SHORT-CUT ABSORBER CALCULATIONS WITH

INCORPORATED HEAT BALANCES

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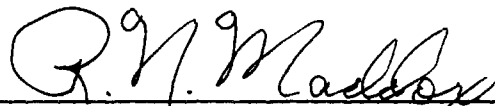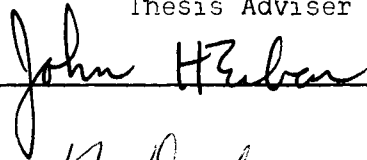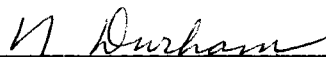1966

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PREFACE

A short-cut absorber calculation method, the MORE method, has been
developed which incorporates heat balances and the theoretical tray
concept. Results from the MORE method were compared with results of
Kremser-Brown, Edmister, and Hull-Raymond short-cut methods. Rigorous
tray-by-tray solutions were provided by the Sujata calculation method.

I wish to thank:

Professor R. N. Maddox, my adviser, for the guidance and counsel through-
out this work;

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CHAPTER I

INTRODUCTION

"Absorption is essentially a vapor pressure phenomenon. The driving force is the difference between the partial pressure of a constituent in the gas and the vapor pressure due to the portion absorbed in the liquid." These were the words of Alois Kremser (8) that started the theoretical analysis of the absorption process in 1930. Since then, many useful and helpful additions have been made in the solution of absorption problems.

The design or evaluation of an absorber represents time and capital investment. Thus, speed and accuracy are plied against one another. The accuracy of a solution, in turn, is a function of the data supplied and the method of calculation.

Design calculations began with little data and easy to use methods. Time brought improved equilibrium and enthalpy data and led to more exact calculation methods. The advent of the computer made possible rigorous calculation methods; however, not everyone has access to a computer and a program for such calculations. The need still exists for a simple hand method that incorporates absorption calculations, heat balance calculations, and a minimum number of assumptions for a broad range of absorber operating conditions.

Such a method would find application in preliminary designs, economic feasibility studies, initial profiles for rigorous calculation, or

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even final designs in the absence of exact methods.

CHAPTER 2

BACKGROUND

Absorption is a mass transfer operation, principally occurring in
one direction. In the petroleum industry absorption describes a multi-
component separation with counter-current flow to increase concentra-
tion driving forces. A gas stream rich in heavy components is fed into
the bottom of the absorber to rise through contacting devices. It is
the in-gas, wet gas, or rich gas. A sponge or absorbing oil is fed in
the top. It is the lean oil. The two streams pass counter-currently
and the gas stream leaving the absorber is denoted the discharge gas,
lean gas, or dry gas; the oil leaving, the rich oil.

A.   DESIGN VARIABLES

From an analysis of design variables (13) for an n tray, C compon-
ent absorber with only two feeds, a simple absorber, a designer is faced
with

$$2C + 2n + 5$$

degrees of freedom, i.e. variables.

A unique absorber could then be described by specifying

PRESSURE IN EACH STAGE		n
HEAT LEAK IN EACH STAGE		n
LEAN OIL COMPOSITION	C	
LEAN OIL RATE AND TEMPERATURE		2
IN-GAS COMPOSITION	C	
IN-GAS RATE AND TEMPERATURE		2
NUMBER OF STAGES		1
		$2C + 2n + 5$

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If a desired recovery of a component is specified, then that specification replaces one in the list above, for instance, the lean oil flow rate. Basic absorber design methods, rigorous and otherwise, begin with these specifications.

B.   ALGEBRAIC DEVELOPMENT

In the engineering of absorption units two basic approaches have been developed which closely resemble the equipment from which they were derived. First, small scale absorption equipment tends to be packed towers which are modeled in transfer units, each unit being an "equivalent" height. Such a model is founded in mass transfer theory. In larger applications, the absorber is built of separate trays. This led to the development of a stagewise treatment of absorbers. Before delving into the history and folklore of stagewise absorber treatment, a background of the algebra and definitions will be presented.

Considering the ith stage with a vapor stream entering the bottom, a liquid stream entering the top, and a liquid and a vapor stream leaving, then material balance equation for each component is, Fig. 1,

$$v_{i+1} + l_{i-1} = v_i + l_i . \tag{1}$$

The equation around the ith tray and the top of the column for a given component is

$$v_1 + l_i = v_{i+1} + l_0 \tag{2}$$

where: v_1 is the moles of component leaving in the dry gas
l_0 is the moles of component entering in the lean oil.

Defining a theoretical stage to have the liquid and vapor leaving in equilibrium, the equilibrium ratio K becomes

$$K = \frac{\text{mole fraction vapor}}{\text{mole fraction liquid}} = \frac{v/V}{l/L} \tag{3}$$
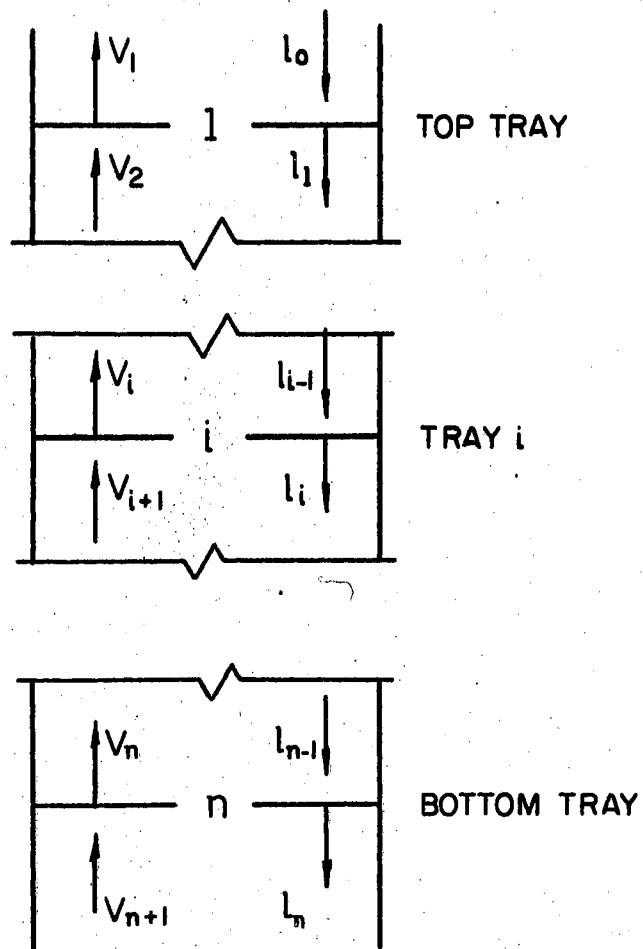
Figure 1.   A Simple Absorber

where V and L are the total streams. Rearranging the equation yields

$$\frac{1}{v} = \frac{L}{VK} = A \qquad (4)$$

for each component on each tray. The ratio A has become known as the absorption factor. So the absorption factor completely defines the absorption phenomenon, irrespective of the conditions of the process.

Rearranging the equation (1) for the top tray of an absorber

$$v_2 = v_1(A_1 + 1) - l_0 \quad ; \qquad (5)$$

then the liquid leaving the tray 2 would be

$$l_2 = v_2 A_2 = v_1(A_1 A_2 + A_2) - l_0 A_2 \quad . \qquad (6)$$

Using equations (2) and (4) to obtain the vapor rising to a given tray and its equilibrium liquid alternately, the equation for the liquid leaving tray n is

$$l_n = v_1(A_1 A_2 A_3 \ldots A_n + A_2 A_3 \ldots A_n + \ldots + A_n) - l_0(A_2 \ldots A_n + \ldots + A_n). \qquad (7)$$

Continuing the convention presented by Edmister (3) defines

$$\pi_A = A_1 A_2 A_3 \ldots A_n \qquad (8)$$

and

$$\Sigma_A = A_1 A_2 \ldots A_n + A_2 A_3 \ldots A_n + \ldots + A_n \quad . \qquad (9)$$

Using these definitions equation (7) becomes

$$l_n = v_1 \Sigma_A - l_0(\Sigma_A - \pi_A) \quad . \qquad (10)$$

Design information usually consists of both feed streams rather than a feed and a product stream. Applying an over-all component balance to equation (10) yields

$$v_1 = v_{n+1} \frac{1}{\Sigma_A + 1} + l_0 \left[1 - \frac{\pi_A}{\Sigma_A + 1} \right] \qquad (11)$$

where v_1 is the moles in the dry gas; v_{n+1} the moles in the wet gas; and l_0 the moles in lean oil. Notice that both quantities included in brackets vary from 0 to 1.0, convenient limits for calculation.

C. LITERATURE SURVEY

Solution of the mathematical model for absorber calculations depends upon the method of evaluating the absorption factor for each individual tray and component. Rigorous solutions for multicomponent systems are difficult and time consuming and, without good data, unwarranted. The simplest method is to assume the absorption factor is constant throughout the column. A refinement of that method is to use an "effective" absorption factor that will give the same value as the rigorous solution. The most difficult method is to evaluate each absorption factor on every tray for all components.

Significant contributions to the average absorption factor methods were made by Kremser (8), Souders and Brown (1), and Landes and Bell (9). The case for "effective" absorption factors has been provided by Horton and Franklin (6), Edmister (3, 4, 5), and Hull and Raymond (7). Horton and Franklin also have provided algebraic background for the rigorous methods. Sujata (4) and Holland (5) have recently presented rigorous methods for computer solution to supplement the Lewis-Matheson and Thiele-Geddes methods for distillation.

THE KREMSER METHOD

In 1930 Kremser (8) presented a mathematical analysis of the relations of the oil absorption process. In order to simplify them the assumption was made that the pressure, oil rate, gas rate, and temperature were constant throughout the absorber. Raoult's Law was also used in the analysis.

Kremser noted these assumptions were not fulfilled with rich gas feed or high pressure plants and recommended theoretical application

at the top and bottom of the column to estimate probable results.

Since the problem at hand was an engineering one, engineering units were used. Kremser defined the absorption factor

$$A = Gq/100 \tag{12}$$

where q was the equilibrium constant $x = qy$ and G was the oil to gas ratio, gallons per 1000 standard cubic feet. Using the material balance similar to that of equation (7), a constant absorption factor, and an algebraic identity

$$\frac{A^{n+1}-1}{A-1} \equiv A^n + A^{n-1} + A^{n-2} + \ldots + A + 1 \tag{13}$$

Kremser derived equation (14) analogous to equation (11),

$$v_1 = \frac{A-1}{A^{n+1}-1} v_{n+1} + \frac{A(A^n-1)}{A^{n+1}-1} v_0 \tag{14}$$

where v_{n+1} was the gasoline content entering the absorber, v_0 was the vapor in equilibrium with the gasoline constituent entering in the lean oil. The number of trays in the absorber was n.

THE SOUDERS AND BROWN MODIFICATION

Brown and Souders (1) introduced several changes to the Kremser method. Their approach being a theoretical one brought molal flow rates and ratios to replace the units of Kremser's derivation. The definition of a new equilibrium ratio K was made as

$$K = y/x. \tag{15}$$

This left the definition of the absorption factor in its present form

$$A = L/VK \quad . \tag{16}$$

Using another algebraic manipulation

$$\frac{A-1}{A^{n+1}-1} = 1 - \frac{A(A^n-1)}{A^{n+1}-1} \quad , \tag{17}$$

Souders and Brown rearranged equation (14) to the form

$$\frac{v_{n+1} - v_1}{v_{n+1} - v_0} = \frac{A^{n+1} - A}{A^{n+1} - 1}$$

(18)

which made it more convenient when changing the composition of the lean oil. The left side of equation (18) is the ratio of the actual change in composition of the gas to the maximum change in composition were it in equilibrium with the lean oil.

The assumptions of this method were substantially valid for moderate pressures and lean gases, hence little absorption. Souders and Brown recommended that with greater absorption the equilibrium values should be evaluated at some intermediate temperature between the top and bottom. This value combined with the oil rate at the top, L, and the gas flow at the bottom, V, produced ultraconservative values for design work in this range.

THE LANDES-BELL METHOD

Recently a method has been presented which incorporates the heat balance into the method of Kremser, Souders, and Brown. Landes and Bell (9) used the Souders and Brown method and an estimated average temperature to provide a first estimate of the average absorption factor. The top tray temperature was assumed and the dew point calculated filling the void with lean oil. A heat balance was made around the top tray using an assumed temperature for the second tray. The same procedure was then followed for the second tray. The assumed temperature for the third tray was left unchecked. An over-all heat balance yielded the temperature of the rich oil stream. After the temperature-tray profile had been plotted, the oil-vapor ratios were cal-

culated. The L/V of the top tray had been found during the top tray analysis. The L/V ratio for the bottom tray was calculated by assuming equal shrinkage on all trays except the top. Using plot estimated values for temperatures and L/V's, the absorption factor for the key component was calculated for each tray and graphically averaged for the second iteration. Absorption factors for other components were found by the ratio equilibrium values and the absorption factor of the key component.

THE HORTON-FRANKLIN METHOD

The previously discussed methods use an average value for the absorption factor, A, for each component. In 1940 Horton and Franklin (6) presented two separate methods to calculate absorber performance. The primary method was based on evaluating the absorption factor on each tray with temperature and vapor profiles calculated by empiricisms

$$\left[\frac{V_1}{V_{n+1}}\right]^{1/n} = \frac{V_i}{V_{i+1}} \tag{19}$$

and

$$\frac{V_{n+1} - V_{i+1}}{V_{n+1} - V_1} = \frac{T_n - T_i}{T_n - T_o} \tag{20}$$

These equations assume constant per cent absorption on each stage and a temperature change proportional to the vapor shrinkage. The authors acknowledged that the predicted material balances and stage temperatures may differ from tray-by-tray results, but their use gave an over-all absorption efficiency which agreed closely.

Horton and Franklin's second method introduced the effective absorption factor as the value which gave the same results as the individual absorption factors. Considering the series expansion similar to

equation (10), they concluded the effective absorption factor for light components (small values of **A**) corresponded to the absorption factor at a position near the bottom and for heavier components, to a position near the middle of the tower. The following table was presented as a guide to the selection of effective factors.

TABLE I

LOCATION OF EFFECTIVE ABSORPTION FACTOR
VIA HORTON-FRANKLIN

ABSORPTION FACTOR	i/n
0.0-0.1	1.0
0.1-0.4	0.9
0.4-1.0	0.8
1.0-4.0	0.8
Above 4.0	0.6

i = plate where L/V and temperature are evaluated by equations (19) and (20)
n = total number of trays

THE EDMISTER METHOD

The method of evaluating an effective absorption factor presented by Horton and Franklin was a discontinuous function and therefore awkward to use. In 1943, Edmister (2) presented a short-cut method based on an exact solution for a two tray absorber. At that time Edmister presented a material balance equation

$$\frac{V_{n+1} - V_1}{V_{n+1}} = \left[1 - \frac{l_o}{A'V_{n+1}} \right] \left[\frac{A_e^{n+1} - A_e}{A_e^{n+1} - 1} \right] \tag{21}$$

defining A_e and A' as

$$\frac{A_e^{n+1} - A_e}{A_e^{n+1} - 1} = \frac{A_1A_2\ldots A_n + A_2\ldots A_n + \ldots + A_n}{A_1A_2\ldots A_n + A_2\ldots A_n + \ldots + A_n + 1} \qquad (22)$$

and

$$\frac{1}{A'} \left| \frac{A_e - A_e}{A_e^{n+1} - 1} \right| = \frac{A_2A_3\ldots A_n + A_3\ldots A_n + \ldots + A_n}{A_1A_2\ldots A_n + A_2\ldots A_n + \ldots + A_n + 1} \quad . \qquad (23)$$

From study, A_e and A' were found to be essentially independent of the number of trays and readily expressed as function of the terminal values of the absorption factor. Solving the system for a two tray absorber, A_e and A' could be expressed as

$$A_e = \sqrt{A_n(A_1 + 1) + 0.25} \quad - 0.5 \qquad (24)$$

and

$$A' = \frac{A_n(A_1 + 1)}{A_n + 1} \quad . \qquad (25)$$

In 1957 Edmister (4) published a new form of the material balance equation to be used in computer application and presented new absorption factor functions as

$$v_1 = v_{n+1} \phi_A' + l_o \psi_A \qquad (26)$$

with

$$\phi_A' = \frac{1}{\sum_A + 1} = \text{fraction not recovered} \qquad (27)$$

and

$$\psi_A = 1 - \frac{\pi_A}{\sum_A + 1} = \text{lean oil fraction lost.} \qquad (28)$$

The value of ϕ_A and ψ_A are bounded between zero and one which makes them more convenient to use. They may be evaluated either rigorously by individual tray absorption factors, or approximately by effective absorption factors as defined by equation (24).

THE HULL-RAYMOND METHOD

Presenting the first short-cut method to incorporate heat balance equations, Hull and Raymond (7) pointed out that the key to over-all absorber heat balance was establishing either the discharge gas or the rich oil temperature. In light hydrocarbon fractionators the problem is solved by dew and bubble point calculations. In absorbers this procedure is complicated by the presence of components with widely varying boiling points. The vapor-liquid equilibrium constant of methane changes slightly with moderate variation in temperature. The vapor-liquid equilibrium constant of a lean oil may change one hundred-fold for small temperature changes. A combination of these properties makes bubble and dew point calculations difficult and very critical with respect to equilibrium data. Thus terminal tray temperatures must be obtained by tedious tray-by-tray heat balances or empirical correlation.

Hull and Raymond presented two methods for determining terminal tray temperatures. The first method, applicable to absorbers with input oil and gas weight ratio from 0.8 to 5.0, was based on the lean oil being the principal heat balance quantity in the top section of the column. For high pressure absorbers where the oil-gas ratio may be very small, a correlation was developed between the in-gas and the rich oil temperatures.

In each of the above cases, the remaining terminal temperature was calculated from the over-all heat balance which included a term for column heat loss to the atmosphere. The column average temperature was correlated as a difference from the average of the terminal temperatures and was used in evaluating the effective absorption factor.

The top, bottom, and average L/V ratios were calculated to be used with respective temperatures. The $(L/V)_{Btm}$ was estimated initially as the sum of the lean oil rate plus estimated shrinkage over the in-gas. This value was corrected in subsequent calculations by a multiplier equal to 1.0 plus fractional shrinkage of propane and heavier components per tray. The average L/V was simply the arithmetic average of the terminal values.

Concluding that the methods of Horton and Franklin and of Edmister were as good as could be developed from theory and still have practical simplicity, Hull and Raymond stated the methods had the following limitations: Horton and Franklin's predicted internal conditions varied from actual conditions; their method for evaluating effective absorption factors was not continuous; and Edmister's two tray model was "of necessity an over-simplification."

The authors then proposed a method of evaluating A_e and A', a term they denoted A_c. The effective absorption factor was in terms of the fractional distance between the bottom and average tower conditions while A' was in terms of the fractional distance between the bottom and top of the column. Using Hull and Raymond's terms in their arrangement of the material balance equation, the fraction absorbed, F, of each component is

$$\frac{v_{n+1} - v_1}{v_{n+1} - l_0/A'} = F = \frac{A_e^{n+1} - A_e}{A_e^{n+1} - 1} \quad . \tag{29}$$

The iteration variable for the calculation scheme was the total moles absorbed.

THE RIGOROUS METHODS

The methods discussed above have been short-cut or approximate solutions to absorber calculations although several are capable of exact solution. With the advent of high speed computers rigorous solutions became more popular and feasible. Lewis and Matheson (10) developed a rigorous multicomponent distillation calculation scheme which could be modified to work on absorbers. For absorbers a top product composition was assumed and temperature and flow rates were calculated down the column from heat and material balances around the top and the tray in question. The initial assumption was checked by comparing it with in-gas feed.

Thiele and Geddes (16) also developed a multicomponent distillation calculation method based on the ratio of the liquid stream to the top product stream. Holland (5) adapted this method to a computer solution for absorbers using the absorption factor approach.

An iterative tray-by-tray method was described by Sujata (15) and programmed for computer application by Spear (14). The Sujata method presents no new equations, but rather applies the absorption factor technique combined with a simultaneous solution for the variables. Temperature and flow profiles are initially assumed. Correct flow profiles are found for given temperature profiles. Individual tray heat balances validate assumed temperature profiles or adjust them as necessary. The major iteration variable is temperature based on heat balance.

In 1959 Ravicz (12) presented a calculation method which eliminated the ideal tray restriction, and the concept of an over-all column effi-

ciency. This method, utilizing the power of the computer, included

non-ideal mass transfer-calculations, enthalpy, equilibrium, and

physical correlations too tedious for hand calculations.

CHAPTER III

DESCRIPTION OF NEW METHOD

The stagewise absorption process can be broken into two operations,
countercurrent mixing of two immiscible fluids and gas absorption.
If an absorption profile can be provided, the operation can be reduced
to countercurrent mixing with a term to correct for absorption on each
stage.

Kremser neglected the absorption operation in his calculation of
the flow model. The L/V ratio was taken as the lean oil rate over the
in-gas rate, the most conservative approach. Acknowledging that no
rule could be devised to give the knock out and temperature on each
tray, Horton and Franklin proposed a constant per cent absorption per
tray accompanied by proportional temperature change. Landes and Bell
used the absorption on the top tray calculated by pseudo-bubble point
technique with the shrinkage for the remaining trays being equal.

The main advantage of a good absorption profile is not in predict-
ing improved L/V ratios throughout the column, but rather in establish-
ing the temperature profile. Once a reasonable absorption profile is
determined, the heats of absorption can be added into straight forward
heat balances to establish temperatures.

In simple absorbers, there is strong tendency for the majority of
the knock out to occur on the ends of the column. The lighter compon-
ents that carry through the column are primarily recovered on the top

stage where the vapors are in equilibrium with denuded oil. The heavier components are absorbed in major quantites at first contact with the lean oil.

In abosrbers with more than three theoretical trays the shrinkage on the two end trays amounts to approximately eighty per cent of the total knock out. The fractional end shrinkage, w, remains quite stable in spite of changes in the shrinkage on one end. Although w may vary slighty with changes in gas composition, lean oil condition, or recovery fraction, a value of eighty per cent knock out on the end trays provides a reasonably accurate absorption profile. For absorbers with three trays w was around eighty-nine per cent. And two tray absorbers necessarily have one hundred per cent absorption on the end trays.

The development of the w factor plays a substantial part in developing the short-cut method associated with this thesis, the MORE method. Not only is the w factor used in determining the terminal tray temperature, but its development led to the three tray model to evaluate absorption.

A. GENERAL DESCRIPTION

A short-cut absorber calculation scheme has been developed with an iterative solution, the total absorption being the iteration variable. Absorber specifications consist of: the number of trays; composition, temperature, and flow rate of in-gas; composition and temperature of the lean oil; and recovery of specified component. Inherent in this model is the assumption of theoretical stages.

The calculation method may be divided into six sections. Figure 2 presents the section sequence. The first section calculates or esti-
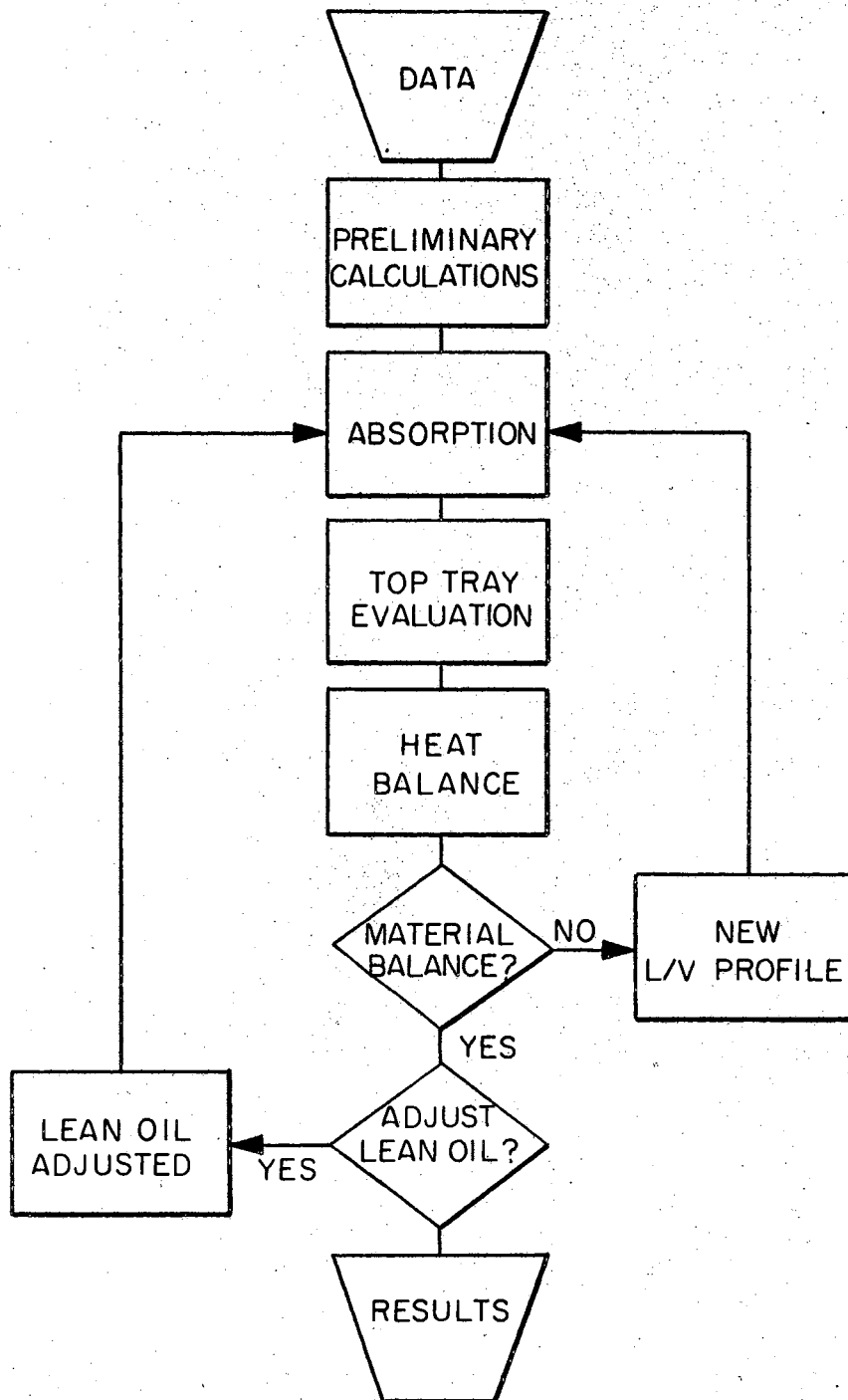
Figure 2.   Proposed Calculation Flowchart

mates the terminal tray temperatures and column average temperature,
along with terminal and average L/V ratios and feed stream enthalpy.
The second section evaluates the absorption factor functions in terms
of the terminal and average absorption factors. The third section com-
putes the temperature and stream flows for one terminal tray. The tem-
perature at the other end of the column is given by the heat balance
section. If the estimated material balance is not satisfied, a new
estimation is made, a new L/V profile calculated, and calculation re-
turns to the absorption section. If the material balance is satisfied,
the recovery of the key is compared with the desired quantity. If this
is satisfactory, solution is reached. If not, the lean oil rate is
adjusted and calculation is returned to the absorption section.

B.   PRELIMINARY CALCULATIONS

As a first approximation L/V ratios are assumed equal for every
tray. The L/V ratio is calculated from the equation

$$(L/V) = (L_o + S)/V_{IG} \qquad (30)$$

where L_o is the lean oil rate and S the total shrinkage. This ratio
is used for the top, the average, and the bottom trays.

A first estimate of the average temperature of the column is made
by assuming the entire heat of absorption is provided by shrinkage of
a pseudo-component usually a little lighter than the key component.
The average temperature is then estimated by mixing the lean oil and
the in-gas stream and adding the total heat of absorption based on the
pseudo-component. Again this value is used as the terminal temperature
on the first iteration.

C. ABSORPTION SECTION

The absorption factors for each component are evaluated at the top, bottom and average conditions. Using equation (11) as the overall material balance equation

$$v_1 = v_{n+1}\left[\frac{1}{\Sigma_A+1}\right] + l_o\left[1-\frac{\pi_A}{\Sigma_A+1}\right] , \qquad (11)$$

the dry gas composition is calculated for the given absorption factors. A study of temperature, liquid, and vapor profiles from the Sujata solution led to the use of three absorption factors, the three tray model. This was done because the L/V ratio and temperature on the ends of an absorber are often quite different from the values of the interior trays. However, the values on the interior trays remain relatively constant. For this reason, the absorption functions become

$$\phi_A = \frac{1}{\Sigma_A + 1} = \frac{A_{AVE} - 1.0}{\pi_A\left(A_{AVE} + \frac{A_{AVE}}{A_{TOP}} - 1.0\right) + \left(A_{AVE} - A_{BTM} - 1.0\right)} \qquad (31)$$

and

$$\psi_A = 1 - \frac{\pi_A}{\Sigma_A + 1} = 1.0 - \frac{A_{AVE} - 1.0}{\left(A_{AVE} + A_{AVE}/A_{TOP} - 1.0\right) + \left(A_{AVE} - A_{BTM} - 1.0\right)/\pi_A} \qquad (32)$$

where ϕ_A and ψ_A are the absorption factor functions. Although these functions are cumberson to write, they are easier to evaluate than the series expression. The value for   is found by the equation

$$\pi_A = A_{TOP} \times A_{BTM} \times A_{AVE}^{n-2} \qquad (33)$$

where n is the number of theoretical trays. The rich oil contribution for each component is found from the over-all material balance knowing three of the four streams involved.

D. TERMINAL TRAY EVALUATION

In absorber calculations temperature and flow rates must be estab-

lished for either the top or bottom tray. In previous methods the top tray temperature was arbitrarily specified ten degrees above the lean oil temperature or some other experience number. Hull and Raymond proposed an empirical relation based on operational data to determine the discharge gas temperature as a function of the heat of absorption released on the top tray. The absorption on the top tray was calculated by a pseudo-bubble point calculation filling the void with lean oil. More recently, Landes and Bell calculated the temperature by heat balance around the top tray. The temperature of the tray below the top was calculated likewise by heat balance based on an assumed temperature for the third tray.

The proposed method of determining a terminal tray temperature is based on a pseudo-bubble point calculation to determine the absorption on the top tray. The end temperature is calculated from either equation (34) or (35);

$$T_{DG} - T_{LO} = \frac{\Delta H_{ABS,TOP} - Cp_{NEXT} \left[T_{DG} - T_{NEXT} \right]}{Cp_{LO}} \qquad (34)$$

and

$$T_{RO} - T_{IG} = \frac{\Delta H_{ABS,BTM} - Cp_{NEXT} \left[T_{RO} - T_{NEXT} \right]}{Cp_{IG}} \qquad (35)$$

where heat capacities are of the total stream and the subscript NEXT represents the adjacent tray. The heat of absorption at the top of the column is determined by the absorption at the top. The heat of absorption at the bottom is part of the difference between total heat of absorption and that of the top tray. The choice of equations is made to minimize the contribution of the temperature difference between the end and adjacent trays. The adjacent tray temperature is empirically estimated (see Figure 3) by correcting the linear temperature profile. The

correction is the difference between the column average and linear average temperatures. The over-all iteration scheme converges rapidly because the pseudo-bubble point portion is relatively temperature insensitive.

E. HEAT BALANCE

Two important quantities are calculated in this section: 1) the temperature of the end tray not yet calculated; 2) the column average temperature. The unknown stream temperature is calculated from a simple heat balance since the enthalpies of the feed streams and one of the product streams have been evaluated. A temperature is assumed and an enthalpy calculated. The Newton-Raphson (11) convergence method

$$T_{NEW} = T - \frac{f(T)}{f'(T)} \tag{36}$$

works easily since $f(T)$ is just a constant minus the stream enthalpy and $f'(T)$ is the stream heat capacity.

The column average temperature has been introduced to indicate the bulge in the temperature profile due to heat of absorption. It is calculated directly from the equation

$$T_{AVE} = T_{DG} + \frac{\left[Cp_{DG}(T_{RO} - T_{DG}) + (1-w)\Delta H_{ABS} \right]}{Cp_{DG} + Cp_{OIL}} \tag{37}$$

where Cp_{DG} and Cp_{OIL} are the stream heat capacities for the dry gas and lean oil and w is the fractional absorption on the end trays. This equation has the inherent assumptions that any material eventually absorbed is returned to its original temperature and the difference in liquid and vapor heat capacities can be neglected.

F. ADJUSTING SECTION

If the estimated shrinkage equals the calculated shrinkage, no
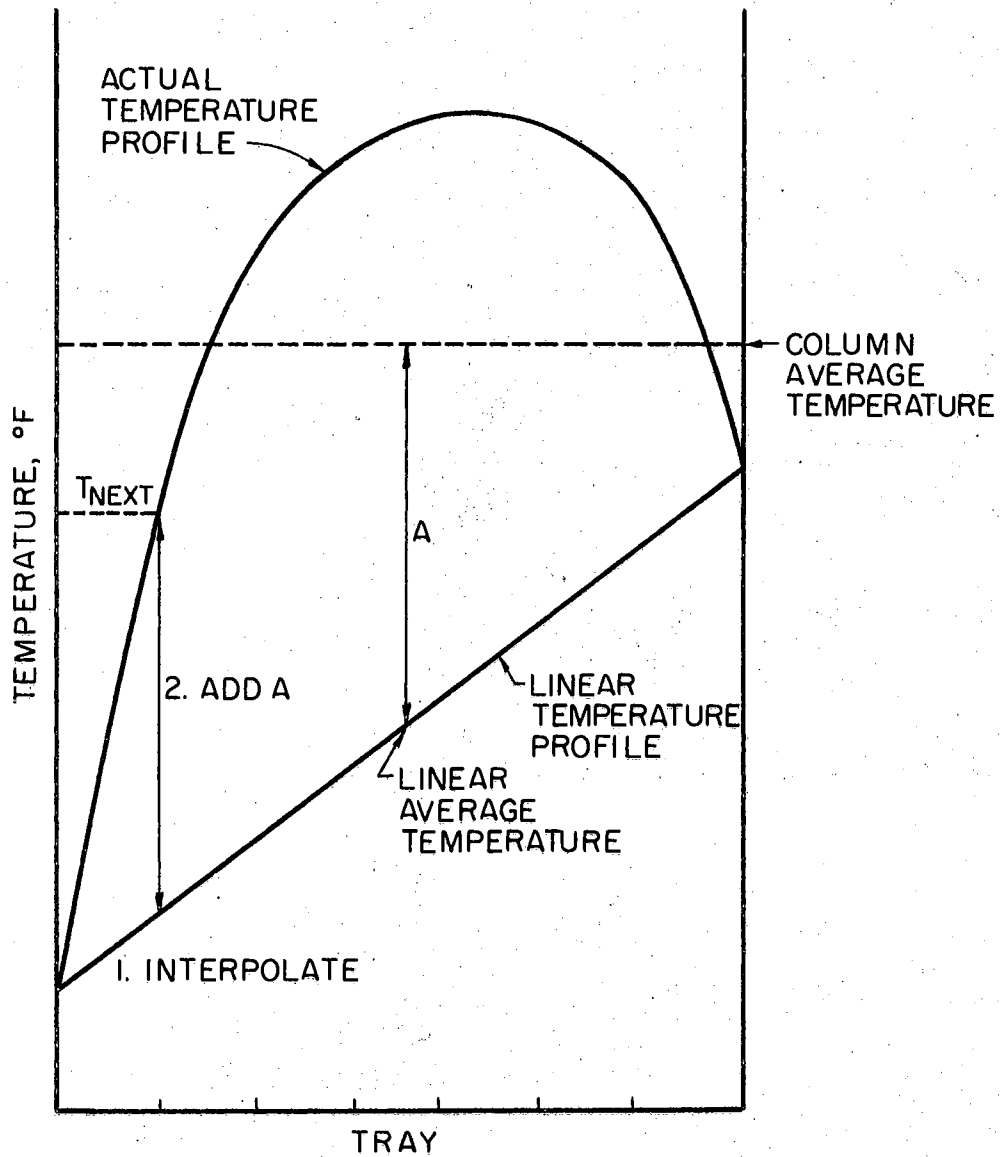
Figure 3. Typical Temperature Profile

calculations are done in this section. If not, new L/V profiles are computed using results of the present iteration. The L/V ratio at the bottom is the rich oil rate divided by the in-gas rate minus the estimated shrinkage on the bottom tray. The top L/V is the liquid leaving the top tray divided by the dry gas rate. The average of the L/V profile is approximated by the equation

$$(L/V)_{AVE} = \frac{L_n - (V_{n+1} - V_n)}{V_n - 0.05S} \tag{38}$$

where L_n is the rich oil; V_{n+1} vapor leaving the bottom tray; and S is the total gas absorbed. The numerator is the oil leaving the tray above the bottom tray. The denominator is an empirical estimate of the vapor leaving that tray. If calculations are done in this section, calculation returns to the absorption section. Otherwise, calculation proceeds to the lean oil adjusting section.

G. LEAN OIL ADJUSTING SECTION

The desired recovery of the key component is tested in this section. If the recovery is equal to that specified the solution has been reached. Otherwise, the lean oil rate is adjusted by the empirical relationship suggested by previous absorption work (14). The new lean oil rate is given by

$$L_{o\ NEW} = L_{o\ OLD} (ED/F)^{1.2} \tag{39}$$

where ED is the specified recovery rate and F is the recovery at the old oil rate, $L_{o\ OLD}$. When the lean oil rate has been adjusted, computation returns to the absorption section.

CHAPTER IV

EVALUATION

The major purpose of this thesis is the development of an absorber short-cut method that yields results comparable with rigorous tray-by-tray results. The rigorous results are supplied by the Sujata method as modified and programmed by Spear. For a new method to be practical its results must surpass those predicted by the classical Edmister and Kremser-Brown methods, as well as those predicted by the Hull-Raymond method. This investigation does not compare results with actual column data, but rather with theoretical results, a procedure used to minimize errors in thermodynamic and equilibrium data and field analysis. Such an evaluation examines each of the short-cut methods to determine how well it predicts the results of tray-by-tray technique.

A description of the program used in evaluating the Edmister and the Kremser-Brown method, as well as a thorough description of the Sujata program can be found in the work by Spear (14). The Hull-Raymond method was adapted to computer solution directly from their outline with the necessary figures curve fitted by least squares to power series.

General Description

Comparison of methods was based on results from a broad range of absorber operating conditions. Adjustable parameters encountered were:

feed stream temperatures, number of theoretical trays, lean oil molecular weight and condition, operating pressure, key component (propane) recovery, and wet gas composition. A short-cut method's effectiveness was monitered by its ability to predict rich oil, discharge gas, and column average temperatures, lean oil rates, and methane and ethane recovery fractions comparable with tray-by-tray results furnished by the Sujata method.

A total of forty-four absorber specifications were evaluated with the MORE method, the Edmister method, and Kremser-Brown method. Product stream temperatures required by Edmister and Kremser-Brown methods were provided directly from Sujata results. The over-all scheme of absorbers was based upon a arbitrary "standard" absorber and variations. Specifications of the standard absorber are described in Table II. Evaluation of the Hull-Raymond calculation method was limited to eight runs, the standard absorber with only feed temperature variation.

Temperature of the Feed Streams

Most absorbers several decades ago operated at or near ambient or plant stream temperatures. Recently, many absorbers have been brought on line around the $0^\circ F$ range. For a thorough evaluation all absorber options were evaluated at two temperatures, $0^\circ F$ and $100^\circ F$; and the standard absorber was evaluated at six other temperatures, 75, 50, 20, 10, -10, and $-20^\circ F$. Another temperature option was a twenty degree temperature difference in the feed streams.

Number of Trays

The number of trays in the absorber was varied from two to twelve

with eight being used in the standard. The tray number was varied primarily to supply information on the shrinkage profile. The number eight was chosen because actual absorber data were reported with twenty to twenty-seven actual trays. Using an estimated efficiency of thirty-three per cent, this gave approximately eight theoretical trays.

TABLE II

DESCRIPTION OF STANDARD ABSORBER

	COLUMN CONDITIONS		
		500.0	Pressure
		8	Trays
		9	Components
		2	Feeds

	COMPONENT	RICH GAS COMPOSITION MOLS	LEAN OIL COMPOSITION MOL FRACTION
1	Methane	89.01	0.000
2	Ethane	6.29	0.000
3	Propane	2.36	0.000
4	i-Butane	0.49	0.000
5	n-Butane	0.68	0.000
6	i-Pentane	0.13	0.000
7	n-Pentane	0.29	0.000
8	Lean Oil	0.00	1.000
9	Nitrogen	0.75	0.000

Product specifications recover seventy per cent of propane.

Lean Oil Molecular Weight

Although thermodynamic and equilibrium data were not under consideration in this evaluation, their availability affected the selection of lean oil. The lean oil of the standard absorber was a 200 molecular weight oil with a normal boiling point of 500°F. Although this oil was too viscous for practical use at lower temperatures, its viscosity had no effect on the numerical solution and it was used anyway. Other oils used were decane and 250 molecular weight oil with 700°F normal boiling point.

Lean Oil Condition

The standard absorber was evaluated with completely denuded lean oil. Non-stripped and methane charged lean oils were also run. The composition of the lean oils can be found in Table III.

TABEL III

RELATIVE LEAN OIL COMPOSITIONS

		LEAN OIL, MOL FRACTION		
	COMPONENT	STANDARD	NON-STRIPPED	METHANE CHARGED
1	Methane	0.000	0.000	0.150
2	Ethane	0.000	0.000	0.000
3	Propane	0.000	0.000	0.000
4	i-Butane	0.000	0.005	0.000
5	n-Butane	0.000	0.005	0.000
6	i-Pentane	0.000	0.010	0.000

TABLE III (continued)

	COMPONENT	LEAN OIL, MOL FRACTION		
		STANDARD	NON-STRIPPED	METHANE CHARGED
7	n-Pentane	0.000	0.010	0.000
8	Lean Oil	1.000	0.970	0.850
9	Nitrogen	0.000	0.000	0.000

Operating Pressure

A pressure of 500 psia was used in the standard absorber. To ensure that the results of the proposed MORE method were valid over the normal absorber pressure range runs were made at 200 and 1000 psia.

Recovery of Key Component

Propane was the key component in all runs. The standard recovery was seventy per cent of the propane. Other recoveries were twenty and ninety per cent of the propane. Such extremes were imposed to open the required lean oil rate to wide ranges.

Gas Composition

The choice of the standard wet gas composition was completely arbitrary. Therefore, the nomenclature rich or lean in-gas is simply relative to the assumed standard. The composition of the standard, rich and lean wet gas is given in Table IV. The choices for lean and rich gas were made to determine the effect of composition on temperature and

shrinkage profiles and on the end tray shrinkage.

TABLE IV

WET GAS COMPOSITION

		COMPOSITION, MOLS		
	COMPONENT	STANDARD	RICH	LEAN
1	Methane	89.01	86.01	92.75
2	Ethane	6.29	6.79	5.00
3	Propane	2.36	3.36	1.75
4	i-Butane	0.49	1.49	0.25
5	n-Butane	0.68	1.18	0.25
6	i-Pentane	0.13	1.13	0.00
7	n-Pentane	0.29	0.29	0.00
8	Lean Oil	0.00	0.00	0.00
9	Nitrogen	0.75	0.75	0.00

TABLE V

LIST OF RUNS

RUN	TRAYS	PRESSURE, PSIA	OIL MW	OIL STRIPPED	OIL TEMP, F	GAS TEMP, F	C3 RECOVERY	GAS COMPOSITION
1	8	500.	200.	YES	100.	100.	0.70	AVERAGE
2	8	500.	200.	YES	50.	50.	0.70	AVERAGE
3	8	500.	200.	YES	0.	0.	0.70	AVERAGE
4	8	500.	200.	YES	100.	120.	0.70	AVERAGE
5	8	500.	200.	YES	120.	100.	0.70	AVERAGE
6	8	500.	200.	YES	0.	20.	0.70	AVERAGE
7	8	500.	200.	YES	20.	0.	0.70	AVERAGE
8	8	500.	200.	YES	100.	100.	0.20	AVERAGE
9	8	500.	200.	YES	0.	0.	0.20	AVERAGE
10	8	500.	200.	YES	100.	100.	0.90	AVERAGE
11	8	500.	200.	YES	0.	0.	0.90	AVERAGE
12	8	500.	200.	NO	100.	100.	0.70	AVERAGE
13	8	500.	200.	NO	0.	0.	0.70	AVERAGE
14	8	500.	200.	YES	100.	100.	0.70	RICH
15	8	500.	200.	YES	0.	0.	0.70	RICH
16	8	500.	200.	YES	100.	100.	0.70	LEAN
17	8	500.	200.	YES	0.	0.	0.70	LEAN
18	8	200.	200.	YES	100.	100.	0.70	AVERAGE
19	8	200.	200.	YES	0.	0.	0.70	AVERAGE
20	8	1000.	200.	YES	100.	100.	0.70	AVERAGE
21	8	1000.	200.	YES	0.	0.	0.70	AVERAGE
22	8	500.	145.	YES	100.	100.	0.70	AVERAGE
23	8	500.	145.	YES	0.	0.	0.70	AVERAGE
24	8	500.	250.	YES	100.	100.	0.70	AVERAGE
25	8	500.	250.	YES	0.	0.	0.70	AVERAGE
26	2	500.	200.	YES	100.	100.	0.70	AVERAGE
27	2	500.	200.	YES	0.	0.	0.70	AVERAGE
28	12	500.	200.	YES	100.	100.	0.70	AVERAGE
29	12	500.	200.	YES	0.	0.	0.70	AVERAGE
30	8	500.	200.	YES	75.	75.	0.70	AVERAGE
31	8	500.	200.	YES	20.	20.	0.70	AVERAGE
32	8	500.	200.	YES	10.	10.	0.70	AVERAGE
33	8	500.	200.	YES	-10.	-10.	0.70	AVERAGE
34	8	500.	200.	YES	-20.	-20.	0.70	AVERAGE
35	3	500.	200.	YES	100.	100.	0.70	AVERAGE
36	3	500.	200.	YES	0.	0.	0.70	AVERAGE
37	4	500.	200.	YES	100.	100.	0.70	AVERAGE
38	4	500.	200.	YES	0.	0.	0.70	AVERAGE
39	5	500.	200.	YES	100.	100.	0.70	AVERAGE
40	5	500.	200.	YES	0.	0.	0.70	AVERAGE
41	8	500.	145.	YES	0.	0.	0.70	RICH
42	8	500.	145.	YES	0.	20.	0.70	AVERAGE
43	8	500.	200.	NO	100.	100.	0.70	AVERAGE
44	8	500.	145.	NO	0.	0.	0.70	AVERAGE

CHAPTER V

RESULTS

The Kremser-Brown, Edmister, and MORE methods were used to determine operational conditions for forty-four absorbers described previously. The Hull-Raymond method was used on the standard absorber at eight temperatures. The results from all methods were compared with Sujata solutions.

The results from the Kremser-Brown and Edmister methods were obtained by a computer program developed by Erbar (18); the Sujata in a program by Spear; and the Hull-Raymond and MORE methods in programs associated with this thesis. Each of the short-cut methods was adapted to use the same enthalpy and equilibrium data as the Sujata program. In the Kremser-Brown and Edmister programs the unknown temperatures were provided by Sujata results. This resulted in a definite test of each method's ability to describe the theoretical tray model.

The evaluation of each calculation method is based on how well that method predicts the absorption of methane and ethane, the lean oil rate required for a specified propane absorption, the product stream temperature, and, in some cases, the column average temperatures. The comments on each method represent a summary of the general trends observed.

TABLE VI

SUMMARY OF RESULTS

KREMSER-BROWN CALCULATION METHOD

Predicted Variable	Remarks
Methane Recovery	Average 10 % low
Ethane Recovery	Average 10 % low
Lean Oil Rate	Average 35 % high
Temperatures: Rich Oil	Specified from Sujata results
Lean Gas	Specified from Sujata results
Column Average	Does not apply

EDMISTER CALCULATION METHOD

Predicted Variable	Remarks
Methane Recovery	Average 1.4 % low
Ethane Recovery	Average 3.0 % low
Lean Oil Rate	Average 2.0 % high
Temperatures: Rich Oil	Average 1.72°F high
Lean Gas	Specified from Sujata results
Column Average	Does not apply

HULL-RAYMOND CALCULATION METHOD

Predicted Variable	Remarks
Methane Recovery	Average 0.4 % low
Ethane Recovery	Average 1.3 % low
Lean Oil Rate	Average 5.1 % high
Temperatures: Rich Oil	Average 2.7°F high
Lean Gas	Average 1.4°F low
Column Average	Average 7.1°F high

TABLE VI (continued)

MORE CALCULATION METHOD

Predicted Variable	Remarks	
Methane Recovery	Average 0.6 %	low
Ethane Recovery	Average 1.0 %	low
Lean Oil Rate	Average 0.4 %	high
Temperatures: Rich Oil	Average 1.8°F	high
Lean Gas	Average 0.2°F	high
Column Average	Average 1.4°F	high

SUMMARY: Kremser-Brown Calculation Method

The Kremser-Brown calculation method is the oldest, simplest, and most conservative of the calculation methods. Its results (Appendix A) are dependent upon good information of product stream temperatures. Even with the best values for these quantities, the resultant absorber is quite conservatively designed; perhaps too conservative for good design.

High oil rates, 35%, and low recoveries, 10%, result from the evaluation of an average absorption factor. In the computer program the average absorption factor is found which gives the designated recovery of the key component. The L/V ratio and then the lean oil rate are backed out of the correct absorption factor. The L/V ratio used is the minimum value attainable with given column conditions, the lean oil rate over the wet gas rate. From this analysis, the Kremser-Brown calculation always over-designs oil rates, but closes in on rigorous solutions when high oil rates are accompanied by small amounts of absorption; phenomena leading to linear temperature distribution and

constant flow ratios. This usually occurs at low pressure operation of
the type used when Kremser and Brown developed the calculation procedure.

Edmister Calculation Method

The results of the Edmister calculation method (Appendix A) indi-
cate it is quite a good method provided accurate values of the dry gas
temperature can be established. The dry gas temperature has greater
influence upon the rich oil temperature than upon the effective absorp-
tion factor because it is inversly coupled to the rich oil temperature.
The effective absorption factor is a function of the product of the two
temperatures and is comparatively insensitive.

The rich oil temperature is consistently higher than Sujata results
by an average of $1.72^{O}F$ in spite of an increase in lean oil rate. This
occurs primarily because the over-all heat balance convergence limit
for the Edmister program is the same as that of the Sujata for each
tray. This allows for the difference (see Appendix D for more detailed
discussion).

The component recoveries are low for a given oil rate. This is
pointed out by the low methane and ethane recoveries and the increased
oil rate for a specified propane recovery. If the two tray model for
the effective absorption factors is going to work, then the terminal
absorption factors must be slightly in error. Since vapor-liquid
equilibrium constants are evaluated very near the correct temperatures
by specification, the deviation in absorption factors must occur in the
L/V ratio. In the computer program the L/V ratios are calculated by
assuming equal absorption on each stage. Such procedure results in
lower L/V ratios than observed in the Sujata results where the major

portion of absorption occurred on the end trays. Figure 4 shows several examples of actual L/V profiles compared with linear approximations.

From Figure 4, the constant absorption per tray model yields good L/V values at the bottom of the column, but often inaccurate, low values at the top of the column. Such a model would produce low absorption factors and a low effective absorption factor.

A possible improvement of the computer program would be the introduction of the end tray absorption factor, $\mathcal{W}$, to provide better L/V values for the end trays. This was attempted but results were not improved.

Hull-Raymond Calculation Method

The Hull-Raymond method was developed empirically from extensive operation data and would be expected to accurately describe absorbers operating within its range. The results from calculation of the standard absorber bear this out. At lower temperatures the column average temperature exceeds the Sujata values by ten degrees, yet the lean oil rate and component recovery rates remain close. At the low temperatures (i.e., low oil rate), the bounds of many of the empirical plots are reached or exceeded. This explains the deviation in column average temperature.

The lean gas temperature averaged $1.4^{\circ}F$ lower than Sujata results. In the Hull-Raymond method the lean gas temperature is found from an empirical plot as a function of the heat of absorption of the top tray per pound of lean oil. Inherent in the plot is the specified lean oil heat capacity of 0.5 Btu per pound. The rich oil temperature is found by over-all heat balance and reflects the oil rate, dry gas temperature,
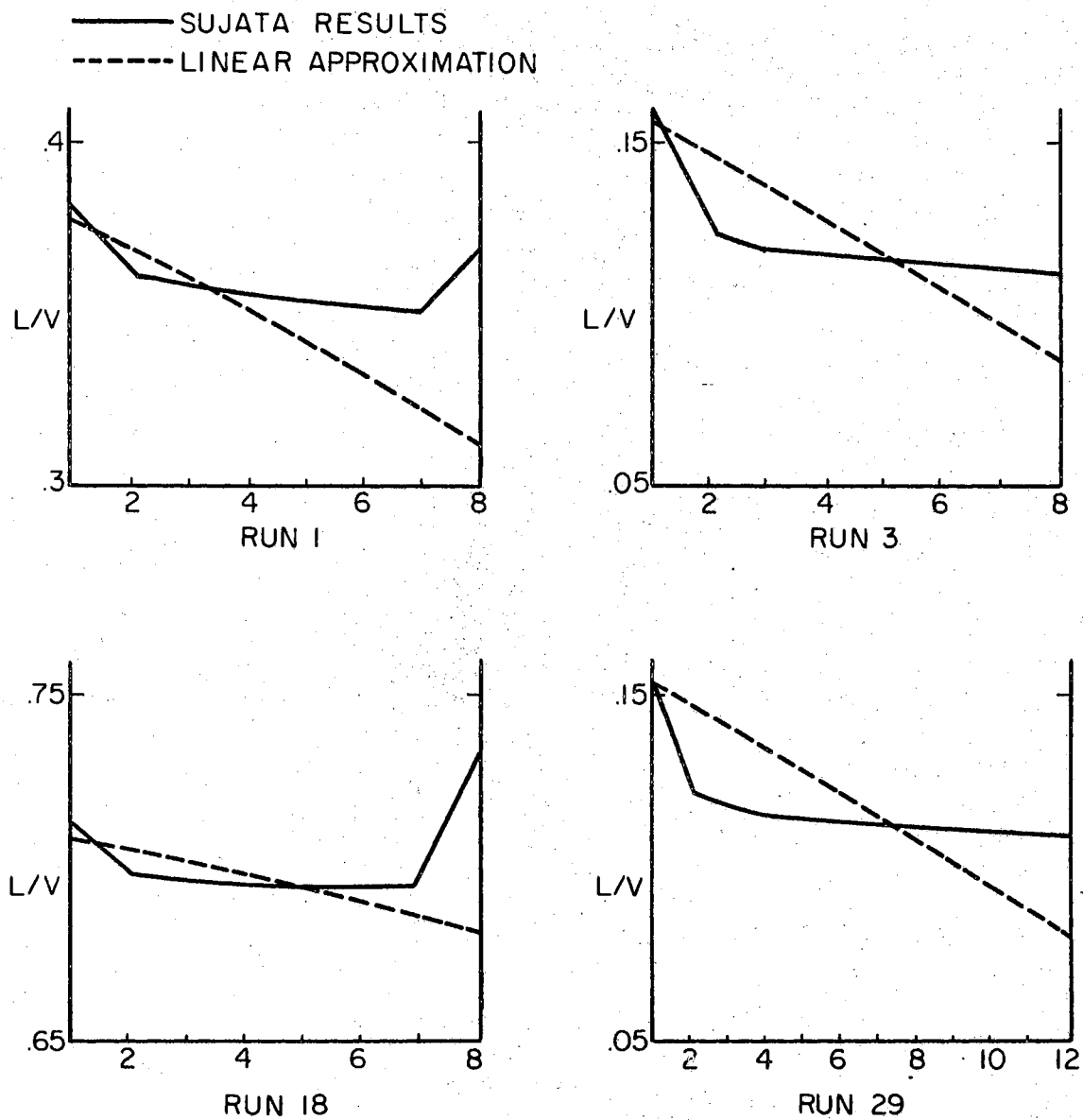
Figure 4. L/V Profile as a Function of
Column Position

and component absorption. The rich oil temperature averaged 2.5°F
higher than Sujata results as a result of low dry gas temperatures and
tighter convergence limits than the Sujata program (see Appendix D).

Within the range of applicability set forth by the authors, the
Hull-Raymond calculation method provides good values with the least
specifications. It is impaired in its ability to describe low tempera-
ture absorber operation because of the low oil rates encountered.
Efforts to extend the Hull-Raymond method to low temperature operation
and to generalize its many empirical plots led to the development of
the absorber calculation method associated with this thesis. This
method is called the MORE method for brevity.

MORE Calculation Method

The short-cut absorber calculation procedure developed in this
thesis, the MORE method, gave the best results of the methods tested.
It did so with neither product stream temperature specified. Component
recoveries, lean oil rates, and column temperatures were consistently
closer to Sujata results than the other short-cut methods. The dry gas
temperature averaged 0.2°F higher than Sujata results for forty-four
runs and varied only 2.06°F below to 1.63°F above as maximum deviations.
The rich oil temperature was 1.70°F higher than Sujata results, with a
range of -0.25 to 3.80°F. A deviation of this size and direction could
have resulted from a tighter over-all convergence in the MORE program.
Both the MORE and Sujata programs solve heat balances with a trial and
error procedure. Convergence occurs when the error in the heat balance
becomes smaller than a specified value. In the Sujata program the
limit is a fractional part of the enthalpy of the streams leaving a

given tray. In the new short-cut program the limit is a fractional part of the total feed enthalpy. The Sujata program employs heat balances on each tray and accrues minor deviations on each tray. The total deviation is the sum of the individual tray errors. The MORE short-cut method has only a single over-all heat balance and a single deviation (see Appendix D).

The column average temperature predicted by the MORE model averaged 1.4 degrees high and ranged from $0.78^\circ F$ below to $3.65^\circ F$ above Sujata results. These values are felt to be accurate enough for this short-cut method.

The lean oil rate and component recovery rates were in good agreement with Sujata results. In forty of the forty-four runs the MORE method most accurately predicted the lean oil rate given by the Sujata program. The average deviation was 0.4%. The greatest deviation by the MORE method between required lean oil rates was 16.5% below Sujata results when the required rate was only 0.314 moles of lean oil per hundred moles of wet gas. The component recovery rates for methane and ethane were 0.6% and 1.0% low respectively, the best values for the short-cut methods.

If more accuracy is needed for component recovery and the temperature profile is sufficiently accurate, the absorption factor method used in the MORE program can be improved. Component recovery is determined by three absorption factors - top, bottom, and interior tray average. The present method calculates the average absorption factor at the column average temperature and an empirically approximated L/V ratio for the interior trays. Still other work could be done explaining the occurence of the terminal tray absorption factor, ω, and its

variation.

CHAPTER VI

CONCLUSIONS

The major purpose of this thesis was the development of an absorber short-cut method capable of yielding results comparable with rigorous tray-by-tray methods starting with the same data. Such a method, the MORE method, has been developed and describes simple absorber operation both externally and internally. The product streams and temperatures compared favorably with rigorous results of the Sujata method. For forty-four runs the maximum temperature deviation was less than 4°F and the maximum deviation in lean oil rate was less than 0.4 moles.

The Kremser-Brown method was also compared with Sujata results. Product stream temperatures were supplied by Sujata results. Even so, the results of the Kremser-Brown calculation were consistently conservative, giving excessive oil rate and low recoveries. Based on this comparison exact temperatures of product streams are not necessary for the application of this method. The recommended use of the Kremser-Brown method would be in early stages of economic feasibility studies, much as an artist uses a sketch, for it is indispensable as a first guess.

The Edmister method gave excellent results compared with Sujata results. In the absence of excellent thermodynamic data, it would give as reliable design as rigorous methods. Dependence upon temperature

specification for the dry gas stream detracted from the method's generality. The Edmister "effective" absorption factor method is a good short-cut method. It can be expected to yield reasonable design data with little specification and good data when accurate temperatures for a terminal product stream are supplied.

The average results of the Edmister method predicted a lean oil rate 2.0% higher than Sujata solution. Methane and ethane recoveries were 1.4 and 3.0% lower than the Sujata results.

The Hull-Raymond calculation method gave good results for absorbers operating in the range from which it was developed. That range was absorbers operating above or around ambient temperature and with the lean oil dominating the heat balances. Attempts to extend empirical temperature plots were unsuccessful. The Hull-Raymond method of evaluating the effective absorption factor was more difficult to use than that of Edmister, but it gave satisfactory results where the rest of the Hull-Raymond method applied.

The method developed in this thesis, the MORE method, provided design information closer to rigorous calculation results than any other short-cut method tested in every respect; temperatures, lean oil rates, and component recoveries. The method incorporated heat balance and absorption factors with no empirical graphs and appeared to give results comparable to rigorous method wherever solution can be reached. The only non-explicit assumption was the introduction of the terminal tray absorption,ω. For absorbers with four or more theoretical stages, eighty per cent of the absorption occurs on the two end trays. Average results of the MORE method predicted all temperatures within $1.8^{\circ}F$ of Sujata results and all component and oil rates within 1.0%. The MORE

method is recommended for use in the space between rough guesses and rigorous calculation for any simple absorber.

LIST OF NOMENCLATURE

A – absorption factor defined as $A = L/KV$

A_e – effective absorption factor defined by equation (22)

A' – absorption factor defined by equation (23)

c – number of components

Cp – heat capacity of specified stream

ED – desired key component absorption

F – component fraction absorbed

ΔH_{ABS} – heat of absorption

K – component equilibrium constant defined by $K = y/x$

L – total liquid rate leaving a tray, moles

l – component liquid rate leaving a tray, moles

n – number of trays in the column

S – total wet gas shrinkage, moles

T – temperature

V – total vapor rate leaving a tray, moles

v – component vapor rate leaving a tray, moles

x – liquid mole fraction

y – vapor mole fraction

Greek Symbols

π_A - $A_1A_2A_3\ldots A_n$

Σ_A - $A_1A_2A_3\ldots A_n + A_2A_3\ldots A_n +\ldots+ A_n$

ϕ_A - fraction of any wet gas component not recovered

ψ_A - fraction of any lean oil component leaving in the dry gas

w - fraction of total gas absorption that occurs on the terminal trays

Subscripts

AVE - column average

BTM - bottom tray

DG   - discharge gas stream

i   - tray reference

IG   - in-gas stream

LO   - lean oil stream

n   - total number of trays (last tray)

NEXT - tray reference of adjacent tray

o   - reference for stream entering tray 1

OIL - average of lean oil and rich oil streams

RO   - rich oil stream

TOP - top tray

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APPENDIX A

TABULATED RESULTS

In the tables that follow the results of each short-cut method are compared with the Sujata results. Results are presented for the dry gas, column average, and rich oil temperatures; the required lean oil rate; and the methane and ethane recovery rates.

TABLE VII

PREDICTED DRY GAS TEMPERATURE

RUN	SUJATA	MORE	HULL—RAYMOND
1	103.73	104.27	104.00
2	58.14	59.12	64.10
3	18.18	18.64	16.26
4	103.87	103.96	...
5	122.84	123.40	...
6	18.97	18.76	...
7	32.60	32.74	...
8	107.48	108.31	...
9	15.44	13.38	...
10	103.11	103.30	...
11	13.58	15.21	...
12	103.87	104.37	...
13	18.41	18.80	...
14	104.84	105.04	...
15	23.24	22.74	...
16	103.22	103.64	...
17	14.10	13.83	...
18	101.93	101.97	...
19	8.37	9.03	...
20	106.21	106.98	...
21	27.35	26.33	...
22	105.48	106.12	...
23	23.39	23.05	...
24	103.82	104.26	...
25	17.83	18.13	...
26	104.84	104.42	...
27	16.99	17.17	...
28	103.82	104.20	...
29	17.62	18.55	...
30	80.54	81.22	80.07
31	33.12	34.59	32.41
32	25.48	25.92	24.20
33	11.21	11.36	8.30
34	4.42	4.13	0.01
35	104.33	104.39	...
36	17.85	17.60	...
37	104.03	104.46	...
38	18.31	18.53	...
39	103.99	104.39	...
40	18.47	18.58	...
41	30.50	30.44	...
42	25.39	25.65	...
43	102.14	102.28	...
44	20.00	20.02	...

TABLE VIII

PREDICTED COLUMN AVERAGE TEMPERATURE

RUN	SUJATA	MORE	HULL-RAYMOND
1	106.31	108.13	106.36
2	61.61	63.78	66.68
3	18.07	20.13	31.61
4	113.01	114.22	...
5	120.35	121.17	...
6	32.23	36.03	...
7	21.76	21.92	...
8	103.43	104.79	...
9	9.64	9.39	...
10	105.94	107.40	...
11	19.85	21.59	...
12	105.81	107.66	...
13	17.73	19.72	...
14	112.15	114.44	...
15	34.44	38.19	...
16	103.34	104.84	...
17	8.08	9.54	...
18	103.50	104.73	...
19	14.95	17.01	...
20	107.84	110.08	...
21	20.10	21.25	...
22	107.84	109.87	...
23	18.09	19.85	...
24	105.57	107.29	...
25	16.03	17.83	...
26	106.19	106.32	...
27	17.75	17.96	...
28	105.79	108.26	...
29	17.40	20.24	...
30	83.66	85.74	82.60
31	35.65	37.44	46.54
32	26.90	29.26	39.25
33	9.16	10.86	23.46
34	0.20	1.53	15.15
35	106.34	107.13	...
36	18.44	19.34	...
37	106.54	107.52	...
38	18.53	19.41	...
39	106.55	107.78	...
40	18.45	19.74	...
41	35.44	38.57	...
42	34.11	37.39	...
43	105.21	107.09	...
44	17.38	19.88	...

TABLE IX

PREDICTED RICH OIL TEMPERATURE

RUN	SUJATA	MORE	EDMISTER	HULL-RAYMOND
1	105.26	106.70	108.05	108.30
2	61.04	63.41	63.82	64.10
3	21.86	23.61	20.07	20.81
4	106.80	107.77	133.70	...
5	123.33	124.21	121.24	...
6	28.28	31.31	34.96	...
7	31.45	30.86	21.37	...
8	106.09	107.63	105.56	...
9	12.06	12.21	*...	...
10	104.46	105.41	107.27	...
11	19.42	22.14	22.11	...
12	105.19	106.57	108.14	...
13	21.74	23.43	20.09	...
14	108.26	109.95	114.03	...
15	34.41	38.06	38.28	...
16	103.84	104.85	104.83	...
17	13.95	13.85	9.02	...
18	102.68	103.19	104.69	...
19	12.79	14.83	17.14	...
20	107.76	109.94	109.91	...
21	28.03	28.24	18.60	...
22	107.41	109.08	110.13	...
23	24.73	25.66	19.04	...
24	105.16	106.36	108.02	...
25	20.45	21.78	20.37	...
26	105.51	104.73	106.28	...
27	17.37	17.53	18.04	...
28	105.02	106.70	108.06	...
29	21.14	23.65	20.52	...
30	82.60	84.54	85.65	85.70
31	37.09	39.39	37.98	37.90
32	29.47	31.43	29.15	29.31
33	14.19	15.58	10.59	12.33
34	6.27	7.35	0.66	4.42
35	105.48	105.69	107.15	...
36	19.03	20.67	19.04	...
37	105.49	106.56	107.57	...
38	20.20	23.05	19.36	...
39	105.51	106.63	107.78	...
40	21.00	23.31	19.54	...
41	39.93	43.14	39.07	...
42	33.88	36.56	37.15	...
43	103.92	104.66	107.29	...
44	22.62	24.19	20.40	...

* DID NOT CONVERGE

TABLE X

PREDICTED LEAN OIL RATE

RUN	SUJATA	MORE	EDMISTER	KREMSER-BROWN	HULL-RAYMOND
1	26.568	26.771	27.574	35.360	26.330
2	14.705	14.907	15.361	20.878	15.361
3	7.006	6.988	6.934	11.174	7.907
4	27.614	27.674	28.880	37.773	...
5	32.018	31.972	32.392	40.227	...
6	8.606	8.643	8.868	12.717	...
7	8.036	7.860	7.607	12.863	...
8	6.146	6.274	6.605	9.918	...
9	0.317	0.265	*...	2.997	...
10	38.679	38.737	39.707	50.661	...
11	11.137	11.056	11.075	15.879	...
12	26.710	26.914	27.610	35.328	...
13	6.996	6.985	6.944	11.170	...
14	25.673	25.886	26.716	36.336	...
15	7.797	7.666	7.283	12.225	...
16	27.875	28.046	28.877	25.054	...
17	6.982	7.042	7.341	10.592	...
18	60.370	60.690	61.094	68.990	...
19	15.765	16.010	16.050	18.030	...
20	16.783	16.873	18.101	28.156	...
21	4.533	4.389	4.436	11.312	...
22	27.259	27.487	28.200	35.650	...
23	7.195	7.192	6.987	11.396	...
24	26.573	26.728	27.578	35.303	...
25	6.785	6.768	6.958	11.074	...
26	40.222	40.204	40.008	54.947	...
27	10.374	10.417	10.498	17.223	...
28	26.021	26.353	27.343	34.756	...
29	6.766	6.916	6.942	10.944	...
30	20.042	20.280	20.938	27.490	20.210
31	9.710	9.759	9.938	14.531	10.713
32	8.311	8.330	8.384	12.771	9.288
33	5.796	5.740	5.566	9.731	5.386
34	4.670	4.597	4.274	8.430	5.386
35	32.474	32.714	32.777	43.581	...
36	8.352	8.453	8.368	13.753	...
37	29.543	29.781	30.070	39.521	...
38	7.660	7.640	7.580	12.469	...
39	28.138	28.304	28.806	37.454	...
40	7.350	7.302	7.223	11.601	...
41	8.374	8.269	7.712	12.601	...
42	9.345	9.350	9.462	13.104	...
43	30.815	31.200	30.863	35.123	...
44	8.218	8.398	7.848	11.222	...

* DID NOT CONVERGE

TABLE XI

PREDICTED METHANE RECOVERY

RUN	SUJATA	MORE	EDMISTER	KREMSER-BROWN	HULL-RAYMOND
1	5.055	5.058	5.108	4.760	4.902
2	3.800	3.801	3.789	3.325	3.787
3	2.998	2.943	2.812	2.226	3.041
4	5.092	5.089	5.221	4.987	...
5	5.669	5.641	5.625	5.215	...
6	3.078	3.005	2.988	2.414	...
7	3.187	3.136	2.948	2.432	...
8	1.376	1.389	1.422	1.334	...
9	0.725	0.717	*...	0.607	...
10	7.188	7.166	7.213	6.825	...
11	4.210	4.138	3.951	3.176	...
12	5.032	5.030	5.111	4.757	...
13	2.987	2.935	2.814	2.225	...
14	5.161	5.208	5.131	4.656	...
15	3.549	3.424	3.126	2.261	...
16	5.044	5.036	5.191	4.930	...
17	2.579	2.570	2.622	2.243	...
18	4.207	4.214	4.210	4.095	...
19	1.936	1.938	1.901	1.632	...
20	7.581	7.530	7.724	7.004	...
21	5.845	5.671	5.343	4.142	...
22	5.128	5.128	5.171	4.788	...
23	3.049	3.004	2.844	2.253	...
24	5.038	5.036	5.108	4.755	...
25	2.950	2.901	2.812	2.213	...
26	7.403	7.396	7.608	7.345	...
27	3.933	3.939	3.978	3.433	...
28	4.972	4.990	5.040	4.681	...
29	2.949	2.923	2.790	2.184	...
30	4.371	4.379	4.404	4.000	4.278
31	3.272	3.246	3.166	2.627	3.339
32	3.129	3.080	2.983	2.420	3.195
33	2.879	2.818	2.650	2.043	2.891
34	2.770	2.707	2.497	1.871	2.738
35	6.063	6.076	6.171	5.863	...
36	3.356	3.359	3.297	2.739	...
37	5.556	5.541	5.627	5.305	...
38	3.165	3.124	3.044	2.482	...
39	5.316	5.304	5.371	5.040	...
40	3.082	3.030	2.926	2.358	...
41	3.661	3.553	3.198	2.305	...
42	3.216	3.142	3.079	2.460	...
43	5.013	5.091	5.487	9.954	...
44	3.008	2.996	2.903	3.899	...

* DID NOT CONVERGE

TABLE XII

PREDICTED ETHANE RECOVERY

RUN	SUJATA	MORE	EDMISTER	KREMSER-BROWN	HULL-RAYMOND
1	1.690	1.684	1.686	1.635	1.649
2	1.513	1.504	1.485	1.394	1.497
3	1.402	1.371	1.300	1.140	1.393
4	1.673	1.670	1.696	1.667	...
5	1.783	1.772	1.757	1.698	...
6	1.378	1.341	1.322	1.190	...
7	1.459	1.434	1.342	1.195	...
8	0.467	0.469	0.475	0.458	...
9	0.358	0.355	*...	0.315	...
10	2.405	2.393	2.398	2.346	...
11	1.947	1.915	1.823	1.632	...
12	1.687	1.680	1.686	1.634	...
13	1.400	1.370	1.300	1.140	...
14	1.871	1.872	1.846	1.774	...
15	1.685	1.624	1.492	1.264	...
16	1.313	1.307	1.327	1.296	...
17	0.992	0.980	0.978	0.890	...
18	1.514	1.511	1.510	1.495	...
19	1.109	1.102	1.078	1.004	...
20	2.009	1.994	2.005	1.918	...
21	1.825	1.776	1.665	1.436	...
22	1.702	1.695	1.694	1.639	...
23	1.422	1.394	1.313	1.148	...
24	1.689	1.682	1.686	1.634	...
25	1.392	1.364	1.299	1.137	...
26	2.277	2.276	2.300	2.273	...
27	1.771	1.772	1.780	1.662	...
28	1.666	1.660	1.661	1.608	...
29	1.385	1.361	1.284	1.120	...
30	1.597	1.591	1.585	1.517	1.565
31	1.436	1.419	1.370	1.243	1.441
32	1.418	1.390	1.334	1.197	1.418
33	1.389	1.355	1.266	1.088	1.363
34	1.376	1.342	1.234	1.036	1.330
35	1.991	1.991	2.008	1.968	...
36	1.559	1.556	1.534	1.391	...
37	1.849	1.844	1.857	1.812	...
38	1.475	1.460	1.419	1.269	...
39	1.774	1.768	1.776	1.728	...
40	1.438	1.415	1.361	1.207	...
41	1.723	1.668	1.515	1.276	...
42	1.422	1.382	1.345	1.202	...
43	1.684	1.693	1.665	1.632	...
44	1.409	1.390	1.290	1.142	...

* DID NOT CONVERGE

APPENDIX B

DATA

Although thermodynamic and equilibrium data do not enter the analysis of the separate absorption calculation methods, their source and values might prove helpful in analysis of this thesis and use of results.

The vapor-liquid equilibruim constant for each component was curve fitted from data taken from N.G.S.M.A. Data Book (16). The equation was of the form

$$\ln K = A + B/T + C/T^2 + D/T^3$$

where $T = \,^{\circ}R/100$.

The liquid and vapor enthalpy were taken from the same source but fitted to the equations

$$H_v = A + BT + CT^2$$

and

$$H_l = A + BT + CT^2$$

where again $T = \,^{\circ}R/100$.

TABLE XIII

K VALUE COEFFICIENTS

COMPONENT	A	B	C	D
− 200 PSIA				
METHANE	0.62936	41.67177	−222.35380	302.69330
ETHANE	1.89355	27.73705	−254.60420	408.75500
PROPANE	1.41560	31.66986	−302.31800	442.47130
I−BUTANE	1.06618	37.21840	−363.29280	531.47560
N−BUTANE	1.70875	28.09457	−337.54400	504.89700
I−PENTANE	1.55110	26.85196	−345.38220	474.47930
N−PENTANE	1.45431	28.93027	−365.60330	500.95320
200 MW OIL	6.27465	−65.07498	−174.09260	245.73240
NITROGEN	−4.32824	−15.77304	84.92576	−151.42850
− 500 PSIA				
METHANE	0.86989	26.59536	−149.53520	180.98960
ETHANE	2.78127	1.13197	−122.21500	211.40340
PROPANE	2.67452	0.07913	−143.93070	205.87790
I−BUTANE	2.10888	6.29061	−189.73140	241.37350
N−BUTANE	2.84696	−3.14933	−166.11700	225.79970
I−PENTANE	2.28437	3.43893	−217.79740	278.51110
N−PENTANE	2.78643	−3.21470	−199.56500	257.36800
200 MW OIL	6.81646	−34.68934	−508.67470	701.43180
NITROGEN	−5.18179	−15.63904	78.55727	−130.90850
DECANE	12.66661	−164.81940	368.43090	−402.67520
250 MW OIL	−5.45264	−12.38642	66.67615	−118.86150
− 1000 PSIA				
METHANE	−0.60247	42.93807	−248.92420	375.15760
ETHANE	1.98596	2.60610	−122.12060	235.75920
PROPANE	1.74780	1.27734	−124.64890	182.44810
I−BUTANE	1.21320	7.51930	−169.46260	222.95100
N−BUTANE	1.71057	1.19572	−155.51380	212.94260
I−PENTANE	1.11933	9.60301	−219.32000	296.40310
N−PENTANE	1.78504	−0.54964	−177.99260	227.70500
200 MW OIL	19.15638	−276.73060	829.38210	−798.32900
NITROGEN	−6.65472	−4.10338	22.03521	−39.18790

TABLE XIV

VAPOR ENTHALPY COEFFICIENTS

COMPONENT	A	B	C
- 200 PSIA			
METHANE	1293.00	636.43	24.000
ETHANE	2808.80	1008.30	39.328
PROPANE	4344.10	1277.50	60.454
I-BUTANE	6590.80	1346.40	92.632
N-BUTANE	6590.80	1346.40	92.632
I-PENTANE	8353.80	1541.10	116.350
N-PENTANE	8353.80	1541.10	116.350
200 MW OIL	28028.00	1311.70	561.760
- 500 PSIA			
METHANE	612.61	777.21	15.010
ETHANE	594.36	1450.00	15.633
PROPANE	4928.90	573.48	136.510
I-BUTANE	7759.90	132.25	218.040
N-BUTANE	7759.90	132.25	218.040
I-PENTANE	9254.40	212.11	251.650
N-PENTANE	9254.40	212.11	251.650
DECANE	12873.00	1413.60	390.560
200 MW OIL	16600.00	1985.20	549.190
250 MW OIL	16600.00	1985.20	549.190
- 1000 PSIA			
METHANE	518.18	716.74	21.001
ETHANE	528.86	1317.40	28.629
PROPANE	5615.70	170.98	166.830
I-BUTANE	8108.50	-190.91	234.360
N-BUTANE	8108.50	-190.91	234.360
I-PENTANE	10630.00	-525.51	297.240
N-PENTANE	10630.00	-525.51	297.240
200 MW OIL	37289.00	-5889.70	1160.600

TABLE XV

LIQUID ENTHALPY COEFFICIENTS

COMPONENT	A	B	C
METHANE	828.12	-821.57	257.710
ETHANE	-1759.90	97.65	235.070
PROPANE	-807.45	-263.30	305.330
I-BUTANE	-3040.00	587.75	279.520
N-BUTANE	-3040.00	587.75	279.520
I-PENTANE	-5114.80	1327.20	261.530
N-PENTANE	-5114.80	1327.20	261.530
DECANE	-10001.00	2420.70	479.370
200 MW OIL	-14782.00	3403.50	673.800
250 MW OIL	-14782.00	3403.50	673.800

APPENDIX C

COMPUTER PROGRAM

The absorption calculation method developed in association with
this thesis was programmed in FORTRAN IV for use on the IBM 7040 compu-
ter. The program handles a maximum of twenty components for a simple,
two feed, non-intercooled absorber consisting of an integral number of
ideal trays. The program has one executive branch with a cabinet of
seven subordinate sections which in turn are supported by nine auxiliary
subroutines. Figure 5 shows the sequence of operations as governed by
the executive program.

Executive

MAIN, the executive program, directs the sequence as shown in
Figure 5. It is a simple director which could be expanded or rearranged
to handle different input, output, and calculation schemes. It contains
the iteration counters for both the shrinkage and lean oil adjustment
sections and will terminate calculations if either exceeds fifty.

Support Cabinet

SUBROUTINE DATA

All input information is read by DATA. Terminal tray absorption,
flow ratios, temperature profile and lean oil rates are calculated or
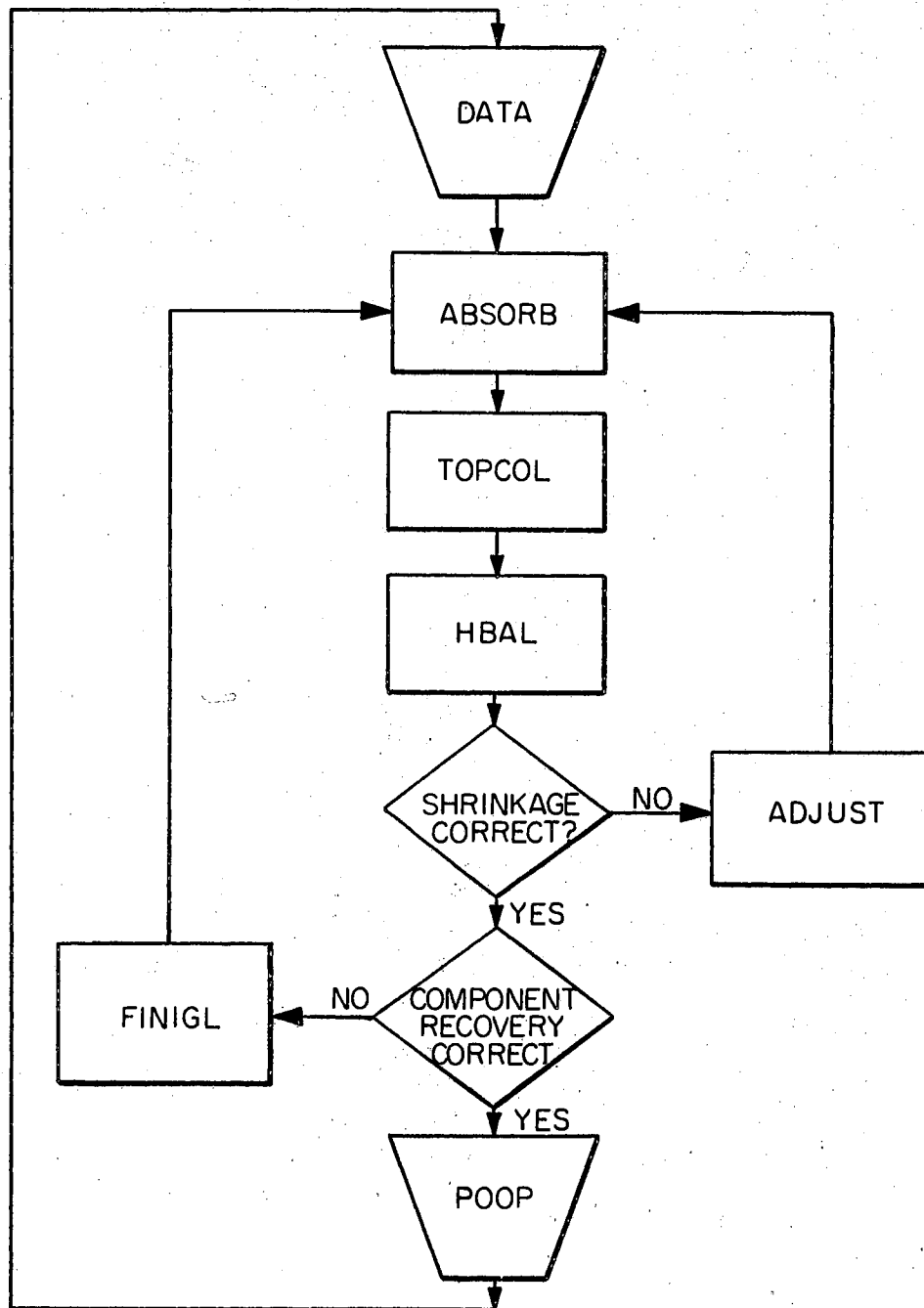set as necessary.

Figure 5. Program Diagram

SUBROUTINE ABSORB

For given temperatures and flow rates for the bottom and middle section, the product streams are calculated.

SUBROUTINE TOPCOL

TOPCOL is the subroutine that evaluates the top tray in the column. After calculating the pseudo-bubble point of the liquid leaving the top tray, TOPCOL chooses the top or bottom tray to minimize the effect of the adjacent tray temperature and finds the initial terminal temperature. The maximum number of iterations to find the temperature is set at fifty. Logic is added to limit changes in the predicted temperature to values less than ten degrees F. After ten iterations succeeding temperature values are averaged to dampen oscillations.

SUBROUTINE HBAL

Given feed stream temperatures and either product stream temperature, HBAL calculates the remaining temperature by the Newton-Raphson method applied to the fundamental heat balance equation. The limit of such iterations is again set at fifty. The column average temperature is also found in this section.

SUBROUTINE ADJUST

ADJUST determines whether or not solution has been reached for a given lean oil rate by comparing estimated and calculated shrinkages. If a solution has not been reached, new flow ratios are calculated based on the calculated shrinkage.

SUBROUTINE FINIGL

FINIGL is the subroutine that adjusts the lean oil flow rate if

necessary. If a change is necessary, the L/V ratios are scaled according to the change in lean oil rate and the enthalpy of the lean oil stream is calculated.

SUBROUTINE POOP

POOP is the major output subroutine called by MAIN after the complete solution has been reached. It also can serve as an intermediate output facility yielding the lean oil rate, estimated shrinkage, temperatures (TAV, TRO, and TDG), and liquid rate leaving the top tray for each major calculation loop (see Figure 5).

Auxiliaries

SUBROUTINE HLIQ

HLIQ is the subroutine that calculates the liquid enthalpy for individual components at a given temperature. HLIQ is called by many subroutines (see Appendix B).

SUBROUTINE HFEED

The enthalpy of each feed stream is calculated as well as total input enthalpy. The maximum deviation in the over-all heat balance is calculated as a per cent of the total feed enthalpy. It can be expanded to handle two phase streams as well as just liquid and vapor. This subroutine is called only by DATA and FINIGL.

SUBROUTINE HBAL

HBAL calculates the heat of absorption for each component at a specified temperature. The heat of absorption used in this program is calculated as the difference in vapor and liquid enthalpy at a tempera-

ture. It is called wherever the need for heat of absorption values arises.

SUBROUTINE CSUBP

CSUBP calculates the heat capacity or the derivative of enthalpy with respect to temperature for each component either as a vapor or a liquid depending upon which is requested.

FUNCTION COMPK

COMPK is the subprogram that calculates the vapor-liquid equilibrium ratio for a specified component and temperatures. COMPK can be called by many subroutines (see Appendix B).

SUBROUTINE ERROR

ERROR terminates calculation for a given problem and prints computational variables at the time of the error. Control returns to MAIN and a new problem is read into the computer by DATA. ERROR can be called from within any iterative calculation loop.

SUBROUTINE NOTE

The subroutine NOTE provides insight directly into the subroutines ABSORB, TOPCOL, HBAL, ADJUST, and FINIGL. NOTE has no use in calculation, but merely serves in error analysis.

Input Data

The input data for the program associated with this thesis is arranged as follows:

Card 1   "Problem Identification"

This card is used for identification of the program. The identification can be either numeric or alphabetic.

    READ: PID
    FORMAT: 12A6

Card 2   "Column Variables"

This card contains column variables which describe the simple absorption system.

    N   Number of Trays
    NCP   Number of Components
    MFD   Number of Feeds (always two)
    P   Column Pressures

    READ: N, NCP, MFD, P
    FORMAT: (3I3, F10.4)

Card 3   "Control Variables"

This card contains the control variables which are discussed below.

KLOOP   Lean Oil Option

    KLOOP = 1   The lean oil rate is specified in the input data.
    KLOOP = 2   The initial estimate of the lean oil rate is given in the input data. The program then adjusts the lean oil rate to the correct values.
    KLOOP = 3   The initial lean oil rate is estimated by the program.

KX   Intermediate Output Variable

    KX = 0   The intermediate output from each major iteration is not printed.
    KX = 1   The intermediate output from each major iteration is printed.

KT   Initial Temperature Profile Variable

    KT = 0   The intial temperature profile is calculated in the pro-
             gram.
    KT = 1   The initial temperature profile is given in the input
             data.

JOB   Inidvidual Subroutine Output Variable

JOB is internally converted to binary mode with the integer 1
causing output and 0 skipping output. There are five subroutines with
this capability, ABSORB, TOPCOL, HBAL, ADJUST, and FINIGL. JOB can
have values from zero to thirty-one $(2^5 - 1)$. Except for error analy-
sis and debugging, JOB is set at zero.

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

Card 4i   "Component Identification"

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

        READ: COMP (J)
        FORMAT: 12A6

Card 5   "Absorption Variables"

This card identifies the key component and specifies the recovery
fraction. For a specified lean oil rate (KLOOP = 1), the recovery
fraction may be left blank.

        READ: KEY, ED
        FORMAT: I3, F10.7

Card 6   "Convergence Limits"

This card contains the principal convergence limits of the program
or rather the maximum error that will be acceptable in a solution. The
variables are listed below with a suggested value included in parenthe-

sis.

ER1 - Heat balance limit, fraction feed enthalpy (0.0001).

ER2 - Material balance limit, fractional difference between succeeding values of shrinkage (0.0001).

ER3 - Temperature agreement limit, degree F (0.01).

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

Card 7i   "Equilibrium Coefficients"

This series of cards (one for each component) contains the coefficients for equilibrium constant. Each card contains the coefficients of one component in the same component order as Card 4i. The equilibrium constant is calculated by the equation of the form

$$\ln K = AK1 + AK2/T + AK3/T^2 + AK4/T^3$$

NOTE: All thermodynamic and equilibrium data must be curve fitted against temperature of the form $^{\circ}R/100$.

READ: AK1, AK2, AK3, AK4
FORMAT: 4E14.8

Card 8i   "Vapor Enthalpy Coefficients"

This series of cards (one for each component) contains the coefficients for component vapor enthalpy as a function of temperature, $^{\circ}R/100$, of the form

$$HV = AV1 + AV2 \times T + AV3 \times T^2$$

READ: AV1, AV2, AV3
FORMAT: 3E12.6

Card 9i   "Liquid Enthalpy Coefficients"

This series of cards (one for each component) contains the coefficients for component liquid enthalpy as a function of temperature,

^{O}R/100, of the form

$$HL = AL1 + AL2 \times T + AL3 \times T^2 \quad .$$

READ: AL1, AL2, AL3
FORMAT: 3E12.6

Card 10i   "Feed Variables"

This series of cards (one for each feed) contains the column feed

position and condition with the lean oil being the last card in the

series. The variables are:

NFD   feed tray number;
MOF   mode of feed;
TFD   feed temperature (^{O}F).

The feed streams presently can only enter in two conditions but

provisions have been made to facilitate expansion. The feed conditions

of MOF are:

MOF = 1   the feed is all liquid at a specified temperature;
MOF = 2   the feed is all vapor at a specified temperature.

READ: NFD, MOF, TFD
FORMAT: 2I3, F10.5

Card 11i   "Component Feed Rates"

This series of cards (one for each feed) contains the component

feed rates for each feed stream with the components in the same order

as Card 4i and the feeds in the order of Card 10i. If the lean oil rate

is to be predicted internally (KLOOP = 3), its feed rate may be in terms

of mole fraction. FD is the component feed variable.

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

NOTE: Each feed begins on a new card.

Card 12   "Operational Variables"

This card contains control variables to over ride those set up by the program.   The variables are:

NOIL   number of the lean oil, unless specified it is assumed to be the last component;

SHRINK   estimated shrinkage for the first iteration;

TABS   terminal tray absorption, unless specified it is set by the program at eighty per cent.

READ: NOIL, SHRINK, TABS
FORMAT: I3, 2F10.7

Card 13   "Initial Temperature Profile"

This card contains the initial estimates for discharge gas, rich oil and average temperatures in $^{\circ}F$ and is present only if KT = 1 in Card 3.

READ: TDG, TRO, TAV
FORMAT: 3F10.5

APPENDIX D

EFFECTS OF VARIOUS HEAT BALANCE LIMITS

ON SUJATA RESULTS

In the Sujata tray-by-tray absorber method, programmed by Spear
(14), material balance and equilibrium relations are used to determine
component absorption on every tray. When correct vapor and liquid rates
are found for given temperature profile, heat balances are used to
correct temperatures on every tray. The calculation continues until
liquid and vapor rates and temperatures no longer change. The itera-
tion variable is tray temperature and convergence is measured by heat
balance.

The criterion of heat balance convergence is an error less than a
specified fraction of exit stream enthalpy for each tray. Convergence
problems occur when severe limits are used, while temperature discrep-
ancies appear when limits are relaxed. The small errors introduced
by approximate convergence may cancel or compound. The simple absorber
initial temperature profiles are provided by linear interpolation of
feed stream temperatures. In the simple adiabatic absorber the final
temperature profile will everywhere be higher than the initial profile.
Thus, successive estimates approach the final temperature from the same
direction. The errors per tray are then additive and significant.

Figures 6 and 7 show the effect of various heat balance limits on
the standard absorber with $100^{\circ}F$ and $0^{\circ}F$ feed respectively. The conver-
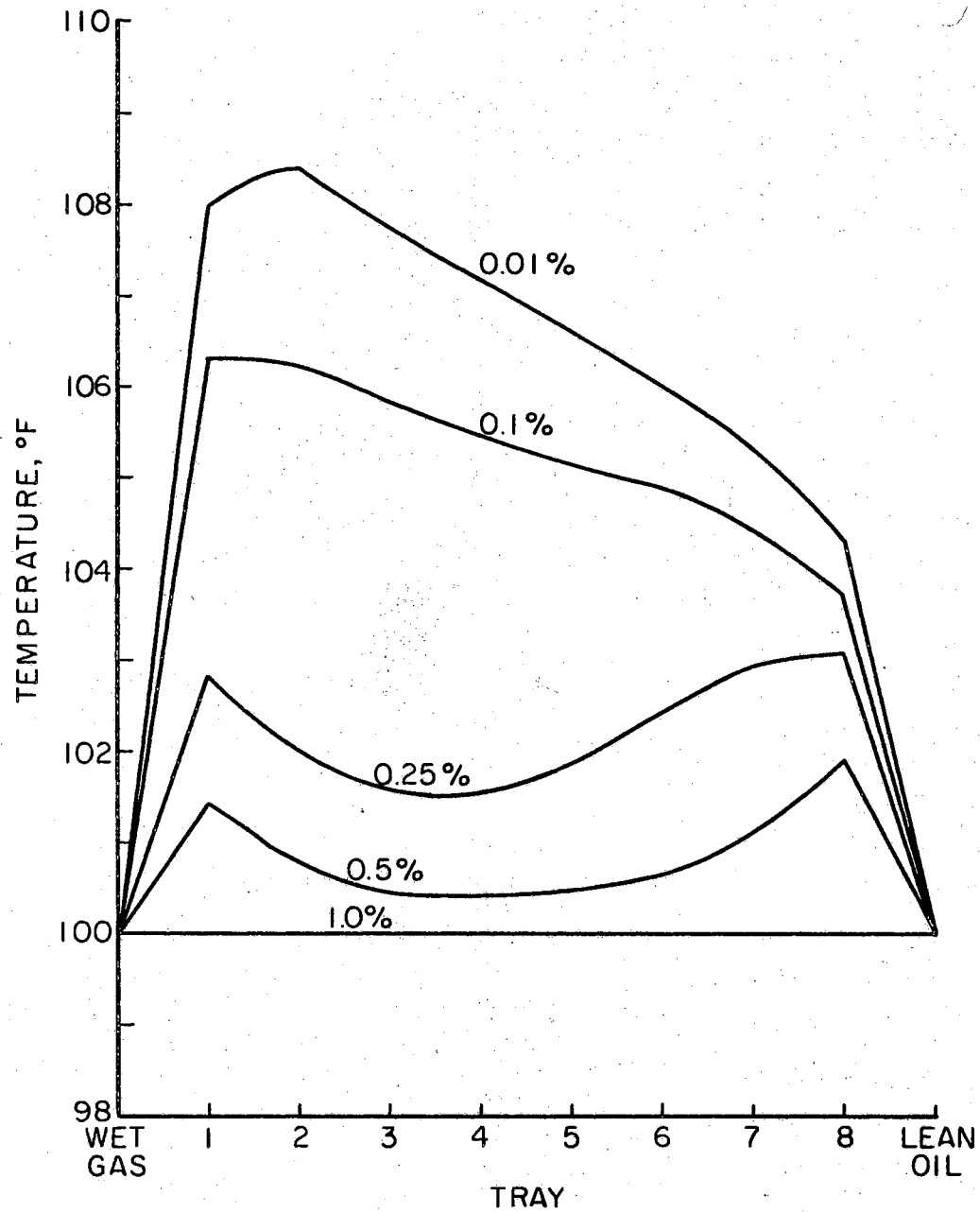
Figure 6. Heat Balance Limit Effect on Sujata Solution
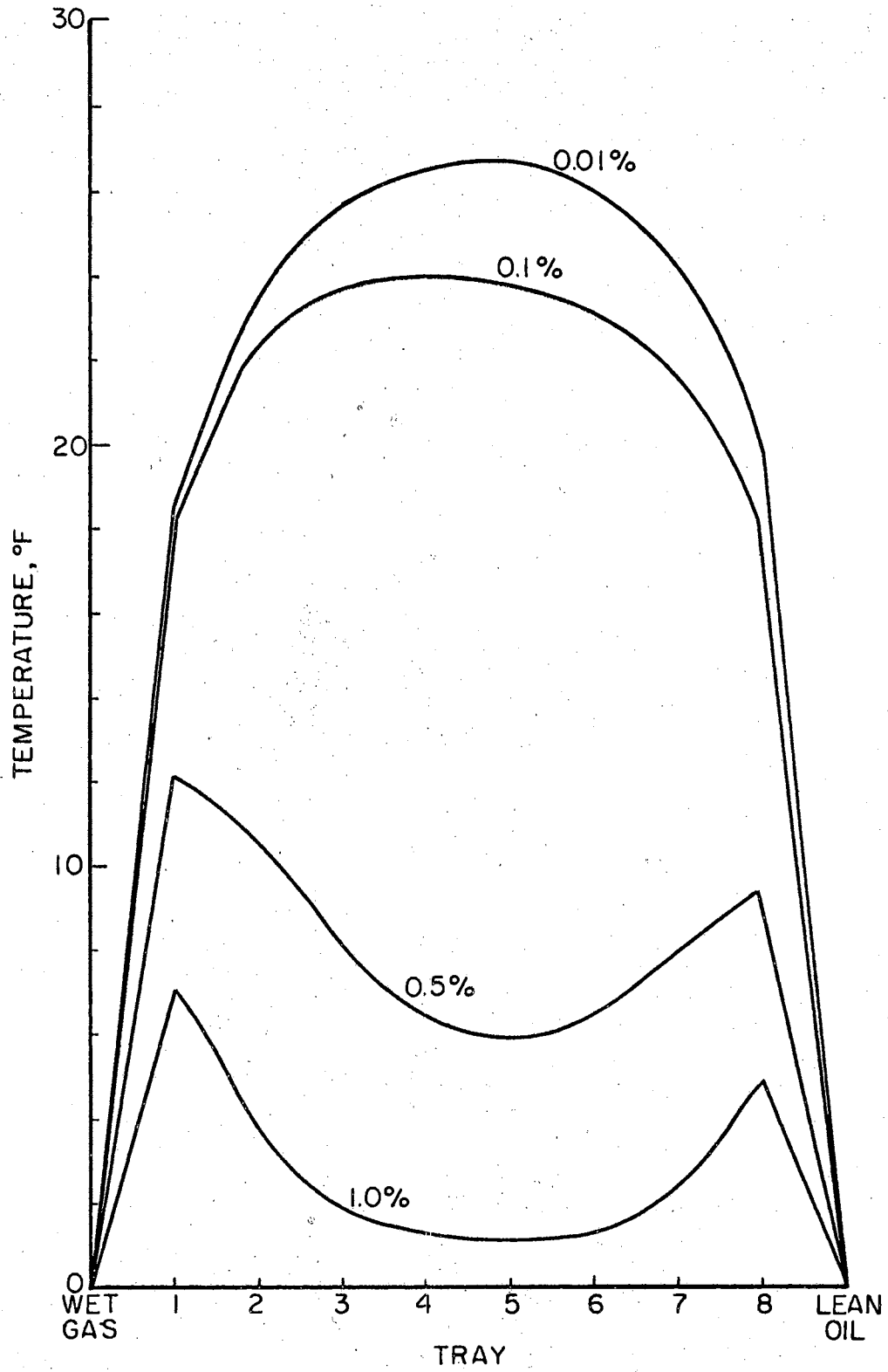of Standard Absorber With 100°F Feeds

Figure 7. Heat Balance Limit Effect on Sujata Solution of Standard Absorber With 0°F Feeds

gence limits are presented as a per cent of the exit stream enthalpy. The same convergence limit does not entail the same temperature accuracy for both systems.

Although the Sujata program written by Spear is an excellent absorber calculation method, there are plausible modifications:

1) since the Sujata iteration variable is temperature, a temperature convergence limit instead of a heat balance convergence limit would be reasonable;

2) computing time might be shortened if the program initially ran with a more relaxed convergence limit than finally desired. As the estimate of the lean oil rate is improved, the convergence limit could be tightened;

3) to diminish over-all error introduced by minor deviations in heat balance on each stage, final temperatures on adjacent stages should be approached from opposite directions.

APPENDIX E

SAMPLE CALCULATION

An absorber operates with eight theoretical trays at 300 psia.
Lean oil, octane, enters at 90°F and a fixed rate of 20 moles per 100
moles of rich gas. The rich gas enters at 90°F and its composition can
be found in column (1) of Table XVI. Determine the product of stream
compositions and temperatures.

BASIS: 100 moles of rich gas

SOLUTION:

I. PRELIMINARY CALCULATIONS

   A. Assume total shrinkage = 15 moles.
      Set end tray shrinkage, ω, at 80%.
      Estimate average L/V and assume constant

$$(L/V) = \frac{\text{lean oil} + \text{shrinkage}}{\text{rich gas}}$$

$$(L/V) = \frac{20 + 15}{100} = 0.35$$

   B. Calculate enthalpy and heat capacity of feed streams.

      Rich gas enthalpy $= \Sigma(1) \times (3) = 735065$ Btu
      Rich gas heat capacity $= \Sigma(1) \times (4) = 1163$ Btu/°F

      Lean oil enthalpy $= \Sigma(2) \times (5) = 486308$ Btu
      Lean oil heat capacity $= \Sigma(2) \times (6) = 2163$ Btu/°F

   C. Estimate total heat of absorption, assuming all 15 moles

      has a heat of absorption between those of ethane and propane.

$$\Delta H_{TOT} = S(\Delta H_{C2} + \Delta H_{C3})/2$$

$$\Delta H_{TOT} = 15\left[(9417-5888)+(12922-6981)\right]/2.0$$

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TABLE XVI

SAMPLE CALCULATIONS

	COMPONENT	1 V_{n+1}	2 l_o	VAPOR - 90°F 3 H_v	4 C_p	LIQUID - 90°F 5 H_L	6 C_p	7 K-111.35°F	8 A	9 V_i	10 l_n	11 K-103.5°F	12 X_i
1	METHANE	70.	0.	5435.	8.95	4105.	20.13	10.3200	0.0339	67.626	2.374	10.080	0.0780
2	ETHANE	15.	0.	9417.	14.89	5888.	26.83	2.1760	0.1608	12.588	2.412	2.053	0.0713
3	PROPANE	10.	0.	12922.	19.40	6981.	30.95	0.7535	0.4645	5.360	4.640	0.695	0.0896
4	N-BUTANE	4.	0.	16165.	23.04	8648.	36.62	0.2724	1.2849	0.133	3.867	0.247	0.0063
5	N-PENTANE	1.	0.	19480.	27.46	10096.	42.04	0.1049	3.3365	0.000	1.000	0.000	0.0000
6	OCTANE	0.	20.	49279.	73.41	24319.	108.15	0.0061	57.3400	0.348	19.692	0.000	0.0000
		100.	20.							86.055	33.945		0.2452

	13 l_1	14 ΔH-103.5°F	15 V_2	16 C_{p_v}-103.5°F	17 H_v-103.5°F	18 H_L-111.35	19 C_{p_L}	20 A_{TOP}	21 A_{BTM}	22 A_{AVE}	23 V_i	24 l_n
1	2.065	1157.	69.691	9.05	5555.	4548.	9.04	0.0305	0.0342	0.0300	67.616	2.384
2	1.888	3346.	14.476	15.08	9618.	6473.	15.06	0.1496	0.1619	0.1430	12.616	2.384
3	2.373	5762.	7.733	19.65	13183.	7657.	19.62	0.4419	0.4675	0.4145	5.562	4.438
4	0.167	7310.	0.300	23.51	16477.	9445.	23.46	1.2467	1.2911	1.1492	0.211	3.789
5	0.000	9163.	0.000	28.03	19810.	11008.	27.89	3.3161	3.1360	3.0000	0.000	1.000
6	20.000	24439.	0.300	75.40	50275.	26665.	73.41	59.5500	57.7900	51.9400	0.337	19.633
											86.342	33.658

$$\Delta H_{TOT} = 71025 \text{ Btu}$$

D. Estimate initial column temperature found by mixing the two feeds and adding the estimated heat of absorption. The equation for this calculation is

$$T = T_{LO} + \underline{/}\, H_{TOT} - CPIG\,(T_{IG} - T_{LO})\,\underline{/}/(CPLO + CPIG)$$

$$T = 90 + 71025/(2163 + 1163)$$

$$T = 90 + 21.35 = 111.35^{\circ}F$$

Assume all temperatures are equal

$$T_{DG} = T_{RO} = T_{AVE} = 111.35^{\circ}F$$

II. ABSORPTION SECTION

A. Find the K values at $111.35^{\circ}F$ $\underline{/}$Engineering Data Book $(16)\,\underline{/}$.

B. Calculate individual absorption factors

$$A = \frac{1}{K}(L/V) \quad .$$

C. Calculate dry gas composition with equation (11) assuming constant absorption factors for the first iteration.

$$A_{TOP} = A_{BTM} = A_{AVE}$$

D. Calculate rich oil rate

$$(1) + (2) - (9) = (10).$$

Total Dry Gas $= \Sigma (9) = 86.055$ moles
Total Rich oil $= \Sigma (10) = 33.945$ moles

Calculate shrinkage $= 100 - 86.055 = 13.944$ moles.

III. TOP TRAY EVALUATION

A. For the first estimate the top tray temperature was assumed to be $111.35^{\circ}F$. This calculation section refines the value by combining pseudo-bubble point and heat balance techniques. The procedure is iterative and could begin with the previous

estimate, $111.35^{\circ}F$. Since the lean oil with a relatively large specific heat enters the top tray at $90^{\circ}F$, a temperature lower than $111.35^{\circ}F$ would be expected. For convenience, assume the top tray temperature, T_{DG}, is $103.5^{\circ}F$ and find the K values.

B. Calculate liquid mole fraction for all components in equilibrium with dry gas except the lean oil.

$$x_i = \frac{v_i}{VK_1} = \frac{(9)}{86.055 \times (11)} = (12)$$

C. Fill the void in the mole fraction with lean oil.

$$x_{lean\ oil} = 1.0 - \mathbf{\Sigma}(12) = 1.0 - 0.2452$$

$$x_{lean\ oil} = 0.7548$$

D. Determine the liquid leaving the top tray.

$$L_1 = \frac{moles\ lean\ oil}{lean\ oil\ mole\ fraction} = \frac{20}{.7548} = 26.48\ moles$$

E. Calculate composition of top tray liquid.

$$l_i = L_i x_i \; ; \quad (13) = 26.48 \times (12)$$

F. Determine the heat of absorption released on the top tray.

$$\mathbf{\Delta} H_{TOP} = \mathbf{\Sigma}(l_1 - l_o)\ H_i = \mathbf{\Sigma}\diagup(13) - (2)\diagup \times (14)$$

$$\mathbf{\Delta} H_{TOP} = 23,600\ Btu$$

G. Since the lean oil heat capacity is greater than that of the in-gas, use equation (34) to determine the dry gas temperature. The first step is to calculate the vapor entering tray 1 from tray 2.

$$v_2 = v_1 + l_1 - l_o$$

$$(15) = (9) + (13) - (2)$$

H. Calculate the heat capacity of V_2.

$$\text{CPNEXT} = \sum Cp_{v2} = \sum (15) \times (16)$$

$$\text{CPNEXT} = 1031 \text{ Btu}/{}^{\circ}\text{F}$$

I.   Estimate temperature on tray 2:

   1.   Linearily interpolate between terminal values;

$$T_1 = 103.5 {}^{\circ}\text{F}$$

$$T_8 = 111.35 {}^{\circ}\text{F}$$

$$T_2(\text{linear}) = 104.48 {}^{\circ}\text{F}$$

   2.   Correct for the difference between the column average and the linear average temperatures;

$$\text{CORRECTION} = 111.35 - (103.5 + 111.35)/2$$

$$\text{CORRECTION} = 111.35 - 107.42 = 3.93 {}^{\circ}\text{F}$$

   3.   The temperature on tray 2 is the linear value plus the correction calculated in step 2;

$$T_2 = 104.48 + 3.93 = 108.41 {}^{\circ}\text{F}$$

   4.   Find the temperature difference, ΔT.

$$\Delta T = T_2 - T_1 = 108.41 - 103.5$$

$$\Delta T = 4.91 {}^{\circ}\text{F}$$

J.   Calculate a new estimate of the top tray temperature, T_{DG}, from equation (34).

$$T_{DG} = 90 + \underline{/}\,23,600 + 1031(4.91)\,\underline{/}/2163 = 103.26 {}^{\circ}\text{F}$$

Ordinarily the calculation scheme outlined in this section would be repeated with the new estimate of T_{DG} until little or no change occurred in successive values. Since the old and new values are very close, the average value is taken for brevity rather than repeat the entire calculation.

$$T_{DG} = (103.26 + 103.5)/2 = 103.4 {}^{\circ}\text{F}$$

IV. HEAT BALANCE SECTION

    A. Calculate the enthalpy of dry gas stream.

$$\sum(9) \times (17) = 633,490 \text{ Btu}$$

    B. Calculate the enthalpy of the rich oil at the assumed temperature 111.35°F.

$$\sum(10) \times (18) = 587,082 \text{ Btu}$$

    C. Check assumed rich oil temperature by over-all heat balance.

	ENTERING		LEAVING
Lean Oil	486,380	Rich Oil	587,082
Rich Gas	735,065	Dry Gas	633,490
	1,221,445		1,221,572

The assumed rich oil temperature is correct. If the temperature were not correct, a new estimate for T_{RO} must be made and computation returns to part B of this section.

    D. Compute the dry gas heat capacity.

$$CPDG = \sum(9) \times (19) = 935 \text{ Btu/°F}$$

    E. Calculate the column average temperature using equation (37).

$$T_{AVE} = \frac{103.4 + \left[935(111.35 - 103.4) + 66479(1.0 - 0.8) \right]}{935 + 2163}$$

$$T_{AVE} = 110.1°F$$

V. ADJUSTING SECTION

The assumed shrinkage was 15 moles while the calculated value was 13.945 moles. For direct iteration the new estimate for the total shrinkage would be 13.945 moles. Experience and insight can over ride direct iteration and the estimate shrinkage is 13.765 moles. With this information new L/V ratios are calculated.

    A. Calculate L/V at the bottom of the column.

$$(L/V)_{BTM} = \frac{\text{rich oil}}{\text{rich gas - gas shrinkage across the bottom tray}}$$

$$(L/V)_{BTM} = \frac{20.0 + 13.675}{100 - \lfloor 0.8(13.675)-(26.48-20) \rfloor}$$

$$(L/V)_{BTM} = \frac{33.675}{95.54} = 0.3525$$

B. Calculate L/V on the top tray.

$$(L/V)_{TOP} = \frac{\text{liquid leaving tray 1}}{\text{dry gas}}$$

$$(L/V)_{TOP} = \frac{26.48}{100-13.675} = 0.3067$$

C. Compute the average L/V using equation (38).

$$(L/V)_{AVE} = \frac{33.675 - (100 - 95.54)}{95.54 - 0.05 \times 13.675}$$

$$(L/V)_{AVE} = 0.308$$

VI. ABSORPTION SECTION

A. Calculate the individual absorption factors for the top

tray, A_{TOP}.

$$A_{TOP} = (L/V)_{TOP} \times 1/K \text{ at } 103.4^{\circ}F = (20)$$

B. Calculate the absorption factors for the bottom tray, A_{BTM}.

$$A_{BTM} = (L/V)_{BTM} \times 1/K \text{ at } 111.35^{\circ}F = (21)$$

C. Calculate the average absorption factors, A_{AVE}.

$$A_{AVE} = (L/V)_{AVE} \times 1/K \text{ at } 110.1^{\circ}F = (22)$$

D. Calculate the dry gas composition from equation (11) using

equations (31) and (32) to evaluate ϕ_A and ψ_A.

E. Determine the rich oil composition.

$$(1) + (2) - (23) = (24)$$

Total Dry Gas $= \Sigma(23) = 86.342$ moles
Total Rich Oil $= \Sigma(24) = 33.945$ moles

Shrinkage $= 100 - 86.342 = 13.653$ moles.

Since the estimate shrinkage, 13.675 moles, and the calculated

shrinkage, 13.653 moles, are close, the latter value is taken as the solution. Had the difference been substantial, then the calculation loop would have been repeated.

VITA

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