

AN EVALUATION OF THE SUJATA ABSORPTION
CALCULATION METHOD

By

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PREFACE

A critical evaluation of the Sujata absorption calculation was made. The results predicted by the Sujata method were compared with results obtained from the classical Kremser-Brown and Edmister short-cut methods and from three operating industrial absorbers. In order to conduct this evaluation, a computer program was written using the Sujata calculation method on a complex column. The complex features of the column included the possibility of an additional feed, liquid side stream, vapor side stream, and intercooler on every tray.

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CHAPTER I

INTRODUCTION

In the natural gas, petroleum, and petro-chemical industries, the separation of complex hydrocarbon mixtures is of particular importance. The separation efficiency and capital outlay for separation equipment are important factors in the economic success or failure of a process in these industries. Thus, the calculation method which describes the process is of the utmost importance in process design.

For many years the hydrocarbon absorption process was described by calculations based on time-saving assumptions and approximations which were either inaccurate or invalid in most cases. With the development of digital computer calculation methods, most of the approximations and assumptions could be discarded. More emphasis was placed on the approach, convergence technique, and generality of the calculation method. The engineering goal is a simple yet completely general calculation method which requires no assumptions, yet

has a simple and rapid convergence technique. Although this goal may never be reached, one of the methods which most closely approaches this goal was developed by Sujata. (16)

The Sujata calculation method has three important and distinct features. 1) A minimum number of primary assumptions are required in the calculation. 2) The method is derived from and uses basic engineering concepts which are familiar to all chemical engineers. 3) The method was derived from general equations and can be applied to a wide variety of complex absorption systems.

The purpose of this study is to examine the Sujata absorption calculation method in detail. Three principal objectives are associated with the evaluation of this method. The first objective is to examine the approach, generality, and scope of the method. If necessary, minor modifications in the basic Sujata method will be suggested. The second objective is to determine the method's reliability and limitations in calculating results for various absorption systems. The third objective is to compare the results obtained from the Sujata method with results from the classical absorption calculations such as the Kremser-Brown and

Edmister methods. In addition the results are compared with data obtained from actual plant operation of three industrial absorption columns.

CHAPTER II

BACKGROUND

A. The Absorption Process

The process of diffusion of a component from a vapor to a liquid phase as a result of a concentration difference between the two phases is known as gaseous absorption. This fundamental mass transfer process results from molecular and eddy diffusion and is often described by some form of the two-film or penetration theories of mass transfer.

The absorption column multiplies the concentration difference existing between the vapor and liquid phases by the countercurrent contacting of the two streams. The result is an increased efficiency in the absorption of the vapor components by the liquid phase. The basic absorption column contains two feed elements as shown in Figure 1. The entering liquid phase is the absorbing medium and is known as the "lean oil." The entering vapor phase is known as the "wet gas" and consists of

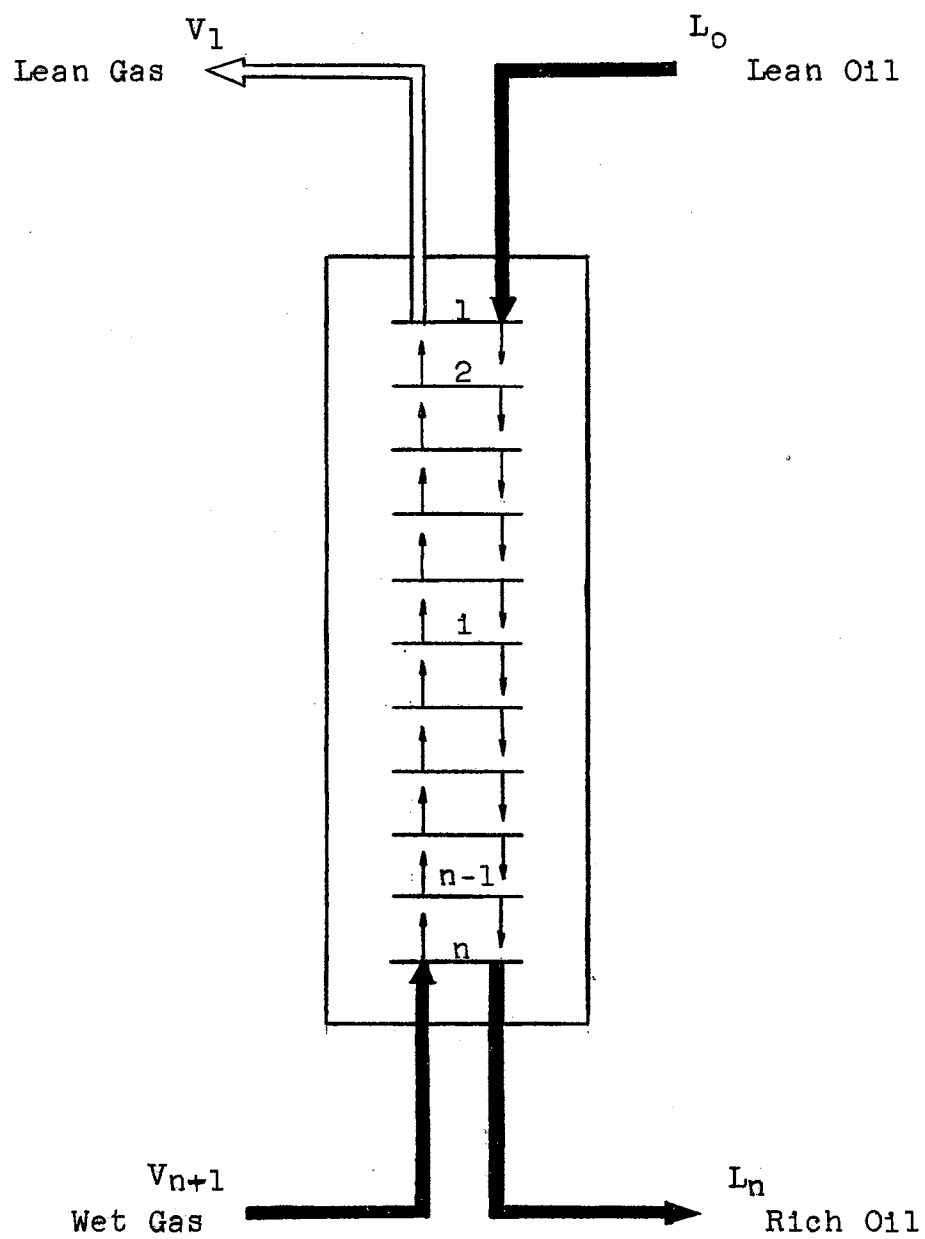


Figure 1. A "Simple" N Tray Absorption Column

those components to be absorbed by the oil and those components which are not absorbed and appear in the exit vapor stream or "lean gas." The absorber oil plus the absorbed vapor components leaving the column is known as the "rich oil."

The rich oil is usually fed to a stripping column which separates the absorbed vapor components from the original absorber oil. The mass transfer is now from the liquid to the vapor phase as a result of the reversed concentration difference. The lean oil leaving the stripper is fed back to the absorption column. The absorber-stripper system as shown in Figure 2 provides for the continuous separation of desired components from a vapor mixture.

B. Absorption Calculations

Absorption calculations are designed to describe, as completely as possible, the operation of absorption columns. The "simple" absorption column with n trays has a single wet gas feed entering the bottom tray and a lean oil entering the top tray as shown in Figure 1. If each tray is considered as a simple equilibrium stage defined by $2C + 6$ possible variables, then the total

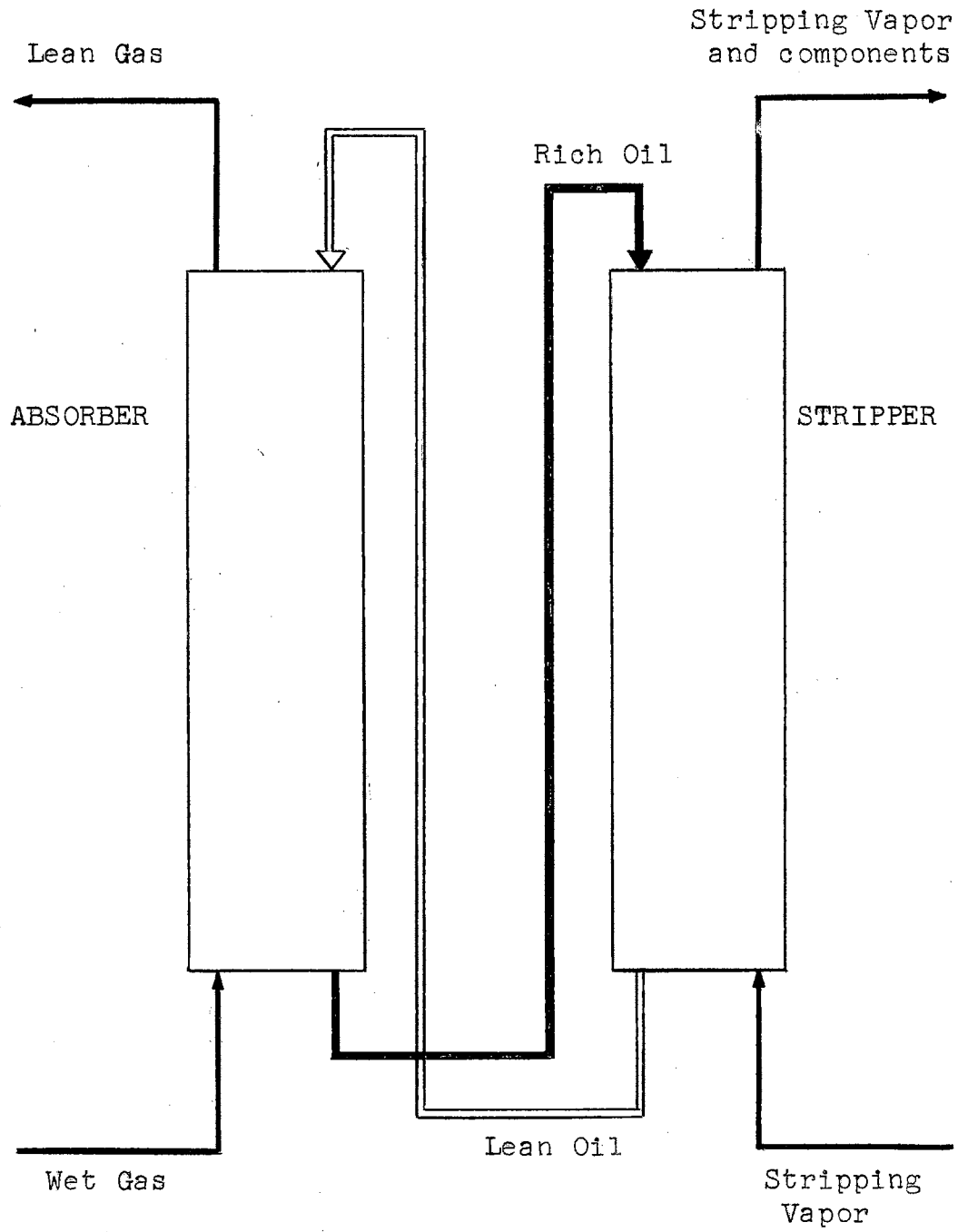


Figure 2. Absorber-Stripper Unit

number of variables associated with an n tray column (the specification of that number of trays represents a single variable) is given by

$$N_v = 1 + n(2C + 6). \quad (1)$$

Some of these variables are not independent and must be subtracted to obtain the degrees of freedom for the column. Each interstream within the column contains $C + 2$ restrictions which must be subtracted. For a column of n trays, the total number of restricted variables is

$$N_c = 2(n - 1)(C + 2). \quad (2)$$

The number of independent variables which completely describes the column is then $N_i = N_v - N_c$ or

$$N_i = 2C + 2n + 5. \quad (3)$$

The most common set of specifications for the degrees of freedom for a simple column is given below.

Pressure for each stage	n
Heat leak for each stage	n
Wet gas feed	$C + 2$
Lean oil feed	$C + 2$
Number of stages	1
TOTAL	$2C + 2n + 5$

The simple absorption column can be modified with a number of complex features. The i^{th} tray in a complex column can have an intercooler, vapor side stream,

liquid side stream, or additional feed. Trays with all these complex features are shown in Figure 3.

The addition of a feed stream to a specified simple tray increases the number of independent variables needed to describe the tray from $2C + 6$ to $3C + 8$. The increase in the number of independent variables resulting from the addition of a feed stream is $C + 2$. In general, the location of the feed tray in a complex column is not fixed so that the location of the feed tray must also be specified. Thus, there are $C + 3$ additional independent variables associated with each feed tray.

The addition of a side stream to a specified simple tray increases the number of independent variables from $2C + 6$ to $2C + 7$. The increase is one. In general, the location of the side stream is not fixed so that the side stream tray location must also be specified. Thus, there are two additional independent variables associated with each side stream tray.

The addition of an intercooler to a simple tray requires no additional independent variables since a heat leak for each stage is already specified in the simple column.

For an n tray, complex column having m feed streams,

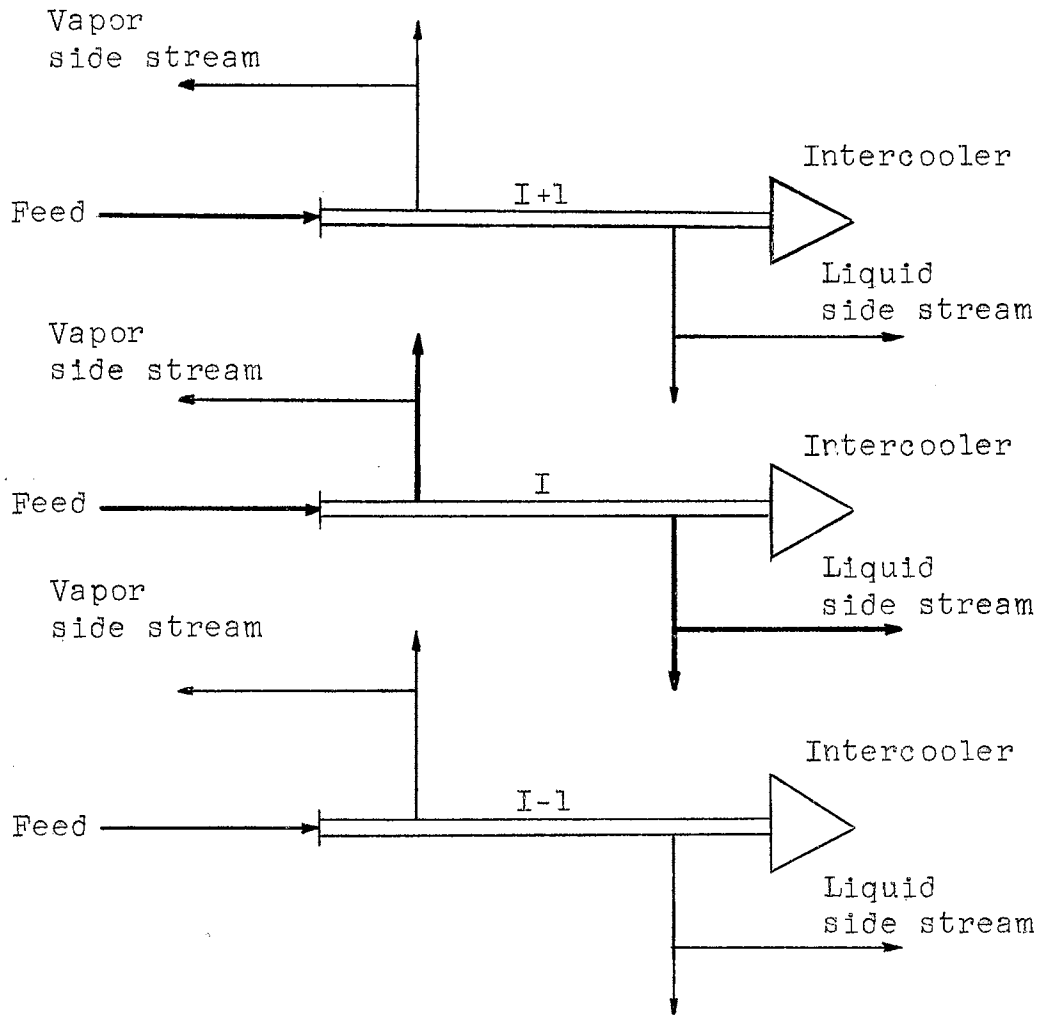


Figure 3. Complex Column Trays

k liquid side streams, and v vapor side streams, the most common set of specifications for the degrees of freedom is given below.

Pressure for each stage	n
Heat leak for each stage	n
Feed streams and location	$m(C + 3)$
Liquid side streams and location	2k
Vapor side streams and location	2v
Number of stages	1
<hr/>	
TOTAL	$2(n + k + v) + m(C + 3) + 1$

A general absorption calculation method must be able to handle each of these complex features.

The engineering analysis of the absorption process has been largely restricted to two basic approaches. The more fundamental mass transfer approach to absorption has been developed from the two-film and the penetration mass transfer theories. This type of absorption calculation usually has been limited to use with packed columns. In this approach the number of transfer units and the "height" of the unit become the basic variables to be evaluated.

A less fundamental but more widely used approach in engineering calculations treats the operation of an absorption column as a stagewise process. Most stage-wise treatments make the primary assumption of an ideal

or equilibrium stage. An accompanying implicit assumption is that an over-all column efficiency can be used to correct the assumption of an ideal stage. A notable exception to both these limiting assumptions is an absorption calculation method developed by Ravicz. (14) This method provides for a non-ideal, vapor-liquid contacting device. As a result of the consideration of a non-ideal stage, individual tray and component efficiencies are also included in this method.

The basic approach which led to the development of the Sujata calculation method treats absorption as a stagewise process using equilibrium or ideal stages. This general approach might be termed the absorption factor approach because of the repeated use of and emphasis on an absorption factor. The development of this absorption factor approach is discussed in the following section.

C. Literature Survey

One of the earliest successful attempts in making a theoretical analysis of the absorption process was made by Kremser (10) in 1930. In this analysis the pressure, temperature, and flow rates of both the liquid and vapor

were assumed to be constant throughout the column.

Having defined the absorption process as a vapor pressure phenomenon, Kremser assumed Raoult's law was valid and using partial pressures defined an absorption factor for each component as

$$A = \frac{G q}{100} \quad (4)$$

This absorption factor, defined in terms of the molal oil-to-gas ratio G and the equilibrium q in terms of partial pressures, completely described the absorption process on an equilibrium tray.

A component material balance made over a theoretical tray as shown in Figure 4 can be expressed in terms of the liquid content X and the vapor content Y as

$$L(X_i - X_{i-1}) = V(Y_{i+1} - Y_i) \quad (5)$$

This equation may be rearranged using the equilibrium relation $X_i = q Y_i$ to give

$$Y_i = \frac{Y_{i+1} + AY_{i-1}}{1 + A} \quad (6)$$

For an absorber having n trays, equation (5) may be applied to each tray to obtain the general expression for the vapor content on the last or n^{th} tray. This equation is

$$Y_n = \frac{Y_{n+1}(A^n - 1) + A^n(A - 1)Y_o}{A^{n+1} - 1} \quad (7)$$

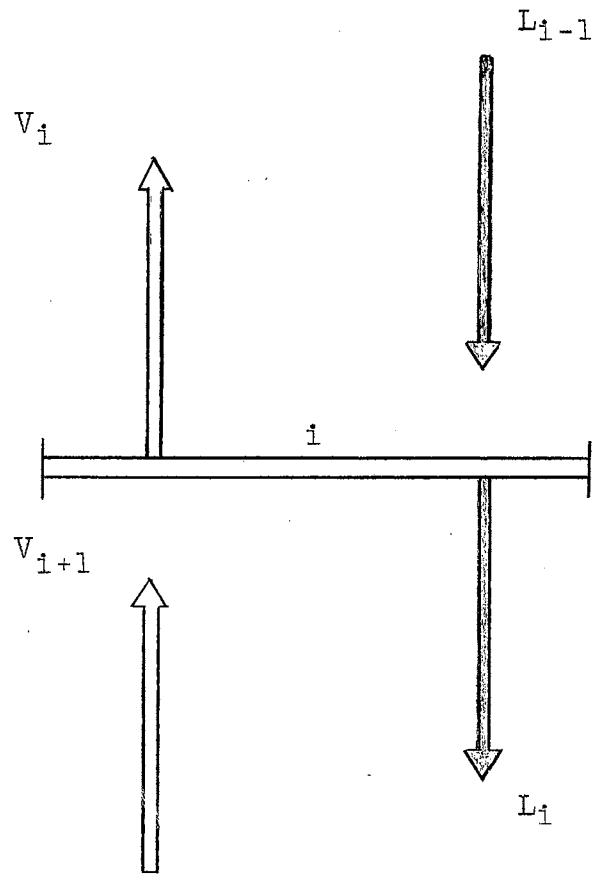


Figure 4. "Simple" Theoretical Tray

From this relationship the rich oil content X_n can be calculated using the equilibrium relation $X_n = q Y_n$. The lean gas leaving the column can be found by combining the equilibrium relation with the over-all material balance to get

$$A(Y_n - Y_o) = Y_{n+1} - Y_1 . \quad (8)$$

Then substituting in for Y_n in equation (8) gives the general expression for the lean gas content.

$$Y_1 = \frac{(A - 1)Y_{n+1}}{A^{n+1} - 1} + \frac{A(A^n - 1)Y_o}{A^{n+1} - 1} \quad (9)$$

Thus, the Kremser equations express the product stream content in terms of the entering streams and column conditions.

The basic absorption factor approach to absorption calculations developed by Kremser was modified by Brown (1) to eliminate the dependence of the absorption factor on the validity of Raoult's law. By assuming ideal solutions and using an equilibrium constant expressed in the form $K = y/x$, Brown redefined the Kremser absorption factor as

$$A = \frac{L}{KV} . \quad (10)$$

Unlike the absorption factor defined by Kremser, this factor is free from any errors introduced by assuming

Raoult's law is valid. Brown also assumed that the pressure, temperature, and liquid and vapor rates remained constant throughout the column. Using these assumptions and the same approach used by Kremser, the equations developed by Brown are completely analogous to those developed by Kremser. The only difference between the two sets of equations is the new definition of the absorption factor.

The assumption of constant liquid and vapor flow rates throughout the column, as made in the Kremser-Brown method, can cause appreciable errors. Horton and Franklin (8) suggested a method in which the limiting assumption of constant column liquid and vapor rates was not made. Individual tray absorption factors were defined for each component on the i^{th} tray as

$$A_i = \frac{L_i}{K_i V_i} \quad (11)$$

By using tray absorption factors and the general approach used by Kremser, a general equation for an absorber with n theoretical trays was developed. This general equation may be expressed as

$$Y_n = (A_1 A_2 \cdots A_{n-1} + A_2 A_3 \cdots A_{n-1} + \cdots + A_{n-1}^{+1}) Y_{n+1} \quad (12)$$

$$+ \frac{L_o X_o}{V_{n+1}} (A_1 A_2 A_3 \cdots A_{n-1})$$

or may be rearranged in the more familiar form

$$\frac{Y_{n+1} - Y_1}{Y_{n+1}} = \frac{(A_1 A_2 \dots A_n + A_2 A_3 \dots A_n + \dots + A_n)}{(A_1 A_2 \dots A_n + A_2 A_3 \dots A_n + \dots + A_{n+1})} \quad (13)$$

$$- \frac{L X_o}{V_{n+1} Y_{n+1}} \frac{(A_2 A_3 \dots A_n + A_3 A_4 \dots A_n + \dots + A_{n+1})}{(A_1 A_2 \dots A_n + A_2 A_3 \dots A_n + \dots + A_{n+1})}$$

The term $\frac{Y_{n+1} - Y_1}{Y_{n+1}}$ defines the absorption efficiency of

the column.

Horton and Franklin noted that if the series of absorption factors was expressed by an average or effective absorption factor A_e in the form

$$\frac{A_e^{n+1} - A_e}{A_e^{n+1} - 1},$$

then their equations would reduce to the Kremser-Brown equation form. If the proper value of the effective absorption factor could be found, then the solution using A_e would correspond to the solution obtained using the individual tray absorption factors. Horton and Franklin suggested the use of the effective factor as a short-cut procedure. They suggested that the effective factor be selected at a position in the column which was dependent on the molecular weight of the component. For very light components the effective factor position would be near the top of the column while for very heavy components the position would be

near the bottom of the column. A table was provided by Horton and Franklin as a guide in selecting empirical effective factors.

The calculation requires the absorption and temperature distributions to be determined for each tray. Horton and Franklin assumed that the percentage absorption on each tray was constant and the temperature was proportional to the "contraction" or reduction in the vapor rate on each tray. These approximations can be expressed mathematically as

$$\frac{(V_1)^{1/n}}{(V_{n+1})} = \frac{V_m}{V_{m+1}} \quad (14)$$

and

$$\frac{V_{n+1} - V_{m+1}}{V_{n+1} - V_1} = \frac{T_n - T_m}{T_n - T_o} \quad (15)$$

The results of this short-cut method may be used as an approximate answer or be refined using the more accurate but time consuming individual tray factor equations.

Edmister (2) found that in many cases that the effective factors were essentially independent of the number of trays and primarily functions of the terminal conditions. By solving for the effective absorption factor A_e in a two tray absorber, the expression

$$A_e = \sqrt{A_n(A_1 + 1) + 0.25} - 0.50 \quad (16)$$

can be used to define A_e in terms of the terminal

tray absorption factors.

Following the development of the Kremser-Brown, Horton-Franklin, and Edmister calculation methods, several short-cut methods were developed.

A different approach to absorption calculations was made in a graphical method first suggested by Lewis (12) and which is commonly referred to as the Sherwood graphical method. (15) This short-cut method is similar to the McCabe-Thiele graphical method since both methods incorporate the equilibrium line, operating line, and tie line concepts. The equilibrium line represents the phase equilibrium on a tray and is defined by the equilibrium equation

$$K = \frac{Y(1 + \sum X)}{X(\sum Y)} \quad (17)$$

The operating line represents the relationship between the passing streams, the vapor leaving and the liquid entering a tray. If it is assumed that the L/V ratio remains constant throughout the column, then the operating line can be defined by a slope (the ratio of lean oil to wet gas) and a point (the wet gas composition). The procedure consists of estimating the component absorption and then checking that assumption

with the graphical results. A successive approximation technique in which the fractional absorption of each component is adjusted is used to determine the final solution.

A short-cut method has been proposed by Landes and Bell. (11) The Kremser-Brown method provides the initial estimates for the lean oil and lean gas rates. Plate-to-plate calculations are carried out over the top two plates. The temperature, L/V ratio, and the absorption factors for these two top trays and the bottom tray are plotted against the tray number. An average absorption factor for the key component is obtained graphically and compared with the specified absorption factor. If the calculated average absorption factor differs greatly from the required absorption factor, then the lean oil and lean gas rates are revised and the calculation is repeated.

Hull and Raymond (9) developed a semi-empirical calculation method for calculating the component yields and temperature conditions of ordinary, nonintercooled, nonreboiled light-hydrocarbon absorbers. The material balance used in the calculations was derived by Horton and Franklin.

This material balance equation can be expressed as

$$\frac{Y_{n+1}V_{n+1} - Y_1V_1}{Y_{n+1}V_{n+1} - L_oX_o/A_c} = \frac{A_e^{n+1} - A_e}{A_e^{n+1} - 1} \quad (18)$$

The lean gas temperature is found by a trial and error procedure in which the difference in the lean gas and lean oil temperatures is correlated with the top-section heat of absorption. A semi-empirical heat balance equation of the form

$$W_oC_p(T_n - T_o) + W_lC_p(T_l - T_{n+1}) + W_sC_p(T_n - T_{n+1}) = H_s - 0.024UA'(T_{av} - T_{amb}) \quad (19)$$

is used to calculate the rich oil temperature. The average tray temperature used in the heat balance is correlated with the weight ratio of lean oil to wet gas feed and the product stream temperatures. The effective absorption factors A_e can be determined by the same methods used by Horton and Franklin or by Edmister. Hull and Raymond developed a correlation between the A_e and the fractional distance between the bottom-section and average column conditions as an alternate procedure.

The various short-cut procedures previously discussed have been gradually replaced by more rigorous but also more time consuming calculation methods. Lewis and Matheson (13) developed a more rigorous multi-component distillation calculation. In general this method may be

applied to absorber calculations as well. The procedure consists of assuming a product distribution and then calculating the temperature and flow rates for each tray. The top-down method assumes the lean gas composition and uses a dew point calculation to determine the temperature of the top tray. The total liquid rate leaving the tray is estimated and the component liquid rates are determined by the equilibrium relationship $l_i = L_i/K_iV_i$ $v_i = A_i v_i$. The component vapor rates from the tray below are determined by a material balance over the top of the column. The general expression for this material balance is

$$v_{i+1} = l_i + v_1 - l_0 \quad (20)$$

The tray temperatures are determined by bubble or dew point calculations. These calculations can become extremely unstable in absorption systems. In a slight modification of the original method, the total liquid rate assumption is checked with a heat balance around the top of the column. The procedure is then repeated on the next lower tray. The initial lean gas composition assumption is checked by comparing the calculated wet gas with the given wet gas. A similar bottom-up method may also be used.

Thiele and Geddes (17) also developed a multi-component distillation calculation method. In this method the product distribution need not be assumed. The products are calculated using l_i/d ratios in the basic equation

$$\frac{l_{i+1}}{d} = A_{i+1} \left[\frac{l_i}{d} + 1 \right] \quad (21)$$

The calculation is based on the l_0/d ratio which is defined as the reflux ratio in the distillation column. In absorption calculations only the l/v ratios are available so that the basic Thiele-Geddes method must be modified.

An absorption calculation based on a modified Thiele-Geddes method was developed for the digital computer by Holland. (7) A material balance around the top of the column down to tray $j-1$ results in

$$v_1 + l_{i-1} = l_0 + v_i \quad (22)$$

Using the equilibrium relation $l_i = A_i v_i$, the material balance equation may be rearranged to give

$$\frac{v_i}{v_1} = A_{i-1} \frac{v_{i-1}}{v_1} + \left(1 - \frac{l_0}{v_1} \right) \quad (23)$$

The equation for an n tray column is obtained by substituting v_i/v_1 into the expression for v_{i+1}/v_1 .

This general equation in terms of the terminal streams

is

$$\frac{v_{n+1}}{v_1} = \omega + \Omega (1 - l_o/v_1) \quad (24)$$

where

$$\omega = A_n A_{n-1} \dots A_3 A_2 A_1$$

and

$$\Omega = 1 + A_n + A_n A_{n-1} + \dots + A_n A_{n-1} \dots A_3 A_2$$

The over-all material balance equation given by

$$v_1 - v_{n+1} = l_o - l_n \quad (25)$$

may be substituted into equation (24) to give

$$\frac{l_n}{v_1} = \frac{l_o + (\Omega + \omega - 1)v_{n+1}}{l_o + v_{n+1}} \quad (26)$$

The component vapor rates for each tray are found by calculating l_n/v_1 from equation (26) and the term $1 - l_o/v_1$ from equation (24) and substituting these values into the material balance equation (23).

The primary assumption of the lean gas rate must be adjusted after each calculation pass. The component vapor rates are adjusted using the relation

$$(v_1)_{co} = \frac{v_{n+1} + l_o}{1 + \theta_o (l_n/v_1)_{cal}} \quad (27)$$

The convergence variable θ_o is defined by

$$(l_n/v_1)_{co} = \theta_o (l_n/v_1)_{cal} \quad (28)$$

The value of θ_o is the positive root of the function

$$g(\theta_o) = \sum (v_1)_{co} - v_1 = 0 \quad (29)$$

Either Newton's method or regula falsi interpolation

is recommended as the procedure for finding the root of

the function.

Edmister (3) also developed a more convenient form for the component distribution equations by introducing the absorption functions. The rich oil equation is given by

$$l_n = v_1 (A_1 A_2 A_3 \dots A_n + A_2 A_3 \dots A_n + \dots + A_n) - l_o (A_2 A_3 \dots A_n + A_3 A_4 \dots A_n + \dots + A_n) \quad (30)$$

and was redefined as

$$l_n = v_1 \Sigma_a - l_o (\Sigma_a - \Pi_a) \quad (31)$$

where

$$\Sigma_a = A_1 A_2 A_3 \dots A_n + A_2 A_3 \dots A_n + \dots + A_n$$

and

$$\Pi_a = A_1 A_2 A_3 \dots A_n$$

Combining the rich oil equation with an over-all material balance results in an equation for the lean gas as given by

$$v_1 = v_{n+1} \left[\frac{1}{1 + \Sigma_a} \right] + l_o \left[1 - \frac{\Pi_a}{1 + \Sigma_a} \right] \quad (32)$$

Two new absorption functions ϕ_a and ϕ_s were defined as

$$\phi_a = \frac{1}{1 + \Sigma_a} \quad (33)$$

and

$$1 - \phi_s = 1 - \frac{\Pi_a}{1 + \Sigma_a} \quad (34)$$

The lean gas equation written in terms of these functions is

$$v_1 = v_{n+1} \phi_a + l_o (1 - \phi_s) \quad (35)$$

The term $v_{n+1}\phi_a$ represents the unabsorbed portion of the wet gas and the term $l_o(1 - \phi_s)$ represents the amount stripped from the lean oil. Thus, ϕ_a is the fraction of the wet gas which is not absorbed and ϕ_s is the fraction which is not stripped from the lean oil. The values of both functions must always be between zero and unity which is a definite advantage in solving for the column products.

This calculation procedure may also use the effective factor concept. The effective absorption factor A_e and the effective stripping factor S_e can be used to define the functions ϕ_a and ϕ_s .

$$\phi_a = \frac{A_e - 1}{A_e^{n+1} - 1} \quad (36)$$

$$\phi_s = \frac{S_e - 1}{S_e^{n+1} - 1} \quad (37)$$

The more rigorous calculation procedure is suitable for computer calculation.

CHAPTER III

THE SUJATA CALCULATION METHOD

A. General Description

The absorber-stripper calculation method described by Sujata (16) is an iterative, tray-by-tray method developed for computer use. The column products for a given absorption system are calculated from the rate, composition, and condition of the column feeds.

The Sujata calculation method may be divided into six major sections. The diagram in Figure 5 shows the relationship between each of these six sections. The method may be briefly described as follows. The initial temperature profile and the total vapor and liquid profiles are assumed. The component flow rates for each tray are calculated using a material balance and the equilibrium relation. A heat balance around each tray is used to determine the validity of the initial temperature assumption. If the heat balance is not satisfied for each tray, then the tray temperatures are adjusted

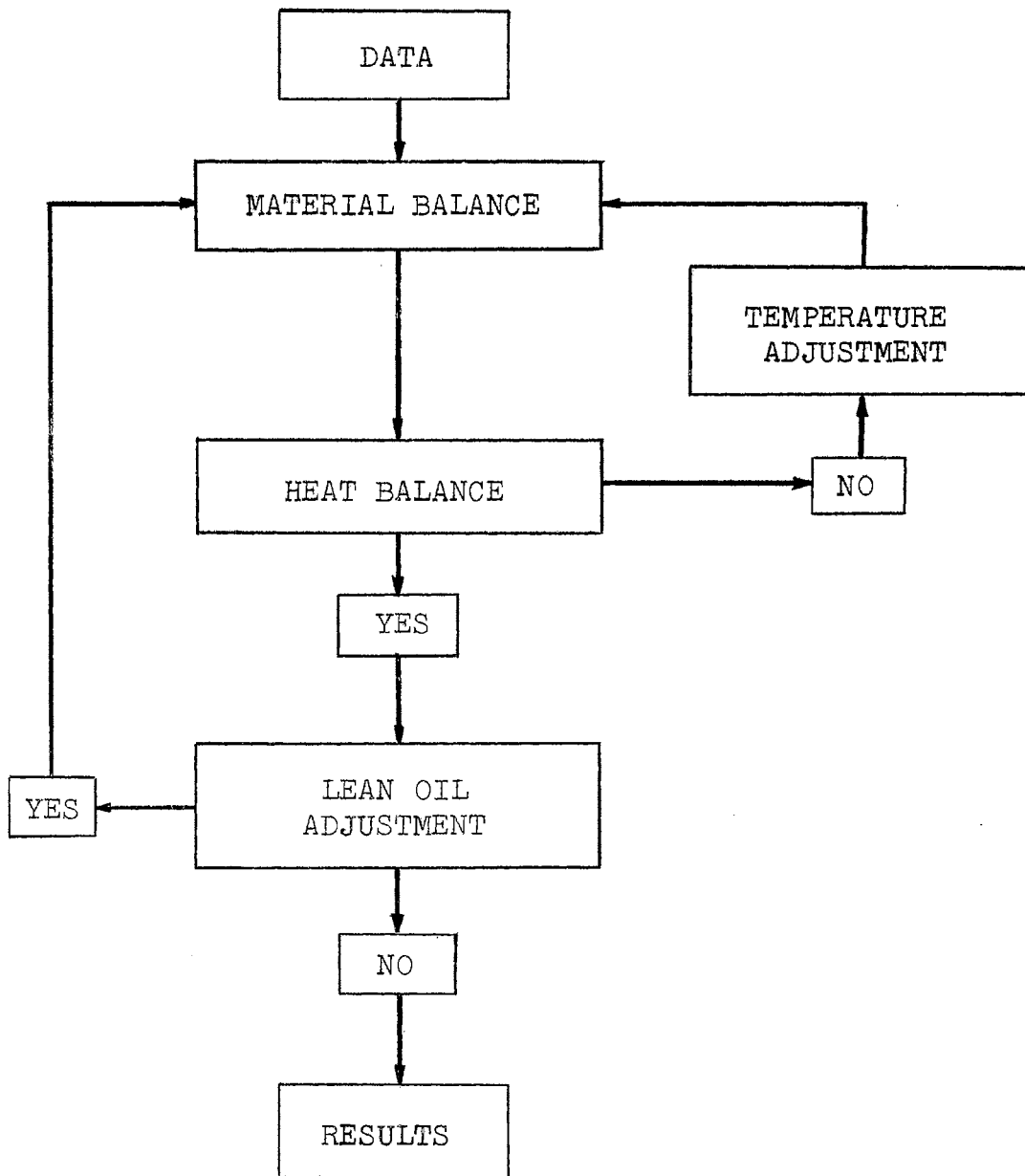


Figure 5. Sujata Absorption Calculation Procedure

and the calculation is repeated. Thus, the tray temperature is the principal iteration variable. When the initial assumptions have been verified, the calculated separation of the key component is compared with the desired separation. If the desired separation has not been obtained, then the lean oil rate is adjusted. The entire calculation is repeated until the desired key component separation has been obtained.

Three basic assumptions are made in nearly every stagewise absorption calculation. 1) Each tray is an equilibrium stage. 2) The vapor-liquid equilibrium is represented by an equilibrium constant in the form $K = y/x$. 3) The column has no unspecified heat losses. One of the advantages of the Sujata method is that these three assumptions are the only primary assumptions made in the calculation. In some cases the assumption of constant column pressure is also made. Most other absorption calculation methods require an excessive number of assumptions such as an average column temperature, vapor rate, liquid rate, or absorption factor.

The Sujata calculation method can be used for both absorption and stripping columns. The calculations are identical with the exception that the stripping vapor rate

is adjusted in the stripping column.

The calculation is divided into six major sections as shown in Figure 5. The procedure is described in detail in the following sections.

B. Material Balance Section

The general n tray complex absorption column for which the calculation method is designed has three distinct types of trays: the bottom or 1st tray, the internal or i^{th} trays, and the top or n^{th} tray. These three types of trays are shown in Figure 6. The i^{th} tray has an entering vapor and liquid stream, an exit vapor and liquid stream, and the possibility of a feed stream, vapor side stream, and liquid side stream. (The original Sujata method did not include the possibility of side streams in the column.) A material balance around each of these three types of trays for a single component results in the following equations:

$$f_1 + (1 - \alpha_2)l_2 = l_1 + v_1 \quad (38)$$

$$f_i + (1 - \beta_{i-1})v_{i-1} + (1 - \alpha_{i+1})l_{i+1} = l_i + v_i \quad (39)$$

$$f_n + (1 - \beta_{n-1})v_{n-1} = l_n + v_n \quad (40)$$

The equilibrium relation between the component liquid and vapor streams leaving the tray is given by

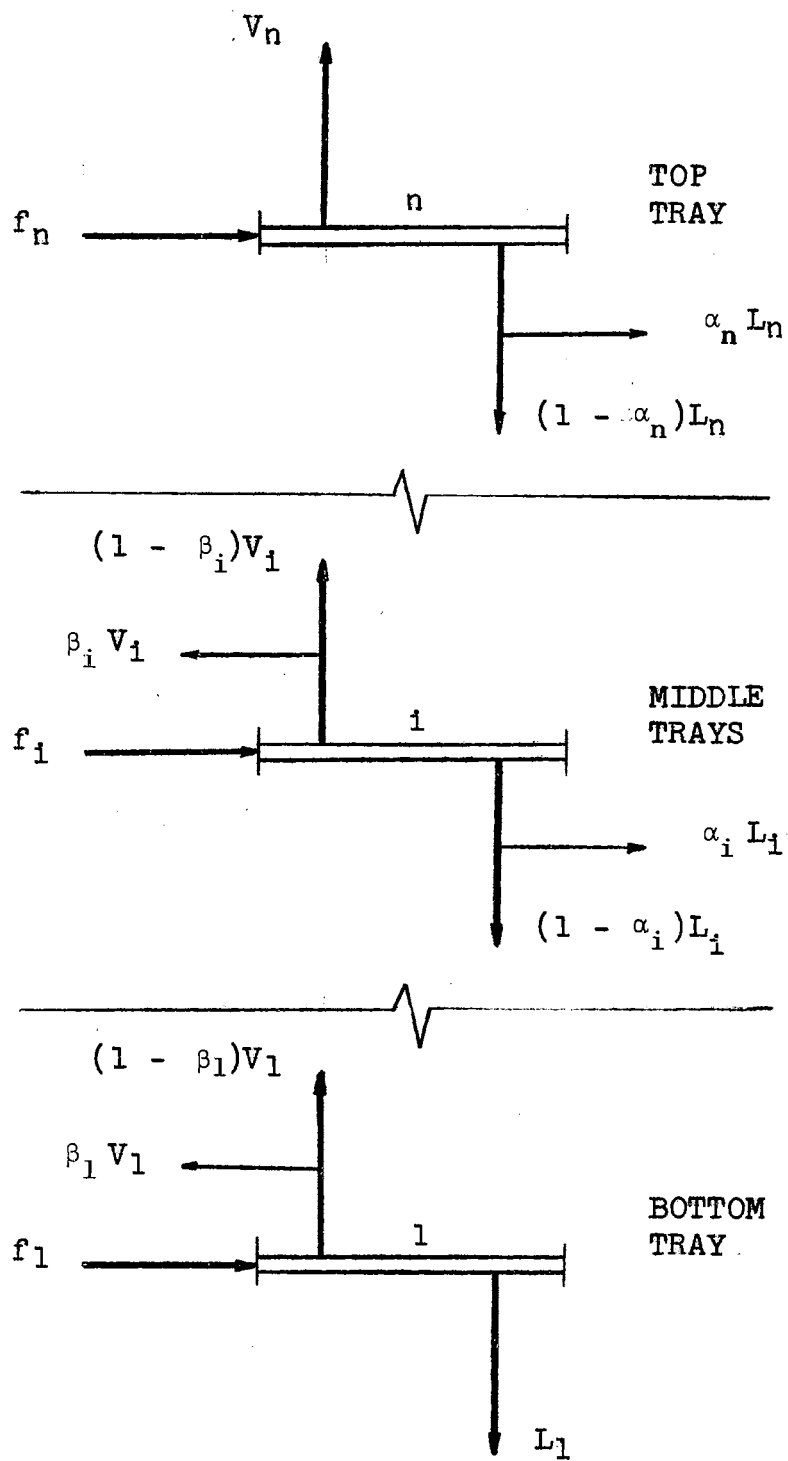


Figure 6. Three Types of Complex Column Trays

$$v_i = \frac{K_i V_i}{L_i} l_i = S_i l_i \quad (41)$$

It is obvious that the stripping factor in the equilibrium relation depends on the initial vapor rate V_i , liquid rate L_i , and the temperature assumptions.

Substituting the equilibrium relation into the three tray material balance equations results in a set of n equations in terms of the liquid component streams l_i . These equations are

$$(1 + S_1)l_1 - (1 - \alpha_2)l_2 = f_1 \quad (42)$$

$$(1 + S_i)l_i - (1 - \alpha_{i+1})l_{i+1} - (1 - \beta_{i-1})S_{i-1}l_{i-1} = f_i \quad (43)$$

$$(1 + S_n)l_n - (1 - \beta_{n-1})S_{n-1}l_{n-1} = f_n \quad (44)$$

This set of n simultaneous equations is written for each component. For any component the set of n equations may be rearranged into the matrix form shown in Figure 7. Matrices of this form are known as tridiagonal matrices.

The set of equations can be solved using a variety of matrix methods. The method selected for solving the matrices in the calculations associated with this thesis is based on a convenient method developed for the tridiagonal matrix. (6) The first step is to define two new quantities. For the first tray in the column

$$F'_1 = \frac{-(1 - \alpha_1)}{(1 + S_1)} \quad (45)$$

$$\begin{bmatrix}
 (1+S_1) & - (1-\alpha_2) & 0 & 0 \\
 - (1-\beta_1)S_1 & (1+S_2) & - (1-\alpha_3) & 0 \\
 0 & - (1-\beta_2)S_2 & (1+S_3) & - (1-\alpha_4) \\
 0 & 0 & - (1-\beta_3)S_3 & (1+S_4)
 \end{bmatrix}
 \begin{bmatrix}
 l_1 \\
 l_2 \\
 l_3 \\
 l_4
 \end{bmatrix}
 =
 \begin{bmatrix}
 f_1 \\
 f_2 \\
 f_3 \\
 f_4
 \end{bmatrix}$$

Figure 7. Tri-diagonal Matrix for a Four Tray Absorption Column

$$G'_1 = \frac{f_1}{(1 + S_1)} \quad (46)$$

and for all remaining trays

$$F'_i = \frac{-(1 - \alpha_i)}{(1 + S_i) + (1 - \beta_{i-1})S_{i-1}F'_{i-1}} \quad (47)$$

$$G'_i = \frac{f_i + (1 - \beta_{i-1})S_{i-1}G'_{i-1}}{(1 + S_i) + (1 - \beta_{i-1})S_{i-1}F'_{i-1}} \quad (48)$$

The unknown component liquid streams leaving the i^{th} tray may be expressed in terms of F_i and G_i by the equations

$$l_n = G'_n \quad (49)$$

$$l_i = G'_i - F'_i l_{i+1} \quad (50)$$

This form of solution is particularly well suited for computer calculations.

When the matrix has been solved for each of the components, the component liquid rates leaving each tray are known. The initial assumptions of the total liquid and vapor rates leaving each tray must be checked. If the sum of the calculated component rates leaving the tray does not equal the assumed rate, then the initial rate assumption must be corrected and the material balance calculation repeated. The initial rate assumption for the next trial is the sum of the calculated component rates calculated in the previous trial. This may be expressed as

$$L_i^{(m+1)} = \sum_j l_i^{(m)}. \quad (51)$$

When the component rates for each tray equal the initial assumption, then the calculation proceeds to the heat balance section.

C. Heat Balance Section

The heat balance section of the calculation is designed to check the initial temperature profile assumption used in the equilibrium relation of the material balance section. This is done by calculating the deviation or residue in the heat balance around each tray. The deviation in the heat balance is defined as the difference between the enthalpy of the exit and entering streams for a given tray. When the deviation G_i is approximately equal to zero for all trays, the initial temperature assumptions are correct. The heat balance deviation for each of the three types of trays is calculated from the following equations:

$$G_1 = Q_1 - f_1 \bar{h}_1 + l_1 (H_1 S_1 + h_1) - (1 - \alpha_2) l_2 h_2 \quad (52)$$

$$G_i = Q_i - f_i \bar{h}_i + l_i (H_i S_i + h_i) - (1 - \alpha_{i+1}) l_{i+1} h_{i+1} \\ - (1 - \beta_{i-1}) H_{i-1} S_{i-1} l_{i-1} \quad (53)$$

$$G_n = Q_n - f_n \bar{h}_n + l_n (H_n S_n + h_n) - (1 - \beta_{n-1}) H_{n-1} S_{n-1} l_{n-1} \quad (54)$$

If the deviation for each tray is not approximately equal to zero, all tray temperatures are adjusted by a procedure outlined in the next section. If all the deviations are approximately equal to zero, then the temperature assumptions are correct and the lean oil rate is adjusted if necessary.

D. Temperature Adjusting Section

The temperature adjusting section of the calculation uses a basic Newton's method to predict the next temperature profile for the material balance calculations.

If the temperature assumptions are reasonable, then the deviation in the heat balance will be small compared to the total enthalpy of the streams entering or leaving the tray. Therefore, the deviation in the heat balance may be considered as a total differential quantity.

That is, $dG_i \approx G_i$. Since each deviation is a function of the temperature on the tray above, the tray below, and the tray itself, the total differential may be expressed for each of the three types of trays as

$$dG_1 = \frac{\partial G_1}{\partial t_2} dt_2 + \frac{\partial G_1}{\partial t_1} dt_1 \quad (55)$$

$$dG_i = \frac{\partial G_i}{\partial t_{i-1}} dt_{i-1} + \frac{\partial G_i}{\partial t_i} dt_i + \frac{\partial G_i}{\partial t_{i+1}} dt_{i+1} \quad (56)$$

$$dG_n = \frac{\partial G_n}{\partial t_{n-1}} dt_{n-1} + \frac{\partial G_n}{\partial t_n} dt_n . \quad (57)$$

A set of n simultaneous equations is formed in which the differential temperature changes dt_i are the unknowns. If it is assumed that the material balances are not changed by the differential change in tray temperature, then dt_i represents the temperature change required to make the heat balance deviation dG_i equal to zero. In reality the differential temperature change results in small changes in the material balances. Thus, dt_i represents a temperature change which will make the heat balance deviation dG_i approach zero in successive approximations.

The set of equations developed from equations (55), (56), and (57) form a tridiagonal matrix. The solution to this system of equations may be obtained using the method developed for the tridiagonal matrix in the material balance section.

The coefficients of the temperature adjusting equations are obtained by differentiating the heat balance equations with respect to the indicated tray temperature. Thus,

$$\frac{\partial G_i}{\partial t_{i+1}} = - \sum_j \left[\frac{\partial h_{i+1}}{\partial t_{i+1}} l_{i+1} \right] \quad (58)$$

$$\frac{\partial G_i}{\partial t_{i+1}} = - \sum_j \left[\frac{\partial H_{i+1}}{\partial t_{i+1}} v_{i-1} \right] \quad (59)$$

$$\frac{\partial G_i}{\partial t_i} = \sum_j \left[\frac{\partial h_i}{\partial t_i} l_i + \frac{\partial H_i}{\partial t_i} v_i \right] \quad (60)$$

The tray temperature for the next iteration in the material balance calculations is given by

$$t_i^{(m+1)} = t_i^{(m)} + dt_i^{(m)} \quad (61)$$

When the correct tray temperatures have been calculated, the separation obtained is compared with the desired separation of the key component.

E. Lean Oil Adjusting Section

The lean oil adjusting section determines the key component separation and, if necessary, adjusts the lean oil rate to give the desired separation. The separation is measured by the fractional absorption of the key component which is given by

$$EA = \frac{l_1}{\sum f_i} \quad (62)$$

If the desired fractional absorption is not obtained, the lean oil rate is adjusted.

The fractional absorption EA also may be expressed in terms of an effective Kremser absorption factor A.

$$EA = \frac{A^{n+1} - A}{A^{n+1} - 1} \quad (63)$$

Rearranging equation (63) to express A in terms of EA results in

$$A^{n+1} - \frac{A}{1 - EA} + \frac{EA}{1 - EA} = 0 \quad (64)$$

An effective absorption factor A^* based on the desired separation ED is evaluated from

$$(A^*)^{n+1} - \frac{A^*}{1 - ED} + \frac{ED}{1 - ED} = 0 \quad (65)$$

The new lean oil rate is defined in terms of A and A^* .

The equation is

$$L_{n+1}^{(m+1)} = L_{n+1}^{(m)} + \left(\frac{A^*}{A} - 1 \right) \sum_j 1_1 \quad (66)$$

where m is the iteration number. The modified Sujata calculation method associated with this thesis does not use the original Sujata lean oil adjusting technique of equation (66). The new lean oil rate is given by

$$L_{n+1}^{(m+1)} = L_{n+1}^{(m)} \left(\frac{ED}{EA} \right)^{1.2} \quad (67)$$

This lean oil adjusting equation is an empirical relation suggested by previous absorption calculation work. (4)

When the lean oil rate has been adjusted, the entire calculation is repeated until the desired fractional absorption has been obtained.

For a stripping column the stripping vapor rate must be adjusted rather than the lean oil rate as in the

absorption column. The procedure is entirely analogous to the lean oil adjusting technique. A fractional stripping factor for the key component is defined as

$$ES = \frac{V_n}{\sum_i f_i} \quad (68)$$

The modified Sujata method uses the empirical relation

$$V_o^{(m+1)} = V_o^{(m)} \left(\frac{ED}{ES} \right)^{1.2} \quad (69)$$

where ED is the desired stripping vapor rate. The stripping vapor rate is adjusted until the desired fractional stripping has been obtained.

CHAPTER IV

EVALUATION PROCEDURE

A. Evaluation Objectives

The primary objective of this thesis is the evaluation of the Sujata calculation method. This evaluation is specifically concerned with the comparison of the Sujata method's results with both actual absorber performance and predictions made by two classical absorption methods. The investigation is an attempt to find answers to three principal questions: 1) How well does each absorption calculation method predict actual column performance? 2) What errors exist in these predictions and what are their relative magnitudes? 3) Why do these errors exist?

B. Calculation Methods

The investigation uses three absorption calculations: the Sujata method, the Kremser-Brown method, and the Edmister method. The Sujata calculation method has already

been described in detail. The two remaining classical calculation methods are described briefly below.

The Kremser-Brown method was the pioneering absorption calculation method. Three primary assumptions are made: 1) The pressure, temperature, liquid rates, and vapor rates are constant throughout the column. 2) The liquid-vapor equilibrium is described by $K = y/x$. 3) The column consists of ideal trays. A series of material balances written around each tray is used to obtain expressions for the product compositions in terms of the feed streams and the column absorption factor A . The column absorption factor is determined by the specified absorption ED of a component by solving

$$ED = \frac{A^{n+1} - A}{A^{n+1} - 1} \quad (70)$$

The lean gas composition is given by the equation

$$y_1 = \frac{A - 1}{A^{n+1} - 1} y_{n+1} + \frac{A(A^n - 1)}{A^{n+1} - 1} y_o \quad (71)$$

and the rich oil composition is given by $x_n = y_n/K_{av}$

where y_n is given by

$$y_n = \frac{A^n - 1}{A^{n+1} - 1} y_{n+1} + \frac{A^n(A - 1)}{A^{n+1} - 1} y_o \quad (72)$$

The average K value K_{av} for the column is based on the average column temperature T_{av} . The average column temperature is defined as

$$T_{av} = 1/4(T_{ro} + T_{lg} + T_{wg} + T_{lo}). \quad (73)$$

In the Kremser-Brown method both the feed and product stream temperatures must be specified. There is no heat balance involved in the calculations.

The lean oil rate is calculated in the following manner. The average L/V for the column is defined by

$$\left(\frac{L}{V}\right)_{av} = K_{av} A \quad (74)$$

so that the lean oil rate can be predicted by

$$L_o = \left(\frac{L}{V}\right)_{av} V_{n+1} \quad (75)$$

The Edmister method was developed after the introduction of the concept of an "effective" absorption factor A_e . If the correct effective absorption factor can be found, the solution of the Kremser-Brown equations using A_e instead of an average column absorption factor will correspond to the solution obtained by considering individual tray absorption factors. Three primary assumptions are associated with this method: 1) The liquid-vapor equilibrium is described by $K = y/x$. 2) The column consists of ideal trays. 3) The effective absorption factors are functions of the terminal trays only. The expression for the effective factor A_e obtained by considering a two tray column is

$$A_e = \sqrt{A_n(A_1 + 1) + 0.25} - 0.50 \quad (75)$$

The feed streams and lean gas temperatures are specified. An over-all heat balance is used to determine the rich oil temperature. The lean oil rate is found by a trial and error procedure in which the calculated key component absorption is compared with the desired absorption.

C. Column Test Data

The test data used in the evaluation of the Sujata calculation method was divided into two sets. The first set consisted of a sample calculation on a test absorber which was presented by Sujata in the article describing the calculation method. The second set of test data consisted of column test data taken from the field analysis of three operating industrial absorbers. The information for all three of these absorbers was obtained from data used in a study of non-theoretical tray absorbers made by Ravicz. (14)

A brief description of each of the test columns appears below. The feed compositions and rates for each column appear in the tables of Appendix A.

Set I: Sujata Sample Calculation

Sujata supplied the set of test data for this 8-tray,

8-component complex absorption column operating at 310 psia. The complex features of the column include an intercooler on tray 2 and an additional feed stream entering tray 5.

Set II: Field Data

Column A

The Phillips Petroleum Company is the source for the test data for this 20-tray, 9-component bubble cap absorption column operating at 232 psia. The available column details indicate that the column diameter was 6.0 ft., plate spacing 27 in., length of the liquid path 3.39 ft., and a fractional cross-section for vapor flow of 0.768. The absorber oil was described as a mineral seal oil fraction having a molecular weight of 223.

Column B

The "X" Petroleum Company (name withheld by request) is the source for the test data for this 27-tray, 15-component Koch Kaskade-type absorption column operating at a pressure of 740 psia. The available column details indicate that the column diameter was 4.5 ft., plate spacing 26 in., and a fractional cross-section for vapor flow of 0.390. The absorber oil consisted of two components. The first component is a light oil having an

average molecular weight of 165. The second component is the absorption oil fraction having a molecular weight of 210.

Column C

This column was designated as Unit 3 of the N.G.A.A. Low Pressure Data and is a 24-tray, 8-component absorption column operating at a pressure of 400 psia. The available column details indicate that the column diameter was 5.0 ft., plate spacing 24 in., liquid path 2.917 ft., weir height 1-7/8 in., and a fractional cross-section for vapor flow of 0.687. The absorber oil was described as an oil having a molecular weight of 207.

D. Evaluation Procedure

The first step in the evaluation of the Sujata method was to test the computer program developed using the Sujata calculation method. This test was made by comparing the results given by the computer program with those given in Sujata's sample calculation. All of the necessary input data was given in the sample calculation except for the source of the equilibrium and enthalpy data. For the evaluation in this thesis, all equilibrium and enthalpy data are obtained from the N.G.S.M.A. Data

Book (18) since it is probably the most readily available source for such information.

The input data needed for the sample calculation appears in Table III of Appendix A. The results for both the Sujata sample calculation and the computer program are listed in Tables IV-V of Appendix A.

The results of the comparison show that the sample calculation and the computer program give virtually the same product predictions. The deviations between the two product streams were very small even for the light components. It was concluded that these deviations were a result of differences in the equilibrium data used in the two calculations. The product stream temperatures and the temperature profile of the column were generally low but followed the same general pattern. The most significant temperature deviation was 10° F which occurred in the rich oil stream. These temperature deviations seem to be a result of significant differences in the enthalpy data used in the two calculations. The small product stream and temperature deviations indicated that the computer program was working properly.

In order to determine how well the Sujata method will predict actual column performance, the program was

run using the column test data supplied by columns A, B, and C. There are two methods for analyzing the performance of a given absorption column. The first method fixes the lean oil rate in the calculation. The second method fixes the absorption of a key component. Both methods were used in this evaluation. When the key component absorption was specified, calculations were made for two, three, five, and ten theoretical trays. In all data cases propane was selected as the key component and equilibrium and enthalpy data used were obtained from the N.G.S.M.A. Data Book.

CHAPTER V

RESULTS

A. Tabulated Results

The Kremser-Brown, Edmister, and Sujata calculation methods were run on each of the absorption systems defined by columns A, B, and C. Two sets of calculations were performed on Column B for which information was also available for a well-stripped lean oil. This second data case for Column B is designated B2 while the first case is B1.

The calculated results for the Kremser-Brown and Edmister methods were obtained from a computer program developed by Erbar. (4) The Sujata calculation results were obtained from a computer program written for this thesis. (See Appendix B for a detailed discussion of the computer program.) The results of all three absorption calculations for each of the three absorption systems appear in Tables VI-XXIX of Appendix A. The first table in each set of tables for columns A, B, and C defines the

absorption system for the column under consideration.

B. Analysis of Results

It is obvious that for a valid evaluation of any calculation method which predicts column performance, the field analysis of the operating column must be accurate. The measurement of feed and product stream temperatures is not difficult and presumably the temperatures given in the field analysis will be reasonably correct. However, the accuracy of the analysis of the component rates in the feed and product streams in an operating absorber is certainly subject to question. If a material balance around the column exists for each component, then the component rates are likely to be reasonably correct. Several components in columns B1 and B2 are not in over-all material balance. Therefore, the predictions made by the calculation methods may not be valid and are not included in the following analysis of results.

The evaluation of the calculation methods is based on how well the method predicts the component product rates, the lean oil rate required for a specified key component absorption, and the product stream temperatures.

The predictions of these variables made by the Kremser-Brown, Edmister, and Sujata methods are listed in Table I. The comments on each method are a summary of the general trend observed in the results of columns A and C as compared with the field analysis of the column.

TABLE I
SUMMARY OF RESULTS

Kremser-Brown Calculation Method	
Predicted Variable	Observations
Lean Gas Product Rates	Within field analysis accuracy
Lean Oil Rate	High by 6 to 13%
Rich Oil Temperature	Specified, not calculated
Lean Gas Temperature	Specified, not calculated
Edmister Calculation Method	
Predicted Variable	Observations
Lean Gas Product Rates	Within field analysis accuracy
Lean Oil Rate	Varied from 5% low to 11% high
Rich Oil Temperature	High by 4 to 28° F
Lean Gas Temperature	Specified, not calculated

I (Continued)

Sujata Calculation Method	
Predicted Variable	Observations
Lean Gas Product Rates	Within field analysis accuracy
Lean Oil Rate	Low by 12 to 15%
Rich Oil Temperature	Varied from 3° low to 4° high
Lean Gas Temperature	High by 6° to 10° F

If the lean oil rate is fixed at the value given by the field analysis, the Sujata calculation method gives the following results.

TABLE II

RESULTS OF SUJATA CALCULATION METHOD
FOR A FIXED LEAN OIL RATE

Sujata Calculation Method	
Predicted Variable	Observations
Lean Gas Product Rates	Slightly low
Lean Oil Rate	Specified, not calculated
Rich Oil Temperature	Low by 0.3° to 2° F
Lean Gas Temperature	High by 6° to 12° F

C. Discussion of Results

The general trends observed in the comparison of the calculation methods and the probable reasons for their existence are discussed for each of the three calculation methods in the following sections.

KREMSER-BROWN METHOD

Although the Kremser-Brown method is the least rigorous of the three calculation methods, the results (Tables VI-XXIX in Appendix A) indicate that this method is capable of predicting column products quite accurately. However, there are two factors which should be considered before the conclusion is made that the Kremser-Brown method is universally accurate. First, both the feed and product stream temperatures, which must be specified, were given the field analysis values which are the best possible estimates. In general the product stream temperatures must be estimated. An error in the temperature estimates may cause a significant error in the predicted column products. The second influencing factor is the fact that both columns A and C have relatively constant temperature, liquid, and vapor profiles. Since the primary assumption of the Kremser-Brown method is

constant temperature, liquid, and vapor profiles, the predicted products are expected to be accurate.

The lean oil rate predicted by the Kremser-Brown method was generally 6 to 13% greater than the lean oil rate given by the field analysis. This overestimate is to be expected since the lean oil rate is predicted by

$$L_o = (L/V)_{av} V_{av} \quad (77)$$

where V_{av} is arbitrarily taken as the wet gas rate. Thus, the vapor rate used in calculating the lean oil rate is the greatest vapor rate in the column and will be greater than any average vapor rate. Therefore, the lean oil rate predicted is larger than actually required for the specified absorption.

EDMISTER METHOD

The results (Tables VI-XXIX in Appendix A) indicate that the Edmister method is capable of predicting column products quite accurately. Again there are two factors which greatly influence the apparent accuracy of the method. First, the feed and lean gas product stream temperatures were given the field analysis values which are the best possible estimates. Since the temperatures of both product streams depend on the lean gas temper-

ature estimate, a significant error in the predicted column products may result if this estimate is in error. The second influencing factor is the fact that the temperature, liquid, and vapor profiles are nearly linear for both columns A and C. This means that any effective factor defined by the terminal tray absorption factors will not differ greatly from the individual tray absorption factors. Therefore, the predicted results are expected to be accurate.

The lean oil rate is determined by a trial and error procedure in which the assumed lean oil rate is checked with an over-all heat balance. This heat balance requires the specification of the lean gas temperature. Since the lean oil rate predicted by the Edmister method was both high and low, it appears that the predicted lean oil rate depends largely on the accuracy of the lean gas temperature estimate.

The Edmister method predicted rich oil temperatures which were consistently greater than those measured in the field. The greatest rich oil temperature error (28° F) occurred when the lean oil rate was 11% high. It appears that the error in the rich oil temperature is probably a direct result of the corresponding error in

the predicted lean oil rate. If the lean oil rate is increased with all other column variables remaining constant, the total absorption will also increase. Therefore, the increase in the rich oil temperature is only a reflection of the increased rich oil enthalpy resulting from the increased lean oil rate.

SUJATA METHOD

The results predicted by the Sujata calculation with a fixed key component absorption were excellent. The difference between the predicted and measured product streams was so small that it was considered to be well within the experimental uncertainty of both the field analysis and the physical data used in the calculation. The excellent results were expected since the calculation involves a minimum number of limiting assumptions. The column products predicted by the Sujata method were slightly more accurate than those predicted by either the Kremser-Brown or Edmister methods.

The lean oil rate prediction made by the Sujata method was from 12 to 15% lower than the measured rate. If the results for the fixed key component absorption

are compared with the results for the fixed lean oil rate, it is apparent that a very small change in the absorption can produce a large change in the predicted lean oil rate. Thus, the major portion of the lean oil error is quite possibly a result of both the equilibrium and enthalpy data used in the calculation.

The temperatures predicted for the product streams were very close to those measured in the field. The error in the rich oil temperature ranged from 2.5° low to 4° F high. This range of errors is considerably better than the 4° to 28° error predicted by the Edmister method. The major portion of the error is probably a result of the enthalpy data used in the calculation. The lean gas temperature was from 6° to 11° high. Since the predicted lean oil rate is lower than the measured rate, the increase in lean gas temperature is probably a reflection of the increased lean gas enthalpy caused by the reduction in absorption throughout the column.

Bubble and dew point calculations were made on the product streams predicted by the Sujata method. The maximum difference between the temperatures obtained by bubble or dew point and the Sujata calculations was less than 1° for both columns A and C.

The results of the Sujata calculation using a fixed lean oil rate showed the same general trend as those described for the calculation using a fixed key component absorption. However, the predicted column products were not as accurate as the predictions made by the fixed key component absorption calculation or by the Kremser-Brown and Edmister methods. The predicted temperatures for the column products were approximately the same as for the fixed key component absorption calculation. A comparison of the two types of Sujata calculations indicates that the predicted lean oil is sensitive to the equilibrium and enthalpy data used in the calculation.

CHAPTER VI

CONCLUSIONS

The primary objective in the evaluation of the Kremser-Brown, Edmister, and Sujata calculation methods was to determine how well the calculation methods predicted actual column performance. Two factors are particularly important if the evaluation is to be meaningful and valid. First, the field analysis which provides the column test data must be accurate since all comparisons of the calculated results are made with this data. The second factor is that accurate equilibrium and enthalpy data are needed for the accurate prediction of column products and temperatures. In the evaluation for this thesis, both these factors seem to be reasonably satisfied.

The analysis of results showed that the classical absorption calculation methods developed by Kremser-Brown and Edmister can accurately predict column products. The accuracy of these predictions is subject to two

principal conditions. The column under consideration must reasonably satisfy the simplifying assumptions made in the calculation theory. The estimates of the product temperatures required for the calculation must also be accurate. If both these conditions are satisfied, then the classical methods are capable of predicting accurate column products. Of the two classical methods, the Edmister method gives slightly better results and requires one less temperature specification. From considerations of the underlying theory, the Edmister method is expected to be the more universally accurate method.

The classical calculation methods have three limitations which seriously affect both their application and usefulness. 1) The columns under consideration must satisfy the simplifying assumptions made by the calculation theory. 2) The column must be a "simple" absorption column with no complex features such as additional feed streams, side streams, or intercoolers. (However, in 1957 Edmister (3) modified his calculation method slightly so that complex features may be included.) 3) The results obtained from the calculations may not accurately predict the internal conditions and state of the column.

The Sujata calculation method is not restricted by these three limitations placed on the classical methods. The only restriction made by the Sujata method is the consideration of each tray as a theoretical stage. The calculation can be used for a complex absorption system having a feed stream, liquid side stream, vapor side stream, or intercooler on any or all trays of the column. The calculation can predict all internal liquid and vapor rates and tray temperatures in the column. The analysis of results showed that the Sujata method was the most accurate of the three methods in predicting both the column products and temperatures. The predicted column products were well within the experimental uncertainty of the column test data and the physical data used in the calculation. The predicted temperatures were reasonably correct but probably could have been improved with the introduction of better equilibrium and enthalpy data. Thus, the Sujata method can be applied to almost any complex absorption system and be expected to give accurate results if given accurate equilibrium and enthalpy data.

The exact nature of the limitations of the Sujata method has not been fully investigated. In all the

operating absorption systems used in this evaluation, the Sujata method converged rapidly and gave excellent results. However, the point at which the calculation does not converge has not been established in this study. Friday and Smith (5) examined the nature of convergence of both distillation and absorption calculations. An analysis of the approach used by Sujata showed that this type of calculation should converge rapidly for column feeds having a wide boiling range. As the boiling range of the feed decreases, the convergence difficulty increases. Therefore, although the Sujata calculation method could be applied to distillation problems, it is most likely that convergence difficulties will appear.

LIST OF NOMENCLATURE

- A - absorption factor defined by $A = L/KV$
- A' - top-section heat transfer area
- A_e - effective absorption factor
- C - number of components in the system
- C_p - component heat capacity
- EA - calculated key component absorption
- ED - desired (specified) key component absorption
- ES - calculated key component stripping
- f - component feed rate to a tray
- F' - variable used in solving a tridiagonal matrix
- G - tray heat balance deviation
- G' - variable used in solving a tridiagonal matrix
- h - component liquid state enthalpy
- \bar{h} - component feed state enthalpy
- H - component vapor state enthalpy
- H_s - component heat of absorption
- K - component equilibrium constant defined by $K = y/x$
- l - component liquid rate leaving a tray
- L - total liquid rate leaving a tray
- n - number of trays in the column

- P - column pressure
 Q - intercooler duty
 S - stripping factor defined by $S = KV/L$
 T - temperature
 U - top-section heat transfer coefficient
 v - component vapor rate leaving a tray
 V - total vapor rate leaving a tray
 W - component mass flow rate leaving a tray
 X - component liquid content in a stream
 Y - component vapor content in a stream
 y - component vapor content in a stream

Greek Symbols

- α - fraction removed by the liquid side stream
 β - fraction removed by the vapor side stream
 θ_0 - convergence variable in the Holland method

Subscripts

- amb- ambient condition
 av - average value
 cal- calculated value
 co - corrected value
 i - tray reference
 j - component reference
 m - tray reference
 n - total number of trays (last tray)
 o - reference for stream entering tray 1

 lg - lean gas stream
 lo - lean oil stream
 ro - rich oil stream
 wg - wet gas stream

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APPENDIX A

CALCULATION RESULTS

TABLE III
SUJATA SAMPLE CALCULATION

Absorption System

Trays: 8
Pressure: 310 psia
Type: Complex absorber
Complex Features: Intercooler, side feed

Column Feed Rates			
Component	Wet Gas	Lean Oil	Side Feed
*			
C ₁	357.846	0.0	13.992
C ₂	19.823	0.0	2.706
C ₃	24.725	0.0	3.944
iC ₄	6.321	0.0	1.155
nC ₄	11.653	0.0	5.399
C ₆	9.632	0.0	5.596
OIL	0.0	245.000	134.409
TOTALS	430.000	245.000	165.000
Temperature	88.0° F	77.5° F	80.0° F
Feed Tray	1	8	5

Rich Oil Temperature: 90.2°
Intercooler Duty: 140,000 BTU/hr

*C₁ contains approximately 7% CO₂

TABLE IV
COMPARISON OF PRODUCT STREAMS FOR
SUJATA SAMPLE CALCULATION

Lean Gas Product Rates		
Component	Sujata Results	Program Results
C ₁	320.22	323.168
C ₂	8.54	8.031
C ₃	0.37	0.403
iC ₄	0.0	0.006
nC ₄	0.0	0.005
C ₆	0.0	0.0
OIL	0.03	0.003
TOTALS	329.20	331.616
Temperature	79.4° F	80.5° F

Rich Oil Product Rates		
Component	Sujata Results	Program Results
C ₁	51.62	48.670
C ₂	13.99	14.498
C ₃	28.30	28.265
iC ₄	7.47	7.470
nC ₄	15.05	15.047
C ₆	15.03	15.027
OIL	379.38	379.406
TOTALS	510.80	508.384
Temperature	90.2° F	79.9° F

TABLE V
COMPARISON OF TRAY TEMPERATURES FOR THE
SUJATA SAMPLE CALCULATION

Temperature Profiles ($^{\circ}$ F)								
TRAY	1	2*	3	4	5	6	7	8
Sujata Results	90.2	81.1	82.5	82.0	81.5	81.3	80.3	79.4
Program Results	79.9	77.2	80.3	80.4	80.4	80.6	80.6	80.5

*Tray 2 intercooler removes 140,000 BTU/hr

TABLE VI
COLUMN A ABSORPTION SYSTEM

Column Specifications

Trays: 20
 Pressure: 232 psia
 Type: Bubble cap
 Diameter: 6.0 ft.
 Plate Spacing: 27 in.
 Source: Phillips Petroleum Company

Comp.	Column Feed Rates		Column Product Rates	
	Wet Gas	Lean Oil	Lean Gas	Rich Oil
N ₂	210.4564	0.0	211.048	0.368
C ₁	985.4553	0.0	971.475	12.032
C ₂	88.8290	0.0	81.152	7.251
C ₃	51.2475	0.0	37.767	13.398
iC ₄	6.1475	0.0	2.744	3.389
nC ₄	14.2126	0.0225	2.091	12.137
C ₅	6.4230	0.5130	0.523	6.410
C ₇	3.8265	0.1778	0.0	3.993
OIL	0.0	203.6867	0.0	203.724
TOTALS	1366.6000	204.4000	1306.800	262.700
Temp.	65.0° F	67.0° F	72.0° F	80.0° F

OIL: Molecular weight of 223.

TABLE VII
CALCULATED RESULTS FOR COLUMN A
TWO THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N2	209.686	209.641	209.633
C1	971.751	970.851	970.747
C2	81.436	81.408	81.202
C3	37.854	37.852	37.849
iC4	2.947	2.776	2.999
nC4	5.160	4.467	5.333
C5	0.812	0.437	1.085
C7	0.006	0.003	0.014
OIL	0.0	0.0	0.028
TOTALS	1309.653	1307.431	1308.891
Temperature	72.0° F	72.0° F	78.6° F
Lean Oil Rate	229.477	198.330	191.412
Lean Oil Temperature	67.0° F	67.0° F	67.0° F
Rich Oil Temperature	80.0° F	82.0° F	78.1° F

TABLE VIII
CALCULATED RESULTS FOR COLUMN A
THREE THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	209.720	209.641	209.658
C ₁	972.340	970.851	971.204
C ₂	81.713	81.408	81.426
C ₃	37.849	37.852	37.850
iC ₄	2.710	2.776	2.802
nC ₄	4.285	4.467	4.579
C ₅	0.391	0.437	0.695
C ₇	0.0	0.0	0.008
OIL	0.0	0.0	0.029
TOTALS	1309.008	1307.432	1308.252
Temperature	72.0° F	72.0° F	79.2° F
Lean Oil Temperature	67.0°	67.0° F	67.0° F
Lean Oil Rate	219.568	192.453	184.109
Rich Oil Temperature	80.0° F	83.0° F	78.5° F

TABLE IX
CALCULATED RESULTS FOR COLUMN A
FIVE THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	209.729	209.643	209.665
C ₁	972.510	970.898	971.315
C ₂	81.802	81.464	81.484
C ₃	37.850	37.854	37.851
iC ₄	2.479	2.573	2.636
nC ₄	3.303	3.563	3.808
C ₅	0.091	0.115	0.388
C ₇	0.0	0.0	0.008
OIL	0.0	0.0	0.029
TOTALS	1307.764	1306.110	1307.183
Temperature	72.0° F	72.0° F	78.9° F
Lean Oil Rate	216.737	192.380	181.528
Lean Oil Temperature	67.0° F	67.0° F	67.0° F
Rich Oil Temperature	80.0° F	84.0° F	78.6° F

TABLE X
CALCULATED RESULTS FOR COLUMN A
TEN THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	209.730	209.639	209.672
C ₁	972.518	970.817	971.449
C ₂	81.806	81.445	81.517
C ₃	37.846	37.852	37.852
iC ₄	2.353	2.473	2.560
nC ₄	2.414	2.782	3.220
C ₅	0.002	0.004	0.259
C ₇	0.0	0.0	0.008
OIL	0.0	0.0	0.028
TOTALS	1306.669	1305.012	1306.564
Temperature	72.0° F	72.0° F	78.3° F
Lean Oil Rate	216.596	194.148	178.071
Lean Oil Temperature	67.0° F	67.0° F	67.0° F
Rich Oil Temperature	80.0° F	84.0° F	77.6° F

TABLE XI
 CALCULATED RESULTS FOR COLUMN A
 TWO THEORETICAL TRAYS WITH A
 FIXED LEAN OIL RATE

Lean Gas Product Rates	
Component	Sujata Method
N ₂	209.580
C ₁	969.802
C ₂	80.716
C ₃	37.070
iC ₄	2.862
nC ₄	5.021
C ₅	1.008
C ₇	0.013
OIL	0.028
TOTALS	1306.100
Temperature	78.4° F
Lean Oil Rate	204.400
Lean Oil Temperature	78.0° F
Rich Oil Temperature	

TABLE XII
COLUMN B1 ABSORPTION SYSTEM

Column Specifications

Trays: 27
 Pressure: 740 psia
 Type: Koch Kaskade
 Diameter: 4.5 ft.
 Plate Spacing: 26 in.
 Source: "X" Petroleum Company

Comp.	Column Feed Rates		Column Product Rates	
	Wet Gas	Lean Oil	Lean Gas	Rich Oil
N ₂	38.228	0.0	43.529	0.0
C ₁	748.344	0.0	723.987	41.524
C ₂	67.413	0.0	35.895	18.960
C ₃	55.664	0.0	7.471	28.544
iC ₄	5.501	0.0	0.568	5.641
nC ₄	12.587	2.909	0.406	15.699
iC ₅	1.492	1.892	0.081	3.397
nC ₅	1.305	2.601	0.081	4.010
C ₆	0.373	2.199	0.081	2.651
C ₇	1.492	0.237	0.0	0.203
C ₈	0.0	0.402	0.0	0.407
C ₉	0.0	3.997	0.0	4.214
C ₁₀	0.0	6.788	0.0	7.136
OIL 1	0.0	37.201	0.0	38.670
OIL 2	0.0	178.274	0.0	185.743
TOTALS	932.400	236.500	812.100	356.800
Temp.	88.0° F	103.0° F	112.0° F	114.0° F

OIL 1: Molecular weight of 165

OIL 2: Molecular weight of 210

TABLE XIII
CALCULATED RESULTS FOR COLUMN B1
TWO THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	37.672	37.606	37.620
C ₁	705.003	699.227	700.442
C ₂	51.232	50.472	50.553
C ₃	27.116	27.125	27.119
iC ₄	1.458	1.515	1.516
nC ₄	2.425	2.573	3.698
iC ₅	0.105	0.118	0.565
nC ₅	0.063	0.073	0.585
C ₆	0.141	0.148	0.209
C ₇	0.003	0.003	0.013
C ₈	0.0	0.0	0.006
C ₉	0.0	0.0	0.027
C ₁₀	0.0	0.0	0.020
OIL 1	0.0	0.0	0.065
OIL 2	0.0	0.0	0.016
TOTALS	825.218	818.860	822.454
Temperature	112.0° F	112.0° F	123.2° F
Lean Oil Rate	252.229	173.172	171.838
Lean Oil Temperature	103.0° F	103.0° F	103.0° F
Rich Oil Temperature	114.0° F	125.0° F	118.8° F

TABLE XIV
CALCULATED RESULTS FOR COLUMN B1
THREE THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	37.741	37.671	37.678
C ₁	710.314	704.245	704.981
C ₂	52.664	51.757	51.714
C ₃	27.120	27.125	27.119
iC ₄	1.214	1.295	1.312
nC ₄	1.757	1.952	3.231
iC ₅	0.045	0.057	0.551
nC ₅	0.022	0.029	0.591
C ₆	0.133	0.142	0.220
C ₇	0.0	0.0	0.010
C ₈	0.0	0.0	0.007
C ₉	0.0	0.0	0.028
C ₁₀	0.0	0.0	0.022
OIL 1	0.0	0.0	0.070
OIL 2	0.0	0.0	0.018
TOTALS	831.012	824.274	827.551
Temperature	112.0° F	112.0° F	125.2° F
Lean Oil Rate	220.643	156.059	152.061
Lean Oil Temperature	103.0° F	103.0° F	103.0° F
Rich Oil Temperature	114.0° F	126.0° F	118.3° F

TABLE XV
CALCULATED RESULTS FOR COLUMN B1
FIVE THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	37.775	37.700	37.703
C ₁	712.905	706.550	706.954
C ₂	53.558	52.562	52.324
C ₃	27.117	27.123	27.120
iC ₄	0.895	1.005	1.077
nC ₄	0.962	1.180	2.707
iC ₅	0.008	0.012	0.551
nC ₅	0.003	0.004	0.607
C ₆	0.122	0.135	0.228
C ₇	0.0	0.0	0.010
C ₈	0.0	0.0	0.007
C ₉	0.0	0.0	0.029
C ₁₀	0.0	0.0	0.022
OIL 1	0.0	0.0	0.072
OIL 2	0.0	0.0	0.019
TOTALS	833.344	826.271	829.430
Temperature	112.0° F	112.0° F	126.2° F
Lean Oil Rate	205.589	149.511	142.571
Lean Oil Temperature	103.0° F	103.0° F	103.0° F
Rich Oil Temperature	114.0° F	127.0° F	117.5° F

TABLE XVI
CALCULATED RESULTS FOR COLUMN B1
TEN THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	37.783	37.703	37.710
C ₁	713.565	706.869	707.619
C ₂	53.812	52.749	52.489
C ₃	27.123	27.124	27.120
iC ₄	0.524	0.664	0.863
nC ₄	0.242	0.394	2.190
iC ₅	0.0	0.0	0.553
nC ₅	0.0	0.0	0.613
C ₆	0.113	0.129	0.229
C ₇	0.0	0.0	0.010
C ₈	0.0	0.0	0.007
C ₉	0.0	0.0	0.029
C ₁₀	0.0	0.0	0.022
OIL 1	0.0	0.0	0.072
OIL 2	0.0	0.0	0.019
TOTALS	833.162	825.633	829.544
Temperature	112.0° F	112.0° F	125.9° F
Lean Oil Rate	201.758	150.532	138.085
Lean Oil Temperature	103.0° F	103.0° F	103.0° F
Rich Oil Temperature	114.0° F	127.0° F	116.1° F

TABLE XVII
 CALCULATED RESULTS FOR COLUMN B1
 TWO THEORETICAL TRAYS WITH A
 FIXED LEAN OIL RATE

Lean Gas Product Rates	
Component	Sujata Method
N ₂	37.273
C ₁	674.860
C ₂	41.060
C ₃	15.842
iC ₄	0.643
nC ₄	1.850
iC ₅	0.333
nC ₅	0.349
C ₆	0.120
C ₇	0.006
C ₈	0.003
C ₉	0.013
C ₁₀	0.010
OIL 1	0.027
OIL 2	0.005
TOTALS	772.393
Temperature	92.5° F
Lean Oil Rate	236.500
Lean Oil Temperature	103.0° F
Rich Oil Temperature	96.0° F

TABLE XVIII

COLUMN B2 ABSORPTION SYSTEM

Column Specifications

Trays: 27
 Pressure: 740 psia
 Type: Koch Kaskade
 Diameter: 4.5 ft.
 Plate Spacing: 26 in.
 Source: "X" Petroleum Company

Comp.	Column Feed Rates		Column Product Rates	
	Wet Gas	Lean Oil	Lean Gas	Rich Oil
N ₂	38.228	0.0	43.529	0.0
C ₁	748.344	0.0	723.987	41.524
C ₂	67.413	0.0	35.895	18.960
C ₃	55.664	0.0	7.471	28.544
iC ₄	5.501	0.0	0.568	5.641
nC ₄	12.587	0.0	0.406	15.699
iC ₅	1.492	0.0	0.081	3.397
nC ₅	1.305	0.0	0.081	4.010
C ₆	0.373	0.236	0.081	2.651
C ₇	1.492	0.236	0.0	0.203
C ₈	0.0	0.402	0.0	0.407
C ₉	0.0	3.997	0.0	4.214
C ₁₀	0.0	6.778	0.0	7.136
OIL 1	0.0	37.201	0.0	38.670
OIL 2	0.0	178.639	0.0	185.743
TOTALS	932.400	236.500	812.100	356.800
Temp.	88.0 ^o F	103.0 ^o F	112.0 ^o F	114.0 ^o F

OIL 1: Molecular weight of 165

OIL 2: Molecular weight of 210

TABLE XIX
CALCULATED RESULTS FOR COLUMN B2
TWO THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N 2	37.672	37.607	37.618
C 1	705.003	699.321	700.272
C 2	51.232	50.480	50.531
C 3	27.116	27.124	27.117
iC 4	1.458	1.514	1.518
nC 4	2.425	2.572	2.586
iC 5	0.105	0.118	0.120
nC 5	0.063	0.073	0.075
C 6	0.141	0.147	0.027
C 7	0.003	0.003	0.013
C 8	0.0	0.0	0.006
C 9	0.0	0.0	0.027
C 10	0.0	0.0	0.020
OIL 1	0.0	0.0	0.065
OIL 2	0.0	0.0	0.017
TOTALS	825.217	818.960	820.011
Temperature	112.0° F	112.0° F	123.3° F
Lean Oil Rate	252.229	172.318	170.383
Lean Oil Temperature	103.0° F	103.0° F	103.0° F
Rich Oil Temperature	114.0° F	124.0° F	119.4° F

TABLE XX
CALCULATED RESULTS FOR COLUMN B2
THREE THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	37.741	37.672	37.675
C ₁	710.314	704.334	704.758
C ₂	52.664	51.765	51.683
C ₃	27.120	27.124	27.119
iC ₄	1.214	1.294	1.315
nC ₄	1.757	1.950	2.004
iC ₅	0.045	0.057	0.061
nC ₅	0.022	0.029	0.032
C ₆	0.133	0.142	0.024
C ₇	0.0	0.0	0.010
C ₈	0.0	0.0	0.007
C ₉	0.0	0.0	0.028
C ₁₀	0.0	0.0	0.021
OIL 1	0.0	0.0	0.069
OIL 2	0.0	0.0	0.019
TOTALS	831.012	824.368	824.823
Temperature	112.0° F	112.0° F	125.2° F
Lean Oil Rate	220.643	155.237	150.887
Lean Oil Temperature	103.0° F	103.0° F	103.0° F
Rich Oil Temperature	114.0° F	125.0° F	119.2° F

TABLE XXI
CALCULATED RESULTS FOR COLUMN B2
FIVE THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	37.775	37.701	37.699
C ₁	712.905	706.642	706.661
C ₂	53.558	52.572	52.280
C ₃	27.117	27.125	27.120
iC ₄	0.895	1.004	1.080
nC ₄	0.962	1.179	1.340
iC ₅	0.008	0.012	0.016
nC ₅	0.003	0.004	0.006
C ₆	0.122	0.135	0.024
C ₇	0.0	0.0	0.010
C ₈	0.0	0.0	0.007
C ₉	0.0	0.0	0.029
C ₁₀	0.0	0.0	0.022
OIL 1	0.0	0.0	0.071
OIL 2	0.0	0.0	0.019
TOTALS	833.344	826.374	826.385
Temperature	112.0° F	112.0° F	126.0° F
Lean Oil Rate	205.589	148.631	141.751
Lean Oil Temperature	103.0° F	103.0° F	103.0° F
Rich Oil Temperature	114.0° F	126.0° F	118.6° F

TABLE XXII
 CALCULATED RESULTS FOR COLUMN B2
 TEN THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
N ₂	37.783	37.704	37.707
C ₁	713.565	706.956	707.267
C ₂	53.812	52.757	52.434
C ₃	27.123	27.124	27.120
iC ₄	0.524	0.663	0.867
nC ₄	0.242	0.393	0.689
iC ₅	0.0	0.0	0.001
nC ₅	0.0	0.0	0.0
C ₆	0.113	0.129	0.024
C ₇	0.0	0.0	0.010
C ₈	0.0	0.0	0.007
C ₉	0.0	0.0	0.029
C ₁₀	0.0	0.0	0.022
OIL 1	0.0	0.0	0.070
OIL 2	0.0	0.0	0.019
TOTALS	833.162	825.727	826.264
Temperature	112.0° F	112.0° F	125.3° F
Lean Oil Rate	201.758	149.690	137.564
Lean Oil Temperature	103.0° F	103.0° F	103.0° F
Rich Oil Temperature	114.0° F	126.0° F	117.5° F

TABLE XXIII

CALCULATED RESULTS FOR COLUMN B2
TWO THEORETICAL TRAYS WITH A
FIXED LEAN OIL RATE

Lean Gas Product Rates	
Component	Sujata Method
N ₂	37.407
C ₁	683.646
C ₂	45.379
C ₃	21.150
iC ₄	1.040
nC ₄	1.688
iC ₅	0.071
nC ₅	0.043
C ₆	0.024
C ₇	0.011
C ₈	0.006
C ₉	0.026
C ₁₀	0.020
OIL 1	0.062
OIL 2	0.016
TOTALS	790.588
Temperature	121.9° F
Lean Oil Rate	236.500
Lean Oil Temperature	103.0° F
Rich Oil Temperature	120.4° F

TABLE XXIV

COLUMN C ABSORPTION SYSTEM

Column Specifications

Trays: 24
 Pressure: 400 psia
 Type: (not specified)
 Diameter: 5.0 ft.
 Plate Spacing: 24 in.
 Source: Unit 3, N.G.A.A. Low Pressure Data

Comp.	Column Feed Rates		Column Product Rates	
	Wet Gas	Lean Oil	Lean Gas	Rich Oil
CO ₂	97.404	0.0	89.802	7.608
C ₁	731.894	0.0	707.479	24.871
C ₂	54.826	0.0	47.343	7.403
C ₃	49.091	0.0	23.811	24.988
iC ₄	6.943	0.0	0.400	8.427
nC ₄	17.595	0.0	0.078	17.293
C ₆	12.346	0.0	0.087	12.055
OIL	0.0	189.500	0.0	189.341
TOTALS	970.100	189.500	869.000	292.600
Temp.	69.0° F	71.0° F	78.0° F	92.0° F

OIL: Molecular weight of 207

TABLE XXV
CALCULATED RESULTS FOR COLUMN C
TWO THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
CO ₂	87.599	88.615	87.793
C ₁	705.085	698.592	701.967
C ₂	43.895	43.199	43.388
C ₃	24.106	24.107	24.104
iC ₄	1.591	1.653	1.658
nC ₄	2.685	2.841	2.859
C ₆	0.053	0.066	0.066
OIL	0.0	0.0	0.005
TOTALS	865.013	859.073	861.841
Temperature	78.0° F	78.0° F	88.6° F
Lean Oil Rate	267.280	243.000	189.735
Lean Oil Temperature	71.0° F	71.0° F	71.0° F
Rich Oil Temperature	92.0° F	118.0° F	89.5° F

TABLE XXVI
CALCULATED RESULTS FOR COLUMN C
THREE THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
CO ₂	88.734	89.554	88.720
C ₁	708.364	701.869	704.527
C ₂	44.954	44.165	44.226
C ₃	24.101	24.107	24.100
iC ₄	1.242	1.326	1.354
nC ₄	1.732	1.914	1.982
C ₆	0.005	0.008	0.008
OIL	0.0	0.0	0.005
TOTALS	869.132	862.942	864.932
Temperature	78.0° F	78.0° F	89.0° F
Lean Oil Rate	234.294	220.250	170.756
Lean Oil Temperature	71.0° F	71.0° F	71.0° F
Rich Oil Temperature	92.0° F	120.0° F	91.0° F

TABLE XXVII
CALCULATED RESULTS FOR COLUMN C
FIVE THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
CO ₂	89.312	90.000	89.107
C ₁	709.947	703.390	705.555
C ₂	45.574	44.733	44.636
C ₃	24.104	24.107	24.102
iC ₄	0.802	0.906	0.986
nC ₄	0.733	0.893	1.025
C ₆	0.0	0.0	0.0
OIL	0.0	0.0	0.005
TOTALS	870.474	864.028	865.416
Temperature	78.0° F	78.0° F	88.3° F
Lean Oil Rate	218.522	210.502	162.425
Lean Oil Temperature	71.0° F	71.0° F	71.0° F
Rich Oil Temperature	92.0° F	121.0° F	91.6° F

TABLE XVIII
CALCULATED RESULTS FOR COLUMN C
TEN THEORETICAL TRAYS

Lean Gas Product Rates			
Component	Kremser-Brown	Edmister	Sujata
CO ₂	89.456	90.077	89.171
C ₁	710.338	703.643	705.866
C ₂	45.738	44.860	44.734
C ₃	24.103	24.107	24.103
iC ₄	0.327	0.430	0.583
nC ₄	0.086	0.139	0.227
C ₆	0.0	0.0	0.0
OIL	0.0	0.0	0.005
TOTALS	870.049	863.257	864.686
Temperature	78.0° F	78.0° F	86.8° F
Lean Oil Rate	214.633	210.724	158.532
Lean Oil Temperature	71.0° F	71.0° F	71.0° F
Rich Oil Temperature	92.0° F	120.0° F	91.2° F

TABLE XXIX

CALCULATED RESULTS FOR COLUMN C
TWO THEORETICAL TRAYS WITH A
FIXED LEAN OIL RATE

Lean Gas Product Rates	
Component	Sujata Method
CO ₂	88.191
C ₁	702.503
C ₂	43.684
C ₃	24.665
iC ₄	1.730
nC ₄	3.007
C ₆	0.072
OIL	0.006
TOTALS	863.858
Temperature	89.7° F
Lean Oil Rate	189.500
Lean Oil Temperature	71.0° F
Rich Oil Temperature	92.3° F

APPENDIX B

COMPUTER PROGRAM

COMPUTER PROGRAM

The Sujata absorption program is written in Fortran IV and was developed for the IBM 7094 computer. The program is written for a general, complex absorption column and has the following size limitations:

Variables	Symbol	Maximum Number
Trays	N	100
Components	NCP	30
Feed streams	MFD	20
Liquid side streams	MSD	10
Vapor side streams	MVSD	10
Intercoolers	MQ	10

The computer program is divided into six major calculation sections. Figure 8 is a block diagram of the calculation procedure.

Main Program

EXEC is the executive program for the entire calculation. The major calculation subroutines are called by EXEC as shown in Figure 9. These major subroutines may in turn call several smaller "support" subroutines. A brief description of the function of each subroutine appears in the following section.

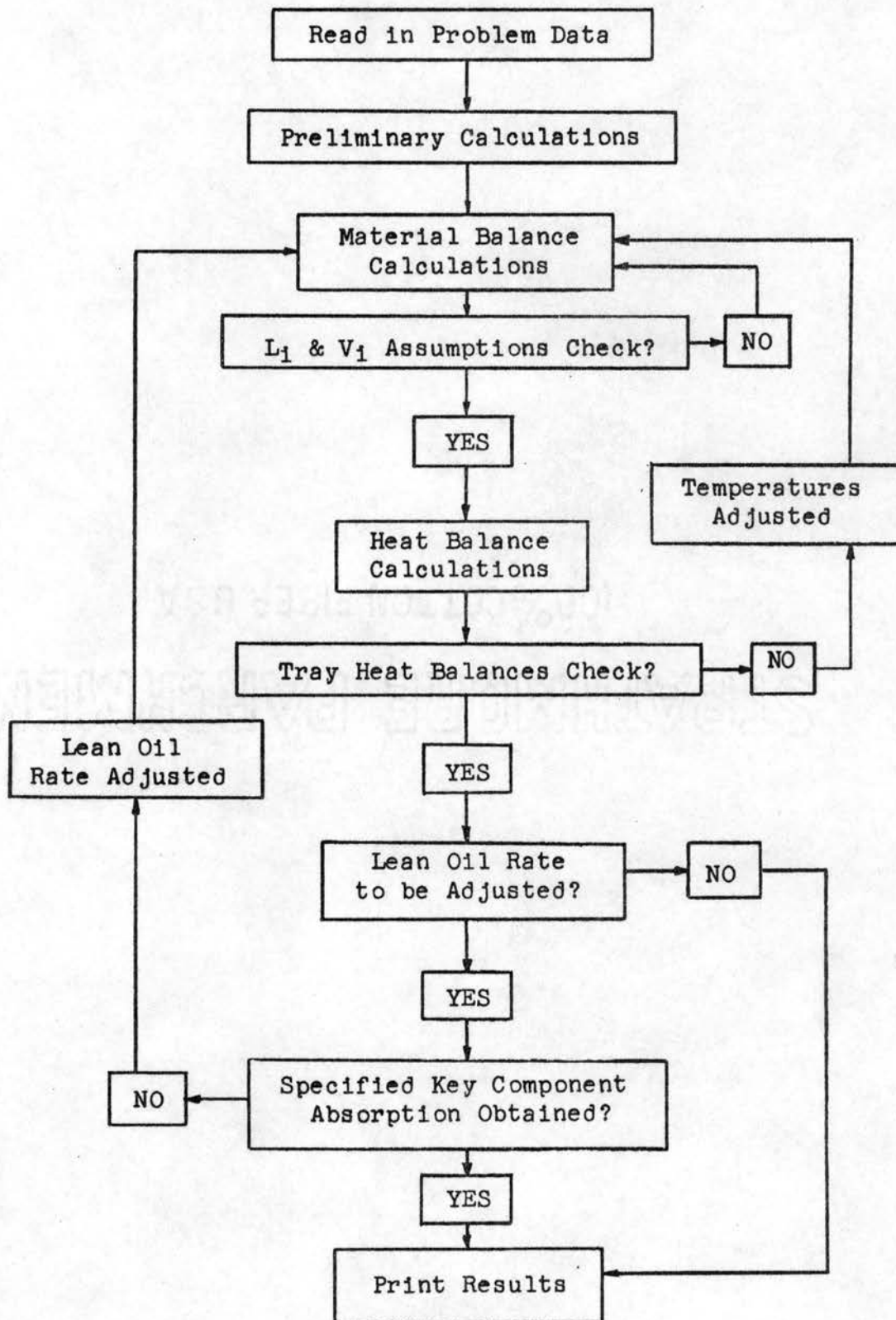
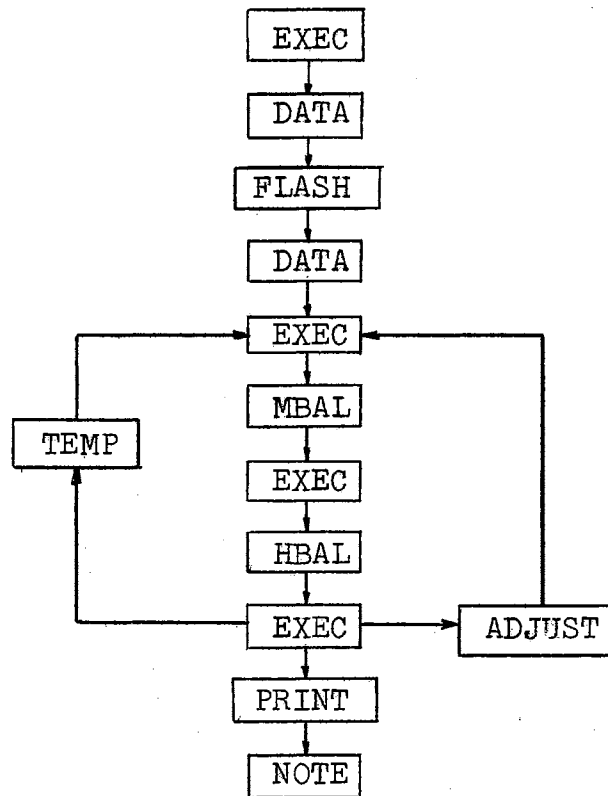


Figure 8. Sujata Program Block Diagram



Support Subroutines

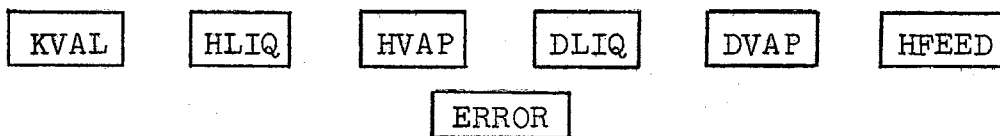


Figure 9. Subroutine Block Diagram

Subroutines

SUBROUTINE ADJUST

ADJUST is the subroutine that determines whether or not the specified key component absorption or stripping has been obtained. If the specified key component absorption has not been obtained, then the subroutine predicts a new lean oil rate. ADJUST is called by the main program EXEC.

SUBROUTINE DATA

DATA is the data input subroutine. All input data is read in by this subroutine. If preliminary calculations (bubble point, dew point, flash, etc.) are required, the subroutine calls the proper calculation subroutine. DATA is called only once by the main program EXEC.

SUBROUTINE DLIQ

DLIQ is the subroutine that calculates the derivative of the liquid component enthalpy at a given temperature. DLIQ is called by numerous subroutines throughout the program.

SUBROUTINE DVAP

DVAP is the subroutine that calculates the derivative of the vapor component enthalpy at a given temperature. DVAP is called by numerous subroutines throughout the program.

SUBROUTINE ERROR

ERROR is the subroutine that prints out the major error messages resulting from major calculation errors. The calculation is terminated with this error message. ERROR may be called by numerous subroutines throughout the program.

SUBROUTINE FLASH

FLASH is the subroutine that checks the validity of the stream conditions given by the input data. It also performs all the necessary bubble point, dew point, and flash calculations associated with the stream conditions. FLASH is called by DATA.

SUBROUTINE HBAL

HBAL is the subroutine that calculates the heat balance around each tray for a given temperature profile. HBAL is called by EXEC.

SUBROUTINE HFEED

HFEED is the subroutine that calculates the enthalpy of the feed streams. HFEED is called by FLASH.

SUBROUTINE HLIQ

HLIQ is the subroutine that calculates the enthalpy for a liquid component at a given temperature. HLIQ is called by numerous subroutines throughout the program.

SUBROUTINE HVAP

HVAP is the subroutine that calculates the enthalpy for a vapor component at a given temperature. HVAP is called by numerous subroutines throughout the program.

SUBROUTINE KVAL

KVAL is the subroutine that calculates the equilibrium constant for a component at a given temperature. KVAL is called by numerous subroutines throughout the program.

SUBROUTINE MBAL

MBAL is the subroutine that calculates the material balance around each tray for a given temperature profile. The initial liquid and vapor assumptions made for each tray are checked and adjusted if necessary. MBAL is

called by the main program EXEC.

SUBROUTINE NOTE

NOTE is the subroutine that prints out the minor error messages resulting from small errors during the calculation. These error messages are warnings that the calculation is not completely correct. NOTE is called by PRINT.

SUBROUTINE OIL

OIL is the subroutine that estimates the lean oil rate required for a specified key component absorption. OIL is called by DATA.

SUBROUTINE PRINT

PRINT is the subroutine that prints out the final results of the calculation. PRINT is called by the main program EXEC.

SUBROUTINE TEMP

TEMP is the subroutine that predicts the new temperature profile for the column if the heat balances are not satisfied. TEMP is called by the main program EXEC.

SUBROUTINE VAPOR

VAPOR is the subroutine that estimates the stripping vapor rate required for a specified key component stripping. VAPOR is called by DATA.

Input Data Specifications

The specific input data requirements and a discussion of each item can be found in the following sections.

Format Specifications

There are four types of format statements used in the program. Each type of format is discussed in detail in the IBM Fortran Manual. (19)

Fw.d This type of format is used for floating point numbers. The total word length is specified by w and the decimal point is located by d which is the number of digits to the right of the decimal. The floating point number 876.32143 would be represented by the format F8.5. If the decimal point is punched on the input data card, the specified decimal point location will be overridden.

Ew.d This type of format is used for floating point numbers with a specified exponent. The terms w and d again refer to the total word length and decimal point location. The E represents the power of ten to which the number preceeding the E is raised. The floating point number -0.010245 would be written as -.10245E-01 and would be represented by the format E11.5.

In This type of format is used for fixed point numbers. The total word length is specified by n. The fixed point number 523 would be represented by the format I3.

An This type of format is used for alphameric information. The field width is specified by n with a maximum n of six spaces. The alphameric information SUJATA ABSORPTION PROGRAM would be represented by 5A6.

Input Data Cards

The input data required for the program is arranged in the following order:

Card 1 "Problem Identification"

This card is used for the alphameric identification of the program. Any short identifying remarks may be used.

```

READ:   WORD(I)
FORMAT: 10A6

```

Card 2 "Column Variables"

This card contains the seven general column variables which define the absorption system. (All these column variables, except the column pressure, have a maximum number as the upper limit. See page 96.)

N	Number of trays
NCP	Number of components
MFD	Number of column feeds
MSD	Number of liquid side streams
MVSD	Number of vapor side streams
MQ	Number of intercoolers
P	Column pressure

```

READ:   N,NCP,MFD,MSD,MVSD,MQ,P
FORMAT: 6I3,F10.4

```

Card 3 "Program Controls"

This card contains the program control variables.

Each variable is discussed below.

KLOOP Lean Oil Prediction Variable

KLOOP = 1 The lean oil rate is specified in the input data.

KLOOP = 2 An initial estimate of the lean oil rate is given in the input data. The program adjusts the lean oil rate to the correct value.

KLOOP = 3 The initial estimate of the lean oil rate is made by the program.

KLOOP = 4 The stripping vapor rate is specified in the input data.

KLOOP = 5 The initial estimate of the stripping vapor rate is given in the input data. The program adjusts the vapor rate to the correct value.

KLOOP = 6 The initial estimate of the stripping vapor rate is made by the program.

KX Intermediate Output Variable

KX = 0 The intermediate calculations are not printed out with the results.

KX \neq 0 The intermediate calculations are printed out with the results.

JOB Output Control Variable

JOB = 2 The component liquid and vapor profiles for each tray are printed out with the column products.

JOB = 3 The total tray and component liquid and vapor profiles are printed out with the column products.

KTX Initial Temperature Profile Variable

KTX = 0 An initial temperature profile is calculated by the program.

KTX \neq 0 The initial temperature profile is specified in the input data.

READ: KLOOP,KX,JOB,KTX
 FORMAT: 4I3

Card 4i "Component Identification"

This series of cards (one for each component) identifies the components used in the calculation.

READ: COMP(J)
 FORMAT: 10A6

Card 5 "Absorption Variables"

This card defines the absorption variables. If the lean oil rate is to be adjusted ($KLOOP \neq 1$), then the desired fractional absorption or the desired product rate for the key component must be specified in the input data. The variables are:

KEY	Key component
ED	Desired fractional absorption
XXX	Desired product rate for key component

READ: KEY,ED,XXX
 FORMAT: I3,F10.7,F12.5

Card 6i "Intercooler Variables"

This series of cards (one for each intercooler) appears in the input data only if at least one intercooler is present in the system. The variables are:

NQ	Tray number
Q	Intercooler duty

READ: NQ,Q
FORMAT: I3,E12.6

Card 7_i "Liquid Side Stream Variables"

This series of cards (one for each liquid side stream) appears in the input data only if at least one liquid side stream is present in the system. The variables are:

NSD Tray number
FR Fraction of the liquid stream removed
by the side stream.

READ: NSD,FR
FORMAT: I3,F10.5

Card 8_i "Vapor Side Stream Variables"

This series of cards (one for each vapor side stream) appears in the input data only if at least one vapor side stream is present in the system. The variables are:

NVSD Tray number
VR Fraction of the vapor stream removed
by the side stream

READ: NVSD,VR
FORMAT: I3,F10.5

Card 9 "Convergence Limits"

This card contains the three principal convergence limits of the program. Each convergence

limit represents the maximum fractional error that can result from incomplete convergence. The variables are:

ER1 Convergence limit in the heat balance
 ER2 Convergence limit in the material balance
 ER3 Convergence limit in the lean oil rate

READ: ER1,ER2,ER3
 FORMAT: 3F10.5

Card 10_i "Equilibrium Coefficients"

This series of cards (one for each component) contains the equilibrium coefficients for the calculation of the equilibrium constant. Each card contains the coefficients for one component. The components must be in the same order as the components listed by Cards 4_i. The equilibrium constant equation in the program is of the form

$$\ln K = A_0 + A_1/T + A_2/T^2 + A_3/T^3.$$

NOTE: All temperatures must be in the form °R/100.

READ: A0,A1,A2,A3
 FORMAT: 4E14.8

Card 11_i "Enthalpy Coefficients for the Vapor"

This series of cards (one for each component) contains the vapor state enthalpy coefficients. Each card contains the coefficients for one component.

The components must be in the same order as the components listed in Cards 4_i. The vapor enthalpy equation is of the form

$$HV = AV + BV*T + CV*T^2 .$$

NOTE: All temperatures must be of the form °R/100.

READ: AV,BV,CV
 FORMAT: 3E12.6

Card 12_i "Enthalpy Coefficients for the Liquid"

This series of cards (one for each component) contains the liquid state enthalpy coefficients. Each contains the coefficients for one component. The components must be in the same order as in Cards 4_i. The enthalpy equation is of the form

$$HL = AL + BL*T + CL*T^2 .$$

NOTE: All temperatures must be of the form °R/100.

READ: AL,BL,CL
 FORMAT: 3E12.6

Card 13_i "Feed Variables"

This series of cards (one for each feed stream) contains the column feed position and conditions.

The variables are:

NFD	Feed tray number
MOD	Feed condition
TFD	Feed temperature (°R/100)
FLK	Flashed feed ratio (L/F)
EN	Feed enthalpy

The feed streams may enter the column in any of seven conditions. The condition of the feed determines whether TFD, FLK, or EN must be specified in the input data. The feed condition is given by MOD.

MOD = 1 The feed is all liquid at a specified temperature. (TFD is specified.)
 MOD = 2 The feed is all vapor at a specified temperature. (TFD is specified.)
 MOD = 3 The feed is flashed at a given L/F ratio. (FLK is specified.)
 MOD = 4 The feed is flashed at a given temperature. (TFD is specified.)
 MOD = 5 The feed is at its bubble point.
 MOD = 6 The feed is at its dew point.
 MOD = 7 The feed is given at a specified enthalpy. (EN is specified.)

READ: NFD,MOD,TFD,FLK,EN
 FORMAT: 2I3,2F10.5,F12.4

Card 14₁ "Component Feed Rates"

This series of cards (one set for each feed stream) contains the component feed rates for each feed stream. Each card contains a maximum of six component feed rates. FD is the component feed rate variable.

READ: FD(I,J)
 FORMAT: 6F12.6

Card 15 "Temperature Limits"

This card contains the maximum and minimum temperature limits of the physical data. The equilibrium

and enthalpy data is fitted over this temperature range. The program will not allow calculation temperatures to exist outside this range. The variables are:

TMAX	Maximum temperature ($^{\circ}\text{R}/100$)
TMIN	Minimum temperature

READ: TMAX,TMIN

FORMAT: 2F10.5

Card 16₁ "Initial Temperature Profile"

This series of cards contains the initial temperature profile used by the program and is present in the input data only if $\text{KTX} \neq 0$ in Card 3. Each card contains six tray temperatures.

READ: T(J)

FORMAT: 6F12.5

Program Output

Intermediate Calculations:

If $\text{KX} = 0$ in Card 3, then the intermediate calculations will be printed out in addition to the final results. These intermediate calculations include the material balance, heat balance, and temperature profile for each pass of the calculation. This information is often useful in locating any errors indicated by the

error messages of the program.

Results:

The program has two major output formats.

- 1) The temperature, liquid, and vapor component rates for each tray are listed along with the total column product rates and their enthalpies.
- 2) The tray temperatures and total and component liquid and vapor rates are listed along with the calculated column product rates and their enthalpies.

Error Comments:

The program contains two types of error comments. The first type of error comment is a warning that indicates the solution contains minor errors resulting from temperatures predicted outside the temperature range defined by TMAX and TMIN. (The equilibrium and enthalpy data is valid only within this range.) The program is allow to continue using either TMAX or TMIN rather than the predicted temperature. The magnitude of the error depends on the difference between the predicted and limiting temperatures. The error comment indicates both the subroutine in which the error occurred and the magnitude of the first correction. Errors of this type

may cause the program to terminate. Error comments of this type appear as

*****PROGRAM ERROR MESSAGES*****

TEMPERATURE IS GREATER THAN TMAX IN SUBROUTINE ____
T EXCEEDS TMAX BY ____

*****WARNING--SOLUTION CONTAINS MINOR ERRORS

In most cases these errors can be corrected by expanding the temperature range of the equilibrium and enthalpy data.

The second type of error comment indicates a major error in the calculation. The program is terminated at that point and passes on to the next data set. This type of error comment is possible in all sections of the program in which a successive approximation technique is used. For most practical absorption systems an error comment of this type is likely to be the result of an error in the input data. Each error comment is listed below with a brief explanation of the error.

HEAT BALANCE DID NOT CONVERGE

The program has made 150 temperature adjusting passes. The deviation in the heat balance still exceeds the convergence limit set by ER1 in the input data.

DEVIATION IN THE HEAT BALANCE EXCEEDS LIMIT

The deviation in the heat balance is extremely large. It is likely that the heat balance calculation is diverging rather converging to the proper values.

MATERIAL BALANCE DID NOT CONVERGE

The program has made 50 material balance passes in subroutine MBAL. The deviation in the material balance still exceeds the convergence limit ER2 for at least one tray.

FINAL SOLUTION DID NOT CONVERGE

The program has made 50 lean oil adjusting passes. The calculated fractional absorption (or stripping) still exceeds the convergence limit ER3. The percentage change in the last lean oil adjustment is printed out with the error comment.

L/F SOLUTION DID NOT CONVERGE IN SUBROUTINE FLASH

The program has made 50 L/F ratio adjusting passes in subroutine FLASH. The correct L/F ratio of the feed could not be found.

DEW POINT DID NOT CONVERGE IN SUBROUTINE FLASH

The program has made 50 calculation passes in

subroutine FLASH. The correct dew point temperature of the feed could not be found.

BUBBLE POINT DID NOT CONVERGE IN SUBROUTINE FLASH

The program has made 50 calculation passes in subroutine FLASH. The correct bubble point temperature of the feed could not be found.

FLASH TEMPERATURE DID NOT CONVERGE IN SUBROUTINE FLASH

The program has made 50 calculation passes in subroutine FLASH. The correct flash temperature of the feed could not be found.

TEMPERATURE WILL NOT CONVERGE IN VAPOR FEED

The program has made 50 calculation passes in subroutine FLASH. The correct feed temperature for the given vapor feed enthalpy could not be found.

TEMPERATURE WILL NOT CONVERGE IN LIQUID FEED

The program has made 50 calculation passes in subroutine FLASH. The correct feed temperature for the given liquid feed enthalpy could not be found.

TEMPERATURE WILL NOT CONVERGE IN FLASHED FEED

The program has made 50 calculation passes in subroutine FLASH. The correct feed temperature for the

flashed feed enthalpy could not be found.

Calculation Variables:

The following is a list of the primary calculation variables used in the program. All these variables appear in COMMON.

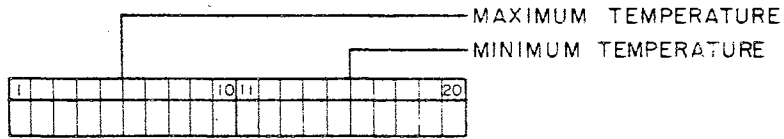
AO	1 st	equilibrium constant coefficient
A1	2 nd	equilibrium constant coefficient
A2	3 rd	equilibrium constant coefficient
A3	4 th	equilibrium constant coefficient
AAA	NOTE	error message variable
AL	1 st	liquid state enthalpy coefficient
AV	1 st	vapor state enthalpy coefficient
BBB	NOTE	error message variable
BL	2 nd	liquid state enthalpy coefficient
BV	2 nd	vapor state enthalpy coefficient
CL	3 rd	liquid state enthalpy coefficient
CV	3 rd	vapor state enthalpy coefficient
ED		desired fractional absorption or stripping
EN		feed enthalpy
ER1		convergence limit in the heat balance
ER2		convergence limit in the material balance
ER3		convergence limit in the lean oil rate
ER4		"spare" variable
ER5		"spare" variable
FD		component feed rate
FR		fraction taken off by a liquid side stream
H		heat balance deviation
HSUM		exit stream enthalpy plus intercooler duty
JOB		output control variable
JX		total number of NOTE error messages
KEY		key component number
KLOOP		lean oil rate control variable
KX		intermediate print out control variable
LX		ERROR message variable
MFD		number of feeds
MOD		condition of feed
MQ		number of intercoolers
MSD		number of liquid side streams
MVSD		number of vapor side streams

MX	lean oil adjustment "pass" variable
N	number of trays
NCP	number of components
NFD	feed tray location
NQ	intercooler tray location
NSD	liquid side stream tray location
NVSD	vapor side stream tray location
PL	total liquid rate leaving the tray
PV	total vapor rate leaving the tray
Q	intercooler duty
SFDH	total feed enthalpy
SMFD	total feed rate
T	tray temperature
TFD	feed temperature
TMAX	maximum temperature
TMIN	minimum temperature
VR	fraction taken off by the vapor side stream
XXX	desired key component product rate
XL	component liquid rate leaving a tray
YYY	a spare variable

ABSORBER PROGRAM
INPUT DATA SHEET

PROJECT NO.	_____
NAME	_____
DATE	_____
PAGE	_____ OF _____ PAGES _____

TEMPERATURE LIMITS



VITA

Robert Ray Spear

Candidate for the Degree of

Master of Science

Thesis: AN EVALUATION OF THE SUJATA ABSORPTION
CALCULATION METHOD

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Southern California Edison Company, Los
Angeles, California, June to September, 1961;
summer employment in the Chemical Division
Engineers section of the Richmond Refinery
of Standard Oil Company of California, June to
September, 1963; summer employment in Inorganic
Research of Monsanto Company, St. Louis,
Missouri, June to September, 1964.