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THE GLC ANALYSIS OF THREE-COMPONENT FAT/OIL MIXTURES  
IN THE DETERMINATION OF COMPONENT  
PROPORTIONS

A thesis presented in fulfilment of the requirements  
for Master in Technology degree at  
Massey University

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1 9 8 3

ABSTRACT

By making use of the fatty acid composition of mixture components and the three-fat(s)/oil(s) mixture, obtained from the gas-liquid chromatographic analysis, the relationship between mixture components and mixture was expressed by the general mixture equation:

$$(A_i - C_i) X_1 + (B_i - C_i) X_2 = (M_i - C_i)$$

where  $A_i$  is the fatty acid percent value of the first mixture component;  $B_i$  is the fatty acid percent value of the second mixture component;  $C_i$  is the fatty acid percent value of the third mixture component;  $M_i$  is the fatty acid percent value of the mixture;  $X_1$  is the fraction of the first component in the mixture; and  $X_2$  is the fraction of the second component in the mixture.

The fraction of first two mixture component can then be estimated by solving simultaneous mixture equations. This can be done either by employing the Cramer's Rule method (McCracken and Dorn, 1964) or by the Gauss-Jordan Elimination method (Dodges, 1978). The third mixture component proportion (i.e.  $X_3$ ) can be obtained by substituting  $X_1$  and  $X_2$  into the following equation:

$$X_3 = 1 - X_1 - X_2$$

The F77 FREQC program, using the Gauss-Jordan Elimination Method to estimate the proportion of each mixture component and the Frequency Method to calculate the weighted mean proportion of each mixture component, gave the best results with almost all of the calculated weighted mean mixture component proportions to be within two calculated standard deviations.

The accuracy of the calculated estimations was dependent upon the accuracy of the experimental and literature component data. In most cases, literature data did not produce as good results as those calculated from experimental data.

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PREFACE

The prohibition of the import of New Zealand pure milk fat into Japan has compelled New Zealand Dairy Board to export milk fat with other fats or oils in the form of a mixture. Nevertheless, for custom declaration purposes, the proportion of each mixture constituent must be stated and determined by a reliable and accurate method. The method must be simple and rapid; and made available to the Japanese authority.

For two components mixture, a computer aided method had been developed by Jebson and Curtis (1981) which proved reliable. However, there was no published article regarding the analysis of three fat(s)/oil(s) mixture available. Hence the analysis, with the aid of computer programs and the gas-liquid chromatograph instrument, was carried out.

The aim of this work was to determine a simple, rapid and accurate method, capable of automation for routine use, for the analysis of three fat(s)/oil(s) mixture.

This research, the analysis of three fat(s)/oil(s) mixture, involved (1) the setting up of mathematical model for three fat(s)/oil(s) mixture; (2) the writing of computer programs using the mathematical model; (3) the Gas Chromatography in analysing the fatty acid compositions of fats, oils and mixtures; (4) the testing of computer programs with data collected from (3); (5) the analysing of results to determine which computer program gave the best results; and (6) the use of the best computer program to test the literature fatty acid values of components to determine the accuracy of the results.

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# **chapter 1**

## 1 LITERATURE REVIEW

### 1.1 Reichert-Meissl, Polenske and Kirschner Methods

Long before the existence of the Gas Liquid Chromatograph instrument and other modern techniques, attempts to determine the mixture component proportions were made by several research workers. Some of the interesting methods are Reichert-Meissl, Polenske, and Kirschner methods (Cocks and Rede, 1966).

In the Reichert-Meissl method, Reichert-Meissl value is calculated, which is the number of ml. of 0.1N alkali required to neutralize the steam-volatile, water-soluble fatty acids. The fatty acids are prepared by first saponifying 5gm of fat and acidifying the soap solution with dilute sulphuric acid, then followed by the distillation of a known volume of distillate under well controlled conditions. After filtering the insoluble acids from the distillate, the soluble fatty acids are titrated with standard alkali.

In the Polenske method, Polenske value, which is the number of ml. of 0.1N alkali required to neutralize the steam-volatile, water-insoluble fatty acids, is calculated. The insoluble acids filtered off from the distillate in the Reichert-Meissl method are dissolved in ethanol and titrated with 0.1N sodium or potassium hydroxide.

Similarly, in the Kirschner method the Kirschner value, which is the number of ml. of 0.1N alkali solution required to neutralize the water-soluble volatile fatty acids which form water-soluble silver salts, is calculated. The fatty acids are prepared by adding silver sulphate to the solution remaining after determination of steam-volatile, water-soluble acids in Reichert-Meissl method.

For a mixture that has milk fat as one of its components, the proportion of milk fat is estimated as follows:

$$\text{Milk fat \%} = \frac{K - (0.1 P + 0.24)}{0.244}$$

where K is the Kirschner value ; and  
P is the Polenske value.

Based on Kirschner and Polenske values of milk fat, coconut oil and palm kernel oil mixture; and Reichert-Meissl and Polenske values of coconut oil and palm kernel oil mixture, two graphs were drawn by Williams (refer to "Laboratory Handbook For Oil And Fat Analyst" page 364). The graphs provide a convenient means of determining the proportions of mixture components in question.

These three methods give a measure respectively of the volatile fatty acids, soluble in water, insoluble in water, and those soluble in water whose silver salts are soluble in water. They do not provide an exact determination of chemical individuals but a quick means of obtaining a reasonable approximation of the contents in a mixture. The accuracy of estimations is dependent upon variations in the component materials. Also errors can occur from overheating during distillation and, in the case of calculating Kirschner value, the impurities in silver sulphate. There is no available method of estimating errors associated with the estimation of mixture components. The accuracy of the estimated values is therefore questionable.

#### 1.2 Timms Triglyceride Method (Timms, 1980)

This method makes use of the triglyceride compositions of mixture and its components in determining the proportion of each mixture component. Mixture components were classified into milk fat and non-milk fats. The non-milk fats involved were cocoa butter, palm kernel oil, coconut oil, beef tallow, lard, sunflower oil and soya bean oil. Seventy six samples of butter were obtained from three Australian factories between September 1975 - September 1976 and their triglyceride compositions were analysed by gas-liquid chromatography. Also the triglyceride compositions of milk and non-milk fats mixtures

and the non-milk fats were determined by gas-liquid chromatography.

As non-milk fats have substantial amounts of diglycerides with carbon number 32-38 and milk fat has substantial amounts of triglycerides with carbon number below 46; by ignoring those triglycerides with carbon numbers less than 32, Timms (1980) was able to use those triglycerides with carbon numbers 40, 42 and 44 to discriminate between milk fat and most non-milk fats. Therefore, when determining a function to discriminate between milk fat and non-milk fats, the non-milk fats equations disappear.

The triglyceride data were fitted to the following equation:

$$\sum ( a_i C_i ) = R + e$$

where  $i$  is the carbon number;  $C_i$  is the percentage of triglyceride with carbon number  $C_i$ ;  $a_i$  is a coefficient to be estimated;  $R$  is a constant defined to be 100 for pure milk and  $e$  is a random error.

Using only triglycerides with carbon numbers 40, 42 and 44 and by multiple linear regression, the equation becomes:

$$100 = 14.197 C_{40} - 36.396 C_{42} + 32.364 C_{44} - e \quad \text{----- (1)}$$

The errors, estimated by Timms, were approximately normally distributed with a standard deviation of 0.7088.

For any mixture of milk fat and non-milk fats, the following equations were used:

$$C_i^{\text{MIX}} = x C_i^{\text{NMF}} + (1 - x) C_i^{\text{MF}}$$

where the superscript MIX, NMF and MF refer to the mixture, non-milk fat and milk fat; and  $x$  is the proportion of non-milk fat in the mixture.

And

$$R = x \left[ \begin{array}{ccc} \text{NMF} & & \text{NMF} \\ a_{40} C_{40} & + a_{42} C_{42} & + a_{44} C_{44} \end{array} \right] + (1-x) \left[ \begin{array}{ccc} \text{MF} & & \text{MF} \\ a_{40} C_{40} & + a_{42} C_{42} & + a_{44} C_{44} \end{array} \right]$$

which reduces to the following form:

$$x = \frac{\begin{array}{c} \text{MF} \quad \text{MIX} \\ R - R \end{array}}{\begin{array}{c} \text{MF} \quad \text{NMF} \\ R - R \end{array}} \quad (2)$$

As  $R(\text{MF}) = 100$  by definition, an estimate of  $x$  can therefore be calculated by the following equation

$$x' = \frac{\begin{array}{c} \text{MIX} \\ 100 - R' \end{array}}{\begin{array}{c} \text{NMF} \\ 100 - R' \end{array}} \quad (3)$$

where  $R'(\text{NMF})$  and  $R'(\text{MIX})$  are estimated from equation (1) when  $C_{40}$ ,  $C_{42}$  and  $C_{44}$  for the non-milk fat and the mixture are substituted.

The lower 99% confidence limit for  $R'(\text{MF})$  is  $100 - 2.65 * 0.7088 = 98.12$  (73 DF) and the upper 99% confidence limit for  $R'(\text{MIX})$  when the mixture has a fraction  $x(D)$  of non-milk fat with  $R(\text{NMF}) = 0$  is  $100(1 - x(D)) + 1.88$ . When  $100(1 - x(D)) + 1.88 > 98.12$  or  $x(D)$  greater than or equal to 0.0376, at least 0.5% of such mixture, at the 1% significant level, is detectable. In general:

$$x(D) \geq \frac{101.88 - 98.12}{\begin{array}{c} \text{NMF} \\ 100 - R \end{array}} \quad (4)$$

Although lauric oils and animal fats had significant amounts of triglycerides with carbon numbers 40-44, the distribution among the three triglycerides was different from that of milk fat, therefore in Timms calculation it showed that the level of detectability of non-milk fat was not affected by the variations.

As little as 5% of any non-milk fat can be detected by this method with better than 99% confidence. Also, when a non-milk fat is involved, its amount can be quantified with 95% confidence limits to better than 2% absolute.

According to Timms (1980), the triglyceride analyses by GLC were more effective than fatty acid analyses for detecting non-milk fat in milk fat. However, the research carried out by Jebson and Curtis had proved otherwise. The levels of contamination down to 5% can be detected by Jebson and Curtis (1981) method (refer to "Computer Aided Gas Liquid Chromatographic Analysis Of Two Component Mixtures").

This method depended entirely on the experimental data obtained from the gas-liquid chromatographic analysis of triglyceride compositions of mixtures and mixture constituents. The accuracy of this method has therefore not been tested by data obtained from literature. Since this method based on the triglyceride percentage of C40, C42 and C44 instead of using all the triglyceride percent distribution, it is doubtful that this method will give as good estimation of mixture component proportions when literature component data are used. Moreover, when three mixture components were involved, this method was not able to estimate the proportion of each component in the mixture. For example, in the case of milk fat, soya bean oil and palm oil mixture, this method only gave the general milk fat and non-milk fat (i.e. soya bean oil and palm oil) proportion estimation.

### 1.3 Computer Aided Gas Liquid Chromatographic Analysis Of Two Component Mixtures

The evolution of new technology has made the development of new analytical techniques in determination of mixture component proportions possible. For instance, since its introduction in 1952, gas chromatography has become one of the most widely used modern analytical techniques. It provides rapid qualitative and quantitative analysis of complex mixture with precision and sensitivity. Also, the falling in price of computer, owing to the invention of cheaper silicon chip, has made the introduction of computer to research affordable. Long, tedious and accurate calculation can now be performed by computer, leaving more time to research workers to concentrate on their research.

The computer aided gas liquid chromatographic analysis of two component mixtures, of which one of the components was milk fat, was carried out by Jebson and Curtis (1981). Based on the mathematical model derived by Jebson and Curtis, a BASIC language program was written. By making use of the results of a gas liquid chromatographic analysis of the proportions of fatty acids present in the mixture and mixture components, the determination of each mixture component was performed by Cromemco computer.

In the analysis, the relation between the proportions of a number of fats in a mixture and their fatty acid composition was expressed as follows:

$$\sum (A_{ij} * X_j) = M_i \quad \text{----- (i)}$$

where  $i = 1$ , to number of fatty acids in the mixture.

$j = 1$ , to number of mixture components.

$A_{ij}$  is the fraction of acid  $i$  in fat  $j$ .

$M_i$  is the proportion of acid  $i$  in the mixture.

$X_j$  is the proportion of fat  $j$  in the mixture.

and 
$$\sum (X_j) = 1$$

For two mixture components case, it becomes:

$$A_{i1} X_1 + A_{i2} (1 - X_1) = M_i \quad \text{----- (ii)}$$

Re-arrange the equation (ii), it gives:

$$X_1 = \frac{M_i - A_{i2}}{A_{i1} - A_{i2}} \quad \text{----- (iii)}$$

where  $X_1$  is the proportion of the first fat in the mixture.

The error in  $X_1$  was determined by the errors in the variables used to determine  $X_1$  as below:

$$x = \frac{1}{(A_{i1} - A_{i2})^2} \left[ \text{abs}\{a_{i1}(A_{i2} - M_i)\} + \text{abs}\{a_{i2}(A_{i1} - M_i)\} + \text{abs}\{m_i(A_{i1} - A_{i2})\} \right] \quad \text{----- (iv)}$$

where  $x$  is the error in  $X_1$ ;  
 $a_{i1}$  is the error of acid  $i$  in the first fat;  
 $a_{i2}$  is the error of acid  $i$  in the second fat;  
 $m_i$  is the error of acid  $i$  in the mixture.

The best overall estimate of the proportion of the two fats was obtained by calculating a weighted average of the estimates from the individual fatty acid analysis. This was done by using following relation:

$$X' = \frac{\sum_2 (X_i/x_i)}{\sum_2 (1/x_i)} \quad \text{----- (v)}$$

where  $X'$  is the weighted average;  
 $X_i$  is the estimate of  $X_1$  from fatty acid  $i$  analysis;  
 $x_i$  is the estimate of error in  $X_i$ .

An estimate of error in X' was given by:

$$x = \frac{\sum_{i=1}^n (1/x_i)}{n} \quad \text{--- (vi)}$$

where n is number of estimates; and  
i varies from 1 to n

The error in the determination of proportion of each fatty acid was assessed either

1. from a standard deviation estimated from the difference in duplicate results; or
2. from a one-way analysis of variance of the results of a number of fatty acids analysis done in duplicate.

In order not to under-estimate the size of the errors, the larger of two estimates of variability was used in the calculation by Jebson and Curtis (1981).

### 1.3.1 Gas-liquid Chromatographic Analysis Of Methyl Esters

Methyl esters of fatty acids were prepared by the method of Shehata, de Man and Alexander (1970). They were then analysed by gas-liquid chromatography employing similar conditions as used by Gray (1973), except that the samples were injected at 40 degrees C and programmed up to 180 degrees C at a rate of 6 degrees C/min. The proportion of methyl esters of fatty acid was determined by Varian model 480 digital integrator and weight response factors of standard methyl esters were determined experimentally. Components and mixtures were analysed in duplicate.

### 1.3.2 Analysis Of Results

The analytical error of the GLC technique was estimated by a one-way analysis of variance, using the BASIC language program, for each fatty acid estimated from analytical results for a number of fats. The analysis of variance was also carried out for each fatty acid present in the mixture. The standard deviations and coefficients of variation for each fatty acid were calculated from the within-sample variances and the mean concentrations.

Calculation of the percentage of milk fat present in the mixtures were made under two sets of condition:

- 1) using the fatty acid compositions of the individual fats obtained experimentally; and
- 2) using the fatty acid compositions of the individual fats obtained from literature (Hildith and Williams, 1964; Codex Committee on Fats and Oils, 1978; Gray, 1973; and Taylor and Hawke, 1975).

There was good agreement between calculated milk fat percentage and the actual percentage of milkfat in the mixtures, and the deviations were generally consistent with the error estimates.

It was pointed out that when using literature fatty acid compositions to determine the milk fat percentage in the mixtures, care must be taken as the composition of oils can vary widely with the variety and with the climate in which the seeds are grown. Also, the composition of milk fat depends upon the stage of lactation, the feeds, and the genetics of the cows. Therefore, it is likely under some circumstances that the fraction of minor components will vary considerably from normal. Hence, when unreasonable results are obtained, that is when the estimated proportion of milk fat is less than 0% or greater than 100%, they are excluded or ignored.

Comparison was made by Jebson and Curtis (1981) between the methods of Cavitt and Weenink (1977) and theirs. It showed that their methods gave results of equivalent precision to the iodine value method, and better than the C14 or C18 methods proposed by Cavitt and Weenink.

The method is suitable for detecting small quantities of other oils in milkfat, and may be used as a means for detecting moderate contamination (i.e. the levels of contamination down to 5% may be detectable by this method).

However, the mathematical model derived by Jebson and Curtis (1981) becomes insufficient and too complicated when dealing with three components mixtures. Therefore, a new mathematical model, which may be similar to the one derived by Jebson and Curtis, was required.

## **chapter 2**

2 MATHEMATICAL MODEL2.1 The General Mixture Equation

It is obvious that any mathematical model used in calculating mixture component proportions will be dependent upon the method(s) and instrument(s) involved. In this three-fat(s)/oil(s) mixture analysis, the fatty acid compositions of mixture and components were analysed by gas-liquid chromatography in duplicate (refer to Chapter 3 for methods and gas-liquid chromatographic analysis). The relationship between mixture and its components can be represented by the following general mixture equation:

$$A_i X_1 + B_i X_2 + C_i X_3 = M_i \quad \text{-- (1)}$$

$i = 1$  to  $N$  (where  $N$  is the number of fatty acids in mixture)

where  $A_i$  is the fatty acid percent value of the first mixture component;  $B_i$  is the fatty acid percent value of the second mixture component;  $C_i$  is the fatty acid percent value of the third mixture component;  $M_i$  is the fatty acid percent value of the mixture;  $X_1$  is the fraction of the first component in the mixture;  $X_2$  is the fraction of the second component in the mixture; and  $X_3$  is the fraction of the third component in the mixture.

However,

$$X_1 + X_2 + X_3 = 1 \quad \text{--(2)}$$

$$X_3 = 1 - X_1 - X_2 \quad \text{--(3)}$$

Therefore, the equation (1) becomes

$$A_i X_1 + B_i X_2 + C_i(1 - X_1 - X_2) = M_i \quad \text{---(4)}$$

$$(A_i - C_i)X_1 + (B_i - C_i)X_2 = (M_i - C_i) \quad \text{---(5)}$$

As there are more than two fatty acids in each fat/oil, more than one two-equation combinations will be available. By choosing two equations at a time,  $X_1$  and  $X_2$  can be obtained by solving the two simultaneous equations.

For example, if there are twenty mixture equations, two equations can be chosen at a time by the following loops (Fortran Programming Language):

```

DO 7 I = 1, 19
DO 8 J = (I+1), 20
DO 9 K = 1, 3
A1(1,K) = A(I,K)
A1(2,K) = A(J,K)
9 CONTINUE
: : : : : : : : {followed by the calculation of X1
: : : : : : : : and X2 if the general equation (5)
: : : : : : : : is used.}
8 CONTINUE
7 CONTINUE

```

where  $A_1(1,1)$ ,  $A_1(1,2)$  and  $A_1(1,3)$  are the terms  $(A_i - C_i)$ ,  $(B_i - C_i)$  and  $(M_i - C_i)$  of the equation (5), when  $i = 1$  (i.e. the first simultaneous equation). Similarly, for the second simultaneous equation,  $A_1(2,1)$ ,  $A_1(2,2)$  and  $A_1(2,3)$  are the coefficients and constant of the equation (5), when  $i = 2$ .

Matrix A is for storing all the average fatty acid percents of components and mixture. For example,  $A(1,1)$  and  $A(2,1)$  are for the first and second fatty acid percent values of the first mixture component;  $A(1,2)$  and  $A(2,2)$  are for the first and second fatty acid percent values of the second mixture component; and  $A(1,3)$  and  $A(2,3)$  are for the first and second fatty acid percent values of the mixture.

By using these loops, there will be 190 sets of two-simultaneous equation available. Therefore, at least one set of X1 and X2 values will be determined at the end of these loops and X3 can be obtained by substituting X1 and X2 into equation (3).

## 2.2 Solving The Simultaneous Equations

The simultaneous equations can be solved by employing (i) Cramer's Rule Method (McCracken and Dorn, 1964; Dickson, 1968; and McCalla, 1967); (ii) Gauss-Jordan Elimination Method (Dodges, 1978); or (iii) Least Squares Method (Scarborough, 1958).

By using Frequency Method (Topping, 1955), estimates calculated by both the Cramer's Rule Method and Gauss-Jordan Elimination Method can be used to calculate weighted mean proportion of each mixture component.

In order to have a better insight of each method, each method will be demonstrated with the help of an example:

### 2.2.1 Cramer's Rule

(McCracken and Dorn, 1964; Dickson, 1968; and McCalla, 1967)

This method makes use of determinants to solve simultaneous linear equations.

## 2.2.1.1 For two unknown case

Assume that the simultaneous linear equations are:

$$a_1X_1 + b_1X_2 = m_1$$

$$a_2X_1 + b_2X_2 = m_2$$

The 2 equations can be expressed in matrix form as below:

$$\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix} \cdot \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} \quad \text{--(6)}$$

$$\text{i.e. } A \cdot X = M$$

The determinant of the coefficient array A is

$$D = a_1 \cdot b_2 - b_1 \cdot a_2 = \begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix} \quad \text{--(7)}$$

In order to solve  $X_1$ ,  $a_1$  and  $a_2$  are replaced by  $m_1$  and  $m_2$  and it becomes

$$D_1 = b_2m_1 - b_1m_2 = \begin{vmatrix} m_1 & b_1 \\ m_2 & b_2 \end{vmatrix} \quad \text{-- (8)}$$

Similarly, to solve  $X_2$ ,  $b_1$  and  $b_2$  are replaced by  $m_1$  and  $m_2$ .

$$D_2 = a_1m_2 - a_2m_1 = \begin{vmatrix} a_1 & m_1 \\ a_2 & m_2 \end{vmatrix} \quad \text{--(9)}$$

The solution is

$$X_1 = D_1 / D \quad \text{-- (10)}$$

$$X_2 = D_2 / D \quad \text{-- (11)}$$

However, when D is very small the calculated results will be inaccurate and when D is equal to zero, there is no solution. As in the work being considered there are more than one two-equation combinations available, when the above stated situation occurs, that combination can be ignored and another one is chosen. Likewise, that set of two-linear simultaneous equation combination is ignored if calculated X1 or X2 value is less than or equal to zero; or greater than or equal to one (i.e. 100%). This is because physically none of the X's value can exceed this range (i.e.  $0.0 < X < 1.0$ ).

Similarly,

2.2.1.2 For three unknown cases

$$a_{11}X_1 + a_{12}X_2 + a_{13}X_3 = K_1$$

$$a_{21}X_1 + a_{22}X_2 + a_{23}X_3 = K_2$$

$$a_{31}X_1 + a_{32}X_2 + a_{33}X_3 = K_3$$

$$D = a_{11}a_{22}a_{33} - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{13}a_{22}a_{31} \quad \text{-- (12)}$$

$$X_1 = (k_1a_{22}a_{33} - k_1a_{23}a_{32} - a_{12}a_{33}k_2 + a_{12}k_3a_{23} + a_{13}k_2a_{32} - a_{13}a_{22}k_3) / D \quad \text{--(13)}$$

$$X_2 = (a_{11}K_2a_{33} - a_{11}a_{23}K_3 - K_1a_{21}a_{33} + K_1a_{23}a_{31} + a_{13}a_{21}K_3 - a_{13}K_2a_{31}) / D \quad \text{--(14)}$$

$$X_3 = (a_{11}a_{22}K_3 - a_{11}K_2a_{32} - a_{12}a_{21}K_3 + a_{12}K_2a_{31} + K_1a_{21}a_{32} - K_1a_{22}a_{31}) / D \quad \text{--(15)}$$

Again, when D is very small, calculated results will be inaccurate and when D is zero, there is no solution. Hence, the next set of simultaneous equations is chosen. Likewise, when X1, or X2, or X3 value is greater than or equal to one (i.e. 100%); or less than or equal to zero, that set of linear simultaneous equations is ignored.

The F77 computer programs using the Cramer's Rule method were named CRAM1, CRAM2, CRAM4, CRAM5, CRA1, CRA2, CRA3, and CRA4. The results produced by these programs will be analysed in Chapter 5.

### 2.2.2 Gauss-Jordan Elimination Method (Dodes, 1978)

Example 1:

Suppose the simultaneous linear equations of four-unknown are:

$$2.630X_1 + 5.210X_2 - 1.694X_3 + 0.938X_4 = 4.230$$

$$3.160X_1 - 2.950X_2 - 0.813X_3 - 4.210X_4 = -0.716$$

$$5.360X_1 + 1.880X_2 - 2.150X_3 - 4.950X_4 = 1.280$$

$$1.340X_1 + 2.980X_2 - 0.432X_3 - 1.768X_4 = 0.419$$

and in matrix form :

$$\begin{bmatrix} 2.630 & 5.210 & -1.694 & 0.938 \\ 3.160 & -2.950 & 0.813 & -4.210 \\ 5.360 & 1.880 & -2.150 & -4.950 \\ 1.340 & 2.980 & -0.432 & -1.768 \end{bmatrix} \cdot \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} = \begin{bmatrix} 4.230 \\ -0.716 \\ 1.280 \\ 0.419 \end{bmatrix}$$

$$A \cdot X = C$$

There are a number of ways to solve this problem. One possible form of the answer is

$$1X_1 = 1.038$$

$$1X_2 = 0.209$$

$$1X_3 = 0.226$$

$$1X_4 = 0.847$$

and in matrix form:

$$\begin{bmatrix} 1000 \\ 0100 \\ 0010 \\ 0001 \end{bmatrix} \cdot \begin{bmatrix} X1 \\ X2 \\ X3 \\ X4 \end{bmatrix} = \begin{bmatrix} 1.038 \\ 0.209 \\ 0.226 \\ 0.847 \end{bmatrix} \quad \text{--(16)}$$

Unfortunately, this is not the only satisfactory form of answer. There are 24 arrangements which are equally satisfactory. One of them is :

$$\begin{array}{rcl} & 1X4 & = 0.847 \\ & 1X2 & = 0.209 \\ 1X1 & & = 1.038 \\ & 1X3 & = 0.226 \end{array}$$

and in Matrix form :

$$\begin{bmatrix} 0001 \\ 0100 \\ 1000 \\ 0010 \end{bmatrix} \cdot \begin{bmatrix} X1 \\ X2 \\ X3 \\ X4 \end{bmatrix} = \begin{bmatrix} 0.847 \\ 0.209 \\ 1.038 \\ 0.226 \end{bmatrix} \quad \text{--(17)}$$

The Optimized Procedure is to choose ,as pivot in each column, the coefficient with maximum absolute value, subject to the condition that there is only one pivot in each row and column. The purpose is to minimize maximum relative error.

From example 1, the augmented matrix :

$$\left[ \begin{array}{cccc|c} 2.630 & 5.210 & -1.694 & 0.938 & 4.230 \\ 3.160 & -2.950 & 0.813 & -4.210 & -0.716 \\ 5.360 & 1.880 & -2.150 & -4.950 & 1.280 \\ 1.340 & 2.980 & -0.432 & -1.768 & 0.419 \end{array} \right]$$

In the first column  $a_{31}$  (i.e. 5.360) is the largest number, so it is chosen as the pivot and that row is divided by  $a_{31}$ , 5.360 ; and it becomes

$$\left[ \begin{array}{cccc|c} 2.630 & 5.210 & -1.694 & 0.938 & 4.230 \\ 3.160 & -2.950 & 0.813 & -4.210 & -0.716 \\ [1] & 0.35075 & -0.40112 & -0.92351 & 0.23881 \\ 1.340 & 2.980 & -0.432 & -1.768 & 0.419 \end{array} \right]$$

In order to make the a11 position 0, the pivot row is first multiplied by -2.630 (i.e. - a11 value) then added to row 1 to obtain :

$$\left[ \begin{array}{cccc|c} 0 & 4.28753 & -0.63906 & 3.36682 & 3.60194 \\ 3.160 & -2.950 & 0.813 & -4.210 & -0.716 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{array} \right]$$

In general, if an augmented matrix is

$$\begin{array}{cccc} 2.630 & \dots\dots\dots & 0.938 & \\ \cdot & & \cdot & \\ \cdot & & \cdot & \\ \cdot & & \cdot & \\ 5.360 & \dots\dots\dots & -4.950 & \end{array}$$

then the pivot row is first divided by 5.360 (the largest number in column 1) to obtain

$$\begin{array}{cccc} 2.630 & \dots\dots\dots & 0.938 & \\ \cdot & & \cdot & \\ \cdot & & \cdot & \\ \cdot & & \cdot & \\ [1] & \dots\dots\dots & -4.950/5.360 & \end{array}$$

In order to make the position a11 zero, the pivot row is multiplied by -2.630 (i.e. negative value of a11) to form a dummy:

$$\begin{array}{cccc} 2.630 & \dots\dots\dots & 0.938 & \\ \cdot & & \cdot & \\ \cdot & & \cdot & \\ \cdot & & \cdot & \\ -2.630 & \dots\dots\dots & (-4.950 * -4.950)/5.360 & \end{array}$$

Then it is added to the first row to obtain the new row 1,

$$0 \dots\dots 0.938 + (-2.630)(-4.950)/5.360$$

Hence, if it starts with a square

$$\begin{array}{r} a(i,q) \dots\dots\dots a(i,j) \\ \cdot \qquad \qquad \qquad \cdot \\ \cdot \qquad \qquad \qquad \cdot \\ \cdot \qquad \qquad \qquad \cdot \\ a(p,q) \dots\dots\dots a(p,j) \end{array}$$

where  $p$  is the pivot row and  $q$  of the pivot column, then  $a(i,q)$  becomes 0 (requiring no computation), and the new  $a(i,j)$  is obtained by

$$a(i,j) = a(i,j) - a(p,j)*a(i,q)/a(p,q)$$

By following this procedure, the solution is:

$$\left[ \begin{array}{l} 0100 : 0.20890 \\ 0010 : 0.22636 \\ 1000 : 1.03835 \\ 0001 : 0.84678 \end{array} \right]$$

which means

$$\left[ \begin{array}{l} 0100 \\ 0010 \\ 1000 \\ 0001 \end{array} \right] \cdot \left[ \begin{array}{l} X1 \\ X2 \\ X3 \\ X4 \end{array} \right] = \left[ \begin{array}{l} 0.20890 \\ 0.22636 \\ 1.03835 \\ 0.84678 \end{array} \right]$$

and  $X1 = 1.03835$ ,  $X2 = 0.20890$ ,  $X3 = 0.22636$ ,  $X4 = 0.84678$

However, unlike the above example, the coefficients and constants of linear simultaneous equations are positive. The linear simultaneous equations are derived from the general mixture equation (5). Therefore, when any of the  $X$ 's values exceed the range :

$$0.0 < X < 1.0$$

this set of solution is ignored and another set of linear simultaneous equations is chosen as in the case of Cramer's Rule method.

The third component fraction (X3) can be determined by substituting X1 and X2 into equation (3).

#### 2.2.2.1 Seidel Iteration (Dodes, 1978)

If the above calculated X's values are substituted in the original equations, a new constant vector can be calculated as follows:

$$A \cdot \begin{bmatrix} 1.03835 \\ 0.20890 \\ 0.22636 \\ 0.84678 \end{bmatrix} = \begin{bmatrix} 4.230055 \\ -0.715982 \\ 1.280053 \\ 0.419016 \end{bmatrix} \quad \{\text{constant vector}\}$$

The calculated constant vector is different from the original constant vector. Obviously, the precision of the results is not known. Nevertheless, by using Seidel Iteration, precision of the results can be improved tremendously even though the starting X's values are quite far out. The original X's value are substituted back into the original equation first as above. The difference between calculated and actual constant is used as the new constant vector and is substituted back into the original equation to obtain the next X's value. After this first iteration, the improved X's values will be the original X's value plus the calculated second X's values. The improved X's values now have become the original X's values and more iterations can be performed until the difference between actual and calculated constants is small; for example  $10^{**}(-7)$ .

Example:

Let  $X_1(0) = 1.035$  instead of 1.03835  
 $X_2(0) = 0.209$  instead of 0.20890  
 $X_3(0) = 0.227$  instead of 0.22636  
 $X_4(0) = 0.846$  instead of 0.84678

Substitute original X's values into original equations to obtain calculated constant.

$$\begin{bmatrix} 2.630 & 5.210 & -1.694 & 0.938 \\ 3.160 & -2.950 & 0.813 & -4.210 \\ 5.360 & 1.880 & -2.150 & -4.950 \\ 1.340 & 2.980 & -0.432 & -1.768 \end{bmatrix} \cdot \begin{bmatrix} 1.035 \\ 0.209 \\ 0.227 \\ 0.846 \end{bmatrix} = \begin{bmatrix} 4.219950 \\ -0.723059 \\ 1.264770 \\ 0.415928 \end{bmatrix}$$

$$\text{i.e. } A \cdot X(0) = C(0)$$

The original problem was ;

$$A \cdot \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} = \begin{bmatrix} -4.230 \\ -0.716 \\ 1.280 \\ 0.419 \end{bmatrix} \quad \{\text{constant vector}\}$$

$$\text{i.e. } A \cdot X = C$$

Let  $E(1)$  be the first error in X

$$X - X(0) = E(1)$$

By Subtraction,

$$C - C(0) = \begin{bmatrix} 0.010050 \\ 0.007059 \\ 0.015230 \\ 0.003072 \end{bmatrix}$$

Using these values as new constants and substituting them into original equations to obtain

$$A \cdot \begin{bmatrix} E1(1) \\ E2(1) \\ E3(1) \\ E4(1) \end{bmatrix} = \begin{bmatrix} 0.010050 \\ 0.007059 \\ 0.015230 \\ 0.003072 \end{bmatrix}$$

Solving by Gauss-Jordan Method, it becomes

$$E1(1) = X1 - X1(0) = +0.003335733$$

$$E2(1) = X2 - X2(0) = -0.000102296$$

$$E3(1) = X3 - X3(0) = -0.000641211$$

$$E4(1) = X4 - X4(0) = +0.000774913$$

and solve for X to obtain new estimate, X(1)

$$X1(1) = X1(0) + E1(1) = 1.038336$$

$$X2(1) = X2(0) + E2(1) = 0.208898$$

$$X3(1) = X3(0) + E3(1) = 0.226359$$

$$X4(1) = X4(0) + E4(1) = 0.846775$$

The size of E(1) gives an estimation of the error.

If the process is repeated once more

$$A \cdot \begin{bmatrix} 1.038336 \\ 0.208898 \\ 0.226359 \\ 0.846775 \end{bmatrix} = \begin{bmatrix} 4.230005064 \\ -0.716000223 \\ 1.280001100 \\ 0.419000992 \end{bmatrix}$$

$$A \cdot \begin{bmatrix} E1(2) \\ E2(2) \\ E3(2) \\ E4(2) \end{bmatrix} = \begin{bmatrix} -0.000005064 \\ 0.000000223 \\ -0.000000100 \\ -0.000000992 \end{bmatrix}$$

Solving by Gauss-Jordan Method, it becomes

$$E1(2) = -0.0000014384$$

$$E2(2) = -0.0000004473$$

$$E3(2) = -0.0000011692$$

$$E4(2) = -0.0000009973$$

which are the errors in X(1).

They are added to obtain

$$\begin{aligned} X1(2) &= 1.038335 \\ X2(2) &= 0.208898 \\ X3(2) &= 0.226358 \\ X4(2) &= 0.846774 \end{aligned}$$

By substituting X(2) values in the original equation, it becomes:

$$A \cdot \begin{bmatrix} 1.038335 \\ 0.208898 \\ 0.226358 \\ 0.846774 \end{bmatrix} = \begin{bmatrix} 4.229999999999996 \\ -0.7160000000000005 \\ 1.279999999999995 \\ 0.418999999999996 \end{bmatrix}$$

The constant vector is almost the same as the original constant vector which implies that the X(2) values are good estimates of the true value.

The F77 computer programs using the Gauss-Jordan Elimination Method were GLC1, GLC2, GLC3, GLC4, and FREQC. Their results will be analysed in Chapter 5.

### 2.2.3 Least Squares Method (Scarborough, 1958)

To solve a two-unknown equation, normally two simultaneous equations are required and they can be solved simply by substitution. However, when there are more than two equations available, the results obtained from solving any two of the simultaneous equations will not represent the actual system. The problem however can be overcome by using Least Squares Method which reduces all the equations to two normal equations in the case of two-unknown equations.

The principle behind this method is that the best representative curve is the one which makes the sum of squares of the residuals a minimum. This insures that the numerical values of the residuals will be small; which implies in the case of a series of plotted points, that the best representative curve will pass as closely as possible to all the points.

In the three-fat/oil mixture analysis, there are about twenty three-unknown equations. For simplicity, four two-unknown equations are used to demonstrate the Least Squares Method (Refer to Scarborough (1958) for detailed derivation.).

Say, four equations are

$$5X_1 + 2X_2 = 10$$

$$3X_1 + 7X_2 = 12$$

$$1X_1 + 4X_2 = 7$$

$$2X_1 + 3X_2 = 5$$

Residuals equations are

$$R_1 = 5X_1 + 2X_2 - 10$$

$$R_2 = 3X_1 + 7X_2 - 12$$

$$R_3 = 1X_1 + 4X_2 - 7$$

$$R_4 = 2X_1 + 3X_2 - 5$$

To obtain the first normal equation, each equation is multiplied by its  $X_1$  constant; then the constants of each column are summed :

$$25 X_1 + 10 X_2 - 50$$

$$9 X_1 + 21 X_2 - 36$$

$$1 X_1 + 4 X_2 - 7$$

$$(+ ) 4 X_1 + 6 X_2 - 10$$

---


$$39 X_1 + 41 X_2 - 103$$

By equating their sum to zero, the first normal equation is

$$39 X_1 + 41 X_2 - 103 = 0$$

Similarly, to obtain the second normal equation, each equation is first multiplied by its  $X_2$  constant then followed by the above procedure to acquire:

$$41 X_1 + 78 X_2 - 147 = 0$$

Hence, normal equations are:

$$39 X_1 + 41 X_2 = 103$$

$$41 X_1 + 78 X_2 = 147$$

The normal equations can be solved by using Gauss-Jordan Elimination Method; or by Cramer's Rule Method; or simply by substitution:

$$X_1 = (103 - 41 X_2)/39$$

substitute  $X_1$  into the second normal equation, it becomes

$$41(103 - 41 X_2) + 78 X_2 = 147$$

---


$$39$$

$$108.3 - 43.1 X_2 + 78 X_2 = 147$$

$$34.9 X_2 = 38.7$$

$$X_2 = 1.11$$

substituting  $X_2$  into one of the normal equations, it becomes

$$X_1 = \frac{103 - 41 * 1.11}{39}$$

$$= 1.47$$

For calculation of standard errors, refer to 'Using Residuals To Calculate Standard Errors'.

The F77 computer program using the Least Squares Method was named LSQ. Its results will be analysed in Chapter 5.

#### 2.2.4 Frequency Method (Topping, 1955)

This method uses frequency as a means of weighting the results when weighted mean is determined, instead of using standard deviations of average fatty acid values.

As mentioned before, there are more than two fatty acids in fat(s) and oil(s); by choosing two or three mixture equations at a time and employing either Cramer's Rule method or Gauss-Jordan Elimination method, there will be more than one set of calculated fat(s) and oil(s) estimates.

By first deciding the class width, the number of calculated fat(s) and oil(s) estimates in each class (i.e. frequency) can be determined. The weighted mean percent of each fat and oil in the mixture, using frequency as weights, can be calculated.

Let  $f_1, f_2, f_3, \dots, f_n$  be the frequencies in the various classes and  $M_1, M_2, M_3, \dots, M_n$  be the mid-values of each class. The mean value of fat or oil is given by:

$$(f_1M_1 + f_2M_2 + f_3M_3 + \dots + f_nM_n)/(f_1 + f_2 + \dots + f_n)$$

which is the weighted mean of  $M_1, M_2, M_3, \dots, M_n$  and the weights being the frequencies of the corresponding classes.

Example:

Assuming the following are fat 1 data:

Class	Frequency
0.0 - 0.099	2
0.1 - 0.199	5
0.2 - 0.299	6
0.3 - 0.399	14
0.4 - 0.499	22
0.5 - 0.599	32
0.6 - 0.699	25
0.7 - 0.799	10
0.8 - 0.899	2
0.9 - 0.999	2

and mid-value of each class is as follows :

$$M_1 = 0.045$$

$$M_2 = 0.145$$

$$M_3 = 0.245$$

$$M_4 = 0.345$$

$$M_5 = 0.445$$

$$M_6 = 0.545$$

$$M_7 = 0.645$$

$$M_8 = 0.745$$

$$M_9 = 0.845$$

$$M_{10} = 0.945$$

The mean value of fat 1 is therefore

$$\begin{aligned}
 &= (0.045 \cdot 2 + 0.145 \cdot 5 + 0.245 \cdot 6 + 0.345 \cdot 14 + 0.445 \cdot 22 + \\
 &\quad 0.545 \cdot 32 + 0.645 \cdot 25 + 0.745 \cdot 10 + 0.845 \cdot 2 + \\
 &\quad 0.945 \cdot 2) / (2 + 5 + 6 + 14 + 22 + 32 + 25 + 10 + 2 + 2) \\
 &= 61.5 / 120
 \end{aligned}$$

= 0.5125

That is, calculated fat 1 mean value indicated that 51.25 % of the fat(s)/oil(s) mixture was made up of fat 1.

By following the above procedure other fat or oil percentage in the mixture can also be calculated.

Standard error of calculated mean fat and oil (%) can be calculated either by Residuals method (refer to 'Using Residuals To Calculate Standard Errors') or simply by standard deviation formula.

The F77 computer program using the FREQC Method was named FREQC; and its results will be analysed in Chapter 5.

Prime Computer provides F77 'Least Squares Problem Solving' subroutines but no detailed information is available and no copy of the subroutines can be listed from the Prime Computer for reference or alteration.

### 2.3 Error Calculation And Error Propagation

There are number of ways to propagate errors or weights in arithmetic operations for final weighted mean calculation. They are the following:

#### 2.3.1 Maximum Error Method (Ribbons, 1969)

Let  $x = a \pm a'$  and  $y = b \pm b'$

where  $a$  and  $b$  are actual values; and  $a'$  and  $b'$  are errors in measurement.

For:

(a) Addition

$$\begin{aligned}x + y &= (a \pm a') + (b \pm b') \\ &= a + b \pm [a' + b']\end{aligned}$$

where x and y are the observed values.

(b) Subtraction

$$\begin{aligned}x - y &= (a \pm a') - (b \pm b') \\ &= a - b \pm [a' + b']\end{aligned}$$

(c) Multiplication

As a' and b' has both + - sign, + sign is chosen for maximum error.

$$\begin{aligned}x * y &= (a + a') (b + b') \\ &= ab + ab' + a'y + a'b'\end{aligned}$$

If a' and b' are small, then a'b' tends to zero.  
Therefore,

$$x * y = ab \pm [ab' + a'b]$$

(d) Division

For maximum error calculation:

$$x/y = (a+a')/(b+b') = (a+a')(b-b')/(b+b')(b-b')$$

$$\begin{aligned}&= \frac{ab - ab' + a'b - a'b'}{a^2 - b'^2}\end{aligned}$$

if a' and b' are small, then a'b' and b'<sup>2</sup>  
(i.e. b' to the power of 2 or b' square) tends to zero.

Therefore,

$$\frac{x}{y} = \frac{ab - ab' + a'b}{b} = \frac{a}{b} +/\- \left[ \frac{a'b - ab'}{b} \right]$$

### 2.3.2 Norris Method (Norris, 1981)

The general equations for Error Propagation is

$$V(z) = (z'x)^2 V(x) + (z'y)^2 V(y) + 2z'x z'y C(x,y)$$

or in the equivalent notation

$$S_z = \left( \frac{\partial z}{\partial x} \right)_m^2 S_x + \left( \frac{\partial z}{\partial y} \right)_m^2 S_y + 2 \left( \frac{\partial z}{\partial x} \right)_m \left( \frac{\partial z}{\partial y} \right)_m S_{xy}$$

for  $z = z(x,y)$ .

where

$$V(z) \text{ and } S_z \text{ are variance of } z$$

$$z'x \text{ is the differential of } z \text{ with respect to } x.$$

If  $x$  and  $y$  are independent then the equations simplify to

$$V(z) = (z'x)^2 V(x) + (z'y)^2 V(y) \quad ; \text{ or}$$

$$S_z = \left( \frac{\partial z}{\partial x} \right)_m^2 S_x + \left( \frac{\partial z}{\partial y} \right)_m^2 S_y$$

In our analysis of fat(s)/oil(s) mixture, the equation required is the latter simplified form.

(For detailed derivation, refer to "Computational Chemistry - An Introduction to Numerical Methods", p52 - 53, A.C.Norris)

For:

(a) Proportionality

(i) If  $z = +/- ax$

$$z' = +/- a$$

$$S_z = a S_x$$

(ii) if  $z = +/- a/x$

$$S_z = a S_x/x$$

(b) Power

$$\text{If } z = ax^{+/-b}$$

$$\text{then } z' = +/- abx^{+/(b-1)} = +/- bz/x$$

and the propagation equation is

$$S_z = b z S_x /x$$

(c) Exponents

$$\text{If } z = ae^{+/-bx}$$

$$\text{then } z' = +/- abe^{+/-bx} = +/- bz$$

Thus,

$$S_z = b z S_x$$

(d) Addition and Subtraction

Let  $z = ax \pm by$  then,

$$z'_x = a, z'_y = \pm b \text{ and}$$

$$S_z = a S_x + b S_y$$

(e) Multiplication and Division

Let  $z = \pm axy$  then

$$z'_x = \pm ay, z'_y = \pm ax \text{ and}$$

$$S_z = a y S_x + a x S_y$$

The simpler relative error form can be used :

$$E_z = E_x + E_y$$

$$\text{i.e. } (S_z/z)^2 = (S_x/x)^2 + (S_y/y)^2$$

If  $z = \pm ax/y$  then

$$S_z = a S_x/y + a x S_y/y$$

and the simpler relative error form is as above.

## 2.3.3 Scarborough Method (Scarborough, 1958)

When using Cramer's Rule to solve simultaneous linear equations, standard errors associated with the calculated fat percent values can be determined as follows:

Say, the simultaneous equations are

$$\begin{array}{r} a_1 X_1 + b_1 X_2 = c_1 \\ a_2 X_1 + b_2 X_2 = c_2 \end{array} \quad ] \quad \text{----- (1)}$$

Let exact values of constants ( $a_1, a_2, b_1, b_2, c_1$ , and  $c_2$ ) be  $a_1+a_1', b_1+b_1'$ , and etc; and the corresponding true values of  $X_1$  and  $X_2$  be  $X_1+X_1'$  and  $X_2+X_2'$ . It becomes

$$\begin{array}{r} (a_1+a_1')(X_1+X_1')+(b_1+b_1')(X_2+X_2') = c_1+c_1' \\ (a_2+a_2')(X_1+X_1')+(b_2+b_2')(X_2+X_2') = c_2+c_2' \end{array} \quad ] \quad \text{----- (2)}$$

where  $a_1', b_1', c_1', a_2', b_2'$  and  $c_2'$  are the errors associated with the coefficients and constants of the simultaneous equations; and  $X_1'$  and  $X_2'$  are the errors associated with the estimated  $X_1$  and  $X_2$  values.

If errors are small, then all those terms involving the products of two errors will tend to zero and are dropped. By making use of (1) it becomes

$$\begin{array}{r} a_1 X_1' + X_1 a_1' + b_1 X_2' + X_2 b_1' = c_1' \\ a_2 X_1' + X_1 a_2' + b_2 X_2' + X_2 b_2' = c_2' \end{array} \quad ] \quad \text{----- (3)}$$

Since the standard errors ( $a_1', a_2', b_1', b_2', c_1'$ , and  $c_2'$ ) can be obtained from experiment or calculation, and  $X_1$  and  $X_2$  can be found from (1), hence the unknowns are  $X_1'$  and  $X_2'$ . By re-arranging the equations, it becomes:

$$\begin{aligned} a_1X_1' + b_1X_2' &= c_1' - (X_1a_1' + X_2b_1') & ] \\ & & ] \text{----- (4)} \\ a_2X_1' + b_2X_2' &= c_2' - (X_1a_2' + X_2b_2') & ] \end{aligned}$$

As errors have both + and - sign, by changing the - sign to + sign, it becomes

$$\begin{aligned} a_1X_1' + b_1X_2' &= k_1 & ] \\ & & ] \text{----- (5)} \\ a_2X_1' + b_2X_2' &= k_2 & ] \end{aligned}$$

where

$$k_1 = c_1' + (X_1a_1' + X_2b_1') \quad ; \text{and}$$

$$k_2 = c_2' + (X_1a_2' + X_2b_2')$$

It is obvious that the system (5) is similar to that of (1). Hence, Cramer's Rule can be used to solve for  $X_1'$  and  $X_2'$ .

$$X_1' = \frac{k_1b_2 - k_2b_1}{a_1b_2 - a_2b_1}$$

$$X_2' = \frac{k_2a_1 - k_1a_2}{a_1b_2 - a_2b_1}$$

Since there are more than one two-linear equation combinations, one will expect to have more than one  $X_1$ ,  $X_2$ ,  $X_1'$ , and  $X_2'$  values. Weighted mean therefore can be calculated (Refer to 'Calculation of Weighted Mean and Weighted Mean Standard Error').

### 2.3.4 Discussion

All the three methods were tested together with Cramer's Rule method (McCracken and Dorn, 1964; Dickson, 1968; and McCalla, 1967) and Gauss-Jordan Elimination method (Dodges, 1978); and the results showed that Maximum Error method (Ribbans, 1969) and Scarborough method (Scarborough, 1958) tended to either underestimate or overestimate the errors, while the Norris method (Norris, 1981) gave a reasonable good error estimation.

## 2.4 Weighted Mean And Arithmetic Mean

### 2.4.1 Weighted Mean and Weighted Mean Standard Error Calculation

(Scarborough, 1958; and Topping, 1955)

#### 2.4.1.1 Weighted Mean

Let  $X(1), X(2), \dots, X(n)$  be the calculated or measured fat 1 values and  $E(1), E(2), \dots, E(n)$  be their propagated standard errors (refer to the 'Error Calculation and Error Propagation').

Then,

Weighted Mean Fat 1 value

$$X' = \frac{X(1)/(E(1))^2 + X(2)/(E(2))^2 + \dots + X(n)/(E(n))^2}{1/(E(1))^2 + 1/(E(2))^2 + \dots + 1/(E(n))^2}$$

## 2.4.1.2 Weighted Mean Standard Error

There are two ways of calculating the weighted mean standard error:

(a) Equation one

$$E_e = \sqrt{\frac{1}{\left( \frac{1}{E(1)^2} + \frac{1}{E(2)^2} + \dots + \frac{1}{E(n)^2} \right)}}$$

(b) Equation two

$$E_i = \sqrt{\frac{\left( \sum \left( \frac{(X(I) - X')^2}{E(I)^2} \right) \right)}{(n-1) \left( \sum \left( \frac{1}{E(I)^2} \right) \right)}}$$

where  $X(i)$  is the calculated or observed values.

$X'$  is the weighted mean percent value.

$I = 1$  to  $n$

$n$  is number of measurements or observations or estimates.

Comment:

Equation one relies entirely on the standard errors of the separate observations, whereas Equation two depends also on the differences between the observations. Equation two is therefore a function of the 'external' consistency of the observations, whereas the Equation one relies on the 'internal' consistency. If samples are collected from an infinite normal population, then  $E_e$  and  $E_i$  may be equal, or the ratio  $E_e/E_i$  is unity with standard error:

$$1 / \sqrt{[2(n-1)]}$$

Therefore,

$$Z = \frac{E_e}{E_i} = \frac{\sqrt{\sum \frac{(X(I) - X')^2}{E(I)^2}}}{(n-1)}$$

where  $I = 1$  to  $n$

$n$  is number of observations or measurements or estimates.

$X'$  is the weighted mean percent value.

$X(I)$  are the calculated or measured percent values.

In practice  $Z$  does not equal unity for it relies on the values of  $E(I)$ , some or all of which may be considerably inaccurate especially if they have been determined from few observations. Moreover,  $Z$  depends also on the  $(X(I) - X')^2$  values and thus will be affected by any systematic errors present.

Nevertheless, if  $Z$  is found not to differ from unity significantly, bearing in mind the uncertainties in the standard errors used, then the observations as a whole may be considered as consistent. In such a situation, the larger of the values of  $E_e$  and  $E_i$  is chosen as the standard error of weighted mean.

If  $Z$  differs significantly from unity, then systematic errors are likely to be present. In such a case, the weights based on the standard errors should be discarded and replaced by others. The decision of assigning new weights depends inevitably upon the experience and judgment of individual concerned.

#### (c) Residual Method

(Using residuals to calculate standard errors)

As mentioned above, when  $E_e$  and  $E_i$  differ significantly, the accuracy of the calculated standard errors become questionable. However, there is another way of calculating standard errors by using the residuals.

Let

$$a_1X_1 + b_1X_2 = c_1$$

$$a_2X_1 + b_2X_2 = c_2$$

After solving the simultaneous equations either by Cramer's Rule or Gauss-Jordan Elimination Method, the  $X_1$  and  $X_2$  values are then substituted back into the equations.

$$a_1A + b_1B = cc_1$$

$$a_2A + b_2B = cc_2$$

where  $A$  and  $B$  are calculated  $X_1$  and  $X_2$  values.

By taking the difference between the calculated constant vector( $cc$ ) and the actual constant vector( $c$ ), the residual equations are:

$$R_1 = cc_1 - c_1$$

$$R_2 = cc_2 - c_2$$

where  $R_1$  and  $R_2$  are the residuals.

Standard errors can then be determined :

$$AE(1) = R_1/c_1$$

$$AE(2) = R_2/c_2$$

where  $AE(1)$  and  $AE(2)$  are the relative errors of  $c$  vector which depends very much upon the accuracy of  $X_1$  and  $X_2$  values.

By borrowing the standard deviation concept, the overall standard deviation (OSD) is calculated as follows:

$$OSD = \sqrt{(AE(1)**2 + AE(2)**2)/(N-1)}$$

where N is number of normal equations.

From above, the residuals equations are:

$$R1 = (a1A + b1B) - c1$$

$$R2 = (a2A + b2B) - c2$$

Since a1,b1,c1,a2,b2,and c2 are constants, then R1 and R2; and consequently OSD are dependent on the calculated X1 and X2 values (i.e. A and B). Therefore by multiplying the calculated X(1) and X(2) values(which can either be weighted mean or arithmetic mean)by OSD, the standard errors of X(1) and X(2) can be obtained:

$$SE(I) = X(I) * OSD$$

where

X(I) are weighted mean or arithmetic mean fat/oil percent values.

SE(I) are standard errors of calculated fat/oil percent values.

I = 1 to number of fat/oil in the fat/oil mixture.

OSD is the Overall Standard Deviation.

Hence, the solutions are

$$X(I) \pm SE(I) \quad \text{where } I = 1,2$$

or

$$X(1) \pm SE(1) \quad \text{and}$$

$$X(2) \pm SE(2)$$

With the exception of CHU2, FREQC and LSQ, all of the F77 computer programs written had made use of Equation one and Equation two in calculating weighted mean standard error. The accuracy of the two methods will be determined in Chapter 5.

Residual Method was tested in the LSQ F77 computer program and the results showed that it provided a reasonably accurate estimation of error when experimental data were involved. Nevertheless, when literature data were involved, in most cases, the LSQ program failed to provide any solution. Therefore, the determination of the accuracy of Residual method was not possible when literature data were involved.

However, when all the three methods fail, one should use standard deviation to estimate the errors associated with the calculated weighted mean proportions of mixture components.

#### 2.5 Calculation of Arithmetic Mean and Probable Error.

(Scarborough, 1958)

Weighted mean becomes arithmetic mean when the weights or standard errors of different measurements or observations are equal; and thus a value of 1.0 replaces all the weights or standard error values.

$$\begin{aligned}
 X' &= \frac{X(1)/1 + X(2)/1 + \dots + X(n)/1}{n(1/1)} \\
 &= \frac{X(1) + X(2) + \dots + X(n)}{n}
 \end{aligned}$$

(which is the arithmetic mean)

For the probable error of arithmetic mean

$$P.E. = 0.6745 * \sqrt{\frac{\sum (X(I) - X')^2}{n(n-1)}}$$

where I = 1 to n

n is number of observations or measurements or estimates.

X(I) are the calculated or measured percent values.

X' is the arithmetic mean.

## 2.6 Standard Deviation (SD) of Weighted Mean and Arithmetic Mean.

Standard deviation can be calculated using the following formula:

$$SD = \sqrt{\frac{\sum (X(I) - X')^2}{(n-1)}}$$

where X(I) are the measured or observed percent values.

X' is either weighted mean or arithmetic mean percent value.

I = 1 to n

n is number of measurements or observations or estimates.

## 2.7 Comparison With The Actual Fat/Oil Percent Values In The Mixtures

(Hinchen, 1969)

After calculating weighted mean or arithmetic mean fat/oil percent values, the significant difference between calculated and actual fat/oil percent values in the mixture can be determined by the following procedures:

- 1) Calculate the weighted mean or arithmetic mean of fat/oil percent values.
- 2) Calculate the standard deviation of the weighted mean or arithmetic mean.

$$SD = \sqrt{\frac{\sum (X(I) - X')^2}{(n-1)}}$$

where

$X(I)$  are the observed or calculated fat percent values.

$X'$  is the weighted mean or arithmetic mean fat/oil percent value.

$I = 1$  to  $n$

$n$  is number of measurements or observations or estimates.

- 3) Calculate the Student's  $t$

$$t = \frac{X_a - X'}{SD/n}$$

where

$X_a$  is the actual fat/oil percent value in the mixture.

$X'$  is the weighted mean or arithmetic mean fat/oil percent value.

$SD$  is the standard deviation.

$n$  is number of observations or measurements or calculated fat/oil percent values.

- 4) Select the probability ( $P'$ ) level or percent of risk that one is willing to take (e.g. 5%).
- 5) Compare the calculated  $t$  value(s) with that of  $t$ -table for  $(n-1)$  degrees of freedom and the probability level selected (i.e. 5%). If calculated  $t$  value is greater than the  $t$ -table value, then the difference is significant.

- 6) Estimate the confidence limits of weighted mean or arithmetic mean, based on n observations or measurements. For 95% confidence limits, use the t(0.975) critical value for (n-1) degrees of freedom.

$$X' \pm tSD/\sqrt{n}$$

where

X' is the weighted mean or arithmetic mean fat/oil percent value.

t is the t - table value.

n is number of measurements or observations or calculated fat/oil percent values.

SD is standard deviation of either weighted mean or arithmetic mean fat/oil percent value.

However, in the practical situation it is not always possible to have the knowledge of actual mixture component proportions. Therefore its use is limited.

## **chapter 3**

### 3 GAS CHROMATOGRAPHY

#### 3.1 Introduction

Chromatography is the separation of chemical species by virtue of their different characteristics of distribution between mobile and stationary phases. Besides Gas Chromatography (mobile phase is a gas), there is liquid chromatography (mobile phase is a liquid).

In gas chromatography, the flow of the mobile phase through the stationary phase induces the separation of chemical species by differential migration. The stationary phase can either be a porous, sorptive solid (gas-solid chromatography) or an involatile liquid which is held in place on an inert solid support (gas-liquid chromatography).

The Gas Chromatography equipment consists of a source of carrier gas, (supplied from a pressurised tank or cylinder which can be argon, helium, hydrogen or nitrogen), an injection port (which provides a means of introducing the sample into the carrier gas by a hypodermic syringe through a rubber septum of the heated injection port), a packed column (about 1 to 3 meters in length and has an internal diameter of 2mm.), a detector and a recorder.

The injection port, column and detector are contained in a thermostatically controlled oven. The gas carries a sample from the injection port through the packed column where the sample is separated into its constituents. On leaving the column, the gas carries with it at different times the separated constituents of the sample which can be detected by a hydrogen flame ionization detector and subsequently recorded in a graphical ionization form (Chromatogram) by a recorder. The proportion of each fatty acid is determined by the areas under the curve.

### 3.2 Sampling and Storage Condition Of Fats and Oils

Milkfat and tallow were provided by Kiwi Bacon Co., Palmerston North while coconut oil, maize oil, cotton seed oil and sunflower oil were provided by Abels Limited, Auckland.

Milkfat and Tallow were placed in beakers and heated in the 40 degrees centigrade oven until all were in liquid form, while the rest in close-lid cans were warmed on a steam bath (making sure that no small solid particles remained in the liquid).

During heating or warming of fats and oils, the temperature should be noted to prevent over-heating as follows (Cock and Rede, 1966):

Coconut oil maximum temperature	42 degrees C
Cotton seed oil maximum temperature	25 degrees C
Soya bean oil maximum temperature	25 degrees C
Sunflower oil maximum temperature	20 degrees C
Tallow and milkfat maximum temperature	58 degrees C
Maize oil maximum temperature	25 degrees C

The fats and oils were first stirred by a glass rod and then poured into several labelled, teflon-lined, screw-cap test tubes with the help of a warm funnel. All teflon-lined screw-cap test tubes were then stored under low temperature (-10 degrees centigrade) until required. A test tube of each fat and oil were stored in a refrigerator and they were used first. After one to two weeks of storage in the refrigerator, they were discarded and a new set of samples (a test tube of each fat and oil) was transferred from cold store to the refrigerator.

### 3.3 Components And Mixtures Code

For simplicity, the following codes were used to represent the components of mixture:

MK - MILKFAT  
TL - TALLOW  
SF - SUNFLOWER OIL  
CCN - COCONUT OIL  
SB - SOYA BEAN OIL  
CS - COTTON SEED OIL  
MZ - MAIZE OIL

The mixture code for the Milkfat, Tallow and Cotton Seed Oil mixture was therefore MKTLCs. When methyl esters of mixture and its components were prepared by the A.O.C.S. Method Ce2-66, a 0 was then placed in front of the mixture code (e.g. OMKTLMZ); otherwise they were prepared by the Chrispherson and Glass Method (1969). All those mixtures treated by the correcting factors- "Weight Response Factors" were coded with a C in front of their usual mixture code (e.g. CMKTLMZ).

### 3.4 Preparation Of Mixtures.

Fat(s) and oil(s), stored in teflon-lined screw-cap test tubes, were warmed in a (40 - 60 degrees C) oven before use; making sure that no "solid particle" was observable. A glass-stopper test tube was first weighed in a beaker on a weighing machine. The first component of the mixture was transferred with care to the test tube with a warm glass dropper. The overall weight was noted. The Second component of the mixture was added in the same manner and weighed. Likewise, the third component was added and weighed.

The percent of each component in the mixture was calculated as below:

Weight of third component, W1

$$= (\text{weight of three components plus the weight of test tube and beaker}) - (\text{weight of first and second components plus the weight of test tube and beaker})$$

Weight of second component, W2

$$= (\text{weight of first and second component plus the weight of test tube and beaker}) - (\text{weight of first component plus the weight of test tube and beaker}).$$

Weight of first component, W3

$$= (\text{weight of first component plus the weight of test tube and beaker}) - (\text{weight of test tube and beaker}).$$

Percent of first component in the mixture

$$= \frac{W3}{W1 + W2 + W3} * 100\%$$

Percent of second component in the mixture

$$= \frac{W2}{W1 + W2 + W3} * 100\%$$

Percent of third component in the mixture

$$= \frac{W1}{W1 + W2 + W3} * 100\%$$

The methyl esters of the fatty acids of the mixture were then prepared either by modified version of A.O.C.S. Method Ce 2-66 or by Christopherson and Glass Method (1969).

### 3.5 Analysis of Fatty Acid

The Fatty Acid composition of fats and oils were determined by preparing methyl esters of them, using either method A or method B, and analysing these esters by gas-liquid chromatography.

#### 3.5.1 Preparation of Methyl Esters

##### 3.5.1.1 Method A (Adapted from A.O.C.S. Method Ce 2-66)

A 0.2 ml sample of fat or oil or mixture was transferred from screw-cap test tube to a 50 ml round bottomed flask. Then 4 ml of 0.5M methanolic sodium hydroxide and a boiling chip were added. A condenser was attached and a steam bath was used to heat the mixture until the fat globules go into solution (about 10 minutes). 5 ml of boron trifluoride-methanol reagent (14% boron trifluoride in methanol) was added through the condenser and boiled for 2 minutes. 5 ml of distilled petroleum ether (bp 30-45 degrees C) was added in the same manner and boiled for a further minute. The condenser was removed with the round-bottomed flask from the steam bath. The condenser was disconnected from the flask and sufficient water was added to float the solution of petroleum ether and fatty acid methyl esters into the neck of the flask. About 2 ml of this solution was transferred to a glass-stopper test tube.

##### 3.5.1.1.1 Analysis of fatty acid methyl esters

One to three ul of fatty acid methyl esters solution was injected into the gas chromatograph to obtain a chromatogram. The area of each methyl ester peak on the chromatogram was determined by measuring the height and width at half height of each peak. The percentage of each fatty acid methyl ester was calculated from its area assuming that peak area was

proportional to mass of ester.

### 3.5.1.2 Method B

Reagents used : (a) Sodium Methoxide  
(b) Petroleum Ether (Distilled at 30 -  
45 degrees centigrade)

#### 3.5.1.2.1 Preparation of Sodium Methoxide

To each of five (100 ml) beakers, 50 - 80 ml of petroleum ether was poured. A desired amount of metallic sodium (in paraffin) was transferred from its container to the first beaker. Extra petroleum ether was added to cover the metallic sodium if necessary. Metallic sodium was agitated by a glass rod to wash away as much paraffin as possible. The Metallic Sodium was then washed as in the same manner in the second and third beakers. The metallic sodium was then transferred to the fourth beaker. Surface layers of metallic sodium (yellow/brown) were cut off to remove those possibly contaminated by paraffin. The fifth beaker with petroleum ether was weighed as accurately as possible and the clean metallic sodium was quickly transferred to the fifth beaker. The fifth beaker was weighed again as accurately as possible. The weight of metallic sodium was determined by the difference in weight of the fifth beaker. The metallic sodium was finally cut into small pieces in petroleum ether. The metallic sodium pieces was dissolved slowly in a desired volume of pure methanol in a beaker to make up 2M of sodium methoxide solution. The solution was then stored in a reagent bottle. (Na AW = 23)

### 3.5.1.2.2 Procedure (Adapted from Christopherson and Glass Method, 1969)

A 2 ml sample of fat, oil or mixture of both was transferred to a glass-stopper test tube. 20 ml of distilled petroleum ether (bp 30 -45 degrees centigrade ) was added. The test tube was stoppered and shaken until all were dissolved in petroleum ether. 1 ml of 2M sodium methoxide was then added. The test tube was re-stoppered and the reactants were mixed by inversion until the solution became clear. (Almost immediately after clearing, the solution again became turbid due to separation of sodium glyceroxide). 1 to 2 ul of the fatty acid methyl was injected into gas liquid chromatograph to obtain a chromatogram. The percentage of each fatty acid methyl ester was calculated from its area assuming that peak area was proportional to the mass of ester.

### 3.6 Weight Response Factors, Fw

(Ackman and Sipos, 1964; and Taylor, 1973)

A known weight of methyl esters of fatty acid were injected into Gas Liquid Chromatograph to obtain a chromatogram. The proportion of each fatty acid was then determined by the areas under the curve. The ratio of the weight and area of methyl esters of fatty acids is the Weight Response Factors.

$$F_w = \frac{\text{Weight of methyl ester}}{\text{Corresponding area under the curve}}$$

Using the calculation of Ackman and Sipos (1964), the theoretical weight response factors were determined by Taylor (1973); assuming that the carbonyl carbon atom gives no response in hydrogen flame ionization detectors and that methyl esters of fatty acids are completely recovered from column.

The following table was obtained from Taylor (1973):

Table 1 :

-----  
 Weight response factors for methyl esters of fatty acids, which were calculated from experimental data and determined from theoretical considerations (methyl caprate assigned a Fw value of 1.00).  
 -----

Methyl esters of fatty acids	<u>Weight Response Factor Values</u>	
	Experimental*1	Theoretical
Methyl butyrate	1.35	1.38
" caproate	1.11	1.17
" caprylate	1.03	1.07
" caprate	1.00	1.00
" myristate	0.96	0.96
" palmitate	0.95	0.91
" stearate	0.99	0.89

-----  
 \*1 -- Methyl esters of fatty acids were prepared by the method of Shehata et al (1970).  
 -----

From above table, it is obvious that theoretical Fw values do not agree with the experimental values especially for methyl butyrate, methyl caproate and methyl caprylate; which means that not all methyl esters of fatty acids are completely recovered from column. To compensate for the difference, their areas under the curve were first multiplied by their correcting factors, Fw of above table under the column of experimental\*1; followed by the determination of fatty acid percents.

### 3.7 EXPERIMENTAL

#### Gas Chromatograph

Model : Varian Aerograph Series 1400  
Column : 1/8" by 5' ; SE30  
Mode Set : Isothermally; 50 - 200 degrees C  
at a rate of 8 degrees C/min.  
Injector Temperature : 180 - 190 degrees C  
Column Temperature : 185 - 200 degrees C  
Detector Temperature : 200 degrees C  
Range (Amp/mv) : 10\*\*(-10)  
Attenuation : 64  
Detector : Hydrogen Flame Ionization Detector.  
Carrier Gas : Nitrogen  
Recorder  
Model : CR652S  
Chart Speed : 10 mm/min

---

The method of preparing methyl esters played an important role in this research work. When milk fat was involved, method A tended to give lower percent values of those low carbon number fatty acids; and there was interference between C4 fatty acid and the petroleum ether peaks. However, similar problems were not observed when method B was employed. Moreover, method B requires no heat energy, and less time and chemicals in preparing methyl esters. Normally, method A requires more than 15 minutes for each sample while method B requires less than 4 minutes for each sample.

Care must be taken when distilling petroleum ether. The distilling temperature must be properly controlled so as not to distill the molecules of high molecular weight over the column. This helps to prevent the interference between C4 fatty acid and petroleum ether peaks.

As mentioned in Chapter 2, the fatty acid compositions of mixture components and mixture, obtained from the gas-liquid chromatographic analysis, were used in determining the proportion of each mixture component. This was done by running the F77 computer programs. One

of the F77 computer programs - FREQC will be documented in Chapter 4 while the rest of the programs are listed in appendix.

## **chapter 4**

4 DOCUMENTATION OF F77 COMPUTER PROGRAM - PROGRAM FREQC

This program has ten subroutines namely GAJOSE, MAT, FAT1, FAT2, FAT3, SS, CONLIMIT and EASE.

When the GAJOSE subroutine is called, the information regarding number of equations (INTS(2)) and columns (INTS(3)) are passed to the subroutine; while coefficients and constant values of the equations are passed by the common block. On returning, the calculated mixture component proportions are stored in vector X. The GAJOSE subroutine will in turn call the MAT subroutine. As the MAT subroutine shares the common block with the main program and the GAJOSE subroutine, it will have the same matrix A, matrix B, vector L6 and vector K6 values. On calling the MAT subroutine, the information regarding which column is used for finding pivot row (J) and the total number of column (IT) are passed to the MAT subroutine. On returning, the variable MI stores the information about pivot row.

After each set of mixture component proportions is calculated by the GAJOSE subroutine, the FAT1, FAT2 and FAT3 subroutines are called to store all the calculated mixture component proportions in vectors M1, M2 and M3 for later calculation of weighted mean and arithmetic mean.

To calculate weighted mean the FREQ subroutine is called. There are altogether three calls. The first call, for the first component, is to pass the information regarding number of mixture component proportion values available (R1) and their values (M1). Similar calls are made for second and third mixture components. The third position of CALL and SUBROUTINE statement, occupied by INTS(1), INTS(2) and INTS(3), helps to indicate which mixture component the subroutine is dealing with. On returning, weighted mean mixture component proportion (X) and its standard deviation (ST) are passed to the main program and printed. Within the FREQ subroutine, it calls the SS subroutine for determining the frequency of each class.

To calculate confidence limit for weighted mean and arithmetic mean of mixture component proportions, the CONLIMIT subroutine is called. On calling, the information concerning number of mixture component estimates stored in vectors M1, M2 and M3; weighted mean mixture component proportion values and their standard deviations are passed to the

subroutine. In order to determine whether calculated mean (both weighted mean and arithmetic mean) mixture component proportions differ significantly from actual values at 95% confidence limit, the subroutine EASE is called by CONLIMIT subroutine. Actual mixture component proportions (AM2), calculated mean values (AM or WMX), calculated T value (T or TS), Table T value (T1), and degrees of freedom (N) are passed to the EASE subroutine.

The FREQC program is explained in detail as below:

Vector CC(I) is used to store mixture components names:

```
CHARACTER*20 CC(5)
```

Common block is shared by the main program, the GAJOSE subroutine and the MAT subroutine:

```
COMMON // A,B,L6,K6
```

To input the mixture components names:

```
READ (1,33) (CC(I),I = 1, 3)
```

M is number of fatty acids in the mixture:

```
READ (1,*) M
```

N is the number of columns or equal to  $((Co + 1) * 2)$  where Co is the number of components in the mixture (only if duplicate data is used):

```
READ (1,*) N
```

Duplicate fatty acid percent values of mixture component and mixture are stored in matrix A:

```
DO 20 I = 1, M
20  READ (1,*) (A(I,J),J=1,N)
```

Calculation of standard deviation of average  
fatty acid values of each component and mixture:

```
V = SQRT (0.5)
DO 10 I = 1, M
BD(I,1)=(DABS(A(I,1)-A(I,2)))*V
BD(I,2)=(DABS(A(I,3)-A(I,4)))*V
BD(I,3)=(DABS(A(I,5)-A(I,6)))*V
BD(I,4)=(DABS(A(I,7)-A(I,8)))*V
```

Calculation of average fatty acid percents for each  
component and mixture:

```
AD(I,1)=(A(I,1)+A(I,2))*0.5
AD(I,2)=(A(I,3)+A(I,4))*0.5
AD(I,3)=(A(I,5)+A(I,6))*0.5
10 AD(I,4)=(A(I,7)+A(I,8))*0.5
```

Average fatty acid percents of each component and mixture  
are printed:

```
WRITE (1,922) ((AD(I,J),J=1,4),I=1,M)
```

Corresponding standard deviation of average fatty acid percents  
are printed:

```
WRITE (1,922) ((BD(I,J),J=1,4),I=1,M)
```

Initialization of variables R1, R2, R3, S1, S2 and S3:

```
R1=0
R2=0
R3=0
S1=0.0
S2=0.0
S3=0.0
```

The following loop is used to choose 2 equations at a time by using  
the equation (5) of Chapter 2:

```

DO 444 PP = 1, (M-1)
HH=PP+1
DO 455 KK = HH, M
A(1,1)=AD(PP,1)-AD(PP,3)
A(1,2)=AD(PP,2)-AD(PP,3)
A(1,3)=AD(PP,4)-AD(PP,3)
A(2,1)=AD(KK,1)-AD(KK,3)
A(2,2)=AD(KK,2)-AD(KK,3)
A(2,3)=AD(KK,4)-AD(KK,3)

```

The GAJOSE subroutine is called for calculation of X(1) and X(2):

```
CALL GAJOSE(INTS(2),INTS(3),X)
```

Calculation of third mixture component fraction in mixture:

```
X(3)=1-X(1)-X(2)
```

X's values are within the range  $0.0 < X_i < 1.0$  as no single mixture component percent in mixture can be 0.0% or 100%.

When any of the calculated X's values is outside the range, that two-equation combination is ignored and another set is chosen.

```

IF (X(1).LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2).LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3).LE.0.0 .OR. X(3) .GE. 1.0) GO TO 466

```

Subroutines FAT1, FAT2 and FAT3 are called for storing calculated mixture component proportions which are within the range and keeping account of number of calculated estimates stored.

```

CALL FAT1 (X(1),R1,M1)
CALL FAT2 (X(2),R2,M2)
CALL FAT3 (X(3),R3,M3)
466 CONTINUE
455 CONTINUE
444 CONTINUE

```

When there is no calculated mixture component estimates stored, the message - "NO SOLUTION FOR THIS MIXTURE" is printed.

```
IF (R1.EQ.0) GO TO 431
```

When there is only one set of calculated mixture component estimates stored, that set of stored estimates is printed.

```
IF (R1.EQ.1) GO TO 4
```

The FREQC subroutine is called to calculate weighted mean mixture component percents and their standard deviations.

```
CALL FREQ (R1,M1,INTS(1),X,ST)
CALL FREQ (R2,M2,INTS(2),X,ST)
CALL FREQ (R3,M3,INTS(3),X,ST)
```

The stored calculated mixture component estimates are printed:

```
WRITE (1,3) (I,1,M1(I),2,M2(I),3,M3(I),I=1,R1)
```

The following statement line makes a warning 'beep' sound:

```
PRINT*,'? '
```

Weighted mean component percentages and their corresponding standard deviations are printed by the following statement:

```
WRITE (1,94) (CC(I),X(I),ST(I),I = 1,3)
```

The CONLIMIT subroutine is called for calculating confidence limit, arithmetic mean, probable error of arithmetic mean, standard deviation of arithmetic mean and t values.

```
CALL CONLIMIT (R1,M1,M2,M3,X,ST)
```

When there is only one set of calculated mixture component proportion, then it is printed by the following statement:

```
WRITE (1,93) M1(1),M2(1),M3(1)
```

When there is no solution:

```
PRINT*, 'NO SOLUTION FOR THIS MIXTURE.'
```

The GAJOSE subroutine is used to solve linear simultaneous equations.

```
SUBROUTINE GAJOSE (IT, JT, X)
```

Common block is shared by the main program, the GAJOSE subroutine and the MAT subroutine.

```
COMMON // A,B,L6,K6
```

Initialization of variable N1:

```
N1=0
```

Initial average fatty acid values are stored in matrix G for later calculation of difference between calculated and actual mixture constants.

```
DO 2100 I = 1, IT
DO 2200 J = 1, JT
2200 G(I,J)=A(I,J)
2100 CONTINUE
```

The maximum allowable difference, between calculated and actual mixture fatty acid percentage, is assigned to variable R.

```
R= 10.0**(-6)
```

Set row indexes - L6(I):

```
DO 1 I = 1, IT
1 L6(I)= I
DO 600 J = 1, IT
```

The MAT subroutine is called to find the pivot row for each column:

```
CALL MAT(J,IT,MI)
K6(J)=MI
```

If the pivot is zero or close to zero this method is inapplicable; hence the command is returned to the main program, otherwise continue the estimation of mixture component proportion.

```
IF(DABS(A(MI,J)).GT.R) GO TO 3850
```

All X's values are assigned 0.0 value before returning to the main program. The main program will then ignore this two-equation combination and choose another set of combination.

```
222 X(1)=0.0
    X(2)=0.0
    X(3)=0.0
    RETURN
```

Reduce row MI, the pivot row, starting at column J+1:

```
3850 J1=J+1
     DO 500 J2 = J1, JT
500  A(MI,J2)=A(MI,J2)/A(MI,J)
```

Reduce other rows, starting in column J1:

```
DO 3000 P1 = 1, IT
```

The next step skips the pivot row:

```
IF(P1.EQ.MI) GO TO 3000
DO 4000 J2 = J1, JT
4000 A(P1,J2)=A(P1,J2)-A(MI,J2)*A(P1,J)
```

This is the equation mentioned in the Chapter of Mathematical Model; that is:

$$a(i,j) = a(i,j) - a(p,j) * a(i,q)/a(p,q)$$

Storage of the answers:

```

DO 4050 I = 1, IT
  MJ=K6(I)
4050  X(I)=A(MJ,IT)

```

Calculation of perturbed constants, using X(I):

```

N1=0
3382  DO 701 I = 1, IT
      C(I)= 0.0
      DO 702 J = 1, IT
702   C(I)=C(I)+G(I,J)*X(J)
      MJ=K6(I)

```

Difference between calculated and actual mixture average fatty acid percent:

```

701   D(I)=G(I,IT)-C(I)

```

Improving The Calculated Answers By Seidel Iteration:

Screen those undesired answers that exceed the above mentioned range:

```

IF (IT .EQ. 2) GO TO 2
IF (X(1).GE.1.0 .OR. X(1).LE.0.0) RETURN
IF (X(2).GE.1.0 .OR. X(2).LE.0.0) RETURN
IF (X(3).GE.1.0 .OR. X(3).LE.0.0) RETURN
GO TO 3
2   IF (X(1).GE.1.0 .OR. X(1).LE.0.0) RETURN
    IF (X(2).GE.1.0 .OR. X(2).LE.0.0) RETURN

```

If the difference between calculated and actual mixture average fatty acids percentage is smaller than or equal to the predetermined limit then the command is returned to the main program; otherwise the seidel iteration is continued until the iteration number is fifteen.

```

      IF (DABS(D(1)).LE.R .AND. DABS(D(2)).LE.R)RETURN
      GO TO 4
3     IF (DABS(D(1)).LE.R .AND. DABS(D(2)).LE.R .AND. DABS(D(3)).LE.R)
      c RETURN

```

A counter to keep account of number of iterations done:

```

4     N1=N1+1

```

The maximum number of iterations is fifteen.

```

      IF(N1.GE.15) GO TO 222
      DO 999 I = 1, IT

```

Replace actual mixture average fatty acids percentage by the difference between calculated and actual mixture average fatty acids percent:

```

      A(I,JT)=D(I)

```

Storing calculated X's values in vector T(I):

```

999   T(I)=X(I)

```

Set row indexes - L6(I)

```

      DO 1217 I = 1, IT
1217  L6(I)=I
      DO 6001 J = 1, IT

```

The MAT subroutine is called to find the pivot row for each column:

```

      CALL MAT(J,IT,MI)
      K6(J)=MI

```

If the pivot row is zero or close to zero then this method is inaplicable; hence all X's values are assigned a 0.0 value before returning to the main program. The main program will therefore ignore that two-equations combination and choose another if there is one.

```

IF(DABS(A(MI,J)).GT.R) GO TO 3851
X(1)=0.0
X(2)=0.0
X(3)=0.0
RETURN

```

Reduce row MI, the pivot row, starting at column J+1:

```

3851   J1=J+1
      DO 5001 J2 = J1, JT
5001   A(MI,J2)=A(MI,J2)/A(MI,J)

```

Reduce other rows, starting in column J1:

```

      DO 3002 P1 = 1, IT

```

The next step skips the pivot row:

```

      IF(P1 .EQ. MI) GO TO 3002
      DO 4002 J2 = J1, JT
      A(P1,J2)=A(P1,J2)-A(MI,J2)*A(P1,J)
4002   CONTINUE
3002   CONTINUE

```

Storage of the answers:

```

      DO 4055 I = 1, IT
      MJ=K6(I)
      Z(I)=A(MJ,JT)

```

Improved mixture component proportions estimation:

```

4055   X(I)=T(I)+Z(I)
      GO TO 3382
      END

```

The MAT subroutine is called for finding the pivot row:

```
SUBROUTINE MAT(J,IT,MI)
```

Common block is shared by the main program, the GAJOSE subroutine and the MAT subroutine.

```
COMMON // A,B,L6,K6
```

For rows which have already been pivoted, set coefficients to zero.

For other rows, find absolute values:

```
DO 433 I = 1, IT
  IF (L6(I).NE.0) GO TO 3130
  Y(I)= 0.0
  GO TO 433
3130  Y(I)=DABS(A(I,J))
433  CONTINUE
```

Set initial values for comparing coefficients:

```
MA=1
MB=2
```

Now compare in pairs:

```
414  IF(Y(MB).GT.Y(MA)) GO TO 616
     MI=MA
     GO TO 717
616  MI=MB
```

Test for termination:

```
717  IF(MB.GE.IT) GO TO 919
     MA=MI
     MB=MB+1
     GO TO 414
919  L6(MI)= 0
     SUBROUTINE FAT1 (F1,R1,M1)
```

Keeping account of the number of calculated component one estimates stored:

R1=R1+1

Storing component one estimates in vector M1:

M1(R1)=F1

SUBROUTINE FAT2 (F2,R2,M2)

Keeping account of the number of calculated component two estimates stored:

R2=R2+1

Storing component two estimates in vector M2:

M2(R2)=F2

SUBROUTINE FAT3 (F3,R3,M3)

Keeping account of the number of calculated component three estimates stored:

R3=R3+1

Storing component three estimates in vector M3:

M3(R3)=F3

The subroutine to calculate weighted mean mixture component proportion and their corresponding standard deviation:

SUBROUTINE FREQ (N,DX,J1,X,ST)

Storing mid-values in vector V:

V(1)=0.045

V(2)=0.145

V(3)=0.245

V(4)=0.345

V(5)=0.445

```

V(6)=0.545
V(7)=0.645
V(8)=0.745
V(9)=0.845
V(10)=0.945

```

Initialization of vectors U and T:

```

DO 18 J= 1,10
  U(J)=0.0
18  T(J)=0

```

To sort out which class each DX's value belongs to and determine the frequency of each class by calling the SS subroutine:

```

DO 17 I= 1,N
  IF (DX(I).GE.0.0 .AND. DX(I).LT.0.1)
c CALL SS(INTS(1),T)
  IF (DX(I).GE.0.1 .AND. DX(I).LT.0.2)
c CALL SS(INTS(2),T)
  IF (DX(I).GE.0.2 .AND. DX(I).LT.0.3)
c CALL SS(INTS(3),T)
  IF (DX(I).GE.0.3 .AND. DX(I).LT.0.4)
c CALL SS(INTS(4),T)
  IF (DX(I).GE.0.4 .AND. DX(I).LT.0.5)
c CALL SS(INTS(5),T)
  IF (DX(I).GE.0.5 .AND. DX(I).LT.0.6)
c CALL SS(INTS(6),T)
  IF (DX(I).GE.0.6 .AND. DX(I).LT.0.7)
c CALL SS(INTS(7),T)
  IF (DX(I).GE.0.7 .AND. DX(I).LT.0.8)
c CALL SS(INTS(8),T)
  IF (DX(I).GE.0.8 .AND. DX(I).LT.0.9)
c CALL SS(INTS(9),T)
  IF (DX(I).GE.0.9 .AND. DX(I).LT.1.0)
c CALL SS(INTS(10),T)
17  CONTINUE

```

Multiplication of each class mid-value by its frequency:

```

      DO 3 I= 1,10
3     U(I)=V(I)*T(I)

```

Initialization of variables UU, TT and S:

```

      TT=0
      UU=0.0
      S=0.0

```

Calculation of weighted mean mixture component percentage:

```

      DO 1 I = 1,10
      UU=UU+U(I)      Sum of product of mid-value and frequency
1     TT=TT+T(I)      Sum of frequency
      X(J1)=UU/TT

```

Calculation of standard deviation of the weighted mean:

```

      DO 2 J = 1,N
2     S=S+(DX(J)-X(J1))**2
      ST(J1)=DSQRT(S/(N-1))

```

The subroutine to determine the frequency of each class.

```

      SUBROUTINE SS(N1,T)
      INTEGER*2 N1,T(20)
      T(N1)=T(N1)+1

```

The subroutine to calculate the confidence limits of each fat:

```

      SUBROUTINE CONLIMIT (N1,XX,XY,XZ,WMX,TS)

```

Initialization of variables S1, S2, S3, D1, D2 and D3:

```

      S1=0.0
      S2=0.0
      S3=0.0
      D1=0.0
      D2=0.0

```

D3=0.0

Convert integer value to real value:

Z1=DBLE(N1)

Calculation of arithmetic mean:

```

DO 1 I = 1, Z1
  S1=S1+XX(I)
  S2=S2+XY(I)
1  S3=S3+XZ(I)
  AM(1)=S1/Z1
  AM(2)=S2/Z1
  AM(3)=S3/Z1

```

Calculation of arithmetic mean probable error:

```

DO 2 I =1, Z1
  D1=D1+(XX(I)-AM(1))**2
  D2=D2+(XY(I)-AM(2))**2
2  D3=D3+(XZ(I)-AM(3))**2
  N= Z1-1.0
  IF((Z1-1).EQ.0) N=1.0
  RR(1)=0.6745*(DSQRT(D1/(Z1*N)))
  RR(2)=0.6745*(DSQRT(D2/(Z1*N)))
  RR(3)=0.6745*(DSQRT(D3/(Z1*N)))

```

Calculation of standard deviation of arithmetic mean:

```

T(1)=DSQRT(D1/N)
T(2)=DSQRT(D2/N)
T(3)=DSQRT(D3/N)
WRITE (1,4) (I,AM(I),RR(I),T(I),I=1,3)
4  FORMAT (5X/5X,'PROBABLE FAT ',I2,' VALUE = ',F9.5/5X,
c 'ITS PROBABLE ERROR = +/- ', F9.5/5X,
c 'ITS STANDARD DEVIATION = +/- ',F9.5//)
  IF (N .LE. 30.0) GO TO 5
  X1=40.0
  X2=40.0
  X3=40.0

```

```

GO TO 10
5  X1=N
   X2=N
   X3=N

```

To calculate confidence limit of weighted mean or arithmetic mean:

```

10  P1=A(X1,2)*T(1)/DSQRT(Z1)
    P2=A(X2,2)*T(2)/DSQRT(Z1)
    P3=A(X3,2)*T(3)/DSQRT(Z1)
    CL(1,1)=AM(1)+P1
    IF (CL(1,1) .GT. 1.0) CL(1,1)=1.0
    CL(1,2)=AM(1)-P1
    IF (P1 .GT. AM(1)) CL(1,2)=0.0
    CL(2,1)=AM(2)+P2
    IF (CL(2,1) .GT. 1.0) CL(2,1)=1.0
    CL(2,2)=AM(2)-P2
    IF (P2 .GT. AM(2)) CL(2,2)=0.0
    CL(3,1)=AM(3)+P3
    IF (CL(3,1) .GT. 1.0) CL(3,1)=1.0
    CL(3,2)=AM(3)-P3
    IF (P3 .GT. AM(3)) CL(3,2)=0.0
    B = 95.00

```

Print out arithmetic mean and its confidence limit:

```

WRITE (1,20) B,AM(1),P1,AM(2),P2,AM(3),P3
WRITE (1,22) (I,(CL(I,J),J=2,1,-1),I=1,3)
T1=A(X1,2)

```

Call the EASE subroutine to find out whether there is any significant difference between actual and calculated arithmetic mean values at 95% confidence limit:

```

CALL EASE(AM2,AM,T,T1,N)

```

The EASE subroutine is called to find out whether there is any significant difference between actual and weighted mean values at 95% confidence limit:

```
CALL EASE(AM2,WMX,TS,T1,N)
```

The EASE Subroutine:

```

SUBROUTINE EASE(AM,X,T,T1,X1)
REAL*8 AM1(5),AM(5),T(10),X(10),T1,X1
INTEGER*2 I
DO 36 I = 1,3
AM1(I)=AM(I)
AM1(I)=(DABS(X(I)-AM1(I)))*DSQRT(X1)/T(I)
WRITE (1,12)
PRINT*, '      FOR FAT',I,' MEAN VALUE:'
PRINT*, '      %%%%'
WRITE (1,35) I,AM1(I),T1
12  FORMAT (5X)
35  FORMAT(5X,'CALCULATED T VALUE FOR FAT',I2,' IS ',F9.5/5X,
c 'T TABLE VALUE IS ',F9.5)

```

If calculated t value is less than that of T - table, there is no significant difference between actual and calculated mean values, be it arithmetic or weighted mean; otherwise there is significant difference at 95% confidence limit.

```

IF (AM1(I)-T1) 38,38,39
38  PRINT*, '      THERE IS NO SIGNIFICANT DIFFERENCE BETWEEN '
PRINT*, 'ACTUAL AND CALCULATED VALUES AT 95
GO TO 37
39  PRINT*, '      THERE IS SIGNIFICANT DIFFERENCE BETWEEN ACTUAL AND'
PRINT*, '      CALCULATED VALUES AT 95
37  PRINT*, '*****'
36  CONTINUE

```

```

PROGRAM FREQC
C USING GAUSS-JORDAN-SEIDEL METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATI
ONS.
C THE GENERAL EQUATION IS: AX = B .
C DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
C ..LOCAL SCALAR..
  INTEGER*2 HH, KK, R1, R2, R3, PP
  REAL*8 D4, D5, D6, T1, T2, V
  INTEGER*2 I, J, M, N, GC
C ..LOCAL ARRAY..
  REAL*8 A(100, 24), B(100, 24), X(10),
  * L6(10), K6(10), M1(700), M3(700), M2(700), ST(10),
  * BD(100, 10), AD(100, 10)
  CHARACTER*20 CC(5)
  INTRINSIC DABS, SQRT
  COMMON // A, B, L6, K6
  READ (1, 33) (CC(I), I = 1, 3)
  READ (1, *) M
  READ (1, *) N
  DO 20 I = 1, M
20  READ (1, *) (A(I, J), J=1, N)
C CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C THE GLC ANALYSIS.
  V = SQRT (0.5)
  DO 10 I = 1, M
    BD(I, 1)=(DABS(A(I, 1)-A(I, 2)))*V
    BD(I, 2)=(DABS(A(I, 3)-A(I, 4)))*V
    BD(I, 3)=(DABS(A(I, 5)-A(I, 6)))*V
    BD(I, 4)=(DABS(A(I, 7)-A(I, 8)))*V
    AD(I, 1)=(A(I, 1)+A(I, 2))*0.5
    AD(I, 2)=(A(I, 3)+A(I, 4))*0.5
    AD(I, 3)=(A(I, 5)+A(I, 6))*0.5
10  AD(I, 4)=(A(I, 7)+A(I, 8))*0.5
    PRINT '(5X//)'
    WRITE (1, 96)
    WRITE (1, 922) ((AD(I, J), J=1, 4), I=1, M)
    WRITE (1, 966)
    WRITE (1, 922) ((BD(I, J), J=1, 4), I=1, M)
    R1=0
    R2=0
    R3=0
    S1=0.0
    S2=0.0
    S3=0.0
C
C MATRIX OPERATION:
  DO 444 PP = 1, (M-1)
    HH=PP+1
    DO 455 KK = HH, M
      A(1, 1)=AD(PP, 1)-AD(PP, 3)
      A(1, 2)=AD(PP, 2)-AD(PP, 3)
      A(1, 3)=AD(PP, 4)-AD(PP, 3)
      A(2, 1)=AD(KK, 1)-AD(KK, 3)
      A(2, 2)=AD(KK, 2)-AD(KK, 3)
      A(2, 3)=AD(KK, 4)-AD(KK, 3)
      B(1, 1)=DSQRT(BD(PP, 1)**2+BD(PP, 3)**2)
      B(1, 2)=DSQRT(BD(PP, 2)**2+BD(PP, 3)**2)
      B(1, 3)=DSQRT(BD(PP, 4)**2+BD(PP, 3)**2)
      B(2, 1)=DSQRT(BD(KK, 1)**2+BD(KK, 3)**2)
      B(2, 2)=DSQRT(BD(KK, 2)**2+BD(KK, 3)**2)
      B(2, 3)=DSQRT(BD(KK, 4)**2+BD(KK, 3)**2)
      CALL GAJOSE(INTS(2), INTS(3), X)
      X(3)=1-X(1)-X(2)

```

```

IF (X(1).LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2).LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3).LE.0.0 .OR. X(3) .GE. 1.0) GO TO 466
CALL FAT1 (X(1),R1,M1)
CALL FAT2 (X(2),R2,M2)
CALL FAT3 (X(3),R3,M3)
466 CONTINUE
455 CONTINUE
444 CONTINUE
IF (R1.EQ.0) GO TO 431
IF (R1.EQ.1) GO TO 4

C
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE AND
C SUM OF SQUARE OF DIFERENCE BETWEEN MEAN VALUE AND INDIVIDUAL.
CALL FREQ (R1,M1,INTS(1),X,ST)
CALL FREQ (R2,M2,INTS(2),X,ST)
CALL FREQ (R3,M3,INTS(3),X,ST)
C *****
C WRITE (1,3) (I,1,M1(I),2,M2(I),3,M3(I),I=1,R1)
C *****
C
PRINT*, '? '
WRITE (1,94) (CC(I),X(I),ST(I),I = 1,3)
CALL CONLIMIT (R1,M1,M2,M3,X,ST)
GO TO 5
4 PRINT*, '? '
PRINT*, 'ONLY ONE SET OF DATAS IS AVAILABLE:'
PRINT*, '-----'
WRITE (1,93) M1(1),M2(1),M3(1)
GO TO 5
431 PRINT*, '? '
PRINT*, 'NO SOLUTION FOR THIS MIXTURE.'
PRINT*, '===== '
5 STOP
3 FORMAT(5X, 'SET NO.', I3/5X, 'FAT', I2, ' =', F9.5, 2X, 'FAT', I2, ' =',
* F9.5, 2X, 'FAT', I2, ' =', F9.5//)
99 FORMAT (6A4, 1A4)
93 FORMAT (5X, 'X(1)= ', F9.5, 5X, 'X(2)= ', F9.5, 5X, 'X(3)= ', F9.5//)
33 FORMAT (A20)
96 FORMAT (10X, 'MATRIX A', 15X, 'VECTOR B'//)
966 FORMAT( 10X, 'STANDARD DEVIATION'//)
922 FORMAT(5X, 4F9.5/)
94 FORMAT (5X, 'WT-MEAN ', A20, '= ', F9.5/5X,
c 'STANDARD DEVIATION =+/- ', F9.5//)
92 FORMAT (5X, 3F9.5/)
END
SUBROUTINE GAJOSE (IT, JT, X)
C SUBROUTINE - FOR THE ANALYSIS OF THREE COMPONENT FAT
C MIXTURES BY SOLVING SIMULTANEOUS EQUATIONS.
REAL*8 X(10), D(10), C(10), Z(10)
REAL*8 T(10), L6(10), K6(10),
* MM(10,5)
REAL*8 G(200, 10), A(100, 24), B(100, 24)
INTEGER*2 I, IT, J, J1, J2, MI, MJ, P1, R, N1, JT
COMMON // A, B, L6, K6
INTRINSIC DABS
N1=0
DO 2100 I = 1, IT
DO 2200 J = 1, JT
2200 G(I, J)=A(I, J)
2100 CONTINUE
R= 10.0**(-6)
C SET ROW INDEXES - L6(I)

```

```

        DO 1 I = 1, IT
1      L6(I)= I
        DO 600 J = 1, IT
C      THE SUBROUTINE FINDS THE PIVOT ROW FOR EACH COLUMN.
C
        CALL MAT(J,IT,MI)
        K6(J)=MI
C      THE PIVOT IS ZERO OR CLOSE TO ZERO;
C      THE METHOD IS INAPPLICABLE.
C
        IF(DABS(A(MI,J)).GT.R) GO TO 3850
C      BECAUSE OF A ZERO PIVOT, THIS SET OF EQUATIONS CANNOT BE
C      SOLVED BY THE GAUSS-JORDAN METHOD.
222    X(1)=0.0
        X(2)=0.0
        X(3)=0.0
        RETURN
C      REDUCE ROW MI, THE PIVOT ROW, STARTING AT COLUMN J+1
3850   J1=J+1
        DO 500 J2 = J1, JT
500    A(MI,J2)=A(MI,J2)/A(MI,J)
C      REDUCE OTHER ROWS, STARTING IN COLUMN J1
        DO 3000 P1 = 1, IT
C      THE NEXT STEP SKIPS THE PIVOT ROW.
        IF(P1.EQ.MI) GO TO 3000
        DO 4000 J2 = J1, JT
4000   A(P1,J2)=A(P1,J2)-A(MI,J2)*A(P1,J)
3000   CONTINUE
600    CONTINUE
C      STORAGE OF THE ANSWERS.
        DO 4050 I = 1, IT
        MJ=K6(I)
4050   X(I)=A(MJ,JT)
C
C      CALCULATION OF PERTURBED CONSTANTS, USING X(I).
C      DISPLAY ERRORS.
        N1=0
3382   DO 701 I = 1, IT
        C(I)= 0.0
        DO 702 J = 1, IT
702    C(I)=C(I)+G(I,J)*X(J)
        MJ=K6(I)
701    D(I)=G(I,JT)-C(I)
C      SEIDEL ITERATION.
        IF (IT .EQ. 2) GO TO 2
        IF (X(1).GE.1.0 .OR. X(1).LE.0.0) RETURN
        IF (X(2).GE.1.0 .OR. X(2).LE.0.0) RETURN
        IF (X(3).GE.1.0 .OR. X(3).LE.0.0) RETURN
        GO TO 3
2      IF (X(1).GE.1.0 .OR. X(1).LE.0.0) RETURN
        IF (X(2).GE.1.0 .OR. X(2).LE.0.0) RETURN
        IF (DABS(D(1)).LE.R .AND. DABS(D(2)).LE.R)RETURN
        GO TO 4
C
3      IF (DABS(D(1)).LE.R .AND. DABS(D(2)).LE.R .AND. DABS(D(3)).LE.R)
c      RETURN
4      N1=N1+1
        IF(N1.GE.15) GO TO 222
        DO 999 I = 1, IT
        A(I,JT)=D(I)
999    T(I)=X(I)
        DO 1217 I = 1, IT
1217   L6(I)=I

```

```

DO 6001 J = 1, IT
CALL MAT(J,IT,MI)
K6(J)=MI
IF(DABS(A(MI,J)).GT.R) GO TO 3851
X(1)=0.0
X(2)=0.0
X(3)=0.0
RETURN
3851 J1=J+1
DO 5001 J2 = J1, JT
5001 A(MI, J2)=A(MI, J2)/A(MI, J)
DO 3002 P1 = 1, IT
IF(P1 .EQ. MI) GO TO 3002
DO 4002 J2 = J1, JT
A(P1, J2)=A(P1, J2)-A(MI, J2)*A(P1, J)
4002 CONTINUE
3002 CONTINUE
6001 CONTINUE
DO 4055 I = 1, IT
MJ=K6(I)
Z(I)=A(MJ, JT)
4055 X(I)=T(I)+Z(I)
GO TO 3382
END
SUBROUTINE MAT(J,IT,MI)
C SUBROUTINE OF THE SUBROUTINE GAJOSE
INTEGER*2 I, IT, J, MI, MA, MB
REAL*8 Y(10), A(100, 24), B(100, 24), L6(10), K6(10)
COMMON // A, B, L6, K6
INTRINSIC DABS
C FOR ROWS WHICH HAVE ALREADY BEEN PIVOTS, SET COEFFICIENTS TO
C ZERO.
C FOR OTHER ROWS, FIND ABSOLUTE VALUES.
DO 433 I = 1, IT
IF (L6(I).NE.0) GO TO 3130
Y(I)= 0.0
GO TO 433
3130 Y(I)=DABS(A(I, J))
433 CONTINUE
C SET INITIAL VALUES FOR COMPARING COEFFICIENTS.
MA=1
MB=2
C NOW COMPARE IN PAIRS.
414 IF(Y(MB).GT.Y(MA)) GO TO 616
MI=MA
GO TO 717
616 MI=MB
C TEST FOR TERMINATION.
717 IF(MB.GE.IT) GO TO 919
MA=MI
MB=MB+1
GO TO 414
919 L6(MI)= 0
RETURN
END
SUBROUTINE FAT1 (F1, R1, M1)
REAL*8 F1, M1(700)
INTEGER*2 R1
R1=R1+1
M1(R1)=F1
RETURN
END
SUBROUTINE FAT2 (F2, R2, M2)

```

```

REAL*8 F2,M2(700)
INTEGER*2 R2
R2=R2+1
M2(R2)=F2
RETURN
END
SUBROUTINE FAT3 (F3,R3,M3)
REAL*8 F3,M3(700)
INTEGER*2 R3
R3=R3+1
M3(R3)=F3
RETURN
END
C
C
SUBROUTINE FREQ (N,DX,J1,X,ST)
REAL*8 DX(700),ST(10),X(10),U(20),V(10)
REAL*8 UU,S
INTEGER*2 T(20),TT
INTEGER*2 I,N,J,J1
C
C
V(1)=0.045
V(2)=0.145
V(3)=0.245
V(4)=0.345
V(5)=0.445
V(6)=0.545
V(7)=0.645
V(8)=0.745
V(9)=0.845
V(10)=0.945
DO 18 J= 1,10
U(J)=0.0
18 T(J)=0
DO 17 I= 1,N
IF (DX(I).GE.0.0 .AND. DX(I).LT.0.1)
c CALL SS(INTS(1),T)
IF (DX(I).GE.0.1 .AND. DX(I).LT.0.2)
c CALL SS(INTS(2),T)
IF (DX(I).GE.0.2 .AND. DX(I).LT.0.3)
c CALL SS(INTS(3),T)
IF (DX(I).GE.0.3 .AND. DX(I).LT.0.4)
c CALL SS(INTS(4),T)
IF (DX(I).GE.0.4 .AND. DX(I).LT.0.5)
c CALL SS(INTS(5),T)
IF (DX(I).GE.0.5 .AND. DX(I).LT.0.6)
c CALL SS(INTS(6),T)
IF (DX(I).GE.0.6 .AND. DX(I).LT.0.7)
c CALL SS(INTS(7),T)
IF (DX(I).GE.0.7 .AND. DX(I).LT.0.8)
c CALL SS(INTS(8),T)
IF (DX(I).GE.0.8 .AND. DX(I).LT.0.9)
c CALL SS(INTS(9),T)
IF (DX(I).GE.0.9 .AND. DX(I).LT.1.0)
c CALL SS(INTS(10),T)
17 CONTINUE
DO 3 I= 1,10
3 U(I)=V(I)*T(I)
TT=0
UU=0.0
S=0.0
DO 1 I = 1,10

```

```

      UU=UU+U(I)
1     TT=TT+T(I)
      X(J1)=UU/TT
      DO 2 J = 1,N
2     S=S+(DX(J)-X(J1))**2
      ST(J1)=DSQRT(S/(N-1))
      RETURN
      END
C
C
      SUBROUTINE SS(N1,T)
      INTEGER*2 N1,T(20)
C
      T(N1)=T(N1)+1
      RETURN
      END
C *****
C THE SUBROUTINE TO CALCULATE THE CONFIDENCE LIMITS OF EACH FAT.
      SUBROUTINE CONLIMIT (N1,XX,XY,XZ,WMX,TS)
      INTEGER*2 I,N1
      REAL*8 XX(700),XY(700),XZ(700),S1,S2,S3,D1,D2,D3,Z1,T1,N,
      * AM(5),A(50,5),RR(5),T(5),X1,X2,X3,CL(5,5),
      * TS(10),AM2(5),WMX(10)
C *****
C T DISTRIBUTION TABLE:
C *****
      A(1,1)=6.314
      A(1,2)=12.71
      A(1,3)=63.66
      A(1,4)=636.6
      A(2,1)=2.920
      A(2,2)=4.303
      A(2,3)=9.925
      A(2,4)=31.60
      A(3,1)=2.353
      A(3,2)=3.182
      A(3,3)=5.841
      A(3,4)=12.94
      A(4,1)=2.132
      A(4,2)=2.776
      A(4,3)=4.604
      A(4,4)=8.610
      A(5,1)=2.015
      A(5,2)=2.571
      A(5,3)=4.032
      A(5,4)=6.859
      A(6,1)=1.943
      A(6,2)=2.447
      A(6,3)=3.707
      A(6,4)=5.959
      A(7,1)=1.895
      A(7,2)=2.365
      A(7,3)=3.499
      A(7,4)=5.405
      A(8,1)=1.860
      A(8,2)=2.306
      A(8,3)=3.355
      A(8,4)=5.041
      A(9,1)=1.833
      A(9,2)=2.262
      A(9,3)=3.250
      A(9,4)=4.781
      A(10,1)=1.812

```

A(10,2)=2.228  
A(10,3)=3.169  
A(10,4)=4.587  
A(11,1)=1.796  
A(11,2)=2.201  
A(11,3)=3.106  
A(11,4)=4.437  
A(12,1)=1.782  
A(12,2)=2.179  
A(12,3)=3.055  
A(12,4)=4.318  
A(13,1)=1.771  
A(13,2)=2.160  
A(13,3)=3.012  
A(13,4)=4.221  
A(14,1)=1.761  
A(14,2)=2.145  
A(14,3)=2.977  
A(14,4)=4.140  
A(15,1)=1.753  
A(15,2)=2.131  
A(15,3)=2.947  
A(15,4)=4.073  
A(16,1)=1.746  
A(16,2)=2.120  
A(16,3)=2.921  
A(16,4)=4.015  
A(17,1)=1.740  
A(17,2)=2.110  
A(17,3)=2.898  
A(17,4)=3.965  
A(18,1)=1.734  
A(18,2)=2.101  
A(18,3)=2.878  
A(18,4)=3.922  
A(19,1)=1.729  
A(19,2)=2.093  
A(19,3)=2.861  
A(19,4)=3.883  
A(20,1)=1.725  
A(20,2)=2.086  
A(20,3)=2.845  
A(20,4)=3.850  
A(21,1)=1.721  
A(21,2)=2.080  
A(21,3)=2.831  
A(21,4)=3.819  
A(22,1)=1.717  
A(22,2)=2.074  
A(22,3)=2.819  
A(22,4)=3.792  
A(23,1)=1.714  
A(23,2)=2.069  
A(23,3)=2.807  
A(23,4)=3.767  
A(24,1)=1.711  
A(24,2)=2.064  
A(24,3)=2.797  
A(24,4)=3.745  
A(25,1)=1.708  
A(25,2)=2.060  
A(25,3)=2.787  
A(25,4)=3.725

```

A(26,1)=1.706
A(26,2)=2.056
A(26,3)=2.779
A(26,4)=3.707
A(27,1)=1.703
A(27,2)=2.052
A(27,3)=2.771
A(27,4)=3.690
A(28,1)=1.701
A(28,2)=2.048
A(28,3)=2.763
A(28,4)=3.674
A(29,1)=1.699
A(29,2)=2.045
A(29,3)=2.756
A(29,4)=3.659
A(30,1)=1.697
A(30,2)=2.042
A(30,3)=2.75
A(30,4)=3.646
C THE FOLLOWING VALUES ARE FOR DF GREATER THAN 30.
A(40,1)=1.645
A(40,2)=1.960
A(40,3)=2.576
A(40,4)=3.291
C *****
S1=0.0
S2=0.0
S3=0.0
D1=0.0
D2=0.0
D3=0.0
Z1=DBLE(N1)
DO 1 I = 1, Z1
S1=S1+XX(I)
S2=S2+XY(I)
1 S3=S3+XZ(I)
AM(1)=S1/Z1
AM(2)=S2/Z1
AM(3)=S3/Z1
DO 2 I =1, Z1
D1=D1+(XX(I)-AM(1))**2
D2=D2+(XY(I)-AM(2))**2
2 D3=D3+(XZ(I)-AM(3))**2
N= Z1-1.0
IF((Z1-1).EQ.0) N=1.0
RR(1)=0.6745*(DSQRT(D1/(Z1*N)))
RR(2)=0.6745*(DSQRT(D2/(Z1*N)))
RR(3)=0.6745*(DSQRT(D3/(Z1*N)))
WRITE (1,11)
11 FORMAT (5X/5X,'ARITHMETIC MEAN AND ITS PROBABLE ERROR:'/5X,
c '#####'//)
T(1)=DSQRT(D1/N)
T(2)=DSQRT(D2/N)
T(3)=DSQRT(D3/N)
WRITE (1,4) (I,AM(I),RR(I),T(I),I=1,3)
4 FORMAT (5X/5X,'PROBABLE FAT ',I2,' VALUE = ',F9.5/5X,
c 'ITS PROBABLE ERROR = +/- ',F9.5/5X,
c 'ITS STANDARD DEVIATION = +/- ',F9.5//)
IF (N .LE. 30.0) GO TO 5
X1=40.0
X2=40.0
X3=40.0

```

```

      GO TO 10
5     X1=N
      X2=N
      X3=N
C     FOR 95
10    P1=A(X1,2)*T(1)/DSQRT(Z1)
      P2=A(X2,2)*T(2)/DSQRT(Z1)
      P3=A(X3,2)*T(3)/DSQRT(Z1)
      CL(1,1)=AM(1)+P1
      IF (CL(1,1) .GT. 1.0) CL(1,1)=1.0
      CL(1,2)=AM(1)-P1
      IF (P1 .GT. AM(1)) CL(1,2)=0.0
      CL(2,1)=AM(2)+P2
      IF (CL(2,1) .GT. 1.0) CL(2,1)=1.0
      CL(2,2)=AM(2)-P2
      IF (P2 .GT. AM(2)) CL(2,2)=0.0
      CL(3,1)=AM(3)+P3
      IF (CL(3,1) .GT. 1.0) CL(3,1)=1.0
      CL(3,2)=AM(3)-P3
      IF (P3 .GT. AM(3)) CL(3,2)=0.0
      B = 95.00
      WRITE (1,20) B,AM(1),P1,AM(2),P2,AM(3),P3
      WRITE (1,22) (I,(CL(I,J),J=2,1,-1),I=1,3)
      T1=A(X1,2)
      PRINT*, '      INPUT ACTUAL MIXTURE COMPONENT VALUES:'
      PRINT*, '      (IF NOT AVAILABLE,INPUT THREE VALUES OF 1.0)'
      READ (1,34) (AM2(I),I=1,3)
      IF (AM2(1).EQ.1.0) RETURN
      PRINT*, '? '
      WRITE(1,*)
      PRINT*, '      ====='
      PRINT*, '      CONSIDERING ARITHMATIC MEAN VALUES:'
      PRINT*, '      ====='
      CALL EASE(AM2,AM,T,T1,N)
      PRINT*, '? '
      WRITE (1,*)
      PRINT*, '      ====='
      PRINT*, '      CONSIDERING WEIGHTED MEAN VALUES:'
      PRINT*, '      ====='
      CALL EASE(AM2,WMX,TS,T1,N)
34    FORMAT (F9.5)
20    FORMAT (5X, '*****'/
* 6X,F5.2, '
* '*****'/5X,
* 'FAT ONE = ',F9.5, ' +/- ',F9.5/5X, 'FAT TWO = ',F9.5,
* ' +/- ',F9.5/5X, 'FAT THREE = ',F9.5, ' +/- ',F9.5//)
22    FORMAT (5X, 'FAT', I2, ' CONFIDENCE LIMIT IS BETWEEN' /
* 5X,F9.5, ' AND ',F9.5//)
      RETURN
      END

C
C
SUBROUTINE EASE(AM,X,T,T1,X1)
REAL*8 AM1(5),AM(5),T(10),X(10),T1,X1
INTEGER*2 I
DO 36 I = 1,3
AM1(I)=AM(I)
AM1(I)=(DABS(X(I)-AM1(I)))*DSQRT(X1)/T(I)
WRITE (1,12)
PRINT*, '      FOR FAT',I, ' MEAN VALUE:'
PRINT*, '      %%%%%%%%%%'
WRITE (1,35) I,AM1(I),T1
12    FORMAT (5X)

```

```
35  FORMAT(5X,'CALCULATED T VALUE FOR FAT',I2,' IS ',F9.5/5X,  
c  'T TABLE VALUE IS ',F9.5)  
38  IF (AM1(I)-T1) 38,38,39  
38  PRINT*,'      THERE IS NO SIGNIFICANT DIFFERENCE BETWEEN '  
PRINT*,'ACTUAL AND CALCULATED VALUES AT 95  
GO TO 37  
39  PRINT*,'      THERE IS SIGNIFICANT DIFFERENCE BETWEEN ACTUAL AND'  
PRINT*,'      CALCULATED VALUES AT 95  
37  PRINT*,'*****'  
36  CONTINUE  
RETURN  
END
```

# chapter 5

## 5 ANALYSIS OF RESULTS

Altogether there were forty nine mixtures and they were tested by the following F77 Fortran programs:

- 1) CRAM1
- 2) CRAM2
- 3) CRAM4
- 4) CRAM5
- 5) CRA1
- 6) CRA2
- 7) CRA3
- 8) CRA4
- 9) GLC1
- 10) GLC2
- 11) GLC3
- 12) GLC4
- 13) FREQC ;and
- 14) CHU2

### 5.1 The Use Of Number Code

The results of each mixture was number-coded as below :

The number 5 was for three calculated component percentages in the mixture to be within two calculated standard errors or deviations (i.e.  $\pm 2SE$  or  $2SD$ );

the number 4 was for two calculated component percentages in the mixture to be within two calculated standard errors or deviations, of which one of them made up the largest proportion of the mixture;

the number 3 was for two calculated component percentages in the mixture to be within two calculated standard errors or deviations, of which none of them was the largest proportion in the mixture;

the number 2 was for one calculated component percentage in the mixture, which made up the largest proportion of the mixture, to be within two calculated standard errors or deviations;

the number 1 was for one calculated component percentage, which did not make up the largest proportion of the mixture, to be within two standard errors or deviations; and

the number 0 was for the no solution situation and for calculated standard error or deviation to be greater than calculated weighted mean mixture component fractions.

Example: For MKTLCS Mixture (Calculated by FREQC program).

WT.MEAN MILKFAT = 0.29875  
STANDARD DEVIATION +/- 0.12851

WT.MEAN TALLOW = 0.40375  
STANDARD DEVIATION +/- 0.18660

WT.MEAN COTTON SEED OIL = 0.29500  
STANDARD DEVIATION +/- 0.14254

ARITHMETIC MEAN AND ITS PROBABLE ERROR:  
#####

PROBABLE FAT 1 VALUE = 0.29796  
ITS PROBABLE ERROR = +/- 0.00969  
ITS STANDARD DEVIATION +/- 0.12851

PROBABLE FAT 2 VALUE = 0.40874  
ITS PROBABLE ERROR = +/- 0.01407  
ITS STANDARD DEVIATION +/- 0.18653

PROBABLE FAT 3 VALUE = 0.29330  
ITS PROBABLE ERROR = +/- 0.01075  
ITS STANDARD DEVIATION +/- 0.14253

- \* Actual milk fat fraction in mixture = 0.3578 (i.e. 35.78%)
- \* Actual Tallow fraction in mixture = 0.34336 (i.e. 34.34%)
- \* Actual Cotton Seed Oil fraction in mixture = 0.29884 (i.e. 29.88%)

By comparing weighted mean values with the actual values of the components of mixture; it showed that all weighted mean values were within one standard deviation. Thus, this mixture was number-coded 5.

However for each program, with the exception of program CHU2, both weighted mean and arithmetic mean components percentage were considered to determine whether they were within two standard errors (or deviations) or two probable errors in the case of arithmetic mean. Therefore, there were two coded numbers for each mixture.

For the ease of understanding the tables that follow, special codes were used. A letter followed by the number 1 (e.g. A1) was used to represent mixture number-coded results obtained by comparing calculated weighted mean values with the actual components percent in the mixture; while a letter followed by the number 2 (e.g. K2) was used to denote mixture number-coded results acquired by comparing calculated arithmetic mean values with the actual components percent in the mixture.

Thus, special codes for the programs results were:

CRA1:	A1,A2
CRA2:	B1,B2
CRA4:	C1,C2
CRA5:	D1,D2
CRA3 :	E1,E2
CRA4 :	F1,F2
GLC1 :	G1,G2
GLC2 :	H1,H2
GLC3 :	I1,I2
GLC4 :	J1,J2
FREQC:	K1,K2
CHU2 :	L1

This ensured that the use of Analysis of Variance to determine the best F77 Fortran program was possible.

The CRA1 and CRA2 programs were omitted from the above list because weighted mean standard errors calculated by using Cramer's Rule were too small to be useful in estimation of error in calculated weighted mean mixture component proportions. Both programs are listed in the appendix.

Table 2 : Number - coded Results Of Mixtures That Had Milkfat As One Of Its Components.

MIXTURE	A1	A2	B1	B2	C1	C2	D1	D2	E1	E2	F1	F2	G1	G2	H1	H2	I1	I2	J1	J2	K1	K2	L1	SUM	SUM OF SQUARE
AMKSBMZ	0	0	2	4	0	0	2	4	5	3	5	3	3	1	1	1	1	1	3	1	5	1	5	51	183
MKTLCN	5	1	5	1	5	1	5	1	1	0	5	0	4	0	4	0	4	0	4	0	5	0	5	56	244
MKSBSF	2	4	2	4	2	4	2	4	5	0	4	0	2	2	4	2	4	2	2	2	5	2	4	64	222
AMKSFSB	0	0	0	0	0	0	0	0	0	1	5	1	0	1	0	1	0	1	0	1	5	1	4	21	73
CSMZMK	0	0	5	3	0	0	2	3	2	1	4	1	4	0	5	0	5	0	4	0	5	0	1	45	177
MKMZCS	0	0	0	0	0	0	0	0	0	2	0	2	0	3	3	0	3	0	4	4	4	5	3	38	142
MZCSMK	2	0	5	1	2	0	5	1	4	1	2	1	1	1	0	4	0	4	1	1	4	4	5	49	175
MKCSMZ	0	0	0	0	0	0	0	0	0	0	2	0	4	0	2	0	0	1	5	0	5	0	5	24	100
AAMKCSMZ	0	0	0	0	0	0	0	0	0	0	2	0	4	0	2	1	2	1	4	0	5	0	5	26	96
MKSBCS	4	4	4	4	4	4	4	5	0	4	4	4	2	2	4	4	4	4	2	2	5	4	4	82	322
CMKSBCS	4	5	4	5	4	5	4	5	1	4	5	4	5	3	4	3	4	3	5	1	5	5	4	92	398
MKSFCs	5	1	5	0	5	1	5	0	1	0	5	0	5	1	5	1	5	1	5	1	5	1	2	60	262
CMKSFCs	5	5	4	4	4	5	4	4	0	0	5	0	5	5	5	5	5	5	5	5	5	5	2	92	434
CMKCCNCS	4	3	0	1	5	5	0	1	1	0	3	0	5	0	5	0	5	0	5	0	5	0	5	53	237
MKCCNCS	2	1	0	1	1	1	0	1	0	0	3	0	5	0	5	2	5	2	5	0	5	2	5	46	180
CMKSFHZ	5	2	1	1	5	2	1	2	4	1	2	1	0	0	0	0	0	0	0	0	5	0	5	37	137
MKSPMZ	4	2	1	2	4	2	1	2	4	1	1	1	0	4	0	1	0	4	0	1	5	1	5	46	154
CMKCCNSB	0	0	3	1	0	0	3	1	1	0	1	0	2	0	0	0	0	0	2	0	5	0	5	24	80
MKCCNSB	0	0	5	1	0	0	5	1	1	1	1	1	0	0	0	0	0	0	0	0	5	0	4	25	97
CMKTLsB	1	1	1	1	1	1	1	1	0	0	3	0	0	1	0	1	0	0	0	0	5	0	5	23	69
MKTLsB	1	1	1	1	1	1	1	1	1	0	3	0	5	0	5	0	5	0	5	0	5	0	5	42	168
MKCCNMZ	0	0	5	1	0	0	5	1	1	0	4	0	2	0	2	0	2	0	4	0	5	0	5	39	159
CMKCCNMZ	0	0	5	1	0	0	5	1	0	0	3	0	2	0	2	2	2	2	2	0	5	0	5	37	135
CMKSFCCN	1	5	3	5	1	5	3	5	0	1	3	1	4	1	4	4	4	4	4	1	5	4	5	73	295
MKSFCcN	3	5	3	5	1	5	3	5	0	1	3	1	4	1	5	1	5	1	4	1	5	1	5	68	276
AMKTLCCN	0	1	3	1	0	1	3	1	0	0	3	0	2	0	1	0	1	0	4	0	5	0	0	26	78
AMKTLCCN	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	5	0	4	12	50
CMKTLMZ	5	5	5	5	3	5	3	5	0	0	3	0	4	0	4	0	4	0	4	0	5	0	5	65	291
MKTLMZ	5	5	5	5	3	5	3	5	0	0	3	0	5	2	4	2	4	2	5	2	5	2	5	77	329
CMKTLsF	4	0	4	0	4	0	4	0	0	0	5	0	4	0	1	0	0	0	1	0	4	0	0	31	123
MKTLsF	4	0	4	0	4	0	4	0	2	0	5	0	4	0	1	0	1	0	4	0	4	0	0	37	143
MKTLCS	1	0	1	0	4	0	4	0	0	0	0	0	5	1	5	1	5	1	5	1	5	1	5	45	189
CMKTLCS	3	0	1	1	4	0	4	1	0	0	0	0	4	1	2	3	4	1	4	1	5	1	5	45	159
SUM	70	51	87	59	67	53	86	61	36	19	102	19	101	29	83	41	82	44	102	25	162	38	134	1551	6177
SS	280	205	355	215	259	221	332	227	118	49	386	49	415	79	337	123	344	138	428	63	790	126	630	86749	

Table 3 : Number - coded Results Of Mixtures With And Without Milkfat As One Of The Mixture Components

MIX	C1	C2	D1	D2	G1	G2	H1	H2	E1	E2	F1	F2	K1	K2	L1	SUM
M1	0	4	0	2	0	4	0	2	4	0	5	0	5	2	5	33
M2	5	1	5	0	4	3	4	5	5	5	4	5	5	5	4	60
M3	5	1	3	3	0	1	0	1	2	1	5	1	5	4	5	37
M4	0	0	4	0	2	0	0	0	4	0	4	0	0	0	4	18
M5	5	5	5	5	4	4	4	4	1	4	1	4	5	4	5	60
M6	0	0	5	5	0	4	0	4	1	1	5	1	5	4	4	39
M7	5	1	4	1	3	4	5	4	1	5	5	5	5	4	4	56
M8	5	4	5	1	3	4	3	5	1	1	5	1	5	5	4	52
M9	5	1	4	1	0	1	3	1	2	1	5	1	5	1	5	36
M10	5	5	4	1	0	4	4	4	0	5	5	5	5	5	5	57
M11	4	2	4	2	0	0	0	2	0	0	5	0	5	2	5	31
M12	5	4	4	4	5	1	3	4	0	5	5	5	5	4	5	59
M13	5	4	4	1	2	5	0	5	4	0	0	0	5	5	5	45
M14	0	0	2	4	3	1	1	1	5	3	5	3	5	1	5	39
M15	5	1	5	1	4	0	4	0	1	0	5	0	5	0	5	36
M16	2	4	2	4	2	2	4	2	5	0	4	0	5	2	4	42
M17	0	0	0	0	0	1	0	1	0	1	5	1	5	1	4	19
M18	0	0	2	3	4	0	5	0	2	1	4	1	5	0	0	27
M19	0	0	0	0	3	3	0	3	2	0	2	0	5	3	5	26
M20	0	0	0	0	4	0	2	0	0	0	2	0	5	0	5	18
M21	0	0	0	0	4	0	2	1	0	0	2	0	5	0	5	19
M22	5	0	5	1	1	0	0	0	1	1	4	1	5	0	5	29
M23	5	1	5	0	0	1	2	1	2	1	2	1	5	1	5	32
M24	4	4	4	5	2	2	4	4	0	4	4	4	5	4	4	54
M25	4	5	4	5	5	3	4	3	1	4	5	4	5	5	4	61
M26	5	1	5	0	5	1	5	1	1	0	5	0	5	1	2	37
M27	4	5	4	4	5	5	5	5	0	0	5	0	5	5	2	54
M28	5	5	0	1	5	0	5	0	1	0	3	0	5	0	5	35
M29	1	1	0	1	5	0	5	2	0	0	3	0	5	2	5	30
M30	5	2	1	2	0	0	0	0	4	1	2	1	5	0	5	28
M31	4	2	1	2	0	4	0	1	4	1	1	1	5	1	5	32
M32	0	0	5	1	4	0	4	1	1	1	4	1	4	1	4	31
M33	0	0	3	1	2	0	0	0	1	0	1	0	5	0	5	18
M34	0	0	5	1	0	0	0	0	1	1	1	1	5	0	4	19
M35	1	1	1	1	0	0	1	0	0	0	3	0	5	0	5	18
M36	1	1	1	1	5	0	5	0	1	0	3	0	5	0	5	27
M37	0	0	5	1	4	0	2	0	1	0	4	0	5	0	5	27
M38	0	0	5	1	2	0	2	2	0	0	3	0	5	0	5	25
M39	1	5	3	5	4	1	4	4	0	1	3	1	5	4	5	46
M40	1	5	3	5	4	1	5	1	0	1	3	1	5	1	5	41
M41	0	1	3	1	2	0	1	0	0	0	3	0	5	0	0	16
M42	0	0	0	0	0	0	0	0	0	0	3	0	5	0	4	12
M43	3	5	3	5	4	0	4	0	0	0	3	0	5	0	5	37
M44	3	5	3	5	5	2	4	2	0	0	3	0	5	2	5	44
M45	4	0	4	0	4	0	1	0	0	0	5	0	4	0	0	22
M46	4	0	4	0	4	0	1	0	2	0	5	0	4	0	0	24
M47	4	0	4	0	5	1	5	1	0	0	0	0	5	1	5	31
M48	4	0	4	1	4	1	2	3	0	0	0	0	5	1	5	30
M49	2	0	5	1	1	1	0	4	4	1	2	1	4	4	5	35
SUM	126	86	152	89	129	65	115	84	65	50	166	50	236	85	207	1704
SS	550	344	628	317	515	213	457	290	209	172	680	172	1164	317	975	67808

Where

M1=OCSCCNMZ	M26=MKSFCS
M2=OMZCSMK	M27=CMKSFCS
M3=OSFMZCCN	M28=CMKCCNCS
M4=OTLMZCS	M29=MKCCNCS
M5=OMZCSSB	M30=CMKSFMZ
M6=OSFSBCCN	M31=MKSFMZ
M7=OSFSBCCN	M32=SBSFMZ
M8=OCCNSFSB	M33=CMKCCNSB
M9=OMZCCNSF	M34=MKCCNSB
M10=OCCNMZSF	M35=CMKTLSE
M11=OCSTMZCCN	M36=MKTLSE
M12=OSFCCNMZ	M37=MKCCNMZ
M13=OCSTMZSB	M38=CMKCCNMZ
M14=AMKSEMZ	M39=CMKSFCCN
M15=MKTLCN	M40=MKSFCCN
M16=MKSBSF	M41=ACMKTLCN
M17=AMKSFBS	M42=AMKTLCN
M18=CSMZMK	M43=CMKTLMZ
M19=MKMZCS	M44=MKTLMZ
M20=MKCSMZ	M45=CMKTLSP
M21=AAMKCSMZ	M46=MKTLCS
M22=CSMZTL	M47=CMKTLCS
M23=MZCSTL	M48=CMKTLCS
M24=MKSBCS	M49=MZCSMK
M25=CMKSBCS	

5.2.1 Case 1: Consider only those mixtures that had milkfat as one of the components

By using Table 2 above, the following calculation was carried out to determine which program produced the best results:

2

$$(1) \text{ Correction Factor C.F.} = (1551) / (33 * 23) \\ = 3169.44$$

(2) Sum of square SS, Programs

$$\begin{aligned}
 & \begin{array}{ccccccc} 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{array} \\
 & = (70 + 51 + 87 + 59 + 67 + 53 + 86 + \\
 & \begin{array}{ccccccc} 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{array} \\
 & 61 + 36 + 19 + 102 + 19 + 101 + 29 + \\
 & \begin{array}{ccccccc} 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{array} \\
 & 83 + 41 + 82 + 44 + 102 + 25 + 162 + \\
 & \begin{array}{cc} 2 & 2 \end{array} \\
 & 38 + 134 )/33 - C.F. \\
 & = 901.26
 \end{aligned}$$

(3) SS, Mixture = (86749/23) - C.F.

$$= 602.26$$

(4) SS, Total = (6177 - C.F.) = 3007.56

(5) SS, Error = (3007.56 - 901.26 - 602.26)

$$= 1504.04$$

(6) Degree of freedom Df, programs = 23 - 1 = 22

(7) Df, Mixture = 33 - 1 = 32

(8) Df, Total = 759 - 1 = 758

(9) Df, Error = 758 - 22 - 32 = 704

(10) Mean Square MS, program = 901.26/22 = 40.97

(11) MS, Mixture = 602.26/32 = 18.82

$$(12) \text{ MS, Error} = 1504.04/704 = 2.14$$

$$(13) \text{ Variance Ratio F, program} = 40.97/2.14$$

$$= 19.15$$

$$(14) \text{ F, Mixture} = 18.82/2.14$$

$$= 8.79$$

Analysis Of Variance Table:

Source of variation	Df	SS	MS	F
Program	22	901.26	40.97	19.15
Mixture	32	602.26	18.82	8.79
Error	704	1504.04	2.14	
Total	758	3007.56		

The calculated F value, with 22 degrees of freedom in the numerator and 32 degrees of freedom in the denominator, must exceed 1.89 to be significant at the 5% level and must exceed 2.47 to be significant at the 1% level (refer to Statistical chart 3 and 4 of "Laboratory Methods for Sensory Evaluation Of Food" - Larmond, 1977).

Since there is a significant difference among the programs, the ones that are different can be determined by using Tukey's Test (Larmond, 1977):

Programs Score:-

A1	A2	B1	B2	C1	C2	D1	D2	E1	E2
70	51	87	59	67	53	86	61	36	19
F1	F2	G1	G2	H1	H2	I1	I2	J1	J2
102	19	101	29	83	41	82	44	102	25

K1	K2	L1
162	38	134

Program Mean:

A1	A2	B1	B2	C1	C2	D1	D2	E1	E2	F1	F2
2.19	1.55	2.72	1.79	2.09	1.61	2.69	1.85	1.09	0.58	3.09	0.58

G1	G2	H1	H2	I1	I2	J1	J2	K1	K2	L1
3.16	0.88	2.59	1.24	2.56	1.33	3.19	0.76	5.06	1.15	4.06

Re-arrange Program Mean according to their magnitude:

K1	L1	F1	J1	G1	B1	D1	H1	I1	A1	C1
5.06	4.06	3.09	3.19	3.16	2.72	2.69	2.59	2.56	2.19	2.09

D2	B2	C2	A2	I2	H2	K2	E1	G2	J2	E2	F2
1.85	1.79	1.61	1.55	1.33	1.24	1.15	1.09	0.88	0.76	0.58	0.58

$$\text{Standard Error SE} = \text{SQRT} (2.14/33)$$

$$= 0.255$$

By using chart of "Laboratory Methods for Sensory Evaluation Of Food", least significant difference was calculated:

$$\text{Least significant difference} = 0.255 * 5.01 = 1.28$$

Hence, any two programs means that differ by 1.28 or more were significantly different at the 5% level.

$$K1 - L1 = 1.00 < 1.28$$

$$K1 - F1 = 1.97 > 1.28$$

$$K1 - J1 > 1.28$$

$$K1 - G1 > 1.28$$

$$K1 - B1 > 1.28$$

$$K1 - D1 > 1.28$$

$$K1 - H1 > 1.28$$

$$K1 - I1 > 1.28$$

K1 - A1 > 1.28  
 K1 - C1 > 1.28  
 K1 - D2 > 1.28  
 K1 - B2 > 1.28  
 K1 - C2 > 1.28  
 K1 - A2 > 1.28  
 K1 - I2 > 1.28  
 K1 - H2 > 1.28  
 K1 - K2 > 1.28  
 K1 - E1 > 1.28  
 K1 - G2 > 1.28  
 K1 - J2 > 1.28  
 K1 - E2 > 1.28  
 K1 - F2 > 1.28

The above results show that the best program is FREQC. The difference between FREQC and CHU2 is not significant; while the rest of the programs differ significantly from FREQC.

To determine whether there is any significant difference between programs using mean coefficient of variation and programs without at 5 % level:

$$\begin{aligned}
 G1 - I1 &= 3.16 - 2.56 = 0.60 \\
 &< 1.28
 \end{aligned}$$

Therefore, there is no significant difference between GLC1 and GLC3 programs.

$$\begin{aligned}
 A1 - C1 &= 2.19 - 2.09 = 0.10 \\
 &< 1.28
 \end{aligned}$$

Thus, there is no significant difference between CRAM1 and CRAM4 programs.

$$\begin{aligned}
 F1 - E1 &= 3.09 - 1.09 = 2.00 \\
 &> 1.28
 \end{aligned}$$

Hence, there is significant difference between CRA4 and CRA3 programs, and CRA4 program gave better results with program mean of 3.09.

5.2.2 Case 2: Consider all mixtures: with or without milkfat as one of the components in mixtures

By using Table 3 above, the following calculation was carried out to determine which program gave the best results:

$$\begin{aligned}
 (1) \text{ Correction Factor C.F.} &= \frac{(1704)^2}{(15 * 49)} \\
 (2) \text{ Sum of square SS, Program} &= \frac{(126^2 + 86^2 + 152^2 + 89^2 + 129^2 + 65^2 + 115^2 + 84^2 + 65^2 + 50^2 + 166^2 + 50^2 + 236^2 + 85^2 + 207^2)}{49} - \text{C.F.} \\
 &= 906.54 \\
 (3) \text{ SS, Mixture} &= (67808/15) - \text{C.F.} = 570.03 \\
 (4) \text{ SS, Total} &= (550 + 344 + 628 + 317 + 515 + 213 + 457 + 290 + 209 + 172 + 680 + 172 + 1164 + 317 + 975) - \text{C.F.} \\
 &= 3052.5 \\
 (5) \text{ SS, Error} &= 3052.5 - 570.03 - 906.54
 \end{aligned}$$

- = 1575.93
- (6) Degree of freedom  
Df, Program =  $15 - 1 = 14$
- (7) Df, Mixture =  $49 - 1 = 48$
- (8) Df, Total =  $(49 * 15) - 1$   
= 734
- (9) Df, Error =  $734 - 14 - 48$   
= 672
- (10) Mean square MS, Program =  $906.54/14 = 64.75$
- (11) MS, Mixture =  $570.03/48 = 11.88$
- (12) MS, Error =  $1575.93/672 = 2.35$
- (13) Variance Ratio  
F, Program =  $64.75/2.35 = 27.55$
- (14) F, Mixture =  $11.88/2.35 = 5.06$

Analysis of Variance Table:

Source of variation	Df	SS	MS	F
Program	14	906.54	64.75	27.55
Mixture	48	570.03	11.88	5.06
Error	672	1575.93	2.35	
Total	734	3052.50		

With 14 degrees of freedom in the numerator and 672 degrees of freedom in the denominator, the calculated F values must exceed 1.71 to be significant at 5% level and must exceed 2.11 to be significant at 1% level.

Since there is a significant difference among the programs, the ones that are different can be determined by Tukey's Test (Larmond, 1977):

Program Score:

C1	C2	D1	D2	G1	G2	H1	H2	E1	E2
126	86	152	89	129	65	115	84	65	50

F1	F2	K1	K2	L1
166	50	236	85	207

Program mean:

C1	C2	D1	D2	G1	G2	H1	H2	E1	E2
2.57	1.76	3.10	1.82	2.63	1.33	2.35	1.71	1.33	1.02

F1	F2	K1	K2	L1
3.39	1.02	4.81	1.74	4.23

Re-arrange the program mean according to their magnitude:

K1	L1	F1	D1	G1	C1	H1	D2	C2	K2
4.81	4.23	3.39	3.10	2.63	2.57	2.35	1.82	1.76	1.74

H2	G2	E1	E2	F2
1.71	1.33	1.33	1.02	1.02

Standard Error SE =  $\text{SQRT}(2.35/49) = 0.219$

Least significant difference =  $4.80 * 0.219 = 1.05$

Any two program means that differ by 1.05 or more are significantly different at the 5% level.

$$K1 - L1 = 0.59 < 1.05$$

$$K1 - F1 = 1.39 > 1.05$$

$$K1 - D1 > 1.05$$

$$K1 - G1 > 1.05$$

$$K1 - C1 > 1.05$$

$$K1 - H1 > 1.05$$

K1 - D2 > 1.05  
 K1 - C2 > 1.05  
 K1 - K2 > 1.05  
 K1 - H2 > 1.05  
 K1 - G2 > 1.05  
 K1 - E1 > 1.05  
 K1 - E2 > 1.05  
 K1 - F2 > 1.05

Again, the program FREQC gives the best results. There is no significant difference between FREQC and CHU2 programs, though FREQC differs significantly from the rest of the programs.

To determine whether there is significant difference between programs using mean coefficient of variation and those without at 5 % level :

$$\begin{aligned}
 F1 - E1 &= 3.39 - 1.33 \\
 &= 2.06 > 1.05
 \end{aligned}$$

Therefore, there is significant difference between CRA4 and CRA3 programs.

FREQC program gave the best results in both cases; hence it will be used to test the literature components data to determine whether there is any difference in accuracy compared with those components data obtained from experiment.

### 5.3 Accuracy Of Error Estimation

The accuracy of error estimation, produced by the FREQC program, can be determined by comparing actual errors (i.e. difference between actual and calculated components percents) with standard deviations of the weighted mean values.

$$\text{Actual Error} = \text{ABS}(\text{Calculated mixture component proportion value} - \text{Actual mixture component proportion value})$$

(where ABS means absolute value)

$$\text{Percentage Actual Error} = \frac{\text{Actual Error}}{\text{Actual component value}} * 100\%$$

$$\text{Coefficient of variation} = \frac{\text{Standard deviation}}{\text{Weighted mean}} * 100\%$$

When coefficient of variation is equal to or greater than the actual error but not greater than 100%, then the error estimation for the calculated component percent is good; otherwise, the estimation is poor.

#### 5.3.1 Determination Of The Accuracy Of Experimental Data

Each mixture component was considered separately by first gathering all those mixtures that had the common component; followed by the calculation of actual error, percentage actual error, standard deviation and coefficient of variation of the component. The results are tabulated in the following tables:

Table 4: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Milkfat Mixture Component

Mixture	Actual Error	Percentage Actual Error	Standard Deviation	Coefficient Of Variation
AMKSBMZ	7.46	9.63	18.99	27.15
MKTLCCN	12.03	13.50	14.78	19.17
MKSBSF	1.70	2.17	12.91	16.90
AMKSFSB	4.07	5.22	11.48	14.70
CSMZMK	16.92	19.57	18.81	21.77
MKMZCS	1.92	2.22	1.36	1.61
MZCSMK	16.92	19.57	33.19	47.76
MKCSMZ	1.92	2.22	2.37	2.81
AAMKCSMZ	1.92	2.22	2.37	2.81
MKSBCS	0.97	1.68	14.54	25.55
CMKSBCS	1.85	3.19	13.38	23.88
MKSFCS	1.08	1.82	9.54	16.40
CMKSFCS	2.17	3.66	11.39	19.21
CMKCCNCS	3.35	6.43	12.66	26.00
MKCCNCS	2.73	5.24	12.71	24.42
CMKSFMZ	7.75	9.94	12.96	18.46
MKSFMZ	0.08	9.94	13.01	16.69
CMKCCNSB	13.91	15.89	15.53	21.10
MKCCNSB	9.70	11.09	16.05	20.62
CMKTLNB	14.88	22.70	15.54	30.67
MKTLNB	16.84	25.70	16.14	33.14
MKCCNMZ	16.23	19.70	14.61	22.09
CMKCCNMZ	17.28	20.99	18.84	27.41
CMKSFCN	4.10	6.23	17.99	27.32
MKSFCN	3.54	5.37	16.95	27.21
ACMKTLCN	33.70	37.79	26.07	47.00
AMKTLCN	31.07	34.84	25.09	43.18
CMKTMZ	2.86	6.25	13.10	30.50
MKTMZ	1.48	3.22	12.73	28.73
MKTLNF	17.83	22.84	29.66	49.25
CMKTLNF	27.11	34.74	27.55	54.10
MKTLCS	5.91	16.50	12.85	43.02
CMKTLCS	6.08	16.99	10.95	36.85
OMZCSMK	1.35	1.67	6.04	7.34
(MEAN		12.37%		15.06%

Table 5: Calculated Actual Errors, Percentage Actual Errors, Standard Deviations and Coefficients Of Variation Of Maize Oil Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
OCSCCNMZ	8.61	32.40	9.75	27.73
OMZCSMK	0.41	10.05	1.85	41.09
OSFMZCCN	3.29	13.77	8.93	32.86
OTLMZCS	ONLY ONE SET OF DATA		AVAILABLE	
OMZCSSB	0.53	2.01	13.04	50.30
OMZCCNSF	3.12	13.07	9.07	33.58
OCCNMZSF	1.25	5.21	8.93	35.55
OCSMZCCN	8.50	31.98	11.56	32.97
OSFCCNMZ	5.06	21.21	8.46	29.24
OCSMZSB	3.39	12.81	11.57	50.14
AMKSBMZ	7.67	129.46	10.43	76.71
CSMZMK	5.13	273.53	4.43	63.34
MKMZCS	7.63	406.94	7.31	76.91
MZCSMK	5.96	317.98	4.73	60.44
MKCSMZ	5.96	317.98	4.18	53.35
AAMKCSMZ	5.96	317.98	4.18	53.35
CSMZTL	14.33	111.13	11.11	40.79
MZCSTL	13.78	106.84	9.83	36.85
CMKSFMZ	2.42	14.32	6.05	41.73
MKSFMZ	1.47	8.86	4.99	32.31
SBSFMZ	6.85	67.42	22.98	135.15
MKCCNMZ	5.72	82.66	10.83	85.67
CMKCCNMZ	5.58	80.64	10.55	84.41
CMKTMZ	5.70	21.42	13.85	66.24
MKTMZ	5.32	19.99	13.61	63.92
(MEAN		27.36	10.01)	

Table 6: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Sunflower Oil Mixture Component

Mixture	Actual Error	Percentage Actual Error	Standard Deviation	Coefficient Of Variation
OSFMZCCN	5.03	9.88	12.16	26.53
OSFSBCCN	0.46	1.85	18.30	71.57
OSFCCNSB	0.61	2.43	17.05	66.35
OCCNSFSB	1.41	5.62	17.91	67.57
OMZCCNSF	6.40	12.51	12.98	29.16
OCCNMZSF	2.61	5.13	9.43	19.54
OSFCCNMZ	7.47	14.69	13.72	31.61
MKSBSF	5.26	47.32	9.84	60.11
AMKSFSB	5.89	52.95	10.93	64.29
MKSFGS	0.17	0.67	11.49	45.50
CMKSFGS	0.73	2.91	12.09	46.86
CMKSFMZ	0.07	136.88	9.12	75.29
MKSFMZ	5.57	108.95	8.94	83.66
SBSFMZ	5.93	26.57	12.10	42.84
CMKSFCCN	4.44	20.07	15.25	57.41
MKSFCCN	4.81	21.74	14.44	53.59
CMKTLSF	9.46	119.74	15.81	91.11
MKTLSF	4.46	56.44	11.02	89.21
(MEAN		18.72	12.92)	

Table 7: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Soya Bean Oil Mixture Component

Mixture	Actual Error	Percentage Actual Error	Standard Deviation	Coefficient Of Variation
OMZCSSB	5.93	12.57	15.25	28.74
OSFSECCN	1.34	2.68	18.46	35.96
OSFCCNSB	0.90	1.80	16.57	32.56
OCCNSFSB	1.90	3.80	19.00	39.51
OCSMZSB	5.93	12.57	17.09	32.20
AMKSEBMZ	0.56	3.36	21.16	122.84
MKSEBF	3.81	35.26	5.39	77.04
AMKSFSB	1.31	12.14	6.01	63.21
MKSECS	2.41	10.27	7.43	35.31
CMKSECS	0.12	0.49	8.07	34.57
SBSFMZ	16.78	24.85	20.01	39.43
CMKCCNSB	2.88	75.86	4.89	73.25
MKCCNSB	3.21	84.45	5.57	79.51
CMKTLNB	5.00	74.17	10.06	51.25
MKTLNB	6.22	42.53	9.27	44.46
(MEAN		23.79	12.28)	

Table 8: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Cotton Seed Oil Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
OCSCCNMZ	8.93	32.56	9.11	49.23
OMZCSMK	2.15	14.34	7.09	55.23
OTLMZCS	ONLY ONE SET OF DATA AVAILABLE			
OMZCSSB	4.75	18.01	4.67	21.58
OCSMZCCN	6.82	24.86	11.54	55.97
OCSMZSB	1.90	7.18	11.60	47.36
CSMZMK	10.29	87.86	15.26	69.36
MKMZCS	2.21	18.88	9.43	99.26
MZCSMK	12.79	109.21	34.55	141.03
MKCSMZ	3.88	33.11	4.87	62.20
AAMKCSMZ	3.88	33.11	4.87	62.20
CSMZTL	6.03	24.96	8.36	46.09
MZCSTL	2.28	9.43	13.97	63.83
MKSBCS	2.43	13.05	15.34	72.86
CMKSBCS	2.80	15.04	15.04	70.20
MKSFCS	1.45	9.26	12.41	72.63
CMKSFCS	1.46	7.36	11.59	67.71
CMKCCNCS	6.31	21.53	14.28	40.07
MKCCNCS	4.81	16.42	13.93	40.82
MKTLCS	0.38	1.29	14.25	48.32
CMKTLCS	0.48	1.62	13.87	45.66
(MEAN		20.52	12.30)	

Table 9: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Coconut Oil Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
OCSCCNMZ	0.49	1.07	8.91	19.16
OSFMZCCN	2.09	8.29	11.67	50.37
OSFSBCCN	2.52	10.10	7.12	11.78
OSFCCNSB	2.01	8.07	5.30	23.16
OCCNSFSB	0.01	0.04	3.84	67.57
OMZCCNSF	0.07	0.29	12.41	48.98
OCCNMZSF	2.01	7.96	11.67	50.19
OCSMZCCN	0.95	2.07	9.97	22.13
OSFCCNMZ	1.87	1.87	12.53	53.57
MKTLCCN	3.85	94.62	5.43	68.57
CMKCCNCS	4.95	26.54	7.87	57.45
MKCCNCS	3.59	19.23	7.47	49.64
CMKCCNSB	10.62	122.46	13.88	71.99
MKCCNSB	7.50	86.51	11.02	68.15
MKCCNMZ	5.87	54.68	8.79	52.94
CMKCCNMZ	6.92	64.47	12.91	73.20
CMKSFCCN	0.98	8.12	5.76	52.07
MKSFCCN	0.46	3.79	6.91	59.72
ACMKTLCCN	7.84	192.65	7.32	61.41
AMKTLCCN	7.63	187.47	11.44	97.80
(MEAN		23.40	9.11)	

Table 10: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Tallow Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
OTLMZCS	ONLY ONE SET OF DATA		AVAILABLE	
MKTLCCN	8.52	126.00	15.12	98.86
CSMZTL	7.53	11.96	15.71	28.36
MZCSTL	11.48	18.24	14.72	28.61
CMKTLSE	6.27	27.46	15.78	54.19
MKTLSE	6.93	30.33	16.41	55.13
ACMKTLCCN	25.48	376.60	25.66	79.59
AMKTLCCN	23.74	350.85	24.46	80.19
CMKTLMZ	7.37	26.70	15.62	44.67
MKTMZ	5.47	19.83	15.53	46.96
CMKTLSE	16.15	114.89	32.20	106.59
MKTLSE	11.15	79.33	28.91	114.67
MKTLCS	6.04	17.59	18.66	46.22
CMKTLCS	4.16	12.13	18.11	47.03
(MEAN		27.06		19.76)

### 5.3.1.1 Discussion

In a normal distribution 68% of the values will be within  $X' \pm 1SD$  (where  $X'$  is the calculated mean value and  $SD$  is its standard deviation), 95% within  $X' \pm 2SD$ , and 99.7% within  $X' \pm 3SD$ . This information will be used as a guide in the discussion that follows.

For those results without solution or having only one set of data, they are omitted in the discussion as they are probably due to the systematic errors.

From above tables, it can be concluded that:

- (i) Milkfat component error estimation is good, as 85.29% of the calculated results are within  $\pm 1SD$  and 100% of the results are within  $\pm 2SD$ ; with mean standard deviation of  $\pm 15.06\%$ , mean percentage actual error  $\pm 12.37\%$  and range  $\pm 1.68\% - 37.79\%$ ;
- (ii) Maize oil component error estimation is good, as 70.83% of the calculated results are within  $\pm 1SD$  and 100% of the results are within  $\pm 2SD$ ; with mean standard deviation  $\pm 10.01\%$ , mean percentage actual error  $\pm 27.36\%$  and range  $\pm 2.01\% - 82.66\%$ ;
- (iii) Sunflower oil component error estimation is good, as 100% of the calculated results are within  $\pm 1SD$ ; with mean standard deviation of  $\pm 12.92\%$ , mean percentage actual error  $\pm 18.72\%$  and range  $\pm 1.85\% - 56.44\%$ ;
- (iv) Soya Bean oil component error estimation is good, as 100% of the calculated results are within  $\pm 1SD$ ; with mean standard deviation of  $\pm 12.28\%$ , mean percentage actual error  $\pm 23.79\%$  and range  $\pm 1.80\% - 84.45\%$ ;
- (v) Cotton Seed oil component error estimation is good, as 95% of the calculated results are within  $\pm 1SD$ ; 100% of the calculated results are within  $\pm 2SD$ ; with mean standard deviation of  $\pm 12.30\%$ , mean percentage actual error  $\pm 20.52\%$  and range  $\pm 1.29\% - 87.86\%$ ;
- (vi) Coconut oil component error estimation is good, as 95% of the calculated results are within  $\pm 1SD$  and 100% of the results are within  $\pm 2SD$ ; with mean standard deviation of  $\pm 9.11\%$ , mean percentage actual error of  $\pm 23.40\%$  and range  $\pm 0.04\% - 94.62\%$ ;
- (vii) Tallow component error estimation is good, as 100% of the calculated results are within  $\pm 1SD$ ; with mean standard deviation of  $\pm 19.76\%$ , mean percentage actual error  $\pm 27.06\%$  and range

+/- 11.96% - 79.33%.

It showed in the Table 5 that when cotton seed oil and maize oil were two of the three mixture components, the determination of maize oil fraction in the mixtures gave poor results. This is due to the fact that their fatty acid distribution are similar.

In fact, according to Jebson and Curtis (1981), coconut oil has a higher proportion of fatty acids present in milk fat than the other oils and many of the acids are present in proportions somewhat similar to milk fat. This explains why the FREQC program did not give satisfactory estimation of the proportion of coconut oil in the MKTLCCN and CMKTLCCN mixtures.

In general, if the fatty acid compositions of two of the three mixture components are similar then their proportions estimation will be inaccurate.

### 5.3.2 Testing Literature Mixture Component Data

Literature data were obtained from Hildith and William (1964); except the sunflower oil data which were acquired from Jebson and Curtis (1981) (refer to Table A1-Table A38 in appendix for experimental component data and Table A39(i)-Table A39(ii) for literature data).

All fatty acid experimental data of mixture components were replaced by literature values and the following results were obtained by running FREQC program :

Table 11: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Literature Milkfat Mixture Component

Mixture	Actual Error	Percentage Actual Error	Standard Deviation	Coefficient Of Deviation
MKTLMZU	4.09	8.93	18.26	36.61
CMKTLMZU	6.89	15.03	17.09	32.45
MKCCNMZU	25.13	30.51	20.78	36.32
CMKCCNMZU	2.85	3.46	11.24	14.13
CMKSFCSU	8.55	14.43	19.75	29.12
MKSFCSU	8.11	13.69	7.08	13.84
CMKSFMZU	ONLY ONE SET OF DATA		AVAILABLE	
MKSFMZU	ONLY ONE SET OF DATA		AVAILABLE	
MKCCNCSU	5.04	9.69	19.68	41.88
CMKCCNCSU	1.55	2.98	16.59	30.96
CMKCCNSBU	35.04	40.03	29.88	56.92
MKCCNSBU	ONLY ONE SET OF DATA		AVAILABLE	
CMKSECSU	3.39	5.85	16.14	29.61
MKSECSU	0.36	0.63	14.19	24.37
CMKSFCCNU	NO SOLUTION			
MKSFCCNU	NO SOLUTION			
ACMKTLCNU	59.67	66.92	23.60	80.01
AMKTLCNU	ONLY ONE SET OF DATA		AVAILABLE	
CMKTLCNU	5.08	14.21	10.96	26.81
MKTLCNU	2.89	8.07	13.50	34.92
CMKTLSBU	11.03	16.83	33.44	61.36
MKTLSBU	1.19	1.82	23.55	35.30
CMKTLSFU	18.54	23.76	41.76	70.18
MKTLSFU	23.54	30.17	41.68	76.47
MKTLCNU	51.33	51.52	21.21	56.05
MKSEMZU	7.91	10.22	11.22	16.14
MZCSMKU	NO SOLUTION			
OMKCSMZU	NO SOLUTION			
MKCSMZU	NO SOLUTION			
MKSFSBU	ONLY ONE SET OF DATA		AVAILABLE	
OMZCSMKU	1.03	1.27	6.28	7.86
(MEAN	17.62		19.90)	

Table 12: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations and Coefficients Of Variation Of  
Literature Cotton Seed Oil Mixture Component

Mixture	Actual Error	Percentage Actual Error	Standard Deviation	Coefficient Of Variation
CMKSFCSU	2.19	13.99	24.64	136.15
MKSFCSU	8.86	56.60	22.18	90.53
MKCCNCSU	1.90	6.48	13.76	50.19
CMKCCNCSU	5.73	19.53	13.41	56.84
CMKSBCSU	15.88	85.27	13.47	39.05
MKSBCSU	12.13	65.13	14.52	47.20
CMKTLCSU	7.34	24.57	7.53	20.21
MKTLCSU	1.22	4.07	10.53	36.72
MZCSMKU	NO SOLUTION			
OMKCSMZU	NO SOLUTION			
MKCSMZU	NO SOLUTION			
OCSCCNMZU	1.70	6.19	19.87	77.22
OCSMZSBU	1.97	4.53	8.91	4.25
OCSMZCCNU	13.96	50.89	10.50	77.95
OTLMZCSU	17.99	106.39	29.12	83.45
OMZCSMKU	0.08	0.55	11.69	78.44
OMZCSSBU	NO SOLUTION			
(MEAN		28.52	15.40)	

Table 13: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Literature Soya Bean Oil Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
CMKCCNSBU	0.71	18.58	1.72	38.13
MKCCNSBU	ONLY ONE SET OF DATA		AVAILABLE	
CMKSBUSU	14.96	63.77	7.97	93.71
MKSBUSU	13.96	59.51	10.28	299.13
CMKTLBSU	0.13	0.88	3.30	22.77
MKTLBSU	0.13	0.88	5.21	35.95
MKSBMZU	4.67	28.00	6.94	57.81
MKSFSBU	ONLY ONE SET OF DATA		AVAILABLE	
SBSFMZU	10.53	15.59	8.39	14.71
OCSMZSBU	3.88	16.24	6.41	23.08
OCCNSFSBU	NO SOLUTION			
OSFCCNSBU	NO SOLUTION			
OSFSBCCNU	NO SOLUTION			
OMZCSSBU	NO SOLUTION			
(MEAN	25.43		6.28)	

Table 14: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Literature Sunflower Oil Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
CMKSFCSU	10.57	42.17	9.41	64.91
MKSFCSU	7.24	28.88	16.22	90.96
CMKSFMZU	ONLY ONE SET OF DATA		AVAILABLE	
MKSFMZU	ONLY ONE SET OF DATA		AVAILABLE	
CMKSFCCNU	NO SOLUTION			
MKSFCCNU	NO SOLUTION			
CMKTLSPU	1.60	20.27	0.88	9.28
MKTLSPU	6.60	83.57	5.94	40.94
MKSFBSU	ONLY ONE SET OF DATA		AVAILABLE	
SBSFMZU	4.68	15.59	21.78	14.71
OCCNMZSFU	3.65	7.18	7.39	15.65
OMZCCNSFU	4.85	9.34	1.70	3.70
OCCNSFSBU	NO SOLUTION			
OSFCCNSBU	NO SOLUTION			
OSFSBCCNU	NO SOLUTION			
OSFMZCCNU	NO SOLUTION			
(MEAN	27.34		9.05)	

Table 15: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Literature Tallow Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
MKTLMZU	0.75	2.71	21.76	76.78
CMKTLMZU	4.17	15.13	19.77	62.21
ACMKTLCCNU	47.74	705.62	11.86	21.76
AMKTLCCNU	ONLY ONE SET OF DATA		AVAILABLE	
CMKTLCSU	14.38	41.88	13.02	65.20
MKTLCSU	6.50	18.94	19.55	70.25
CMKTLSEBU	9.16	40.09	35.81	111.91
MKTLSEBU	2.79	12.20	25.31	126.21
CMKTLSEFU	15.44	109.82	41.45	140.51
MKTLSEFU	20.44	145.38	41.28	119.64
MKTLCCNU	47.74	705.62	10.55	19.36
OTLMZCSU	33.85	44.88	33.15	79.76
(MEAN		25.12	24.87)	

Table 16: Calculated Actual Errors, Percentage Actual Errors,  
Standard Deviations And Coefficients Of Variation Of  
Literature Maize Oil Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
MKTLMZU	6.72	25.26	19.10	96.05
CMKTLMZU	9.38	35.25	15.16	88.02
MKCCNMZU	3.04	43.86	11.52	115.71
CMKCCNMZU	2.42	34.97	1.01	22.49
CMKSFMZU	ONLY ONE SET OF DATA		AVAILABLE	
MKSFMZU	ONLY ONE SET OF DATA		AVAILABLE	
MKSBMZU	11.08	187.02	8.64	50.82
MZCSMKU	NO SOLUTION			
OMKCSMZU	NO SOLUTION			
MKCSMZU	NO SOLUTION			
SBSFMZU	6.85	67.42	14.18	83.41
OCSCCNMZU	6.67	25.12	18.41	55.41
OCSMZSBU	0.36	1.43	6.38	25.63
OCSMZCCNU	18.34	69.05	9.79	21.80
OCCNMZSFU	3.33	13.94	8.06	29.61
OMZCCNSFU	6.58	27.54	3.39	11.13
OTLMZCSU	13.89	180.93	15.05	69.77
OMZCSSBU	NO SOLUTION			
OSFMZCCNU	3.88	16.24	7.37	26.55
OMZCSMKU	5.81	142.11	5.17	52.21
(MEAN		32.74	10.23)	

Table 17: Calculated Actual Errors, Percentage Actual Errors, Standard Deviations And Coefficients Of Variation Of Literature Coconut Oil Mixture Component

Mixture	Actual Error	Percentage Error	Actual Standard Deviation	Coefficient Of Variation
MKCCNMZU	20.14	187.72	15.43	50.00
CMKCCNMZU	1.27	11.87	10.83	90.27
MKCCNCSU	5.03	26.96	8.69	36.71
CMKCCNCSU	3.13	16.80	9.00	41.32
CMKCCNSBU	35.83	413.38	28.83	64.78
MKCCNSBU	ONLY ONE SET OF DATA		AVAILABLE	
MKSFCCNU	NO SOLUTION			
ACMKTLCNU	10.43	256.27	12.04	83.06
AMKTLCNU	ONLY ONE SET OF DATA		AVAILABLE	
MKTLCNU	7.10	174.37	11.01	98.57
OCSCCNMZU	6.67	13.28	18.41	10.64
OCSMZCCNU	5.39	11.72	3.63	8.93
OCCNMZSFU	0.41	1.62	7.37	28.70
OMZCCNSFU	2.58	10.22	3.82	16.83
OCCNSFSBU	NO SOLUTION			
OSFCCNSBU	NO SOLUTION			
OSFSBCCNU	NO SOLUTION			
OSFMZCCNU	0.36	1.43	6.54	26.28
(MEAN		11.74	11.30)	

#### 5.3.2.1 Discussion

From the above tables, it can be concluded that:

- (i) Literature Milkfat component error estimation is good, as 76.19% of the calculated results are within  $\pm 1SD$ ; 90.48% of the calculated results are within  $\pm 2SD$ ; 100% of the calculated results are within  $\pm 3SD$ ; with mean standard deviation of  $\pm 19.90\%$ , mean percentage actual error  $\pm 17.62$  and range  $\pm 0.63\% - 37.79\%$ ;

- (ii) Literature Cotton Seed oil component error estimation is good, as 84.62% of the calculated results are within  $\pm 1SD$ ; 100% of the calculated results are within  $\pm 2SD$ ; with mean standard deviation of  $\pm 15.40\%$ , mean percentage actual error of  $\pm 28.52\%$  and range  $\pm 0.55\% - 85.27\%$ ;
- (iii) Literature Soya Bean oil component error estimation is fairly good, as 62.50% of the calculated results are within  $\pm 1SD$ ; 100% of the calculated results are within  $\pm 2SD$ ; with mean standard deviation of  $\pm 6.28\%$ , mean percentage actual error  $\pm 25.43\%$  and range  $\pm 0.88\% - 63.77\%$ ;
- (iv) Literature Sunflower oil component error estimation is fair, as 42.86% of the calculated results are within  $\pm 1SD$ ; 85.72% of the calculated results are within  $\pm 2SD$ ; 100% of the calculated results are within  $\pm 3SD$ ; with mean standard deviation of  $\pm 9.05\%$ , mean percentage actual error  $\pm 27.34\%$  and range  $\pm 7.18\% - 83.57\%$ ;
- (v) Literature Tallow component error estimation is fair, as 63.64% of the calculated results are within  $\pm 1SD$ ; 81.82% of the calculated results are within  $\pm 2SD$ ; with mean standard deviation of  $\pm 24.87\%$ , mean percentage actual error  $\pm 25.12\%$  and range  $\pm 2.71\% - 44.88\%$ ;
- (vi) Literature Maize oil component error estimation is fair, as 64.29% of the calculated results are within  $\pm 1SD$ ; 92.86% of the calculated results are within  $\pm 2SD$ ; 100% of the calculated results are within  $\pm 3SD$ ; with mean standard deviation of  $\pm 10.23\%$ , mean percentage actual error  $\pm 32.74\%$  and range  $\pm 1.43\% - 69.05\%$ ;
- (vii) Literature Coconut oil component error estimation is good, as 75% of the calculated results are within  $\pm 1SD$ ; 100% of the calculated results are within  $\pm 2SD$ ; with mean standard deviation of  $\pm 11.30\%$ ,

mean percentage actual error +/- 11.74% and range  
+/- 1.43% - 26.96%.

From above results, it is obvious that the FREQC F77 computer program can be used in determining the proportion of milk fat component in a three-component mixture using experimental and literature data. However, experimental data gave more accurate results than literature data.

#### 5.3.2.2 A Few Words About The LSQ Program

The LSQ program, listed in the appendix, was tested by both experimental and literature data. The results showed that the program did not give as good overall estimation of mixture component proportions as the FREQC program. Results calculated using experimental data gave program mean of 3.78 while literature data, in most cases, gave no solution. Provided the experimental data is used, the LSQ program can still be used in estimation of mixture component proportions.

# chapter 6

## 6 FINAL DISCUSSION

### 6.1 The Effect Of Weight Response Factors Treatment

From Table 2 and Table 3, under the column of K1, it is obvious that there is no significant difference between results obtained from data corrected by weight response factors Fw and results obtained from untreated data. This may be due to the fact that the systematic errors in the mixture fatty acid values, especially those of low carbon number saturated fatty acids, had cancelled out those in the component fatty acid values. Another possible explanation is that the systematic errors in the fatty acid values were too small, owing to the use of an improved model of Gas Liquid Chromatograph instrument, to show any effect on the calculated weighted mean values.

### 6.2 The Effect Of The Use Of Mean Coefficient Of Variation

The mean coefficient of variation of each fatty acid of components and mixtures (that had milkfat as one of its components), calculated from several sets of experimental fatty acid data, were used to compare with the calculated standard deviation of average value of duplicate fatty acid percent in some programs. They are CRAM1, CRAM2, GLC3, GLC4 and CRA4 programs. For comparison purposes, GLC3, CRAM1 and CRA4 programs were considered. If the calculated standard deviation of average fatty acid percent is less than the standard deviation calculated by multiplying average fatty acid percent by mean coefficient of variation of that fatty acid, then it will be replaced by the latter. From the analysis of variance calculation, it showed that the use of mean coefficient of variation in GLC3 and CRAM1 programs did not make any significant difference from GLC1 and CRAM4 programs. The use of mean coefficient of variation in CRA4 program did make a significant difference from CRA3 program. However, both CRA3 and CRA4 programs did not make use of the equation (3) in calculation; thus were ignored. The use of mean coefficient of variation therefore did not give any significant difference from those without.

### 6.3 Accuracy Of Weighted Mean Standard Error And Calculated Weighted Mean Component Proportions

Weighted mean standard error calculated by using Scarborough and Topping method did not give a good error estimation. As weighted mean standard error (which is  $E_i$ ) differed significantly from the alternative weighted mean standard error (which is  $E_e$ ), systematic errors were therefore likely involved. Hence, the calculated weighted mean and alternative weighted mean standard errors could not be used in error estimation.

### 6.4 Accuracy Of Standard Deviation

However, standard deviations of weighted mean mixture component proportions gave good error estimations, particularly for the FREQC program with actual errors of calculated weighted mean mixture component proportions within two standard deviations. The program mean of the FREQC program for mixtures that had milkfat as one of its components was 5.06 and the program mean for mixtures with and without milkfat as one of its components was 4.81. The average of the two program means is approximately equal to 5, which implies that almost all the calculated results had actual errors of three weighted mean mixture component proportions within two standard deviations. Therefore, the FREQC program gave good results; and the calculated results agreed with the Mathematical Model.

### 6.5 Comparison Of Results Obtained From Literature And Experimental Data

From the tables of Chapter 5, they showed that results calculated from experimental data were better than those calculated from literature data, especially for sunflower oil and tallow component data. This may be due to the fact that fatty acid compositions of oils vary greatly with climate and the strain that is grown. For example, the proportion of linoleic acid of sunflower oil can vary from 45% to 70% (Hildith and William, 1964). Also, the fatty acid

composition of milk fat relies upon the stage of lactation, the feeds, and the genetics of the cows. The new improved model of Gas Liquid Chromatograph instrument will also give more accurate results than those results obtained by old model of Gas Liquid Chromatograph instrument (i.e. literature data). Moreover, different methods of preparing fatty acid methyl esters for Gas Liquid Chromatographic analysis, in most cases, gives different results. For example, methyl esters of fatty acids prepared by A.O.C.S. method Ce 2-66 did not give as good results as those prepared by Christopherson and Glass method (1969), especially for the low carbon number saturated fatty acid values. This is because part of the Boron Trifluoride-methanol reagent dissolved in water instead of converting fatty acids to esters; worse still when water-soluble fatty acids are involved. The Shehata et al method will give the similar good results to the Christopherson and Glass method though more work is involved.

#### 6.6 Comparison Of Two Component Program With The FREQC Program

The FREQC program gave as good weighted mean estimation of milkfat component proportion in the mixtures as the program used by Jebson and Curtis (1981), though the FREQC program involved three component mixtures. Nevertheless, the estimation of second and third components in the mixtures did not always render good results. This may be owing to the presence of similarity between second and third components in fatty acid composition. Also, Gas Liquid Chromatographic analysis does not provide any detailed information on the unsaturated fatty acids, thus cis-configurations may have been treated as trans-configurations or vice versa. The existence of branched chain configuration can further complicate the situation.

The levels of contamination down to 4% can be detected quite accurately by the FREQC F77 program when experimental data are used (refer to Table A40 in appendix).

## 6.7 The Probable Areas Of Application

The FREQC program can be used in a quality assurance program. For example, in the production of seed oils, there exist the contamination of grease from machines. If the composition of grease is known and is similar to that of seed oils, the percent of contaminant in the final product can be estimated by the FREQC program.

Another probable area of application of the FREQC program is the detection of adulteration of expensive oils, such as safflower oil, for the benefit of consumers. This makes sure that consumers get what they pay for.

The problem of identifying a piece of unknown meat can also be solved by the FREQC program by first extracting fat from the meat. One possible extraction method is to heat or 'cook' the piece of meat under pressure at low temperature. The fat can be separated from meat by solidifying the fat through cooling. The fat can then be used, with another two oils of known fatty acid composition, to form a mixture. If one suspects that the unknown meat is beef then the fatty acid composition of beef is treated as the fatty acid composition of unknown meat. The estimation of mixture component proportions can then be carried out by the FREQC program. If the estimated unknown fat proportion agrees with the actual value, one can conclude that the unknown meat is beef, otherwise it is something else.

The aim of most hydrogenation reaction is to saturate fatty acids selectively, which means reducing the six double bonds to five, the five to four and so on. However, the ideal is not achieved in practice, a mixture of unsaturated, mono-saturated and saturated fatty acids is formed instead. The proportion of each mixture component (i.e. unsaturated, mono-saturated and saturated fatty acids) can be determined in the similar manner as in the analysis of three fat(s)/oil(s) mixture. For example, if the unsaturated fatty acids composition of oil, determined by gas-liquid chromatographic analysis, is as follows:

<u>Carbon Number</u>	<u>Percentage</u>
16:0	10
16:1	2
18:0	20
18:1	30
18:2	30
18:3	8

assuming that during hydrogenation, unsaturated fatty acids are all converted to mono-saturated fatty acids, then its composition will be:

<u>Carbon Number</u>	<u>Percentage</u>
16:0	10
16:1	2
18:0	20
18:1	68

Likewise, if all the mono-saturated fatty acids are converted to saturated fatty acids, its composition is:

<u>Carbon Number</u>	<u>Percentage</u>
16:0	12
18:0	88

Therefore, we know the fatty acids composition of each mixture component; and the fatty acids composition of the mixture after hydrogenation can be determined by the gas-liquid chromatographic analysis. Similarly, their fatty acids compositions can be expressed by the general mixture equations (1), (3) and (5). The FREQC F77 program can therefore be employed to estimate the fraction of each mixture component (i.e. unsaturated, mono-saturated and saturated fatty acids).

As mentioned above, almost all of the calculated weighted mean mixture component proportions are within two calculated standard deviations, therefore the accuracy of the FREQC program can be used in unlimited areas provided that each component or unknown has similar characteristic to that of oils and fats. Even in the mathematical field, the FREQC program can be modified to solve more than three three-unknown linear equations for the unknowns.

# APPENDIX

\*Note: values enclosed within the brackets are actual mixture component percent values.

Table A1: Fatty Acid Composition Of OSBSFCCN Mixture And Its Components

Fatty Acids	Soya Bean Oil (50.17%)		Sunflower Oil 25.00%		Coconut oil 24.83%		Mixture	
8:0	0.00	0.00	0.00	0.00	7.54	7.61	5.76	4.22
10:0	0.00	0.00	0.00	0.00	10.01	8.77	4.13	3.50
12:0	0.00	0.00	3.83	3.73	16.58	19.94	6.75	5.34
14:0	2.59	0.00	5.50	3.78	11.28	11.90	6.93	5.86
16:0	8.21	8.95	10.54	10.43	9.07	9.67	7.54	6.62
16:1	10.94	10.75	23.89	24.57	20.74	16.14	7.13	16.94
18:0	14.47	6.67	9.10	9.49	7.47	7.96	6.79	5.73
18:1	11.24	13.66	13.44	13.08	9.14	9.33	9.16	7.86
18:2	16.15	17.63	23.67	24.80	8.17	8.68	11.95	11.00
18:3	10.01	10.34	0.00	0.00	0.00	0.00	8.55	8.03
20:0	26.39	32.00	10.03	10.12	0.00	0.00	25.31	24.90

Table A2: Fatty Acid Composition Of OSBMZCS Mixture And Its Components

Fatty Acids	Soya Bean Oil (47.14%)		Maize Oil 26.46%		Cotton Seed Oil Mixture 26.40%			
16:0	10.98	11.15	11.48	11.29	19.24	20.02	12.96	12.77
18:0	4.48	4.54	2.25	2.58	2.91	3.30	3.45	2.99
18:1	23.30	24.09	31.17	33.49	22.05	22.76	25.50	25.61
18:0	52.77	52.29	53.12	51.34	55.07	51.66	53.34	51.96
20:0	8.47	7.93	1.97	1.30	0.73	2.27	4.75	6.68

Table A3: Fatty Acid Composition Of OSFCCNMZ Mixture And Its Components

Fatty Acids	Sunflower Oil (50.86%)		Coconut Oil 25.26%		Maize Oil 23.88%		Mixture	
8:0	0.00	0.00	4.60	4.22	0.00	0.00	2.15	2.02
10:0	0.00	0.00	9.43	8.73	0.00	0.00	1.83	1.77
12:0	0.00	0.00	46.50	44.78	0.00	0.00	10.60	10.32
14:0	0.00	0.00	18.49	21.12	0.00	0.00	3.63	3.84
16:0	7.17	6.69	9.40	9.85	11.48	11.29	9.06	8.85
18:0	4.58	4.31	2.68	3.21	2.25	2.58	3.86	2.91
18:1	17.31	17.08	6.99	6.14	31.17	33.49	17.21	18.60
18:2	69.22	69.50	1.91	1.95	53.12	51.34	51.09	51.23
20:0	1.72	2.42	0.00	0.00	1.97	1.30	0.55	0.45

Table A4: Fatty Acid Composition Of OCSCCNMZ Mixture And Its Components

Fatty Acids	Cotton Seed Oil (27.43%)	Coconut Oil 46.01%	Maize Oil 26.56%	Mixture				
8:0	0.00	0.00	4.60	4.22	0.00	0.00	2.91	2.96
10:0	0.00	0.00	9.43	8.73	0.00	0.00	2.83	2.77
12:0	0.00	0.00	46.50	44.78	0.00	0.00	22.58	19.14
14:0	0.58	0.55	18.49	21.12	0.00	0.00	8.23	8.22
16:0	18.66	19.46	9.40	9.85	11.48	11.29	11.49	12.27
18:0	2.91	3.30	2.69	3.21	2.25	2.58	2.46	3.08
18:1	22.05	22.76	6.99	6.14	31.17	33.49	17.61	19.06
18:2	55.07	51.66	1.91	1.95	53.12	51.34	31.12	31.08
20:0	0.73	2.27	0.00	0.00	1.97	1.30	0.78	1.43

Table A5: Fatty Acid Composition Of OMKCSMZ Mixture And Its Components

Fatty Acids	Milkfat (80.93%)	Cotton Seed Oil 14.98%	Maize Oil 4.09%	Mixture				
4:0	1.55	1.79	0.00	0.00	0.00	0.00	1.84	1.01
6:0	1.44	1.59	0.00	0.00	0.00	0.00	1.25	1.07
8:0	1.17	1.27	0.00	0.00	0.00	0.00	1.20	0.87
10:0	3.09	3.56	0.00	0.00	0.00	0.00	2.99	2.35
11:0	0.28	0.26	0.00	0.00	0.00	0.00	0.20	0.14
12:0	3.73	3.79	0.00	0.00	0.00	0.00	3.33	2.94
14:0	10.66	11.02	0.00	0.00	0.00	0.00	9.05	9.04
14:1	1.73	1.90	0.00	0.00	0.00	0.00	1.42	1.47
15:0	0.89	1.15	0.00	0.00	0.00	0.00	0.83	0.93
16:0Br	0.16	0.22	0.00	0.00	0.00	0.00	0.13	0.19
16:0	26.60	26.68	19.24	20.02	11.48	11.29	25.33	25.43
16:1	7.06	4.72	0.00	0.00	0.00	0.00	8.55	6.69
18:0	13.63	13.09	2.91	3.30	2.25	2.58	10.90	12.14
18:1	20.89	19.86	22.05	22.76	31.17	33.49	20.44	22.04
18:2	5.81	7.09	55.07	51.66	53.12	51.34	11.36	11.35
20:0	1.32	2.01	0.73	2.27	1.97	1.30	1.19	2.34

Table A6: Fatty Acid Composition Of SBSFMZ Mixture And Its Components

Fatty Acids	Soya Bean Oil (67.53%)	Sunflower Oil 22.32%	Maize Oil 10.15%	Mixture				
12:0	0.26	0.28	0.25	0.16	0.11	0.12	0.21	0.22
14:0	0.09	0.08	0.06	0.06	0.00	0.00	0.07	0.07
16:0	9.87	8.70	5.84	5.75	9.42	11.42	8.91	9.25
18:0	3.97	3.94	4.04	4.23	2.32	2.16	4.19	3.89
18:1	24.11	23.90	16.23	17.66	33.63	32.26	22.99	21.91
18:2	52.75	54.68	72.53	69.37	53.45	52.64	57.63	58.50
18:3	8.08	7.80	0.53	1.24	0.90	0.98	5.16	4.90
20:0	0.89	0.63	0.47	1.48	0.17	0.43	0.84	1.25

Table A7: Fatty Acid Composition Of MZCSTL Mixture And Its Components

Fatty Acids	Maize Oil (12.90%)		Cotton Seed Oil 24.17%		Tallow 62.94%		Mixture	
12:0	0.38	0.50	0.43	0.38	1.26	0.92	0.30	0.02
14:0	0.00	0.00	0.73	0.92	2.77	3.21	1.70	1.49
14:1	0.00	0.00	0.00	0.00	0.95	1.22	0.70	0.62
15:0	0.00	0.00	0.00	0.00	0.54	0.69	0.16	0.23
16:0Br	0.00	0.00	0.00	0.00	0.15	0.37	0.20	0.22
16:0	10.91	9.18	18.56	21.25	24.36	22.22	18.37	20.96
16:1	0.06	0.09	0.37	0.73	2.26	3.34	1.61	1.51
16:2	0.00	0.00	0.00	0.00	0.90	1.11	0.90	0.60
18:0Br	0.00	0.00	0.00	0.00	0.99	0.61	0.26	0.49
18:0	2.06	2.51	2.84	2.42	30.74	29.71	21.58	20.65
18:1	32.23	33.49	21.65	21.63	30.92	30.39	30.80	28.61
18:2	52.92	53.14	53.43	49.87	1.29	2.17	21.23	22.00
18:3	1.00	0.91	1.48	2.81	1.42	1.75	1.44	1.54
20:0	0.44	0.17	0.52	0.00	1.48	2.08	0.60	0.64

Table A8: Fatty Acid Composition Of OTLMZCS Mixture And Its Components

Fatty Acids	Tallow Oil (75.41%)		Maize Oil 7.68%		Cotton Seed Oil 16.91%		Mixture	
14:0	2.65	3.25	0.00	0.00	0.00	0.00	2.24	2.46
14:1	1.06	0.64	0.00	0.00	0.00	0.00	0.61	0.78
15:0	0.71	0.59	0.00	0.00	0.00	0.00	0.38	0.61
16:0Br	0.46	0.28	0.00	0.00	0.00	0.00	0.27	0.28
16:0	22.81	21.91	11.48	11.29	19.24	20.02	22.06	23.43
16:1	2.69	2.43	0.00	0.00	0.00	0.00	3.31	2.70
16:2	1.64	1.84	0.00	0.00	0.00	0.00	1.49	1.20
18:0Br	0.46	0.74	0.00	0.00	0.00	0.00	0.60	0.57
18:0	30.52	30.45	2.25	2.58	2.91	3.30	24.75	23.33
18:1	33.51	32.18	31.17	33.49	22.05	22.76	29.89	29.38
18:2	2.82	4.46	53.12	51.34	55.07	51.66	13.33	14.45
20:0	0.63	1.21	1.97	1.30	0.73	2.27	1.06	0.81

Table A9: Fatty Acid Composition Of MKCSMZ Mixture And Its Components

Fatty Acids	Milkfat (86.42%)		Cotton Seed Oil 11.71%		Maize Oil 1.87%		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	3.20	3.05
6:0	2.21	2.35	0.00	0.00	0.00	0.00	2.35	2.55
8:0	1.53	1.28	0.00	0.00	0.00	0.00	1.52	1.60
10:0	2.84	3.18	0.00	0.00	0.00	0.00	3.11	3.34
10:1	0.35	0.40	0.00	0.00	0.00	0.00	0.18	0.14
12:0	3.56	3.67	0.32	0.32	0.11	0.12	3.77	2.86
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.09	0.08
14:0	10.32	11.17	0.69	0.73	0.00	0.00	9.99	11.47
14:1	2.05	2.01	0.00	0.00	0.00	0.00	1.55	1.73
15:0	0.89	0.86	0.00	0.00	0.00	0.00	1.10	0.78
16:0Br	0.25	0.23	0.00	0.00	0.00	0.00	0.11	0.14
16:0	31.01	28.30	16.53	16.79	9.34	11.37	24.03	24.92
16:1	2.37	2.18	0.46	0.46	0.09	0.06	1.87	2.16
16:2	0.68	0.46	0.00	0.00	0.00	0.00	0.68	0.71
18:0Br	0.45	0.35	0.00	0.00	0.00	0.00	0.33	0.37
18:0	13.51	12.83	2.41	2.97	2.32	2.16	12.77	11.35
18:1	21.14	22.55	21.80	21.76	33.63	32.26	21.25	21.44
18:2	1.45	2.06	55.80	54.97	53.45	52.64	9.89	8.85
18:3	2.24	2.23	1.77	1.48	0.90	0.98	1.96	2.16
20:0	0.47	0.71	0.23	0.52	0.17	0.43	0.25	0.31

Table A10: Fatty Acid Composition Of MKCCNSB Mixture And Its Components

Fatty Acids	Milkfat (87.54%)		Coconut Oil 8.67%		Soya Bean Oil 3.80%		Mixture	
4:0	3.41	3.36	0.00	0.00	0.00	0.00	4.42	3.52
6:0	1.99	2.17	1.07	1.14	0.17	0.23	3.33	2.15
8:0	1.36	1.18	11.03	11.11	0.00	0.00	2.75	2.03
10:0	2.66	3.02	6.60	6.58	0.00	0.00	4.15	3.81
10:1	0.23	0.27	0.00	0.00	0.00	0.00	0.23	0.18
12:0	3.38	3.71	46.31	45.18	0.27	0.28	7.81	7.85
14:0Br	0.12	0.11	0.00	0.00	0.00	0.00	0.12	0.13
14:0	11.21	10.39	16.41	15.69	0.10	0.08	10.48	11.28
14:1	2.15	1.94	0.00	0.00	0.00	0.00	2.01	1.71
15:0	0.89	0.82	0.00	0.00	0.00	0.00	0.77	0.76
16:0Br	0.20	0.17	0.00	0.00	0.00	0.00	0.22	0.18
16:0	30.32	28.66	7.08	7.00	9.53	8.51	25.54	24.82
16:1	2.36	2.25	0.00	0.00	0.17	0.05	2.64	2.71
16:2	0.68	0.87	0.00	0.00	0.08	0.60	1.47	1.50
18:0Br	0.53	0.40	0.00	0.00	0.00	0.00	0.75	0.70
18:0	13.04	12.78	2.67	2.34	3.90	3.83	10.07	11.19
18:1	20.56	22.67	5.53	5.46	23.75	23.87	18.01	18.72
18:2	1.81	1.48	1.84	2.41	53.31	55.00	0.85	0.98
18:3	2.14	2.44	1.46	3.09	7.83	7.45	1.19	2.16
20:0	0.47	0.91	0.00	0.00	0.91	0.64	0.37	0.00

Table A11: Fatty Acid Composition Of OMKCSMZ Mixture And Its Components

Fatty Acids	Milkfat (86.42%)		Cotton Seed Oil (11.71%)		Maize Oil (1.87%)		Mixture	
4:0	4.02	4.64	0.00	0.00	0.00	0.00	4.36	3.45
6:0	2.51	2.89	0.00	0.00	0.00	0.00	2.10	2.08
8:0	1.64	1.78	0.00	0.00	0.00	0.00	1.40	1.41
10:0	3.49	3.29	0.00	0.00	0.00	0.00	2.81	2.96
10:1	0.34	0.30	0.00	0.00	0.00	0.00	0.24	0.23
12:0	3.39	3.92	0.63	0.33	0.00	0.00	2.67	3.80
14:0Br	0.38	0.12	0.00	0.00	0.00	0.00	0.29	0.26
14:0	12.13	11.23	0.55	0.65	0.00	0.00	10.75	9.32
14:1	2.08	1.97	0.00	0.00	0.00	0.00	1.95	1.59
15:0	0.92	1.15	0.00	0.00	0.00	0.00	0.79	1.13
16:0Br	28.57	25.12	17.70	18.20	10.76	11.29	24.94	24.46
16:1	2.37	2.08	0.38	0.20	0.00	0.00	2.16	1.92
16:2	0.66	0.62	0.00	0.00	0.00	0.00	0.71	0.70
18:0Br	0.73	0.51	0.00	0.00	0.00	0.00	0.39	0.40
18:0	12.04	14.30	2.74	2.41	1.96	2.04	11.11	12.76
18:1	17.92	20.60	21.39	21.22	32.67	32.52	20.36	20.96
18:2	1.64	1.46	55.46	55.19	53.69	53.33	1.18	0.80
18:3	2.60	1.78	0.00	0.00	0.92	0.83	0.04	9.37
20:0	2.36	2.06	1.16	1.81	0.00	0.00	2.28	2.28

Table A12: Fatty Acid Composition Of MKSFBS Mixture And Its Components

Fatty Acids	Milkfat (78.07%)		Sunflower Oil (11.12%)		Soya Bean Oil (10.81%)		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	2.49	2.84
6:0	2.21	2.35	0.00	0.00	0.00	0.00	1.69	1.69
8:0	1.53	1.28	0.00	0.00	0.00	0.00	1.13	1.20
10:0	2.84	3.18	0.00	0.00	0.00	0.00	2.39	2.70
10:1	0.35	0.40	0.00	0.00	0.00	0.00	0.25	0.26
12:0	3.56	3.67	0.25	0.16	0.26	0.28	2.77	3.15
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.12	0.19
14:0	10.32	11.17	0.06	0.06	0.09	0.08	8.26	7.33
14:1	2.05	2.01	0.00	0.00	0.00	0.00	1.55	1.43
15:0	0.89	0.86	0.00	0.00	0.00	0.00	0.75	0.73
16:0Br	0.25	0.23	0.00	0.00	0.00	0.00	0.19	0.34
16:0	31.01	28.30	5.84	5.75	9.63	8.59	22.52	24.39
16:1	2.37	2.18	0.00	0.00	0.16	0.50	2.07	1.35
16:2	0.68	0.46	0.00	0.00	0.08	0.06	0.33	0.98
18:0Br	0.45	0.35	0.00	0.00	0.00	0.00	0.25	0.16
18:0	13.51	12.83	4.04	4.23	3.97	3.94	11.67	11.16
18:1	21.14	22.55	16.23	17.66	24.11	23.90	20.19	20.58
18:2	1.45	2.06	72.53	69.37	52.75	54.68	16.12	16.06
18:3	2.24	2.23	0.53	1.24	8.07	7.79	2.94	1.89
20:0	0.47	0.71	0.47	1.48	0.89	0.63	1.96	1.30

Table A13: Fatty Acid Composition Of MKCCNSB Mixture And Its Components

Fatty Acids	Milkfat (87.54%)		Coconut Oil 8.67%		Soya Bean Oil 3.80%		Mixture	
4:0	3.41	3.36	0.00	0.00	0.00	0.00	4.42	3.52
6:0	1.99	2.17	0.79	0.68	0.00	0.00	3.33	2.15
8:0	1.36	1.18	11.06	11.28	0.00	0.00	2.75	2.03
10:0	2.66	3.02	6.62	6.60	0.00	0.00	4.15	3.81
10:1	0.23	0.27	0.00	0.00	0.00	0.00	0.23	0.18
12:0	3.38	3.71	46.45	45.34	0.27	0.28	7.81	7.85
14:0Br	0.12	0.11	0.00	0.00	0.00	0.00	0.12	0.13
14:0	11.21	10.34	16.46	15.73	0.09	0.08	10.48	11.28
14:1	2.15	1.94	0.00	0.00	0.00	0.00	2.01	1.71
15:0	0.89	0.82	0.00	0.00	0.00	0.00	0.77	0.76
16:0Br	0.20	0.17	0.00	0.00	0.00	0.00	0.22	0.18
16:0	30.32	28.66	7.10	7.02	9.54	8.53	25.54	24.82
16:1	2.36	2.25	0.00	0.00	0.17	0.05	2.64	2.71
16:2	0.68	0.87	0.00	0.00	0.08	0.06	1.47	1.50
18:0Br	0.53	0.40	0.00	0.00	0.00	0.00	0.75	0.70
18:0	13.04	12.78	2.68	2.35	3.90	3.84	10.07	11.19
18:1	20.56	22.67	5.55	5.48	23.79	23.94	18.01	18.72
18:2	1.81	1.48	1.85	2.42	53.40	55.11	0.85	0.98
18:3	2.14	2.44	0.00	0.00	7.84	7.47	1.19	2.16
20:0	0.47	0.91	1.46	3.10	0.91	0.65	0.37	0.00

Table A14: Fatty Acid Composition Of CMKCCNSB Mixture And Its Components

Fatty Acids	Milkfat (87.54%)		Coconut Oil 8.67%		Soya Bean Oil 3.80%		Mixture	
4:0	3.87	3.49	0.00	0.00	0.00	0.00	4.51	5.79
6:0	2.58	2.42	0.71	0.93	0.00	0.00	2.75	3.90
8:0	1.30	1.57	11.92	11.84	0.00	0.00	2.30	2.82
10:0	3.13	2.80	6.93	6.72	0.00	0.00	3.83	4.07
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.18	0.22
12:0	3.81	3.52	43.49	45.44	0.27	0.28	8.03	7.82
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.12	0.11
14:0	11.03	10.19	16.00	16.41	0.09	0.08	11.08	10.34
14:1	1.99	2.02	0.00	0.00	0.00	0.00	1.64	1.90
15:0	0.85	0.88	0.00	0.00	0.00	0.00	0.73	0.73
16:0Br	0.23	0.25	0.00	0.00	0.00	0.00	0.17	0.21
16:0	27.93	30.64	7.09	7.27	9.54	8.53	24.23	25.02
16:1	2.15	2.34	0.00	0.00	0.17	0.05	2.59	2.49
16:2	0.46	0.67	0.00	0.00	0.08	0.06	1.44	1.39
18:0Br	0.35	0.44	0.00	0.00	0.00	0.00	0.67	0.71
18:0	12.66	13.35	2.33	2.59	3.90	3.84	11.13	10.03
18:1	22.25	20.89	5.39	5.60	23.79	23.94	18.76	18.03
18:2	2.03	1.43	2.76	1.79	53.40	55.11	3.78	2.96
18:3	2.20	2.21	3.39	1.41	7.84	7.47	2.07	1.13
20:0	0.70	0.46	0.00	0.00	0.91	0.65	0.00	0.35

Table A15: Fatty Acid Composition Of MZCSMK Mixture And Its Components

Fatty Acids	Maize Oil (1.87%	Cotton Seed Oil 11.71%	Milkfat 86.42%)	Mixture
4:0	0.00	0.00	0.00	3.41 3.36 3.45 4.36
6:0	0.00	0.00	0.00	1.99 2.17 2.08 2.10
8:0	0.00	0.00	0.00	1.36 1.18 1.41 1.40
10:0	0.00	0.00	0.00	2.66 3.02 2.96 2.81
10:1	0.00	0.00	0.00	0.23 0.27 0.23 0.24
12:0	0.16	0.20	0.31 0.32	3.38 3.71 3.80 2.67
14:0Br	0.00	0.00	0.00	0.12 0.11 0.26 0.29
14:0	0.00	0.00	0.64 0.73	11.21 10.34 9.32 10.75
14:1	0.00	0.00	0.00	2.15 1.94 1.59 1.95
15:0	0.00	0.00	0.00	0.89 0.82 1.13 0.79
16:0Br	0.00	0.00	0.00	0.20 0.17 0.11 0.31
16:0	10.94	9.21	18.16 18.67	30.32 28.66 24.46 24.94
16:1	0.06	0.09	0.20 0.37	2.36 2.25 1.92 2.16
16:2	0.00	0.00	0.00	0.68 0.87 0.70 0.71
18:0Br	0.00	0.00	0.00	0.53 0.40 0.40 0.39
18:0	2.06	2.52	2.41 2.85	13.04 12.78 12.76 11.11
18:1	32.31	33.59	21.17 21.27	20.56 22.67 20.96 20.36
18:2	53.04	53.30	55.06 53.77	1.81 1.48 9.37 9.04
18:3	1.00	0.92	1.81 1.49	2.14 2.44 2.03 2.16
20:0	0.44	0.17	0.24 0.53	0.47 0.91 0.25 0.31

Table A16: Fatty Acid Composition Of MKTLCN Mixture And Its Components

Fatty Acids	Milkfat (89.17%	Tallow Oil 6.77%	Coconut Oil 4.07%)	Mixture
4:0	3.41	3.36	0.00 0.00	0.00 0.00 3.13 3.95
6:0	1.99	2.17	0.00 0.00	0.79 0.68 2.19 2.46
8:0	1.36	1.18	0.00 0.00	11.06 11.28 1.69 1.91
10:0	2.66	3.02	0.00 0.00	6.62 6.60 3.00 3.19
10:1	0.23	0.27	0.00 0.00	0.00 0.00 0.26 0.37
12:0	3.38	3.71	0.62 0.27	46.45 45.34 5.12 5.27
14:0	11.21	10.34	2.78 3.23	16.46 15.73 13.48 13.17
14:1	2.15	1.94	0.95 1.22	0.00 0.00 1.92 2.14
15:0	0.89	0.82	0.54 0.69	0.00 0.00 0.92 0.86
16:0Br	0.20	0.17	0.15 0.37	0.00 0.00 0.16 0.17
16:0	30.32	28.66	24.51 22.36	7.10 1.02 24.73 22.81
16:1	2.36	2.25	2.28 3.37	0.00 0.00 2.26 3.16
16:2	0.68	0.87	0.91 1.12	0.00 0.00 0.89 0.77
18:0Br	0.53	0.40	0.99 0.62	0.00 0.00 0.44 0.41
18:0	13.04	12.78	30.94 29.90	2.68 2.35 13.66 13.66
18:1	20.56	22.67	31.12 30.59	5.55 5.48 19.93 20.48
18:2	1.81	1.48	1.04 1.31	1.85 2.42 3.64 3.35
18:3	2.14	2.44	1.43 1.76	0.00 0.00 2.08 1.66
20:0	0.47	0.91	1.49 2.10	1.46 3.10 0.48 0.23

Table A17: Fatty Acid Composition Of MKSFBSB Mixture And Its Components

Fatty Acids	Milk Fat (78.07%)		Sunflower Oil 11.12%		Coconut Oil 10.81%		Mixture	
4:0	2.63	3.00	0.00	0.00	0.00	0.00	2.84	2.49
6:0	2.01	2.18	0.00	0.00	0.00	0.00	1.69	1.69
8:0	1.37	1.18	0.00	0.00	0.00	0.00	1.20	1.13
10:0	2.68	3.03	0.00	0.00	0.00	0.00	2.70	2.40
10:1	0.23	0.27	0.00	0.00	0.00	0.00	0.26	0.25
12:0	3.41	3.72	0.25	0.16	0.27	0.28	3.15	2.77
14:OBr	0.12	0.11	0.00	0.00	0.00	0.00	0.19	0.12
14:0	11.30	10.43	0.06	0.06	0.09	0.08	7.33	8.26
14:1	2.17	1.95	0.00	0.00	0.00	0.00	1.43	1.55
15:0	0.89	0.82	0.00	0.00	0.00	0.00	0.73	0.75
16:OBr	0.21	0.17	0.00	0.00	0.00	0.00	0.34	0.19
16:0	30.56	28.77	5.84	5.75	9.54	8.53	24.39	22.52
16:1	2.38	2.25	0.00	0.00	0.17	0.05	1.35	2.07
16:2	0.69	0.87	0.00	0.00	0.08	0.06	0.98	0.33
18:OBr	0.53	0.40	0.00	0.00	0.00	0.00	0.16	0.25
18:0	13.15	12.83	4.04	4.23	3.90	3.84	11.16	11.67
18:1	20.73	22.76	16.23	17.66	23.79	23.94	20.58	20.19
18:2	1.83	1.48	72.53	69.37	53.40	55.11	16.06	16.12
18:3	2.16	2.45	0.53	1.24	7.84	7.47	1.89	2.94
20:0	0.47	0.91	0.47	1.48	0.91	0.65	1.30	1.96

Table A18: Fatty Acid Composition Of MKSFCS Mixture And Its Components

Fatty Acids	Milk Fat (59.28%)		Sunflower oil 25.07%		Cotton Seed Oil 15.65%		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	1.97	1.65
6:0	2.21	2.36	0.00	0.00	0.00	0.00	1.57	1.23
8:0	1.53	1.28	0.00	0.00	0.00	0.00	0.84	0.97
10:0	2.84	3.18	0.00	0.00	0.00	0.00	1.89	1.85
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.13	0.12
12:0	3.56	3.86	0.25	0.16	0.33	0.32	2.42	2.70
14:OBr	0.09	0.11	0.00	0.00	0.00	0.00	0.08	0.10
14:0	10.32	11.17	0.06	0.06	0.64	0.73	6.53	7.08
14:1	2.05	2.01	0.00	0.00	0.00	0.00	1.14	1.05
15:0	0.89	0.86	0.00	0.00	0.00	0.00	0.65	0.65
16:OBr	0.25	0.23	0.00	0.00	0.00	0.00	0.15	0.09
16:0	30.01	28.30	5.84	5.75	18.16	18.67	21.35	18.97
16:1	2.37	2.18	0.00	0.00	0.20	0.37	1.46	1.64
16:2	0.68	0.46	0.00	0.00	0.00	0.00	0.41	0.54
18:OBr	0.45	0.35	0.00	0.00	0.00	0.00	0.13	0.22
18:0	13.51	12.83	4.04	4.23	2.41	2.85	9.32	9.47
18:1	21.14	22.55	16.23	17.66	21.17	21.27	19.81	20.31
18:2	1.45	2.06	72.53	69.37	55.06	53.77	28.30	28.76
18:3	2.24	2.23	0.53	1.24	1.81	1.49	1.10	1.90
20:0	0.47	0.71	0.47	1.48	0.24	0.53	0.62	0.74

Table A19: Fatty Acid Composition Of CMKSFCS Mixture And Its Components

Fatty Acids	Milk Fat (59.28%)		Sunflower Oil 25.07%		Cotton Seed Oil 15.65%			Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	2.21	2.63	
6:0	2.58	2.42	0.00	0.00	0.00	0.00	1.35	1.73	
8:0	1.30	1.56	0.00	0.00	0.00	0.00	0.99	0.85	
10:0	3.13	2.80	0.00	0.00	0.00	0.00	1.84	1.87	
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.11	0.12	
12:0	3.81	3.52	0.25	0.16	0.33	0.32	2.68	2.41	
14:OBr	0.10	0.08	0.00	0.00	0.00	0.00	0.10	0.08	
14:0	11.03	10.19	0.06	0.06	0.64	0.73	7.02	6.53	
14:1	1.99	2.02	0.00	0.00	0.00	0.00	1.04	1.13	
15:0	0.85	0.88	0.00	0.00	0.00	0.00	0.64	0.64	
16:OBr	0.23	0.25	0.00	0.00	0.00	0.00	0.09	0.14	
16:0	27.93	30.64	5.84	5.75	18.16	18.67	18.83	21.17	
16:1	2.15	2.34	0.00	0.00	0.20	0.37	1.63	1.45	
16:2	0.46	0.67	0.00	0.00	0.00	0.00	0.53	0.41	
18:OBr	0.35	0.44	0.00	0.00	0.00	0.00	0.22	0.12	
18:0	12.66	13.35	4.04	4.23	2.41	2.85	9.40	9.32	
18:1	22.25	20.89	16.23	17.66	21.17	21.27	20.16	19.64	
18:2	2.03	1.43	72.53	69.37	55.06	53.77	28.54	28.05	
18:3	2.20	2.21	0.53	1.24	1.81	1.49	1.89	1.10	
20:0	0.70	0.46	0.47	1.48	0.24	0.53	0.73	0.62	

Table A20: Fatty Acid Composition Of MKSFCCN Mixture And Its Components

Fatty Acids	Milk Fat (65.84%)		Sunflower Oil 22.13%		Coconut Oil 12.03%		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	2.15	1.72
6:0	2.21	2.36	0.00	0.00	0.84	0.64	1.40	1.47
8:0	1.54	1.28	0.00	0.00	11.55	11.62	2.31	1.76
10:0	2.84	3.18	0.00	0.00	6.72	6.96	2.81	2.42
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.10	0.16
12:0	3.56	3.86	0.25	0.16	45.64	43.49	8.84	9.22
14:OBr	0.09	0.11	0.00	0.00	0.00	0.00	0.11	0.12
14:0	10.32	11.17	0.06	0.06	16.48	16.07	7.29	7.87
14:1	2.05	2.01	0.00	0.00	0.00	0.00	1.21	1.26
15:0	0.89	0.86	0.00	0.00	0.00	0.00	0.68	0.93
16:OBr	0.25	0.23	0.00	0.00	0.00	0.00	0.12	0.19
16:0	30.01	28.30	5.84	5.75	7.30	7.12	19.14	20.96
16:1	2.37	2.182	0.00	0.00	0.00	0.00	1.77	1.89
16:2	0.68	0.46	0.00	0.00	0.00	0.00	0.52	0.56
18:OBr	0.45	0.35	0.00	0.00	0.00	0.00	0.15	0.35
18:0	13.51	12.83	4.04	4.23	2.60	2.34	9.51	10.30
18:1	21.14	22.55	16.23	17.66	5.63	5.42	21.93	19.30
18:2	1.45	2.06	72.53	69.37	1.80	2.77	18.22	17.58
18:3	2.24	2.23	0.53	1.24	1.42	3.41	1.44	1.27
20:0	0.47	0.71	0.47	1.48	0.00	0.00	0.31	0.70

Table A21: Fatty Acid Composition Of CMKSFCCN Mixture And Its Components

Fatty Acids	Milk Fat (65.84%)		Sunflower Oil 22.13%		Coconut Oil 12.03%		Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	2.31	2.87
6:0	2.58	2.42	0.00	0.00	0.71	0.93	1.61	1.54
8:0	1.30	1.56	0.00	0.00	11.92	11.84	1.80	2.36
10:0	3.13	2.80	0.00	0.00	6.93	6.72	2.40	2.78
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.16	0.10
12:0	3.81	3.52	0.25	0.16	43.45	45.44	9.14	8.76
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.12	0.11
14:0	11.03	10.19	0.06	0.06	16.00	16.41	7.81	7.22
14:1	1.99	2.02	0.00	0.00	0.00	0.00	1.25	1.20
15:0	0.85	0.88	0.00	0.00	0.00	0.00	0.93	0.67
16:0Br	0.23	0.25	0.00	0.00	0.00	0.00	0.19	0.12
16:0	27.93	30.64	5.84	5.75	7.09	7.27	20.79	18.96
16:1	2.15	2.34	0.00	0.00	0.00	0.00	1.87	1.76
16:2	0.46	0.67	0.00	0.00	0.00	0.00	0.55	0.51
18:0Br	0.35	0.44	0.00	0.00	0.00	0.00	0.35	0.15
18:0	12.66	13.35	4.04	4.23	2.33	2.59	10.21	9.42
18:1	22.25	20.89	16.23	17.66	5.39	5.60	19.13	21.72
18:2	2.03	1.43	72.53	69.37	2.76	1.79	17.43	18.04
18:3	2.20	2.21	0.53	1.24	3.40	1.41	1.26	1.43
20:0	0.70	0.46	0.47	1.48	0.00	0.00	0.69	0.31

Table A22: Fatty Acid Composition Of AMKTLCCN Mixture And Its Components

Fatty Acids	Milk Fat (89.17%)		Tallow 6.77%		Coconut Oil 4.07%		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	3.37	4.05
6:0	2.21	2.36	0.00	0.00	0.84	0.64	2.35	2.81
8:0	1.53	1.28	0.00	0.00	11.55	11.62	1.78	2.12
10:0	2.84	3.18	0.00	0.00	6.72	6.96	3.15	3.52
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.26	0.36
12:0	3.56	3.86	0.61	0.25	45.64	43.49	5.28	5.33
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.17	0.26
14:0	10.32	11.17	2.91	3.52	16.48	16.07	13.39	13.05
14:1	2.05	2.01	0.93	0.95	0.00	0.00	1.89	2.08
15:0	0.89	0.86	0.52	0.68	0.00	0.00	0.91	0.83
16:0Br	0.25	0.23	0.15	0.16	0.00	0.00	0.16	0.17
16:0	30.01	28.30	24.48	22.53	7.30	7.12	24.62	22.73
16:1	2.37	2.18	2.22	3.33	0.00	0.00	2.22	3.07
16:2	0.68	0.46	0.88	1.45	0.00	0.00	0.88	0.75
18:0Br	0.45	0.35	0.54	0.61	0.00	0.00	0.43	0.40
18:0	13.51	12.83	31.34	30.32	2.60	2.34	13.83	13.63
18:1	21.14	22.55	31.52	31.17	5.63	5.42	20.33	20.89
18:2	1.45	2.06	0.81	0.93	1.80	2.77	2.48	2.13
18:3	2.24	2.23	1.39	1.74	1.42	3.41	2.05	1.61
20:0	0.47	0.71	1.45	2.07	0.00	0.00	0.48	0.22

Table A23: Fatty Acid Composition Of ACMKTLCCN Mixture And Its Components

Fatty Acids	Milk Fat (89.17%)		Tallow (6.77%)		Coconut Oil (4.07%)		Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	5.37	4.48
6:0	2.58	2.42	0.00	0.00	0.71	0.93	3.07	2.57
8:0	1.30	1.56	0.00	0.00	11.92	11.84	2.15	1.81
10:0	3.13	2.80	0.00	0.00	6.93	6.72	3.46	3.10
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.36	0.25
12:0	3.81	3.52	0.61	0.25	43.49	45.44	5.23	5.20
14:OBr	0.10	0.08	0.00	0.00	0.00	0.00	0.25	0.16
14:0	11.03	10.19	2.91	3.52	16.00	16.41	12.82	13.19
14:1	1.99	2.02	0.93	0.95	0.00	0.00	2.04	1.86
15:0	0.85	0.88	0.52	0.68	0.00	0.00	0.82	0.90
16:OBr	0.23	0.25	0.15	0.16	0.00	0.00	0.16	0.16
16:0	27.93	30.64	24.48	22.53	7.09	7.27	22.33	24.25
16:1	2.15	2.34	2.22	3.33	0.00	0.00	3.01	2.19
16:2	0.46	0.67	0.88	1.45	0.00	0.00	0.73	0.86
18:OBr	0.35	0.44	0.54	0.61	0.00	0.00	0.39	0.42
18:0	12.66	13.35	31.34	30.32	2.33	2.59	13.39	13.63
18:1	22.25	20.89	31.52	31.17	5.39	5.60	20.53	20.03
18:2	2.03	1.43	0.81	0.93	2.76	1.79	2.09	2.45
18:3	2.20	2.21	1.39	1.74	3.39	1.41	1.58	2.02
20:0	0.70	0.46	1.45	2.07	0.00	0.00	0.22	0.47

Table A24: Fatty Acid Composition Of MKSBCS Mixture And Its Components

Fatty Acid	Milk Fat (57.89%)		Soya Bean Oil (23.46%)		Cotton Seed Oil (18.62%)		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	2.07	2.07
6:0	2.21	2.36	0.00	0.00	0.00	0.00	1.31	1.49
8:0	1.53	1.28	0.00	0.00	0.00	0.00	0.89	0.99
10:0	2.84	3.18	0.00	0.00	0.00	0.00	1.86	2.26
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.06	0.05
12:0	3.56	3.86	0.26	0.27	0.33	0.32	2.53	2.26
14:OBr	0.09	0.11	0.00	0.00	0.00	0.00	0.11	0.06
14:0	10.32	11.17	0.09	0.08	0.64	0.73	5.50	7.91
14:1	2.05	2.01	0.00	0.00	0.00	0.00	1.22	1.02
15:0	0.89	0.86	0.00	0.00	0.00	0.00	0.64	0.55
16:OBr	0.25	0.23	0.00	0.00	0.00	0.00	0.16	0.18
16:0	30.01	28.30	9.63	8.59	18.16	18.67	19.54	21.60
16:1	2.37	2.18	0.16	0.05	0.20	0.37	1.43	1.19
16:2	0.68	0.46	0.08	0.06	0.00	0.00	0.21	0.11
18:OBr	0.45	0.35	0.00	0.00	0.00	0.00	0.13	0.16
18:0	13.51	12.83	3.97	3.94	2.41	2.85	9.19	9.34
18:1	21.14	22.55	24.11	23.90	21.17	21.27	23.26	20.93
18:2	1.45	2.06	52.75	54.68	55.06	53.77	25.64	23.46
18:3	2.24	2.23	8.07	7.79	1.81	1.49	3.70	3.32
20:0	0.47	0.71	0.89	0.63	0.24	0.53	0.57	1.07

Table A25: Fatty Acid Composition Of CMKSBCS Mixture And Its Components

Fatty Acids	Milk Fat (57.89%)		Soya Bean Oil 23.46%		Cotton Seed Oil 18.62%		Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	2.77	2.77
6:0	2.58	2.42	0.00	0.00	0.00	0.00	1.44	1.63
8:0	1.30	1.56	0.00	0.00	0.00	0.00	0.90	1.01
10:0	3.13	2.80	0.00	0.00	0.00	0.00	1.84	2.24
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.06	0.05
12:0	3.81	3.52	0.26	0.28	0.33	0.32	2.51	2.24
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.11	0.06
14:0	11.03	10.19	0.09	0.08	0.64	0.73	5.45	7.83
14:1	1.99	2.02	0.00	0.00	0.00	0.00	1.21	1.01
15:0	0.85	0.88	0.00	0.00	0.00	0.00	0.63	0.55
16:0Br	0.23	0.25	0.00	0.00	0.00	0.00	0.16	0.18
16:0	27.93	30.64	9.63	8.59	18.16	18.67	19.37	21.41
16:1	2.15	2.34	0.16	0.05	0.20	0.37	1.41	1.18
16:2	0.46	0.67	0.08	0.06	0.00	0.00	0.21	0.11
18:0Br	0.35	0.44	0.00	0.00	0.00	0.00	0.13	0.16
18:0	12.66	13.35	3.98	3.94	2.41	2.85	9.11	9.25
18:1	22.25	20.89	24.11	23.90	21.17	21.27	23.06	20.74
18:2	2.03	1.43	52.75	54.68	55.06	53.77	25.41	23.25
18:3	2.20	2.21	8.07	7.79	1.81	1.49	3.67	3.29
20:0	0.70	0.46	0.89	0.63	0.24	0.53	0.56	1.05

Table A26: Fatty Acid Composition Of MKSFMZ Mixture And Its Components

Fatty Acids	Milk Fat (77.96%)		Sunflower Oil 5.12%		Maize Oil 16.92%		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	2.27	2.52
6:0	2.21	2.36	0.00	0.00	0.00	0.00	2.01	1.63
8:0	1.53	1.28	0.00	0.00	0.00	0.00	0.99	1.20
10:0	2.84	3.18	0.00	0.00	0.00	0.00	2.34	2.46
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.14	0.13
12:0	3.56	3.86	0.25	0.16	0.12	0.11	2.95	2.59
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.15	0.58
14:0	10.32	11.17	0.06	0.06	0.00	0.00	7.15	9.31
14:1	2.05	2.01	0.00	0.00	0.00	0.00	1.41	1.44
15:0	0.89	0.86	0.00	0.00	0.00	0.00	0.86	0.85
16:0Br	0.25	0.23	0.00	0.00	0.00	0.00	0.14	0.13
16:0	30.01	28.30	5.84	5.75	11.37	9.34	23.96	25.71
16:1	2.37	2.18	0.00	0.00	0.06	0.09	1.97	1.82
16:2	0.68	0.46	0.00	0.00	0.00	0.00	0.74	0.30
18:0Br	0.45	0.35	0.00	0.00	0.00	0.00	0.36	0.09
18:0	13.51	12.83	4.04	4.23	2.16	2.32	11.56	10.19
18:1	21.14	22.55	16.23	17.66	32.26	33.63	23.68	22.72
18:2	1.45	2.06	72.53	69.37	52.64	53.45	14.71	13.41
18:3	2.24	2.23	0.53	1.24	0.98	0.90	1.63	1.49
20:0	0.47	0.71	0.47	1.48	0.43	0.17	0.99	1.44

Table A27: Fatty Acid Composition Of MKSFMZ Mixture And Its Components

Fatty Acids	Milk Fat (77.96%)		Sunflower Oil 5.12%		Maize Oil 16.92)		Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	3.04	3.37
6:0	2.58	2.42	0.00	0.00	0.00	0.00	2.21	1.79
8:0	1.30	1.56	0.00	0.00	0.00	0.00	1.01	1.23
10:0	3.13	2.80	0.00	0.00	0.00	0.00	2.32	2.43
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.14	0.13
12:0	3.81	3.52	0.25	0.16	0.12	0.11	2.92	2.56
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.14	0.57
14:0	11.03	10.19	0.06	0.06	0.00	0.00	7.07	9.21
14:1	1.99	1.02	0.00	0.00	0.00	0.00	1.40	1.42
15:0	0.85	0.88	0.00	0.00	0.00	0.00	0.85	0.84
16:0Br	0.23	0.25	0.00	0.00	0.00	0.00	0.14	0.13
16:0	27.93	30.64	5.84	5.75	11.37	9.34	23.71	25.43
16:1	2.15	2.34	0.00	0.00	0.06	0.09	1.95	1.80
16:2	0.46	0.67	0.00	0.00	0.00	0.00	0.73	0.30
18:0Br	0.35	0.44	0.00	0.00	0.00	0.00	0.36	0.08
18:0	12.66	13.35	4.04	4.23	2.16	2.32	11.44	10.08
18:1	22.25	20.89	16.23	17.66	32.26	33.63	23.43	22.48
18:2	2.03	1.43	72.53	69.37	52.64	53.45	14.55	13.27
18:3	2.20	2.21	0.53	1.24	0.98	0.90	1.61	1.48
20:0	0.70	0.46	0.47	1.48	0.43	0.17	0.98	1.42

Table A28: Fatty Acid Composition Of MKCCNMZ Mixture And Its Components

Fatty Acids	Milk Fat (82.35%)		Coconut Oil 10.73%		Maize Oil 6.92%)		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	2.33	2.03
6:0	2.21	2.36	0.84	0.64	0.00	0.00	1.54	1.41
8:0	1.53	1.28	11.55	11.62	0.00	0.00	2.00	2.07
10:0	2.84	3.18	6.72	6.96	0.00	0.00	3.11	3.44
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.10	0.23
12:0	3.56	3.86	45.64	43.49	0.12	0.11	9.43	8.67
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.12	0.14
14:0	10.32	11.17	16.48	16.07	0.00	0.00	10.91	10.25
14:1	2.05	2.01	0.00	0.00	0.00	0.00	1.59	1.52
15:0	0.89	0.86	0.00	0.00	0.00	0.00	0.75	1.03
16:0Br	0.25	0.23	0.00	0.00	0.00	0.00	0.18	0.31
16:0	30.01	28.30	7.30	7.12	11.37	9.34	23.70	27.28
16:1	2.37	2.18	0.00	0.00	0.06	0.09	3.31	1.80
16:2	0.68	0.46	0.00	0.00	0.00	0.00	0.41	0.28
18:0Br	0.45	0.35	0.00	0.00	0.00	0.00	0.12	0.09
18:0	13.51	12.83	2.60	2.34	2.16	2.32	11.25	10.22
18:1	21.14	22.55	5.63	5.42	32.26	33.63	20.65	20.53
18:2	1.45	2.06	1.80	2.77	52.64	53.45	6.04	5.47
18:3	2.24	2.23	1.42	3.41	0.98	0.90	1.59	2.05
20:0	0.47	0.71	0.00	0.00	0.43	0.17	0.86	1.19

Table A29: Fatty Acid Composition Of CMKCCNMZ Mixture And Its Components

Fatty Acids	Milk Fat (82.35%)		Coconut Oil 10.73%		Maize Oil 6.92%		Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	2.72	3.11
6:0	2.58	2.42	0.71	0.93	0.00	0.00	1.55	1.69
8:0	1.30	1.56	11.92	11.84	0.00	0.00	2.12	2.04
10:0	3.13	2.80	6.93	6.72	0.00	0.00	3.41	3.08
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.23	0.10
12:0	3.81	3.52	43.49	45.44	0.12	0.11	8.35	9.33
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.14	0.12
14:0	11.03	10.19	16.00	16.41	0.00	0.00	10.15	10.80
14:1	1.99	2.02	0.00	0.00	0.00	0.00	1.51	1.58
15:0	0.85	0.88	0.00	0.00	0.00	0.00	1.02	0.75
16:0Br	0.23	0.25	0.00	0.00	0.00	0.00	0.31	0.18
16:0	27.93	30.64	7.09	7.27	11.37	9.34	27.03	23.45
16:1	2.15	2.34	0.00	0.00	0.06	0.09	1.78	3.27
16:2	0.46	0.67	0.00	0.00	0.00	0.00	0.27	0.40
18:0Br	0.35	0.44	0.00	0.00	0.00	0.00	0.09	0.12
18:0	12.66	13.35	2.33	2.59	2.16	2.32	10.13	11.13
18:1	22.25	20.89	5.39	5.60	32.26	33.63	20.34	20.44
18:2	2.03	1.43	2.76	1.79	52.64	53.45	5.42	5.98
18:3	2.20	2.21	3.39	1.41	0.98	0.90	2.03	1.58
20:0	0.70	0.46	0.00	0.00	0.43	0.17	1.17	0.85

Table A30: Fatty Acid Composition Of MKTLSB Mixture And Its Components

Fatty Acids	Milk Fat (65.53%)		Tallow 22.84%		Soya Bean Oil 14.63%		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	1.92	2.36
6:0	2.21	2.36	0.00	0.00	0.00	0.00	1.27	1.69
8:0	1.53	1.28	0.00	0.00	0.00	0.00	0.80	0.77
10:0	2.84	3.18	0.00	0.00	0.00	0.00	1.80	2.17
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.11	0.16
12:0	3.56	3.86	0.61	0.25	0.26	0.28	2.55	2.20
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.09	0.12
14:0	10.32	11.17	2.91	3.52	0.09	0.08	6.63	6.83
14:1	2.05	2.01	0.93	0.95	0.00	0.00	1.24	1.21
15:0	0.89	0.86	0.52	0.68	0.00	0.00	0.59	0.57
16:0Br	0.25	0.23	0.15	0.16	0.00	0.00	0.11	0.14
16:0	30.01	28.30	24.48	22.53	9.63	8.59	23.51	21.19
16:1	2.37	2.18	2.22	3.33	0.16	0.05	2.13	2.14
16:2	0.68	0.46	0.88	1.45	0.08	0.06	0.64	0.85
18:0Br	0.45	0.35	0.54	0.61	0.00	0.00	0.27	0.34
18:0	13.51	12.83	31.34	30.32	3.97	3.94	15.84	16.59
18:1	21.14	22.55	31.52	31.17	24.11	23.90	27.07	23.90
18:2	1.45	2.06	0.81	0.93	52.75	54.68	10.08	14.01
18:3	2.24	2.23	1.39	1.74	8.07	7.79	2.72	2.33
20:2	0.47	0.71	1.45	2.07	0.89	0.63	0.64	0.45

Table A31: Fatty Acid Composition Of CMKTL5B Mixture And Its Components

Fatty Acids	Milk Fat (65.53%)		Tallow (22.84%)		Soya Bean Oil (14.63%)		Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	3.16	2.57
6:0	2.58	2.42	0.00	0.00	0.00	0.00	1.85	1.40
8:0	1.30	1.56	0.00	0.00	0.00	0.00	0.78	0.82
10:0	3.13	2.80	0.00	0.00	0.00	0.00	2.14	1.78
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.15	0.11
12:0	3.81	3.52	0.61	0.25	0.26	0.28	2.18	2.53
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.12	0.09
14:0	11.03	10.19	2.91	3.52	0.09	0.08	6.76	6.58
14:1	2.00	2.02	0.93	0.95	0.00	0.00	1.20	1.23
15:0	0.85	0.88	0.52	0.68	0.00	0.00	0.56	0.59
16:0Br	0.23	0.25	0.15	0.16	0.00	0.00	0.14	0.11
16:0	27.93	30.64	24.48	22.53	9.63	8.59	20.97	23.32
16:1	2.15	2.34	2.22	3.33	0.16	0.05	2.12	2.12
16:2	0.46	0.67	0.88	1.45	0.08	0.06	0.85	0.63
18:0Br	0.35	0.44	0.54	0.61	0.00	0.00	0.34	0.27
18:0	12.66	13.35	31.34	30.32	3.97	3.94	16.42	15.71
18:1	22.25	20.89	31.52	31.17	24.11	23.90	23.65	26.85
18:2	2.03	1.43	0.81	0.93	52.75	54.68	13.87	9.99
18:3	2.20	2.21	1.39	1.74	8.07	7.79	2.31	2.70
20:0	0.70	0.46	1.45	2.07	0.89	0.63	0.45	0.63

Table A32: Fatty Acids Of MKCCNCS Mixture And Its Components

Fatty Acids	Milk Fat (52.04%)		Coconut Oil (18.64%)		Cotton Seed Oil (29.32%)		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	1.68	1.09
6:0	2.21	2.36	0.84	0.64	0.00	0.00	1.42	1.28
8:0	1.53	1.28	11.55	11.62	0.00	0.00	2.67	2.17
10:0	2.84	3.18	6.72	6.96	0.00	0.00	2.65	2.47
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.08	0.11
12:0	3.56	3.86	45.64	43.49	0.33	0.32	11.06	9.98
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.07	0.10
14:0	10.32	11.19	16.48	16.07	0.64	0.73	9.41	7.71
14:1	2.05	2.01	0.00	0.00	0.00	0.00	0.84	0.89
15:0	0.89	0.86	0.00	0.00	0.00	0.00	0.53	0.65
16:0Br	0.25	0.23	0.00	0.00	0.00	0.00	0.10	0.14
16:0	30.01	28.30	7.30	7.12	18.16	18.67	18.22	21.70
16:1	2.37	2.18	0.00	0.00	0.20	0.37	1.36	1.32
16:2	0.68	0.46	0.00	0.00	0.00	0.00	0.27	0.29
18:0Br	0.45	0.35	0.00	0.00	0.00	0.00	0.15	0.26
18:0	13.51	12.83	2.60	2.34	2.41	2.85	8.69	8.17
18:1	21.14	22.55	5.63	5.42	21.17	21.27	20.21	20.08
18:2	1.45	2.06	1.80	2.77	55.06	53.77	18.32	18.98
18:3	2.24	2.23	1.42	3.41	1.81	1.49	1.73	1.88
20:0	0.47	0.71	0.00	0.00	0.24	0.53	0.54	0.72

Table A33: Fatty Acid Composition Of CMKCCNCS Mixture And Its Components

Fatty Acids	Milk Fat (52.04%)		Coconut Oil (18.64%)		Cotton Seed Oil Mixture (29.31%)			
4:0	3.87	3.48	0.00	0.00	0.00	0.00	1.46	2.25
6:0	2.58	2.42	0.71	0.93	0.00	0.00	1.16	1.57
8:0	1.30	1.56	11.92	11.84	0.00	0.00	2.23	2.73
10:0	3.13	2.80	6.93	6.72	0.00	0.00	2.47	2.62
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.11	0.08
12:0	3.81	3.52	43.45	45.44	0.33	0.32	9.94	10.97
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.10	0.07
14:0	11.03	10.19	16.00	16.41	0.64	0.73	7.69	9.33
14:1	1.99	2.02	0.00	0.00	0.00	0.00	0.89	0.84
15:0	0.85	0.88	0.00	0.00	0.00	0.00	0.65	0.53
16:0Br	0.23	0.25	0.00	0.00	0.00	0.00	0.14	0.10
16:0	27.93	30.64	7.09	7.27	18.16	18.67	21.63	18.07
16:1	2.15	2.34	0.00	0.00	0.20	0.37	1.31	1.35
16:2	0.46	0.67	0.00	0.00	0.00	0.00	0.29	0.27
18:0Br	0.35	0.44	0.00	0.00	0.00	0.00	0.26	0.15
18:0	12.66	13.35	2.33	3.59	2.41	2.85	8.15	8.62
18:1	22.25	20.89	5.39	5.60	21.17	21.27	20.02	20.04
18:2	2.03	1.43	2.76	1.79	55.06	53.77	18.92	18.17
18:3	2.20	2.21	3.39	1.41	1.81	1.49	1.87	1.72
20:0	0.70	0.46	0.00	0.00	0.24	0.53	0.72	0.51

Table A34: Fatty Acid Composition Of MKTLCS Mixture And Its Components

Fatty Acids	Milk Fat (35.78%)		Tallow (34.34%)		Cotton Seed Oil Mixture (29.88%)			
4:0	2.61	2.90	0.00	0.00	0.00	0.00	0.68	0.81
6:0	2.21	2.36	0.00	0.00	0.00	0.00	0.67	0.57
8:0	1.53	1.28	0.00	0.00	0.00	0.00	0.47	0.42
10:0	2.84	3.18	0.00	0.00	0.00	0.00	1.16	0.93
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.07	0.04
12:0	3.56	3.86	0.61	0.25	0.33	0.32	1.34	1.31
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.05	0.06
14:0	10.32	11.17	2.91	3.52	0.64	0.73	5.12	5.18
14:1	2.05	2.01	0.93	0.95	0.00	0.00	0.93	0.92
15:0	0.89	0.86	0.52	0.68	0.00	0.00	0.57	0.46
16:0Br	0.25	0.23	0.15	0.16	0.00	0.00	0.12	0.15
16:0	30.01	28.30	24.48	22.53	18.16	18.67	21.79	23.03
16:1	2.37	2.18	2.22	3.33	0.20	0.37	2.27	1.80
16:2	0.68	0.46	0.88	1.45	0.00	0.00	0.91	0.62
18:0Br	0.45	0.35	0.54	0.61	0.00	0.00	0.65	0.20
18:0	13.51	12.83	31.34	30.32	2.41	2.85	15.61	16.33
18:1	21.14	22.55	31.52	31.17	21.17	21.27	26.52	26.38
18:2	1.45	2.06	0.81	0.93	55.06	53.77	18.96	18.74
18:3	2.24	2.23	1.39	1.74	1.81	1.49	1.53	1.65
20:0	0.47	0.71	1.45	2.07	0.24	0.53	0.59	0.41

Table A35: Fatty Acid Composition Of CMKTLCS Mixture And Its Components

Fatty Acids	Milk Fat (35.78%)		Tallow 34.34%		Cotton Seed Oil Mixture 29.88%)			
4:0	3.87	3.48	0.00	0.00	0.00	0.00	1.09	0.92
6:0	2.58	2.42	0.00	0.00	0.00	0.00	0.63	0.75
8:0	1.30	1.56	0.00	0.00	0.00	0.00	0.43	0.48
10:0	3.13	2.80	0.00	0.00	0.00	0.00	0.92	1.16
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.04	0.07
12:0	3.81	3.52	0.61	0.25	0.33	0.32	1.30	1.33
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.06	0.05
14:0	11.03	10.19	2.91	3.52	0.64	0.73	5.16	5.10
14:1	1.99	2.02	0.93	0.95	0.00	0.00	0.91	0.93
15:0	0.85	0.88	0.52	0.68	0.00	0.00	0.46	0.57
16:0Br	0.23	0.25	0.15	0.16	0.00	0.00	0.15	0.12
16:0	27.93	30.64	24.48	22.53	18.16	18.67	22.95	21.72
16:1	2.15	2.34	2.22	3.33	0.20	0.37	1.79	2.26
16:2	0.46	0.67	0.88	1.45	0.00	0.00	0.61	0.90
18:0Br	0.35	0.44	0.54	0.61	0.00	0.00	0.20	0.65
18:0	12.66	13.35	31.34	30.32	2.41	2.85	16.27	15.56
18:1	22.25	20.89	31.52	31.17	21.17	21.27	26.29	26.43
18:2	2.03	1.43	0.81	0.93	55.06	53.77	18.68	18.90
18:3	2.20	2.21	1.39	1.74	1.81	1.49	1.65	1.53
20:0	0.70	0.46	1.45	2.07	0.24	0.53	0.40	0.59

Table A36: Fatty Acid Composition Of MKTSLF Mixture And Its Components

Fatty Acids	Milk Fat (78.04%)		Tallow 14.06%		Sunflower Oil Mixture 7.90%)			
4:0	2.61	2.90	0.00	0.00	0.00	0.00	2.48	3.18
6:0	2.21	2.36	0.00	0.00	0.00	0.00	1.92	2.51
8:0	1.53	1.28	0.00	0.00	0.00	0.00	1.18	1.34
10:0	2.84	3.18	0.00	0.00	0.00	0.00	3.06	3.86
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.15	0.26
12:0	3.56	3.86	0.61	0.25	0.25	0.16	3.44	2.87
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.17	0.08
14:0	10.32	11.17	2.91	3.52	0.06	0.06	10.41	10.39
14:1	2.05	2.01	0.93	0.95	0.00	0.00	1.91	1.62
15:0	0.89	0.86	0.52	0.68	0.00	0.00	1.08	1.20
16:0Br	0.25	0.23	0.15	0.16	0.00	0.00	0.25	0.47
16:0	30.01	28.30	24.48	22.53	5.84	5.75	30.27	26.98
16:1	2.37	2.18	2.22	3.33	0.00	0.00	2.74	2.28
16:2	0.68	0.46	0.88	1.45	0.00	0.00	1.00	1.50
18:0Br	0.45	0.35	0.54	0.61	0.00	0.00	0.19	0.47
18:0	13.51	12.83	31.34	30.32	4.04	4.23	2.23	4.90
18:1	21.14	22.55	31.52	31.17	16.23	17.66	26.00	24.07
18:2	1.45	2.06	0.81	0.93	72.53	69.37	9.23	7.88
18:3	2.24	2.23	1.39	1.74	0.53	1.24	1.64	1.68
20:0	0.47	0.71	1.45	2.07	0.47	1.48	0.65	2.43

Table A37: Fatty Acid Composition Of CMKTLSE Mixture And Its Components

Fatty Acids	Milk Fat (78.04%)		Tallow (14.06%)		Sunflower Oil (7.90%)		Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	3.31	4.23
6:0	2.58	2.42	0.00	0.00	0.00	0.00	2.11	2.75
8:0	1.30	1.56	0.00	0.00	0.00	0.00	1.21	1.36
10:0	3.13	2.80	0.00	0.00	0.00	0.00	3.03	3.81
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.15	0.26
12:0	3.81	3.52	0.61	0.25	0.25	0.16	3.41	2.87
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.17	0.08
14:0	11.03	10.19	2.91	3.52	0.06	0.06	10.30	10.24
14:1	1.99	2.02	0.93	0.95	0.00	0.00	1.89	1.60
15:0	0.85	0.88	0.52	0.68	0.00	0.00	1.07	1.18
16:0Br	0.23	0.25	0.15	0.16	0.00	0.00	0.25	0.46
16:0	27.93	30.64	24.48	22.53	5.84	5.75	29.93	26.60
16:1	2.15	2.34	2.22	3.33	0.00	0.00	2.71	2.24
16:2	0.46	0.67	0.88	1.45	0.00	0.00	0.99	1.48
18:0Br	0.35	0.44	0.54	0.61	0.00	0.00	0.19	0.46
18:0	12.66	13.35	31.34	30.32	4.04	4.23	2.20	4.83
18:1	22.25	20.89	31.52	31.17	16.23	17.66	25.72	23.73
18:2	2.03	1.43	0.81	0.93	72.53	69.37	9.13	7.77
18:3	2.20	2.21	1.39	1.74	0.53	1.24	1.62	1.66
20:0	0.70	0.46	1.45	2.07	0.47	1.48	0.65	2.40

Table A38: Fatty Acid Composition Of MKTLMZ Mixture And Its Components

Fatty Acids	Milk Fat (45.80%)		Tallow (27.60%)		Maize Oil (26.60%)		Mixture	
4:0	2.61	2.90	0.00	0.00	0.00	0.00	0.97	1.10
6:0	2.21	2.35	0.00	0.00	0.00	0.00	0.76	0.83
8:0	1.53	1.28	0.00	0.00	0.00	0.00	0.53	0.64
10:0	2.84	3.18	0.00	0.00	0.00	0.00	1.48	1.55
10:1	0.35	0.39	0.00	0.00	0.00	0.00	0.14	0.11
12:0	3.56	3.86	0.61	0.25	0.12	0.11	1.79	1.88
14:0Br	0.09	0.11	0.00	0.00	0.00	0.00	0.12	0.07
14:0	10.32	11.17	2.91	3.52	0.00	0.00	7.15	7.14
14:1	2.05	2.01	0.93	0.95	0.00	0.00	0.95	0.32
15:0	0.89	0.86	0.52	0.68	0.00	0.00	0.56	0.70
16:0Br	0.25	0.23	0.15	0.16	0.00	0.00	0.10	0.25
16:0	30.01	28.30	24.48	22.53	11.37	9.34	20.60	25.77
16:1	2.37	2.18	2.22	3.33	0.06	0.09	2.19	2.00
16:2	0.68	0.46	0.88	1.45	0.00	0.00	0.98	0.64
18:0Br	0.45	0.35	0.54	0.61	0.00	0.00	0.43	0.10
18:0	13.51	12.83	31.34	30.32	2.16	2.32	14.84	15.01
18:1	21.14	22.55	31.52	31.17	32.26	33.63	28.67	26.12
18:2	1.45	2.06	0.81	0.93	52.64	53.45	15.95	14.41
18:3	2.24	2.23	1.39	1.74	0.98	0.90	1.37	0.93
20:0	0.47	0.71	1.45	2.07	0.43	0.17	0.43	0.31

Table A39: Fatty Acid Composition Of CMKTLMZ Mixture And Its Components

Fatty Acids	Milk Fat (45.80%)		Tallow (27.60%)		Maize Oil (26.60%)		Mixture	
4:0	3.87	3.48	0.00	0.00	0.00	0.00	1.48	1.31
6:0	2.58	2.42	0.00	0.00	0.00	0.00	0.92	0.84
8:0	1.30	1.56	0.00	0.00	0.00	0.00	0.66	0.54
10:0	3.13	2.80	0.00	0.00	0.00	0.00	1.54	1.48
10:1	0.39	0.35	0.00	0.00	0.00	0.00	0.11	0.13
12:0	3.81	3.52	0.61	0.25	0.12	0.11	1.88	1.78
14:0Br	0.10	0.08	0.00	0.00	0.00	0.00	0.07	0.12
14:0	11.03	10.29	2.91	3.52	0.00	0.00	7.10	7.12
14:1	1.99	2.02	0.93	0.95	0.00	0.00	0.32	0.95
15:0	0.85	0.88	0.52	0.68	0.00	0.00	0.70	0.56
16:0Br	0.23	0.25	0.15	0.16	0.00	0.00	0.25	0.10
16:0	27.93	30.64	24.48	22.53	11.37	9.34	25.77	20.51
16:1	2.15	2.34	2.22	3.33	0.06	0.09	1.90	2.18
16:2	0.46	0.67	0.88	1.45	0.00	0.00	0.64	0.98
18:0Br	0.35	0.44	0.54	0.61	0.00	0.00	0.10	0.42
18:0	12.66	13.35	31.34	30.32	2.16	2.32	14.93	14.78
18:1	22.25	20.89	31.52	31.17	32.26	33.63	25.99	28.54
18:2	2.03	1.43	0.81	0.93	52.64	53.45	14.34	15.88
18:3	2.20	2.21	1.39	1.74	0.98	0.90	0.92	1.37
20:0	0.70	0.46	1.45	2.07	0.43	0.17	0.31	0.43

Table A40(i): Literature Fatty Acid Compositions Of Cotton Seed Oil, Soya Bean Oil, Tallow And Sunflower Oil

Fatty Acids	Cotton Seed Oil		Soya Bean Oil		Tallow		Sunflower Oil	
12:0	0.00	0.00	0.00	0.00	1.30	0.20	0.00	0.00
14:0	3.30	2.00	0.30	0.40	3.50	4.10	0.04	0.06
14:1	0.00	0.00	0.00	0.00	0.50	0.50	0.00	0.00
16:0	19.90	19.60	9.80	10.60	25.00	24.60	6.73	6.50
16:1	0.00	0.00	0.50	1.00	1.70	2.60	0.00	0.00
18:0	1.30	2.70	2.40	2.40	22.20	15.40	4.52	4.52
18:1	29.60	24.60	28.90	23.50	42.00	45.10	23.24	23.12
18:2	45.30	50.40	50.70	51.20	2.20	5.00	65.06	65.40
18:3	0.00	0.00	6.50	8.50	0.00	0.00	0.00	0.00
20:0	0.60	0.70	0.90	2.40	1.60	2.50	0.40	0.58

Table A40(ii) Literature Fatty Acid Compositions Of Milk Fat, Coconut Oil And Maize Oil

Fatty Acids	Milk Fat		Coconut Oil		Maize Oil	
4:0	3.10	3.40	0.00	0.00	0.00	0.00
6:0	1.90	1.80	0.00	0.00	0.00	0.00
8:0	0.80	0.90	7.90	7.80	0.00	0.00
10:0	2.00	1.90	7.20	7.60	0.00	0.00
12:0	3.90	3.10	48.00	44.80	0.00	0.00
14:0	10.60	9.70	17.50	18.10	0.40	0.00
16:0	28.10	27.60	9.00	9.50	12.70	12.00
18:0	8.50	12.20	2.10	2.40	2.70	2.30
18:1	36.40	34.30	5.70	8.20	30.70	28.30
18:2	3.70	4.40	2.60	1.50	53.50	56.60
18:3	0.00	0.00	0.00	0.00	0.00	0.80
20:0	1.00	0.70	0.00	0.00	0.00	0.00

Table A41: Mixture Component Proportions And Their Standard Deviation  
 Calculated By The FREQC F77 Program Using Experimental Data

Mixtures	Fat	Standard	Fat	Standard	Fat	Standard
	One	Deviation	Two	Deviation	Three	Deviation
	+/-%	+/-%	+/-%	+/-%	+/-%	+/-%
OCSCCNMZ	18.50	9.11	46.50	8.91	35.17	9.75
(Actual Val.	27.43		46.01		26.56)	
OMZCSMK	4.50	1.85	12.83	7.09	82.28	6.04
(Actual Val.	4.09		14.98		80.93	
OSFMZCCN	45.83	12.16	27.17	8.93	23.17	11.67
(Actual Val.	50.86		23.88		25.26)	
OTIMZCS	(Only One Set Of Data Is Available)					
	75.78		- 27.57		51.79	
(Actual Val.	75.41		7.68		16.91)	
OMZCSSB	25.93	13.04	21.64	4.67	53.07	15.25
(Actual Val.	26.46		26.40		47.14)	
OSFSBCCN	25.55	18.29	51.34	18.46	22.40	7.12
(Actual Val.	25.09		50.00		24.91)	
OSFCCNSB	25.70	17.05	22.90	5.30	50.90	16.57
(Actual Val.	25.09		24.91		50.00)	
OCCNSFSB	24.90	3.84	26.50	17.91	48.10	19.00
(Actual Val.	24.91		25.09		50.00)	
OMZCCNSF	27.00	9.07	25.33	12.41	44.50	12.98
(Actual Val.	23.88		25.26		50.86)	
OCCNMZSF	23.25	11.67	25.13	8.93	48.25	9.43
(Actual Val.	25.26		23.88		50.86)	
OCSMZCCN	20.61	11.54	35.06	11.56	45.06	9.97
(Actual Val.	27.43		26.56		46.01)	
OSFCCNMZ	43.39	13.72	23.39	12.53	28.94	8.46
(Actual Val.	50.86		25.26		23.88)	
OCSMZSB	24.50	11.60	23.07	11.57	53.07	17.09
(Actual Val.	26.40		26.46		47.14)	
AMKSBMZ	69.96	18.99	17.23	21.16	13.59	10.43
(Actual Val.	77.41		16.67		5.92)	
MKPLCCN	77.13	14.78	15.29	15.12	7.92	5.43
(Actual Val.	89.17		6.77		4.07)	
MKSBSF	76.38	12.91	7.00	5.39	16.38	9.84
(Actual Val.	78.07		10.81		11.12)	
AMKSFSB	74.00	11.48	17.00	10.93	9.50	6.01
(Actual Val.	78.07		11.12		10.81)	
CSMZMK	22.00	15.26	7.00	4.43	69.50	18.81
(Actual Val.	11.71		1.87		86.42)	
MKMZCS	84.50	1.36	9.50	7.31	9.50	9.43
(Actual Val.	86.42		1.87		11.71)	
MZCSMK	7.83	4.73	24.50	34.55	69.50	33.19
(Actual Val.	1.87		11.72		86.42)	
MKCSMZ	84.50	2.37	7.83	4.87	7.83	4.18
(Actual Val.	86.42		11.71		1.87)	
AAMKCSMZ	84.50	2.37	7.83	4.87	7.83	4.18
(Actual Val.	86.42		11.71		1.87)	
CSMZTL	18.14	8.36	27.23	11.11	55.41	15.71
(Actual Val.	24.17		12.90		62.94)	
MZCSTL	26.67	9.83	21.89	13.97	51.46	14.72
(Actual Val.	12.90		24.17		62.94)	
MKSBCS	56.91	14.54	21.05	7.43	21.05	15.34
Actual Val.	57.89		23.46		18.62)	
CMKSBCS	56.04	13.38	23.35	8.07	21.42	15.04
(Actual Val.	57.89		23.46		18.62)	

Table A41 ..... continue

Mixture	Fat	Standard	Fat	Standard	Fat	Standard
	One	Deviation	Two	Deviation	Three	Deviation
	+/-%	+/-%	+/-%	+/-%	+/-%	+/-%
MKSFCS	58.20	9.54	25.24	11.49	17.09	12.41
(Actual Val.	59.28		25.07		15.65)	
CMKSFCS	57.11	11.39	25.80	12.09	17.11	11.59
Actual Val.	59.28		25.07		15.65)	
CMKCCNCS	48.69	12.66	13.69	7.87	35.63	14.28
(Actual Val.	52.04		18.64		29.32)	
MKCCNCS	49.32	12.71	15.06	7.47	34.13	13.93
(Actual Val.	52.04		18.64		29.32)	
CMKSFMZ	70.21	12.96	12.12	9.12	14.50	6.05
(Actual Val.	77.96		5.12		16.92)	
MKSFMZ	70.21	13.01	10.69	8.94	15.45	4.99
(Actual Val.	77.96		5.12		16.92)	
SBSFMZ	50.75	20.01	28.25	12.10	17.00	22.98
(Actual Val.	67.53		22.32		10.15)	
CMKCCNSB	73.63	15.53	19.28	13.88	6.67	4.89
(Actual Val.	87.54		8.67		3.80)	
MKCCNSB	77.83	16.05	16.17	11.02	7.00	5.57
(Actual Val.	87.54		8.67		3.80)	
CMKTLSB	50.65	15.54	29.12	15.78	19.63	10.06
(Actual Val.	65.53		22.84		14.63)	
MKTLSB	48.69	16.14	29.77	16.41	20.85	9.27
(Actual Val.	65.53		22.84		14.63)	
MKCCNMZ	66.13	14.61	16.59	8.79	12.64	10.83
(Actual Val.	82.35		10.73		6.92)	
CMKCCNMZ	65.07	17.84	17.64	12.91	12.50	10.55
(Actual Val.	82.35		10.73		6.92)	
CMKSFCCN	61.74	17.99	26.57	15.25	11.05	5.76
(Actual Val.	65.84		22.13		12.03)	
MKSFCCN	62.31	16.95	26.94	14.44	11.57	6.91
(Actual Val.	65.84		22.13		12.03)	
ACMKTLCN	55.47	26.07	32.24	25.66	11.91	7.32
(Actual Val.	89.17		6.77		4.07)	
AMKTLCN	58.10	25.09	30.50	24.46	11.70	11.44
Actual Val.	89.17		6.77		4.07)	
CMKTLMZ	42.94	13.10	34.97	15.62	20.91	13.85
(Actual Val.	45.80		27.60		26.60)	
MKTLMZ	44.32	12.73	33.07	15.53	21.29	13.61
(Actual Val.	45.80		27.60		26.60)	
CMKTLSF	50.93	27.55	30.21	32.20	17.36	15.81
(Actual Val.	78.04		14.06		7.90)	
MKTLSF	60.21	29.66	25.21	28.91	12.36	11.02
(Actual Val.	78.04		14.06		7.90)	
MKT LCS	29.88	12.85	40.38	18.66	29.50	14.25
(Actual Val.	35.78		34.34		29.88)	
CMKT LCS	29.70	10.95	38.50	18.11	30.37	13.87
(Actual Val.	35.78		34.34		29.88)	

Table A42: Mixture Component Proportions And Their Standard Deviation  
Calculated By The FREQC F77 Program Using Literature Data

Mixtures	Fat One	Standard Deviation	Fat Two	Standard Deviation	Fat Three	Standard Deviation
MKTLMZU	49.89	18.26	28.35	21.76	19.89	19.10
(Actual Val.	45.80		27.60		26.60)	
CMKTLMZU	52.68	17.09	31.77	19.77	17.23	15.16
(Actual Val.	45.80		27.60		26.60)	
MKCCNMZU	57.23	20.78	30.86	15.43	9.96	11.52
(Actual Val.	82.35		10.73		6.92)	
CMKCCNMZU	79.50	11.24	12.00	10.83	4.50	1.01
(Actual Val.	82.35		10.73		6.92)	
CMKSFCU	67.83	19.75	14.50	9.41	17.83	24.64
(Actual Val.	59.28		25.07		15.65)	
MKSFCU	51.17	7.08	17.83	16.22	24.50	22.18
(Actual Val.	59.28		25.07		15.65)	
CMKSFMZU	78.29		2.47		19.24	
	(Only One Set Of Data Is Available)					
(Actual Val.	77.96		5.12		16.92)	
MKSFMZU	79.11		8.53		12.36	
	(Only One Set Of Data Is Available)					
(Actual Val.	77.96		5.12		16.92)	
MKCCNCU	47.00	19.68	23.67	8.69	27.42	13.76
(Actual Val.	52.04		18.64		29.32)	
CMKCCNCU	53.59	16.59	21.77	9.00	23.59	13.41
(Actual Val.	52.04		18.64		29.32)	
CMKCCNSBU	52.50	29.88	44.50	28.83	4.50	1.72
(Actual Val.	87.54		8.67		3.80)	
MKCCNSBU	21.13		78.66		0.21	
	(Only One Set Of Data Is Available)					
(Actual Val.	87.54		8.67		3.80)	
CMKSBCU	54.50	16.14	8.50	7.97	34.50	13.47
(Actual Val.	57.89		23.46		18.62)	
MKSBCU	58.25	14.19	9.50	10.28	30.75	14.52
(Actual Val.	57.89		23.46		18.62)	
CMKSFCNU	NO SOLUTION FOR THIS MIXTURE					
MKSFCNU	NO SOLUTION FOR THIS MIXTURE					
ACMKTLCNU	29.50	23.60	54.50	11.86	14.50	12.04
(Actual Val.	89.17		6.77		4.07)	
AMKTLCNU	53.52		45.69		0.80	
	(Only One Set Of Data Is Available)					
(Actual Val.	89.17		6.77		4.07)	
CMKTLCU	40.86	10.96	19.96	13.01	37.23	7.53
(Actual Val.	35.78		34.34		29.88)	
MKTLCU	38.67	13.50	27.83	19.55	28.67	10.53
(Actual Val.	35.78		34.34		29.88)	
CMKTLSBU	54.50	33.44	32.00	35.81	14.50	3.30
(Actual Val.	65.53		22.84		14.63)	
MKTLSBU	66.72	23.55	20.06	25.31	14.50	5.21
(Actual Val.	65.53		22.84		14.63)	
CMKTLSFU	59.50	41.76	29.50	41.45	9.60	0.88
(Actual Val.	78.04		14.06		7.90)	
MKTLSFU	54.50	41.68	34.50	41.28	14.50	5.94
(Actual Val.	78.04		14.06		7.90)	
MKTLCNU	37.83	21.21	54.50	10.55	11.17	11.01
(Actual Val.	89.17		6.77		4.07)	
MKSMBZU	69.50	11.22	12.00	6.94	17.00	8.64
(Actual Val.	77.41		16.67		5.92)	
MZCSMKU	NO SOLUTION FOR THIS MIXTURE					

Table A42 ..... continue

Mixture	Fat One +/-%	Standard Deviation +/-%	Fat Two +/-%	Standard Deviation +/-%	Fat Three +/-%	Standard Deviation +/-%
OMKCSMZU	NO SOLUTION FOR THIS MIXTURE					
MKCSMZU	NO SOLUTION FOR THIS MIXTURE					
MKSFSBU	NO SOLUTION FOR THIS MIXTURE					
SBSFMZU	57.00 (Actual Val. 67.53)	8.39	27.00 22.32	21.78	17.00 10.15)	14.18
OCSCNMZU	25.73 (Actual Val. 27.43)	19.87	39.90 46.01	4.25	33.23 26.56)	18.41
OCSMZSBU	46.33 (Actual Val. 50.86)	1.97	24.90 25.26	6.38	27.76 23.88)	6.41
OCSMZCCNU	13.47 (Actual Val. 27.43)	10.50	44.90 26.56	9.79	40.61 46.01)	3.63
OCCNMZSFU	25.67 (Actual Val. 25.26)	7.37	27.21 23.88	8.06	47.21 50.86)	7.39
OMZCCNSFU	30.46 (Actual Val. 23.88)	3.39	22.68 25.26	3.82	46.01 50.86)	1.70
OCCNSFSBU	NO SOLUTION FOR THIS MIXTURE					
OSFCCNSBU	NO SOLUTION FOR THIS MIXTURE					
OSFSECCNU	NO SOLUTION FOR THIS MIXTURE					
OTLMZCSU	41.57 (Actual Val. 75.41)	33.15	21.57 7.68	15.05	34.90 16.91)	29.12
OMZCCSSBU	NO SOLUTION FOR THIS MIXTURE					
OSFMZCCNU	44.90 (Actual Val. 50.86)	2.37	27.76 23.88	7.37	24.90 25.26)	6.54
OMZCCSMKU	9.90 (Actual Val. 4.09)	5.17	14.90 14.98	11.69	79.90 80.93)	6.28

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PROGRAM CRA4
C USING CRAMER'S RULE METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C THE GENERAL EQUATION IS: AX = B .
C DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
  INTEGER*2 M,N,NIN,NOUT,PP,HH,KK,GG,JL,I,N1,N2,N3,N4
  REAL*8 AA(30,10),BB(30,10), TITLE(20), X(10)
  REAL*8 A(30,10),B(30,10),T(50),EE(50),ER(50),C(50),
  * G(30,10),AE(30),DE(30),XX(600),XY(600),XZ(600),ST(10),
  * ET(5),D4(600),D5(600),D6(600)
  REAL*8 V,D,R,A8,B8,C8,F8,D8,E8,ED,A1,A2,A3,A4,A5,A6,A7,
  * C1,C2,C3,C4,C5,C6,C7,X1,X2,X3,Y1,Y2,Y3,G1,G2,G3,Z1,
  * E1,E2,E3,D1,D2,D3,S1,H1,H2,H3,B1,B2,B3,B4,B5,B6,B7
  INTRINSIC DABS, SQRT, DSQRT
  CHARACTER*16 CC(5)

C
  DATA NIN/1/, NOUT/1/
  READ (1,52) (CC(I),I=1,3)
  READ (NIN,*) M
  READ (NIN,*) N

C INPUT CODE NUMBER FOR EACH FAT OR OIL AND MIXTURE:
C 1 FOR MILKFAT; 2 FOR TALLOW; 3 FOR SUNFLOWER OIL;
C 4 FOR MAIZE OIL; 5 FOR COTTON SEED OIL; 6 FOR SOYA
C BEAN OIL; 7 FOR COCONUT OIL; 8 FOR MIXTURE THAT HAS
C MILKFAT AS ONE OF THE COMPONENTS.
  READ (1,*) N1,N2,N3,N4
  READ(NIN,99) TITLE
  WRITE (NOUT,98) (TITLE(I),I=1,7)
  DO 20 I=1,M
20  READ (NIN,*) (A(I,J),J=1,N)
C CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C THE GLC ANALYSIS.
  V = SQRT(0.5)
  R = 10.0 ** (-6)
  DO 10 I = 1, M
    BB(I,1)=DABS(A(I,1)-A(I,2))*V
    BB(I,2)=DABS(A(I,3)-A(I,4))*V
    BB(I,3)=DABS(A(I,5)-A(I,6))*V
    BB(I,4)=DABS(A(I,7)-A(I,8))*V
    AA(I,1)=(A(I,1)+A(I,2))*0.5
    AA(I,2)=(A(I,3)+A(I,4))*0.5
    AA(I,3)=(A(I,5)+A(I,6))*0.5
10  AA(I,4)=(A(I,7)+A(I,8))*0.5
    CALL COEFV (BB,AA,N1,N2,N3,N4)
    DO 100 I = 1,M
    DO 101 J = 1,4
101  G(I,J)=AA(I,J)
100  CONTINUE
  WRITE (NOUT,22)
  WRITE (NOUT,96)
  WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
  WRITE (NOUT,90)
  WRITE (NOUT,91) ((BB(I,J),J=1,4),I=1,M)
  X1=0.0
  X2=0.0
  X3=0.0
  Y1=0.0
  Y2=0.0
  Y3=0.0
  G1=0.0
  G2=0.0
  G3=0.0
  Z1=0

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D1=0.0
D2=0.0
D3=0.0
H1=0.0
H2=0.0
H3=0.0
LL= 0
DO 444 PP= 1, (M-2)
HH=PP+1
DO 455 KK=HH, (M-1)
GG=KK+1
DO 466 LI= GG, M
DO 477 JL= 1,4
A(1,JL)=AA(PP,JL)
B(1,JL)=BB(PP,JL)
A(2,JL)=AA(KK,JL)
B(2,JL)=BB(KK,JL)
A(3,JL)=AA(LI,JL)
477 B(3,JL)=BB(LI,JL)
D=A(1,1)*A(2,2)*A(3,3)-A(1,1)*A(2,3)*A(3,2)-A(1,2)*A(2,1)*A(3,3)+
* A(1,2)*A(2,3)*A(3,1)+A(1,3)*A(2,1)*A(3,2)-A(1,3)*A(2,2)*A(3,1)
IF (D-R) 466, 51, 51
51 T(1)=(A(1,4)*A(2,2)*A(3,3))-(A(1,4)*A(2,3)*A(3,2))-
* (A(1,2)*A(2,4)*A(3,3))+(A(1,2)*A(2,3)*A(3,4))+
* (A(1,3)*A(2,4)*A(3,2))-(A(1,3)*A(2,2)*A(3,4))
X(1)=T(1)/D
T(2)=(A(1,1)*A(2,4)*A(3,3))-(A(1,1)*A(2,3)*A(3,4))
* -(A(1,4)*A(2,1)*A(3,3))+(A(1,4)*A(2,3)*A(3,1))
* +(A(1,3)*A(2,1)*A(3,4))-(A(1,3)*A(2,4)*A(3,1))
X(2)=T(2)/D
T(3)=(A(1,1)*A(2,2)*A(3,4))-(A(1,1)*A(2,4)*A(3,2))
* -(A(1,2)*A(2,1)*A(3,4))+(A(1,2)*A(2,4)*A(3,1))
* +(A(1,4)*A(2,1)*A(3,2))-(A(1,4)*A(2,2)*A(3,1))
X(3)=T(3)/D
A8=B(1,1)*A(2,2)*A(3,3)+B(2,2)*A(1,1)*A(3,3)+B(3,3)*A(1,1)*A(2,2)
B8=B(1,1)*A(2,3)*A(3,2)+B(2,3)*A(1,1)*A(3,2)+B(3,2)*A(1,1)*A(2,3)
C8=B(1,2)*A(2,1)*A(3,3)+B(2,1)*A(1,2)*A(3,3)+B(3,3)*A(1,2)*A(2,1)
D8=B(1,2)*A(2,3)*A(3,1)+B(2,3)*A(1,2)*A(3,1)+B(3,1)*A(2,3)*A(1,2)
E8=B(1,3)*A(2,1)*A(3,2)+B(2,1)*A(1,3)*A(3,2)+B(3,2)*A(1,3)*A(2,1)
F8=B(1,3)*A(2,2)*A(3,1)+B(2,2)*A(1,3)*A(3,1)+B(3,1)*A(1,3)*A(2,2)
ED=A8+B8+C8+D8+E8+F8
A2=B(1,4)*A(2,2)*A(3,3)+B(2,2)*A(1,4)*A(3,3)+B(3,3)*A(1,4)*A(2,2)
A3=B(1,4)*A(2,3)*A(3,2)+B(2,3)*A(1,4)*A(3,2)+B(3,2)*A(1,4)*A(2,3)
A4=B(1,2)*A(2,4)*A(3,3)+B(2,4)*A(1,2)*A(3,3)+B(3,3)*A(1,2)*A(2,4)
A5=B(1,2)*A(2,3)*A(3,4)+B(2,3)*A(1,2)*A(3,4)+B(3,4)*A(1,2)*A(2,3)
A6=B(1,3)*A(2,4)*A(3,2)+B(2,4)*A(1,3)*A(3,2)+B(3,2)*A(1,3)*A(2,4)
A7=B(1,3)*A(2,2)*A(3,4)+B(2,2)*A(1,3)*A(3,4)+B(3,4)*A(1,3)*A(2,2)
A1=A2+A3+A4+A5+A6+A7
B2=B(1,1)*A(2,4)*A(3,3)+B(2,4)*A(1,1)*A(3,3)+B(3,3)*A(1,1)*A(2,4)
B3=B(1,1)*A(2,3)*A(3,4)+B(2,3)*A(1,1)*A(3,4)+B(3,4)*A(1,1)*A(2,3)
B4=B(1,4)*A(2,1)*A(3,3)+B(2,1)*A(1,4)*A(3,3)+B(3,3)*A(1,4)*A(2,1)
B5=B(1,4)*A(2,3)*A(3,1)+B(2,3)*A(1,4)*A(3,1)+B(3,1)*A(1,4)*A(2,3)
B6=B(1,3)*A(2,1)*A(3,4)+B(2,1)*A(1,3)*A(3,4)+B(3,4)*A(1,3)*A(2,1)
B7=B(1,3)*A(2,4)*A(3,1)+B(2,4)*A(1,3)*A(3,1)+B(3,1)*A(1,3)*A(2,4)
B1=B2+B3+B4+B5+B6+B7
C2=B(1,1)*A(2,2)*A(3,4)+B(2,2)*A(1,1)*A(3,4)+B(3,4)*A(1,1)*A(2,2)
C3=B(1,1)*A(2,4)*A(3,2)+B(2,4)*A(1,1)*A(3,2)+B(3,2)*A(1,1)*A(2,4)
C4=B(1,2)*A(2,1)*A(3,4)+B(2,1)*A(1,2)*A(3,4)+B(3,4)*A(1,2)*A(2,1)
C5=B(1,2)*A(2,4)*A(3,1)+B(2,4)*A(1,2)*A(3,1)+B(3,1)*A(1,2)*A(2,4)
C6=B(1,4)*A(2,1)*A(3,2)+B(2,1)*A(1,4)*A(3,2)+B(3,2)*A(1,4)*A(2,1)
C7=B(1,4)*A(2,2)*A(3,1)+B(2,2)*A(1,4)*A(3,1)+B(3,1)*A(1,4)*A(2,2)
C1=C2+C3+C4+C5+C6+C7
IF (X(1) .LE. 0.0 .OR. X(1) .GE. 1.0) GO TO 466

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IF (X(2) .LE. 0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3) .LE. 0.0 .OR. X(3).GE.1.0) GO TO 466
EE(1)=ABS(A1/D)+ABS((T(1)*ED)/D**2)
EE(2)=ABS(B1/D)+ABS((T(2)*ED)/D**2)
EE(3)=ABS(C1/D)+ABS((T(3)*ED)/D**2)
IF (EE(1) .EQ. 0.0) GO TO 466
IF (EE(2) .EQ. 0.0) GO TO 466
IF (EE(3) .EQ. 0.0) GO TO 466
Z1=Z1+1
X1=X1+X(1)/(EE(1)**2)
X2=X2+X(2)/(EE(2)**2)
X3=X3+X(3)/(EE(3)**2)
Y1=Y1+1/EE(1)**2
Y2=Y2+1/EE(2)**2
Y3=Y3+1/EE(3)**2
G1=G1+(EE(1)**2)
G2=G2+(EE(2)**2)
G3=G3+(EE(3)**2)
D4(Z1)=EE(1)**2
D5(Z1)=EE(2)**2
D6(Z1)=EE(3)**2
XX(Z1)=X(1)
XY(Z1)=X(2)
XZ(Z1)=X(3)
466 CONTINUE
455 CONTINUE
444 CONTINUE
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE.
C FAT ONE:
X(1)=X1/Y1
C FAT TWO:)
X(2)=X2/Y2
C FAT THREE:
X(3)=X3/Y3
DO 77 I= 1,M
C(I)= 0.0
DO 770 J= 1,3
770 C(I)=C(I)+G(I,J)*X(J)
AE(I)=G(I,4)-C(I)
DE(I)= AE(I)/G(I,4)
77 CONTINUE
DO 11 I= 1, Z1
E1=DABS(XX(I)-X(1))
D1=D1+(E1**2)
H1=H1+(E1**2)/(D4(I))
E2=DABS(XY(I)-X(2))
D2=D2+(E2**2)
H2=H2+(E2**2)/(D5(I))
E3=DABS(XZ(I)-X(3))
D3=D3+(E3**2)
H3=H3+(E3**2)/(D6(I))
11 CONTINUE
S1=Z1-1
ST(1)=DSQRT(D1/S1)
ST(2)=DSQRT(D2/S1)
ST(3)=DSQRT(D3/S1)
C DETERMINE THE STANDARD ERROR OF EACH WEIGHTED MEAN
C FAT VALUE:
C FAT ONE:
ER(1)=DSQRT(H1/(S1*Y1))
ET(1)=DSQRT(1/Y1)
C FAT TWO:
ER(2)=DSQRT(H2/(S1*Y2))

```

```

      ET(2)=DSQRT(1/Y2)
C   FAT THREE:
      ER(3)=DSQRT(H3/(S1*Y3))
      ET(3)=DSQRT(1/Y3)
      WRITE (NOUT, 234) Z1
      WRITE (NOUT,2) (I,XX(I),XY(I),XZ(I),I=1,Z1)
      WRITE (NOUT,93) (G(I,4),C(I),AE(I),DE(I),I=1,M)
      PRINT*, '???'
      WRITE (1,94) (CC(I),X(I),ER(I),ET(I),ST(I),I=1,3)
      CALL CONLIMIT (Z1,XX,XY,XZ,X,ST)
22   FORMAT (15X, '          ' //)
52   FORMAT (A16)
2   FORMAT (5X, 'SET ', I3//5X, 'X(1) =', F9.5, 2X,
*   'X(2) =', F9.5, 2X, 'X(3) =', F9.5//)
93   FORMAT(5X, 'ACTUAL MIXTURE VALUE =', F9.5/5X
*   'CALCULATED VALUE =', F9.5, 5X, 'DIFFERENCE=', F9.5/5X,
*   'ACTUAL ERROR =', F9.5//)
94   FORMAT (5X/5X, 'WT. MEAN ', A16, '= ', F9.5/5X,
c   'WT. MEAN STANDARD ERROR =+/- ', F9.5/5X,
c   'ALTERNATIVE WT. MEAN STANDARD ERROR =+/- ', F9.5/5X,
c   'STANDARD DEVIATION =+/- ', F9.5//)
98   FORMAT (4(1X/), 1H 5A4, 1A3, 7HRESULTS/1X)
96   FORMAT(7X, 'MATRIX A', 18X, 'VECTOR B'//)
92   FORMAT (1X, 3F9.5//)
99   FORMAT (6A4, 1A4)
90   FORMAT(15X, 'STANDARD DEVIATION'//)
91   FORMAT (5X, 4F9.5//)
234  FORMAT (5X, 'NUMBER OF COMBINATIONS USED =', I3//)
      STOP
      END

```

## PROGRAM LSQ

```

C   USING LEAST SQUARE AND CRAMER'S RULE METHODS TO SOLVE SIMULTANEOUS
C   LINEAR EQUATIONS.
C   THE GENERAL EQUATION IS: AX = B .
C   DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
      INTEGER*2 M, N, NIN, NOUT, PP, I, K1, K2
      REAL*8 AA(50,10), BB(50,10), X(10)
      REAL*8 A(50,10), EE(50), ER(50), C(50), AX(50),
*   G(50,10), AE(50), DE(50), V1(50,10), A22(50,10)
      REAL*8 V, R, Y1, Y2
      CHARACTER*16 CC(5)
      INTRINSIC DABS, SQRT, DSQRT
C
      DATA NIN/1/, NOUT/1/
      READ (NIN,33) (CC(I), I = 1, 3)
      READ (NIN,*) M
      READ (NIN,*) N
      DO 20 I=1, M
20   READ (NIN,*) (A(I, J), J=1, N)
C   CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C   THE GLC ANALYSIS.
      V = SQRT(0.5)
      R = 10.0 ** (-6)
      DO 10 I = 1, M
      BB(I,1)=DABS(A(I,1)-A(I,2))*V
      BB(I,2)=DABS(A(I,3)-A(I,4))*V
      BB(I,3)=DABS(A(I,5)-A(I,6))*V
      BB(I,4)=DABS(A(I,7)-A(I,8))*V
      AA(I,1)=(A(I,1)+A(I,2))*0.5
      AA(I,2)=(A(I,3)+A(I,4))*0.5
      AA(I,3)=(A(I,5)+A(I,6))*0.5
10   AA(I,4)=(A(I,7)+A(I,8))*0.5

```

```

DO 100 I = 1,M
DO 101 J = 1,4
101 G(I,J)=AA(I,J)
100 CONTINUE
WRITE (NOUT,22)
WRITE (NOUT,96)
WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
WRITE (NOUT,90)
WRITE (NOUT,91) ((BB(I,J),J=1,4),I= 1,M)
Y1=0.0
Y2=0.0
DO 444 PP=1, M
A(PP,1)=AA(PP,1)-AA(PP,3)
A(PP,2)=AA(PP,2)-AA(PP,3)
444 A(PP,3)=AA(PP,4)-AA(PP,3)
DO 1 I=1,M
DO 2 J=1,3
2 V1(I,J)=A(I,J)
1 CONTINUE
CALL LEASQ(V1,INTS(1),M,INTS(3),A22)
CALL LEASQ(V1,INTS(2),M,INTS(3),A22)
N = 3
DO 231 K1=1,M
DO 231 K2=1,N
231 A(K1,K2)=A22(K1,K2)
X(2)=(A(2,1)*A(1,3)-A(1,1)*A(2,3))/
c (A(2,1)*A(1,2)-A(1,1)*A(2,2))
X(1)=(A(1,3)-A(1,2)*X(2))/A(1,1)
X(3)=1.0 - X(1) - X(2)
DO 711 I = 1,M
C(I)=0.0
DO 770 J= 1,3
770 C(I)=C(I)+G(I,J)*X(J)
AE(I)=G(I,4)-C(I)
DE(I)=ABS(AE(I)/G(I,4))*100.0
Y1=Y1+(DE(I)/100.0)**2
711 CONTINUE
Y2=SQRT(Y1)
DO 7 J=1,3
7 EE(J)=X(J)*Y2
IF (X(1).LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2).LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3).LE.0.0 .OR. X(3).GE.1.0) GO TO 466
WRITE (NOUT,93) (G(I,4),C(I),AE(I),DE(I),I=1,M)
PRINT*,'?'
WRITE (NOUT,94) (CC(I),X(I),EE(I),I=1,N)
22 FORMAT (5X/)
33 FORMAT (A16)
90 FORMAT (15X,'STANDARD DEVIATION'//)
91 FORMAT (5X,4F9.5/)
93 FORMAT(5X,'ACTUAL MIXTURE VALUE =',F9.5/5X
* 'CALCULATED VALUE =',F9.5,5X,'DIFFERENCE=',F9.5/5X,
* 'ACTUAL DEVIATION =',F9.5,1X,'
94 FORMAT (5X/5X,A16,' = ',F10.6/5X,
c 'STANDARD ERROR =',F10.6)
96 FORMAT (7X,'MATRIX A',18X,'VECTOR B'//)
GO TO 111
466 PRINT*,'NO SOLUTION FOR THIS MIXTURE.'
111 STOP
END
C
C
SUBROUTINE LEASQ(A1,NM,M,NN,A2)

```

```

REAL*8 T(50,10),F(10)
REAL*8 A(50,10),A1(50,10),A2(50,10)
INTEGER*2 I,J,M,NN,K,NM,I1
DO 10 I= 1,NN
10  F(I)=0.0
    DO 1 I = 1,M
      DO 2 I1 = 1, NN
2    A(I,I1)=A1(I,I1)
1    CONTINUE
      DO 11 J=1,NN
        DO 12 I=1,M
          T(I,J)=A(I,NM)*A(I,J)
12    F(J)=F(J)+T(I,J)
11    CONTINUE
        DO 13 K=1,NN
13    A2(NM,K)=F(K)
      RETURN
    END

PROGRAM CRA1
C USING CRAMER'S RULE METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C THE GENERAL EQUATION IS: AX = B .
C DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
  INTEGER*2 M,N,NIN,NOUT,PP,HH,KK,GG,JL,I,Z1
  REAL*8 AA(100,10),BB(100,10), TITLE(20), X(10)
  REAL*8 A(30,10),B(30,10),EE(10),ER(50),C(50),
  * G(30,10),AE(30),DE(30),XX(600),XY(600),XZ(600),ST(10)
  REAL*8 D4(100),D5(100),D6(100),ET(10)
  REAL*8 V,R,X1,X2,X3,Y1,Y2,Y3,G1,G2,G3
  REAL*8 E1,E2,E3,D1,D2,D3,S1,H1,H2,H3
  INTRINSIC DABS, SQRT, DSQRT
  CHARACTER*16 CC(5)

C
  DATA NIN/1/, NOUT/1/
  READ (1,52) (CC(I),I=1,3)
  READ (NIN,*) M
  READ (NIN,*) N
  READ(NIN,99) TITLE
  WRITE (NOUT,98) (TITLE(I),I=1,7)
  DO 20 I=1,M
20  READ (NIN,*) (A(I,J),J=1,N)
C CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C THE GLC ANALYSIS.
  V = SQRT(0.5)
  R = 10.0 ** (-6)
  DO 10 I = 1, M
    BB(I,1)=DABS(A(I,1)-A(I,2))*V
    BB(I,2)=DABS(A(I,3)-A(I,4))*V
    BB(I,3)=DABS(A(I,5)-A(I,6))*V
    BB(I,4)=DABS(A(I,7)-A(I,8))*V
    IF (BB(I,1) .LT. 0.7 .AND. BB(I,1).NE.0.0) BB(I,1)=0.7
    IF (BB(I,2) .LT. 0.7 .AND. BB(I,2).NE. 0.0) BB(I,2)=0.7
    IF (BB(I,3) .LT. 0.7 .AND. BB(I,3).NE. 0.0) BB(I,3)=0.7
    IF (BB(I,4) .LT. 0.7 .AND. BB(I,4).NE. 0.0) BB(I,4)=0.7
    AA(I,1)=(A(I,1)+A(I,2))*0.5
    AA(I,2)=(A(I,3)+A(I,4))*0.5
    AA(I,3)=(A(I,5)+A(I,6))*0.5
10  AA(I,4)=(A(I,7)+A(I,8))*0.5
    DO 100 I = 1,M
      DO 101 J = 1,4
101  G(I,J)=AA(I,J)
100  CONTINUE
  WRITE (NOUT,22)

```

```

WRITE (NOUT,96)
WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
WRITE (NOUT,90)
WRITE (NOUT,91) ((BB(I,J),J=1,4),I= 1,M)
X1=0.0
X2=0.0
X3=0.0
Y1=0.0
Y2=0.0
Y3=0.0
G1=0.0
G2=0.0
G3=0.0
Z1=0
D1=0.0
D2=0.0
D3=0.0
H1=0.0
H2=0.0
H3=0.0
DO 444 PP= 1, (M-2)
HH=PP+1
DO 455 KK=HH, (M-1)
GG=KK+1
DO 466 LI= GG, M
DO 477 JL= 1,4
A(1,JL)=AA(PP,JL)
B(1,JL)=BB(PP,JL)
A(2,JL)=AA(KK,JL)
B(2,JL)=BB(KK,JL)
A(3,JL)=AA(LI,JL)
B(3,JL)=BB(LI,JL)
477 CALL CRAMER (A,R,X)
IF (X(1) .LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2) .LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3) .LE.0.0 .OR. X(3).GE.1.0) GO TO 466
A(1,4)=B(1,4)+(X(1)*B(1,1)+X(2)*B(1,2)+X(3)*B(1,3))
A(2,4)=B(2,4)+(X(1)*B(2,1)+X(2)*B(2,2)+X(3)*B(2,3))
A(3,4)=B(3,4)+(X(1)*B(3,1)+X(2)*B(3,2)+X(3)*B(3,3))
CALL CRAMER (A,R,EE)
IF (EE(1) .EQ. 0.0) GO TO 466
IF (EE(2) .EQ. 0.0) GO TO 466
IF (EE(3) .EQ. 0.0) GO TO 466
Z1=Z1+1
X1=X1+X(1)/(EE(1)**2)
X2=X2+X(2)/(EE(2)**2)
X3=X3+X(3)/(EE(3)**2)
Y1=Y1+1/EE(1)**2
Y2=Y2+1/EE(2)**2
Y3=Y3+1/EE(3)**2
G1=G1+(EE(1)**2)
G2=G2+(EE(2)**2)
G3=G3+(EE(3)**2)
D4(Z1)=EE(1)**2
D5(Z1)=EE(2)**2
D6(Z1)=EE(3)**2
XX(Z1)=X(1)
XY(Z1)=X(2)
XZ(Z1)=X(3)
466 CONTINUE
455 CONTINUE
444 CONTINUE

```

C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE.

```

C  FAT ONE:
    X(1)=X1/Y1
C  FAT TWO:)
    X(2)=X2/Y2
C  FAT THREE:
    X(3)=X3/Y3
    DO 77 I= 1,M
    C(I)= 0.0
    DO 770 J= 1,3
770  C(I)=C(I)+G(I,J)*X(J)
    AE(I)=G(I,4)-C(I)
    DE(I)= AE(I)/G(I,4)
77  CONTINUE
    DO 11 I= 1, Z1
    E1=DABS(XX(I)-X(1))
    D1=D1+(E1**2)
    H1=H1+(E1**2)/(D4(I))
    E2=DABS(XY(I)-X(2))
    D2=D2+(E2**2)
    H2=H2+(E2**2)/(D5(I))
    E3=DABS(XZ(I)-X(3))
    D3=D3+(E3**2)
    H3=H3+(E3**2)/(D6(I))
11  CONTINUE
    S1=Z1-1
    IF (S1 .EQ. 0.0) S1=1.0
    ST(1)=DSQRT(D1/S1)
    ST(2)=DSQRT(D2/S1)
    ST(3)=DSQRT(D3/S1)
C  DETERMINE THE STANDARD ERROR OF EACH WEIGHTED MEAN
C  FAT VALUE:
C  FAT ONE:
    ER(1)=DSQRT(H1/(S1*Y1))
    ET(1)=SQRT(1/Y1)
C  FAT TWO:
    ER(2)=DSQRT(H2/(S1*Y2))
    ET(2)=SQRT(1/Y2)
C  FAT THREE:
    ER(3)=DSQRT(H3/(S1*Y3))
    ET(3)=SQRT(1/Y3)
    WRITE (NOUT, 234) Z1
    WRITE (NOUT, 2) (I, XX(I), XY(I), XZ(I), I=1, Z1)
    WRITE (NOUT, 93) (G(I,4), C(I), AE(I), DE(I), I=1, M)
    PRINT*, '???'
    WRITE (1, 94) (CC(I), X(I), ER(I), ET(I), ST(I), I=1, 3)
    CALL CONLIMIT (Z1, XX, XY, XZ, X, ST)
22  FORMAT (15X, '          '/')
52  FORMAT (A16)
2   FORMAT (5X, 'SET ', I3//5X, 'X(1) =', F9.5, 2X,
*   'X(2) =', F9.5, 2X, 'X(3) =', F9.5//)
93  FORMAT(5X, 'ACTUAL MIXTURE VALUE =', F9.5/5X
*   'CALCULATED VALUE =', F9.5, 5X, 'DIFFERENCE=', F9.5/5X,
*   'ACTUAL ERROR =', F9.5//)
94  FORMAT (5X/5X, 'WT. MEAN ', A16, '= ', F9.5/5X,
c   'WT. MEAN STANDARD ERROR =+/- ', F9.5/5X,
c   'ALTERNATIVE WT. MEAN STANDARD ERROR =+/- ', F9.5/5X,
c   'STANDARD DEVIATION =+/- ', F9.5//)
98  FORMAT (4(1X/), 1H 5A4, 1A3, 7HRESULTS/1X)
96  FORMAT(7X, 'MATRIX A', 18X, 'VECTOR B'//)
92  FORMAT (1X, 3F9.5/)
99  FORMAT (6A4, 1A4)
90  FORMAT(15X, 'STANDARD DEVIATION'//)
91  FORMAT (5X, 4F9.5/)

```

```

234   FORMAT (5X,'NUMBER OF COMBINATIONS USED =',I3//)
      STOP
      END
      SUBROUTINE CRAMER (A,R,X)
      REAL*8 A(30,10),X(10),T(10),R
      D=A(1,1)*A(2,2)*A(3,3)-A(1,1)*A(2,3)*A(3,2)-A(1,2)*A(2,1)*A(3,3)+
*   A(1,2)*A(2,3)*A(3,1)+A(1,3)*A(2,1)*A(3,2)-A(1,3)*A(2,2)*A(3,1)
      IF (D-R) 122, 51, 51
51    T(1)=(A(1,4)*A(2,2)*A(3,3))-(A(1,4)*A(2,3)*A(3,2))-
*   (A(1,2)*A(2,4)*A(3,3))+(A(1,2)*A(2,3)*A(3,4))+
*   (A(1,3)*A(2,4)*A(3,2))-(A(1,3)*A(2,2)*A(3,4))
      X(1)=T(1)/D
      T(2)=(A(1,1)*A(2,4)*A(3,3))-(A(1,1)*A(2,3)*A(3,4))
*   -(A(1,4)*A(2,1)*A(3,3))+(A(1,4)*A(2,3)*A(3,1))
*   +(A(1,3)*A(2,1)*A(3,4))-(A(1,3)*A(2,4)*A(3,1))
      X(2)=T(2)/D
      T(3)=(A(1,1)*A(2,2)*A(3,4))-(A(1,1)*A(2,4)*A(3,2))
*   -(A(1,2)*A(2,1)*A(3,4))+(A(1,2)*A(2,4)*A(3,1))
*   +(A(1,4)*A(2,1)*A(3,2))-(A(1,4)*A(2,2)*A(3,1))
      X(3)=T(3)/D
      GO TO 121
122   X(1)=0.0
121   RETURN
      END

```

```

      PROGRAM CRA2
C     USING CRAMER'S RULE METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C     THE GENERAL EQUATION IS: AX = B .
C     DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
      INTEGER*2 M,N,NIN,NOUT,PP,HH,KK,GG,JL,I
      REAL*8 AA(30,10),BB(30,10), TITLE(20), X(10)
      REAL*8 A(30,10),B(30,10),EE(10),ER(50),C(50),
*   G(30,10),AE(30),DE(30),XX(600),XY(600),XZ(600),ST(10),
*   ET(5),D4(600),D5(600),D6(600)
      REAL*8 V,R,X1,X2,X3,Y1,Y2,Y3,G1,G2,G3,Z1,
*   E1,E2,E3,D1,D2,D3,S1,H1,H2,H3
      INTRINSIC DABS, SQRT, DSQRT
      CHARACTER*16 CC(5)
C
      DATA NIN/1/, NOUT/1/
      READ (1,52) (CC(I),I=1,3)
      READ (NIN,*) M
      READ (NIN,*) N
C     INPUT CODE NUMBER FOR EACH FAT OR OIL AND MIXTURE:
C     1 FOR MILKFAT; 2 FOR TALLOW; 3 FOR SUNFLOWER OIL;
C     4 FOR MAIZE OIL; 5 FOR COTTON SEED OIL;6 FOR SOYA
C     BEAN OIL; 7 FOR COCONUT OIL; 8 FOR MIXTURE THAT
C     HAS MILKFAT AS ONE OF THE COMPONENTS.
      READ (1,*) N1,N2,N3,N4
      READ(NIN,99) TITLE
      WRITE (NOUT,98) (TITLE(I),I=1,7)
      DO 20 I=1,M
20    READ (NIN,*) (A(I,J),J=1,N)
C     CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C     THE GLC ANALYSIS.
      V = SQRT(0.5)
      R = 10.0 ** (-6)
      DO 10 I = 1, M
      BB(I,1)=DABS(A(I,1)-A(I,2))*V
      BB(I,2)=DABS(A(I,3)-A(I,4))*V
      BB(I,3)=DABS(A(I,5)-A(I,6))*V
      BB(I,4)=DABS(A(I,7)-A(I,8))*V
      CALL COEFV (BB,AA,N1,N2,N3,N4)

```

```

AA(I,1)=(A(I,1)+A(I,2))*0.5
AA(I,2)=(A(I,3)+A(I,4))*0.5
AA(I,3)=(A(I,5)+A(I,6))*0.5
10 AA(I,4)=(A(I,7)+A(I,8))*0.5
DO 100 I = 1,M
DO 101 J = 1,4
101 G(I,J)=AA(I,J)
100 CONTINUE
WRITE (NOUT,22)
WRITE (NOUT,96)
WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
WRITE (NOUT,90)
WRITE (NOUT,91) ((BB(I,J),J=1,4),I= 1,M)
X1=0.0
X2=0.0
X3=0.0
Y1=0.0
Y2=0.0
Y3=0.0
G1=0.0
G2=0.0
G3=0.0
Z1=0
D1=0.0
D2=0.0
D3=0.0
H1=0.0
H2=0.0
H3=0.0
LL= 0
DO 444 PP= 1, (M-2)
HH=PP+1
DO 455 KK=HH, (M-1)
GG=KK+1
DO 466 LI= GG, M
DO 477 JL= 1,4
A(1,JL)=AA(PP,JL)
B(1,JL)=BB(PP,JL)
A(2,JL)=AA(KK,JL)
B(2,JL)=BB(KK,JL)
A(3,JL)=AA(LI,JL)
477 B(3,JL)=BB(LI,JL)
CALL CRAMER (A,R,X)
IF (X(1) .LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2) .LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3) .LE.0.0 .OR. X(3).GE.1.0) GO TO 466
A(1,4)=B(1,4)+(X(1)*B(1,1)+X(2)*B(1,2)+X(3)*B(1,3))
A(2,4)=B(2,4)+(X(1)*B(2,1)+X(2)*B(2,2)+X(3)*B(2,3))
A(3,4)=B(3,4)+(X(1)*B(3,1)+X(2)*B(3,2)+X(3)*B(3,3))
CALL CRAMER (A,R,EE)
IF (EE(1) .EQ. 0.0) GO TO 466
IF (EE(2) .EQ. 0.0) GO TO 466
IF (EE(3) .EQ. 0.0) GO TO 466
Z1=Z1+1
X1=X1+X(1)/(EE(1)**2)
X2=X2+X(2)/(EE(2)**2)
X3=X3+X(3)/(EE(3)**2)
Y1=Y1+1/EE(1)**2
Y2=Y2+1/EE(2)**2
Y3=Y3+1/EE(3)**2
G1=G1+(EE(1)**2)
G2=G2+(EE(2)**2)
G3=G3+(EE(3)**2)

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D4(Z1)=EE(1)**2
D5(Z1)=EE(2)**2
D6(Z1)=EE(3)**2
XX(Z1)=X(1)
XY(Z1)=X(2)
XZ(Z1)=X(3)
466 CONTINUE
455 CONTINUE
444 CONTINUE
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE.
C FAT ONE:
  X(1)=X1/Y1
C FAT TWO:
  X(2)=X2/Y2
C FAT THREE:
  X(3)=X3/Y3
  DO 77 I= 1,M
  C(I)= 0.0
  DO 770 J= 1,3
770  C(I)=C(I)+G(I,J)*X(J)
      AE(I)=G(I,4)-C(I)
      DE(I)= AE(I)/G(I,4)
77  CONTINUE
  DO 11 I= 1, Z1
  E1=DABS(XX(I)-X(1))
  D1=D1+(E1**2)
  H1=H1+(E1**2)/(D4(I))
  E2=DABS(XY(I)-X(2))
  D2=D2+(E2**2)
  H2=H2+(E2**2)/(D5(I))
  E3=DABS(XZ(I)-X(3))
  D3=D3+(E3**2)
  H3=H3+(E3**2)/(D6(I))
11  CONTINUE
  S1=Z1-1
  ST(1)=DSQRT(D1/S1)
  ST(2)=DSQRT(D2/S1)
  ST(3)=DSQRT(D3/S1)
C DETERMINE THE STANDARD ERROR OF EACH WEIGHTED MEAN
C FAT VALUE:
C FAT ONE:
  ER(1)=DSQRT(H1/(S1*Y1))
  ET(1)=DSQRT(1/Y1)
C FAT TWO:
  ER(2)=DSQRT(H2/(S1*Y2))
  ET(2)=DSQRT(1/Y2)
C FAT THREE:
  ER(3)=DSQRT(H3/(S1*Y3))
  ET(3)=DSQRT(1/Y3)
  WRITE (NOUT, 254) Z1
  WRITE (NOUT, 2) (I, XX(I), XY(I), XZ(I), I=1, Z1)
  WRITE (NOUT, 93) (G(I, 4), C(I), AE(I), DE(I), I=1, M)
  PRINT*, '???'
  WRITE (1, 94) (CC(I), X(I), ER(I), ET(I), ST(I), I=1, 3)
  CALL CONLIMIT (Z1, XX, XY, XZ, X, ST)
22  FORMAT (15X, '          ' //)
52  FORMAT (A16)
2   FORMAT (5X, 'SET ', I3//5X, 'X(1) =', F9.5, 2X,
*   'X(2) =', F9.5, 2X, 'X(3) =', F9.5//)
93  FORMAT(5X, 'ACTUAL MIXTURE VALUE =', F9.5/5X
*   'CALCULATED VALUE =', F9.5, 5X, 'DIFFERENCE=', F9.5/5X,
*   'ACTUAL ERROR =', F9.5//)
94  FORMAT (5X/5X, 'WT. MEAN ', A16, '= ', F9.5/5X,

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c 'WT. MEAN STANDARD ERROR =+/- ',F9.5/5X,
c 'ALTERNATIVE WT. MEAN STANDARD ERROR =+/- ',F9.5/5X,
c 'STANDARD DEVIATION =+/- ',F9.5//)
98 FORMAT (4(1X/),1H 5A4, 1A3,7HRESULTS/1X)
96 FORMAT(7X,'MATRIX A',18X,'VECTOR B'//)
92 FORMAT (1X,3F9.5/)
99 FORMAT (6A4,1A4)
90 FORMAT(15X,'STANDARD DEVIATION'//)
91 FORMAT (5X,4F9.5/)
234 FORMAT (5X,'NUMBER OF COMBINATIONS USED =',I3//)
STOP
END

```

## PROGRAM CRA3

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C USING CRAMER'S RULE METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C THE GENERAL EQUATION IS: AX = B .
C DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
  INTEGER*2 M,N,NIN,NOUT,PP,HH,KK,GG,JL,I
  REAL*8 AA(30,10),BB(30,10), TITLE(20), X(10)
  REAL*8 A(30,10),B(30,10),T(50),EE(50),ER(50),C(50),
  * G(30,10),AE(30),DE(30),XX(600),XY(600),XZ(600),ST(10),
  * ET(5),D4(600),D5(600),D6(600)
  REAL*8 V,D,R,A8,B8,C8,F8,D8,E8,ED,A1,A2,A3,A4,A5,A6,A7,
  * C1,C2,C3,C4,C5,C6,C7,X1,X2,X3,Y1,Y2,Y3,G1,G2,G3,Z1,
  * E1,E2,E3,D1,D2,D3,S1,H1,H2,H3,B1,B2,B3,B4,B5,B6,B7
  INTRINSIC DABS, SQRT, DSQRT
  CHARACTER*16 CC(5)

C
  DATA NIN/1/, NOUT/1/
  READ (1,52) (CC(I),I=1,3)
  READ (NIN,*) M
  READ (NIN,*) N
  READ(NIN,99) TITLE
  WRITE (NOUT,98) (TITLE(I),I=1,7)
  DO 20 I=1,M
20  READ (NIN,*) (A(I,J),J=1,N)
C CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C THE GLC ANALYSIS.
  V = SQRT(0.5)
  R = 10.0 ** (-6)
  DO 10 I = 1, M
  BB(I,1)=DABS(A(I,1)-A(I,2))*V
  BB(I,2)=DABS(A(I,3)-A(I,4))*V
  BB(I,3)=DABS(A(I,5)-A(I,6))*V
  BB(I,4)=DABS(A(I,7)-A(I,8))*V
  AA(I,1)=(A(I,1)+A(I,2))*0.5
  AA(I,2)=(A(I,3)+A(I,4))*0.5
  AA(I,3)=(A(I,5)+A(I,6))*0.5
10  AA(I,4)=(A(I,7)+A(I,8))*0.5
  DO 100 I = 1,M
  DO 101 J = 1,4
101  G(I,J)=AA(I,J)
100  CONTINUE
  WRITE (NOUT,22)
  WRITE (NOUT,96)
  WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
  WRITE (NOUT,90)
  WRITE (NOUT,91) ((BB(I,J),J=1,4),I= 1,M)
  X1=0.0
  X2=0.0
  X3=0.0
  Y1=0.0
  Y2=0.0

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```

Y3=0.0
G1=0.0
G2=0.0
G3=0.0
Z1=0
D1=0.0
D2=0.0
D3=0.0
H1=0.0
H2=0.0
H3=0.0
LL= 0
DO 444 PP= 1, (M-2)
HH=PP+1
DO 455 KK=HH, (M-1)
GG=KK+1
DO 466 LI= GG, M
DO 477 JL= 1,4
A(1,JL)=AA(PP,JL)
B(1,JL)=BB(PP,JL)
A(2,JL)=AA(KK,JL)
B(2,JL)=BB(KK,JL)
A(3,JL)=AA(LI,JL)
477 B(3,JL)=BB(LI,JL)
D=A(1,1)*A(2,2)*A(3,3)-A(1,1)*A(2,3)*A(3,2)-A(1,2)*A(2,1)*A(3,3)+
* A(1,2)*A(2,3)*A(3,1)+A(1,3)*A(2,1)*A(3,2)-A(1,3)*A(2,2)*A(3,1)
IF (D-R) 466, 51, 51
51 T(1)=(A(1,4)*A(2,2)*A(3,3))-(A(1,4)*A(2,3)*A(3,2))-
* (A(1,2)*A(2,4)*A(3,3))+(A(1,2)*A(2,3)*A(3,4))+
* (A(1,3)*A(2,4)*A(3,2))-(A(1,3)*A(2,2)*A(3,4))
X(1)=T(1)/D
T(2)=(A(1,1)*A(2,4)*A(3,3))-(A(1,1)*A(2,3)*A(3,4))
* -(A(1,4)*A(2,1)*A(3,3))+(A(1,4)*A(2,3)*A(3,1))
* +(A(1,3)*A(2,1)*A(3,4))-(A(1,3)*A(2,4)*A(3,1))
X(2)=T(2)/D
T(3)=(A(1,1)*A(2,2)*A(3,4))-(A(1,1)*A(2,4)*A(3,2))
* -(A(1,2)*A(2,1)*A(3,4))+(A(1,2)*A(2,4)*A(3,1))
* +(A(1,4)*A(2,1)*A(3,2))-(A(1,4)*A(2,2)*A(3,1))
X(3)=T(3)/D
A8=B(1,1)*A(2,2)*A(3,3)+B(2,2)*A(1,1)*A(3,3)+B(3,3)*A(1,1)*A(2,2)
B8=B(1,1)*A(2,3)*A(3,2)+B(2,3)*A(1,1)*A(3,2)+B(3,2)*A(1,1)*A(2,3)
C8=B(1,2)*A(2,1)*A(3,3)+B(2,1)*A(1,2)*A(3,3)+B(3,3)*A(1,2)*A(2,1)
D8=B(1,2)*A(2,3)*A(3,1)+B(2,3)*A(1,2)*A(3,1)+B(3,1)*A(2,3)*A(1,2)
E8=B(1,3)*A(2,1)*A(3,2)+B(2,1)*A(1,3)*A(3,2)+B(3,2)*A(1,3)*A(2,1)
F8=B(1,3)*A(2,2)*A(3,1)+B(2,2)*A(1,3)*A(3,1)+B(3,1)*A(1,3)*A(2,2)
ED=A8-B8-C8+D8+E8-F8
A2=B(1,4)*A(2,2)*A(3,3)+B(2,2)*A(1,4)*A(3,3)+B(3,3)*A(1,4)*A(2,2)
A3=B(1,4)*A(2,3)*A(3,2)+B(2,3)*A(1,4)*A(3,2)+B(3,2)*A(1,4)*A(2,3)
A4=B(1,2)*A(2,4)*A(3,3)+B(2,4)*A(1,2)*A(3,3)+B(3,3)*A(1,2)*A(2,4)
A5=B(1,2)*A(2,3)*A(3,4)+B(2,3)*A(1,2)*A(3,4)+B(3,4)*A(1,2)*A(2,3)
A6=B(1,3)*A(2,4)*A(3,2)+B(2,4)*A(1,3)*A(3,2)+B(3,2)*A(1,3)*A(2,4)
A7=B(1,3)*A(2,2)*A(3,4)+B(2,2)*A(1,3)*A(3,4)+B(3,4)*A(1,3)*A(2,2)
A1=A2-A3-A4+A5+A6-A7
B2=B(1,1)*A(2,4)*A(3,3)+B(2,4)*A(1,1)*A(3,3)+B(3,3)*A(1,1)*A(2,4)
B3=B(1,1)*A(2,3)*A(3,4)+B(2,3)*A(1,1)*A(3,4)+B(3,4)*A(1,1)*A(2,3)
B4=B(1,4)*A(2,1)*A(3,3)+B(2,1)*A(1,4)*A(3,3)+B(3,3)*A(1,4)*A(2,1)
B5=B(1,4)*A(2,3)*A(3,1)+B(2,3)*A(1,4)*A(3,1)+B(3,1)*A(1,4)*A(2,3)
B6=B(1,3)*A(2,1)*A(3,4)+B(2,1)*A(1,3)*A(3,4)+B(3,4)*A(1,3)*A(2,1)
B7=B(1,3)*A(2,4)*A(3,1)+B(2,4)*A(1,3)*A(3,1)+B(3,1)*A(1,3)*A(2,4)
B1=B2-B3-B4+B5+B6-B7
C2=B(1,1)*A(2,2)*A(3,4)+B(2,2)*A(1,1)*A(3,4)+B(3,4)*A(1,1)*A(2,2)
C3=B(1,1)*A(2,4)*A(3,2)+B(2,4)*A(1,1)*A(3,2)+B(3,2)*A(1,1)*A(2,4)
C4=B(1,2)*A(2,1)*A(3,4)+B(2,1)*A(1,2)*A(3,4)+B(3,4)*A(1,2)*A(2,1)

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C5=B(1,2)*A(2,4)*A(3,1)+B(2,4)*A(1,2)*A(3,1)+B(3,1)*A(1,2)*A(2,4)
C6=B(1,4)*A(2,1)*A(3,2)+B(2,1)*A(1,4)*A(3,2)+B(3,2)*A(1,4)*A(2,1)
C7=B(1,4)*A(2,2)*A(3,1)+B(2,2)*A(1,4)*A(3,1)+B(3,1)*A(1,4)*A(2,2)
C1=C2-C3-C4+C5+C6-C7
IF (X(1) .LE. 0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2) .LE. 0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3) .LE. 0.0 .OR. X(3).GE.1.0) GO TO 466
EE(1)=(A1/D)+((T(1)*ED)/D**2)
EE(2)=(B1/D)+((T(2)*ED)/D**2)
EE(3)=(C1/D)+((T(3)*ED)/D**2)
IF (EE(1) .EQ. 0.0) GO TO 466
IF (EE(2) .EQ. 0.0) GO TO 466
IF (EE(3) .EQ. 0.0) GO TO 466
Z1=Z1+1
X1=X1+X(1)/(EE(1)**2)
X2=X2+X(2)/(EE(2)**2)
X3=X3+X(3)/(EE(3)**2)
Y1=Y1+1/EE(1)**2
Y2=Y2+1/EE(2)**2
Y3=Y3+1/EE(3)**2
G1=G1+(EE(1)**2)
G2=G2+(EE(2)**2)
G3=G3+(EE(3)**2)
D4(Z1)=EE(1)**2
D5(Z1)=EE(2)**2
D6(Z1)=EE(3)**2
XX(Z1)=X(1)
XY(Z1)=X(2)
XZ(Z1)=X(3)
466 CONTINUE
455 CONTINUE
444 CONTINUE
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE.
C FAT ONE:
X(1)=X1/Y1
C FAT TWO:)
X(2)=X2/Y2
C FAT THREE:
X(3)=X3/Y3
DO 77 I= 1,M
C(I)= 0.0
DO 770 J= 1,3
770 C(I)=C(I)+G(I,J)*X(J)
AE(I)=G(I,4)-C(I)
DE(I)= AE(I)/G(I,4)
77 CONTINUE
DO 11 I= 1, Z1
E1=DABS(XX(I)-X(1))
D1=D1+(E1**2)
H1=H1+(E1**2)/(D4(I))
E2=DABS(XY(I)-X(2))
D2=D2+(E2**2)
H2=H2+(E2**2)/(D5(I))
E3=DABS(XZ(I)-X(3))
D3=D3+(E3**2)
H3=H3+(E3**2)/(D6(I))
11 CONTINUE
S1=Z1-1
ST(1)=DSQRT(D1/S1)
ST(2)=DSQRT(D2/S1)
ST(3)=DSQRT(D3/S1)
C DETERMINE THE STANDARD ERROR OF EACH WEIGHTED MEAN
C FAT VALUE:

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C   FAT ONE:
      ER(1)=DSQRT(H1/(S1*Y1))
      ET(1)=DSQRT(1/Y1)
C   FAT TWO:
      ER(2)=DSQRT(H2/(S1*Y2))
      ET(2)=DSQRT(1/Y2)
C   FAT THREE:
      ER(3)=DSQRT(H3/(S1*Y3))
      ET(3)=DSQRT(1/Y3)
      WRITE (NOUT, 234) Z1
      WRITE (NOUT,2) (I,XX(I),XY(I),XZ(I),I=1,Z1)
      WRITE (NOUT,93) (G(I,4),C(I),AE(I),DE(I),I=1,M)
      PRINT*, '???'
      WRITE (1,94) (CC(I),X(I),ER(I),ET(I),ST(I),I=1,3)
      CALL CONLIMIT (Z1,XX,XY,XZ,X,ST)
22   FORMAT (15X, '          ' //)
52   FORMAT (A16)
2   FORMAT (5X, 'SET ', I3//5X, 'X(1) =', F9.5, 2X,
*   'X(2) =', F9.5, 2X, 'X(3) =', F9.5//)
93   FORMAT(5X, 'ACTUAL MIXTURE VALUE =', F9.5/5X
*   'CALCULATED VALUE =', F9.5, 5X, 'DIFFERENCE=', F9.5/5X,
*   'ACTUAL ERROR =', F9.5//)
94   FORMAT (5X/5X, 'WT. MEAN ', A16, '= ', F9.5/5X,
c   'WT. MEAN STANDARD ERROR =+/- ', F9.5/5X,
c   'ALTERNATIVE WT. MEAN STANDARD ERROR =+/- ', F9.5/5X,
c   'STANDARD DEVIATION =+/- ', F9.5//)
98   FORMAT (4(1X/), 1H 5A4, 1A3, 7HRESULTS/1X)
96   FORMAT(7X, 'MATRIX A', 18X, 'VECTOR B'//)
92   FORMAT (1X, 3F9.5/)
99   FORMAT (6A4, 1A4)
90   FORMAT(15X, 'STANDARD DEVIATION'//)
91   FORMAT (5X, 4F9.5/)
234   FORMAT (5X, 'NUMBER OF COMBINATIONS USED =', I3//)
      STOP
      END

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## PROGRAM CRAM1

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C   USING CRAMER'S RULE METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C   THE GENERAL EQUATION IS: AX = B .
C   DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
      INTEGER*2 M,N,NIN,NOUT,PP,HH,KK,I,N1,N2,N3,N4
      REAL*8 AA(30,10),BB(30,10), TITLE(20), X(10)
      REAL*8 A(30,10),B(30,10),EE(50),ER(50),C(50),
*   G(30,10),AE(30),DE(30),XX(600),XY(600),XZ(600),ST(10),
*   ET(5),D4(600),D5(600),D6(600)
      REAL*8 V,D,R,AS,B8,ED,A1,A2,A3,Z1,
*   X1,X2,X3,Y1,Y2,Y3,T1,T2,
*   E1,E2,E3,D1,D2,D3,S1,H1,H2,H3,B1,B2,B3
      CHARACTER*16 CC(5)
      INTRINSIC DABS, SQRT, DSQRT
C
      DATA NIN/1/, NOUT/1/
      READ (NIN,33) (CC(I), I = 1,3)
      READ (NIN,*) M
      READ (NIN,*) N
C   INPUT CODE NUMBER FOR EACH FAT OR OIL. 1 FOR MILKFAT; 2 FOR TALLOW;
C   3 FOR SUNFLOWER OIL; 4 FOR MAIZE OIL; 5 FOR COTTON SEED OIL;
C   6 FOR SOYA BEAN OIL; 7 FOR COCONUT OIL; 8 FOR MIXTURE THAT HAS
C   MILKFAT AS ONE OF THE COMPONENTS.
      READ (NIN,*) N1,N2,N3,N4
      READ(NIN,99) TITLE
      WRITE (NOUT,98) (TITLE(I),I=1,7)
      DO 20 I=1,M

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20   READ (NIN,*) (A(I,J),J=1,N)
C    CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C    THE GLC ANALYSIS.
      V = SQRT(0.5)
      R = 10.0 ** (-6)
      DO 10 I = 1, M
        BB(I,1)=DABS(A(I,1)-A(I,2))*V
        BB(I,2)=DABS(A(I,3)-A(I,4))*V
        BB(I,3)=DABS(A(I,5)-A(I,6))*V
        BB(I,4)=DABS(A(I,7)-A(I,8))*V
        AA(I,1)=(A(I,1)+A(I,2))*0.5
        AA(I,2)=(A(I,3)+A(I,4))*0.5
        AA(I,3)=(A(I,5)+A(I,6))*0.5
10   AA(I,4)=(A(I,7)+A(I,8))*0.5
      DO 100 I = 1,M
        DO 101 J = 1,4
101   G(I,J)=AA(I,J)
100  CONTINUE
      CALL COEFV(BB,AA,N1,N2,N3,N4)
      WRITE (NOUT,22)
      WRITE (NOUT,96)
      WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
      WRITE (NOUT,90)
      WRITE (NOUT,91) ((BB(I,J),J=1,4),I= 1,M)
      X1=0.0
      X2=0.0
      X3=0.0
      Y1=0.0
      Y2=0.0
      Y3=0.0
      Z1=0.0
      D1=0.0
      D2=0.0
      D3=0.0
      H1=0.0
      H2=0.0
      H3=0.0
      DO 444 PP=1, (M-1)
        HH=PP+1
        DO 455 KK= HH, M
          A(1,1)=AA(PP,1)-AA(PP,3)
          A(1,2)=AA(PP,2)-AA(PP,3)
          A(1,3)=AA(PP,4)-AA(PP,3)
          A(2,1)=AA(KK,1)-AA(KK,3)
          A(2,2)=AA(KK,2)-AA(KK,3)
          A(2,3)=AA(KK,4)-AA(KK,3)
          B(1,1)=DSQRT(BB(PP,1)**2+BB(PP,3)**2)
          B(1,2)=DSQRT(BB(PP,2)**2+BB(PP,3)**2)
          B(1,3)=DSQRT(BB(PP,4)**2+BB(PP,3)**2)
          B(2,1)=DSQRT(BB(KK,1)**2+BB(KK,3)**2)
          B(2,2)=DSQRT(BB(KK,2)**2+BB(KK,3)**2)
          B(2,3)=DSQRT(BB(KK,4)**2+BB(KK,3)**2)
          D=A(1,1)*A(2,2)-A(1,2)*A(2,1)
          IF (D-R) 466,51,51
51   T1=A(2,2)*A(1,3)-A(1,2)*A(2,3)
          T2=A(2,2)*A(2,3)-A(2,1)*A(1,3)
          X(1)=T1/D
          X(2)=T2/D
          X(3)=1-X(1)-X(2)
          IF (X(1) .LE. 0.0 .OR. X(1) .GE. 1.0) GO TO 466
          IF (X(2) .LE. 0.0 .OR. X(2) .GE. 1.0) GO TO 466
          IF (X(3) .LE. 0.0 .OR. X(3) .GE. 1.0) GO TO 466
C    ERROR PROPAGATION:

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AS=A(2,2)**2*B(1,1)**2+A(1,1)**2*B(2,2)**2
BS=A(2,1)**2*B(1,2)**2+A(1,2)**2*B(2,1)**2
ED=AS+BS
A2=A(1,3)**2*B(2,2)**2+A(2,2)**2*B(1,3)**2
A3=A(2,3)**2*B(1,2)**2+A(1,2)**2*B(2,3)**2
A1=A2+A3
B2=A(2,3)**2*B(2,2)**2+A(2,2)**2*B(2,3)**2
B3=A(1,3)**2*A(2,1)**2+A(2,1)**2*B(1,3)**2
B1=B2+B3
EE(1)=DSQRT((1/D)**2*A1+(T1/D**2)**2*ED)
EE(2)=DSQRT((1/D)**2*B1+(T2/D**2)**2*ED)
EE(3)=DSQRT(EE(1)**2+EE(2)**2)
IF (EE(1) .EQ. 0.0) GO TO 466
IF (EE(2) .EQ. 0.0) GO TO 466
IF (EE(3) .EQ. 0.0) GO TO 466
Z1=Z1+1.0
X1=X1+X(1)/(EE(1)**2)
X2=X2+X(2)/(EE(2)**2)
X3=X3+X(3)/(EE(3)**2)
Y1=Y1+1/EE(1)**2
Y2=Y2+1/EE(2)**2
Y3=Y3+1/EE(3)**2
D4(Z1)=EE(1)**2
D5(Z1)=EE(2)**2
D6(Z1)=EE(3)**2
XX(Z1)=X(1)
XY(Z1)=X(2)
XZ(Z1)=X(3)
466 CONTINUE
455 CONTINUE
444 CONTINUE
IF (Z1 .GT. 1.0) GO TO 9
IF (Z1 .EQ. 0.0) GO TO 19
WRITE (1,14)
X(1)=XX(1)
X(2)=XY(1)
X(3)=XZ(1)
WRITE (1,23) (I,X(I),EE(I),I= 1,3)
23 FORMAT (5X/5X,'FAT ',I2,' = ',F9.5,5X,'STD. ERROR =+/-',F9.5/)
33 FORMAT (A16)
STOP
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE.
C FAT ONE:
9 X(1)=X1/Y1
C FAT TWO:)
X(2)=X2/Y2
C FAT THREE:
X(3)=X3/Y3
DO 77 I= 1,M
C(I)= 0.0
DO 770 J= 1,3
770 C(I)=C(I)+G(I,J)*X(J)
AE(I)=G(I,4)-C(I)
DE(I)= AE(I)/G(I,4)
77 CONTINUE
DO 11 I= 1, Z1
E1=DABS(XX(I)-X(1))
D1=D1+(E1**2)
H1=H1+(E1**2)/(D4(I))
E2=DABS(XY(I)-X(2))
D2=D2+(E2**2)
H2=H2+(E2**2)/(D5(I))
E3=DABS(XZ(I)-X(3))

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D3=D3+(E3**2)
H3=H3+(E3**2)/(D6(I))
11 CONTINUE
S1=Z1-1
ST(1)=DSQRT(D1/S1)
ST(2)=DSQRT(D2/S1)
ST(3)=DSQRT(D3/S1)
C DETERMINE THE STANDARD ERROR OF EACH WEIGHTED MEAN
C FAT VALUE:
C FAT ONE:
ER(1)=DSQRT(H1/(S1*Y1))
ET(1)=DSQRT(1/Y1)
C FAT TWO:
ER(2)=DSQRT(H2/(S1*Y2))
ET(2)=DSQRT(1/Y2)
C FAT THREE:
ER(3)=DSQRT(H3/(S1*Y3))
ET(3)=DSQRT(1/Y3)
WRITE (NOUT, 234) Z1
WRITE (NOUT, 2) (I, XX(I), XY(I), XZ(I), I=1, Z1)
WRITE (NOUT, 93) (G(I, 4), C(I), AE(I), DE(I), I=1, M)
PRINT*, '? ? '
WRITE (NOUT, 94) (CC(I), X(I), ER(I), ET(I), ST(I), I=1, 3)
CALL CONLIMIT (Z1, XX, XY, XZ, X, ST)
14 FORMAT(5X/5X, 'ONLY ONE SET OF DATAS AVAILABUE: '/')
15 FORMAT(5X/5X, 'NO SOLUTION FOR THIS SET OF MIXTURE DATAS.'/5X,
C '*****')
22 FORMAT (15X, ' ' //)
2 FORMAT (5X, 'SET ', I3//5X, 'X(1) =', F9.5, 2X,
* 'X(2) =', F9.5, 2X, 'X(3) =', F9.5//)
93 FORMAT(5X, 'ACTUAL MIXTURE VALUE =', F9.5/5X
* 'CALCULATED VALUE =', F9.5, 5X, 'DIFFERENCE=', F9.5/5X,
* 'ACTUAL ERROR =', F9.5//)
94 FORMAT(5X, 'WT. MEAN ', A16, ' =', F9.5, /5X, 'WT.MEAN STD. ERROR =+/-',
* F9.5/5X, 'ALTERNATIVE STD.ERROR =+/-', F9.5/5X,
* 'STANDARD DEVIATION =+/- ', F9.5//)
98 FORMAT (4(1X/), 1H 5A4, 1A3, 7HRESULTS/1X)
96 FORMAT(7X, 'MATRIX A', 18X, 'VECTOR B'//)
92 FORMAT (1X, 3F9.5//)
99 FORMAT (6A4, 1A4)
90 FORMAT(15X, 'STANDARD DEVIATION'//)
91 FORMAT (5X, 4F9.5//)
234 FORMAT (5X, 'NUMBER OF COMBINATIONS USED =', I3//)
STOP
19 WRITE (1, 15)
STOP
END
C THE SUBROUTINE TO COMPARE CALCULATED STANDARD DEVIATION WITH
C THE STANDARD VALUE OF COEFFICIENT OF VARIATION TIMES THE
C MEAN VALUE AND CHOOSE WHICHEVER IS THE LARGEST AS STANDARD DEVIATION.
SUBROUTINE COEFV(BB, A, T1, T2, T3, T4)
REAL*8 A(30, 10), B(30, 10), BB(30, 10), C(30, 10)
INTEGER*2 T1, T2, T3, T4
DATA (B(I, 1), I=1, 20)/0.0555, 0.0623, 0.114, 0.0774, 0.114,
c 0.0225, 0.102, 0.0551,
c 0.0538, 0.0668, 0.0888, 0.0547, 0.0506, 0.169, 0.197, 0.0394,
c 0.0689, 0.197, 0.0573, 0.501/
DATA (B(I, 2), I=1, 20)/5*0.0, 0.41, 0.0, 0.131, 0.180, 0.164,
c 0.331, 0.0457, 0.181, 0.192, 0.250, 0.0166,
c 0.0194, 0.263, 0.3, 0.244/
DATA (B(I, 3), I=1, 20)/5*0.0, 0.287, 0.0, 0.0599, 3*0.0,
c 0.026, 3*0.0, 0.0375,
c 0.0442, 0.202, 0.46, 0.731/

```

```

DATA (B(I,4),I=1,20)/5*0.0,0.159,5*0.0,0.104,0.285,2*0.0,
c 0.11,0.032,0.00956,
c 0.107,0.61/
DATA (B(I,5),I=1,20)/5*0.0,0.133,0.0,0.0831,3*0.0,0.0317,0.444,
c 2*0.0,0.115,0.0224,0.0289,0.373,0.76/
DATA (B(I,6),I=1,20)/5*0.0,0.0443,0.0,0.0831,3*0.0,0.0651,
c 0.725,0.211,0.0,0.0364,0.0127,0.0221,0.0494,0.144/
DATA (B(I,7),I=1,20)/0.0,0.107,0.0267,0.0192,0.0,0.0195,
c 0.0,0.0527,3*0.0,0.0165,3*0.0,0.104,0.611,0.131,0.0,0.508/
DATA (B(I,8),I=1,20)/0.13,0.0639,0.0682,0.0477,0.119,0.136,
c 0.116,0.0787,0.105,
c 0.132,0.354,0.0355,0.14,0.0413,0.0852,0.0513,0.0153,
c 0.0468,0.17,0.452/
DO 3 I = 1, 20
  C(I,1)=B(I,T1)*A(I,1)
  C(I,2)=B(I,T2)*A(I,2)
  C(I,3)=B(I,T3)*A(I,3)
  C(I,4)=B(I,T4)*A(I,4)
3 CONTINUE
DO 7 I = 1, 20
  DO 8 J = 1, 4
    IF (BB(I,J) .GE. C(I,J) ) GO TO 8
    BB(I,J) = C(I,J)
8 CONTINUE
7 CONTINUE
RETURN
END

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PROGRAM CRAM2
C USING CRAMER'S RULE METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C THE GENERAL EQUATION IS: AX = B .
C DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
  INTEGER*2 M,N,NIN,NOUT,PP,KK,L,N1,N2,N3,N4
  REAL*3 AA(30,10),BB(30,10), TITLE(20), X(10)
  REAL*3 A(30,10),B(30,10),EE(50),ER(50),C(50),
  * G(30,10),AE(30),DE(30),XX(600),XY(600),XZ(600),ST(10),
  * ET(5),D4(600),D5(600),D6(600)
  REAL*8 V,D,R,A8,B8,ED,A1,A2,A3,Z1,
  * X1,X2,X3,Y1,Y2,Y3,T1,T2,
  * E1,E2,E3,D1,D2,D3,S1,H1,H2,H3,B1,B2,B3
  CHARACTER*16 CC(5)
  INTRINSIC DABS, SQRT, DSQRT
C
  DATA N1N/1/, NOUT/1/
  READ (NIN,33) (CC(I), I = 1,3)
  READ (NIN,*) M
  READ (NIN,*) N
C INPUT CODE NUMBER FOR EACH FAT OR OIL. 1 FOR MILKFAT; 2 FOR TALLOW;
C 3 FOR SUNFLOWER OIL; 4 FOR MAIZE OIL; 5 FOR COTTON SEED OIL;
C 6 FOR SOYA BEAN OIL; 7 FOR COCONUT OIL; 8 FOR MIXTURE THAT HAS
C MILKFAT AS ONE OF THE COMPONENTS.
  READ (NIN,*) N1,N2,N3,N4
  READ(NIN,99) TITLE
  WRITE (NOUT,98) (TITLE(I),I=1,7)
  DO 20 I=1,M
20 READ (NIN,*) (A(I,J),J=1,N)
C CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C THE GLC ANALYSIS.
  V = SQRT(0.5)
  R = 10.0 ** (-6)
  DO 10 I = 1, M
  BB(I,1)=DABS(A(I,1)-A(I,2))*V
  BB(I,2)=DABS(A(I,3)-A(I,4))*V

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BB(I,3)=DABS(A(I,5)-A(I,6))*V
BB(I,4)=DABS(A(I,7)-A(I,8))*V
AA(I,1)=(A(I,1)+A(I,2))*0.5
AA(I,2)=(A(I,3)+A(I,4))*0.5
AA(I,3)=(A(I,5)+A(I,6))*0.5
10 AA(I,4)=(A(I,7)+A(I,8))*0.5
DO 100 I = 1,M
DO 101 J = 1,4
101 G(I,J)=AA(I,J)
100 CONTINUE
CALL CDEPV(BB,AA,N1,N2,N3,N4)
WRITE (NOUT,22)
WRITE (NOUT,96)
WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
WRITE (NOUT,90)
WRITE (NOUT,91) ((BB(I,J),J=1,4),I= 1,M)
X1=0.0
X2=0.0
X3=0.0
Y1=0.0
Y2=0.0
Y3=0.0
Z1=0.0
D1=0.0
D2=0.0
D3=0.0
H1=0.0
H2=0.0
H3=0.0
DO 444 PP=1, M
DO 455 KK= 1, M
IF (PP .EQ. KK) GO TO 466
A(1,1)=AA(PP,1)-AA(PP,5)
A(1,2)=AA(PP,2)-AA(PP,3)
A(1,3)=AA(PP,4)-AA(PP,3)
A(2,1)=AA(KK,1)-AA(KK,3)
A(2,2)=AA(KK,2)-AA(KK,3)
A(2,3)=AA(KK,4)-AA(KK,3)
B(1,1)=DSQRT(BB(PP,1)**2+BB(PP,3)**2)
B(1,2)=DSQRT(BB(PP,2)**2+BB(PP,3)**2)
B(1,3)=DSQRT(BB(PP,4)**2+BB(PP,3)**2)
B(2,1)=DSQRT(BB(KK,1)**2+BB(KK,3)**2)
B(2,2)=DSQRT(BB(KK,2)**2+BB(KK,3)**2)
B(2,3)=DSQRT(BB(KK,4)**2+BB(KK,3)**2)
D=A(1,1)*A(2,2)-A(1,2)*A(2,1)
IF (D-R) 466,51,51
51 T1=A(2,2)*A(1,3)-A(1,2)*A(2,3)
T2=A(2,2)*A(2,3)-A(2,1)*A(1,3)
X(1)=T1/D
X(2)=T2/D
X(3)=1-X(1)-X(2)
IF (X(1) .LE. 0.0 .OR. X(1) .GE. 1.0) GO TO 466
IF (X(2) .LE. 0.0 .OR. X(2) .GE. 1.0) GO TO 466
IF (X(3) .LE. 0.0 .OR. X(3) .GE. 1.0) GO TO 466
C ERROR PROPAGATION:
A8=A(2,2)**2*B(1,1)**2+A(1,1)**2*B(2,2)**2
B8=A(2,1)**2*B(1,2)**2+A(1,2)**2*B(2,1)**2
ED=A8+B8
A2=A(1,3)**2*B(2,2)**2+A(2,2)**2*B(1,3)**2
A3=A(2,3)**2*B(1,2)**2+A(1,2)**2*B(2,3)**2
A1=A2+A3
B2=A(2,3)**2*B(2,2)**2+A(2,2)**2*B(2,3)**2
B3=A(1,3)**2*A(2,1)**2+A(2,1)**2*B(1,3)**2

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B1=B2+B3
EE(1)=DSQRT((1/D)**2*A1+(T1/D**2)**2*ED)
EE(2)=DSQRT((1/D)**2*B1+(T2/D**2)**2*ED)
EE(3)=DSQRT(EE(1)**2+EE(2)**2)
IF (EE(1) .EQ. 0.0) GO TO 466
IF (EE(2) .EQ. 0.0) GO TO 466
IF (EE(3) .EQ. 0.0) GO TO 466
Z1=Z1+1.0
X1=X1+X(1)/(EE(1)**2)
X2=X2+X(2)/(EE(2)**2)
X3=X3+X(3)/(EE(3)**2)
Y1=Y1+1/EE(1)**2
Y2=Y2+1/EE(2)**2
Y3=Y3+1/EE(3)**2
D4(Z1)=EE(1)**2
D5(Z1)=EE(2)**2
D6(Z1)=EE(3)**2
XX(Z1)=X(1)
XY(Z1)=X(2)
XZ(Z1)=X(3)
466 CONTINUE
455 CONTINUE
444 CONTINUE
IF (Z1 .GT. 1.0) GO TO 9
IF (Z1 .EQ. 0.0) GO TO 19
WRITE (1,14)
X(1)=XX(1)
X(2)=XY(1)
X(3)=XZ(1)
WRITE (1,23) (I,X(I),EE(I),I= 1,3)
23 FORMAT (5X/5X,'FAT ',I2,' =',F9.5,5X,'STD.ERROR =+/- ',F9.5/)
33 FORMAT (A16)
STOP
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE.
C FAT ONE:
9 X(1)=X1/Y1
C FAT TWO:)
X(2)=X2/Y2
C FAT THREE:
X(3)=X3/Y3
DO 77 I= 1,M
C(I)= 0.0
DO 770 J= 1,3
770 C(I)=C(I)+G(I,J)*X(J)
AE(I)=G(I,4)-C(I)
DE(I)= AE(I)/G(I,4)
77 CONTINUE
DO 11 I= 1, Z1
E1=DABS(XX(I)-X(1))
D1=D1+(E1**2)
H1=H1+(E1**2)/(D4(I))
E2=DABS(XY(I)-X(2))
D2=D2+(E2**2)
H2=H2+(E2**2)/(D5(I))
E3=DABS(XZ(I)-X(3))
D3=D3+(E3**2)
H3=H3+(E3**2)/(D6(I))
11 CONTINUE
S1=Z1-1
ST(1)=DSQRT(D1/S1)
ST(2)=DSQRT(D2/S1)
ST(3)=DSQRT(D3/S1)
C DETERMINE THE STANDARD ERROR OF EACH WEIGHTED MEAN

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C  FAT VALUE:
C  FAT ONE:
      ER(1)=DSQRT(H1/(S1*Y1))
      ET(1)=DSQRT(1/Y1)
C  FAT TWO:
      ER(2)=DSQRT(H2/(S1*Y2))
      ET(2)=DSQRT(1/Y2)
C  FAT THREE:
      ER(3)=DSQRT(H3/(S1*Y3))
      ET(3)=DSQRT(1/Y3)
      WRITE (NOUT, 234) Z1
      WRITE (NOUT, 2) (I, XX(I), XY(I), XZ(I), I=1, Z1)
      WRITE (NOUT, 93) (G(I, 4), C(I), AE(I), DE(I), I=1, M)
      PRINT*, '? ? '
      WRITE (NOUT, 94) (CC(I), X(I), ER(I), ET(I), ST(I), I=1, 3)
      CALL CONLIMIT (Z1, XX, XY, XZ, X, ST)
14  FORMAT(5X/5X, 'ONLY ONE SET OF DATAS AVAILABLE: '/')
15  FORMAT(5X/5X, 'NO SOLUTION FOR THIS SET OF MIXTURE DATAS.'/5X,
C    '*****')
22  FORMAT (15X, ' ' //)
2   FORMAT (5X, 'SET ', I3//5X, 'X(1) =', F9.5, 2X,
*   'X(2) =', F9.5, 2X, 'X(3) =', F9.5/)
93  FORMAT(5X, 'ACTUAL MIXTURE VALUE =', F9.5/5X
*   'CALCULATED VALUE =', F9.5, 5X, 'DIFFERENCE=', F9.5/5X,
*   'ACTUAL ERROR =', F9.5//)
94  FORMAT(5X, 'WT. MEAN ', A16, ' =', F9.5, /5X, 'WT. MEAN STD. ERROR =+/-',
*   F9.5/5X, 'ALTERNATIVE STD. ERROR =+/-', F9.5/5X,
*   'STANDARD DEVIATION =+/- ', F9.5//)
98  FORMAT (4(1X/), 1H 5A4, 1A3, 7HRESULTS/1X)
96  FORMAT(7X, 'MATRIX A', 13X, 'VECTOR B'//)
92  FORMAT (1X, 3F9.5/)
99  FORMAT (6A4, 1A4)
90  FORMAT(15X, 'STANDARD DEVIATION'//)
91  FORMAT (5X, 4F9.5/)
234 FORMAT (5X, 'NUMBER OF COMBINATIONS USED =', I3//)
STOP
19  WRITE (1, 15)
STOP
END

PROGRAM CRAM4
C  USING CRAMER'S RULE METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C  THE GENERAL EQUATION IS: AX = B .
C  DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
      INTEGER*2 M, N, NIN, NOUT, PP, HH, KK, I
      REAL*8 AA(30, 10), BB(30, 10), TITLE(20), X(10)
      REAL*8 A(30, 10), B(30, 10), EE(50), ER(50), C(50),
*   G(30, 10), AE(30), DE(30), XX(600), XY(600), XZ(600), ST(10),
*   ET(5), D4(600), D5(600), D6(600)
      REAL*8 V, D, R, AS, BS, ED, A1, A2, A3, Z1,
*   X1, X2, X3, Y1, Y2, Y3, T1, T2,
*   E1, E2, E3, D1, D2, D3, S1, H1, H2, H3, B1, B2, B3
      CHARACTER*16 CC(5)
      INTRINSIC DABS, SQRT, DSQRT
C
      DATA NIN/1/, NOUT/1/
      READ (NIN, 33) (CC(I), I = 1, 3)
      READ (NIN, *) M
      READ (NIN, *) N
      READ(NIN, 99) TITLE
      WRITE (NOUT, 98) (TITLE(I), I=1, 7)
      DO 20 I=1, M
20  READ (NIN, *) (A(I, J), J=1, N)

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C   CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C   THE GLC ANALYSIS.
      V = SQRT(0.5)
      R = 10.0 ** (-6)
      DO 10 I = 1, M
        BB(I,1)=DABS(A(I,1)-A(I,2))*V
        BB(I,2)=DABS(A(I,3)-A(I,4))*V
        BB(I,3)=DABS(A(I,5)-A(I,6))*V
        BB(I,4)=DABS(A(I,7)-A(I,8))*V
        AA(I,1)=(A(I,1)+A(I,2))*0.5
        AA(I,2)=(A(I,3)+A(I,4))*0.5
        AA(I,3)=(A(I,5)+A(I,6))*0.5
10   AA(I,4)=(A(I,7)+A(I,8))*0.5
      DO 100 I = 1, M
        DO 101 J = 1, 4
101   G(I,J)=AA(I,J)
100  CONTINUE
      WRITE (NOUT,22)
      WRITE (NOUT,96)
      WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
      WRITE (NOUT,90)
      WRITE (NOUT,94) ((BB(I,J),J=1,4),I=1,M)
      X1=0.0
      X2=0.0
      X3=0.0
      Y1=0.0
      Y2=0.0
      Y3=0.0
      Z1=0.0
      D1=0.0
      D2=0.0
      D3=0.0
      H1=0.0
      H2=0.0
      H3=0.0
      DO 444 PP=1, (M-1)
        HH=PP+1
        DO 455 KK= HH, M
          A(1,1)=AA(PP,1)-AA(PP,3)
          A(1,2)=AA(PP,2)-AA(PP,3)
          A(1,3)=AA(PP,4)-AA(PP,3)
          A(2,1)=AA(KK,1)-AA(KK,3)
          A(2,2)=AA(KK,2)-AA(KK,3)
          A(2,3)=AA(KK,4)-AA(KK,3)
          B(1,1)=DSQRT(BB(PP,1)**2+BB(PP,3)**2)
          B(1,2)=DSQRT(BB(PP,2)**2+BB(PP,3)**2)
          B(1,3)=DSQRT(BB(PP,4)**2+BB(PP,3)**2)
          B(2,1)=DSQRT(BB(KK,1)**2+BB(KK,3)**2)
          B(2,2)=DSQRT(BB(KK,2)**2+BB(KK,3)**2)
          B(2,3)=DSQRT(BB(KK,4)**2+BB(KK,3)**2)
          D=A(1,1)*A(2,2)-A(1,2)*A(2,1)
          IF (D-R) 466,51,51
51   T1=A(2,2)*A(1,3)-A(1,2)*A(2,3)
          T2=A(2,2)*A(2,3)-A(2,1)*A(1,3)
          X(1)=T1/D
          X(2)=T2/D
          X(3)=1-X(1)-X(2)
          IF (X(1) .LE. 0.0 .OR. X(1) .GE. 1.0) GO TO 466
          IF (X(2) .LE. 0.0 .OR. X(2) .GE. 1.0) GO TO 466
          IF (X(3) .LE. 0.0 .OR. X(3) .GE. 1.0) GO TO 466
C   ERROR PROPAGATION:
      AS=A(2,2)**2*B(1,1)**2+A(1,1)**2*B(2,2)**2
      BS=A(2,1)**2*B(1,2)**2+A(1,2)**2*B(2,1)**2

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```

ED=A8+B8
A2=A(1,3)**2*B(2,2)**2+A(2,2)**2*B(1,3)**2
A3=A(2,3)**2*B(1,2)**2+A(1,2)**2*B(2,3)**2
A1=A2+A3
B2=A(2,3)**2*B(2,2)**2+A(2,2)**2*B(2,3)**2
B3=A(1,3)**2*A(2,1)**2+A(2,1)**2*B(1,3)**2
B1=B2+B3
EE(1)=DSQRT((1/D)**2*A1+(T1/D**2)**2*ED)
EE(2)=DSQRT((1/D)**2*B1+(T2/D**2)**2*ED)
EE(3)=DSQRT(EE(1)**2+EE(2)**2)
IF (EE(1) .EQ. 0.0) GO TO 466
IF (EE(2) .EQ. 0.0) GO TO 466
IF (EE(3) .EQ. 0.0) GO TO 466
Z1=Z1+1.0
X1=X1+X(1)/(EE(1)**2)
X2=X2+X(2)/(EE(2)**2)
X3=X3+X(3)/(EE(3)**2)
Y1=Y1+1/EE(1)**2
Y2=Y2+1/EE(2)**2
Y3=Y3+1/EE(3)**2
D4(Z1)=EE(1)**2
D5(Z1)=EE(2)**2
D6(Z1)=EE(3)**2
XX(Z1)=X(1)
XY(Z1)=X(2)
XZ(Z1)=X(3)
466 CONTINUE
455 CONTINUE
444 CONTINUE
IF (Z1 .GT. 1.0) GO TO 9
IF (Z1 .EQ. 0.0) GO TO 19
PRINT*, 'ONLY ONE SET OF DATA AVAILABLE:'
X(1)=XX(1)
X(2)=XY(1)
X(3)=XZ(1)
WRITE (1,23) (I,X(I),EE(I), I=1,3)
23  FORMAT (5X/5X,'FAT ',I2,' =', P9.5,5X,'STD. ERROR =+/-',P9.5/)
GO TO 13
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE.
C FAT ONE:
9 X(1)=X1/Y1
C FAT TWO:)
X(2)=X2/Y2
C FAT THREE:
X(3)=X3/Y3
DO 77 I= 1,M
C(I)= 0.0
DO 770 J= 1,3
770 C(I)=C(I)+G(I,J)*X(J)
AE(I)=G(I,4)-C(I)
DE(I)= AE(I)/G(I,4)
77 CONTINUE
DO 11 I= 1, Z1
E1=DABS(XX(I)-X(1))
D1=D1+(E1**2)
H1=H1+(E1**2)/(D4(I))
E2=DABS(XY(I)-X(2))
D2=D2+(E2**2)
H2=H2+(E2**2)/(D5(I))
E3=DABS(XZ(I)-X(3))
D3=D3+(E3**2)
H3=H3+(E3**2)/(D6(I))
11 CONTINUE

```

```

S1=Z1-1
ST(1)=DSQRT(D1/S1)
ST(2)=DSQRT(D2/S1)
ST(3)=DSQRT(D3/S1)
C DETERMINE THE STANDARD ERROR OF EACH WEIGHTED MEAN
C FAT VALUE:
C FAT ONE:
  ER(1)=DSQRT(H1/(S1*Y1))
  ET(1)=DSQRT(1/Y1)
C FAT TWO:
  ER(2)=DSQRT(H2/(S1*Y2))
  ET(2)=DSQRT(1/Y2)
C FAT THREE:
  ER(3)=DSQRT(H3/(S1*Y3))
  ET(3)=DSQRT(1/Y3)
  WRITE (NOUT, 234) Z1
  WRITE (NOUT,2) (I,XX(I),XY(I),XZ(I),I=1,Z1)
  WRITE (NOUT,93) (G(I,4),C(I),AE(I),DE(I),I=1,M)
  PRINT*, '?'
  WRITE (NOUT,94) (CC(I),X(I),ER(I),ET(I),ST(I),I= 1,3)
  CALL CONLIMIT (Z1,XX,XY,XZ,X,ST)
22  FORMAT (15X, '          ' //)
33  FORMAT (A16)
2   FORMAT (5X, 'SET ', I3//5X, 'X(1) =', F9.5, 2X,
*   'X(2) =', F9.5, 2X, 'X(3) =', F9.5/)
93  FORMAT(5X, 'ACTUAL MIXTURE VALUE =', F9.5/5X
*   'CALCULATED VALUE =', F9.5, 5X, 'DIFFERENCE =', F9.5/5X,
*   'ACTUAL ERROR =', F9.5//)
94  FORMAT(5X, 'WT. MEAN ', A16, ' =', F9.5, /5X,
*   'WT. MEAN STD. ERROR =+/- ', F9.5/5X,
*   'ALTERNATIVE STD.ERROR =+/- ', F9.5 /5X,
*   'STANDARD DEVIATION =+/- ', F9.5//)
98  FORMAT (4(1X/), 1H 5A4, 1A3, 7HRESULTS/1X)
96  FORMAT(7X, 'MATRIX A', 18X, 'VECTOR B'//)
92  FORMAT (1X, 3F9.5/)
99  FORMAT (6A4, 1A4)
90  FORMAT(15X, 'STANDARD DEVIATION'//)
91  FORMAT (5X, 4F9.5/)
234  FORMAT (5X, 'NUMBER OF COMBINATIONS USED =', I3//)
    GO TO 13
19  PRINT*, 'NO SOLUTION FOR THIS SET OF MIXTURE DATAS.'
    PRINT*, '#####'
13  STOP
    END

```

## PROGRAM GRAM5

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C USING CRAMER'S RULE METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C THE GENERAL EQUATION IS: AX = B .
C DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
  INTEGER*2 M,N,NIN,NOUT,PP,HH,KK,I
  REAL*8 AA(30,10),BB(30,10), TITLE(20), X(10)
  REAL*8 A(30,10),B(30,10),EE(50),ER(50),C(50),
*   G(30,10),AE(30),DE(30),XX(600),XY(600),XZ(600),ST(10),
*   ET(5),D4(600),D5(600),D6(600)
  REAL*8 V,D,R,A8,B8,ED,A1,A2,A3,Z1,
*   X1,X2,X3,Y1,Y2,Y3,T1,T2,
*   E1,E2,E3,D1,D2,D3,S1,H1,H2,H3,B1,B2,B3
  CHARACTER*16 CC(5)
  INTRINSIC DABS, SQRT, DSQRT
C
  DATA NIN/1/, NOUT/1/
  READ (NIN,33) (CC(I),I = 1, 3)
  READ (NIN,*) M

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READ (NIN,*) N
READ(NIN,99) TITLE
WRITE (NOUT,98) (TITLE(I),I=1,7)
DO 20 I=1,M
20  READ (NIN,*) (A(I,J),J=1,N)
C  CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C  THE GLC ANALYSIS.
  V = SQRT(0.5)
  R = 10.0 ** (-6)
  DO 10 I = 1, M
    BB(I,1)=DABS(A(I,1)-A(I,2))*V
    BB(I,2)=DABS(A(I,3)-A(I,4))*V
    BB(I,3)=DABS(A(I,5)-A(I,6))*V
    BB(I,4)=DABS(A(I,7)-A(I,8))*V
    AA(I,1)=(A(I,1)+A(I,2))*0.5
    AA(I,2)=(A(I,3)+A(I,4))*0.5
    AA(I,3)=(A(I,5)+A(I,6))*0.5
10  AA(I,4)=(A(I,7)+A(I,8))*0.5
    DO 100 I = 1,M
      DO 101 J = 1,4
101  G(I,J)=AA(I,J)
100  CONTINUE
    WRITE (NOUT,22)
    WRITE (NOUT,96)
    WRITE (NOUT,91) ((AA(I,J),J=1,4),I=1,M)
    WRITE (NOUT,90)
    WRITE (NOUT,91) ((BB(I,J),J=1,4),I= 1,M)
    X1=0.0
    X2=0.0
    X3=0.0
    Y1=0.0
    Y2=0.0
    Y3=0.0
    Z1=0.0
    D1=0.0
    D2=0.0
    D3=0.0
    H1=0.0
    H2=0.0
    H3=0.0
    DO 444 PP=1, M
      DO 455 KK= 1, M
        IF (PP .EQ. KK) GO TO 466
        A(1,1)=AA(PP,1)-AA(PP,3)
        A(1,2)=AA(PP,2)-AA(PP,3)
        A(1,3)=AA(PP,4)-AA(PP,3)
        A(2,1)=AA(KK,1)-AA(KK,3)
        A(2,2)=AA(KK,2)-AA(KK,3)
        A(2,3)=AA(KK,4)-AA(KK,3)
        B(1,1)=DSQRT(BB(PP,1)**2+BB(PP,3)**2)
        B(1,2)=DSQRT(BB(PP,2)**2+BB(PP,3)**2)
        B(1,3)=DSQRT(BB(PP,4)**2+BB(PP,3)**2)
        B(2,1)=DSQRT(BB(KK,1)**2+BB(KK,3)**2)
        B(2,2)=DSQRT(BB(KK,2)**2+BB(KK,3)**2)
        B(2,3)=DSQRT(BB(KK,4)**2+BB(KK,3)**2)
        D=A(1,1)*A(2,2)-A(1,2)*A(2,1)
        IF (D-R) 466,51,51
51  T1=A(2,2)*A(1,3)-A(1,2)*A(2,3)
        T2=A(2,2)*A(2,3)-A(2,1)*A(1,3)
        X(1)=T1/D
        X(2)=T2/D
        X(3)=1-X(1)-X(2)
        IF (X(1) .LE. 0.0 .OR. X(1) .GE. 1.0) GO TO 466

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      IF (X(2) .LE. 0.0 .OR. X(2) .GE. 1.0) GO TO 466
      IF (X(3) .LE. 0.0 .OR. X(3) .GE. 1.0) GO TO 466
C   ERROR PROPAGATION:
      A8=A(2,2)**2*B(1,1)**2+A(1,1)**2*B(2,2)**2
      B8=A(2,1)**2*B(1,2)**2+A(1,2)**2*B(2,1)**2
      ED=A8+B8
      A2=A(1,3)**2*B(2,2)**2+A(2,2)**2*B(1,3)**2
      A3=A(2,3)**2*B(1,2)**2+A(1,2)**2*B(2,3)**2
      A1=A2+A3
      B2=A(2,3)**2*B(2,2)**2+A(2,2)**2*B(2,3)**2
      B3=A(1,3)**2*A(2,1)**2+A(2,1)**2*B(1,3)**2
      B1=B2+B3
      EE(1)=DSQRT((1/D)**2*A1+(T1/D**2)**2*ED)
      EE(2)=DSQRT((1/D)**2*B1+(T2/D**2)**2*ED)
      EE(3)=DSQRT(EE(1)**2+EE(2)**2)
      IF (EE(1) .EQ. 0.0) GO TO 466
      IF (EE(2) .EQ. 0.0) GO TO 466
      IF (EE(3) .EQ. 0.0) GO TO 466
      Z1=Z1+1.0
      X1=X1+X(1)/(EE(1)**2)
      X2=X2+X(2)/(EE(2)**2)
      X3=X3+X(3)/(EE(3)**2)
      Y1=Y1+1/EE(1)**2
      Y2=Y2+1/EE(2)**2
      Y3=Y3+1/EE(3)**2
      D4(Z1)=EE(1)**2
      D5(Z1)=EE(2)**2
      D6(Z1)=EE(3)**2
      XX(Z1)=X(1)
      XY(Z1)=X(2)
      XZ(Z1)=X(3)
466   CONTINUE
455   CONTINUE
444   CONTINUE
      IF (Z1 .GT. 1.0) GO TO 9
      IF (Z1 .EQ. 0.0) GO TO 19
      PRINT*, 'ONLY ONE SET OF DATAS AVAILABLE:'
      X(1)=XX(1)
      X(2)=XY(1)
      X(3)=XZ(1)
      WRITE (1,23) (I,X(I),EE(I), I=1,3)
23   FORMAT (5X/5X,'FAT ',I2,' =', F9.5,5X,'STD. ERROR =+/-',F9.5/)
      GO TO 13
C   DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE.
C   FAT ONE:
9     X(1)=X1/Y1
C   FAT TWO:)
      X(2)=X2/Y2
C   FAT THREE:
      X(3)=X3/Y3
      DO 777 I= 1,M
      G(I)= 0.0
      DO 770 J= 1,3
770   C(I)=C(I)+G(I,J)*X(J)
      AE(I)=G(I,4)-C(I)
      DE(I)= AE(I)/G(I,4)
77   CONTINUE
      DO 11 I= 1, Z1
      E1=DABS(XX(I)-X(1))
      D1=D1+(E1**2)
      H1=H1+(E1**2)/(D4(I))
      E2=DABS(XY(I)-X(2))
      D2=D2+(E2**2)

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H2=H2+(E2**2)/(D5(I))
E3=DABS(XZ(I)-X(3))
D3=D3+(E3**2)
H3=H3+(E3**2)/(D6(I))
11  CONTINUE
    S1=Z1-1
    ST(1)=DSQRT(D1/S1)
    ST(2)=DSQRT(D2/S1)
    ST(3)=DSQRT(D3/S1)
C   DETERMINE THE STANDARD ERROR OF EACH WEIGHTED MEAN
C   FAT VALUE:
C   FAT ONE:
    ER(1)=DSQRT(H1/(S1*Y1))
    ET(1)=DSQRT(1/Y1)
C   FAT TWO:
    ER(2)=DSQRT(H2/(S1*Y2))
    ET(2)=DSQRT(1/Y2)
C   FAT THREE:
    ER(3)=DSQRT(H3/(S1*Y3))
    ET(3)=DSQRT(1/Y3)
    WRITE (NOUT, 234) Z1
    WRITE (NOUT,2) (I,XX(I),XY(I),XZ(I),I=1,Z1)
    WRITE (NOUT,93) (G(I,4),C(I),AE(I),DE(I),I=1,M)
    PRINT*,'? '
    WRITE (NOUT,94) (CC(I),X(I),ER(I),ET(I),ST(I),I= 1,3)
    CALL CONLIMIT (Z1,XX,XY,XZ,X,ST)
22  FORMAT (15X,'          '///)
33  FORMAT (A16)
2   FORMAT (5X,'SET ',I3//5X,'X(1) =',F9.5,2X,
*   'X(2) =',F9.5,2X,'X(3) =',F9.5/)
93  FORMAT(5X,'ACTUAL MIXTURE VALUE =',F9.5/5X
*   'CALCULATED VALUE =',F9.5,5X,'DIFFERENCE=',F9.5/5X,
*   'ACTUAL ERROR =',F9.5//)
94  FORMAT(5X,'WT. MEAN ', A16,' =',F9.5,/5X,
*   'WT. MEAN STD. ERROR =+/- ', F9.5/5X,
*   'ALTERNATIVE STD. ERROR =+/- ',F9.5 /5X,
*   'STANDARD DEVIATION =+/- ',F9.5//)
98  FORMAT (4(1X/),1H 5A4, 1A3,7HRESULTS/1X)
96  FORMAT(7X,'MATRIX A',18X,'VECTOR B'///)
92  FORMAT (1X,3F9.5/)
99  FORMAT (6A4,1A4)
90  FORMAT(15X,'STANDARD DEVIATION'///)
91  FORMAT (5X,4F9.5/)
234  FORMAT (5X,'NUMBER OF COMBINATIONS USED =',I3//)
    GO TO 13
19  PRINT*,'NO SOLUTION FOR THIS SET OF MIXTURE DATAS.'
    PRINT*,'#####'
13  STOP
    END

PROGRAM GLC2
C   USING GAUSS-JORDAN-SEIDEL METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATION
S.
C   THE GENERAL EQUATION IS: AX = B .
C   DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
C   ..LOCAL SCALAR..
    REAL*8 V,X1,X2,X3,H1,H2,H3,E4,E5,E6,
*   S1,S2,S3,S4,S5,S6,S7,S8,S9
    INTEGER*2 LL,HH,KK,R1,R2,R3,PP
    REAL*8 D4,D5,D6,T1,T2,T3
    INTEGER*2 I, J, M,N,NIN,NOUT,
*   GG,LI,JL
    REAL*8 D1,D2,D3

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C  ..LOCAL ARRAY..
   REAL*8  A(100,24),B(100,24), TITLE(20), X(10),
   *  L6(10),K6(10),M1(700),M3(700),M2(700),ST(10),ET(10),
   *  W1(700),W3(700),W2(700),BD(100,10),
   *  AD(100,10),ER(10),E(10),A1(700),A3(700),A2(700),AM(10),RR(10)
   CHARACTER*16 CC(5)
   INTRINSIC DABS, SQRT
   COMMON //  A,B,L6,K6
   DATA NIN/1/, NOUT/1/
   READ (NIN,33) (CC(I),I = 1, 3)
   READ (NIN,*) M
   READ (NIN,*) N
   READ(NIN,99) TITLE
   WRITE (NOUT,98) (TITLE(I),I=1,7)
   DO 20 I = 1, M
20  READ (NIN,*) (A(I,J),J=1,N)
C  CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C  THE GLC ANALYSIS.
   V = SQRT (0.5)
   DO 10 I = 1, M
   BD(I,1)=(DABS(A(I,1)-A(I,2)))*V
   BD(I,2)=(DABS(A(I,3)-A(I,4)))*V
   BD(I,3)=(DABS(A(I,5)-A(I,6)))*V
   BD(I,4)=(DABS(A(I,7)-A(I,8)))*V
   AD(I,1)=(A(I,1)+A(I,2))*0.5
   AD(I,2)=(A(I,3)+A(I,4))*0.5
   AD(I,3)=(A(I,5)+A(I,6))*0.5
10  AD(I,4)=(A(I,7)+A(I,8))*0.5
   PRINT '(5X//)'
   WRITE (NOUT,96)
   WRITE (NOUT,922) ((AD(I,J),J=1,4),I=1,M)
   WRITE (NOUT,966)
   WRITE (NOUT,922) ((BD(I,J),J=1,4),I=1,M)
   S1=0.0
   S2=0.0
   S3=0.0
   S4=0.0
   S5=0.0
   S6=0.0
   S7=0.0
   S8=0.0
   S9=0.0
   D1=0.0
   D2=0.0
   D3=0.0
   D4=0.0
   D5=0.0
   D6=0.0
   R1=0
   R2=0
   R3=0
   X1= 0.0
   X2= 0.0
   X3= 0.0
   E4= 0.0
   E5= 0.0
   E6= 0.0
   H1= 0.0
   H2= 0.0
   H3= 0.0
C
C  MATRIX OPERATION:
   DO 444 PP = 1, (M-1)

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HH = PP + 1
DO 455 KK = HH, M
A(1,1)=AD(PP,1)-AD(PP,3)
A(1,2)=AD(PP,2)-AD(PP,3)
A(1,3)=AD(PP,4)-AD(PP,3)
A(2,1)=AD(KK,1)-AD(KK,3)
A(2,2)=AD(KK,2)-AD(KK,3)
A(2,3)=AD(KK,4)-AD(KK,3)
B(1,1)=DSQRT(BD(PP,1)**2+BD(PP,3)**2)
B(1,2)=DSQRT(BD(PP,2)**2+BD(PP,3)**2)
B(1,3)=DSQRT(BD(PP,4)**2+BD(PP,3)**2)
B(2,1)=DSQRT(BD(KK,1)**2+BD(KK,3)**2)
B(2,2)=DSQRT(BD(KK,2)**2+BD(KK,3)**2)
B(2,3)=DSQRT(BD(KK,4)**2+BD(KK,3)**2)
CALL GAJOSE(INTS(2),INTS(3),X,E)
X(3)=1-X(1)-X(2)
E(3)=DSQRT(E(1)**2+E(2)**2)
IF (X(1).LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2).LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3).LE.0.0 .OR. X(3).GE.1.0) GO TO 466
IF (E(1).EQ.0.0 .OR. E(2).EQ.0.0 .OR. E(3).EQ.0.0) GO TO 466
CALL FAT1 (X(1),E(1),R1,M1,A1)
CALL FAT2 (X(2),E(2),R2,M2,A2)
CALL FAT3 (X(3),E(3),R3,M3,A3)
X1=X1+X(1)/(E(1)**2)
X2=X2+X(2)/(E(2)**2)
X3=X3+X(3)/(E(3)**2)
H1=H1+1/(E(1)**2)
H2=H2+1/(E(2)**2)
H3=H3+1/(E(3)**2)
E4=E4+E(1)**2
E5=E5+E(2)**2
E6=E6+E(3)**2
466 CONTINUE
455 CONTINUE
444 CONTINUE
GO TO 37

C
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE AND
C SUM OF SQUARE OF DIFERENCE BETWEEN MEAN VALUE AND INDIVIDUAL.
C FAT ONE:
37 X(1)=X1/H1
DO 9 I = 1, R1
S4=S4+M1(I)
S7=S7+M1(I)**2
D1=D1+(M1(I)-X(1))**2/(A1(I)**2)
9 S1=S1+(M1(I)-X(1))**2
ST(1)=DSQRT(S1/(R1-1))
ER(1)=DSQRT(D1/((R1-1)*H1))
ET(1)=DSQRT(1/H1)

C
C FAT TWO:
X(2)= X2/H2
DO 17 I = 1, R2
S5=S5+M2(I)
S8=S8+M2(I)**2
D2=D2+(M2(I)-X(2))**2/(A2(I)**2)
17 S2=S2+(M2(I)-X(2))**2
ST(2)=DSQRT(S2/(R2-1))
ER(2)=DSQRT(D2/((R2-1)*H2))
ET(2)=DSQRT(1/H2)

C
C FAT THREE:

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X(3)= X3/H3
DO 18 I = 1, R3
S6=S6+M3(I)
S9=S9+M3(I)**2
D3=D3+(M3(I)-X(3))**2/(A3(I)**2)
18 S3=S3+(M3(I)-X(3))**2
ST(3)=DSQRT(S3/(R3-1))
ER(3)=DSQRT(D3/((R3-1)*H3))
ET(3)=DSQRT(1/H3)
C *****
WRITE (NOUT,3) (I,1,M1(I),2,M2(I),3,M3(I),I=1,R1)
C *****
C
PRINT*, '?'
WRITE (NOUT,94) (CC(I),X(I),ER(I),ET(I),ST(I),I = 1,3)
CALL CONLIMIT (R1,M1,M2,M3,X,ST)
STOP
3 FORMAT(5X,'SET NO.',I3/5X,'FAT',I2,' =',F9.5,2X,'FAT',I2,' =',
* F9.5,2X,'FAT',I2,' =',F9.5//)
99 FORMAT (6A4,1A4)
33 FORMAT (A16)
98 FORMAT (4(1X/),1H 5A4,1A3,7HRESULTS/1X)
96 FORMAT (10X,'MATRIX A',15X,'VECTOR B'//)
966 FORMAT( 10X,'STANDARD DEVIATION'//)
922 FORMAT(5X,4F9.5/)
94 FORMAT (5X,'WT.MEAN ',A16,' = ',F9.5/5X,
c 'WT. MEAN STANDARD ERROR = +/-',F9.5/5X,
c 'ALTERNATIVE WT.MEAN STANDARD ERROR = +/-',F9.5/5X,
c 'STANDARD DEVIATION = +/- ',F9.5//)
92 FORMAT (5X,3F9.5/)
END
SUBROUTINE GAJOSE (IT,JT,X,E)
C SUBROUTINE - FOR THE ANALYSIS OF THREE COMPONENT FAT
C MIXTURES BY SOLVING SIMULTANEOUS EQUATIONS.
REAL*8 X(10),D(10),C(10),E(10),Z(10),MR(200,10)
REAL*8 T(10),H9,R9,L6(10),K6(10),E1(200),
* E2(200,10),MM(10,5)
REAL*8 A4(200,10),G(200,10),A(100,24),B(100,24)
INTEGER*2 I,IT,J,J1,J2,ML,MJ,P1,R,N1,JT
COMMON // A,B,L6,K6
INTRINSIC DABS
N1=0
DO 2100 I = 1, IT
DO 2200 J = 1, JT
2200 G(I,J)=A(I,J)
2100 CONTINUE
R= 10.0**(-6)
C SET ROW INDEXES - L6(I)
DO 1 I = 1, IT
1 L6(I)= I
DO 600 J = 1, JT
C THE SUBROUTINE FINDS THE PIVOT ROW FOR EACH COLUMN.
C
CALL MAT(J,IT,MI)
K6(J)=MI
C THE PIVOT IS ZERO OR CLOSE TO ZERO;
C THE METHOD IS INAPPLICABLE.
C
IF(DABS(A(MI,J)).GT.R) GO TO 3850
C BECAUSE OF A ZERO PIVOT, THIS SET OF EQUATIONS CANNOT BE
C SOLVED BY THE GAUSS-JORDAN METHOD.
222 X(1)=0.0
X(2)=0.0

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```

X(3)=0.0
RETURN
C REDUCE ROW MI, THE PIVOT ROW, STARTING AT COLUMN J+1
3850 J1=J+1
DO 500 J2 = J1, JT
A(MI, J2)=A(MI, J2)/A(MI, J)
H9=(1/A(MI, J))**2*B(MI, J2)**2
R9=((A(MI, J2)/A(MI, J)**2)**2*B(MI, J)**2
500 E2(MI, J2)=SQRT(H9+R9)
C REDUCE OTHER ROWS, STARTING IN COLUMN J1
DO 3000 P1 = 1, IT
C THE NEXT STEP SKIPS THE PIVOT ROW.
IF(P1.EQ.MI) GO TO 3000
DO 4000 J2 = J1, JT
A(P1, J2)=A(P1, J2)-A(MI, J2)*A(P1, J)
4000 MR(P1, J2)=DSQRT(B(P1, J2)**2+A(P1, J)**2*E2(MI, J2)**2+
c A(MI, J2)**2*B(P1, J)**2)
3000 CONTINUE
600 CONTINUE
C STORAGE OF THE ANSWERS.
DO 4050 I = 1, IT
MJ=K6(I)
A4(MJ, JT)=MR(MJ, JT)
4050 X(I)=A(MJ, JT)
C
C CALCULATION OF PERTURBED CONSTANTS, USING X(I).
C DISPLAY ERRORS.
N1=0
3382 DO 701 I = 1, IT
C(I)=0.0
E1(1)=0.0
E1(2)=0.0
E1(3)=0.0
DO 702 J = 1, IT
C(I)=C(I)+G(I, J)*X(J)
702 E1(I)=E1(I)+DSQRT(G(I, J)**2*A4(MJ, JT)**2+
c X(J)**2*B(I, J)**2)
MJ=K6(I)
D(I)=G(I, JT)-C(I)
701 MR(MJ, JT)=DSQRT(B(I, JT)**2+E1(I)**2)
C SEIDEL ITERATION.
IF (IT .EQ. 2) GO TO 2
IF (X(1).GE.1.0 .OR. X(1).LE.0.0) RETURN
IF (X(2).GE.1.0 .OR. X(2).LE.0.0) RETURN
IF (X(3).GE.1.0 .OR. X(3).LE.0.0) RETURN
GO TO 3
2 IF (X(1).GE.1.0 .OR. X(1).LE.0.0) RETURN
IF (X(2).GE.1.0 .OR. X(2).LE.0.0) RETURN
IF (DABS(D(1)).LE.R .AND. DABS(D(2)).LE.R)RETURN
GO TO 4
C
3 IF (DABS(D(1)).LE.R .AND. DABS(D(2)).LE.R .AND. DABS(D(3)).LE.R)
c RETURN
4 N1=N1+1
IF(N1.GE.15) GO TO 222
DO 999 I = 1, IT
A(I, JT)=D(I)
999 T(I)=X(I)
DO 1217 I = 1, IT
1217 L6(I)=I
DO 6001 J = 1, IT
CALL MAT(J, IT, MI)
K6(J)=MI

```

```

      IF(DABS(A(MI,J)).GT.R) GO TO 3851
      X(1)=0.0
      X(2)=0.0
      X(3)=0.0
      RETURN
3851   J1=J+1
      DO 5001 J2 = J1, JT
      A(MI,J2)=A(MI,J2)/A(MI,J)
      H9=(1/A(MI,J))**2*MR(MI,J)**2
      R9=(A(MI,J2)/A(MI,J)**2)**2*MR(MI,J)**2
5001   E2(MI,J2)=SQRT(H9+R9)
      DO 3002 P1 = 1, IT
      IF(P1.EQ.MI) GO TO 3002
      DO 4002 J2 = J1, JT
      A(P1,J2)=A(P1,J2)-A(MI,J2)*A(P1,J)
      MR(P1,J2)=DSQRT(MR(P1,J2)**2+A(P1,J)**2*E2(MI,J2)**2+
c     A(MI,J2)**2*MR(P1,J)**2)
4002   CONTINUE
3002   CONTINUE
6001   CONTINUE
      DO 4055 I = 1, IT
      MJ=K6(I)
      Z(I)=A(MJ,JT)
      X(I)=T(I)+Z(I)
      E(I)=DSQRT(A4(MJ,JT)**2+MR(MJ,JT)**2)
4055   A4(MJ,JT)= E(I)
      GO TO 3382
      END
      SUBROUTINE MAT(J,IT,MI)
c     SUBROUTINE OF THE SUBROUTINE GAJOSE
      INTEGER*2 I,IT,J,MI,MA,MB
      REAL*8 Y(10),A(100,24),B(100,24),L6(10),K6(10)
      COMMON // A,B,L6,K6
      INTRINSIC DABS
c     FOR ROWS WHICH HAVE ALREADY BEEN PIVOTS, SET COEFFICIENTS TO
c     ZERO.
c     FOR OTHER ROWS, FIND ABSOLUTE VALUES.
      DO 433 I = 1, IT
      IF (L6(I).NE.0) GO TO 3130
      Y(I)= 0.0
      GO TO 433
3130   Y(I)=DABS(A(I,J))
433    CONTINUE
c     SET INITIAL VALUES FOR COMPARING COEFFICIENTS.
      MA=1
      MB=2
c     NOW COMPARE IN PAIRS.
414   IF(Y(MB).GT.Y(MA)) GO TO 616
      MI=MA
      GO TO 717
616   MI=MB
c     TEST FOR TERMINATION.
717   IF(MB.GE.IT) GO TO 919
      MA=MI
      MB=MB+1
      GO TO 414
919   L6(MI)= 0
      RETURN
      END
      SUBROUTINE FAT1 (F1,E1,R1,M1,A1)
      REAL*8 F1,M1(700),A1(700),E1
      INTEGER*2 R1
      R1=R1+1

```

```

M1(R1)=F1
A1(R1)=E1
RETURN
END
SUBROUTINE FAT2 (F2,E2,R2,M2,A2)
REAL*8 F2,M2(700),A2(700),E2
INTEGER*2 R2
R2=R2+1
M2(R2)=F2
A2(R2)=E2
RETURN
END
SUBROUTINE FAT3 (F3,E3,R3,M3,A3)
REAL*8 F3,M3(700),A3(700),E3
INTEGER*2 R3
R3=R3+1
M3(R3)=F3
A3(R3)=E3
RETURN
END

PROGRAM GLC1
C USING GAUSS-JORDAN-SEIDEL METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATION
S.
C THE GENERAL EQUATION IS: AX = B .
C DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
C ..LOCAL SCALAR..
REAL*8 V,X1,X2,X3,H1,H2,H3,E4,E5,E6,
* S1,S2,S3,S4,S5,S6,S7,S8,S9
INTEGER*2 LL,HH,KK,R1,R2,R3,PP
REAL*8 D4,D5,D6,T1,T2,T3
INTEGER*2 I, J, M,N,NIN,NOU,
* GC,LI, JL
REAL*8 D1,D2,D3
C ..LOCAL ARRAY..
REAL*8 A(100,24),B(100,24), TITLE(20), X(10),
* L6(10),K6(10),M1(700),M3(700),M2(700),ST(10),ET(10),
* W1(700),W3(700),W2(700),BD(100,10),
* AD(100,10),ER(10),E(10),A1(700),A3(700),A2(700),AM(10),RR(10)
CHARACTER*16 CC(5)
INTRINSIC DABS, SQRT
COMMON // A,B,L6,K6
DATA NIN/1/, NOU/1/
READ (NIN,33) (CC(I),I = 1, 3)
READ (NIN,*) M
READ (NIN,*) N
READ(NIN,99) TITLE
WRITE (NOU,98) (TITLE(I),I=1,7)
DO 20 I = 1, M
20 READ (NIN,*) (A(I,J),J=1,N)
C CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C THE GLC ANALYSIS.
V = SQRT (0.5)
DO 10 I = 1, M
BD(I,1)=(DABS(A(I,1)-A(I,2)))*V
BD(I,2)=(DABS(A(I,3)-A(I,4)))*V
BD(I,3)=(DABS(A(I,5)-A(I,6)))*V
BD(I,4)=(DABS(A(I,7)-A(I,8)))*V
AD(I,1)=(A(I,1)+A(I,2))*0.5
AD(I,2)=(A(I,3)+A(I,4))*0.5
AD(I,3)=(A(I,5)+A(I,6))*0.5
10 AD(I,4)=(A(I,7)+A(I,8))*0.5
PRINT '(5X//)'

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```

WRITE (NOUT,96)
WRITE (NOUT,922) ((AD(I,J),J=1,4),I=1,M)
WRITE (NOUT,966)
WRITE (NOUT,922) ((BD(I,J),J=1,4),I=1,M)
S1=0.0
S2=0.0
S3=0.0
S4=0.0
S5=0.0
S6=0.0
S7=0.0
S8=0.0
S9=0.0
D1=0.0
D2=0.0
D3=0.0
D4=0.0
D5=0.0
D6=0.0
R1=0
R2=0
R3=0
X1= 0.0
X2= 0.0
X3= 0.0
E4= 0.0
E5= 0.0
E6= 0.0
H1= 0.0
H2= 0.0
H3= 0.0

```

C

C

MATRIX OPERATIONS:

```

D) 444 PP = 1, M
DO 455 KK = 1, M
IF(PP.EQ.KK) GO TO 466
A(1,1)=AD(PP,1)-AD(PP,3)
A(1,2)=AD(PP,2)-AD(PP,3)
A(1,3)=AD(PP,4)-AD(PP,3)
A(2,1)=AD(KK,1)-AD(KK,3)
A(2,2)=AD(KK,2)-AD(KK,3)
A(2,3)=AD(KK,4)-AD(KK,3)
B(1,1)=DSQRT(BD(PP,1)**2+BD(PP,3)**2)
B(1,2)=DSQRT(BD(PP,2)**2+BD(PP,3)**2)
B(1,3)=DSQRT(BD(PP,4)**2+BD(PP,3)**2)
B(2,1)=DSQRT(BD(KK,1)**2+BD(KK,3)**2)
B(2,2)=DSQRT(BD(KK,2)**2+BD(KK,3)**2)
B(2,3)=DSQRT(BD(KK,4)**2+BD(KK,3)**2)
CALL GAJOSE(INTS(2),INTS(3),X,E)
X(3)=1-X(1)-X(2)
E(3)=DSQRT(E(1)**2+E(2)**2)
IF (X(1).LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2).LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3).LE.0.0 .OR. X(3).GE.1.0) GO TO 466
IF (E(1).EQ.0.0 .OR. E(2).EQ.0.0 .OR. E(3).EQ.0.0) GO TO 466
CALL FAT1 (X(1),E(1),R1,M1,A1)
CALL FAT2 (X(2),E(2),R2,M2,A2)
CALL FAT3 (X(3),E(3),R3,M3,A3)
X1=X1+X(1)/(E(1)**2)
X2=X2+X(2)/(E(2)**2)
X3=X3+X(3)/(E(3)**2)
H1=H1+1/(E(1)**2)
H2=H2+1/(E(2)**2)

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H3=H3+1/(E(3)**2)
E4=E4+E(1)**2
E5=E5+E(2)**2
E6=E6+E(3)**2
466 CONTINUE
455 CONTINUE
444 CONTINUE
GO TO 37

C
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE AND
C SUM OF SQUARE OF DIFERENCE BETWEEN MEAN VALUE AND INDIVIDUAL.
C FAT ONE:
37 X(1)=X1/H1
DO 9 I = 1, R1
S4=S4+M1(I)
S7=S7+M1(I)**2
D1=D1+(M1(I)-X(1))**2/(A1(I)**2)
9 S1=S1+(M1(I)-X(1))**2
ST(1)=DSQRT(S1/(R1-1))
ER(1)=DSQRT(D1/((R1-1)*H1))
ET(1)=DSQRT(1/H1)

C
C FAT TWO:
X(2)= X2/H2
DO 17 I = 1, R2
S5=S5+M2(I)
S8=S8+M2(I)**2
D2=D2+(M2(I)-X(2))**2/(A2(I)**2)
17 S2=S2+(M2(I)-X(2))**2
ST(2)=DSQRT(S2/(R2-1))
ER(2)=DSQRT(D2/((R2-1)*H2))
ET(2)=DSQRT(1/H2)

C
C FAT THREE:
X(3)= X3/H3
DO 18 I = 1, R3
S6=S6+M3(I)
S9=S9+M3(I)**2
D3=D3+(M3(I)-X(3))**2/(A3(I)**2)
18 S3=S3+(M3(I)-X(3))**2
ST(3)=DSQRT(S3/(R3-1))
ER(3)=DSQRT(D3/((R3-1)*H3))
ET(3)=DSQRT(1/H3)

C *****
WRITE (NOUT,3) (I,1,M1(I),2,M2(I),3,M3(I),I=1,R1)
C *****
C
PRINT*, '? '
WRITE (NOUT,94) (CC(I),X(I),ER(I),ET(I),ST(I),I = 1,3)
CALL CONLIMIT (R1,M1,M2,M3,X,ST)
STOP
3 FORMAT(5X,'SET NO.',I3/5X,'FAT',I2,' = ',F9.5,2X,'FAT',I2,' = ',
* F9.5,2X,'FAT',I2,' = ',F9.5//)
99 FORMAT (6A4,1A4)
33 FORMAT (A16)
98 FORMAT (4(1X/),1H 5A4,1A3,7HRESULTS/1X)
96 FORMAT (10X,'MATRIX A',15X,'VECTOR B'//)
966 FORMAT( 10X,'STANDARD DEVIATION'//)
922 FORMAT(5X,4F9.5/)
94 FORMAT (5X,'WT.MEAN ',A16,' = ',F9.5/5X,
c 'WT. MEAN STANDARD ERROR = +/-',F9.5/5X,
c 'ALTERNATIVE WT.MEAN STANDARD ERROR = +/-',F9.5/5X,
c 'STANDARD DEVIATION = +/- ',F9.5//)

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92     FORMAT (5X,3F9.5/)
      END

      PROGRAM GLC3
C     USING GAUSS-JORDAN-SEIDEL METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATION
S.
C     THE GENERAL EQUATION IS: AX = B .
C     DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
C     ..LOCAL SCALAR..
      DOUBLE PRECISION V,X1,X2,X3,H1,H2,H3,
      * S1,S2,S3,S4,S5,S6,S7,S8,S9
      INTEGER*2 LL,HH,KK,R1,R2,R3,PP,C1,C2,C3,C4
      DOUBLE PRECISION D4,D5,D6,T1,T2,T3
      INTEGER*2 I, J, M,N,NIN,NOU,
      * GG,LI, JL
      DOUBLE PRECISION D1,D2,D3
C     ..LOCAL ARRAY..
      DOUBLE PRECISION A(100,24),B(100,24), TITLE(20), X(10),
      * L6(10),K6(10),M1(700),M3(700),M2(700),ST(10),ET(10),
      * W1(700),W3(700),W2(700),BD(100,10),
      * AD(100,10),ER(10),E(10),A1(700),A3(700),A2(700)
      CHARACTER*16 CC(5)
      INTRINSIC DABS, SQRT
      COMMON // A,B,L6,K6
      DATA NIN/1/, NOU/1/
      READ (NIN,33) (CC(I),I = 1,3)
      READ (NIN,*) M
      READ (NIN,*) N
      READ (NIN,*) C1,C2,C3,C4
      READ(NIN,99) TITLE
      WRITE (NOU,98) (TITLE(I),I=1,7)
      DO 20 I = 1, M
20     READ (NIN,*) (A(I,J),J=1,N)
C     CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C     THE GLC ANALYSIS.
      V = SQRT (0.5)
      DO 10 I = 1, M
      BD(I,1)=(DABS(A(I,1)-A(I,2)))*V
      BD(I,2)=(DABS(A(I,3)-A(I,4)))*V
      BD(I,3)=(DABS(A(I,5)-A(I,6)))*V
      BD(I,4)=(DABS(A(I,7)-A(I,8)))*V
      AD(I,1)=(A(I,1)+A(I,2))*0.5
      AD(I,2)=(A(I,3)+A(I,4))*0.5
      AD(I,3)=(A(I,5)+A(I,6))*0.5
10     AD(I,4)=(A(I,7)+A(I,8))*0.5
      CALL COEFV (BD,A,C1,C2,C3,C4)
      PRINT '(5X//)'
      WRITE (NOU,96)
      WRITE (NOU,922) ((AD(I,J),J=1,4),I=1,M)
      WRITE (NOU,966)
      WRITE (NOU,922) ((BD(I,J),J=1,4),I=1,M)
      S1=0.0
      S2=0.0
      S3=0.0
      S4=0.0
      S5=0.0
      S6=0.0
      S7=0.0
      S8=0.0
      S9=0.0
      D1=0.0
      D2=0.0
      D3=0.0

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```

D4=0.0
D5=0.0
D6=0.0
R1=0
R2=0
R3=0
X1= 0.0
X2= 0.0
X3= 0.0
H1= 0.0
H2= 0.0
H3= 0.0
C
C MATRIX OPERATION:
DO 444 PP = 1, (M-1)
HH=PP+1
DO 455 KK = HH, M
A(1,1)=AD(PP,1)-AD(PP,3)
A(1,2)=AD(PP,2)-AD(PP,3)
A(1,3)=AD(PP,4)-AD(PP,3)
A(2,1)=AD(KK,1)-AD(KK,3)
A(2,2)=AD(KK,2)-AD(KK,3)
A(2,3)=AD(KK,4)-AD(KK,3)
B(1,1)=DSQRT(BD(PP,1)**2+BD(PP,3)**2)
B(1,2)=DSQRT(BD(PP,2)**2+BD(PP,3)**2)
B(1,3)=DSQRT(BD(PP,4)**2+BD(PP,3)**2)
B(2,1)=DSQRT(BD(KK,1)**2+BD(KK,3)**2)
B(2,2)=DSQRT(BD(KK,2)**2+BD(KK,3)**2)
B(2,3)=DSQRT(BD(KK,4)**2+BD(KK,3)**2)
CALL GAJOSE(INTS(2),INTS(3),X,E)
X(3)=1-X(1)-X(2)
E(3)=DSQRT(E(1)**2+E(2)**2)
IF (X(1).LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2).LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3).LE.0.0 .OR. X(3).GE.1.0) GO TO 466
IF (E(1).EQ.0.0 .OR. E(2).EQ.0.0 .OR. E(3).EQ.0.0) GO TO 466
CALL FAT1 (X(1),E(1),R1,M1,A1)
CALL FAT2 (X(2),E(2),R2,M2,A2)
CALL FAT3 (X(3),E(3),R3,M3,A3)
X1=X1+X(1)/(E(1)**2)
X2=X2+X(2)/(E(2)**2)
X3=X3+X(3)/(E(3)**2)
H1=H1+1/(E(1)**2)
H2=H2+1/(E(2)**2)
H3=H3+1/(E(3)**2)
466 CONTINUE
455 CONTINUE
444 CONTINUE
GO TO 37
C
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE AND
C SUM OF SQUARE OF DIFFERENCE BETWEEN MEAN VALUE AND INDIVIDUAL.
C FAT ONE:
37 X(1)=X1/H1
DO 9 I = 1, R1
S4=S4+M1(I)
S7=S7+M1(I)**2
D1=D1+(M1(I)-X(1))**2/(A1(I)**2)
9 S1=S1+(M1(I)-X(1))**2
ST(1)=DSQRT(S1/(R1-1))
ER(1)=DSQRT(D1/((R1-1)*H1))
ET(1)=DSQRT(1/H1)
C

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C   FAT TWO:
      X(2)= X2/H2
      DO 17 I = 1, R2
      S5=S5+M2(I)
      S8=S8+M2(I)**2
      D2=D2+(M2(I)-X(2))**2/(A2(I)**2)
17   S2=S2+(M2(I)-X(2))**2
      ST(2)=DSQRT(S2/(R2-1))
      ER(2)=DSQRT(D2/((R2-1)*H2))
      ET(2)=DSQRT(1/H2)

C
C   FAT THREE:
      X(3)= X3/H3
      DO 18 I = 1, R3
      S6=S6+M3(I)
      S9=S9+M3(I)**2
      D3=D3+(M3(I)-X(3))**2/(A3(I)**2)
18   S3=S3+(M3(I)-X(3))**2
      ST(3)=DSQRT(S3/(R3-1))
      ER(3)=DSQRT(D3/((R3-1)*H3))
      ET(3)=DSQRT(1/H3)

C *****
      WRITE (NOUT,3) (I,1,M1(I),2,M2(I),3,M3(I),I=1,R1)
C *****
C
      PRINT*, '? '
      WRITE (NOUT,94) (CC(I),X(I),ER(I),ET(I),ST(I),I=1,3)
      CALL CONLIMIT(R1,M1,M2,M3,X,ST)
      STOP

3   FORMAT(5X,'SET NO.',I3/5X,'FAT',I2,' = ',F9.5,2X,'FAT',I2,' = ',
*   F9.5,2X,'FAT',I2,' = ',F9.5//)
99  FORMAT (6A4,1A4)
98  FORMAT (4(1X/),1H 5A4,1A3,7HRESULTS/1X)
96  FORMAT (10X,'MATRIX A',15X,'VECTOR B'//)
33  FORMAT (A16)
966 FORMAT( 10X,'STANDARD DEVIATION'//)
922 FORMAT(5X,4F9.5/)
94  FORMAT (5X,'WT. MEAN ',A16,' = ',F9.5/5X,
*   'WT. MEAN STD. ERROR =+/-',F9.5/5X,
*   'ALTERNATIVE WT. MEAN ERROR =+/-',F9.5/5X,
*   'STANDARD DEVIATION =+/-',F9.5//)
      END

      PROGRAM GLC4
C   USING GAUSS-JORDAN-SEIDEL METHOD TO SOLVE SIMULTANEOUS LINEAR EQUATION
S.
C   THE GENERAL EQUATION IS: AX = B .
C   DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
C   ..LOCAL SCALAR..
      DOUBLE PRECISION V,X1,X2,X3,H1,H2,H3,
*   S1,S2,S3,S4,S5,S6,S7,S8,S9
      INTEGER*2 LL,HH,KK,R1,R2,R3,PP,C1,C2,C3,C4
      DOUBLE PRECISION D4,D5,D6,T1,T2,T3
      INTEGER*2 I, J, M,N,NIN,NOUT,
*   GG,LI,JL
      DOUBLE PRECISION D1,D2,D3
C   ..LOCAL ARRAY..
      DOUBLE PRECISION A(100,24),B(100,24), TITLE(20), X(10),
*   L6(10),K6(10),M1(700),M3(700),M2(700),ST(10),ET(10),
*   W1(700),W3(700),W2(700),BD(100,10),
*   AD(100,10),ER(10),E(10),A1(700),A3(700),A2(700)
      CHARACTER*16 CC(5)
      INTRINSIC DABS, SQRT

```

```

COMMON // A,B,L6,K6
DATA NIN/1/, NOUT/1/
READ (NIN,33) (CC(I),I = 1,3)
READ (NIN,*) M
READ (NIN,*) N
READ (NIN,*) C1,C2,C3,C4
READ(NIN,99) TITLE
WRITE (NOUT,98) (TITLE(I),I=1,7)
DO 20 I = 1, M
20 READ (NIN,*) (A(I,J),J=1,N)
C CALCULATE STD DEV AND AVERAGE VALUES OF DUPLICATES OBTAINED FROM
C THE GLC ANALYSIS.
V = SQRT (0.5)
DO 10 I = 1, M
BD(I,1)=(DABS(A(I,1)-A(I,2)))*V
BD(I,2)=(DABS(A(I,3)-A(I,4)))*V
BD(I,3)=(DABS(A(I,5)-A(I,6)))*V
BD(I,4)=(DABS(A(I,7)-A(I,8)))*V
AD(I,1)=(A(I,1)+A(I,2))*0.5
AD(I,2)=(A(I,3)+A(I,4))*0.5
AD(I,3)=(A(I,5)+A(I,6))*0.5
10 AD(I,4)=(A(I,7)+A(I,8))*0.5
CALL COEFV (BD,A,C1,C2,C3,C4)
PRINT '(5X//)'
WRITE (NOUT,96)
WRITE (NOUT,922) ((AD(I,J),J=1,4),I=1,M)
WRITE (NOUT,966)
WRITE (NOUT,922) ((BD(I,J),J=1,4),I=1,M)
S1=0.0
S2=0.0
S3=0.0
S4=0.0
S5=0.0
S6=0.0
S7=0.0
S8=0.0
S9=0.0
D1=0.0
D2=0.0
D3=0.0
D4=0.0
D5=0.0
D6=0.0
R1=0
R2=0
R3=0
X1= 0.0
X2= 0.0
X3= 0.0
H1= 0.0
H2= 0.0
H3= 0.0
C
C MATRIX OPERATION:
DO 444 PP = 1, M
DO 455 KK = 1, M
IF (PP .EQ. KK) GO TO 466
A(1,1)=AD(PP,1)-AD(PP,3)
A(1,2)=AD(PP,2)-AD(PP,3)
A(1,3)=AD(PP,4)-AD(PP,3)
A(2,1)=AD(KK,1)-AD(KK,3)
A(2,2)=AD(KK,2)-AD(KK,3)
A(2,3)=AD(KK,4)-AD(KK,3)

```

```

B(1,1)=DSQRT(BD(PP,1)**2+BD(PP,3)**2)
B(1,2)=DSQRT(BD(PP,2)**2+BD(PP,3)**2)
B(1,3)=DSQRT(BD(PP,4)**2+BD(PP,3)**2)
B(2,1)=DSQRT(BD(KK,1)**2+BD(KK,3)**2)
B(2,2)=DSQRT(BD(KK,2)**2+BD(KK,3)**2)
B(2,3)=DSQRT(BD(KK,4)**2+BD(KK,3)**2)
CALL GAJOSE(INTS(2),INTS(3),X,E)
X(3)=1-X(1)-X(2)
E(3)=DSQRT(E(1)**2+E(2)**2)
IF (X(1).LE.0.0 .OR. X(1).GE.1.0) GO TO 466
IF (X(2).LE.0.0 .OR. X(2).GE.1.0) GO TO 466
IF (X(3).LE.0.0 .OR. X(3).GE.1.0) GO TO 466
IF (E(1).EQ.0.0 .OR. E(2).EQ.0.0 .OR. E(3).EQ.0.0) GO TO 466
CALL FAT1 (X(1),E(1),R1,M1,A1)
CALL FAT2 (X(2),E(2),R2,M2,A2)
CALL FAT3 (X(3),E(3),R3,M3,A3)
X1=X1+X(1)/(E(1)**2)
X2=X2+X(2)/(E(2)**2)
X3=X3+X(3)/(E(3)**2)
H1=H1+1/(E(1)**2)
H2=H2+1/(E(2)**2)
H3=H3+1/(E(3)**2)
466 CONTINUE
455 CONTINUE
444 CONTINUE
GO TO 37
C
C DETERMINE THE PROPORTION OF EACH FAT IN A FAT MIXTURE AND
C SUM OF SQUARE OF DIFFERENCE BETWEEN MEAN VALUE AND INDIVIDUAL.
C FAT ONE:
37 X(1)=X1/H1
DO 9 I = 1, R1
S4=S4+M1(I)
S7=S7+M1(I)**2
D1=D1+(M1(I)-X(1))**2/(A1(I)**2)
9 S1=S1+(M1(I)-X(1))**2
ST(1)=DSQRT(S1/(R1-1))
ER(1)=DSQRT(D1/((R1-1)*H1))
ET(1)=DSQRT(1/H1)
C
C FAT TWO:
X(2)= X2/H2
DO 17 I = 1, R2
S5=S5+M2(I)
S8=S8+M2(I)**2
D2=D2+(M2(I)-X(2))**2/(A2(I)**2)
17 S2=S2+(M2(I)-X(2))**2
ST(2)=DSQRT(S2/(R2-1))
ER(2)=DSQRT(D2/((R2-1)*H2))
ET(2)=DSQRT(1/H2)
C
C FAT THREE:
X(3)= X3/H3
DO 18 I = 1, R3
S6=S6+M3(I)
S9=S9+M3(I)**2
D3=D3+(M3(I)-X(3))**2/(A3(I)**2)
18 S3=S3+(M3(I)-X(3))**2
ST(3)=DSQRT(S3/(R3-1))
ER(3)=DSQRT(D3/((R3-1)*H3))
ET(3)=DSQRT(1/H3)
C *****
WRITE (NOJP,3) (I,1,M1(I),2,M2(I),3,M3(I),I=1,R1)

```

```

C *****
C
  PRINT*, '? '
  WRITE (NOUT,94) (CC(I),X(I),ER(I),ET(I),ST(I),I=1,3)
  CALL CONLIMIT(R1,M1,M2,M3,X,ST)
  STOP
3   FORMAT(5X,'SET NO.',I3/5X,'FAT',I2,'=',F9.5,2X,'FAT',I2,'=',
*   F9.5,2X,'FAT',I2,'=',F9.5//)
99  FORMAT(6A4,1A4)
98  FORMAT(4(1X/),1H 5A4,1A3,7HRESULTS/1X)
96  FORMAT(10X,'MATRIX A',15X,'VECTOR B')
33  FORMAT(A16)
966 FORMAT(10X,'STANDARD DEVIATION'//)
922 FORMAT(5X,4F9.5/)
94  FORMAT(5X,'WT. MEAN ',A16,'=',F9.5/5X,
*   'WT. MEAN STD. ERROR =+/-',F9.5/5X,
*   'ALTERNATIVE WT. MEAN ERROR =+/-',F9.5/5X,
*   'STANDARD DEVIATION =+/-',F9.5//)
  END

  PROGRAM CHU2
C   USING FO4JAF PROGRAM TO SOLVE SIMULTANEOUS LINEAR EQUATIONS.
C   DATAS ARE OBTAINED FROM GLC ANALYSIS OF 3-FATS MIXTURES.
C   MARK 8 RELEASE. NAG COPYRIGHT 1979
C   ..LOCAL SCALAR..
  REAL*8 SIGMA, TOL
  INTEGER*2 I, IFAIL, IRANK, J, LWORK,M,N,NIN,NOUT,NRA
C   ..LOCAL ARRAY..
  REAL*8 A(200,24), B(250), TITLE(7),WORK(200),AA(40,10),D(5)
C   ..SUBROUTINE REFERENCES..
C   FO4JAF
C
  CHARACTER*16 CC(5)
  DATA NIN/1/, NOUT/1/
  READ (NIN,33) (CC(I),I=1,3)
  READ (NIN,*) M
  READ (NIN,*) N
  READ(NIN,99) TITLE
  WRITE (NOUT,98) (TITLE(I),I=1,7)
  NRA= 200
  LWORK = 200
  IFAIL = 0
  TOL = 5.0E-4
  READ (NIN,*) ((AA(I,J),J=1,N),I=1,M)
  DO 1 I = 1,M
  A(I,1)=(AA(I,1)+AA(I,2))*0.5
  A(I,2)=(AA(I,3)+AA(I,4))*0.5
  A(I,3)=(AA(I,5)+AA(I,6))*0.5
  1  B(I) =(AA(I,7)+AA(I,8))*0.5
  WRITE (NOUT,96)
  WRITE (NOUT,92) ((A(I,J),J=1,3),B(I),I=1,M)
  DO 444 PP = 1, M
  A(PP,1)=A(PP,1)-A(PP,3)
  A(PP,2)=A(PP,2)-A(PP,3)
  444 B(PP) =B(PP)-A(PP,3)
  N = 2
  CALL FO4JAF(M,N,A,NRA,B,TOL,SIGMA,IRANK,WORK,LWORK,IFAIL)
  B(3)=1-B(1)-B(2)
  DO 11 K = 1, 3
  11 D(K) = B(K)*SIGMA
  WRITE (NOUT,94)
  WRITE (NOUT,12) (CC(I),B(I),I=1,3)
  WRITE (NOUT,15) (CC(I),D(I),I=1,3)

```

```

WRITE (NOUT,93) IRANK
STOP
99  FORMAT (6A4,1A3)
15  FORMAT (5X,A16,'STANDARD ERROR =+/- ',F9.5/)
12  FORMAT (5X,A16,' = ',F9.5/)
33  FORMAT (A16)
98  FORMAT (4(1X/),1H 5A4,1A3,7HRESULTS/1X)
96  FORMAT (5X/7X, 'MATRIX A',20X,'VECTOR B'/)
94  FORMAT (5X/5X,'SOLUTION VECTOR'/)
93  FORMAT (10X,'*****'/12X,'RANK = ',I2/10X,
c   '*****'/)
92  FORMAT (5X,4F9.5)
END

```

C THE SUBROUTINE TO CALCULATE THE CONFIDENCE LIMITS OF EACH FAT.  
SUBROUTINE CONLIMIT (N1,XX,XY,XZ,WMX,TS)

```

INTEGER*2 I,N1
REAL*8 XX(700),XY(700),XZ(700),S1,S2,S3,D1,D2,D3,Z1,T1,N,
* AM(5),A(50,5),RR(5),T(5),X1,X2,X3,CL(5,5),
* TS(10),AM2(5),WMX(10)
C *****
C T DISTRIBUTION TABLE:
C *****

```

```

A(1,1)=6.314
A(1,2)=12.71
A(1,3)=63.66
A(1,4)=636.6
A(2,1)=2.920
A(2,2)=4.303
A(2,3)=9.925
A(2,4)=31.60
A(3,1)=2.353
A(3,2)=3.182
A(3,3)=5.841
A(3,4)=12.94
A(4,1)=2.132
A(4,2)=2.776
A(4,3)=4.604
A(4,4)=8.610
A(5,1)=2.015
A(5,2)=2.571
A(5,3)=4.032
A(5,4)=6.859
A(6,1)=1.943
A(6,2)=2.447
A(6,3)=3.707
A(6,4)=5.959
A(7,1)=1.895
A(7,2)=2.365
A(7,3)=3.499
A(7,4)=5.405
A(8,1)=1.860
A(8,2)=2.306
A(8,3)=3.355
A(8,4)=5.041
A(9,1)=1.833
A(9,2)=2.262
A(9,3)=3.250
A(9,4)=4.781
A(10,1)=1.812
A(10,2)=2.228
A(10,3)=3.169
A(10,4)=4.587

```

A(11,1)=1.796  
A(11,2)=2.201  
A(11,3)=3.106  
A(11,4)=4.437  
A(12,1)=1.782  
A(12,2)=2.179  
A(12,3)=3.055  
A(12,4)=4.318  
A(13,1)=1.771  
A(13,2)=2.160  
A(13,3)=3.012  
A(13,4)=4.221  
A(14,1)=1.761  
A(14,2)=2.145  
A(14,3)=2.977  
A(14,4)=4.140  
A(15,1)=1.753  
A(15,2)=2.131  
A(15,3)=2.947  
A(15,4)=4.073  
A(16,1)=1.746  
A(16,2)=2.120  
A(16,3)=2.921  
A(16,4)=4.015  
A(17,1)=1.740  
A(17,2)=2.110  
A(17,3)=2.898  
A(17,4)=3.965  
A(18,1)=1.734  
A(18,2)=2.101  
A(18,3)=2.878  
A(18,4)=3.922  
A(19,1)=1.729  
A(19,2)=2.093  
A(19,3)=2.861  
A(19,4)=3.883  
A(20,1)=1.725  
A(20,2)=2.086  
A(20,3)=2.845  
A(20,4)=3.850  
A(21,1)=1.721  
A(21,2)=2.080  
A(21,3)=2.831  
A(21,4)=3.819  
A(22,1)=1.717  
A(22,2)=2.074  
A(22,3)=2.819  
A(22,4)=3.792  
A(23,1)=1.714  
A(23,2)=2.069  
A(23,3)=2.807  
A(23,4)=3.767  
A(24,1)=1.711  
A(24,2)=2.064  
A(24,3)=2.797  
A(24,4)=3.745  
A(25,1)=1.708  
A(25,2)=2.060  
A(25,3)=2.787  
A(25,4)=3.725  
A(26,1)=1.706  
A(26,2)=2.056  
A(26,3)=2.779

```

A(26,4)=3.707
A(27,1)=1.703
A(27,2)=2.052
A(27,3)=2.771
A(27,4)=3.690
A(28,1)=1.701
A(28,2)=2.048
A(28,3)=2.763
A(28,4)=3.674
A(29,1)=1.699
A(29,2)=2.045
A(29,3)=2.756
A(29,4)=3.659
A(30,1)=1.697
A(30,2)=2.042
A(30,3)=2.75
A(30,4)=3.646
C THE FOLLOWING VALUES ARE FOR DF GREATER THAN 30.
A(40,1)=1.645
A(40,2)=1.960
A(40,3)=2.576
A(40,4)=3.291
C *****
S1=0.0
S2=0.0
S3=0.0
D1=0.0
D2=0.0
D3=0.0
Z1=DBLE(N1)
DO 1 I = 1, Z1
S1=S1+XX(I)
S2=S2+XY(I)
1 S3=S3+XZ(I)
AM(1)=S1/Z1
AM(2)=S2/Z1
AM(3)=S3/Z1
DO 2 I =1, Z1
D1=D1+(XX(I)-AM(1))**2
D2=D2+(XY(I)-AM(2))**2
2 D3=D3+(XZ(I)-AM(3))**2
N= Z1-1.0
IF((Z1-1).EQ.0) N=1.0
RR(1)=0.6745*(DSQRT(D1/(Z1*N)))
RR(2)=0.6745*(DSQRT(D2/(Z1*N)))
RR(3)=0.6745*(DSQRT(D3/(Z1*N)))
WRITE (1,11)
11 FORMAT (5X/5X,'ARITHMETIC MEAN AND ITS PROBABLE ERROR:'/5X,
c '#####'//)
T(1)=DSQRT(D1/N)
T(2)=DSQRT(D2/N)
T(3)=DSQRT(D3/N)
WRITE (1,4) (I,AM(I),RR(I),T(I),I=1,3)
4 FORMAT (5X/5X,'PROBABLE FAT ',I2,' VALUE = ',F9.5/5X,
c 'ITS PROBABLE ERROR = +/- ', F9.5/5X,
c 'ITS STANDARD DEVIATION =+/- ',F9.5//)
IF (N .LE. 30.0) GO TO 5
X1=40.0
X2=40.0
X3=40.0
GO TO 10
5 X1=N
X2=N

```

```

X3=N
C   FOR 95% LEVEL OF CONFIDENCE
10  P1=A(X1,2)*T(1)/DSQRT(Z1)
    P2=A(X2,2)*T(2)/DSQRT(Z1)
    P3=A(X3,2)*T(3)/DSQRT(Z1)
    CL(1,1)=AM(1)+P1
    IF (CL(1,1) .GT. 1.0) CL(1,1)=1.0
    CL(1,2)=AM(1)-P1
    IF (P1 .GT. AM(1)) CL(1,2)=0.0
    CL(2,1)=AM(2)+P2
    IF (CL(2,1) .GT. 1.0) CL(2,1)=1.0
    CL(2,2)=AM(2)-P2
    IF (P2 .GT. AM(2)) CL(2,2)=0.0
    CL(3,1)=AM(3)+P3
    IF (CL(3,1) .GT. 1.0) CL(3,1)=1.0
    CL(3,2)=AM(3)-P3
    IF (P3 .GT. AM(3)) CL(3,2)=0.0
    B = 95.00
    WRITE (1,20) B,AM(1),P1,AM(2),P2,AM(3),P3
    WRITE (1,22) (I,(CL(I,J),J=2,1,-1),I=1,3)
    T1=A(X1,2)
    PRINT*, '      INPUT ACTUAL MIXTURE COMPONENT VALUES:'
    PRINT*, '      (IF NOT AVAILABLE, INPUT THREE VALUES OF 1.0)'
    READ (1,34) (AM2(I),I=1,3)
    IF (AM2(1).EQ.1.0) RETURN
    PRINT*, '^207 '
    WRITE(1,*)
    PRINT*, '====='
    PRINT*, '      CONSIDERING ARITHMETIC MEAN VALUES:'
    PRINT*, '====='
    CALL EASE(AM2,AM,T,T1,N)
    PRINT*, '^207 '
    WRITE (1,*)
    PRINT*, '====='
    PRINT*, '      CONSIDERING WEIGHTED MEAN VALUES:'
    PRINT*, '====='
    CALL EASE(AM2,WMX,TS,T1,N)
34  FORMAT (F9.5)
20  FORMAT (5X, '*****')
*   3A, F5.2,
*   '*****' /5X,
*   'FAT ONE = ',F9.5, ' +/- ',F9.5/5X, 'FAT TWO = ',F9.5,
*   ' +/- ',F9.5/5X, 'FAT THREE = ',F9.5, ' +/- ',F9.5//)
22  FORMAT (5X, 'FAT', I2, ' CONFIDENCE LIMIT IS BETWEEN' /
*   5X, F9.5, ' AND ', F9.5//)
    RETURN
    END

C
C
SUBROUTINE EASE(AM,X,T,T1,X1)
REAL*8 AM1(5),AM(5),T(10),X(10),T1,X1
INTEGER*2 I
DO 36 I = 1,3
AM1(I)=AM(I)
AM1(I)=(DABS(X(I)-AM1(I)))*DSQRT(X1)/T(I)
WRITE (1,12)
PRINT*, '      FOR FAT', I, ' MEAN VALUE:'
PRINT*, '      %%%%%%%%%%'
WRITE (1,35) I,AM1(I),T1
12  FORMAT (5X)
35  FORMAT(5X, 'CALCULATED T VALUE FOR FAT', I2, ' IS ', F9.5/5X,
C   'T TABLE VALUE IS ', F9.5)
    IF (AM1(I)-T1) 38,38,39

```

```
38 PRINT*, '   THERE IS NO SIGNIFICANT DIFFERENCE BETWEEN '
PRINT*, 'ACTUAL AND CALCULATED VALUES AT 95
GO TO 37
39 PRINT*, '   THERE IS SIGNIFICANT DIFFERENCE BETWEEN ACTUAL AND'
PRINT*, '   CALCULATED VALUES AT 95
37 PRINT*, '*****'
36 CONTINUE
RETURN
END
```

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