK(K'K)^{-1})C^{p-1}H_0'$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.1.3)$$

Due to the feasibility of $\eta(\alpha)$, we have $\Re(K) = \Re(M)$.

Now the right-hand side of equation (4.1.3) simplifies to $traceH_0 C_k(M(\eta(\beta)))C^{p-1}H_0'$ and the equation turns into $traceH_0 C_k(M(\eta(\beta)))C^{p-1}H_0' \leq traceH_0 C^p H_0'$ for all $\beta \in T_m$.

Since the information matrix is a linear mapping then it can be expressed as $C_k(M(\eta(\alpha))) = \sum_{j\in\partial(\alpha)}^{m} \alpha_j C_k(M(\eta_j))$, with $\partial(\alpha) = \{j = (1,2,\cdots,m : \alpha_j > 0)\}$. We then can write the left-hand side as $\sum_{j=1}^{m} \beta_j traceH_0 C_j C^{p-1}H_0'$. Giving

$$traceH_0\, C_j C^{p-1}H_0' \leq traceH_0 C^p H_0' \text{ for all } 1 \leq j \leq m.$$

Finally, is the assertion that equality must hold for any $j \in \partial(\alpha)$ ▪

In addition, the weighted centroid designs with first and second weights being positive are unique, Klein (2004).

4.1.1 A- Optimal Slope Weighted Centroid Design

This section presents the slope optimal weighted centroid designs for the average variance criterion, ϕ_{-1}.

4.1.1.1 A- Optimal Slope Weighted Centroid Design with Two Ingredients

The first case is a mixture experiment with two ingredients. According to (3.2), the weighted centroid design has three support points (1, 0), (0, 1) and (½, ½). The slope weighted centroid design $\eta(\alpha)=\sum_{j=1}^{2}\alpha_j\eta_j=\alpha_1\eta_1+\alpha_2\eta_2$ with $\alpha=(\alpha_1,\alpha_2,0,0)\in T_2$ and $\alpha_1+\alpha_2=1$, encompassing (from (3.3)) two elementary centroid designs;

$$\eta_1=\left\{\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix}\right\} \text{ and } \eta_2=\left\{\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\end{pmatrix}\right\}.$$

The Kronecker model (as defined in 3.5) has four parameters which are not all estimable. We chose the maximal parameter subsystem by using the coefficient (K) matrix for the design. Using the unit vectors $e_1=\begin{pmatrix}1\\0\end{pmatrix}$, $e_2=\begin{pmatrix}0\\1\end{pmatrix}$ and $E_{12}=(1)$, we have for m=2 in (3.7) and (3.8);

$$K_1=e_{11}e_1'+e_{22}e_2'=\begin{pmatrix}1&0\\0&0\\0&0\\0&1\end{pmatrix}$$

and

$$K_2=\begin{pmatrix}0\\\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix}$$

which when substituted into (3.6), gave the coefficient matrix,

$$K = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 \end{bmatrix} \qquad (4.2)$$

The moment matrix for the weighted centroid design with two ingredients from (3.10) is

$$M(\eta(\alpha)) = \begin{bmatrix} \mu_4 & \mu_{31} & \mu_{31} & \mu_{22} \\ \mu_{31} & \mu_{22} & \mu_{22} & \mu_{31} \\ \mu_{31} & \mu_{22} & \mu_{22} & \mu_{31} \\ \mu_{22} & \mu_{31} & \mu_{31} & \mu_4 \end{bmatrix}.$$

Using the definition of the fourth order moments (3.11), for m=2 these moment matrices for two centroids η_1 and η_2 are respectively;

$$M(\eta_1) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} \qquad (4.3)$$

and

$$M(\eta_2) = \begin{bmatrix} \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \end{bmatrix} \qquad (4.4)$$

We obtained the left inverse of the coefficient matrix (4.2) using (3.15) as;

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \qquad \text{(4.5)}$$

Then, for the design η_1, the information matrix using (4.5) and (4.3) in (3.18) is;

$$C_1 = \begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \text{(4.6)}$$

For the design η_2, the information matrix was obtained using (4.5) and (4.4) in (3.18) as

$$C_2 = \begin{pmatrix} 1/16 & 1/16 & 2/16 \\ 1/16 & 1/16 & 2/16 \\ 2/16 & 2/16 & 4/16 \end{pmatrix} \qquad \text{(4.7)}$$

From equations (4.6) and (4.7) we got the information matrix for the design $\eta(\alpha)$ using the linear function (3.17) that was to be adjusted for slope as;

$$C_0 = \begin{pmatrix} \frac{8\alpha_1 + \alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1 + \alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{4} \end{pmatrix} \qquad \text{(4.8)}$$

To get the A- optimal slope design we proceeded as follows. First by condition (3.21), putting p=-1, we have that $\eta(\alpha)$ is $\phi_{-1} - slope\ optimal$ for $K'\theta$ in T if and only if

$$trace H_0 C_j C_0^{-2} H_0' = trace H_0 C_0^{-1} H_0' \text{ for all } j \in \{1,2\} \qquad \text{(4.9)}$$

The inverse of the information matrix (4.8) is;

$$C_0^{-1} = [C(M(\eta(\alpha)))]^{-1} = \begin{pmatrix} \frac{2}{\alpha_1} & 0 & \frac{-1}{\alpha_1} \\ 0 & \frac{2}{\alpha_1} & \frac{-1}{\alpha_1} \\ \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{4\alpha_1+\alpha_2}{\alpha_1\alpha_2} \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.10)$$

which on squaring yields,

$$C_0^{-2} = \begin{pmatrix} \frac{5}{\alpha_1^2} & \frac{1}{\alpha_1^2} & \frac{-(4\alpha_1+3\alpha_2)}{\alpha_1^2\alpha_2} \\ \frac{1}{\alpha_1^2} & \frac{5}{\alpha_1^2} & \frac{-(4\alpha_1+3\alpha_2)}{\alpha_1^2\alpha_2} \\ \frac{-(4\alpha_1+3\alpha_2)}{\alpha_1^2\alpha_2} & \frac{-(4\alpha_1+3\alpha_2)}{\alpha_1^2\alpha_2} & \frac{16\alpha_1^2+8\alpha_1\alpha_2+3\alpha_2^2}{\alpha_1^2\alpha_2^2} \end{pmatrix} \quad \ldots\ldots\ldots(4.11)$$

The slope matrix for the design with two ingredients using equation (3.12) is

$$D = \begin{pmatrix} 2t_1 & t_2 & t_2 & 0 \\ 0 & t_1 & t_1 & 2t_2 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(4.12)$$

This using equation (3.13) gave an adjusted slope matrix

$$H_0 = DK = \begin{pmatrix} 2t_1 & 0 & t_2 \\ 0 & 2t_2 & t_1 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(4.13)$$

For j=1 in equation (4.9),

$$trace H_0 C_1 C_0^{-2} H_0' = trace H_0 C_0^{-1} H_0' . \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (4.14)$$

We have from equations (4,6), (4.11) and (4.13);

$$H_0C_1C_0^{-2}H_0' = \frac{1}{2\alpha_1^2}\begin{pmatrix} 20t_1^2 - \frac{2(4\alpha_1+3\alpha_2)}{\alpha_2}t_1t_2 & 4t_1t_2 - \frac{2(4\alpha_1+3\alpha_2)}{\alpha_2}t_1^2 \\ 4t_1t_2 - \frac{2(4\alpha_1+3\alpha_2)}{\alpha_2}t_2^2 & 20t_2^2 - \frac{2(4\alpha_1+3\alpha_2)}{\alpha_2}t_1t_2 \end{pmatrix} \quad \text{……...(4.15a)}$$

The trace of (4.15a) is;

$$traceH_0C_1C_0^{-2}H_0' = \frac{1}{2\alpha_1^2}\left[20(t_1^2+t_2^2) - \frac{4(4\alpha_1+3\alpha_2)}{\alpha_2}t_1t_2\right] = \frac{47\alpha_2 - 4\alpha_1}{2\alpha_1^2\alpha_2} \quad \text{………(4.15b)}$$

after substituting for $t_i^2 = \frac{5}{4}, i = 1,2$ and $t_1t_2 = \frac{1}{4}$.

Also, from equations (4.10) and (4.13);

$$H_0C_0^{-1}H_0' = \frac{1}{\alpha_1}\begin{pmatrix} 8t_1^2 - 4t_1t_2 + bt_2^2 & -2t_2^2 + (b-2)t_1t_2 \\ -2t_1^2 + (b-2)t_1t_2 & 8t_2^2 - 4t_1t_2 + bt_1^2 \end{pmatrix} \quad \text{…………………………..(4.16a)}$$

where

$b = \frac{4\alpha_1 + \alpha_2}{\alpha_2}$, $t_i^2 = \frac{5}{4}, i = 1,2$ and $t_1t_2 = \frac{1}{4}$.

The trace of (4.16a) is;

$$traceH_0C_0^{-1}H_0' = \frac{1}{\alpha_1}\left[8(t_1^2+t_2^2) - 8t_1t_2 + b(t_1^2+t_2^2)\right] = \frac{41\alpha_2 + 20\alpha_1}{2\alpha_1\alpha_2} \quad \text{……………….(4.16b)}$$

Using equations (4.15b) and (4.16b) in condition (4.14) gives;

$$\frac{47\alpha_2 - 4\alpha_1}{2\alpha_1^2\alpha_2} = \frac{41\alpha_2 + 20\alpha_1}{2\alpha_1\alpha_2}$$

This after employing the strict relation $\alpha_2 = 1 - \alpha_1$, yielded the equation,

$$21\alpha_1^2 - 92\alpha_1 + 47 = 0$$

with solutions; 3.790504535 and 0.590447846. Therefore, $\alpha_1 = 0.590447846$ since $\alpha_1 \in (0,1)$.

Similarly, for j=2, in condition (4.9) we obtained the necessary condition as,

$$traceH_0C_2C_0^{-2}H_0' = traceH_0C_0^{-1}H_0'. \qquad (4.17)$$

The left hand side of this condition was gotten by evaluating the product of (4.7), (4.11) and (4.13);

$$H_0C_2C_0^{-2}H_0' = \frac{-1}{2\alpha_1\alpha_2}\begin{pmatrix} 4t_1^2+(4+2a)t_1t_2+2at_2^2 & 4t_2^2+(4+2a)t_1t_2+2at_1^2 \\ 4t_1^2+(4+2a)t_1t_2+2at_2^2 & 4t_2^2+(4+2a)t_1t_2+2at_1^2 \end{pmatrix} \qquad (4.18a)$$

where

$$a = -\frac{4\alpha_1+\alpha_2}{\alpha_2},\ t_i^2 = \frac{5}{4},\ i=1,2 \text{ and } t_1t_2 = \frac{1}{4}.$$

The trace of (4.18a) is;

$$traceH_0C_2C_k^{-2}H_0' = \frac{12\alpha_1-3\alpha_2}{\alpha_1\alpha_2^2} \qquad (4.18b)$$

Using equations (4.16b) and (4.18b) in condition (4.17) led to the equation;

$$\frac{12\alpha_1-3\alpha_2}{\alpha_1\alpha_2^2} = \frac{41\alpha_2+20\alpha_1}{2\alpha_1\alpha_2}.$$

From this equation together with the relation $\alpha_1 = 1-\alpha_2$ resulted in the quadratic equation

$$21\alpha_2^2+50\alpha_2-24=0,$$

with solutions -2.790504535 and 0.409552154. Hence, $\alpha_2 = 0.409552154$ since $\alpha_2 \in (0,1)$

Thus for m=2 ingredients, we have the A- optimal slope weight vector;

$$\alpha_1 = 0.590447846 \text{ and } \alpha_2 = 0.409552154 \ldots\ldots\ldots\ldots\ldots (4.19)$$

Therefore, in the second-degree Kronecker model for mixture experiments with two ingredients, the unique A- optimal slope design for $K'\theta$ is $\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.590447846\eta_1 + 0.409552154\eta_2$

From equation (3.22), the average-variance criterion, for a nonnegative definite matrix C of order s is given by;

$$v(\phi_{-1}) = \left(\frac{1}{s} traceC^{-1}\right)^{-1} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.20)$$

At present the average-variance criterion, is obtained for the information matrices of order m=2 from the relation;

$$v(\phi_{-1}) = \left(\frac{1}{2} traceH_0 C_0^{-1} H_0'\right)^{-1} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.20)$$

Now, from (4.10), (4.13) and (4.19) we obtained;

$$H_0 C_0^{-1} H_0' = \frac{1}{4\alpha_1\alpha_2}\begin{bmatrix} 20\alpha_1 + 41\alpha_2 & 4\alpha_1 - 11\alpha_2 \\ 4\alpha_1 - 11\alpha_2 & 20\alpha_1 + 41\alpha_2 \end{bmatrix} = \begin{bmatrix} 29.56816162 & -2.215790169 \\ -2.215790169 & 29.56816162 \end{bmatrix} \ldots (4.21)$$

Hence using (4.20) and (4.21), we got;

$$v(\phi_{-1}) = (29.56816162)^{-1} = 0.033820161 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.22)$$

4.1.1.2 A- Optimal Slope Weighted Centroid Design with Three Ingredients

The second case is a mixture experiment with three ingredients. From (3.2) this weighted centroid design has seven support points are as shown in table 1.

Table 1: Support points for the three ingredients centroid design

Design point	Ingredients		
	t_1	t_2	t_3
1	1	0	0
2	0	1	0
3	0	0	1
4	½	½	0
5	½	0	½
6	0	½	½
7	⅓	⅓	⅓

The optimal slope weighted centroid design is $\eta(\alpha)=\sum_{j=1}^{3}\alpha_j\eta_j=\alpha_1\eta_1+\alpha_2\eta_2$ with $\alpha=(\alpha_1,\alpha_2,0,0)\in T_3$ and $\alpha_1+\alpha_2=1$. According to (3.3), the design with m=3 ingredients has three centroids. These are:

$$\eta_1=\left\{\begin{pmatrix}1\\0\\0\end{pmatrix},\ \begin{pmatrix}0\\1\\0\end{pmatrix},\ \begin{pmatrix}0\\0\\1\end{pmatrix}\right\},\eta_2=\left\{\begin{pmatrix}1/2\\1/2\\0\end{pmatrix},\begin{pmatrix}1/2\\0\\1/2\end{pmatrix},\begin{pmatrix}0\\1/2\\1/2\end{pmatrix}\right\} \text{ and } \eta_3=\left\{\begin{pmatrix}1/3\\1/3\\1/3\end{pmatrix}\right\}.$$

The Kronecker model as defined in (3.5) has nine parameters all of which are not all estimable simultaneously. We chose the maximal parameter subsystem (consisting of six parameters) by using the coefficient (K) matrix. This matrix was arrived at using by using the unit vectors

$e_1=(1\quad 0\quad 0)'$, $e_2=(0\quad 1\quad 0)'$, $e_3=(0\quad 0\quad 1)$, $E_{12}=(1\quad 0\quad 0)'$, $E_{13}=(0\quad 1\quad 0)'$ and $E_{23}=(0\quad 0\quad 1)'$.

With these vectors for m=3 in (3.7) and (3.8), we got the submatrices for the coefficient matrix as;

$$K_1 = e_{11}e_1' + e_{22}e_2' + e_{33}e_3' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and

$$K_2 = (e_{12} + e_{21})E_{12}' + (e_{13} + e_{31})E_{13}' + (e_{23} + e_{32})E_{23}' = \begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 \end{pmatrix}$$

The two matrices were then substituted into (3.6), to give the coefficient matrix,

$$K = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.23)$$

The moment matrix the weighted centroid design which has all moments being of order four is from (3.10);

$$M(\eta(\alpha)) = \begin{pmatrix} \mu_4 & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} \\ \mu_{31} & \mu_{22} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} \\ \mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} \\ \mu_{31} & \mu_{22} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} \\ \mu_{22} & \mu_{31} & \mu_{211} & \mu_{31} & \mu_4 & \mu_{31} & \mu_{211} & \mu_{31} & \mu_{22} \\ \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{22} & \mu_{31} \\ \mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} \\ \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{22} & \mu_{31} \\ \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_4 \end{pmatrix}$$

Using the definition of the fourth order moments (3.11), for m=3 ingredients the moment matrices for two centroids η_1 and η_2 are respectively;

$$M(\eta_1)=\begin{pmatrix}1/3&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0\\0&0&0&0&1/3&0&0&0&0\\0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&1/3\end{pmatrix}\ldots\ldots\ldots\ldots\ldots(4.24)$$

and

$$M(\eta_2)=\begin{pmatrix}1/24&1/48&1/48&1/48&1/48&0&1/48&0&1/48\\1/48&1/48&0&1/48&1/48&0&0&0&0\\1/48&0&1/48&0&0&0&1/48&0&1/48\\1/48&1/48&0&1/48&1/48&0&0&0&0\\1/48&1/48&0&1/48&1/24&1/48&0&1/48&1/48\\0&0&0&0&1/48&1/48&0&1/48&1/48\\1/48&0&1/48&0&0&0&1/48&0&1/48\\0&0&0&0&1/48&1/48&0&1/48&1/48\\1/48&0&1/48&0&1/48&1/48&1/48&1/48&1/24\end{pmatrix}\ldots..(4.25)$$

The left inverse of the coefficient matrix using the coefficient matrix (4.23) is;

$$L=(K'K)^{-1}K'=\begin{pmatrix}1&0&0&0&0&0&0&0&0\\0&0&0&0&1&0&0&0&0\\0&0&0&0&0&0&0&0&1\\0&3/2&0&3/2&0&0&0&0&0\\0&0&3/2&0&0&0&3/2&0&0\\0&0&0&0&0&3/2&0&3/2&0\end{pmatrix}\ldots\ldots\ldots(4.26)$$

Then, we obtained for the design η_1, the information matrix using (4.24) and (4.26) in (3.18) as;

$$C_1 = \begin{pmatrix} 1/3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots(4.27)$$

For the design η_2, the information matrix was obtained using (4.25) and (4.26) in (3.18) as

$$C_2 = \begin{pmatrix} 1/24 & 1/48 & 1/48 & 1/16 & 1/16 & 0 \\ 1/48 & 1/24 & 1/48 & 1/16 & 0 & 1/16 \\ 1/48 & 1/48 & 1/24 & 0 & 1/16 & 1/16 \\ 1/16 & 1/16 & 0 & 3/16 & 0 & 0 \\ 1/16 & 0 & 1/16 & 0 & 3/16 & 0 \\ 0 & 1/16 & 1/16 & 0 & 0 & 3/16 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots (4.28)$$

From equations (4.27) and (4.28) we got the information matrix for the design $\eta(\alpha)$ using the linear function (3.17) that was later adjusted for slope as;

$$C_0 = C_k(M(\eta(\alpha))) = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{16} & 0 & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 & \frac{3\alpha_2}{16} & 0 & 0 \\ \frac{\alpha_2}{16} & 0 & \frac{\alpha_2}{16} & 0 & \frac{3\alpha_2}{16} & 0 \\ 0 & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 & 0 & \frac{3\alpha_2}{16} \end{pmatrix} \ldots(4.29)$$

To get the A- optimal slope design with three ingredients we proceeded as follows. First by condition (3.21), putting p=-1, we have that $\eta(\alpha)$ is $\phi_{-1} - slope\ optimal$ for $K'\theta$ in T if and only if

$$traceH_0C_jC_k^{-2}H_0' = traceH_0C_k^{-1}H_0' \text{ for all } j \in \{1,2\} \qquad (4.30)$$

The inverse of the information matrix (4.29) for the design with three ingredients is;

$$C_0^{-1} = \begin{pmatrix} \frac{3}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 \\ 0 & \frac{3}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} \\ 0 & 0 & \frac{3}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} \\ \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} & \frac{1}{3\alpha_1} & \frac{1}{3\alpha_1} \\ \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{1}{3\alpha_1} & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} & \frac{1}{3\alpha_1} \\ 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{1}{3\alpha_1} & \frac{1}{3\alpha_1} & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} \end{pmatrix} \qquad (4.31)$$

which on squaring yielded the matrix;

$$[C(\alpha)]^{-2} = \begin{pmatrix} a & b & b & c & c & d \\ b & a & b & c & d & c \\ b & b & a & d & c & c \\ c & c & d & e & f & f \\ c & d & c & f & e & f \\ d & c & c & f & f & e \end{pmatrix} \qquad (4.32)$$

where:

$a = \frac{11}{\alpha_1^2}$, $b = \frac{1}{\alpha_1^2}$, $c = \frac{-4(4\alpha_1 + 3\alpha_2)}{3\alpha_1^2\alpha_2}$, $d = \frac{-2}{3\alpha_1^2}$, $e = \frac{8(27\alpha_1^2 + 2\alpha_1 + 3)}{9\alpha_1^2\alpha_2^2}$ and

$$f = \frac{2(16\alpha_1 + 7\alpha_2)}{9\alpha_1^2\alpha_2}$$

The slope matrix for the design with three (m=3) ingredients using equation (3.12) is

$$D = \begin{pmatrix} 2t_1 & t_2 & t_3 & t_2 & 0 & 0 & t_3 & 0 & 0 \\ 0 & t_1 & 0 & t_1 & 2t_2 & t_3 & 0 & t_3 & 0 \\ 0 & 0 & t_1 & 0 & 0 & t_2 & t_1 & t_2 & 2t_3 \end{pmatrix}, \ldots\ldots\ldots\ldots \quad (4.33)$$

We then got the adjusted slope matrix using (3.13) as;

$$H_0 = \begin{pmatrix} 2t_1 & 0 & 0 & \frac{2}{3}t_2 & \frac{2}{3}t_3 & 0 \\ 0 & 2t_2 & 0 & \frac{2}{3}t_1 & 0 & \frac{2}{3}t_3 \\ 0 & 0 & 2t_3 & 0 & \frac{2}{3}t_1 & \frac{2}{3}t_2 \end{pmatrix} \ldots\ldots\ldots\ldots (4.34)$$

when j=1 in (4.30), the necessary condition is;

$$traceH_0C_1C_k^{-2}H_0' = traceH_0C_k^{-1}H_0'. \ldots\ldots\ldots\ldots \quad (4.35)$$

We used (4.27), (4.32) and (4.34) to obtain;

$$H_0C_1C_0^{-2}H_0' = \frac{1}{3\alpha_1^2}\begin{pmatrix} 44t_1^2 + \frac{4}{3}c(t_1t_2 + t_1t_3) & 4t_1t_2 + \frac{4}{3}(ct_2^2 + dt_2t_3) & 4t_1t_3 + \frac{4}{3}(ct_3^2 + dt_2t_3) \\ 4t_1t_2 + \frac{4}{3}(ct_1^2 + dt_1t_3) & 44t_2^2 + \frac{4}{3}c(t_1t_2 + t_2t_3) & 4t_1t_3 + \frac{4}{3}(ct_3^2 + dt_1t_3) \\ 4t_1t_3 + \frac{4}{3}(ct_1^2 + dt_1t_2) & 4t_2t_3 + \frac{4}{3}(ct_2^2 + dt_1t_2) & 44t_3^2 + \frac{4}{3}c(t_1t_3 + t_2t_3) \end{pmatrix} \ldots (4.36a)$$

where:

$$c = \frac{-4(4\alpha_1 + 3\alpha_2)}{3\alpha_2}, \quad d = \frac{-2}{3} \quad t_i^2 = \frac{29}{18}, i = 1,2,3 \text{ and } t_it_j = \frac{13}{36}, i \neq j = 1,2,3.$$

The trace of (4.36a) is;

$$traceH_0C_1C_0^{-2}H_0' = \frac{5430\alpha_2 - 416\alpha_1}{81\alpha_1^2\alpha_2} \ldots\ldots\ldots\ldots (4.36b)$$

Also, from (4.31) and (4.34) we got;

$$H_0C_0^{-1}H_0' = \frac{-1}{\alpha_1}\begin{bmatrix} -12t_1^2+\frac{8}{3}(t_1t_2+t_1t_3)+\frac{4}{9}a(t_2^2+t_3^2)+\frac{8}{9}bt_2t_3 & \frac{4}{3}(t_1^2+t_2^2)+\frac{4}{9}bt_3^2+\frac{4}{9}(at_1t_2+bt_1t_3+bt_2t_3) & \frac{4}{3}(t_1^2+t_3^2)+\frac{4}{9}bt_2^2+\frac{4}{9}(bt_1t_2+at_1t_3+bt_2t_3) \\ \frac{4}{3}(t_1^2+t_2^2)+\frac{4}{9}bt_2^2+\frac{4}{9}(at_1t_2+bt_2t_3+bt_1t_3) & -12t_2^2+\frac{8}{3}(t_1t_2+t_2t_3)+\frac{4}{9}a(t_1^2+t_3^2)+\frac{8}{9}bt_1t_3 & \frac{4}{3}(t_2^2+t_3^2)+\frac{4}{9}bt_1^2+\frac{4}{9}(bt_1t_3+bt_1t_2+at_2t_3) \\ \frac{4}{3}(t_1^2+t_3^2)+\frac{4}{9}bt_2^2+\frac{4}{9}(at_1t_3+bt_2t_3+bt_1t_2) & \frac{4}{3}(t_2^2+t_3^2)+\frac{4}{9}bt_1^2+\frac{4}{9}(bt_1t_2+bt_1t_3+at_2t_3) & -12t_3^2+\frac{8}{3}(t_1t_3+t_2t_3)+\frac{4}{9}a(t_1^2+t_2^2)+\frac{8}{9}bt_1t_2 \end{bmatrix} \quad \text{....(4.37a)}$$

where:

$$a=\frac{-2(8\alpha_1+\alpha_2)}{3\alpha_2},\ b=\frac{-1}{3},\ t_i^2=\frac{29}{18}, i=1,2,3 \text{ and } t_it_j=\frac{13}{36}, i\neq j=1,2,3 .$$

Trace of (4.37a) is;

$$traceH_0C_0^{-1}H'=\frac{-1}{\alpha_1}\left[(-12+\tfrac{8}{9}a)(t_1^2+t_2^2+t_3^2)+(\tfrac{16}{3}+\tfrac{8}{9}b)(t_1t_2+t_1t_3+t_2t_3)\right]=\frac{1856\alpha_1+4488\alpha_2}{81\alpha_1\alpha_2} \text{ .(4.37b)}$$

Using (4.36b) and (4.37b) in condition (4.35) gave the equality relation;

$$\frac{5430\alpha_2-416\alpha_1}{81\alpha_1^2\alpha_2}=\frac{1856\alpha_1+4488\alpha_2}{81\alpha_1\alpha_2} .$$

This after using the equality, $\alpha_2 = 1-\alpha_1$, yielded the quadratic equation,

$$2632\alpha_1^2-10334\alpha_1+5430=0,$$

with solutions 0.6249112749 and 3.301380518. But since $\alpha_1 \in (0, 1)$ the definite choice is $\alpha_1 = 0.6249112749$.

Similarly, when j=2 in condition (4.30), we got the relation,

$$traceH_0C_2C_k^{-2}H_0' = traceH_0C_k^{-1}H_0' . \text{ .... (4.38)}$$

We first worked out the product on the left hand side of condition (4.38) using equations (4.28), (4.31) and (4.34). That is

$$H_0C_2C_0^{-1}H_0' =$$

$$\frac{-1}{3\alpha_1\alpha_2}\begin{bmatrix} 8t_1^2+\frac{4}{9}d(t_2^2+t_3^2)+(4+\frac{4}{3}c)(t_1t_2+t_1t_3)-\frac{16}{9}t_2t_3 & 4t_2^2+\frac{4}{3}ct_1^2-\frac{8}{9}t_3^2+(4+\frac{4}{9}d)t_1t_2-\frac{16}{9}t_1t_3-\frac{8}{9}t_2t_3 & 4t_3^2+\frac{4}{3}ct_1^2-\frac{8}{9}t_2^2+(4+\frac{4}{9}d)t_1t_3-\frac{16}{9}t_1t_2-\frac{8}{9}t_2t_3 \\ 4t_1^2+\frac{4}{3}ct_2^2-\frac{8}{9}t_3^2+(4+\frac{4}{9}d)t_1t_2-\frac{16}{9}t_2t_3-\frac{8}{9}t_1t_3 & 8t_2^2+\frac{4}{9}d(t_1^2+t_3^2)+(4+\frac{4}{3}c)(t_1t_2+t_2t_3)-\frac{16}{9}t_2t_3 & 4t_3^2+\frac{4}{3}ct_2^2-\frac{8}{9}t_1^2+(4+\frac{4}{9}d)t_2t_3-\frac{16}{9}t_1t_2-\frac{8}{9}t_1t_3 \\ 4t_1^2+\frac{4}{3}ct_3^2-\frac{8}{9}t_2^2+(4+\frac{4}{9}d)t_1t_3-\frac{16}{9}t_2t_3-\frac{8}{9}t_1t_2 & 4t_2^2+\frac{4}{3}ct_3^2-\frac{8}{9}t_1^2+(4+\frac{4}{9}d)t_2t_3-\frac{16}{9}t_1t_3-\frac{8}{9}t_1t_2 & 8t_3^2+\frac{4}{9}d(t_1^2+t_2^2)+(4+\frac{4}{3}c)(t_1t_3+t_2t_3)-\frac{16}{9}t_1t_2 \end{bmatrix} \quad \ldots(4.39a)$$

where:

$$c=\frac{-(3+13\alpha_1)}{3\alpha_2}, d=\frac{-(2+14\alpha_1)}{\alpha_2}, t_i^2=\frac{29}{18}, i=1,2,3 \text{ and } t_it_j=\frac{13}{36}, i\neq j=1,2,3 .$$

The trace of this matrix (4.39a) being,

$$\begin{aligned} traceH_0C_2C_0^{-1}H' &= \frac{-1}{3\alpha_1\alpha_2}\left[(8+\tfrac{8}{9}d)(t_1^2+t_2^2+t_3^2)+(8+\tfrac{8}{3}c-\tfrac{16}{9})(t_1t_2+t_1t_3+t_2t_3)\right] \\ &= \frac{310+1962\alpha_1-1226\alpha_2}{81\alpha_1\alpha_2^2} \end{aligned} \quad \ldots (4.39b)$$

Using (4.37b) and (4.39b) in condition (4.38) gave the conditional equation,

$$\frac{310+1962\alpha_1-1226\alpha_2}{81\alpha_1\alpha_2^2}=\frac{1856\alpha_1+4488\alpha_2}{81\alpha_1\alpha_2} .$$

From which after using the relation, $\alpha_1 = 1-\alpha_2$ narrowed to the quadratic equation;

$$2632\alpha_2^2+5044\alpha_2-2272=0$$

with solutions 0.3764775227 and -2.292890897. Therefore, $\alpha_2 = 0.3764775227$ since $\alpha_2 \in (0, 1)$.

Thus for m=3 ingredients, we have the A- optimal slope weight vector;

$\alpha_1 = 0.6249112749$ and $\alpha_2 = 0.3764775227$……………………………(4.40)

Therefore, in the second-degree Kronecker model for mixture experiments with three ingredients, the unique A- optimal slope design for $K'\theta$ is

$$\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.6249112749\eta_1 + 0.3750887251\eta_2 .$$

From equation (3.22), the average-variance criterion, for a nonnegative definite matrix C of order s is given by;

$$v(\phi_{-1}) = \left(\frac{1}{s} traceC^{-1}\right)^{-1} \quad \text{……………………………………………..….. (4.41)}$$

Presently the average-variance criterion, is obtained for the information matrix of order m=3 from the relation;

$$v(\phi_{-1}) = \left(\frac{1}{3} traceH_0C_0^{-1}H_0'\right)^{-1} \quad \text{……………………………..……..…(4.42)}$$

Now, from (4.31), (4.34) and (4.40) we obtained;

$$H_0C_0^{-1}H_0' = \frac{1}{243\alpha_1\alpha_2}\begin{bmatrix} 1856\alpha_1 + 4488\alpha_2 & 208\alpha_1 - 934\alpha_2 & 208\alpha_1 - 934\alpha_2 \\ 208\alpha_1 - 934\alpha_2 & 1856\alpha_1 + 4488\alpha_2 & 208\alpha_1 - 934\alpha_2 \\ 208\alpha_1 - 934\alpha_2 & 208\alpha_1 - 934\alpha_2 & 1856\alpha_1 + 4488\alpha_2 \end{bmatrix}$$

$$H_0C_0^{-1}H_0' = \begin{bmatrix} 49.9176 & -3.8686 & -3.8686 \\ -3.8686 & 49.9176 & 3.8686 \\ -3.8686 & -3.8686 & 49.9176 \end{bmatrix} \quad \text{…………..………………(4.43)}$$

The average variance criterion for the design with m=3 ingredients using (4.42) and (4.43) is given by;

$$v(\phi_{-1}) = (49.9176)^{-1} = 0.020033014 \blacksquare$$

4.1.1.3 A- Optimal Slope Weighted Centroid Design with Four Ingredients

For a mixture experiment with four ingredients, we consider the weighted centroid design with the following fifteen points of support (in table 2) arrived at using the definition of points (3.2).

Table 2: Support points for the four ingredients centroid design

Design points	Ingredients			
	t_1	t_2	t_3	t_4
1	1	0	0	0
2	0	1	0	0
3	0	0	1	0
4	0	0	0	1
5	½	½	0	0
6	½	0	½	0
7	½	0	0	½
8	0	½	½	0
9	0	½	0	½
10	0	0	½	½
11	⅓	⅓	⅓	0
12	⅓	⅓	0	⅓
13	⅓	0	⅓	⅓
14	0	⅓	⅓	⅓
15	¼	¼	¼	¼

The optimal slope weighted centroid design is

$\eta(\alpha) = \sum_{j=1}^{4} \alpha_j \eta_j = \alpha_1\eta_1 + \alpha_2\eta_2 + \alpha_3\eta_3 + \alpha_4\eta_4$ with $\alpha = (\alpha_1, \alpha_2, 0, 0) \in T_2$ and $\alpha_1 + \alpha_2 = 1$. There are four-elementary centroid designs as directed from (3.3) are;

$$\eta_1 = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\}, \eta_2 = \left\{ \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \\ 0 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 0 \\ 0 \\ 1/2 \end{pmatrix}, \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1/2 \\ 0 \\ 1/2 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1/2 \\ 1/2 \end{pmatrix} \right\},$$

$$\eta_3 = \left\{ \begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \\ 0 \end{pmatrix}, \begin{pmatrix} 1/3 \\ 1/3 \\ 0 \\ 1/3 \end{pmatrix}, \begin{pmatrix} 1/3 \\ 0 \\ 1/3 \\ 1/3 \end{pmatrix}, \begin{pmatrix} 0 \\ 1/3 \\ 1/3 \\ 1/3 \end{pmatrix} \right\} \text{ and } \eta_4 = \left\{ \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{pmatrix} \right\}.$$

The Kronecker model using m=4 ingredients (according to (3.3)) has sixteen parameters which are not all estimable. We chose the maximal parameter subsystem (consisting of ten parameters) by using the coefficient (K) matrix for the design. To construct this matrix, we relied on the unit vectors:

$$e_1 = (1 \quad 0 \quad 0 \quad 0)', \quad e_2 = (0 \quad 1 \quad 0 \quad 0)', \quad e_3 = (0 \quad 0 \quad 1 \quad 0)', \quad e_4 = (0 \quad 0 \quad 0 \quad 1)',$$

$$E_{12} = (1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)', \ E_{13} = (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0)', \ E_{14} = (0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0)',$$

$$E_{23} = (0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0)', \quad E_{24} = (0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0)' \text{ and}$$

$$E_{34} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1)'$$

we have for m=4 in (3.7) and (3.8);

$$K_1 = e_{11}e_1' + e_{22}e_2' + e_{33}e_3' + e_{44}e_4' = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$K_2 = \frac{1}{4}[(e_{12} + e_{21})E_{12}' + (e_{13} + e_{31})E_{13}' + (e_{14} + e_{41})E_{14}' + (e_{23} + e_{32})E_{23}' + (e_{24} + e_{42})E_{24}' + (e_{34} + e_{43})E_{34}']$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/4 & 0 & 0 & 0 \\ 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

which when substituted into (3.6), gave the coefficient matrix,

$$K = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.45)$$

The moment matrix for the weighted centroid design $\eta(\alpha)$ with four ingredients from (3.10) is given by;

$$M(\eta(\alpha)) =$$

$$\begin{pmatrix}
\mu_{4} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{31} \\
\mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} \\
\mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} \\
\mu_{31} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} \\
\mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} \\
\mu_{22} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{4} & \mu_{31} & \mu_{31} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} \\
\mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} \\
\mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} \\
\mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} \\
\mu_{211} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} \\
\mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{211} & \mu_{31} & \mu_{31} & \mu_{4} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} \\
\mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{21} & \mu_{22} & \mu_{31} \\
\mu_{31} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} \\
\mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} \\
\mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{1111} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{22} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} \\
\mu_{22} & \mu_{211} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{22} & \mu_{211} & \mu_{31} & \mu_{211} & \mu_{211} & \mu_{22} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{31} & \mu_{4}
\end{pmatrix}$$

Using the definition of the fourth order moments (3.11), for m=4 these moment matrices for two centroids η_1 and η_2 are respectively;

$$M(\eta_1) = \begin{pmatrix}
1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4
\end{pmatrix} \ldots (4.46)$$

and

$$M(\eta_2)=\begin{pmatrix}
\frac{1}{32}&\frac{1}{96}&\frac{1}{96}&\frac{1}{96}&\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&0&\frac{1}{96}&0&\frac{1}{96}&0&0&\frac{1}{96}\\
\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}&0&0&0&0&0&0&0&0&0&0\\
\frac{1}{96}&0&\frac{1}{96}&0&0&0&0&0&\frac{1}{96}&0&\frac{1}{96}&0&0&0&0&0\\
\frac{1}{96}&0&0&\frac{1}{96}&0&0&0&0&0&0&0&0&\frac{1}{96}&0&0&\frac{1}{96}\\
\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}&0&0&0&0&0&0&0&0&0&0\\
\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{32}&\frac{1}{96}&\frac{1}{96}&0&\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&0&\frac{1}{96}\\
0&0&0&0&0&\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}&0&0&0&0&0\\
0&0&0&0&0&\frac{1}{96}&0&\frac{1}{96}&0&0&0&0&0&\frac{1}{96}&0&\frac{1}{96}\\
\frac{1}{96}&0&\frac{1}{96}&0&0&0&0&0&\frac{1}{96}&0&\frac{1}{96}&0&0&0&0&0\\
0&0&0&0&0&\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}&0&0&0&0&0\\
\frac{1}{96}&0&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}&0&\frac{1}{96}&\frac{1}{96}&\frac{1}{32}&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}\\
\frac{1}{96}&0&0&\frac{1}{96}&0&0&0&0&0&0&0&0&\frac{1}{96}&0&0&\frac{1}{96}\\
0&0&0&0&0&\frac{1}{96}&0&\frac{1}{96}&0&0&0&0&0&\frac{1}{96}&0&\frac{1}{96}\\
0&0&0&0&0&0&0&0&0&0&\frac{1}{96}&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}\\
\frac{1}{96}&0&0&\frac{1}{96}&0&\frac{1}{96}&0&\frac{1}{96}&0&0&\frac{1}{96}&\frac{1}{96}&\frac{1}{96}&\frac{1}{96}&\frac{1}{96}&\frac{1}{32}
\end{pmatrix}\text{..(4.47)}$$

Then, we obtained the left inverse of the coefficient matrix using (4.45) as;

$$L=\begin{pmatrix}
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
0&2&0&0&2&0&0&0&0&0&0&0&0&0&0&0\\
0&0&2&0&0&0&0&0&2&0&0&0&0&0&0&0\\
0&0&0&2&0&0&0&0&0&0&0&0&2&0&0&0\\
0&0&0&0&0&0&2&0&0&2&0&0&0&0&0&0\\
0&0&0&0&0&0&0&2&0&0&0&0&0&2&0&0\\
0&0&0&0&0&0&0&0&0&0&0&2&0&0&2&0
\end{pmatrix}\text{....................(4.48)}$$

The design η_1, has the information matrix obtained using (4.46) and (4.48) in (3.18) as;

$$C_1 = \begin{pmatrix} 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.49)$$

Then for the design η_2, the information matrix was obtained using (4.47) and (4.48) in (3.18) as;

$$C_2 = \begin{pmatrix} \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{24} & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 \\ \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{24} & 0 & 0 & \frac{1}{24} & \frac{1}{24} & 0 \\ \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & 0 & \frac{1}{24} & 0 & \frac{1}{24} & 0 & \frac{1}{24} \\ \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & 0 & 0 & \frac{1}{24} & 0 & \frac{1}{24} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{24} & 0 & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 \\ \frac{1}{24} & 0 & 0 & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 \\ 0 & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 & 0 & \frac{1}{6} & 0 & 0 \\ 0 & \frac{1}{24} & 0 & \frac{1}{24} & 0 & 0 & 0 & 0 & \frac{1}{6} & 0 \\ 0 & 0 & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 & 0 & 0 & \frac{1}{6} \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.50)$$

From equations (4.49) and (4.50) we got the information matrix for the design $\eta(\alpha)$ using the linear function (3.17) that was to be adjusted for slope as;

$$C_0 = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0 \\ \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} \\ \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha}{6} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0 \\ 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6} & 0 \\ 0 & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6} \end{pmatrix} \quad \ldots (4.51)$$

From condition (3.21), putting p=-1, we have that $\eta(\alpha)$ is $\phi_{-1} - slope\,optimal$ for $K'\theta$ in T if and only if,

$$trace H_0 C_j C_k^{-2} H_0' = trace H_0 C_k^{-1} H_0' \text{ for all } j \in \{1,2\} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.52)$$

The inverse of the information matrix (4.51) is;

$$C_0^{-1} = \begin{pmatrix} \frac{4}{\alpha_1} & 0 & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & 0 & 0 \\ 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 \\ 0 & 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} \\ 0 & 0 & 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} \\ \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & 0 & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0 \\ \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{1}{4\alpha_1} \\ \frac{-1}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} \\ 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} \\ 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} \\ 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} \end{pmatrix} \quad \text{.........(4.53)}$$

which on squaring yields,

$$C_0^{-2} = \begin{pmatrix} a & b & b & b & c & c & c & d & d & d \\ b & a & b & b & c & d & d & c & c & d \\ b & b & a & b & d & c & d & c & d & c \\ b & b & b & a & d & d & c & d & c & c \\ c & c & d & d & e & f & f & f & f & g \\ c & d & c & d & f & e & f & f & g & f \\ c & d & d & c & f & f & e & g & f & f \\ d & c & c & d & f & f & g & e & f & f \\ d & c & d & c & f & g & f & f & e & f \\ d & d & c & c & g & f & f & f & f & e \end{pmatrix} \quad \text{..............................(4.54)}$$

where:

$$a = \frac{19}{\alpha_1^2},\ b = \frac{1}{\alpha_1^2},\ c = \frac{-(6\alpha_1 + 5\alpha_2)}{\alpha_1^2\alpha_2},\ d = \frac{-1}{2\alpha_1^2},\ e = \frac{65\alpha_1^2 + 2\alpha_1 + 5}{2\alpha_1^2\alpha_2^2},$$

$$f = \frac{24\alpha_1 + 11\alpha_2}{8\alpha_1^2\alpha_2} \text{ and } g = \frac{1}{4\alpha_1^2}$$

The slope matrix for the design with four ingredients using equation (3.12) is

$$D=\begin{pmatrix} 2t_1 & t_2 & t_3 & t_4 & t_2 & 0 & 0 & 0 & t_3 & 0 & 0 & 0 & t_4 & 0 & 0 & 0 \\ 0 & t_1 & 0 & 0 & t_1 & 2t_2 & t_3 & t_4 & 0 & t_3 & 0 & 0 & 0 & t_4 & 0 & 0 \\ 0 & 0 & t_1 & 0 & 0 & 0 & t_2 & 0 & t_1 & t_2 & 2t_3 & t_4 & 0 & 0 & t_4 & 0 \\ 0 & 0 & 0 & t_4 & 0 & 0 & 0 & t_2 & 0 & 0 & 0 & t_3 & t_1 & t_2 & t_3 & 2t_4 \end{pmatrix}, \quad \text{……(4.55)}$$

This making us of equation (3.13) led to an adjusted slope matrix;

$$H_0=\begin{pmatrix} 2t_1 & 0 & 0 & 0 & \frac{1}{2}t_2 & \frac{1}{2}t_3 & \frac{1}{2}t_4 & 0 & 0 & 0 \\ 0 & 2t_2 & 0 & 0 & \frac{1}{2}t_1 & 0 & 0 & \frac{1}{2}t_3 & \frac{1}{2}t_4 & 0 \\ 0 & 0 & 2t_3 & 0 & 0 & \frac{1}{2}t_1 & 0 & \frac{1}{2}t_2 & 0 & \frac{1}{2}t_4 \\ 0 & 0 & 0 & 2t_4 & 0 & 0 & \frac{1}{2}t_1 & 0 & \frac{1}{2}t_2 & \frac{1}{2}t_3 \end{pmatrix} \quad \text{…………………..(4.56)}$$

when j=1 in (4.52) results in the relation,

$$traceH_0C_1C_0^{-2}H_0' = traceH_0C_0^{-1}H_0'. \quad \text{……………………………………..… (4.57)}$$

We have from equations (4.49), (4.54) and (4.56);

$$H_0C_1C_o^{-2}H_0'=\frac{1}{4\alpha_1^2}\begin{bmatrix} 76t_1^2+A(t_1t_2+t_1t_3+t_1t_4) & 4t_1t_2+At_1^2-\frac{1}{2}(t_1t_3+t_1t_4) & 4t_1t_3+At_1^2-\frac{1}{2}(t_1t_2+t_1t_4) & 4t_1t_4+At_1^2-\frac{1}{2}(t_1t_2+t_1t_3) \\ 4t_1t_2+At_2^2-\frac{1}{2}(t_2t_3+t_2t_4) & 76t_2^2+A(t_1t_2+t_2t_3+t_2t_4) & 4t_2t_3+At_2^2-\frac{1}{2}(t_1t_2+t_2t_4) & 4t_2t_4+At_2^2-\frac{1}{2}(t_1t_2+t_2t_3) \\ 4t_1t_3+At_3^2-\frac{1}{2}(t_2t_3+t_3t_4) & 4t_2t_3+At_3^2-\frac{1}{2}(t_1t_3+t_3t_4) & 76t_3^2+A(t_1t_3+t_2t_3+t_3t_4) & 4t_3t_4+At_3^2-\frac{1}{2}(t_1t_3+t_2t_3) \\ 4t_1t_4+At_4^2-\frac{1}{2}(t_2t_4+t_3t_4) & 4t_2t_4+At_4^2-\frac{1}{2}(t_1t_4+t_3t_4) & 4t_3t_4+At_4^2-\frac{1}{2}(t_1t_4+t_2t_4) & 76t_4^2+A(t_1t_4+t_2t_4+t_3t_4) \end{bmatrix} \quad \text{……….(4.58a)}$$

where:

$$A=\frac{-(6\alpha_1+5\alpha_2)}{\alpha_2},\ t_i^2=\frac{103}{48}, i=1,2,3,4 \text{ and } t_it_j=\frac{77}{144},\ i\neq j=1,2,3,4$$

The trace of (4.58a) is;

$$\begin{aligned} traceH_0C_1C_0^{-2}H_0' &= \frac{1}{4\alpha_1^2}\left[76(t_1^2+t_2^2+t_3^2+t_4^2)-\frac{2(6\alpha_1+5\alpha_2)}{\alpha_2}(t_1t_2+t_1t_3+t_1t_4+t_2t_3+t_2t_4+t_3t_4)\right] \\ &= \frac{7443\alpha_2-462\alpha_1}{48\alpha_1^2\alpha_2} \end{aligned} \quad \text{………(4.58b)}$$

Also, from equations (4.53) and (4.56);

$$H_0 C_0^{-1} H_0' = \frac{-1}{\alpha_1}\begin{bmatrix}
-16t_1^2 + \tfrac{a}{4}(t_2^2+t_3^2+t_4^2) + 2(t_1t_2+t_1t_3+t_1t_4) - \tfrac{1}{8}(t_2t_3+t_2t_4+t_3t_4) & t_1^2+t_2^2-\tfrac{1}{16}(t_3^2+t_4^2+t_1t_3+t_1t_4+t_2t_3+t_2t_4)+\tfrac{a}{4}t_1t_2 & t_1^2+t_3^2-\tfrac{1}{16}(t_2^2+t_4^2+t_1t_2+t_1t_4+t_2t_3+t_3t_4)+\tfrac{a}{4}t_1t_3 & t_1^2+t_4^2-\tfrac{1}{16}(t_2^2+t_3^2+t_1t_2+t_1t_3+t_2t_4+t_3t_4)+\tfrac{a}{4}t_1t_4 \\
t_2^2+t_1^2-\tfrac{1}{16}(t_3^2+t_4^2+t_1t_3+t_1t_4+t_2t_3+t_3t_4)+\tfrac{a}{4}t_1t_2 & -16t_2^2 + \tfrac{a}{4}(t_1^2+t_3^2+t_4^2) + 2(t_1t_2+t_2t_3+t_2t_4) - \tfrac{1}{8}(t_1t_3+t_1t_4+t_3t_4) & t_2^2+t_3^2-\tfrac{1}{16}(t_1^2+t_4^2+t_1t_2+t_1t_3+t_2t_4+t_3t_4)+\tfrac{a}{4}t_2t_3 & t_2^2+t_4^2-\tfrac{1}{16}(t_1^2+t_3^2+t_1t_2+t_1t_4+t_2t_3+t_3t_4)+\tfrac{a}{4}t_2t_4 \\
t_3^2+t_1^2-\tfrac{1}{16}(t_2^2+t_4^2+t_1t_2+t_1t_4+t_2t_3+t_3t_4)+\tfrac{a}{4}t_1t_3 & t_3^2+t_2^2-\tfrac{1}{16}(t_1^2+t_4^2+t_1t_2+t_1t_3+t_2t_4+t_3t_4)+\tfrac{a}{4}t_2t_3 & -16t_3^2 + \tfrac{a}{4}(t_1^2+t_2^2+t_4^2) + 2(t_1t_3+t_2t_3+t_3t_4) - \tfrac{1}{8}(t_1t_2+t_1t_4+t_2t_4) & t_3^2+t_4^2-\tfrac{1}{16}(t_1^2+t_2^2+t_1t_3+t_1t_4+t_2t_3+t_2t_4)+\tfrac{a}{4}t_3t_4 \\
t_4^2+t_1^2-\tfrac{1}{16}(t_2^2+t_3^2+t_1t_2+t_1t_3+t_2t_4+t_3t_4)+\tfrac{a}{4}t_1t_4 & t_4^2+t_2^2-\tfrac{1}{16}(t_1^2+t_3^2+t_1t_2+t_1t_4+t_2t_3+t_3t_4)+\tfrac{a}{4}t_2t_4 & t_4^2+t_3^2-\tfrac{1}{16}(t_1^2+t_2^2+t_1t_3+t_1t_4+t_2t_3+t_2t_4)+\tfrac{a}{4}t_3t_4 & -16t_4^2 + \tfrac{a}{4}(t_1^2+t_2^2+t_3^2) + 2(t_1t_4+t_2t_4+t_3t_4) - \tfrac{1}{8}(t_1t_2+t_1t_3+t_2t_3)
\end{bmatrix} \quad \ldots\ldots(4.59a)$$

where:

$$a = \frac{-(12\alpha_1+\alpha_2)}{2\alpha_2}, \; t_i^2 = \frac{103}{48}, i = 1,2,3,4 \text{ and } t_i t_j = \frac{77}{144}, \; i \neq j = 1,2,3,4$$

Trace of (4.59a) is;

$$trace H_0 C_k^{-1} H_0' = \frac{-1}{\alpha_1}\left[(-16+\tfrac{3}{4}a)(t_1^2+t_2^2+t_3^2+t_4^2) + \tfrac{15}{4}(t_1t_2+t_1t_3+t_1t_4+t_2t_3+t_2t_4+t_3t_4)\right] \quad \ldots\ (4.59b)$$

$$= \frac{1854\alpha_1 + 6169\alpha_2}{48\alpha_1\alpha_2}$$

Using (4.58b) and (4.59b) in (4.47) gave the equality relation

$$\frac{7443\alpha_2 - 462\alpha_1}{48\alpha_1^2\alpha_2} = \frac{1854\alpha_1 + 6169\alpha_2}{48\alpha_1\alpha_2} \,,$$

that after substituting for $\alpha_2 = 1 - \alpha_1$ led to the quadratic equation,

$$4315\alpha_1^2 - 14074\alpha_1 + 7443 = 0$$

with solutions 0.66403958 and 2.597605842. But since $\alpha_1 \in (0, 1)$, the right choice is

$\alpha_1 = 0.664039581$.

When j=2 in (4.52), we obtained the relation,

$$traceH_0C_2C_0^{-2}H_0' = traceH_0C_0^{-1}H_0'. \qquad \text{………………..…………} \ (4.60)$$

To work out the trace on the left hand side of this condition, we first multiplied

(4.50), (4.53) and (4.56), to get;

$$H_0C_2C_0^{-1}H_0' = \frac{-1}{4\alpha_1\alpha_2}\begin{bmatrix} 12t_1^2+\frac{1}{4}d(t_2^2+t_3^2+t_4^2)+(4+a)t_1(t_2+t_3+t_4)-\frac{1}{2}(t_2t_3+t_2t_4+t_3t_4) & 4t_2(t_2+t_1)+2t_1(2at_1-t_3-t_4)+\frac{1}{4}t_2(dt_1-t_3-t_4)-\frac{1}{4}t_3(t_1+t_3)-\frac{1}{4}t_4(t_1+t_4) & 4t_3(t_3+t_1)+2t_1(2at_1-t_2-t_4)+\frac{1}{4}t_3(dt_1-t_2-t_4)-\frac{1}{4}t_2(t_1+t_2)-\frac{1}{4}t_4(t_1+t_4) & 4t_4(t_4+t_1)+2t_1(2at_1-t_2-t_3)+\frac{1}{4}t_4(dt_1-t_2-t_3)-\frac{1}{4}t_2(t_1+t_2)-\frac{1}{4}t_3(t_1+t_3) \\ 4t_1(t_1+t_2)+2t_2(2at_2-t_3-t_4)+\frac{1}{4}t_1(dt_2-t_3-t_4)-\frac{1}{4}t_3(t_2+t_3)-\frac{1}{4}t_4(t_2+t_4) & 12t_2^2+\frac{1}{4}d(t_1^2+t_3^2+t_4^2)+(4+a)t_2(t_1+t_3+t_4)-\frac{1}{2}(t_1t_3+t_1t_4+t_3t_4) & 4t_3(t_3+t_2)+2t_2(2at_2-t_1-t_4)+\frac{1}{4}t_3(dt_2-t_1-t_4)-\frac{1}{4}t_1(t_1+t_2)-\frac{1}{4}t_4(t_2+t_4) & 4t_4(t_4+t_2)+2t_2(2at_2-t_1-t_3)+\frac{1}{4}t_4(dt_2-t_1-t_3)-\frac{1}{4}t_1(t_1+t_2)-\frac{1}{4}t_3(t_2+t_3) \\ 4t_1(t_1+t_3)+2t_3(2at_3-t_2-t_4)+\frac{1}{4}t_1(dt_3-t_2-t_4)-\frac{1}{4}t_2(t_2+t_3)-\frac{1}{4}t_4(t_3+t_4) & 4t_2(t_2+t_3)+2t_3(2at_3-t_1-t_4)+\frac{1}{4}t_2(dt_3-t_1-t_4)-\frac{1}{4}t_1(t_1+t_3)-\frac{1}{4}t_4(t_3+t_4) & 12t_3^2+\frac{1}{4}d(t_1^2+t_2^2+t_4^2)+(4+a)t_3(t_1+t_2+t_4)-\frac{1}{2}(t_1t_2+t_1t_4+t_2t_4) & 4t_4(t_4+t_3)+2t_3(2at_3-t_1-t_2)+\frac{1}{4}t_4(dt_3-t_1-t_2)-\frac{1}{4}t_1(t_1+t_3)-\frac{1}{4}t_2(t_2+t_3) \\ 4t_1(t_1+t_4)+2t_4(2at_4-t_2-t_3)+\frac{1}{4}t_1(dt_4-t_2-t_3)-\frac{1}{4}t_2(t_2+t_4)-\frac{1}{4}t_3(t_3+t_4) & 4t_2(t_2+t_4)+2t_4(2at_4-t_1-t_3)+\frac{1}{4}t_2(dt_4-t_1-t_3)-\frac{1}{4}t_1(t_1+t_4)-\frac{1}{4}t_3(t_3+t_4) & 4t_3(t_3+t_4)+2t_4(2at_4-t_1-t_2)+\frac{1}{4}t_3(dt_4-t_1-t_2)-\frac{1}{4}t_1(t_1+t_4)-\frac{1}{4}t_2(t_2+t_4) & 12t_4^2+\frac{1}{4}d(t_1^2+t_2^2+t_3^2)+(4+a)t_4(t_1+t_2+t_3)-\frac{1}{2}(t_1t_2+t_1t_3+t_2t_3) \end{bmatrix} \text{………}(4.61a)$$

where:

$$a = \frac{-(5\alpha_1+1)}{\alpha_2},\ d = \frac{-2(11\alpha_1+1)}{\alpha_2},\ t_i^2 = \frac{103}{48}, i = 1,2,3,4 \text{ and}$$

$$t_it_j = \frac{77}{144},\ i \neq j = 1,2,3,4$$

The trace of matrix (4.61a) being,

$$traceH_0C_2C_0^{-2}H' = \frac{-1}{4\alpha_1\alpha_2}\left[(12+\tfrac{3}{4}d)(t_1^2+t_2^2+t_3^2+t_4^2)+(7+2a)(t_1t_2+t_1t_3+t_1t_4+t_2t_3+t_2t_4+t_3t_4)\right] \quad \ldots(4.61b)$$
$$= \frac{463+4169\alpha_1-3011\alpha_2}{96\alpha_1\alpha_2^2}$$

Using (4.51b) and (4.61b) in (4.60) gave,

$$\frac{1854\alpha_1+6169\alpha_2}{48\alpha_1\alpha_2} = \frac{463+4169\alpha_1-3011\alpha_2}{96\alpha_1\alpha_2^2} \ ,$$

That after substituting for $\alpha_1 = 1-\alpha_2$ led to the quadratic equation;

$$4515\alpha_2^2+5444\alpha_2-2316=0$$

with solutions 0.335960419 and -1.597605842. But since $\alpha_2 \in (0,\ 1)$ the only acceptable choice is $\alpha_2 = 0.335960419$.

Thus for m=4 ingredients, we have the A- optimal slope weight vector;

$$\alpha_1 = 0.664039581 \text{ and } \alpha_2 = 0.335960419 \ldots\ldots\ldots\ldots(4.62)$$

Therefore, in the second-degree Kronecker model for mixture experiments with four ingredients, the unique A-optimal slope design for $K'\theta$ is $\eta(\alpha^A) = \alpha_1\eta_1 + \alpha_2\eta_2 = 0.664039581\eta_1 + 0.335960419\eta_2$.

From equation (3.22), the average-variance criterion, for a nonnegative definite matrix C of order s is given by;

$$v(\phi_{-1}) = \left(\frac{1}{s}traceC^{-1}\right)^{-1} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.63)$$

At present the average-variance criterion, is obtained for the information matrices of order m=4 ingredients from the relation;

$$v(\phi_{-1}) = \left(\frac{1}{4} trace H_0 C_0^{-1} H_0' \right)^{-1} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.64)$$

Now, the product of (4.53) and (4.56) together with the use of the weight vector (4.62) gave;

$$H_0 C_0^{-1} H_0' = \frac{1}{348\alpha_1\alpha_2} \begin{bmatrix} 3708\alpha_1 + 1233\alpha_2 & 308\alpha_1 - 1468\alpha_2 & 308\alpha_1 - 1468\alpha_2 & 308\alpha_1 - 1468\alpha_2 \\ 308\alpha_1 - 1468\alpha_2 & 3708\alpha_1 + 1233\alpha_2 & 308\alpha_1 - 1468\alpha_2 & 308\alpha_1 - 1468\alpha_2 \\ 308\alpha_1 - 1468\alpha_2 & 308\alpha_1 - 1468\alpha_2 & 3708\alpha_1 + 1233\alpha_2 & 308\alpha_1 - 1468\alpha_2 \\ 308\alpha_1 - 1468\alpha_2 & 308\alpha_1 - 1468\alpha_2 & 308\alpha_1 - 1468\alpha_2 & 3708\alpha_1 + 1233\alpha_2 \end{bmatrix}$$

$$H_0 C_0^{-1} H_0' = \begin{bmatrix} 77.1282 & -3.3696 & -3.3696 & -3.3696 \\ -3.3696 & 77.1282 & -3.3696 & -3.3696 \\ -3.3696 & -3.3696 & 77.1282 & -3.3696 \\ -3.3696 & -3.3696 & -3.3696 & 77.1282 \end{bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots (4.65)$$

The average variance criterion for the design with m=4 ingredients from (4.65) and (4.64) is given by

$$v(\phi_{-1}) = (77.1282)^{-1} = 0.012965426 \blacksquare$$

4.1.1.4 A- Optimal Slope Weighted Centroid Design with m Ingredients

Now, following are relations that can be used to get the A- optimal slope weight vector and the optimal value for a design with $m \geq 2$ ingredients for the A-criterion. This development was motivated by the realization that there is a trend in the numerical values for the weight vector and the A-slope optimality values linking the values to the number of ingredients.

The information matrices for weighted centroid designs are contained in the quadratic subspace, $C \in sym(s, H)$ and by (3.25) can be uniquely represented in the form

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.66)$$

with coefficients $a,\cdots,g \in \Re$, Klein (2004). The terms containing V_2, W_2 and W_3 only occur for $m \geq 3$ and $m \geq 4$ respectively.

The matrix (4.66) according to (3.25a) can be partitioned according to the block structure,

$$C = \begin{pmatrix} C_{11} & C'_{21} \\ C_{21} & C_{22} \end{pmatrix} \qquad (4.67)$$

with $C_{11} \in sym(m)$, $C_{21} \in \Re^{\binom{m}{2}\times m}$ and $C_{22} \in sym\left(\binom{m}{2}\right)$.

For j=1,2, …, m, from (3.25c) we obtain

$$C_j = \begin{pmatrix} C_{11,j} & C'_{21,j} \\ C_{21,j} & C_{22,j} \end{pmatrix} \qquad (4.68)$$

with blocks obtained using (3.25d) as follows:

i) for j=1;

$$C_{11,1} = \frac{1}{m} I_m, \; C_{21,1}=0 \text{ and } C_{22,1}=0 .$$

ii) for j=2;

$$C_{11,2} = \frac{1}{8m} I_m + \frac{1}{8(m-1)} U_2, \; C_{21,2} = \frac{1}{8(m-1)} V_1 \text{ and } C_{22,2} = \frac{m}{8(m-1)} I_{\binom{m}{2}},$$

Thus we have

$$C_1 = \begin{pmatrix} \frac{1}{m} I_m & 0 \\ 0 & 0 \end{pmatrix} \qquad (4.69)$$

and

$$C_2 = \begin{pmatrix} \frac{1}{8m} I_m + \frac{1}{8m(m-1)} U_2 & \frac{1}{8(m-1)} V_1' \\ \frac{1}{8(m-1)} V_1 & \frac{m}{8(m-1)} I\binom{m}{2} \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(4.70)$$

From (4.69) and (4.70) in equation (3.17) which we obtained the information matrix to be adjusted for slope as,

$$C_0 = \begin{pmatrix} \frac{8\alpha_1 + \alpha_2}{8m} I_m + \frac{\alpha_2}{8m(m-1)} U_2 & \frac{\alpha_2}{8(m-1)} V_1' \\ \frac{\alpha_2}{8(m-1)} V_1 & \frac{m\alpha_2}{8(m-1)} I_{\binom{m}{2}} \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.71)$$

An inverse of a matrix in $sym(s, H)$ can be computed by solving a system of linear equations. By the same approach we obtained the blocks of the inverse matrix partitioned as,

$$C_0^{-1} = \begin{pmatrix} \frac{m}{\alpha_1} I_m & \frac{-1}{\alpha_1} V_1' \\ \frac{-1}{\alpha_1} V_1 & \frac{2[4(m-1)\alpha_1 + \alpha_2]}{m\alpha_1\alpha_2} I_{\binom{m}{2}} + \frac{1}{m\alpha_1} W_2 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.72)$$

The square of this inverse matrix was algebraically obtained as;

$$C_0^{-2} = \begin{pmatrix} \frac{m^2 + m - 1}{\alpha_1^2} I_m + \frac{1}{\alpha_1^2} U_2 & -\left(\frac{8(m-1)\alpha_1 + m(m+1)\alpha_2}{m\alpha_1^2\alpha_2}\right) V_1' - \frac{2}{m\alpha_1^2} V_2' \\ -\left(\frac{8(m-1)\alpha_1 + m(m+1)\alpha_2}{m\alpha_1^2\alpha_2}\right) V_1 - \frac{2}{m\alpha_1^2} V_2 & \begin{matrix} \frac{2[32(m-1)^2\alpha_1^2 + 16(m-1)\alpha_1\alpha_2 + m(m+1)\alpha_2^2]}{m^2\alpha_1^2\alpha_2^2} I_{\binom{m}{2}} \\ + \frac{16(m-1)\alpha_1 + (m^2 + m + 2)\alpha_2}{m^2\alpha_1^2\alpha_2} W_2 + \frac{4}{m^2\alpha_1^2} W_3 \end{matrix} \end{pmatrix} \ldots\ldots.(4.73)$$

From the Kronecker second order regression function we got the slope matrix D using (3.12) as

$$D = \left(\frac{\partial f'(t)}{\partial t_1}, \frac{\partial f'(t)}{\partial t_2}, ..., \frac{\partial f'(t)}{\partial t_m} \right)' \qquad (4.74)$$

This slope matrix was then adjusted using (3.13) to get the adjusted slope matrix

$$H_0 = DK = \begin{pmatrix} 2t_i I_m & \frac{2}{m} t_j V_1' \end{pmatrix} \qquad (4.75)$$

This is an $m \times \begin{pmatrix} m+1 \\ 2 \end{pmatrix}$ matrix with K being the coefficient matrix as defined in (3.6)

Now a design that is A-slope optimal if and only if it satisfies condition (3.21). That is, a design is A-slope optimal if,

$$trace H_0 C_j C_0^{-2} H_0' = trace H_0 C_0^{-1} H_0' \quad for\ all\ j \in \partial(\alpha) \qquad (4.76)$$

For j=1;

we employed the matrices (4.69), (4.73) and (4.75) to get the product:

$$H_o C_1 C_0^{-2} H_0' = \left[\frac{4(m^2+m-1)}{m\alpha_1^2} t_i^2 - \frac{4(m-1)[8(m-1)\alpha_1 + m(m+1)\alpha_2]}{m^3\alpha_1^2\alpha_2} t_i t_j \right] I_m + \left[\frac{2}{m\alpha_1^2} t_i^2 - \frac{4(m-1)[8\alpha_1 + (m+4)\alpha_2]}{m^3\alpha_1^2\alpha_2} t_i t_j \right] U_2 \qquad (4.77a)$$

The trace of (4.77a) is;

$$\begin{aligned} trace(H_o C_1 C_0^{-2} H') &= m\left[\frac{4(m^2+m-1)}{m\alpha_1^2} t_i^2 - \frac{4(m-1)[8(m-1)\alpha_1 + m(m+1)\alpha_2]}{m^3\alpha_1^2\alpha_2} t_i t_j \right] \\ &= m\left[\frac{4(m^2+m-1)}{m\alpha_1^2} A - \frac{4(m-1)[8(m-1)\alpha_1 + m(m+1)\alpha_2]}{m^3\alpha_1^2\alpha_2} B \right] \end{aligned} \qquad (4.77b)$$

where $A = t_i^2 = \sum_{i=0}^{m-1} \begin{pmatrix} m-1 \\ i \end{pmatrix} \frac{1}{(i+1)^2}$ and $B = t_i t_j = \sum_{i=0}^{m-2} \begin{pmatrix} m-2 \\ i \end{pmatrix} \frac{1}{(i+2)^2}$

From the matrices (4.72) and (4.75) we got the product;

$$H_o C_0^{-1} H_0' = \left[\frac{4m}{\alpha_1} t_i^2 - \frac{8(m-1)}{m\alpha_1} t_i t_j + \frac{4(m-1)[8(m-1)\alpha_1 + m\alpha_2]}{m^3 \alpha_1 \alpha_2} t_j^2\right] I_m + \left[\frac{-8}{m\alpha_1} t_i t_j + \frac{32(m-1)\alpha_1 + 4(3m-4)\alpha_2}{m^3 \alpha_1 \alpha_2} t_j^2\right] U_2 \quad \text{........(4.78a)}$$

The trace of (4.78a) is;

$$trace(H_o C_0^{-1} H_0') = m\left[\frac{4m}{\alpha_1} t_i^2 - \frac{8(m-1)}{m\alpha_1} t_i t_j + \frac{4(m-1)[8(m-1)\alpha_1 + m\alpha_2]}{m^3 \alpha_1 \alpha_2} t_j^2\right]$$
$$= m\left[\frac{4[8(m-1)^2 \alpha_1 + m(m^3 + m - 1)\alpha_2]}{m^3 \alpha_1 \alpha_2} A - \frac{8(m-1)}{m\alpha_1} B\right] \quad \text{..... (4.78b)}$$

$$A = t_i^2 = \sum_{i=0}^{m-1} \binom{m-1}{i} \frac{1}{(i+1)^2} \text{ and } B = t_i t_j = \sum_{i=0}^{m-2} \binom{m-2}{i} \frac{1}{(i+2)^2}$$

after employing the ordinates of the support points in the m-ingredient mixture design.

Using (4.77b) and (4.78b) in condition (4.76) we obtained the relation,

$$m\left[\frac{4(m^2+m-1)}{m\alpha_1^2} A - \frac{4(m-1)[8(m-1)\alpha_1 + m(m+1)\alpha_2]}{m^3 \alpha_1^2 \alpha_2} B\right] = m\left[\frac{4[8(m-1)^2 \alpha_1 + m(m^3+m-1)\alpha_2]}{m^3 \alpha_1 \alpha_2} A - \frac{8(m-1)}{m\alpha_1} B\right]$$

That after substituting for $\alpha_2 = 1 - \alpha_1$ led to the quadratic equation;

$$[(-m^4 + 7m^2 - 15m + 8)A + 2m^2(m-1)B]\alpha_1^2 + [(m^4 + 2m^2 - 1)A - m(3m^2 - 10m + 15)B]\alpha_1$$
$$-(m^2 + m - 1)A + m(m^2 - 1)B = 0$$

The only acceptable solution being;

$$\alpha_1 = \frac{-[(m^4 + 2m^2 - 1)A - m(3m^2 - 10m + 15)B] + \sqrt{gA^2 + hB^2 + qAB}}{2[(-m^4 + 7m^2 - 15m + 8)A + 2m^2(m-1)B]}$$

where:

$$g = m^8 - 4m^5 + 34m^4 - 32m^3 - 92m^2 + 92m - 31,$$

$$h = m^2(-8m^4 + 8m^3 + 11m^2 - 18m + 15)$$

$$q = 2m(-m^6 + 10m^5 - 33m^4 + 50m^3 - 37m^2 - 36m + 31).$$

Similarly, for j=2, we worked out the product of the matrices (4.70), (4.73) and (4.75) to get;

$$H_o C_2 C_0^{-2} H_0' = \left[\frac{-4(m-1)}{m\alpha_1\alpha_2} t_i^2 + \frac{4(m-1)^2(8\alpha_1 + m\alpha_2)}{m^3\alpha_1\alpha_2^2} t_i t_j + \frac{16(m-1)^2\alpha_1^2 + 16(m-1)^2\alpha_1\alpha_2 + m(m+1)(m-2)\alpha_2^2}{2m^3\alpha_1^2\alpha_2^2} t_j^2 \right] I_m \quad \text{...(4.79a)}$$
$$+ \left[\frac{-4}{m\alpha_1\alpha_2} t_i^2 + \frac{4[8(m-1)\alpha_1 - (m^3 - 3m + 4)\alpha_2}{m^3\alpha_1\alpha_2^2} t_i t_j + \frac{16(m-1)^2\alpha_1^2 - 16(m-1)^2\alpha_1\alpha_2 + m(m+1)(3m-4)\alpha_2^2}{2m^3(m-1)\alpha_1^2\alpha_2^2} \right] U_2$$

where;

$$A = t_i^2 = \sum_{i=0}^{m-1} \binom{m-1}{i} \frac{1}{(i+1)^2} \text{ and } B = t_i t_j = \sum_{i=0}^{m-2} \binom{m-2}{i} \frac{1}{(i+2)^2}$$

The trace of (4.79a) is;

$$trace(H_o C_2 C_0^{-2} H_0') = m \left[\begin{array}{l} \frac{-4(m-1)}{m\alpha_1\alpha_2} t_i^2 + \frac{4(m-1)^2(8\alpha_1 + m\alpha_2)}{m^3\alpha_1\alpha_2^2} t_i t_j + \\ \frac{16(m-1)^2\alpha_1^2 + 16(m-1)^2\alpha_1\alpha_2 + m(m+1)(m-2)\alpha_2^2}{2m^3\alpha_1^2\alpha_2^2} t_j^2 \end{array} \right] \quad \text{..(4.79b)}$$
$$= m \left[\frac{16(m-1)^2\alpha_1^2 - 8(m-1)(m^2 - 2m + 2)\alpha_1\alpha_2 + m(m+1)(m-2)\alpha_2^2}{2m^3\alpha_1^2\alpha_2^2} A + \frac{4(m-1)^2(8\alpha_1 + m\alpha_2)}{m^3\alpha_1\alpha_2^2} B \right]$$

Using (4.78b) and (4.79b) in condition (4.76) we obtained the equivalence relation;

$$m\left[\frac{16(m-1)^2\alpha_1^2-8(m-1)(m^2-2m+2)\alpha_1\alpha_2+m(m+1)(m-2)\alpha_2^2}{2m^3\alpha_1^2\alpha_2^2}A+\frac{4(m-1)^2(8\alpha_1+m\alpha_2)}{m^3\alpha_1\alpha_2^2}B\right]=$$
$$m\left[\frac{4(m-1)[8(m-1)^2\alpha_1+m(m^3+m-1)\alpha_2]}{m^3\alpha_1\alpha_2}A-\frac{8(m-1)}{m\alpha_1}B\right]$$

This alongside the conditional relation $\alpha_1 = 1-\alpha_2$ gave the equation;

$$[(m^4+63m^2+127m-64)A-16m^2(m-1)B]\alpha_2^3+$$
$$[(-m^4+9m^3+118m^2-257m+128)A+8(m-1)(m^2+9m-8)B]\alpha_2^2+$$
$$[8(m-1)(m^2-14m+14)A+8(m-1)(m-16)B]\alpha_2+16(m-1)^2A+64(m-1)^2B=0$$

with a feasible solution;

$$\alpha_2=\frac{-(m-1)(m^3+m^2-15m+15)A+m(7m^2-14m+15)B-\sqrt{gA^2+hB^2+qAB}}{2[(-m^4+7m^2-15m+8)A+2m^2(m-1)B]}$$

where:

$$g=m^8-4m^5+34m^4-32m^3-92m^2+92m-31,$$

$$h=m^2(-8m^4+8m^3+11m^2-18m+15)$$

$$q=2m(-m^6+10m^5-33m^4+50m^3-37m^2-36m+31).$$

Thus for a design with m≥2 ingredients, we have the A- optimal slope weight vector;

$$\alpha_1=\frac{-[(m^4+2m^2-1)A-m(3m^2-10m+15)B]+\sqrt{gA^2+hB^2+qAB}}{2[(-m^4+7m^2-15m+8)A+2m^2(m-1)B]}$$

and

$$\alpha_2=\frac{-(m-1)(m^3+m^2-15m+15)A+m(7m^2-14m+15)B-\sqrt{gA^2+hB^2+qAB}}{2[(-m^4+7m^2-15m+8)A+2m^2(m-1)B]}\quad\ldots\ldots\ldots(4.80)$$

Therefore, in the second-degree Kronecker model for mixture experiments with $m \geq 2$ ingredients, the unique A- optimal slope design for $K'\theta$ is $\eta(\alpha^{(A)}) = \alpha_1\eta_1 + \alpha_2\eta_2$, with the weight vector as provided for in (4.80).

From equation (3.22), the average-variance criterion, for a nonnegative definite matrix C of order s is given by;

$$v(\phi_{-1}) = \left(\frac{1}{s} traceC^{-1}\right)^{-1} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.81)}$$

At present the average-variance criterion, is obtained for the information matrices of order s=m from the relation;

$$v(\phi_{-1}) = \left(\frac{1}{m} traceH_0 C_0^{-1} H_0'\right)^{-1} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.82)}$$

Using the trace value from (4.78) we got;

$$v(\phi_{-1}) = \frac{m^3\alpha_1\alpha_2}{4[8(m-1)^2\alpha_1 + m(m^3+m-1)\alpha_2]A - 8m^2(m-1)\alpha_2 B} \,\blacksquare\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.80a)}$$

4.1.2 D- Optimal Slope Weighted Centroid Design

We then derived optimal slope weighted centroid designs for the determinant criterion, ϕ_0. We started this section by adapting equation (3.21). This equation provides necessary and sufficient condition for the derivation of the D- optimal slope designs for a specific number of ingredients. We got the obligatory relation by putting p=0 in equation (3.21), to get the condition that a design is D-slope optimal for $K'\theta$ if and only if;

$$traceH_0 C_j C_0^{-1} H_0' \begin{cases} = traceH_0 H_0' & for\ all\ j \in \partial(\alpha) \\ \leq traceH_0 H_0' & otherwise \end{cases} \quad \text{.............................. (4.83)}$$

where, H_0 is an adjusted slope matrix according to (3.13).

We then proceeded to demonstrating the D- optimal slope designs for specific number of ingredients.

4.1.2.1 D- Optimal Slope Weighted Centroid Design with Two Ingredients

To obtain the D- optimal slope weighted centroid design with two ingredients, we proceeded by first assembling the necessary matrices as follows:

The information matrix to be adjusted for slope and optimized for the D-criterion from (4.11) is;

$$C_0 = \begin{bmatrix} \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{16} & \frac{8\alpha_1+\alpha_2}{16} & \frac{\alpha_2}{8} \\ \frac{\alpha_2}{8} & \frac{\alpha_2}{8} & \frac{\alpha_2}{4} \end{bmatrix} \quad \text{..(4.84)}$$

The information matrices employed for the two centroids η_1 and η_2 are provided in (4.6) and (4.7). These are respectively;

$$C_1 = \begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{...(4.85)}$$

and

$$C_2 = \begin{pmatrix} 1/16 & 1/16 & 2/16 \\ 1/16 & 1/16 & 2/16 \\ 2/16 & 2/16 & 4/16 \end{pmatrix} \quad \text{..(4.86)}$$

The inverse of the information matrix for the design with two ingredients is provided in (4.7) as,

$$C_0^{-1} = \begin{pmatrix} \frac{2}{\alpha_1} & 0 & \frac{-1}{\alpha_1} \\ 0 & \frac{2}{\alpha_1} & \frac{-1}{\alpha_1} \\ \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{4\alpha_1 + \alpha_2}{\alpha_1\alpha_2} \end{pmatrix} \quad \text{(4.87)}$$

We also needed to use the adjusted slope matrix as is from (4.13). That is;

$$H_0 = DK = \begin{pmatrix} 2t_1 & 0 & t_2 \\ 0 & 2t_2 & t_1 \end{pmatrix} \quad \text{(4.88)}$$

From condition (3.21), we have that a weighted centroid design $\eta(\alpha)$ is $\phi_0 - slope\,optimal$ for $K'\theta$ in T if and only if

$$trace H_0 C_j C_0^{-1} H_0' = trace H_0 H_0' \quad for\ all\ j \in \partial(\alpha) \quad \text{(4.89)}$$

For $j \in \{1,2\}$ we begin with the case j=1. Using the information matrices (4.85), (4.87) and (4.88), We calculated the following products:

i) $$H_0 C_1 C_0^{-1} H_0' = \frac{1}{2\alpha_1}\begin{pmatrix} 8t_1^2 - 2t_1t_2 & -2t_1^2 \\ -2t_2^2 & 8t_2^2 - 2t_1t_2 \end{pmatrix} = \frac{1}{4\alpha_1}\begin{pmatrix} 19 & -5 \\ -5 & 19 \end{pmatrix} \quad \text{(4.90a)}$$

where;

$t_i^2 = \frac{5}{4}$ and $t_1 t_2 = \frac{1}{4}$

The trace of (4.90a) is,

$$traceH_0C_1C^{-1}H_0' = \frac{19}{2\alpha_1}$$ ………………….. …………………………… (4.90b)

ii) $H_0H_0' = \begin{pmatrix} 4t_1^2 + t_2^2 & t_1t_2 \\ t_1t_2 & 4t_2^2 + t_1^2 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 25 & 1 \\ 1 & 25 \end{pmatrix}$.

The trace of (4.91a) is;

$$traceH_0H_0' = \frac{25}{2}$$ ……………………………………… ………………… (4.91b)

Using (4.90b) and (4.91b) in the relation (4.89) we got,

$$\alpha_1 = \frac{19}{25} \ .$$

Similarly, when j=2, first a product of the matrices (4.86), (4.87) and (4.88) is;

$$H_0C_2C_0^{-1}H_0' = \frac{1}{\alpha_2}\begin{pmatrix} t_2^2 + t_1t_2 & t_1^2 + t_1t_2 \\ t_2^2 + t_1t_2 & t_1^2 + t_1t_2 \end{pmatrix} = \frac{1}{2\alpha_2}\begin{pmatrix} 3 & 3 \\ 3 & 3 \end{pmatrix}$$ ……………………(4.92a)

The trace of (4.92a) is;

$$traceH_0C_2C_0^{-1}H_0' = \frac{3}{\alpha_2}$$ ……………………………………………….(4.92b)

Second, using (4.91b) and (4.92b) in (4.89) we got,

$$\alpha_2 = \frac{6}{25}.$$

Hence, the D- optimal slope weight vector is;

$$\alpha_1 = \frac{19}{25} \text{ and } \alpha_2 = \frac{6}{25}$$ ………………………………………………(4.93)

Therefore in the second-degree Kronecker model for mixture experiments with two ingredients, the unique D- optimal slope design for $K'\theta$ is $\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{19}{25}\eta_1 + \frac{6}{25}\eta_2$.

To obtain the optimal value $v(\phi_0)$, first we adjusted the information matrix (4.84) for slope by pre- and post-multiplying by the adjusted slope matrix (4.88). This led to the matrix;

$$H_0C_0H_0' = \frac{1}{4}\begin{pmatrix} 8(\alpha_1+\alpha_2)t_1^2 + 2\alpha_2t_1t_2 + \alpha_2t_2^2 & \alpha_2(t_1^2 + 2t_1t_2 + t_2^2) \\ \alpha_2(t_1^2 + 2t_1t_2 + t_2^2) & 8(\alpha_1+\alpha_2)t_2^2 + 2\alpha_2t_1t_2 + \alpha_2t_1^2 \end{pmatrix}$$
$$= \frac{1}{4}\begin{pmatrix} 10\alpha_1 + 3\alpha_2 & 3\alpha_2 \\ 3\alpha_2 & 10\alpha_1 + 3\alpha_2 \end{pmatrix} = \frac{1}{100}\begin{pmatrix} 208 & 18 \\ 18 & 208 \end{pmatrix} \quad \text{……….(4.94)}$$

after employing the ordinates of the support points where $t_i^2 = \frac{5}{4}$ and $t_1t_2 = \frac{1}{4}$ and the values for α_1 and α_2 from (4.93).

From equation (3.22), the determinant criterion, for a nonnegative definite matrix C of order s is given by;

$$v(\phi_{-1}) = (traceC)^{\frac{1}{s}} \quad \text{…………………………………………..….. (4.95)}$$

At present the determinant criterion, is obtained for the information matrix of order m=2 from the relation;

$$v(\phi_0) = \left(traceH_0C_0^{-1}H_0'\right)^{\frac{1}{2}} \quad \text{……………………………………………(4.96)}$$

The optimum slope value for the determinant criterion was then obtained using (4.94) and (4.96) as

$$v(\phi_0) = \left(\frac{42940}{10000}\right)^{\frac{1}{2}} = 2.072196902.$$

4.1.2.2 D- Optimal Slope Weighted Centroid Design with Three Ingredients

To derive the D- optimal slope design with three ingredients, we begun be assembling the necessary matrices. These are as outlined:

The information matrix to be adjusted for slope and optimized for the D-criterion is from (4.13);

$$C_0 = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 \\ \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & \frac{\alpha_2}{48} & \frac{\alpha_2}{16} & 0 & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{48} & \frac{\alpha_2}{48} & \frac{8\alpha_1+\alpha_2}{24} & 0 & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} \\ \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 & \frac{3\alpha_2}{16} & 0 & 0 \\ \frac{\alpha_2}{16} & 0 & \frac{\alpha_2}{16} & 0 & \frac{3\alpha_2}{16} & 0 \\ 0 & \frac{\alpha_2}{16} & \frac{\alpha_2}{16} & 0 & 0 & \frac{3\alpha_2}{16} \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.97)$$

The information matrices employed for the two centroids η_1 and η_2 are available from (4.27) and (4.28) respectively as:

$$C_1 = \begin{pmatrix} 1/3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.98)$$

and

$$C_2 = \begin{pmatrix} 1/24 & 1/48 & 1/48 & 1/16 & 1/16 & 0 \\ 1/48 & 1/24 & 1/48 & 1/16 & 0 & 1/16 \\ 1/48 & 1/48 & 1/24 & 0 & 1/16 & 1/16 \\ 1/16 & 1/16 & 0 & 3/16 & 0 & 0 \\ 1/16 & 0 & 1/16 & 0 & 3/16 & 0 \\ 0 & 1/16 & 1/16 & 0 & 0 & 3/16 \end{pmatrix} \quad \text{.....................................(4.99)}$$

The inverse of the information matrix for the design with three ingredients is from (4.31),

$$C_0^{-1} = \begin{pmatrix} \frac{3}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 \\ 0 & \frac{3}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} \\ 0 & 0 & \frac{3}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} \\ \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} & \frac{1}{3\alpha_1} & \frac{1}{3\alpha_1} \\ \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{1}{3\alpha_1} & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} & \frac{1}{3\alpha_1} \\ 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{1}{3\alpha_1} & \frac{1}{3\alpha_1} & \frac{2(8\alpha_1+\alpha_2)}{3\alpha_1\alpha_2} \end{pmatrix} \quad \text{.................(4.100)}$$

We also needed the adjusted slope matrix for the Kronecker model with three ingredients as is from (4.34). That is;

$$H_0 = \begin{pmatrix} 2t_1 & 0 & 0 & \frac{2}{3}t_2 & \frac{2}{3}t_3 & 0 \\ 0 & 2t_2 & 0 & \frac{2}{3}t_1 & 0 & \frac{2}{3}t_3 \\ 0 & 0 & 2t_3 & 0 & \frac{2}{3}t_1 & \frac{2}{3}t_2 \end{pmatrix} \quad \text{...(4.101)}$$

From condition (3.21), we have that a weighted centroid design $\eta(\alpha)$ is $\phi_0 - slope\,optimal$ for $K'\theta$ in T if and only if

$$traceH_0 C_j C_0^{-1} H_0' = traceH_0 H_0' \quad for\ all\ j \in \partial(\alpha) \quad \text{................................ (4.102)}$$

For j=1, the products of the matrices (4.98), (4.100) and (4.101):

$$H_0C_1C^{-1}H_0' = \frac{1}{9\alpha_1}\begin{pmatrix} 36t_1^2 - 4(t_1t_2 + t_1t_3) & t_1^2 & t_1^2 \\ t_2^2 & 36t_2^2 - 4(t_1t_2 + t_2t_3) & t_2^2 \\ t_3^2 & t_3^2 & 36t_3^2 - 4(t_1t_3 + t_2t_3) \end{pmatrix} \ldots(4.103a)$$

where;

$$t_i^2 = \frac{29}{18}, i = 1,2,3 \text{ and } t_it_j = \frac{13}{36}, i \neq j = 1,2,3$$

The trace of (4.103a) is;

$$traceH_0C_1C^{-1}H_0' = \frac{1}{9\alpha_1}\left[36(t_1^2 + t_2^2 + t_3^2) - 8(t_1t_2 + t_1t_3 + t_2t_3)\right] = \frac{496}{27\alpha_1} \ldots\ldots\ldots\ldots (4.103b)$$

and from (4.101) we got the product,

$$H_0H_0' = \frac{1}{9}\begin{pmatrix} 36t_1^2 + 4(t_2^2 + t_3^2) & 4t_1t_2 & 4t_1t_3 \\ 4t_1t_2 & 36t_2^2 + 4(t_1^2 + t_3^2) & 4t_2t_3 \\ 4t_1t_3 & 4t_2t_3 & 36t_3^2 + 4(t_1^2 + t_2^2) \end{pmatrix} \ldots\ldots\ldots\ldots(4.104a)$$

where;

$$t_i^2 = \frac{29}{18}, i = 1,2,3 \text{ and } t_it_j = \frac{13}{36}, i \neq j = 1,2,3$$

the trace of (4.104a) is;

$$traceH_0H_0' = \frac{44}{9}(t_1^2 + t_2^2 + t_3^2) = \frac{638}{27} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.104b)$$

Using the (4.103b) and (4.104b) in the condition (4.102) we have $\alpha_1 = \frac{248}{319}$.

Similarly, when j=2 and using (4.99), (4.100) and (4.101) we got a matrix product,

$$H_0C_2C_0^{-1}H_0' = \frac{4}{9\alpha_2}\begin{pmatrix} t_2^2+t_3^2+t_1t_2+t_1t_3 & t_1^2+t_1t_2 & t_1^2+t_1t_3 \\ t_2^2+t_1t_2 & t_1^2+t_3^2+t_1t_2+t_2t_3 & t_2^2+t_2t_3 \\ t_3^2+t_1t_3 & t_3^2+t_2t_3 & t_1^2+t_2^2+t_1t_3+t_2t_3 \end{pmatrix} \ldots(4.105a)$$

where;

$$t_i^2 = \frac{29}{18}, i = 1,2,3 \text{ and } t_it_j = \frac{13}{36}, i \neq j = 1,2,3$$

The trace of the matrix product (4.105a) was elementary obtained as;

$$traceH_0C_2C^{-1}H_0' = \frac{8}{9\alpha_2}\left(t_1^2+t_2^2+t_3^2+t_1t_2+t_1t_3+t_2t_3\right) = \frac{142}{27\alpha_2} \ldots.(4.105b)$$

Using the (4.104b) and (4.105b) in the condition (4.102) we have $\alpha_2 = \frac{71}{319}$.

Hence, the D-optimal slope weight vector for the weighted centroid design with three ingredients is;

$$\alpha_1 = \frac{248}{319} \text{ and } \alpha_2 = \frac{71}{319} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.106)$$

Therefore, in the second-degree Kronecker model for mixture experiments with three ingredients, the unique D- optimal slope design for $K'\theta$ is

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{248}{319}\eta_1 + \frac{71}{319}\eta_2.$$

To obtain the optimal value $v(\phi_0)$, first we adjusted the information matrix (4.97) for slope by pre- and post-multiplying by the adjusted slope matrix (4.101). This led to the matrix;

$$H_0C_0H_0' = \frac{1}{48}\begin{pmatrix} 8(8\alpha_1+\alpha_2)t_1^2+8\alpha_2(t_1t_2+t_1t_3) \\ +4\alpha_2(t_2^2+t_3^2) & 4\alpha_2(t_1^2+2t_1t_2+t_2^2) & 4\alpha_2(t_1^2+2t_1t_3+t_3^2) \\ 4\alpha_2(t_1^2+2t_1t_2+t_2^2) & 8(8\alpha_1+\alpha_2)t_2^2+8\alpha_2(t_1t_2+t_2t_3) \\ +4\alpha_2(t_1^2+t_3^2) & 4\alpha_2(t_2^2+2t_2t_3+t_3^2) \\ 4\alpha_2(t_1^2+2t_1t_3+t_3^2) & 4\alpha_2(t_2^2+2t_2t_3+t_3^2) & 8(8\alpha_1+\alpha_2)t_3^2+8\alpha_2(t_1t_3+t_2t_3) \\ +4\alpha_2(t_1^2+t_2^2) \end{pmatrix} \quad \ldots..(4.107)$$

$$= \frac{1}{432}\begin{pmatrix} 4(232\alpha_1+71\alpha_2) & 142\alpha_2 & 142\alpha_2 \\ 142\alpha_2 & 4(232\alpha_1+71\alpha_2) & 142\alpha_2 \\ 142\alpha_2 & 142\alpha_2 & 4(232\alpha_1+71\alpha_2) \end{pmatrix}$$

after employing the ordinates of the support points.

where;

$$t_i^2 = \frac{29}{18}, i = 1,2,3 \text{ and } t_it_j = \frac{13}{36}, \; i \neq j = 1,2,3$$

From equation (3.22), the determinant criterion, for a nonnegative definite matrix C of order s is given by;

$$v(\phi_0) = (traceC)^{\frac{1}{s}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.\ldots.. (4.108)$$

At present the determinant criterion, is obtained for the information matrix of order m=3 from the equation;

$$v(\phi_0) = \left(traceH_0C_0^{-1}H_0'\right)^{\frac{1}{3}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.109)$$

The optimum slope value for the determinant criterion was then obtained using (4.107) and (4.109) while taking note the numerical values for α_1 and α_2, (from 4.106). The determinant criterion was obtained as;

$$v(\phi_0) = 5.964019334^{\frac{1}{3}} = 1.813481018$$

4.1.2.3 D- Optimal Slope Weighted Centroid Design with Four Ingredients

The task here was to derive the D- optimal slope design for a mixture experiment with four ingredients. The information matrix to be adjusted for slope and optimized for the D-criterion is from (4.33);

$$C_0 = \begin{pmatrix} \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0 \\ \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & \frac{\alpha_2}{96} & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} \\ \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{\alpha_2}{96} & \frac{8\alpha_1+\alpha_2}{32} & 0 & 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} \\ \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0 & 0 & 0 \\ \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha_2}{24} & 0 & 0 & \frac{\alpha}{6} & 0 & 0 & 0 \\ 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6} & 0 & 0 \\ 0 & \frac{\alpha_2}{24} & 0 & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6} & 0 \\ 0 & 0 & \frac{\alpha_2}{24} & \frac{\alpha_2}{24} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha_2}{6} \end{pmatrix} \quad \ldots(4.110)$$

The information matrices employed for the two centroids η_1 and η_2 are respectively from (4.49) and (4.50);

$$C_1 = \begin{pmatrix} 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(4.111)$$

and

$$C_2 = \begin{pmatrix} \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{24} & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 \\ \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & \frac{1}{96} & \frac{1}{24} & 0 & 0 & \frac{1}{24} & \frac{1}{24} & 0 \\ \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & \frac{1}{96} & 0 & \frac{1}{24} & 0 & \frac{1}{24} & 0 & \frac{1}{24} \\ \frac{1}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{32} & 0 & 0 & \frac{1}{24} & 0 & \frac{1}{24} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{24} & 0 & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 \\ \frac{1}{24} & 0 & 0 & \frac{1}{24} & 0 & 0 & \frac{1}{6} & 0 & 0 & 0 \\ 0 & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 & 0 & \frac{1}{6} & 0 & 0 \\ 0 & \frac{1}{24} & 0 & \frac{1}{24} & 0 & 0 & 0 & 0 & \frac{1}{6} & 0 \\ 0 & 0 & \frac{1}{24} & \frac{1}{24} & 0 & 0 & 0 & 0 & 0 & \frac{1}{6} \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.112)$$

The inverse of the information matrix (4.110) for the design with four ingredients is,

$$C_0^{-1} = \begin{pmatrix} \frac{4}{\alpha_1} & 0 & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & 0 & 0 \\ 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 \\ 0 & 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} \\ 0 & 0 & 0 & \frac{4}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} \\ \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & 0 & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0 \\ \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{1}{4\alpha_1} \\ \frac{-1}{\alpha_1} & 0 & 0 & \frac{-1}{\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} \\ 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} \\ 0 & \frac{-1}{\alpha_1} & 0 & \frac{-1}{\alpha_1} & \frac{1}{4\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} & \frac{1}{4\alpha_1} \\ 0 & 0 & \frac{-1}{\alpha_1} & \frac{-1}{\alpha_1} & 0 & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{1}{4\alpha_1} & \frac{12\alpha_1+\alpha_2}{2\alpha_1\alpha_2} \end{pmatrix} \ldots.(4.113)$$

We also utilized the adjusted slope matrix as is from (4.56). That is;

$$H_0 = \begin{pmatrix} 2t_1 & 0 & 0 & 0 & \frac{1}{2}t_2 & \frac{1}{2}t_3 & \frac{1}{2}t_4 & 0 & 0 & 0 \\ 0 & 2t_2 & 0 & 0 & \frac{1}{2}t_1 & 0 & 0 & \frac{1}{2}t_3 & \frac{1}{2}t_4 & 0 \\ 0 & 0 & 2t_3 & 0 & 0 & \frac{1}{2}t_1 & 0 & \frac{1}{2}t_2 & 0 & \frac{1}{2}t_4 \\ 0 & 0 & 0 & 2t_4 & 0 & 0 & \frac{1}{2}t_1 & 0 & \frac{1}{2}t_2 & \frac{1}{2}t_3 \end{pmatrix}, \ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.114)$$

From condition (3.21), we have that a weighted centroid design $\eta(\alpha)$ is $\phi_0 - slope\,optimal$ for $K'\theta$ in T if and only if

$$trace H_0 C_j C_0^{-1} H_0' = trace H_0 H_0' \quad for\ all\ j \in \partial(\alpha) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.115)$$

For the case j=1, we have the following requisite products using (4.111), (4.113) and (4.114)

$$H_0 C_1 C_0^{-1} H_0' = \frac{1}{4\alpha_1}\begin{pmatrix} 16t_1^2 - t_1(t_2+t_3+t_3) & -t_1^2 & -t_1^2 & -t_1^2 \\ -t_2^2 & 16t_2^2 - t_2(t_1+t_3+t_4) & -t_2^2 & -t_2^2 \\ -t_3^2 & -t_3^2 & 16t_3^2 - t_3(t_1+t_2+t_4) & -t_3^2 \\ -t_4^2 & -t_4^2 & -t_4^2 & 16t_4^2 - t_4(t_1+t_2+t_3) \end{pmatrix} \ldots(4.116a)$$

The trace of (4.116a) is;

$$\begin{aligned} trace H_0 C_1 C_0^{-1} H_0' &= \frac{1}{4\alpha_1}\left[16(t_1^2+t_2^2+t_3^2+t_4^2) + 2(t_1t_2+t_1t_3+t_1t_4+t_2t_3+t_2t_4+t_3t_4)\right] \\ &= \frac{1571}{48\alpha_1} \end{aligned} \quad \ldots (4.116b)$$

where;

$$t_i^2 = \frac{103}{48}, i = 1,2,3,4 \text{ and } t_it_j = \frac{77}{144},\ i \neq j = 1,2,3,4$$

and

$$H_0H_0' = \frac{1}{4}\begin{pmatrix} 16t_1^2+t_2^2+t_3^2+t_4^2) & t_1t_2 & t_1t_3 & t_1t_4 \\ t_1t_2 & 16t_2^2+t_1^2+t_3^2+t_4^2) & t_2t_3 & t_2t_4 \\ t_1t_3 & t_2t_3 & 16t_3^2+t_1^2+t_2^2+t_4^2) & t_3t_4 \\ t_1t_4 & t_2t_4 & t_3t_4 & 16t_4^2+t_1^2+t_2^2+t_3^2) \end{pmatrix} \text{........(4.117a)}$$

The trace of (4.117a) is;

$$traceH_0H_0' = \frac{19}{4}(t_1^2+t_2^2+t_3^2+t_4^2) = \frac{1957}{48} \quad \text{....................................... (4.117b)}$$

where;

$$t_i^2 = \frac{103}{48}, i = 1,2,3,4 \text{ and } t_it_j = \frac{77}{144},\ i \neq j = 1,2,3,4$$

Using the (4.116b) and (4.117b) in the relation (4.115) we have, $\alpha_1 = \frac{1571}{1957}$.

Similarly, when j=2 and using (4.112), (4.113) and (4.114), we have,

$$H_0C_2C_0^{-1}H_0' =$$

$$\frac{1}{4\alpha_2}\begin{pmatrix} t_2^2+t_3^2+t_4^2+t_1(t_2+t_3+t_4) & t_2^2+t_1t_2 & t_3^2+t_1t_3 & t_1^2+t_1t_4 \\ t_2^2+t_1t_2 & t_1^2+t_3^2+t_4^2+t_2(t_1+t_3+t_4) & t_2^2+t_2t_3 & t_2^2+t_2t_4 \\ t_3^2+t_1t_3 & t_3^2+t_2t_3 & t_1^2+t_2^2+t_4^2+t_3(t_1+t_2+t_4) & t_3^2+t_3t_4 \\ t_4^2+t_1t_4 & t_4^2+t_2t_4 & t_4^2+t_3t_4 & t_1^2+t_2^2+t_3^2+t_4(t_1+t_2+t_3) \end{pmatrix} \text{..(4.118a)}$$

The trace of this matrix product (4.118a) was elementary obtained as;

$$traceH_0C_2C_0^{-1}H_0' = \frac{1}{4\alpha_2}\left[3(t_1^2+t_2^2+t_3^2+t_4^2) + 2(t_1t_2+t_1t_3+t_1t_4+t_2t_3+t_2t_4+t_3t_4\right] = \frac{193}{24\alpha_2} \quad \text{...(4.118b)}$$

where;

$$t_i^2 = \frac{103}{48}, i = 1,2,3,4 \text{ and } t_it_j = \frac{77}{144},\ i \neq j = 1,2,3,4$$

Using the (4.117b) and (4.118b) in the relation (4.115) we got $\alpha_2 = \frac{386}{1957}$.

Hence, the D- optimal slope weight vector is;

$$\alpha_1 = \frac{1571}{1957} \text{ and } \alpha_2 = \frac{386}{1957} \quad \ldots\ldots(4.119)$$

Therefore, in the second-degree Kronecker model for mixture experiments with four ingredients, the unique D-optimal slope design for $K'\theta$ is,

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{1571}{1957}\eta_1 + \frac{386}{1957}\eta_2 .$$

To obtain the optimal value $v(\phi_0)$, first we adjusted the information matrix (4.110) for slope by pre- and post-multiplying by the adjusted slope matrix (4.114). This led to the matrix;

$$H_0C_0H_0' = \frac{1}{96}\begin{pmatrix} \begin{matrix}16(8\alpha_1+\alpha_2)t_1^2 \\ +8\alpha_2(t_1t_2+t_1t_3+t_1t_4) \\ +4\alpha_2(t_2^2+t_3^2+t_4^2)\end{matrix} & 4\alpha_2(t_1^2+2t_1t_2+t_2^2) & 4\alpha_2(t_1^2+2t_1t_3+t_3^2) & 4\alpha_2(t_1^2+2t_1t_4+t_4^2) \\ 4\alpha_2(t_1^2+2t_1t_2+t_2^2) & \begin{matrix}16(8\alpha_1+\alpha_2)t_2^2 \\ +8\alpha_2(t_1t_2+t_2t_3+t_2t_4) \\ +4\alpha_2(t_1^2+t_3^2+t_4^2)\end{matrix} & 4\alpha_2(t_2^2+2t_2t_3+t_3^2) & 4\alpha_2(t_2^2+2t_2t_4+t_4^2) \\ 4\alpha_2(t_1^2+2t_1t_3+t_3^2) & 4\alpha_2(t_2^2+2t_2t_3+t_3^2) & \begin{matrix}16(8\alpha_1+\alpha_2)t_3^2 \\ +8\alpha_2(t_1t_3+t_2t_3+t_3t_4) \\ +4\alpha_2(t_1^2+t_2^2+t_4^2)\end{matrix} & 4\alpha_2(t_3^2+2t_3t_4+t_4^2) \\ 4\alpha_2(t_1^2+2t_1t_4+t_4^2) & 4\alpha_2(t_2^2+2t_2t_4+t_4^2) & 4\alpha_2(t_3^2+2t_3t_4+t_4^2) & \begin{matrix}16(8\alpha_1+\alpha_2)t_4^2 \\ +8\alpha_2(t_1t_4+t_2t_4+t_3t_4) \\ +4\alpha_2(t_1^2+t_2^2+t_3^2)\end{matrix} \end{pmatrix}$$

$$= \frac{1}{3456}\begin{pmatrix} 3(3296\alpha_1+875\alpha_2) & 772\alpha_2 & 772\alpha_2 & 772\alpha_2 \\ 772\alpha_2 & 3(3296\alpha_1+875\alpha_2) & 772\alpha_2 & 772\alpha_2 \\ 772\alpha_2 & 772\alpha_2 & 3(3296\alpha_1+875\alpha_2) & 772\alpha_2 \\ 772\alpha_2 & 772\alpha_2 & 772\alpha_2 & 3(3296\alpha_1+875\alpha_2) \end{pmatrix} \ldots\ldots(4.120)$$

after employing the ordinates of the support points, where;

$$t_i^2 = \frac{103}{48}, i = 1,2,3,4 \text{ and } t_it_j = \frac{77}{144},\ i \neq j = 1,2,3,4$$

From equation (3.22), the determinant criterion, for a nonnegative definite matrix C of order s is given by;

$$v(\phi_0) = (traceC)^{\frac{1}{s}} \quad \text{(4.121)}$$

At present the determinant criterion, is obtained for the information matrix of order m=4 from the relation;

$$v(\phi_0) = \left(traceH_0 C_0^{-1} H_0'\right)^{\frac{1}{4}} \quad \text{(4.122)}$$

The optimum slope value for the determinant criterion was then obtained using (4.120) , (4.122) and the numerical values for α_1 and α_2 (from (4.119)). The slope optimal value for the determinant criterion was obtained as;

$$v(\phi_0) = (35.7622)^{\frac{1}{4}} = 2.4454 \blacksquare$$

4.1.2.4 D- Optimal Slope Weighted Centroid Design with m Ingredients

This section presents the general expressions that can be used to derive the D- optimal slope weight vector and the optimal value for the D-criterion for a mixture experiment with at least two ingredients.

The information matrices of the weighted centroid designs involved in this study belong to the quadratic subspace, $C \in sym(s, H)$. According to (3.25), they can be uniquely represented in the form

$$C = \begin{pmatrix} aI_m + bU_2 & cV_1' + dV_2' \\ cV_1 + dV_2 & eI_{\binom{m}{2}} + fW_2 + gW_3 \end{pmatrix} \quad \text{(4.124)}$$

with coefficients $a, \cdots, g \in \Re$, Klein (2004). The terms containing V_2, W_2 and W_3 only occur for $m \geq 3$ and $m \geq 4$ respectively.

The matrix (4.124) according to (3.25a) can be partitioned according to the block structure,

$$C = \begin{pmatrix} C_{11} & C'_{21} \\ C_{21} & C_{22} \end{pmatrix} \quad \text{……………………………………………….… ……(4.125)}$$

with $C_{11} \in sym(m)$, $C_{21} \in \Re^{\binom{m}{2} \times m}$ and $C_{22} \in sym\left(\binom{m}{2}\right)$.

For j=1,2, …, m, from (3.25c) we obtain

$$C_j = \begin{pmatrix} C_{11,j} & C'_{21,j} \\ C_{21,j} & C_{22,j} \end{pmatrix} \quad \text{………………………………………….......... (4.126)}$$

with blocks obtained using (3.25d) as follows:

i) for j=1;

$$C_{11,1} = \frac{1}{m} I_m, \ C_{21,1}=0 \text{ and } C_{22,1}=0.$$

ii) for j=2;

$$C_{11,2} = \frac{1}{8m} I_m + \frac{1}{8(m-1)} U_2, \ C_{21,2} = \frac{1}{8(m-1)} V_1 \text{ and } C_{22,2} = \frac{m}{8(m-1)} I_{\binom{m}{2}},$$

Thus we have

$$C_1 = \begin{pmatrix} \frac{1}{m} I_m & 0 \\ 0 & 0 \end{pmatrix} \quad \text{………………………………………………………... (4.127)}$$

and

$$C_2 = \begin{pmatrix} \frac{1}{8m} I_m + \frac{1}{8m(m-1)} U_2 & \frac{1}{8(m-1)} V_1' \\ \frac{1}{8(m-1)} V_1 & \frac{m}{8(m-1)} I\binom{m}{2} \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots (4.128)$$

From (4.127) and (4.128) in equation (3.17) which we obtained the information matrix to be adjusted for slope as,

$$C_0 = \begin{pmatrix} \frac{8\alpha_1 + \alpha_2}{8m} I_m + \frac{\alpha_2}{8m(m-1)} U_2 & \frac{\alpha_2}{8(m-1)} V_1' \\ \frac{\alpha_2}{8(m-1)} V_1 & \frac{m\alpha_2}{8(m-1)} I_{\binom{m}{2}} \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots (4.129)$$

An inverse of a matrix in $sym(s, H)$ can be computed by solving a system of linear equations. By the same approach we obtained the blocks of the inverse C_0^{-1} partitioned as,

$$C^{-1} = \begin{pmatrix} \frac{m}{\alpha_1} I_m & \frac{-1}{\alpha_1} V_1' \\ \frac{-1}{\alpha_1} V_1 & \frac{2[4(m-1)\alpha_1 + \alpha_2]}{m\alpha_1\alpha_2} I_{\binom{m}{2}} + \frac{1}{m\alpha_1} W_2 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots (4.130)$$

From the Kronecker second order regression function we get the slope matrix D using (3.12) as

$$D = \left(\frac{\partial f'(t)}{\partial t_1}, \frac{\partial f'(t)}{\partial t_2}, \ldots, \frac{\partial f'(t)}{\partial t_m} \right)', \quad \ldots\ldots\ldots\ldots\ldots\ldots (4.131)$$

The adjusted slope matrix was then obtained using (3.13) and written as;

$$H_0 = DK = \begin{pmatrix} 2t_i I_m & \frac{2}{m} t_j V_1' \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots (4.132)$$

This is an $m \times \binom{m+1}{2}$ matrix with K being the coefficient matrix as defined in (3.6).

Now a design that is D-slope optimal if and only if it satisfies condition (3.21). That is, a design is D-slope optimal for $K'\theta$ in T if,

$$traceH_0C_jC_0^{-1}H_0' = traceH_0H_0' \quad for\ all\ j \in \partial(\alpha) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.133)}$$

For j=1 we evaluated the following requisite products of matrices:

i) a product of (4.127), (4.130) and (4.132),

$$H_oC_1C_0^{-1}H_0' = \frac{4}{m^2\alpha_1}\begin{bmatrix} m^2t_1^2 - t_1(t_2+t_3+\cdots+t_m) & -t_1^2 & \cdots & -t_1^2 \\ -t_2^2 & m^2t_2^2 - t_2(t_1+t_3+\cdots+t_m)\cdots & & -t_2^2 \\ \vdots & \vdots & \ddots & \vdots \\ -t_m^2 & -t_m^2 & \cdots m^2t_m^2 - t_m(t_1+t_2+\cdots+t_{m-1}) & \end{bmatrix}$$

$$H_oC_1C_0^{-1}H_0' = \frac{4}{m^2\alpha_1}\begin{bmatrix} m^2A-(m-1)B & -A & \cdots & -A \\ -A & m^2A-(m-1)B & \cdots & -A \\ \vdots & \vdots & \ddots & \vdots \\ -A & -A & \cdots & m^2A-(m-1)B \end{bmatrix} \ldots\ldots\ldots\ldots \text{(4.134a)}$$

with

$$trace(H_oC_1C_0^{-1}H_0') = \frac{4[m^2A-(m-1)B]}{m\alpha_1} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4.134b)}$$

where,

$$A = t_i^2 = \sum_{i=0}^{m-1}\binom{m-1}{i}\frac{1}{(i+1)^2}, i = 1,2,...,m$$

$$B = t_it_j = \sum_{i=0}^{m-2}\binom{m-2}{i}\frac{1}{(i+2)^2},\ i \neq j = 1,2,...,m$$

ii) a product of (4.132) and its transpose,

$$H_oH_0' = \frac{4}{m^2}\begin{bmatrix} m^2t_1^2+t_2^2+t_3+\cdots+t_m^2 & t_1t_2 & \cdots & t_1t_m \\ t_2t_1 & m^2t_2^2+t_1^2+t_3+\cdots+t_m^2\cdots & & t_2t_m \\ \vdots & \vdots & \ddots & \vdots \\ t_mt_1 & t_mt_2 & \cdots m^2t_m^2+t_1+t_2^2+\cdots+t_{m-1}^2 & \end{bmatrix}$$

$$H_oH_0' = \frac{4}{m^2}\begin{bmatrix} (m^2+m-1)A & B & \cdots & B \\ B & (m^2+m-1)A & \cdots & B \\ \vdots & \vdots & \ddots & \vdots \\ B & B & \cdots & (m^2+m-1)A \end{bmatrix} \ldots\ldots\ldots\ldots\ldots(4.135a)$$

The trace of (4.135a) is,

$$trace(H_oH_0') = \frac{4(m^2+m-1)A}{m} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.135b)$$

after employing the ordinates of the support points in the m-ingredient mixture design, where,

$$A = t_i^2 = \sum_{i=0}^{m-1}\binom{m-1}{i}\frac{1}{(i+1)^2}, i = 1,2,\ldots,m$$

$$B = t_it_j = \sum_{i=0}^{m-2}\binom{m-2}{i}\frac{1}{(i+2)^2}, \ i \neq j = 1,2,\ldots,m$$

Using (4.134b) and (4.135b) in condition (4.133) we obtained the equivalence relation,

$$\frac{4[m^2A-(m-1)B]}{m\alpha_1} = \frac{4(m^2+m-1)A}{m} .$$

This implies that,

$$\alpha_1 = \frac{m^2A-(m-1)B}{(m^2+m-1)A} .$$

Similarly, for j=2, we worked out the product of matrices (4.128), (4.130) and (4.132) getting,

$$H_oC_2C_0^{-1}H_0' = \frac{4}{m^2\alpha_2}\begin{bmatrix} t_2^2+t_3^2+\cdots t_m^2 - t_1(t_2+t_3+\cdots+t_m) & t_1^2+t_1t_2 & \cdots & t_1^2+t_1t_m \\ t_2^2+t_2t_1 & t_1^2+t_3^2+\cdots t_m^2-t_2(t_1+t_3+\cdots+t_m) & \cdots & t_2^2+t_2t_m \\ \vdots & \vdots & \ddots & \vdots \\ t_m^2+t_mt_1 & t_m^2+t_mt_2 & \cdots & t_1^2+t_2^2+\cdots t_m^2-t_m(t_1+t_2+\cdots+t_{m-1}) \end{bmatrix}$$

$$H_oC_2C_0^{-1}H_0' = \frac{4}{m^2\alpha_2}\begin{bmatrix} (m-1)(A+B) & A+B & \cdots & A+B \\ A+B & (m-1)(A+B) & \cdots & A+B \\ \vdots & \vdots & \ddots & \vdots \\ A+B & A+B & \cdots & (m-1)(A+B) \end{bmatrix} \text{.........(4.136a)}$$

where,

$$A = t_i^2 = \sum_{i=0}^{m-1}\binom{m-1}{i}\frac{1}{(i+1)^2}, i = 1,2,...,m$$

$$B = t_it_j = \sum_{i=0}^{m-2}\binom{m-2}{i}\frac{1}{(i+2)^2},\ i \neq j = 1,2,...,m$$

The trace of (4.136a) is;

$$trace(H_oC_2C_0^{-1}H_0') = \frac{4(m-1)(A+B)}{m\alpha_2} \text{ ....(4.136b)}$$

Using (4.135b) and (4.136b) in condition (4.133), we obtained the equivalence relation,

$$\frac{4(m-1)(A+B)}{m\alpha_2} = \frac{4(m^2+m-1)A}{m}.$$

This led to the solution,

$$\alpha_2 = \frac{(m-1)(A+B)}{(m^2+m-1)A}$$

Therefore, for a design with m≥2 ingredients, we have the optimal slope weight vector for the D-criterion as;

$$\alpha_1 = \frac{m^2A-(m-1)B}{(m^2+m-1)A} \text{ and } \alpha_2 = \frac{(m-1)(A+B)}{(m^2+m-1)A} \quad \ldots\ldots\ldots\ldots\ldots\ldots..(4.137)$$

Therefore, in the second-degree Kronecker model for mixture experiments with $m \geq 2$ ingredients, the unique D- optimal slope design for $K'\theta$ is

$$\eta(\alpha^{(D)}) = \alpha_1\eta_1 + \alpha_2\eta_2 = \frac{m[mA-(m-1)B]}{(m^2+m-1)A}\eta_1 + \frac{(m-1)(A+B)}{(m^2+m-1)A}\eta_2 .$$

To obtain the optimal value $v(\phi_0)$, first we adjusted the information matrix (4.129) for slope by pre- and post-multiplying by the adjusted slope matrix (4.132). This led to the matrix;

$$H_0C_0H_0' = \frac{1}{m(m-1)}\begin{bmatrix} 2^{m-3}(8\alpha_1+\alpha_2)A+(m-1)\alpha_2B & \alpha_2(A+B) & \cdots & \alpha_2(A+B) \\ \alpha_2(A+B) & 2^{m-3}(8\alpha_1+\alpha_2)A+(m-1)\alpha_2B & \cdots & \alpha_2(A+B) \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_2(A+B) & \alpha_2(A+B) & \cdots & 2^{m-3}(8\alpha_1+\alpha_2)A+(m-1)\alpha_2B \end{bmatrix} \quad \ldots.(4.138a)$$

after employing the ordinates of the support points, where,

$$A = t_i^2 = \sum_{i=0}^{m-1}\binom{m-1}{i}\frac{1}{(i+1)^2}, i = 1,2,\ldots,m$$

$$B = t_it_j = \sum_{i=0}^{m-2}\binom{m-2}{i}\frac{1}{(i+2)^2}, \; i \neq j = 1,2,\ldots,m$$

The adjusted information matrix has the determinant;

$$\det H_0 C_0 H_0' = \frac{1}{[2m(m-1)]^m}\left\{[2^{m-2}(8\alpha_1+\alpha_2)+(m-3)\alpha_2]A+2(m-2)\alpha_2 B\right\}^{m-1}\times \left\{[2^{m-2}(8\alpha_1+\alpha_2)+3(m-1)\alpha_2]A+4(m-1)\alpha_2 B\right\} \quad \text{...(4.138b)}$$

From equation (3.22), the determinant criterion, for a nonnegative definite matrix C of order s is given by;

$$v(\phi_0) = (traceC)^{\frac{1}{s}} \quad \text{... (4.139)}$$

At present the determinant criterion, is obtained for the information matrices of order s=m from the relation;

$$v(\phi_0) = (\det H_0 C_0 H_0')^{\frac{1}{m}} \quad \text{...(4.140a)}$$

Using the determinant value (4.138b) and the equation (4.140) we got the maximum of the D criterion as,

$$v(\phi_0) = (\det H_0 C_0 H_0')^{\frac{1}{m}} = \frac{1}{2m(m-1)}\left\{[2^{m-2}(8\alpha_1+\alpha_2)+(m-3)\alpha_2]A+2(m-2)\alpha_2 B\right\}^{\frac{m-1}{m}}\times \left\{[2^{m-2}(8\alpha_1+\alpha_2)+3(m-1)\alpha_2]A+4(m-1)\alpha_2 B\right\}^{\frac{1}{m}} \quad \text{...(4.140b)}$$

4.2 Numerical Slope Optimal Weighted Centroid Designs

We generated numerical ϕ_p – optimal slope weighted centroid designs for A- and D-criteria for $m \subseteq [5,20]$. To do this, we employed the analytical results for the case of a design with m ingredients.

4.2.1 Numerical D-Optimal Slope Weighted Centroid Designs

The numerical ϕ_p – optimal designs presented here are as a result of proper utilization of the findings on the D-optimal slope design with m ingredients. In particular, we present the values of D-optimal slope weight vector and the maximum of the determinant criterion for each of the values $m \subseteq [5, 20]$. Going with these are values of the sums of the squares and cross products of the ordinates of the support points for each particular m ingredients design. These squares and cross products are gotten from the definitions of A and B in equation (4.134). The D-optimal slope weight vector is as given in (4.137) with corresponding maximum of the D-criterion as shown in (4.140b). They are as shown in table 3 below:

Table 3: Numerical D-slope optimal weighted centroid designs

Number of ingredients m	Sum of Squares A	Sum of Cross-products B	Optimal Weight Vector α_1	α_2	Optimal value $v(\phi_0)$
5	2.956666667	0.810833333	0.824242895	0.175757105	4.083088547
6	4.213888889	1.257222222	0.841664389	0.158335611	7.832687801
7	6.203741497	1.989852608	0.855918137	0.144081863	16.62771156
8	9.412648810	3.208907313	0.867797174	0.132202826	38.18245748
9	14.67544092	5.262792108	0.877877555	0.122122445	93.37814928
10	23.43789683	8.762455908	0.886562146	0.113437854	240.4342067
11	38.22453430	14.78663748	0.894134633	0.105865367	646.0738788
12	63.47665645	25.25212214	0.900800051	0.099199949	1799.201131
13	107.0612923	43.58463589	0.906711612	0.093288388	5163.871038
14	183.0007919	75.93949953	0.911987627	0.088012373	15206.46235
15	316.4318502	133.4310583	0.916722030	0.083277970	45779.14297
16	552.6509533	236.2191031	0.920991009	0.079008991	140480.2054
17	973.6749457	421.0239924	0.924857331	0.075142669	438351.1759
18	1728.665226	754.9902808	0.928373290	0.071626710	1388105.141
19	3090.001406	1361.336179	0.931582823	0.068417177	4453420.629
20	5556.938835	2466.937430	0.934523089	0.065476911	14455379.73

As seen from the results, generally the first centroid η_1 is more weighted (α_1) than the second centroid, η_2 . This implies that the response is principally a function of the pure ingredients. As the number of ingredients increase the weight value α_1 increases while α_2 decreases. This is an indication that in presence of many factors the response is dominated by the main effects concurring with the sparsity-of-effects principle. This principle sometimes referred to as the hierarchical ordering principle, Wu et. al. (2000). The main factor effects dominate the two factor interaction effects. The D-optimal slope values increase with increase in the number of ingredients.

4.2.2 Numerical A- Optimal Slope Weighted Centroid Designs

The numerical ϕ_p – optimal designs presented here are as a result of proper utilization of the findings on the A-optimal slope design with m ingredients. We present the values of A-optimal slope weight vector and the maximum of the average variance criterion for each of the values $m \subseteq [5,20]$. Together with these are values of the sums of the squares and cross products of the ordinates of the support points for each particular case of m ingredient design, since they are included in the working. These squares and cross products are gotten from the definitions of A and B in equation (4.134). The A-optimal slope weight vector is as given in (4.80) with corresponding maximum of the A-criterion as shown in (4.80a). They are as shown in table 4.

Table 4: Numerical A-slope optimal weighted centroid designs

Number of ingredients m	**Sum of Squares A**	**Sum of Cross-products B**	**Optimal Weight Vector**		**Optimal value**
			α_1	α_2	$v(\phi_{-1})$
5	2.956666667	0.810833333	0.829201318	0.170798682	0.007233662
6	4.213888889	1.257222222	0.845920916	0.154079084	0.004679335
7	6.203741497	1.989852608	0.859735778	0.140264222	0.002956347
8	9.41264881	3.208907313	0.871127459	0.128872541	0.001823532
9	14.67544092	5.262792108	0.880686693	0.119313307	0.001099475
10	23.43789683	8.762455908	0.888873427	0.111126573	0.000649383
11	38.2245343	14.78663748	0.896007767	0.103992233	0.000376665
12	63.47665645	25.25212214	0.902307370	0.09769263	0.000215101
13	107.0612923	43.58463589	0.907923173	0.092076827	0.000121219
14	183.0007919	75.93949953	0.912964364	0.087035636	6.75484E-05
15	316.4318502	133.4310583	0.917513889	0.082486111	3.72831E-05
16	552.6509533	236.2191031	0.921637573	0.078362427	2.04114E-05
17	973.6749457	421.0239924	0.925389399	0.074610601	1.10969E-05
18	1728.665226	754.9902808	0.928814627	0.071185373	5.99664E-06
19	3090.001406	1361.336179	0.931951732	0.068048268	3.22354E-06
20	5556.938835	2466.93743	0.934833707	0.065166293	1.72487E-06

As seen from the results in table 4, generally the first centroid η_1 is more weighted than the second centroid, η_2 , since the weight candidate α_1 is greater than α_2 . This implies that the response is predominantly a function of the pure ingredients. As the number of ingredients increase the weight value α_1 increases while α_2 decreases. This is an indication that in presence of many factors the response is dominated by the main effects. In this case, the main factor effects dominate the two factor interaction effects.

The findings here concur with the sparsity-of-effects principle. The A-optimal slope values decrease with increase in the number of ingredients.

4.3 Sensory Evaluation Experiment

We now present the analysis of the sensory experiment data for two, three and four selected fruits. Development of fruit blends is an important task to nutritionists. It is therefore important to have polynomial functions that describe accurately mixture properties in terms of compositions and pure blends that meet nutritional demands or taste preferences of consumers. The empirical models assist in coming up with formulations that attain optimal desired qualities of the fruit punch. Each fruit was taken individually and in combination with each of the other fruits.

4.3.1 Two Ingredients Experiment

We begin with the experiment with two fruits namely pine apple and pawpaw. The response was taken as the average score for the four attributes: taste, colour, texture and smell. Since each of the attributes are on the 1-15 scale, so is the response. The twelve data values are from three support points each replicated four times. The points comprised two pure blends and one binary blend.

4.3.1.1 Fitted Model

The estimates of the coefficients for the Kronecker model were obtained using SAS software package. The model is;

$$\hat{y} = E(y) = 10.125(pineapple)^2 + 9(pawpaw)^2 + 20.375 peneapple(pawpaw)$$

4.3.1.2 Model Validity

An analysis of the model validity was performed to examine the fitted model if it provides an adequate approximation of the true response surface. Analysis of variance

(ANOVA) was used to examine the Kronecker model. As is evident from the output below, 98.2% of the variation in the response is accounted for by the purposeful changes made on the ingredients. The overall model is highly significant with an estimated probability value less than 0.0001 (from table 5), much lower than the 0.05 and 0.01 significant levels.

Table 5: ANOVA for two ingredients Kronecker model

The GLM Procedure

Dependent Variable: yield

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	3	1124.125000	374.708333	163.51	<.0001
Error	9	20.625000	2.291667		
Uncorrected Total	12	1144.750000			

R-Square	Coeff Var	Root MSE	yield Mean
0.981983	15.66026	1.513825	9.666667

NOTE: No intercept term is used: R-square is not corrected for the mean.

The t-test values were used to test for the significance of the individual parameters (hence factors) in the model. The test involves testing the hypothesis $H_o : \beta_{ij} = 0$ against the alternative hypothesis $H_1 : \beta_{ij} \neq 0$ From table 6 below, all the coefficients are highly significant with very low estimated probability (Pr > |t|) values.

Table 6: T-test Values for coefficients of the two ingredients Kronecker model

Parameter	Estimate	Standard Error	t Value	Pr > |t|
pine*pine	10.12500000	0.75691259	13.38	<.0001
paw*paw	9.00000000	0.75691259	11.89	<.0001
pine*paw	20.37500000	3.21130814	6.34	0.0001

The assumption of normality on the errors, clearly points to a similar distribution on the observations. By examination of the P-P and Q-Q plots from figure 1 below, there is no indication of any serious deviation from normality.

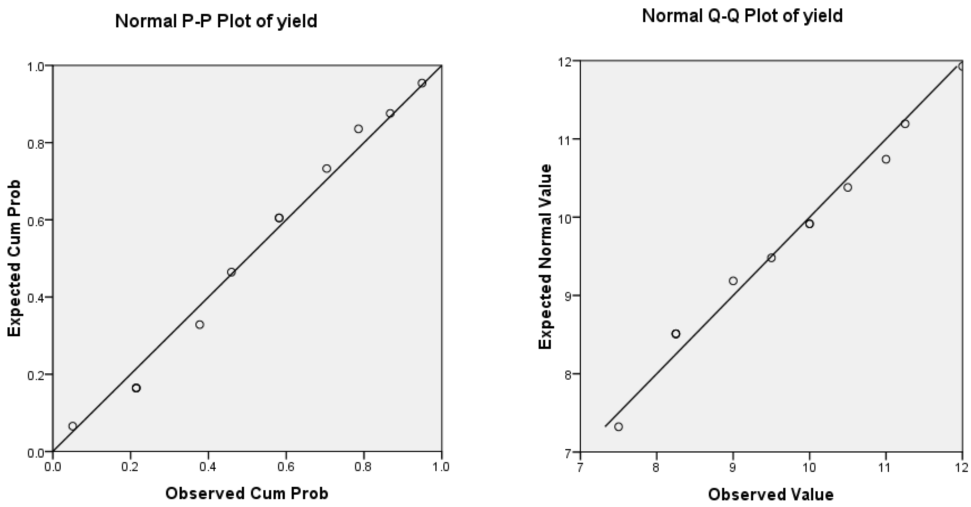

Figure 1: P-P and Q-Q plots

4.3.1.3 Slope Information for the D-optimal Criterion

The fitted model for the design with two ingredients can be written in a way to coincide with the Kronecker product as follows;

$$\hat{y} = E(y) = 10.125t_1^{\,2} + 10.1875t_1t_2 + 10.1875t_2t_1 + 9t_2^{\,2}, \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.141)$$

where the two ingredients are symbolized as t_1 represent pineapple and t_2 represent pawpaw.

Using the definition of slope matrix (equation 3.12) and the regression function (4.141) the slope matrix for the design with two ingredients was obtained as;

$$D = \begin{pmatrix} 20.25t_1 & 10.1875t_2 & 10.1875t_2 & 0 \\ 0 & 10.1875t_1 & 10.1875t_1 & 18t_2 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.142)$$

The coefficient matrix (4.2) was then used in the definition for the adjusted slope matrix (3.13) to get the adjusted slope matrix;

$$H_0 = DK = \begin{pmatrix} 20.25t_1 & & 10.1875t_2 \\ & 18t_2 & 10.1875t_1 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.143)$$

To derive the D-optimal slope information matrix the information matrix (4.8) was pre- and post-multiplied with the slope matrix (4.143) to get the square information matrix (as defined in (3.19)),

$$C = H_0 C_0 H_0' = \frac{1}{16}\begin{pmatrix} 20.25^2(8\alpha_1+\alpha_2)t_1^2 + (40.5(20.375)t_1t_2 + 20.375^2 t_2^2)\alpha_2 & (18(20.375)t_2^2 + (364.5 + 20.375^2)t_1t_2 + 20.25(20.375)t_1^2)\alpha_2 \\ (20.25(20.375)t_1^2 + (364.5 + 20.375^2)t_1t_2 + 18(20.375)t_2^2)\alpha_2 & 18^2(8\alpha_1+\alpha_2)t_2^2 + (36(20.375)t_1t_2 + 20.375^2 t_1^2)\alpha_2 \end{pmatrix}$$

After using the coordinates of the support points and the values of the D-optimal slope weight vector as from (4.93), simplified to;

$$C = \frac{1}{1600}\begin{pmatrix} 34135.471875 & 28058.15625 \\ 28058.15625 & 27281.521875 \end{pmatrix} \quad \text{.........................(4.144)}$$

Then the information function definition (3.22) was used with $p = 0$, $m = 2$ and the information matrix (4.144) to obtain the D-optimal slope information as;

$$v(\phi_0) = (\det C)^{\frac{1}{2}} = 189.9213469.$$

4.3.1.4 Slope Information for the A-optimal Criterion

To get the A- optimal slope value for the design with the two ingredients, first pre- and post-multiplication of the inverse of information matrix (4.10) with the adjusted slope matrix (4.143) was done, to get the requisite slope information matrix;

$$C = H_0 C_0^{-1} H_0' = \begin{pmatrix} \frac{20.25(40.5)}{\alpha_1} t_1^2 - \frac{20.25(20.375)}{\alpha_1} t_1 t_2 + \frac{20.375^2(4\alpha_1+\alpha_2)}{4\alpha_1\alpha_2} t_2^2 & -\frac{20.25(20.375)}{2\alpha_1} t_1^2 - \frac{18(20.375)}{2\alpha_1} t_2^2 + \frac{20.375^2(4\alpha_1+\alpha_2)}{4\alpha_1\alpha_2} t_1 t_2 \\ -\frac{18(20.375)}{2\alpha_1} t_2^2 - \frac{20.25(20.375)}{2\alpha_1} t_1^2 + \frac{20.375^2(4\alpha_1+\alpha_2)}{4\alpha_1\alpha_2} t_1 t_2 & \frac{18(36)}{\alpha_1} t_2^2 - \frac{18(20.375)}{\alpha_1} t_1 t_2 + \frac{20.375^2(4\alpha_1+\alpha_2)}{4\alpha_1\alpha_2} t_1^2 \end{pmatrix}$$

which after utilizing the ordinates of the support points led to the matrix;

$$C = \begin{pmatrix} \frac{5(20.25)(40.5)}{4\alpha_1} - \frac{20.25(20.375)}{4\alpha_1} + \frac{5(20.375^2)(4\alpha_1+\alpha_2)}{16\alpha_1\alpha_2} & -\frac{5(20.25)(20.375)}{8\alpha_1} - \frac{5(18)(20.375)}{8\alpha_1} + \frac{20.375^2(4\alpha_1+\alpha_2)}{16\alpha_1\alpha_2} \\ -\frac{5(18)(20.375)}{8\alpha_1} - \frac{5(20.25)(20.375)}{8\alpha_1} + \frac{20.375^2(4\alpha_1+\alpha_2)}{16\alpha_1\alpha_2} & \frac{5(18)(36)}{4\alpha_1} - \frac{5(18)(20.375)}{4\alpha_1} + \frac{5(20.375^2)(4\alpha_1+\alpha_2)}{16\alpha_1\alpha_2} \end{pmatrix} \quad \ldots\ldots(4.145)$$

with

$$traceC = \frac{6561.28125}{4\alpha_1} + \frac{5(20.375^2)(4\alpha_1+\alpha_2)}{8\alpha_1\alpha_2} = 5751.642535, \quad \ldots\ldots\ldots\ldots\ldots\ldots(4.146)$$

where the A- optimal slope weight vector is available from (4.19).

The A- optimal slope information was gotten by using equation (3.22) with $p = -1$, $m = 2$ and the trace (4.146) of the information matrix (4.145) as;

$$v(\phi_{-1}) = \left(\frac{1}{2} traceC\right)^{-1} = \left(\frac{5751.642535}{2}\right)^{-1} = 3.47726756 \times 10^{-4}.$$

4.3.2 Three Ingredients Experiment

The three fruits that were involved in the experiment were: pine apple, pawpaw and banana. The response on a scale 1-15 was taken as the average score for the four attributes: taste, colour, texture and smell. The twenty-eight data values are from seven support points for weighted design each replicated four times. The points comprised the three pure blends, three binary blends and a ternary blend.

4.3.2.1 Fitted Model

The estimates of the coefficients for the Kronecker model were obtained using SAS software package. The model is;

$$\hat{y} = E(y) = 10.54(pineapple)^2 + 9.35(pawpaw)^2 + 11.92(banana)^2 + 17.70\, peneapple * pawpaw + 10.39\, pineapple * banana + 17.83\, pawpaw * banana$$

4.3.2.2 Model Validity

Analysis of the model validity was performed to examine the fitted model if it provides an adequate approximation of the true response surface. Analysis of variance (ANOVA) was used to examine the Kronecker model. As is evident from the output below, 96.3% of the variation in the response is accounted for by the purposeful changes made on the amounts of each fruit in the mixture. The overall model is highly significant with an estimated probability value less than 0.0001 (as is seen from table 7), much lower than the 0.05 and 0.01 levels of significance.

Table 7: ANOVA for three ingredients Kronecker model

The GLM Procedure

Dependent Variable: yield

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	6	2664.738593	444.123099	95.60	<.0001
Error	22	102.198907	4.645405		
Uncorrected Total	28	2766.937500			

R-Square	Coeff Var	Root MSE	yield Mean
0.963064	22.24847	2.155320	9.687500

NOTE: No intercept term is used: R-square is not corrected for the mean.

Student t-test values were used to test for the significance of the individual coefficients (hence fruits) in the model. A choice between the hypothesis $H_o : \beta_{ij} = 0$ and the alternative hypothesis $H_1 : \beta_{ij} \neq 0$ was made as guided by the rejection rule. From table

8 below, all the coefficients but that for the interaction between pineapple and banana, are highly significant with very low estimated probability (Pr > |t|) values at the 0.01 level of significance. The interaction between pineapple and banana, unlike all the other coefficients, is insignificant at the 0.05 level of significance.

Table 8: T-test Values for coefficients of the three ingredients Kronecker model

Parameter	Estimate	Standard Error	t Value	Pr > |t|
pine*pine	10.54083600	1.07358032	9.82	<.0001
paw*paw	9.35333600	1.07358032	8.71	<.0001
ban*ban	11.91583600	1.07358032	11.10	<.0001
pine*paw	17.70245194	4.24979173	4.17	0.0004
pine*ban	10.38995194	4.24979173	2.44	0.0230
paw*ban	17.82745194	4.24979173	4.19	0.0004

The assumption of normality on the errors, clearly points to a similar distribution on the observations. By examination of the P-P and Q-Q plots from figure 2 below, there is no indication of any serious deviation from normality.

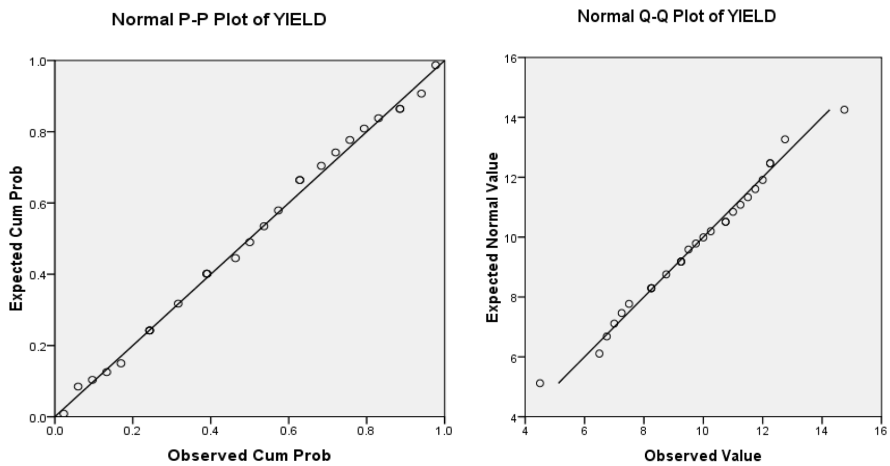

Figure 2: P-P and Q-Q plots

4.3.2.3 Slope Information for the D-optimal Criterion

The fitted model for the design with three ingredients can be written as follows;

$$\hat{y} = E(y) = at_1^2 + bt_2^2 + ct_3^2 + dt_1t_2 + et_1t_3 + ft_2t_3 \quad \text{.................................(4.147)}$$

where the three ingredients are $t_1 = pineapple,\ t_2 = pawpaw,\ t_3 = banana$ and the coefficients assigned as:

$a = 10.540836$, $b = 9.353336$, $c = 11.915836$, $d = 17.70245194$, $e = 10.38995194$ and $f = 17.82745194$.

The definition of slope matrix (equation 3.12) and the regression function (4.147) were used to get the slope matrix for the design with three ingredients as;

$$D = \begin{pmatrix} 2at_1 & \frac{d}{2}t_2 & \frac{e}{2}t_3 & \frac{d}{2}t_2 & 0 & 0 & \frac{e}{2}t_3 & 0 & 0 \\ 0 & \frac{d}{2}t_1 & 0 & \frac{d}{2}t_1 & 2bt_2 & \frac{f}{2}t_3 & 0 & \frac{f}{2}t_3 & 0 \\ 0 & 0 & \frac{e}{2}t_1 & 0 & 0 & \frac{f}{2}t_2 & \frac{e}{2}t_1 & \frac{f}{2}t_2 & 2ct_3 \end{pmatrix}$$

The coefficient matrix (4.23) was then used in the definition for the adjusted slope matrix (3.13) to get the adjusted slope matrix;

$$H_0 = DK = \begin{pmatrix} 2at_1 & & & \frac{d}{3}t_2 & \frac{e}{3}t_3 & 0 \\ & 2bt_2 & & \frac{d}{3}t_1 & 0 & \frac{f}{3}t_3 \\ & & 2ct_3 & 0 & \frac{e}{3}t_1 & \frac{f}{3}t_2 \end{pmatrix} \quad \text{..........................(4.148)}$$

To derive the D- optimal slope information matrix, the information matrix (4.29) was pre- and post-multiplied with the slope matrix (4.148) to get the square information matrix,

$$C = H_0 C_0 H_0' = \begin{pmatrix} \frac{(8\alpha_1+\alpha_2)a^2}{6}t_1^2 + \frac{(4adt_1t_2 + 4aet_1t_3 + d^2t_2^2 + e^2t_3^2)\alpha_2}{48} & \frac{[2adt_1^2 + (4ab+d^2)t_1t_2 + 2bdt_2^2]\alpha_2}{48} & \frac{[2aet_1^2 + (4ac+e^2)t_1t_3 + 2cet_3^2]\alpha_2}{48} \\ \frac{[2bdt_2^2 + (4ab+d^2)t_1t_2 + 2adt_1^2]\alpha_2}{48} & \frac{(8\alpha_1+\alpha_2)b^2}{6}t_2^2 + \frac{(4bdt_1t_2 + 4bft_2t_3 + d^2t_1^2 + f^2t_3^2)\alpha_2}{48} & \frac{[2cft_3^2 + (4bc+f^2)t_2t_3 + 2bft_2^2]\alpha_2}{48} \\ \frac{[2cet_3^2 + (4ac+e^2)t_1t_3 + 2aet_1^2]\alpha_2}{48} & \frac{[2bft_2^2 + (4bc+f^2)t_2t_3 + 2cft_3^2]\alpha_2}{48} & \frac{(8\alpha_1+\alpha_2)c^2}{6}t_1^2 + \frac{(4cet_1t_3 + 4cft_2t_3 + e^2t_1^2 + f^2t_2^2)\alpha_2}{48} \end{pmatrix} \ldots\ldots(4.149)$$

When coordinates of the support points for the three ingredients design and the values of the D-optimal slope weight vector from (4.106) are employed, (4.149) simplified to;

$$C = \frac{1}{551232}\begin{pmatrix} 108773160.706 & 3553766.82088 & 2485019.01972 \\ 3553766.82088 & 8724479.38143 & 3827716.32331 \\ 2485019.01972 & 3827716.32331 & 138382278.064 \end{pmatrix} \ldots.(4.150)$$

Equation (3.22) was the used with $p = 0$, $m = 3$ and the information matrix (4.150) to obtain the D- optimal slope information as;

$$v(\phi_0) = (\det C)^{\frac{1}{3}} = (7817642.8861)^{\frac{1}{3}} = 198.468662331.$$

4.3.2.4 Slope Information for the A-optimal Criterion

To get the A-optimal slope value for the design with the three ingredients, first the inverse of information matrix (4.31) was pre- and post-multiplied with the adjusted slope matrix (4.148), to get the necessary slope information matrix;

$$C = H_0 C_0^{-1} H_0' = \begin{pmatrix} \frac{12a^2}{\alpha_1}t_1^2 - \frac{4ad}{3\alpha_1}t_1t_2 - \frac{4ae}{3\alpha_1}t_1t_3 + \frac{2de}{27\alpha_1}t_2t_3 + \frac{2(8\alpha_1+\alpha_2)(d^2t_2^2+e^2t_3^2)}{27\alpha_1\alpha_2} & -\frac{2bd}{3\alpha_1}t_2^2 - \frac{2ad}{3\alpha_1}t_1^2 + \frac{ef}{27\alpha_1}t_3^2 + \frac{de}{27\alpha_1}t_1t_3 + \frac{df}{27\alpha_1}t_2t_3 + \frac{2(8\alpha_1+\alpha_2)d^2}{27\alpha_1\alpha_2}t_1t_2 & -\frac{2ce}{3\alpha_1}t_3^2 - \frac{2ae}{3\alpha_1}t_1^2 + \frac{df}{27\alpha_1}t_2^2 + \frac{de}{27\alpha_1}t_1t_2 + \frac{ef}{27\alpha_1}t_2t_3 + \frac{2(8\alpha_1+\alpha_2)e^2}{27\alpha_1\alpha_2}t_1t_3 \\ -\frac{2bd}{3\alpha_1}t_2^2 - \frac{2ad}{3\alpha_1}t_1^2 + \frac{ef}{27\alpha_1}t_3^2 + \frac{de}{27\alpha_1}t_1t_3 + \frac{df}{27\alpha_1}t_2t_3 + \frac{2(8\alpha_1+\alpha_2)d^2}{27\alpha_1\alpha_2}t_1t_2 & \frac{12b^2}{\alpha_1}t_1^2 - \frac{4bd}{3\alpha_1}t_1t_2 - \frac{4bf}{3\alpha_1}t_2t_3 + \frac{2df}{27\alpha_1}t_1t_3 + \frac{2(8\alpha_1+\alpha_2)(d^2t_1^2+f^2t_3^2)}{27\alpha_1\alpha_2} & -\frac{2cf}{3\alpha_1}t_3^2 - \frac{2bf}{3\alpha_1}t_2^2 + \frac{de}{27\alpha_1}t_1^2 + \frac{df}{27\alpha_1}t_1t_2 + \frac{ef}{27\alpha_1}t_1t_3 + \frac{2(8\alpha_1+\alpha_2)f^2}{27\alpha_1\alpha_2}t_2t_3 \\ -\frac{2ce}{3\alpha_1}t_3^2 - \frac{2ae}{3\alpha_1}t_1^2 + \frac{df}{27\alpha_1}t_2^2 + \frac{de}{27\alpha_1}t_1t_2 + \frac{ef}{27\alpha_1}t_2t_3 + \frac{2(8\alpha_1+\alpha_2)e^2}{27\alpha_1\alpha_2}t_1t_3 & -\frac{2cf}{3\alpha_1}t_3^2 - \frac{2bf}{3\alpha_1}t_2^2 + \frac{de}{27\alpha_1}t_1^2 + \frac{df}{27\alpha_1}t_1t_2 + \frac{ef}{27\alpha_1}t_1t_3 + \frac{2(8\alpha_1+\alpha_2)f^2}{27\alpha_1\alpha_2}t_2t_3 & \frac{12c^2}{\alpha_1}t_1^2 - \frac{4ce}{3\alpha_1}t_1t_3 - \frac{4cf}{3\alpha_1}t_2t_3 + \frac{2ef}{27\alpha_1}t_1t_2 + \frac{2(8\alpha_1+\alpha_2)(e^2t_1^2+f^2t_2^2)}{27\alpha_1\alpha_2} \end{pmatrix} \quad ...(4.151)$$

After using the coordinates of the support points for the design with three ingredients simplified to the matrix;

$$C = \begin{pmatrix} \frac{58a^2}{3\alpha_1} + \frac{13(de-18ad-18ae)}{486\alpha_1} + \frac{29(8\alpha_1+\alpha_2)(d^2+e^2)}{243\alpha_1\alpha_2} & \frac{13(8\alpha_1+\alpha_2)d^2}{486\alpha_1\alpha_2} + \frac{29(ef-18bd-18ad)}{486\alpha_1} + \frac{13(de+df)}{972\alpha_1} & \frac{13(8\alpha_1+\alpha_2)e^2}{486\alpha_1\alpha_2} + \frac{29(df-18ce-18ae)}{486\alpha_1} + \frac{13(de+ef)}{972\alpha_1} \\ \frac{13(8\alpha_1+\alpha_2)d^2}{486\alpha_1\alpha_2} + \frac{29(ef-18bd-18ad)}{486\alpha_1} + \frac{13(de+df)}{972\alpha_1} & \frac{58b^2}{3\alpha_1} + \frac{13(df-18bd-18bf)}{486\alpha_1} + \frac{29(8\alpha_1+\alpha_2)(d^2+f^2)}{243\alpha_1\alpha_2} & \frac{13(8\alpha_1+\alpha_2)f^2}{486\alpha_1\alpha_2} + \frac{29(de-18cf-18bf)}{486\alpha_1} + \frac{13(df+ef)}{972\alpha_1} \\ \frac{13(8\alpha_1+\alpha_2)e^2}{486\alpha_1\alpha_2} + \frac{29(df-18ce-18ae)}{486\alpha_1} + \frac{13(de+ef)}{972\alpha_1} & \frac{13(8\alpha_1+\alpha_2)f^2}{486\alpha_1\alpha_2} + \frac{29(de-18cf-18bf)}{486\alpha_1} + \frac{13(df+ef)}{972\alpha_1} & \frac{58c^2}{3\alpha_1} + \frac{13(ef-18ce-18cf)}{486\alpha_1} + \frac{29(8\alpha_1+\alpha_2)(e^2+f^2)}{243\alpha_1\alpha_2} \end{pmatrix} \quad ....(4.152)$$

with

$$traceC = \frac{58(a^2+b^2+c^2)}{3\alpha_1} + \frac{13[de+df+ef-18(ad+ae+bd+bf+ce+cf)]}{486\alpha_1} + \frac{58(8\alpha_1+\alpha_2)(d^2+e^2+f^2)}{243\alpha_1\alpha_2} = 13867.9442 \quad , \ldots(4.153)$$

where the A- optimal slope weight vector entries are available from (4.40).

The A- optimal slope information was gotten by using equation (3.22) with $p = -1$, $m = 3$ and the trace value (4.153) as;

$$v(\phi_{-1}) = \left(\frac{1}{3}traceC\right)^{-1} = \left(\frac{13867.9442}{3}\right)^{-1} = 2.163262237 \times 10^{-4}.$$

4.3.3 Four Ingredients Experiment

The four fruits that were involved in the experiment were: pine apple, pawpaw, banana and coconut. The response on a scale 1-15 was taken as the average score for the four attributes: taste, colour, texture and smell. The sixty data values are from fifteen support points for weighted design each replicated four times. The points comprised the four pure blends, six binary blends, four ternary blend and the four fruits together in the mixture.

4.3.3.1 Fitted Model

The estimates of the parameters for the Kronecker model were obtained using SAS software package. The model is;

$$\begin{aligned}\hat{y} = E(y) = {} & 11.17(pineapple)^2 + 10.50(pawpaw)^2 + 10.12(banana)^2 + 9.31(coconut)^2 + \\ & 24.68 peneapple * pawpaw + 21.54 pineapple * banana + 16.40 pineapple * coconut + \\ & 19.25 pawpaw * banana + 10.86 pawpaw * coconut + 16.72 banana * coconut\end{aligned}$$

4.3.3.2 Model Validity

The analysis on the model validity was done to examine the fitted model if it provides a good approximation of the true response surface. Analysis of variance (ANOVA) was used to examine the Kronecker model. As is evident from the output table 9 below, 96.67% of the variation in the response is accounted for by the purposeful changes made on the amounts of each fruit in the mixture. The overall model is highly significant with an estimated probability value less than 0.0001, much lower than the 0.05 and 0.01 levels of significance.

Table 9: ANOVA for the four ingredients Kronecker model

The GLM Procedure

Dependent Variable: yield

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	10	5794.907380	579.490738	145.17	<.0001
Error	50	199.592620	3.991852		
Uncorrected Total	60	5994.500000			

R-Square	Coeff Var	Root MSE	yield Mean
0.966704	20.43951	1.997962	9.775000

NOTE: No intercept term is used: R-square is not corrected for the mean.

The t-test values were also used to test for the significance of the individual coefficients (hence fruits) in the model. The tested hypothesis was $H_o : \beta_{ij} = 0$ against the alternative hypothesis $H_1 : \beta_{ij} \neq 0$. From the information below (in table 10), all the coefficients significant with small estimated probability (Pr > |t|) values at the 0.05 and 0.01 levels of significance. The interaction between pawpaw and coconut, compared to the other coefficients, is the least significant.

Table 10: T-test Values for coefficients of the four ingredients Kronecker model

The GLM Procedure

Dependent Variable: yield

Parameter	Estimate	Standard Error	t Value	Pr > |t|
pine*pine	11.16953443	0.98751632	11.31	<.0001
paw*paw	10.49541136	0.98751632	10.63	<.0001
ban*ban	10.12119869	0.98751632	10.25	<.0001
coco*coco	9.30566494	0.98751632	9.42	<.0001
pine*paw	24.67598681	3.63911375	6.78	<.0001
pine*ban	21.53760215	3.63911375	5.92	<.0001
pine*coco	16.40167588	3.63911375	4.51	<.0001
paw*ban	19.24769445	3.63911375	5.29	<.0001
paw*coco	10.86176818	3.63911375	2.98	0.0044
ban*coco	16.72338352	3.63911375	4.60	<.0001

The assumption of normality on the errors, clearly points to a similar distribution on the observations. By examination of the P-P and Q-Q plots in figure 3 below, there is no indication of any serious deviation from normality.

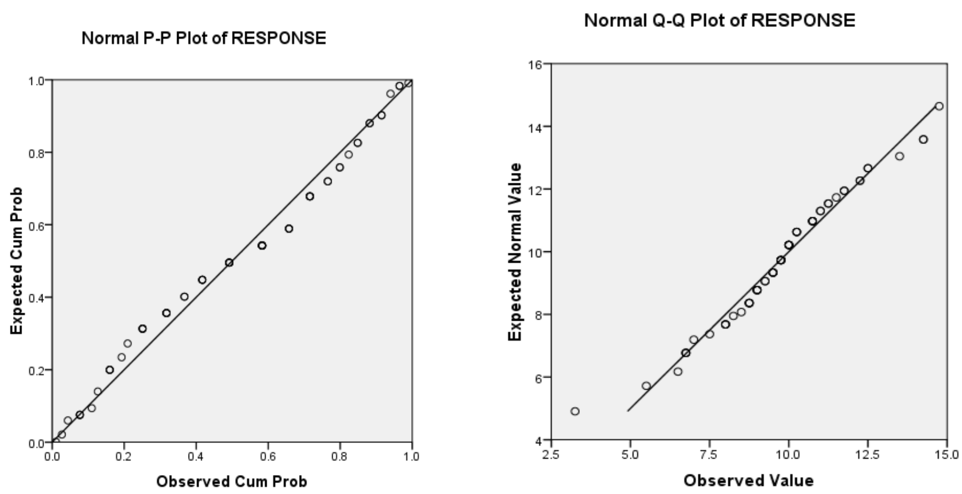

Figure 3: P-P and Q-Q plots

4.3.3.3 Slope Information for the D-optimal Criterion

The fitted model for the design with four ingredients can be written as follows;

$$\hat{y} = E(y) = at_1^2 + bt_2^2 + ct_3^2 + dt_4^2 + et_1t_2 + ft_1t_3 + gt_1t_4 + ht_2t_3 + kt_2t_4 + mt_3t_4, \ldots\ldots(4.154)$$

where;

the four ingredients are $t_1 = pineapple,\ t_2 = pawpaw,\ t_3 = banana$ and $t_4 = coconut$

the coefficients are assigned as:

$a = 11.16953443;\ b = 10.49541136;\ c = 10.12119869;\ d = 9.305664494;$

$e = 24.67598681;\ f = 21.53760215;\ g = 16.40167588;\ h = 19.24769445;\ k = 10.86176818$

$m = 16.72338352$

The definition of the slope matrix (equation 3.12) was invoked to give the slope matrix for the design with four ingredients as;

$$D = \begin{pmatrix} 2at_1 & \frac{e}{2}t_2 & \frac{f}{2}t_3 & \frac{g}{2}t_4 & \frac{e}{2}t_2 & 0 & 0 & 0 & \frac{f}{2}t_3 & 0 & 0 & 0 & \frac{g}{2}t_4 & 0 & 0 & 0 \\ 0 & \frac{e}{2}t_1 & 0 & 0 & \frac{e}{2}t_1 & 2bt_2 & \frac{h}{2}t_3 & \frac{k}{2}t_4 & 0 & \frac{h}{2}t_3 & 0 & 0 & 0 & \frac{k}{2}t_4 & 0 & 0 \\ 0 & 0 & \frac{f}{2}t_1 & 0 & 0 & 0 & \frac{h}{2}t_2 & 0 & \frac{f}{2}t_1 & \frac{h}{2}t_2 & 2ct_3 & \frac{m}{2}t_4 & 0 & 0 & \frac{m}{2}t_4 & 0 \\ 0 & 0 & 0 & \frac{g}{2}t_1 & 0 & 0 & 0 & \frac{k}{2}t_2 & 0 & 0 & 0 & \frac{m}{2}t_3 & \frac{g}{2}t_1 & \frac{k}{2}t_2 & \frac{m}{2}t_3 & 2dt_4 \end{pmatrix}$$

The coefficient matrix (4.45) was then used in the definition for the adjusted slope matrix (3.13) to get the adjusted slope matrix;

$$H_0 = DK = \begin{pmatrix} 2at_1 & 0 & 0 & 0 & \frac{e}{4}t_2 & \frac{f}{4}t_3 & \frac{g}{4}t_4 & 0 & 0 & 0 \\ 0 & 2bt_2 & 0 & 0 & \frac{e}{4}t_1 & 0 & 0 & \frac{h}{4}t_3 & \frac{k}{4}t_4 & 0 \\ 0 & 0 & 2ct_3 & 0 & 0 & \frac{f}{4}t_1 & 0 & \frac{h}{4}t_2 & 0 & \frac{m}{4}t_4 \\ 0 & 0 & 0 & 2dt_4 & 0 & 0 & \frac{g}{4}t_1 & 0 & \frac{k}{4}t_2 & \frac{m}{4}t_3 \end{pmatrix} \ldots\ldots (4.155)$$

To derive the D-optimal slope information matrix, the information matrix (4.51) was pre- and post-multiplied with the slope matrix (4.155) to give the square information matrix,

$$C = H_0 C_0 H_0' = \begin{pmatrix} \frac{(8\alpha_1+\alpha_2)a^2}{8}t_1^2 + \frac{at_1(et_2+ft_3+gt_4)\alpha_2}{24} + \frac{(e^2t_2^2+f^2t_3^2+g^2t_4^2)\alpha_2}{96} & \frac{[2aet_1^2+(4ab+e^2)t_1t_2+2bet_2^2]\alpha_2}{96} & \frac{[2aft_1^2+(4ac+f^2)t_1t_3+2cft_3^2]\alpha_2}{96} & \frac{[2agt_1^2+(4ad+g^2)t_1t_4+2dgt_4^2]\alpha_2}{96} \\ \frac{[2bet_2^2+(4ab+e^2)t_1t_2+2aet_1^2]\alpha_2}{96} & \frac{(8\alpha_1+\alpha_2)b^2}{8}t_2^2 + \frac{bt_2(et_1+ht_3+kt_4)\alpha_2}{24} + \frac{(e^2t_1^2+h^2t_3^2+k^2t_4^2)\alpha_2}{96} & \frac{[2bht_2^2+(4bc+h^2)t_2t_3+2cht_3^2]\alpha_2}{96} & \frac{[2bkt_2^2+(4bd+k^2)t_2t_4+2dkt_4^2]\alpha_2}{96} \\ \frac{[2cft_3^2+(4ac+f^2)t_1t_3+2aft_1^2]\alpha_2}{96} & \frac{[2cht_3^2+(4bc+h^2)t_2t_3+2bht_2^2]\alpha_2}{96} & \frac{(8\alpha_1+\alpha_2)c^2}{8}t_3^2 + \frac{ct_3(ft_1+ht_2+mt_4)\alpha_2}{24} + \frac{(f^2t_1^2+h^2t_2^2+m^2t_4^2)\alpha_2}{96} & \frac{[2cmt_3^2+(4cd+m^2)t_3t_4+2dmt_4^2]\alpha_2}{96} \\ \frac{[2dgt_4^2+(4ad+g^2)t_1t_4+2agt_1^2]\alpha_2}{96} & \frac{[2dkt_4^2+(4bd+k^2)t_2t_4+2bkt_2^2]\alpha_2}{96} & \frac{[2dmt_4^2+(4cd+m^2)t_3t_4+2cmt_3^2]\alpha_2}{96} & \frac{(8\alpha_1+\alpha_2)d^2}{8}t_4^2 + \frac{dt_4(gt_1+kt_2+mt_3)\alpha_2}{24} + \frac{(g^2t_1^2+k^2t_2^2+m^2t_3^2)\alpha_2}{96} \end{pmatrix} \quad \ldots\ldots(4.156)$$

After using the coordinates of the support points for the design with four ingredients, the coefficients from the model (4.154) and the D-slope optimal values of the derived weight vector (4.119), simplified to;

$$C = \begin{pmatrix} 230.4970 & 5.8981 & 5.0498 & 3.7135 \\ 5.8981 & 202.9420 & 4.3729 & 2.4553 \\ 5.0498 & 4.3729 & 189.3485 & 3.5858 \\ 3.7135 & 2.4553 & 3.5858 & 158.4876 \end{pmatrix} \quad \ldots\ldots\ldots\ldots\ldots (4.157)$$

Equation (3.22) was then employed with $p = 0$, $m = 4$ and the matrix (4.157) to obtain the D-slope optimal information as;

$$v(\phi_0) = (\det C)^{\frac{1}{4}} = (1.399 \times 10^9)^{\frac{1}{4}} = 193.4307 .$$

4.3.3.4 Slope Information for the A-optimal Criterion

To get the A- optimal slope value for the design with the four ingredients, first the inverse of information matrix (4.53) was pre- and post-multiplied with the adjusted slope matrix (4.155), to derive the necessary slope information matrix;

$$C = \begin{pmatrix}
\frac{16a^2}{\alpha_1}t_1^2 + \frac{(12\alpha_1+\alpha_2)(e^2t_2^2+f^2t_3^2+g^2t_4^2)}{32\alpha_1\alpha_2} - \frac{at_1(et_2+ft_3+gt_4)}{\alpha_1} + \frac{eft_2t_3+egt_2t_4+fgt_3t_4}{32\alpha_1} &
-\frac{be}{2\alpha_1}t_2^2 - \frac{ae}{2\alpha_1}t_1^2 + \frac{fh}{64\alpha_1}t_3^2 + \frac{gk}{64\alpha_1}t_4^2 + \frac{e(ft_1t_3+gt_1t_4+ht_2t_3+kt_2t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)e^2t_1t_2}{32\alpha_1\alpha_2} &
-\frac{cf}{2\alpha_1}t_3^2 - \frac{af}{2\alpha_1}t_1^2 + \frac{eh}{64\alpha_1}t_2^2 + \frac{gm}{64\alpha_1}t_4^2 + \frac{f(et_1t_2+gt_1t_4+ht_2t_3+mt_3t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)f^2t_1t_3}{32\alpha_1\alpha_2} &
-\frac{dg}{2\alpha_1}t_4^2 - \frac{ag}{2\alpha_1}t_1^2 + \frac{ek}{64\alpha_1}t_2^2 + \frac{fm}{64\alpha_1}t_3^2 + \frac{g(et_1t_2+ft_1t_3+kt_2t_4+mt_3t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)g^2t_1t_4}{32\alpha_1\alpha_2} \\
-\frac{be}{2\alpha_1}t_2^2 - \frac{ae}{2\alpha_1}t_1^2 + \frac{fh}{64\alpha_1}t_3^2 + \frac{gk}{64\alpha_1}t_4^2 + \frac{e(ft_1t_3+gt_1t_4+ht_2t_3+kt_2t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)e^2t_1t_2}{32\alpha_1\alpha_2} &
\frac{16b^2}{\alpha_1}t_2^2 + \frac{(12\alpha_1+\alpha_2)(e^2t_1^2+h^2t_3^2+k^2t_4^2)}{32\alpha_1\alpha_2} - \frac{bt_2(et_1+ht_3+kt_4)}{\alpha_1} + \frac{eht_1t_3+ekt_1t_4+hkt_3t_4}{32\alpha_1} &
-\frac{ch}{2\alpha_1}t_3^2 - \frac{bh}{2\alpha_1}t_2^2 + \frac{ef}{64\alpha_1}t_1^2 + \frac{km}{64\alpha_1}t_4^2 + \frac{h(et_1t_2+ft_1t_3+kt_2t_4+mt_3t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)h^2t_2t_3}{32\alpha_1\alpha_2} &
-\frac{dk}{2\alpha_1}t_4^2 - \frac{bk}{2\alpha_1}t_2^2 + \frac{eg}{64\alpha_1}t_1^2 + \frac{hm}{64\alpha_1}t_3^2 + \frac{k(et_1t_2+gt_1t_4+ht_2t_3+mt_3t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)k^2t_2t_4}{32\alpha_1\alpha_2} \\
-\frac{cf}{2\alpha_1}t_3^2 - \frac{af}{2\alpha_1}t_1^2 + \frac{eh}{64\alpha_1}t_2^2 + \frac{gm}{64\alpha_1}t_4^2 + \frac{f(et_1t_2+gt_1t_4+ht_2t_3+mt_3t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)f^2t_1t_3}{32\alpha_1\alpha_2} &
-\frac{ch}{2\alpha_1}t_3^2 - \frac{bh}{2\alpha_1}t_2^2 + \frac{ef}{64\alpha_1}t_1^2 + \frac{km}{64\alpha_1}t_4^2 + \frac{h(et_1t_2+ft_1t_3+kt_2t_4+mt_3t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)h^2t_2t_3}{32\alpha_1\alpha_2} &
\frac{16c^2}{\alpha_1}t_3^2 + \frac{(12\alpha_1+\alpha_2)(f^2t_1^2+h^2t_2^2+m^2t_4^2)}{32\alpha_1\alpha_2} - \frac{ct_3(ft_1+ht_2+mt_4)}{\alpha_1} + \frac{fht_1t_2+fmt_1t_4+hmt_2t_4}{32\alpha_1} &
-\frac{dm}{2\alpha_1}t_4^2 - \frac{cm}{2\alpha_1}t_3^2 + \frac{fg}{64\alpha_1}t_1^2 + \frac{hk}{64\alpha_1}t_2^2 + \frac{m(ft_1t_3+gt_1t_4+ht_2t_3+kt_2t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)m^2t_3t_4}{32\alpha_1\alpha_2} \\
-\frac{dg}{2\alpha_1}t_4^2 - \frac{ag}{2\alpha_1}t_1^2 + \frac{ek}{64\alpha_1}t_2^2 + \frac{fm}{64\alpha_1}t_3^2 + \frac{g(et_1t_2+ft_1t_3+kt_2t_4+mt_3t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)g^2t_1t_4}{32\alpha_1\alpha_2} &
-\frac{dk}{2\alpha_1}t_4^2 - \frac{bk}{2\alpha_1}t_2^2 + \frac{eg}{64\alpha_1}t_1^2 + \frac{hm}{64\alpha_1}t_3^2 + \frac{k(et_1t_2+gt_1t_4+ht_2t_3+mt_3t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)k^2t_2t_4}{32\alpha_1\alpha_2} &
-\frac{dm}{2\alpha_1}t_4^2 - \frac{cm}{2\alpha_1}t_3^2 + \frac{fg}{64\alpha_1}t_1^2 + \frac{hk}{64\alpha_1}t_2^2 + \frac{m(ft_1t_3+gt_1t_4+ht_2t_3+kt_2t_4)}{64\alpha_1} + \frac{(12\alpha_1+\alpha_2)m^2t_3t_4}{32\alpha_1\alpha_2} &
\frac{16d^2}{\alpha_1}t_4^2 + \frac{(12\alpha_1+\alpha_2)(g^2t_1^2+k^2t_2^2+m^2t_3^2)}{32\alpha_1\alpha_2} - \frac{dt_4(gt_1+kt_2+mt_3)}{\alpha_1} + \frac{gkt_1t_2+gmt_1t_3+kmt_2t_3}{32\alpha_1}
\end{pmatrix} \quad ....(4.158)$$

After using the coordinates of the support points for the four ingredients design (4.158) simplified to the matrix;

$$C=\begin{pmatrix}
\frac{103a^2}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(e^2+f^2+g^2)}{1536}-\frac{77a(e+f+g)}{144\alpha_1}+\frac{77(ef+eg+fg)}{4608\alpha_1} &
-\frac{103e(b+a)}{972\alpha_1}+\frac{103(fh+gk)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)e^2}{4608\alpha_1\alpha_2}+\frac{77e(f+g+h+k)}{9216\alpha_1} &
-\frac{103f(c+a)}{972\alpha_1}+\frac{103(eh+gm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)f^2}{4608\alpha_1\alpha_2}+\frac{77f(e+g+h+m)}{9216\alpha_1} &
-\frac{103g(d+a)}{972\alpha_1}+\frac{103(ek+fm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)g^2}{4608\alpha_1\alpha_2}+\frac{77g(e+f+k+m)}{9216\alpha_1} \\
-\frac{103e(b+a)}{972\alpha_1}+\frac{103(fh+gk)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)e^2}{4608\alpha_1\alpha_2}+\frac{77e(f+g+h+k)}{9216\alpha_1} &
\frac{103b^2}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(e^2+h^2+k^2)}{1536}-\frac{77b(e+h+k)}{144\alpha_1}+\frac{77(eh+kg+hk)}{4608\alpha_1} &
-\frac{103h(c+b)}{972\alpha_1}+\frac{103(ef+km)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)h^2}{4608\alpha_1\alpha_2}+\frac{77h(e+f+k+m)}{9216\alpha_1} &
-\frac{103k(d+b)}{972\alpha_1}+\frac{103(eg+hm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)k^2}{4608\alpha_1\alpha_2}+\frac{77k(e+g+h+m)}{9216\alpha_1} \\
-\frac{103f(c+a)}{972\alpha_1}+\frac{103(eh+gm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)f^2}{4608\alpha_1\alpha_2}+\frac{77f(e+g+h+m)}{9216\alpha_1} &
-\frac{103h(c+b)}{972\alpha_1}+\frac{103(ef+km)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)h^2}{4608\alpha_1\alpha_2}+\frac{77h(e+f+k+m)}{9216\alpha_1} &
\frac{103c^2}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(f^2+h^2+m^2)}{1536}-\frac{77c(f+h+m)}{144\alpha_1}+\frac{77(fh+fm+hm)}{4608\alpha_1} &
-\frac{103m(c+d)}{972\alpha_1}+\frac{103(fg+hk)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)m^2}{4608\alpha_1\alpha_2}+\frac{77m(f+g+h+k)}{9216\alpha_1} \\
-\frac{103g(d+a)}{972\alpha_1}+\frac{103(ek+fm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)g^2}{4608\alpha_1\alpha_2}+\frac{77g(e+f+k+m)}{9216\alpha_1} &
-\frac{103k(d+b)}{972\alpha_1}+\frac{103(eg+hm)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)k^2}{4608\alpha_1\alpha_2}+\frac{77k(e+g+h+m)}{9216\alpha_1} &
-\frac{103m(c+d)}{972\alpha_1}+\frac{103(fg+hk)}{3072\alpha_1}+\frac{77(12\alpha_1+\alpha_2)m^2}{4608\alpha_1\alpha_2}+\frac{77m(f+g+h+k)}{9216\alpha_1} &
\frac{103d^2}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(g^2+k^2+m^2)}{1536}-\frac{77d(g+k+m)}{144\alpha_1}+\frac{77(gk+gm+km)}{4608\alpha_1}
\end{pmatrix} \quad \ldots (4.159)$$

With

$$\begin{aligned} traceC &= \frac{103(a^2+b^2+c^2+d^2)}{3\alpha_1}+\frac{103(12\alpha_1+\alpha_2)(e^2+f^2+g^2+h^2+k^2+m^2)}{768} \\ &\quad -\frac{77(ae+af+ag+be+bh+bk+cf+ch+cm+dg+dk+dm)}{486\alpha_1} \\ &\quad +\frac{77(ef+eg+fg+eh+ek+hk+fh+fm+hm+gk+gm+km)}{243\alpha_1\alpha_2} \\ &= 2.2545\times10^4 \end{aligned} \quad , \ldots\ldots (4.160)$$

where the A- optimal slope weight vector entries are from (4.62) and coefficient values from (4.154).

The A- optimal slope information was gotten by using equation (3.22) with $p = -1$, $m = 4$ and the trace value from (4.160) as;

$$v(\phi_{-1}) = \left(\frac{1}{4} traceC\right)^{-1} = \left(\frac{2.2545 \times 10^{4}}{4}\right)^{-1} = 1.7742 \times 10^{-4} .$$

CHAPTER FIVE

CONCLUSIONS AND RECOMMENDATIONS

5.0 Introduction

This chapter covers the conclusions, recommendations and suggestions on arears of further research.

5.1 Concluding Remarks

The study has presented the necessary and sufficient condition for existence of ϕ_p – optimal slope mixture designs. The equivalence theorem was presented for the maximal parameter subsystem. For these cases the moment matrices are of full column rank. The unique parameter least squares estimates for the designs involved are the best. With this condition, optimal slope weighted centroid designs were derived for second degree Kronecker model for mixture experiments for the D- and A-optimal criteria. The designs were constructed for experiments with two, three and four ingredients.

Analytically a general optimal slope design was constructed using the general forms of moment and information matrices for weighted centroid designs with m ingredients. It is important to note that the information functions for these designs are finite mappings on the real line. For the slope optimal models presented one has to take keen interest on the scaling of parameter estimates to compensate for the shielding effect between ingredients in any particular mixture experiment.

One of the key task in this study was to establish numerical values of the restricted weight vector. It is evidently noted that both for A- optimal and D- optimal slope designs, the first weight is relatively larger than the second, for designs with two, three and four ingredients. This could be interpreted to mean the pure blends plays a major role in determining the response optimality values. They are therefore relatively more significant. This is an indication that in presence of many factors the response is dominated by the main effects. In this case, the main factor effects dominate the two factor interaction effects. This definitely is in concurrence with the sparsity-of-effects principle.

The statistical analysis of the sensory experiment data revealed that the Kronecker model adequately describes the data. This means the model fit is good for this kind of mixture experiments. Indeed, the Kronecker model with the weighted centroid design is very efficient considering the few support points that are necessary for a particular number of ingredients experiment. However, caution has to be exercised in determining the number of replications for two reasons. First, to allow for precise estimation of error variance. Second, to guarantee a good precision level for parameter estimates.

5.2 Recommendations

This study established that optimal slope designs are efficient in explaining the response for mixture experiments. It is recommended that the form of the Kronecker model discussed be utilized for analysis of simplex centroid designs. Least squares estimators are to be embraced since they are unique and unbiased for the maximal parameter subsystem.

The analysis of the sensory experiment data revealed that the Kronecker model is a highly effective model to describe the response. The model is therefore recommended for situations where decisions are made on the amounts of the various components have to be decided to give desired properties of the mixture.

5.3 Areas of Further Research

This study concentrated on weighted centroid design to analyze the slope for the second degree Kronecker model for mixture experiments. A maximal parameter subsystem was considered. Further analysis could be done for non-maximal parameter subsets of the full parameter vector. One may also consider other forms of the Kronecker model.

The concept of optimal slope could also be extended to other mixture model forms like for axial designs, symmetric-simplex designs, extreme vertices designs, mixture amount and mixture process variable designs, among others. The underlying regression models may also be varied from the Kronecker model like the use of cox regression models.

Further a need is here expressed on the research to analyze categorical responses in mixture experiments. It would also be interesting to explore nonlinear models.

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APPENDICES

Appendix 1: Questionnaire Used for Experimental Data Collection

SAMPLE QUESTIONNAIRE

Sensory evaluation and consumer acceptability

You are invited in a study to taste the sensory attributes of items presented. You will be required to taste samples and rate the samples for intensity of each characteristic. If you have any prior experience of allergic reactions, you should not participate in the study.

There is no direct benefit to you for participating in the study. You are free to withdraw from the study at any time.

I understand the above information and voluntarily consent to participate in the study.

Signature………………………. Date………………………………….

(TICK (APPROPRIATELY)

Socio- demographic characteristics

1. Gender

   Male ☐ Female ☐

2. Age

   Below 20 ☐ 20-22 ☐ 23- 24 ☐ 25-26 ☐ above 26 ☐

3. Do you take any medication that may affect senses especially smell and taste?
   ……………………………………………………………………………………..
4. Do you have any food allergies? If so, please state

   Yes ☐ No ☐

5. What is your year of study?
   Year 3 ☐ Year 4 ☐

6. Have you participated in a tasting panel another time?

   Yes ☐ No ☐

   If yes, how many times? …………

7.
8. Do you smoke
   Yes ☐ No ☐

Sample Characteristics

SAMPLE LABEL: ………………………...

You are expected to describe your likeness of the product in the table using the scale below.

Scale	Description	ATTRIBUTE			
		Texture (mouth feel)	**Appearance (Colour)**	**Taste**	**Aroma (Smell)**
15	Greatest imaginable like				
14	Greater imaginable like				
13	Great imaginable like				
12	Like extremely				
11	Like very much				
10	Like moderately				
9	Like slightly				
8	Neither like nor dislike				
7	Dislike slightly				
6	Dislike moderately				
5	Dislike very much				
4	Dislike extremely				
3	Great imaginable dislike				
2	Greater imaginable dislike				
1	Greatest imaginable dislike				

Would you recommend this product to a friend? Give reason

……………………………………………………………………………………………

……………………………………………………………………………………………

Would you buy this product in the market? Give reason

……………………………………………………………………………………………

……………………………………………………………………………………………

Appendix 2: Sensory Data for the Two Ingredients Experiment

	Combinations		ATTRIBUTES				TOTAL	MEAN
Label	pine apple	paw paw	texture	colour	Taste	smell	yield 1	yield 2
2.11	1	0	11	10	12	13	46	11.5
2.11	1	0	6	8	10	9	33	8.25
2.11	1	0	8	9	10	11	38	9.5
2.11	1	0	14	15	5	11	45	11.25
2.12	0	1	10	11	7	5	33	8.25
2.12	0	1	7	11	7	11	36	9
2.12	0	1	11	12	7	12	42	10.5
2.12	0	1	13	15	1	4	33	8.25
2.13	0.5	0.5	9	10	10	11	40	10
2.13	0.5	0.5	8	7	8	7	30	7.5
2.13	0.5	0.5	10	11	9	10	40	10
2.13	0.5	0.5	13	15	5	15	48	12

Appendix 3: Sensory Data for the Three Ingredients Experiment

	Combinations			ATTRIBUTES				TOTAL	MEAN
Label	pineapple	paw paw	banana	texture	colour	taste	smell	yield 1	yield 2
3.11	1	0	0	13	11	12	10	46	11.5
3.11	1	0	0	6	5	9	10	30	7.5
3.11	1	0	0	8	14	13	12	47	11.75
3.11	1	0	0	9	12	10	13	44	11
3.12	0	1	0	2	12	11	4	29	7.25
3.12	0	1	0	11	10	5	11	37	9.25
3.12	0	1	0	9	11	4	9	33	8.25
3.12	0	1	0	13	13	11	12	49	12.25
3.13	0	0	1	14	15	9	11	49	12.25
3.13	0	0	1	11	10	8	12	41	10.25
3.13	0	0	1	10	13	11	14	48	12
3.13	0	0	1	14	10	13	14	51	12.75
3.14	0.5	0.5	0	9	11	12	11	43	10.75
3.14	0.5	0.5	0	5	11	6	11	33	8.25
3.14	0.5	0.5	0	7	12	8	11	38	9.5
3.14	0.5	0.5	0	11	12	9	11	43	10.75
3.15	0.5	0	0.5	11	9	10	10	40	10
3.15	0.5	0	0.5	4	1	6	7	18	4.5
3.15	0.5	0	0.5	10	11	12	12	45	11.25
3.15	0.5	0	0.5	12	9	6	8	35	8.75
3.16	0	0.5	0.5	9	11	9	8	37	9.25
3.16	0	0.5	0.5	10	11	7	11	39	9.75
3.16	0	0.5	0.5	6	11	4	7	28	7
3.16	0	0.5	0.5	14	15	15	15	59	14.75
3.17	0.333333	0.333333	0.333333	1	6	7	13	27	6.75
3.17	0.333333	0.333333	0.333333	9	7	9	12	37	9.25
3.17	0.333333	0.333333	0.333333	7	7	9	10	33	8.25
3.17	0.333333	0.333333	0.333333	5	1	9	11	26	6.5

Appendix 4: Sensory Data for the Four Ingredients Experiment

	combinations				ATTRIBUTES				TOTAL	MEAN
Label	pine apple	pawpaw	banana	coconut	texture	colour	taste	smell	Yield 1	yield 2
4.01	1	0	0	0	10	8	10	12	40	10
4.01	1	0	0	0	12	15	11	9	47	11.75
4.01	1	0	0	0	8	9	11	11	39	9.75
4.01	1	0	0	0	14	14	14	15	57	14.25
4.02	0	1	0	0	9	12	8	12	41	10.25
4.02	0	1	0	0	13	14	2	14	43	10.75
4.02	0	1	0	0	12	15	9	14	50	12.5
4.02	0	1	0	0	10	12	9	8	39	9.75
4.03	0	0	1	0	4	5	5	13	27	6.75
4.03	0	0	1	0	10	11	10	14	45	11.25
4.03	0	0	1	0	8	6	11	10	35	8.75
4.03	0	0	1	0	15	15	14	13	57	14.25
4.04	0	0	0	1	10	12	9	9	40	10
4.04	0	0	0	1	9	10	8	9	36	9
4.04	0	0	0	1	15	10	10	8	43	10.75
4.04	0	0	0	1	10	7	10	5	32	8
4.05	0.5	0.5	0	0	10	10	10	9	39	9.75
4.05	0.5	0.5	0	0	10	9	5	11	35	8.75
4.05	0.5	0.5	0	0	9	7	10	9	35	8.75
4.05	0.5	0.5	0	0	14	15	15	15	59	14.75
4.06	0.5	0	0.5	0	13	9	12	10	44	11
4.06	0.5	0	0.5	0	9	8	9	10	36	9
4.06	0.5	0	0.5	0	9	9	10	11	39	9.75
4.06	0.5	0	0.5	0	14	5	13	15	47	11.75
4.07	0.5	0	0	0.5	10	13	4	14	41	10.25
4.07	0.5	0	0	0.5	5	6	7	8	26	6.5
4.07	0.5	0	0	0.5	9	8	8	15	40	10
4.07	0.5	0	0	0.5	6	10	9	10	35	8.75
4.08	0	0.5	0.5	0	10	11	12	10	43	10.75
4.08	0	0.5	0.5	0	12	10	12	12	46	11.5
4.08	0	0.5	0.5	0	6	8	7	9	30	7.5
4.08	0	0.5	0.5	0	6	7	6	13	32	8
4.09	0	0.5	0	0.5	10	8	7	12	37	9.25
4.09	0	0.5	0	0.5	4	9	8	15	36	9
4.09	0	0.5	0	0.5	5	9	5	9	28	7
4.09	0	0.5	0	0.5	1	1	1	10	13	3.25
4.10	0	0	0.5	0.5	4	8	11	14	37	9.25
4.10	0	0	0.5	0.5	8	3	7	15	33	8.25
4.10	0	0	0.5	0.5	10	7	12	11	40	10
4.10	0	0	0.5	0.5	10	6	7	15	38	9.5
4.11	0.333333	0.333333	0.333333	0	13	10	12	15	50	12.5
4.11	0.333333	0.333333	0.333333	0	9	10	9	10	38	9.5
4.11	0.333333	0.333333	0.333333	0	15	15	9	15	54	13.5
4.11	0.333333	0.333333	0.333333	0	11	10	11	11	43	10.75
4.12	0.333333	0.333333	0	0.333333	11	10	9	10	40	10
4.12	0.333333	0.333333	0	0.333333	14	13	10	8	45	11.25
4.12	0.333333	0.333333	0	0.333333	4	9	9	12	34	8.5
4.12	0.333333	0.333333	0	0.333333	10	7	9	15	41	10.25
4.13	0.333333	0	0.333333	0.333333	5	5	10	7	27	6.75

4.13	0.333333	0	0.333333	0.333333	9	6	10	7	32	8
4.13	0.333333	0	0.333333	0.333333	9	9	10	10	38	9.5
4.13	0.333333	0	0.333333	0.333333	5	13	7	15	40	10
4.14	0	0.333333	0.333333	0.333333	6	9	6	15	36	9
4.14	0	0.333333	0.333333	0.333333	5	7	4	6	22	5.5
4.14	0	0.333333	0.333333	0.333333	12	9	10	13	44	11
4.14	0	0.333333	0.333333	0.333333	3	7	5	12	27	6.75
4.15	0.25	0.25	0.25	0.25	11	13	10	15	49	12.25
4.15	0.25	0.25	0.25	0.25	9	8	11	10	38	9.5
4.15	0.25	0.25	0.25	0.25	10	13	12	14	49	12.25
4.15	0.25	0.25	0.25	0.25	9	7	10	13	39	9.75

Appendix 5: SAS Program Codes (Two Ingredients)

```
DATA twoingredients;
input pine paw yield;
cards;
1 0 11.5
1 0 8.25
1 0 9.5
1 0 11.25
0 1 8.25
0 1 9.0
0 1 10.5
0 1 8.25
0.5 0.5 10.0
0.5 0.5 7.5
0.5 0.5 10.0
0.5 0.5 12.0
;
run;
proc print data=twoingredients;
run;
proc glm;
model yield=pine*pine paw*paw pine*paw/NOINT solution;
estimate 'pine*pine paw*paw pine*paw' pine*pine 2 paw*paw 2 pine*paw
1/divisor=2;
run;
```

Appendix 6: SAS Program Codes (Three Ingredients)

```
DATA threeingredients;
input pine paw ban yield;
cards;
1 0 0 11.5
1 0 0 7.5
1 0 0 11.75
1 0 0 11
0 1 0 7.25
0 1 0 9.25
0 1 0 8.25
0 1 0 12.25
0 0 1 12.25
0 0 1 10.25
0 0 1 12
0 0 1 12.75
0.5 0.5 0 10.75
0.5 0.5 0 8.25
0.5 0.5 0 9.5
0.5 0.5 0 10.75
0.5 0 0.5 10
0.5 0 0.5 4.5
0.5 0 0.5 11.25
0.5 0 0.5 8.75
0 0.5 0.5 9.25
0 0.5 0.5 9.75
0 0.5 0.5 7
0 0.5 0.5 14.75
0.333 0.333 0.333 6.75
0.333 0.333 0.333 9.25
0.333 0.333 0.333 8.25
0.333 0.333 0.333 6.5
```

```
;
run;
proc print data=threeingredients;
run;
proc glm;
model yield=pine*pine paw*paw ban*ban pine*paw pine*ban paw*ban/NOINT
solution;
estimate 'pine*pine paw*paw ban*ban pine*paw pine*ban paw*ban'
pine*pine 3 paw*paw 3 ban*ban 3 pine*paw 1 pine*ban 1 paw*ban
1/divisor=3;
run;
```

Appendix 7: SAS Program Codes (Four Ingredients)

```
DATA fouringredients;
input pine paw ban coco yield;
cards;
1 0 0 0 10
1 0 0 0 11.75
1 0 0 0 9.75
1 0 0 0 14.25
0 1 0 0 10.25
0 1 0 0 10.75
0 1 0 0 12.5
0 1 0 0 9.75
0 0 1 0 6.75
0 0 1 0 11.25
0 0 1 0 8.75
0 0 1 0 14.25
0 0 0 1 10.0
0 0 0 1 9.0
0 0 0 1 10.75
0 0 0 1 8.0
0.5 0.5 0 0 9.75
0.5 0.5 0 0 8.75
0.5 0.5 0 0 8.75
0.5 0.5 0 0 14.75
0.5 0 0.5 0 11.0
0.5 0 0.5 0 9.0
0.5 0 0.5 0 9.75
0.5 0 0.5 0 11.75
0.5 0 0 0.5 10.25
0.5 0 0 0.5 6.5
0.5 0 0 0.5 10.0
0.5 0 0 0.5 8.75
0 0.5 0.5 0 10.75
0 0.5 0.5 0 11.5
0 0.5 0.5 0 7.5
0 0.5 0.5 0 8.0
0 0.5 0 0.5 9.25
0 0.5 0 0.5 9.0
0 0.5 0 0.5 7.0
0 0.5 0 0.5 3.25
0 0 0.5 0.5 9.25
0 0 0.5 0.5 8.25
0 0 0.5 0.5 10.0
0 0 0.5 0.5 9.5
0.333 0.333 0.333 0 12.5
0.333 0.333 0.333 0 9.5
0.333 0.333 0.333 0 13.5
```

```
0.333 0.333 0.333 0 10.75
0.333 0.333 0 0.333 10.0
0.333 0.333 0 0.333 11.25
0.333 0.333 0 0.333 8.5
0.333 0.333 0 0.333 10.25
0.333 0 0.333 0.333 6.75
0.333 0 0.333 0.333 8.0
0.333 0 0.333 0.333 9.5
0.333 0 0.333 0.333 10.0
0 0.333 0.333 0.333 9.0
0 0.333 0.333 0.333 5.5
0 0.333 0.333 0.333 11.0
0 0.333 0.333 0.333 6.75
0.25 0.25 0.25 0.25 12.25
0.25 0.25 0.25 0.25 9.5
0.25 0.25 0.25 0.25 12.25
0.25 0.25 0.25 0.25 9.75
;
run;
proc print data=fouringredients;
run;
proc glm;
model yield=pine*pine paw*paw ban*ban coco*coco pine*paw pine*ban
pine*coco paw*ban paw*coco ban*coco/NOINT solution;
estimate 'pine*pine paw*paw ban*ban coco*coco pine*paw pine*ban
pine*coco paw*ban paw*coco ban*coco' pine*pine 4 paw*paw 4 ban*ban 4
coco*coco 4 pine*paw 1 pine*ban 1 pine*coco 1 paw*ban 1 paw*coco 1
ban*coco 1/divisor=4;
run;
```