SHORTCUT METHODS FOR COMPLEX DISTILIATION COLUMNS:
PART 1 — MINIMUM REFLUX

by

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Abstract

Shortcut Methods for Complex Distillation Columns:
Part 1 -- Minimum Reflux

This two-part paper presents in detail the theory for calculating via shortcut methods the minimum reflux conditions and the number of stages and feed tray location for ordinary and thermally coupled columns. Nonadjacent key components are permitted.

In this paper, part 1, the approximations made to estimate minimum reflux are similar to earlier methods such as those by Underwood and Colburn. However, some novel manipulations lead to particularly simple equations requiring only a few minutes to use, particularly for ordinary distillation columns.

Several example problems demonstrate that the method compares favorably with these other approaches.

I. Introduction

Although thermally coupled distillation schemes were known for many years, only recently, because of the huge rise in the energy cost which made them economically more attractive, they have become the subject of several papers.

Thus, Petlyuk et al. (1965)', for instance, made a study to compare the performance of a thermally coupled distillation system to that of conventional schemes. They used the amount of liquid to be vaporized in the reboilers and the thermodynamic work required to separate a ternary mixture as criteria for comparison. Each of these criteria is a measurement of the amount of energy demanded by the separation process. Their results showed that the thermally coupled system consumes much less energy than the conventional schemes at any concentration level of the middle component, at least for a ternary mixture formed by very close boiling components.

Stupin and Lockhart (1971) proposed an approximate design method to find initial designs for the thermally coupled scheme studied by Petlyuk et al.. Based on Underwood's equations, they developed a procedure to find the limiting flow conditions. For a ternary mixture formed by not-close boiling components, they conclude that this distillation system is definitely a lower cost alternative to the conventional schemes.

Finally, Tedder and Rudd (1978) developed a similar study which also included other kinds of non-conventional distillation schemes. They found the optimality region with respect to the feed composition for each of them, in the separation of various types of hydrocarbon ternary mixtures into their pure components. According to their results, the conventional schemes seem to be the best choice for a rather wide range of feed compositions.

In Part I of the present two part paper, a general method is proposed to find approximate values for the operating parameters at limiting flow conditions in complex distillation systems. The method involves relatively straightforward calculations and is illustrated through its application to several example problems.

Part II of this paper will provide a shortcut method for estimating the number of stages needed in each section within a complex column. This shortcut method includes a new approach to locating the feedtrays in a complex column. Again, the computations required are straightforward and are illustrated through their application to several example problems.

II. Conventional Distillation Columns

A conventional distillation column can carry out the separation between any two selected components of the feed mixture (adjacent or not-adjacent in volatility), which are usually called light and heavy keys, respectively. This type of separation equipment consists of two column sections, commonly called rectifying and exhausting sections, respectively. Each of them accomplishes one specific goal which is defined by its own design specification. Thus, the rectifying section washes the heavy key from the vapor phase by means of a liquid reflux stream created by a condenser. If y_{iIV} is the fraction of the amount of heavy key contained in the feed to be recovered in the bottom product, the removal of all but $(1-Y^{™}_{UK})$ of the heavy key can be regarded as the rectifying section design specification.

On the other hand, the exhausting section serves to strip the light key out of the falling liquid stream with a vapor reflux stream generated by a reboiler. Such a stripping process is carried out until the desired fraction of light key in the bottom product, $(1-Y_{tt}.)$, is achieved.

When the recovery fractions $Y_{ut,\,tils.}$ and $Y_{T\_,\,U\backslash.}$ are close to one, the separation between the keys is nearly complete and is called a sharp separation. For this type of separation, the expressions giving the number of ideal stages required and the limiting flows are much simpler, with the additional advantage that the results for limiting flows can usually be extended to other non-sharp situations $(Y_w, Y_{Tlr}$ ^ $0.90)$ without making a significant error.

In the present paper, a shortcut approach to get fast, good estimations of the limiting flows in complex separation systems is proposed <u>for sharp separations</u> between the key components (which are not adjacent in volatility if distributed components are present). However, it will be introduced through particular cases, the first of them is the conventional distillation column. In the last section, we will describe the algorithm for a general complex column.

In a distillation column, the interstage liquid and vapor flows, which are assumed to be <u>invariant</u> in each column section, can be expressed in terms of two parameters, R « (L/D) and $R^1 = (L^f/B)$, and of the product flowrates D and B:

$$L > RD$$

$$V = (R+1)D$$

$$L^f - (R^f+1)B$$

$$V^I - R^fB$$

However, under any flow conditions, R and R^1 are not independent parameters. They are related through the thermal condition of the feed q in the following way,

$$R^f+1 = R(D/B) + q(F/B) \tag{1}$$

Therefore, in a separation structure composed by only <u>a pair</u> of column sections, the limiting flow conditions can be described through the value of a <u>single</u> parameter R, usually called reflux ratio.

At minimum reflux, there must be a zone in <u>each</u> of the two sections of the column, where the composition change between two plates becomes negligible and the operating line becomes "pinched" at the equilibrium curve (Colburn, 1941). Based on this fact, a system of equations relating the composition at the pinch zone and the composition of one of the products can be derived (Underwood, 1946).

Rectifying Section

A material balance for the heavy key over the entire rectifying section at minimum reflux, gives

$$(y_{HK})_{UP} = (K_{HK})_{UP}(x_{HK})_{UP} = \frac{R_m}{R_m+1}(x_{HK})_{UP} + \frac{(x_{HK})_D}{R_m+1}$$

where the subscript UP stands for the upper pinch zone, located somewhere in the rectifying section. Then,

$$(K_{HK})_{UP} = \frac{R_m}{R_m+1} + \frac{(x_{HK})_D}{(R_m+1)(x_{HK})_{UP}}$$

For sharp separations,

$$\begin{matrix} R \\ m \end{matrix} \qquad (2)$$

because $(x_{HK})_D$ is negligible while the pinch mole fraction $(x_{HK})_{UP}$ is not.

In a similar way, a material balance for any other jth-component over the rectifying section at minimum reflux, after replacing equation (2), gives

$$\alpha_j (K_{HK})_{UP} (x_j)_{UP} = (K_{HK})_{UP} \cdot (x_j)_{UP} + \frac{(x_j)_D}{R_m} \qquad (3)$$

where α_j is the relative volatility of jth-component, with reference to the heavy key, at the upper pinch zone temperature. Rearranging equation (3) and then replacing $(K_{HK})_{UP}$ by (2), one obtains

$$(x_j)_{UP} = \left(\frac{1}{R_m}\right) \frac{(x_j)_D}{\alpha_j - 1} \quad \text{for any } j \neq HK \qquad (4)$$

and

$$\sum_{j \neq HK} (x_j)_{UP} + (x_{HK})_{UP} = 1 \qquad (5)$$

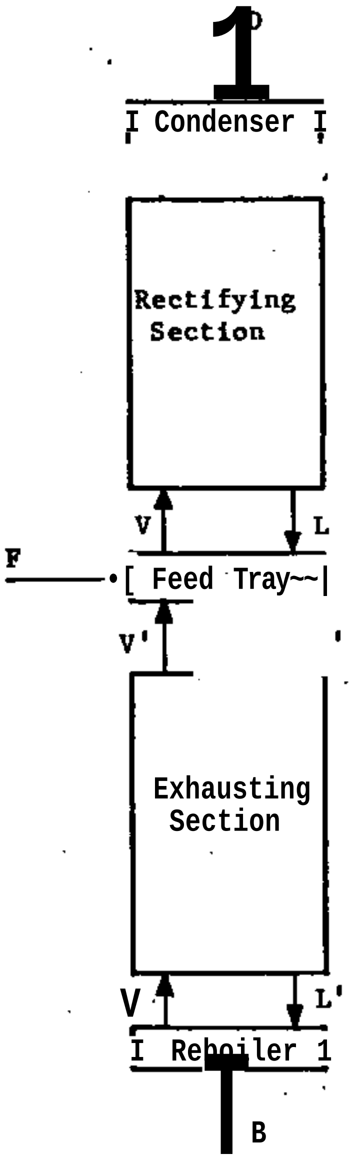

Figure 1: Standard Distillation Column

Equation (4) shows that the upper pinch zone contains only those components present in the top product (the heavy key and all components lighter than it) for sharp separations. Since all components are present on the feed tray, a relatively small number of plates should separate it from the upper pinch zone in order to reduce all components heavier than the heavy key to a negligible amount.

After fixing (or guessing) R_m, equations (4) and (5) represent a system of <u>linear</u> equations which enables us to determine the upper pinch zone composition in terms of the distillate composition. For sharp separations, the composition of the top product can be known beforehand, unless distributed components are contained in the feed (the keys are not adjacent in volatility). In this case, the split of each distributed component between the two products at minimum reflux as well as R_m are indeed unknowns, whose values should be predicted by means of a <u>similar number of additional equations</u>.

<u>Exhausting Section</u>

A material balance for the light key over the entire exhausting section at minimum reflux, gives

$$(K_{LK})_{LP} \approx \frac{R'_m+1}{R'_m} \qquad (6)$$

for sharp separations.

A material balance for any other component over the exhausting section at minimum reflux, leads to the following equation,

$$(x_i)_{LP} = \frac{\alpha_{LK}\,(x_i)_B}{(R'_m+1)(\alpha_{LK}-\alpha_i)} \qquad \text{for any } i \neq LK \qquad (7)$$

where the subscript LP stands for lower pinch zone, located somewhere in the exhausting section. We can also write

$$\sum_{i \neq LK} (x_i)_{LP} + (x_{LK})_{LP} = 1 \qquad (8)$$

Through equation (7) one can conclude that the lower pinch zone is located a small number of plates below the top tray of the exhausting section in such a way that all components lighter than the light key are present in that zone in negligible amounts.

Equations (7) and (8) are linear relationships between the lower pinch zone and the bottom product compositions, after R_m has been fixed. They would allow us to predict the composition at the lower pinch zone, if and only if a number of additional equations as large as the number of distributed components plus one is available*

Additional Equation for Predicting Minimum Reflux R_m

An additional equation for predicting the minimum reflux, R_m, will be obtained by assuming that the upper pinch zone is located at the bottom tray of the rectifying section while the lower pinch occurs at the top tray of the exhausting section. (See Figure 2).

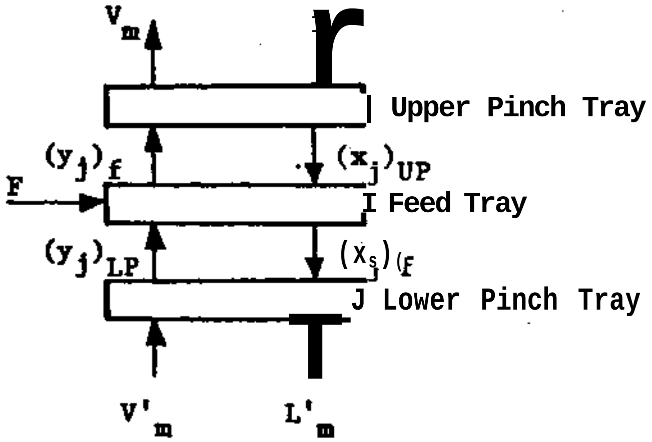

Figure 2: Assumed Picture Around the Feed Tray of a Distillation Column at Minimum Reflux

A material balance for the heavy key over the entire rectifying section gives

$$V_m(y_{HK})_f - L_m(x_{HK})_{UP} = D(x_{HK})_D \qquad (9)$$

From equations (4) and (5), one can derive the following expression for $(x_{HK})_{UP}$:

$$(x_{HK})_{UP} = \frac{R_m - \sigma_D}{m} \qquad (10)$$

where

$$\sigma_D = \sum_{j \neq HK} \frac{(x_j)_D}{\alpha_j - 1} \qquad (11)$$

By substituting (10) into (9) and neglecting the value of $(x_{HK})_D$ because sharp separations between the keys are considered, we get

$$(R_m+1)(K_{HK})_f(x_{HK})_f = R_m - \sigma_D \qquad (12)$$

An expression for the heavy key mole fraction at the feed tray, $(x_{HK})_f$, can be developed through a material balance for the heavy key over the entire exhausting section (see Figure 2).

$$(R'_m+1)(x_{HK})_f - R'_m(y_{HK})_{LP} = (x_{HK})_B \qquad (13)$$

From equations (6), (7) and (8)

$$(y_{HK})_{LP} = \frac{(x_{HK})_B}{R'_m(\alpha_{LK}-1)} \qquad (14)$$

which when substituted into (13) gives

$$(x_{HK})_f = \frac{\alpha_{LK}\, x_{HKB}}{(R'_m+1)(\alpha_{LK}-1)} \qquad (15)$$

Replacing (15)in (12), we obtain

$$(R_m+1)(K_{HK})_f = \frac{(\alpha_{LK}-1)(R\ [illegible]}{\alpha_{LK}(x_{HK})_B} \qquad (16)$$

On the other hand, a material balance for the light key over the entire rectifying section at minimum reflux, gives

$$({}^{R}{}_{m}{}^{+1}>\wedge LK>f \;- {}^{R}m({}^{x}LK>UP={}({}^{x}LK>D \qquad (17)$$

Substituting (4) into (17), an expression for $(y_{LR})_f$ is derived.

$$({}^{y}LK>f = (K_{LK})_f(x_{LK})_f = \frac{\alpha_{LK}(x_{LK})_D}{(\alpha_{LK}-1)(R_m+1)} \qquad (18)$$

In turn, a material balance for the light key over the exhausting section leads to an expression for fcrr^f

$$\wedge \;\; X \;\; \wedge \;\; f \;\; " \; {}^{Rl}m({}yLK>LP = {}({}^{X}LK>B \qquad (19)$$

From equations (6), (7) and (8):

$$\begin{array}{c} R'_{m}-\sigma \\ \mathrm{VL\bar{P}IT} \\ m \end{array} \qquad <^{2O}>$$

where

$${}^{c}\bar{B} \;.\, y\, L \;\frac{\alpha_i(x_i)_B}{\alpha r \;\; -a} \qquad (21)$$

Therefore

$$<{}^{X}LK>f \;-\; \frac{R'_m\wedge}{R_m}H\,\frac{R}{F} \qquad (22)$$

which is valid for sharp separations between the keys because $(x_{\pi}r)r$, was neglected. Combining equations (18) and (22); we get

$$(R_m+1)(K_{LK})_f = \frac{\alpha_{LK}(x_{LK})_D(R'_m+1)}{(\alpha_{LK}-1)(R'_m-\sigma_B)} \qquad (23)$$

Finally, dividing (23) by (16) one can obtain

$$R'_m-\sigma_B = \frac{\omega}{R_m-\sigma_D} \qquad (24)$$

where

$$\omega = \frac{\alpha_{LK}(x_{HK})_B(x_{LK})_D}{(\alpha_{LK}-1)^2} \qquad (25)$$

However, there is another easier way to derive equation (24). From equations (4) and (10)

$$\left(\frac{x_{LK}}{x_{HK}}\right)_{UP} = \frac{(x_{LK})_D}{(\alpha_{LK}-1)(R_m-\sigma_D)}$$

while the mole ratio between the keys at the lower pinch zone can be found from equations (20), (6) and (7)

$$\left(\frac{x_{LK}}{x_{HK}}\right)_{LP} = \frac{\alpha_{LK}(R'_m-\sigma_B)}{(\alpha_{LK}-1)(x_{HK})_B}$$

Defining the parameter Y (Colburn, 1941) as

$$\Psi = \frac{(x_{LK}/x_{HK})_{LP}}{(x_{LK}/x_{HK})_{UP}} \qquad (26)$$

Then

$$\Psi = \frac{(R'_m-\sigma_B)(R_m-\sigma_D)}{\omega}$$

When the mole ratie between the keys at both pinch zones is the same (Y=1), equation (24) is also obtained.

In absence of distributed components, the substitution of equation (1), which accounts for the thermal state of the feed, into the additional equation (24) leads us to a quadratic equation in R_m (Gilliland, 1940).

$$R = -\frac{\Delta_1}{2} \pm \left[\left(\frac{\Delta_1}{2}\right)^2 + \Delta_2\right]^{\frac{1}{2}} \qquad (27)$$

where

$$\Delta_1 = \left(\frac{F}{D}-1\right)\sigma_B + (1-q)\frac{F}{D} - (1-\sigma_D) \qquad (28)$$

$$\Delta_2 = (\omega-\sigma_B\sigma_D)\left(\frac{F}{D}-1\right) + \sigma_D\left[1-(1-q)\frac{F}{D}\right] \qquad (29)$$

In equation (27) the sign (+) was chosen because we are interested in the largest R_m• Equation (27) is really useful in the absence of distributed components. Otherwise, we need to have additional equations available to predict the split of each distributeddcomponent between the products so as to evaluate the product flowrate D.

Several examples have been included in the Appendix to illustrate the performance of equation (27) where sharp separations between adjacent keys are studied. Note how easy equation (27) is to use. With no distributed components and assuming sharp separation, D/F is readily determined. Then evaluating a_g (equation (21)), *o^* (equation (11)) and u> (equation (25)) allows A_l and A_z to be calculated (equations (28) and (29)) and then R_m (equation (27)). Only a few minutes is needed using a hand calculator. The agreement with results provided by Underwood's method is completely satisfactory when the reduction of heavies and/or lights to negligible amounts is not difficult.

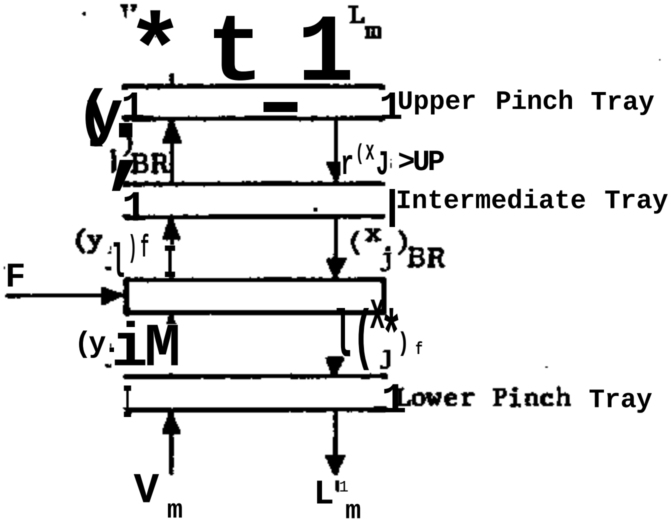

Figure 3: Assumed Picture of the Conditions Around the Feed Tray at Minimum Reflux where Relatively Volatile Heavies are Present in the Feed.

However, for cases involving large amounts of heavies and/or lights (not quite non-volatile and/or volatile) or normal amounts of those components but with relatively close volatiles to the keys, equation (27) predicts R_m-values smaller than the ones indicated by the other methods, as expected (Gilliland, 1940).

~~Variation in Y as Pinch Zones Move Apart~~

Where the reduction of heavies or lights to negligible amounts is somewhat difficult, Y is no longer nearly equal 1. In order to establish the kind of variation that the parameter Y undergoes, a similar treatment to that already described in the previous section was developed, but assuming now that the upper pinch zone is located on the plate right above the bottom tray of the rectifying section (see Figure 3). The following result was obtained.

$$Y = 1 + - i\pounds \frac{(0f\, LK''1)}{\alpha\, LK}(e-1) \qquad (30)$$

where

$$e = \frac{(K_H)_{K\,BR}}{(K_{HK})_{UP}} > 1 \qquad (31)$$

The subscript BR stands for bottom tray of the rectifying section.

Therefore, Y > 1 results as the pinch zones move away from the feed plate. In the general case, definition (29) can be written in the following way.

$$A_2 = (U)\ Y - cr_B a_D)(| - 1) + a_D\ [1 - (l-q)|l \qquad (32)$$

while definition (28) remains unchanged. Since the ratio (F/D) is always greater than one, it follows from equations (32) and (27), that the asssumption Y=l leads to smaller values than the real ones, when the reduction of heavies and/or lights is rather difficult, as expected (Gilliland, 1940).

Expression for the Parameter Y

When the reduction of heavies and/or lights to negligible amounts is rather difficult, Y is no longer equal 1. In order to get an expression for Y which enables us to predict its value for those kinds of situations, we shall assume that the upper and lower pinch zones are located two trays above and below the feed plate, respectively.

Following an analogous treatment to that described in a previous section, one can derive the equation

$$R'_m - \sigma_B = \frac{\omega}{R_m - \sigma_D}\left[1 + \frac{(\alpha_{LK}-1)(\epsilon-1)}{\alpha_{LK}}\right]\left[1 + \frac{(\alpha_{LK}-1)(\epsilon'-1)}{\alpha_{LK}}\right]$$

where σ_B, σ_D, ω and ϵ have already been defined through equations (21), (11), (25) and (31), respectively, while ϵ' is given by

$$\epsilon' = \frac{(K_{HK})_{TX}}{(K_{HK})_{LP}} > 1 \qquad (33)$$

where the subscript TX stands for top tray of the exhausting section. Therefore,

$$\Psi = \left[1 + \frac{(\alpha_{LK}-1)(\epsilon-1)}{\alpha_{LK}}\right]\left[1 + \frac{(\alpha_{LK}-1)(\epsilon'-1)}{\alpha_{LK}}\right]$$

Then,

$$\Psi = 1 + \frac{\alpha_{LK}-1}{\alpha_{LK}}(\epsilon-1) + \frac{\alpha_{LK}-1}{\alpha_{LK}}(\epsilon'-1) + \left(\frac{\alpha_{LK}-1}{\alpha_{LK}}\right)^2(\epsilon-1)(\epsilon'-1)$$

Since e and e' are relatively close to 1, the last term can be neglected.

Now, assuming a common value $\bar{\epsilon}$ for them, one obtains

$$\Psi = 1 + \frac{2(\alpha_{LK}-1)}{\alpha_{LK}}(\bar{\epsilon}-1) \qquad (34)$$

An upper bound for $\bar{\epsilon}$ can be chosen as

$$\bar{\epsilon} \leq \frac{(K_{HK})_{LP}}{(K_{HK})_{UP}} = \frac{(R'_m+1)(R_m+1)}{\alpha_{LK} R_m R'_m}$$

or

r-K^-r^f^s^-i]
LK^{w} ^{R}m^{R} *m*

where the expressions of (K^^p^{and} ^R^UP' $^{for sharp}$ s^{e}P^{arations}. given by equations (6) and (2), respectively, have been substituted. A fair estimation of Y can be obtained replacing ($\bar{e}$-1) by its upper bound in equation (34).

$$\Psi = 1 + 2(\alpha_{LK} - 1)\left[\frac{(R_m+1)(R'_m+1)}{m\,m} - 1\right] \qquad \text{<35>}$$

which can be used when the reduction of some lights <u>and</u> heavies present in the feed to negligible amounts are rather difficult. On the other hand, in the case when the reduction of some lights <u>or</u> of some heavies (but not of both kinds) is difficult, it follows from equation (30) by making a similar analysis,

$$\Psi = 1 + \text{or} \; -l_r \; (+M \;\; R' \; +)_{m} \; , \qquad (36)$$

which differs from equation (35) in the factor 2.

The use of equation (32) is suggested instead of (29) to estimate the parameter A_2 when either the volatilities of some heavies *(ci$_{h}$ < $^{a}u_{K}$)* and/or lights (Of$_{J6}$ > O.f$_{LK}$) are relatively close to those of the keys or their mole fractions in the feed are rather large. A more precise criterion can be given in this way:

(1) Use equation (32) when the ratios (<*/«$_{riJs.\ n}$) and/or *(otja$_{Xf\ LK}$)*, for a certain heavy or light component, is less than 1.70.

(2) When those volatility ratios are between 1.70 and 2.20 and the mole fraction of that heavy or light component in the feed is greater than 0.20 also use equation (32) to evaluate A_2.

(3) Otherwise, A_9 is determined by equation (29).

According to the case, equation (35) or (36) should be used to approximate the value of Y. Estimation of Y using the R_m-value given by equations (29)and (27) have shown to be quite satisfactory. In other words, new evaluations of Y by the iterative use of equations (32) and (27) produce little improvement (see example 1,2.1). In the Appendix three examples illustrate the performance of these expressions proposed for Y. The agreement with R_m-values provided by Underwood's method is very satisfactory.

<u>Distributed Components</u>

As suggested by Colburn (1941), the division of a distributed component between the tops and bottoms is made in such a way that the value of the ratio $[(x_u)_{1Tt)}/(x.)_{TT}]$ lies between the values of that ratio for the keys. Mathematically,

$$\frac{(x_{LK})_{UP}}{(x_{LK})_{LP}} < \frac{(x_k)_{UP}}{(x_k)_{UP}} < \frac{(x_{HK})_{UP}}{(x_{HK})_{LP}}$$

where the subscript k denotes a distributed component. But,

$$= \frac{(x_{HK})_{UP}/(x_{HK})_{LP}}{(x_{LK})_{UP}/(x_{LK})_{LP}} = \frac{(x_{LK})_{LP}/(x_{HK})_{LP}}{(x_{LK})_{UP}/(x_{HK})_{UP}}$$

In many cases Y is equal or close to 1, from which it follows that

$$\frac{(x_k)_{UP}}{(x_k)_{LP}} = \frac{(x_{HK})_{UP}}{(x_{HK})_{LP}} \tag{37}$$

whose range of validity is undoubtedly larger than the assumption Y=1. We can use one equation (37) for each distributed component.

By means of equations (4), (7) and (10), equation (37) can be written

$$\frac{d_k}{b_k} = \frac{(\quad)}{(a_{LK} - Y(x_{HK})_B} \tag{38}$$

Therefore, when distributed components are contained in the feed, their splits should be guessed so that R can be evaluated. Then , such guesses are checked out through (37) or (38), which act as error functions.

Algorithm

(i) Guess R_m and the split $(d/f)_k$ for each distributed component.

(ii) Solve the system of linear equations (4), (5), (7) and (8) to determine the composition at both pinch zones,

(iii) Check out the guesses with equations (26) and (37) acting as error functions. According to the particular case, Y can be assumed equal to 1 or given by equation (35) or (36).

(iv) If the error functions are smaller than a certain small value, the final results have been achieved. Otherwise, re-guess R_m and $(d/f)_k$ using, for example, a secant method. Then, return to step (ii).

III. Distillation System with a Side-Stream Stripping Section

A single pair of appropriate column sections can carry out the separation between two components in the feed, called the light and heavy keys, respectively. As illustrated in Figure 4, we shall now consider a distillation column structure composed of two pairs of column sections. This unit requires four specifications for its design.

Any three selected components in the feed (adjacent or non-adjacent in volatility) can be separated in this unit, which will be called light key (LK), middle key (MK) and heavy key (HK), respectively. Each pair of column sections accomplishes the separation between two of the keys; thus, pair (1,2) carries out the separation (LK/MK) while (3,4) separates (MK/HK). The design specifications are given in the same way described before for a conventional distillation column. For example, column section 1 which is indeed a

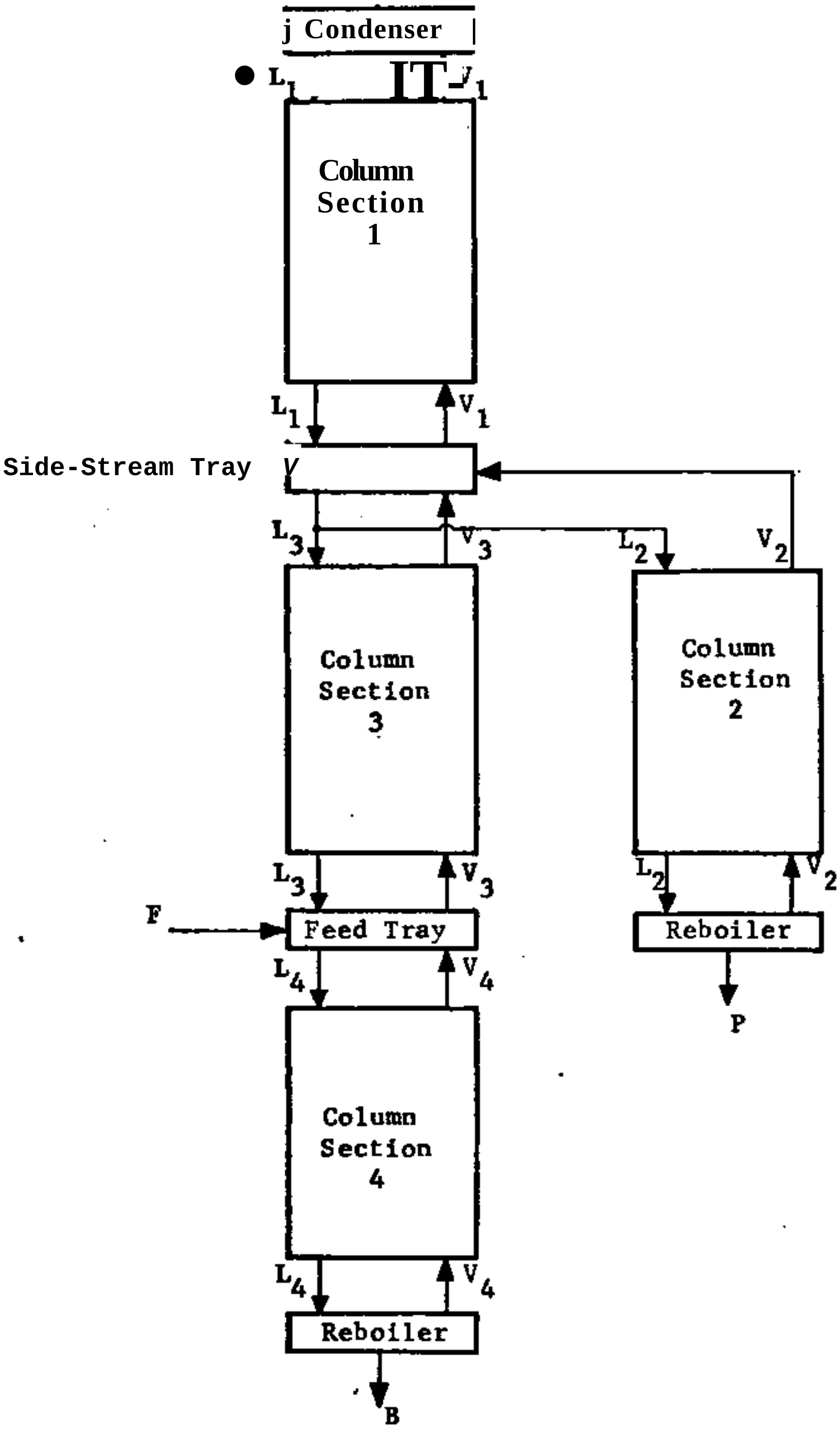

Figure 4. Distillation System with a Side-stream Stripping Section

rectifying section serves to wash the middle key from the vapor phase almost completely when sharp separations among the keys are considered.

Again, only sharp separations are studied here; that is, the recovery fraction of each key in one of the product streams is very close to 1. However, the results can be extended to other non-sharp situations.

In this distillation system, assuming constant molar overflows in each column section, all the internal liquid and vapor stream flowrates can be expressed in terms of three operating parameters.

$$»>! - - \overset{L}{\pounds} \quad ; \quad <R' >_4 - - \overset{V}{f} \quad ; \quad <R')_2 - - \overset{V}{f}$$

where the subscripts stand for the numbers identifying each column section (see Figure 4). Thus,

$$\backslash - C(R^f)_4 + l3 B$$

$$V_A = (R«)_4 B$$

$$V_3 = [(R)_x + l] D - (R^f)_2 P$$

$$L_3 = (R)_x D - C(R')_2 + 1] P$$

$$L_2 = [R^1)_2 + l] P$$

$$V_2 = (R^f)_2 P$$

$$L_x - (R)_x D$$

$$V_x = C(R)_x + l] D$$

Accounting for the thermal condition of the feed, the following equation can be written:

$$L_3 = E(R')_4 + 1\} B - qF$$

Therefore

$$[(R')_4 + 1]\,B - qF = (R')_1\,D - [(R')_2 + 1]\,P$$

or

$$(R')_2 + 1 = (R')_1\,(D/P) + q(F/P) - [(R')_4 + 1]\,(B/P) \qquad (39)$$

which indicates that under any flow conditions, only two of the three operating parameters are independent. Thus the limiting flow conditions in a separation structure composed by <u>two</u> pairs of column sections are described through the values of two parameters, for instance, $(R')_1$ and $(R')_4$.

As shown earlier for a conventional distillation column, a pair of zones of constant composition are generated by decreasing the single independent parameter R until it reaches a certain value called minimum reflux. Generalizing this fact for the complex distillation system now being studied, the continuous reduction of the independent parameters $(R')_1$ and $(R')_4$ generates finally the formation of <u>two</u> pairs of constant composition zones, each of them located around the plate connecting the two corresponding column sections of the system, (1,2) and (3,4).

<u>Pinch Zones in Column Sections (1,2)</u>

The goal for column sections (1,2) is to achieve the separation (LK/MK). The expressions for the pinch equations can be derived from those obtained for a conventional distillation column by replacing HK by MK. Thus, at the upper pinch zone,

$$(x_j)_{up_{1-2}} = \frac{1}{(R')_1}\,\frac{(x_j)_D}{(\alpha_j/\alpha_{MK} - 1)} \quad \text{for any } j \neq MK, \qquad (40)$$

and

$$\sum_{j \neq MK} (x_j)_{up_{1-2}} + (x_{MK})_{up_{1-2}} = 1 \qquad (41)$$

where equation (40) is the type of pinch equation always obtained for a rectifying section. On the other hand, in the lower pinch zone located in the column section 2,

$$(x_i)_{LP_{1-2}} = \frac{\alpha_{LK}(x_i)_P}{[(R'_m)_2 + 1](\alpha_{LK}-\alpha_i)} \quad , \quad \text{for any } i \neq LK, \tag{42}$$

and

$$\sum_{i \neq LK} (x_i)_{LP_{1-2}} + (x_{LK})_{LP_{1-2}} = 1 \tag{43}$$

where (42) is the characteristic exhausting section pinch equation. The only difference from the result obtained in a conventional column is that the bottom product composition $(x_i)_B$ is replaced by the composition of the product stream coming from column section 2, $(x_i)_P$.

After fixing (or guessing) $(R_m)_1$ and $(R'_m)_4$, equations (40), (41), (42) and (43) are linear relationships which enables us to calculate the pinch compositions in terms of product compositions.

Equations for Pinch Zones in Column Sections (3,4)

The goal for column sections (3,4) is to carry out the separation (MK/HK). The expression for the lower pinch zone composition is easily written by noting that column section 4 is an exhausting section whose design key component is MK and its product stream is B. Thus,

$$(x_i)_{LP_{3-4}} = \frac{\alpha_{MK}(x_i)_B}{[(R'_m)_4 + 1](\alpha_{MK}-\alpha_i)} \quad , \quad \text{for any } i \neq MK, \tag{44}$$

and

$$\sum_{i \neq MK} (x_i)_{LP_{3-4}} + (x_{MK})_{LP_{3-4}} = 1 \tag{45}$$

However, the derivation of pinch equations for a column section like CS-3 is more difficult because no real product stream is coming out of it. In such a case, one should express the composition of the net flow (V_3-L_3) in terms of product compositions. Since

$$\begin{pmatrix}\text{Net flow of jth-component}\\ \text{coming out of CS-3}\end{pmatrix} = D(x_j)_D + P(x_j)_P$$

and

$$V_3 - L_3 = D + P,$$

then the reflux ratio at CS-3 is given by

$$\frac{L_3}{V_3-L_3} = \frac{[(R'_m)_4 + 1]B - qF}{D + P}$$

Now, an equation for the upper pinch zone composition similar to equation (4) can be written:

$$(x_j)_{UP_{3-4}} = \frac{1}{(\alpha_j - 1)}\left\{\frac{(P/B)(x_j)_P + (D/B)(x_j)_D}{[(R'_m)_4 + 1] - q(F/B)}\right\}, \quad j \neq HK \qquad (46)$$

and finally

$$\sum_{j \neq HK} (x_j)_{UP_{3-4}} + (x_{HK})_{UP_{3-4}} = 1 \qquad (47)$$

Again, after guessing $(R_m)_1$, $(R'_m)_4$, and the split of each distributed component among the products, equations (44), (45), (46) and (47) are linear relationships between pinch zone and product compositions.

Predicting Liquid Reflux Ratio ($(R_m)_1$)

Calling

$$\Psi_{1-2} = \left[\frac{(x_{LK}/x_{MK})_{LP}}{(x_{LK}/x_{MK})_{UP}}\right]_{1-2}, \qquad (48)$$

one can show that Ψ_{1-2} is close to 1 when the reduction of lights and/or heavies involved in the separation (LK/MK) to negligible amounts is not difficult, using a derivation similar to that for a conventional distillation column. Otherwise, the value of Ψ_{1-2} (greater than 1) can be predicted by

$$\Psi_{1-2} = 1 + \frac{\theta[(\alpha_{LK}/\alpha_{MK}) - 1]}{(\alpha_{LK}/\alpha_{MK})^2}\left\{\frac{[(R_m)_1 + 1][(R'_m)_2 + 1]}{\quad} - 1\right\} \qquad (49)$$

with 6 = 1 or 2, as described earlier. Equation (48) with Y given by (49) provides us an additional relationship to predict $(R_m)_1$.

Predicting Vapor Reflux Rates $(R^f_m)_4$

An equation to predict $(R_m)_4$ is given by

$$Y_{3-4} = \left[\frac{(x_{MK}/x_{HK})_{LP}}{(x_{MK}/x_{HK})_{UP}}\right]_{3-4} \tag{50}$$

with $Y_{3-4} = 1$ or evaluated by

$$\Psi_{3-4} = 1 + \frac{\theta(\alpha_{MK}-1)}{\alpha_{MK}^2}\left\{\frac{}{[[(R'_m)_4 + 1]B - qF](R'_m)_4} - 1\right\} \tag{51}$$

with 6 = 1 or 2.

Simple Case: Adjacent Keys and $Y_{1-2} = Y_{3-4} = 1$

If the three keys are adjacent in volatility and $Y_{1-2} = Y_{3-4} = 1$ is a good approximation, then analytical solutions can be derived to determine $(R_m)_1$ and $(R^f_m)_4$. Equation (50) leads to a quadratic equation in $(R^f_m)_4$ whose solution is given by

$$(R'_m)_4 = \frac{(\Delta_1)_{3-4}}{2} + \left\{\left[\frac{(\Delta_1)_{3-4}}{2}\right]^2 + (\Delta_2)_{3-4}\right\}^{\frac{1}{2}}$$

where

$$(A_1)_{3-4} = a_3 + a_4 + q(F/B) - 1$$

$$(A_2)_{3-4} = (P/B)\omega_{3-4} - \sigma_4[\sigma_3 + q(F/B) - 1]$$

and where

$$\sigma_3 = \sum_{j \neq HK} \frac{(P/B)(x_j) + (D/B)(x_j)_D}{\alpha_j - 1}$$

$$\sigma_4 = \sum_{i \neq MK} \frac{\alpha_i (x_i)_B}{\alpha - a_i}$$

$$\omega_{3-4} = \frac{\alpha_{MK}(x_{MK})_P(x_{HK})_B}{(\alpha_{MK}-1)^2}$$

Equation (48) enables us to derive a quadratic equation in $(R_m)_1$, whose analytical solution is

$$(R_m)_1 = \frac{(\Delta_1)_{1-2}}{2} + \sqrt{\left\{\left[\frac{(\Delta_1)_{1-2}}{2}\right]^2 + (\Delta_2)_{1-2}\right\}}$$

where

$$(\Delta_1)_{1-2} = [(R'_m)_4 + 1](B/D) + \sigma_1 + (P/D)\sigma_2 - q(F/D)$$

$$(\Delta_2)_{1-2} = \omega_{1-2}(P/D) + \sigma_1\left\{q(F/D) - \sigma_2(P/D) - [(R'_m)_4 + 1](B/D)\right\}$$

$$\sigma_1 = \sum_{j \neq MK} \frac{(x_j)_D}{\left(\frac{\alpha_j}{\alpha_{MK}} - 1\right)}$$

$$\sigma_2 = \sum_{i \neq LK} \frac{\alpha_{LK}(x_i)_P}{\alpha - \alpha_i}$$

$$\omega_{1-2} = \frac{\alpha_{MK}\alpha_{LK}(x_{LK})_D(x_{MK})_P}{(\alpha_{LK}-\alpha_{MK})^2}$$

Distributed Components in the Separation (LK/MK)

Since γ_{1-2} is frequently close to 1, for the same argument already explained for a conventional distillation column, one can write

$$\left[\frac{(x_k/x_{MK})_{LP}}{(x_k/x_{MK})_{UP}}\right]_{1-2} = 1 \qquad (52)$$

where the subscript k stands for any distributed component in the separation (LK/MK). Equation (52) can also be written in this way:

$$\frac{d_k}{p_k} = \frac{(\alpha_{LK}-\alpha_{MK})(\alpha_k-\alpha_{MK})(D/P)[(R_m)_1-\sigma_1]}{(\alpha_{LK}-\alpha_k)(x_{MK})_P}$$

Distributed Components in the Separation (MK/HK)

For analogous reasons,

$$\left[\frac{(x_m/x_{HK})_{LP}}{(x_m/x_{HK})_{UP}}\right]_{3-4} = 1 \tag{53}$$

where the subscript m denotes any distributed component in the separation (MK/HK). By appropriate substitutions, equation (53) can be written

$$\frac{p_m}{b_m} = \frac{(\alpha_{MK}-1)(\alpha_k-1)[(R'_m)_4 + 1 - q(F/B) - \sigma_3]}{(\alpha_{MK}-\alpha_k)(x_{HK})_B}$$

General Algorithm

1. Guess $(R_m)]$» $({}^{R}m$^4 and the split: of each distributed component.
2. Solve the system of linear equations (40), (41), (42), (43), (44), (45), (46), and (47) to find the compositions at both pairsof pinch zones•
3. Evaluate the error functions obtained from equations (48), (50), (52) and (53), respectively. If their all values are small enough the values of (R^j and $(R^f_m)A$ have been found. Otherwise, go to step 4.
4. Update the guesses through, for instead, the secant method and return to step *2.*

IV. Arbitrary Thermally Coupled Distillation System

Like conventional schemes, any thermally coupled distillation system can be regarded as being formed by a certain number of two-section fractionators, each carrying out a specific separation between its design components. However, some of the fractionators in the system can be single-product ones or even nonproductive. Those fractionators do not have their own condensers or reboilers so that their liquid and/or vapor reflux streams are obtained by drawing them out of adjacent fractionators.

In general, the internal liquid and vapor stream flowrates in any distillation system can be expressed in terms of a certain number of independent operating parameters and of the product flowrates, if constant molal overflows are assumed in each column section.

In a conventional scheme and in some thermally coupled distillation systems too (i.e. a distillation structure with a side stripping section), at limiting flow conditions, a pair of pinch zones shows up around each fractionator feed tray. In such cases, the number of independent operating parameters is equal to the number of two-section fractionators composing the distillation system. The way one can determine their limiting values was already described in sections (II) and (III) and its generalization should be evident.

However, the distillation system shown in Figure 5 represents a different situation. Although it is composed by three two-section fractionators (one non-productive and the other two single-product ones), the unit accomplishes only two net separations because of the way the three pairs of column sections (or fractionators) are arranged. Pair (1,2) carries out the separation between two non-adjacent keys LK and HK, while pairs (3,4) and (5,6) complete the separations between adjacent keys (LK/MK) and (MK/HK), respectively; Like the distillation unit depicted in Figure 4, this one only has three overall key components.

Looking at Figure 5, one can identify four operating parameters, given by

$R = (L_3/D)$

$X_L = (L_1/L_3)$

*V " (W (54)

$R^1 = (V_6/B)$

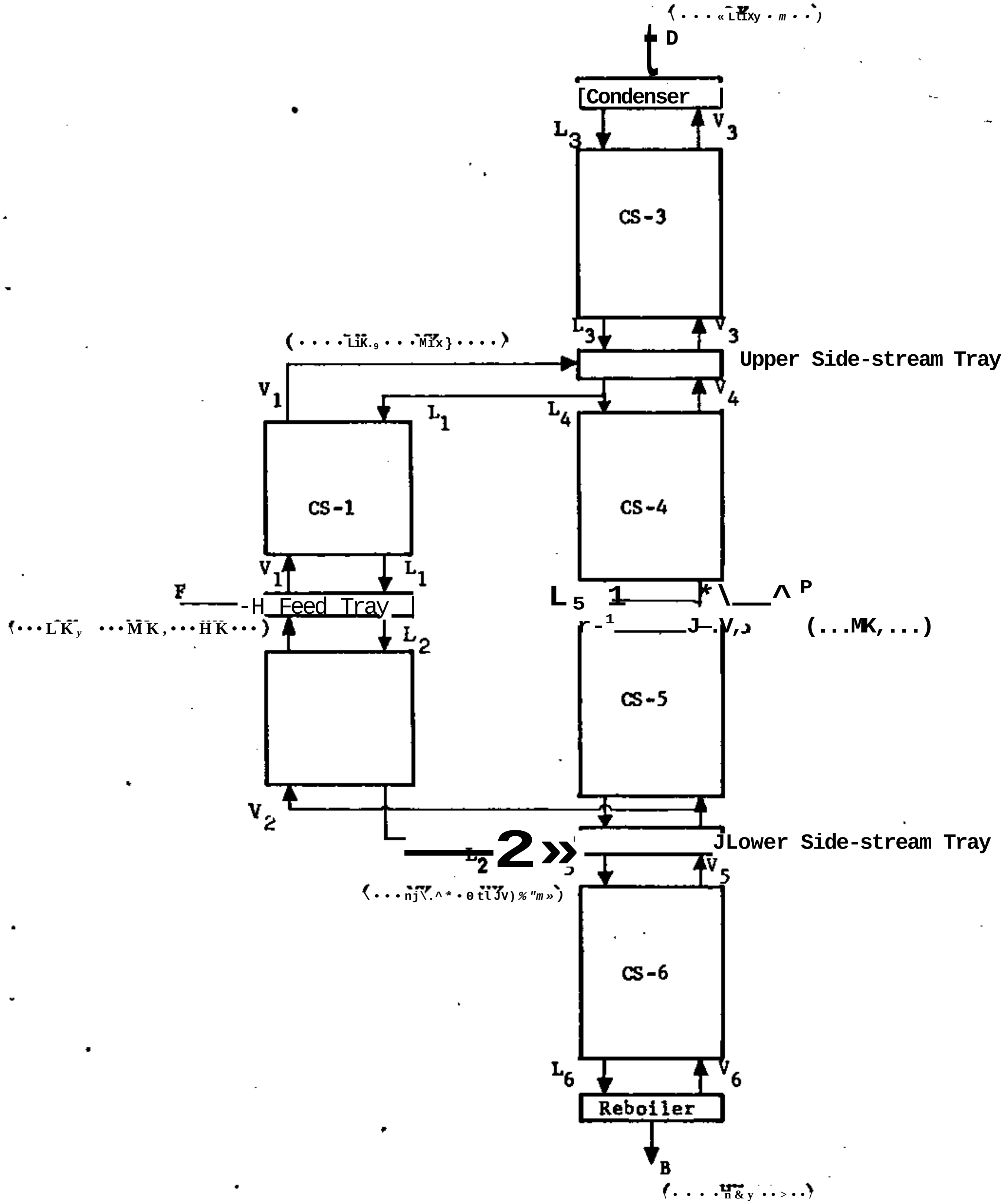

Figure 5: Petlyuk's thermally coupled distillation system

Since the distillation system is formed by three fractionators, one could expect that it has three independent operating parameters, but it only possesses two. One of the operating parameters, i.e. R', as usual, is fixed by the thermal state of the feed

$$R' = (R+1)(D/B) + (1-q)(F/B)$$

On the other hand, limiting flow conditions at the fractionators (1,2) can be achieved by decreasing X_T (or RX_T), while the reduction in the value of R finally generates a pair of pinch zones around the feed plate of either fractionator (3,4) or (5,6). In that situation, the splits of distributed components (any jth-component such as $1 < \alpha_j < \alpha_{LK}$) in the pair (1,2) between the net flows (V_1-L_1) and (L_2-V_2) are perfectly defined and so also is the other operating parameter $(RX_L)_m$,

$$(R')_m = [(RX_L)_m(D/B) + (F/B) - \frac{[illegible]}{B}]$$

so that only two operating parameters are independent.

Keeping in mind that the goal of fractionator (1,2) is the separation of the keys LK and HK, the expressions of its pinch equations can be derived following the procedure already described in previous sections. They are

$$(x_j)_{UP_{1-2}} = \frac{[(v_{T1}-\ell_{T1})_j/D]}{(\alpha_j-1)(RX_L)_m} \quad \text{for any } j \neq HK$$

$$(x_{HK})_{UP_{1-2}} = \frac{(RX_L)_m - \sigma_1}{(RX_L)_m}$$

where

$$\sigma_1 = \sum_j \frac{[(v_{T1}-\ell_{T1})_j/D]}{\alpha_j - 1}$$

and

$$(x_i)_{LP_{1-2}} = \frac{\alpha_{LK}[(\ell_{B2}-v_{B2})_i/B]}{(\alpha_{LK}-\alpha_i)[(RX_L)_m(D/B)+q(F/B)]}, \quad i \neq LK$$

$$(x_{LK})_{LP_{1-2}} = \frac{(RX_L)_m(D/B) + q(F/B) - \sigma_2}{(RX_L)_m(D/B) + q(F/B)}$$

where

$$\sigma_2 = \sum_i \frac{\alpha_{LK}[(\ell_{B2} - v_{B2})_i/B]}{\alpha_{LK} - \alpha_i}$$

Defining,

$$\Psi_{1-2} = \frac{(x_{LK}/x_{HK})_{LP_{1-2}}}{(x_{LK}/x_{HK})_{UP_{1-2}}}$$

and substituting the expressions for the key mole fraction ratios at both pinch zones, one can finally find an algebraic quadratic equation whose analytical solution is given by

$$(RX_L)_m = \frac{(\Delta_1)_{1-2}}{2} + \left\{\left[\frac{(\Delta_1)_{1-2}}{2}\right]^2 + (\Delta_2)_{1-2}\right\}^{\frac{1}{2}}$$

where

$$(\Delta_1)_{1-2} = \sigma_1 + \sigma_2(B/D) - q(F/D)$$

$$(\Delta_2)_{1-2} = \Psi_{1-2}\omega_{1-2} + \sigma_1[q(F/D) - \sigma_2(B/D)]$$

$$\omega_{1-2} = \frac{\alpha_{LK}(x_{LK})_D(x_{HK})_B}{(\alpha_{LK}-1)^2}$$

Ψ_{1-2} can be assumed equal 1 or given by

$$\Psi_{1-2} = 1 + \frac{\theta(\alpha_{LK}-1)}{\alpha_{LK}^2}\left\{\frac{[(RX_L)_m + q(F/D)][(R'X_V)_m(B/D) + (1-q)(F/D)]}{(RX_L)_m(R'X_V)_m(B/D)} - 1\right\}$$

$(\theta = 1 \text{ or } 2)$

In order to evaluate σ_1 and σ_2, one should know the splits of the distributed components in the fractionator (1,2). As written before

$$\left(\frac{x_k}{x_{HK}}\right)_{UP_{1-2}} = \left(\frac{x_k}{x_{HK}}\right)_{LP_{1-2}} \quad , \quad \text{for any } \alpha_{HK} < \alpha_k < \alpha_{LK}$$

which leads to

$$(v_{Tl}-\ell_{Tl})_k = \frac{\rho_k}{1+\rho_k} f_k$$

where

$$\rho_k = \frac{(\alpha_k-1)(\alpha_{LK}-1)(D/B)[(RX_L)_m-\sigma_1]}{(\alpha_{LK}-\alpha_k)(x_{HK})_B}$$

The other pair of pinch zones can show up around the feed tray of the fractionator (3,4) or (5,6), whichever gives the largest R_m. Proceeding as before, one can find for fractionator (3,4)

$$R_B = \frac{(\Delta_1)_{3-4}}{2} + \left\{\left[\frac{(\Delta_1)_{3-4}}{2}\right]^2 + (\Delta_2)_{3-4}\right\}^{\frac{1}{2}}$$

where

$$(\Delta_1)_{3-4} = \sigma_3 + \sigma_4 + (RX_L)_m$$

$$(\Delta_2)_{3-4} = \gamma_{3-4} + \beta_{3-4} - \sigma_3[(RX_L)_m + \sigma_4]$$

$$\sigma_3 = \sum_{i \geq m} \frac{(x_i)_D}{(\alpha_i/\alpha_{MK} - 1)}$$

$$\sigma_4 = \sum_{i \leq LK} \frac{\alpha_{LK}[(v_{T1}-\ell_{T1})_i/D]}{(\alpha_{LK}-\alpha_i)}$$

$$\gamma_{3-4} = \frac{\alpha_{LK}\alpha_{MK}(x_{LK})_D[(v_{T1}-\ell_{T1})_{MK}/D]}{(\alpha_{LK}-\alpha_{MK})^2}$$

For fractionator (5,6)

$$R_m = \frac{(\Delta_1)_{5-6}}{2} + \left\{\left[\frac{(\Delta_1)_{5-6}}{2}\right]^2 + (\Delta_2)_{5-6}\right\}^{\frac{1}{2}}$$

where

$$({}^{A}l\}5\text{-}6 = \wedge I \wedge m + 2 < {}^{P/D)} + <{}^{CT}{}_{5}\text{-}{}^{HT}{}_{6}{}^{)(B/D)} \;\; " \;\; q(F/D)$$

$$(\Delta_2)_{5-6} = (B/D)^2\left\{(\Psi\omega)_{5-6} + [q\frac{F}{B} - \frac{P}{B} - \sigma_6][\,|\;(RX_L)_m + f + \sigma_5]\right\}$$

$$a_5 = \sum_j \frac{[\frac{(\ell_{B2}-v_{B2})_j}{B} - (x_j)_B]}{a_j - l}$$

$$a_6 = \sum_i \frac{\alpha_{MK}(x_i)_B}{\alpha_{MK}-\alpha_i}$$

$$\bullet 3\text{-}6 = \frac{\alpha_{MK}(x_{HK})_B}{{}_{MK}}\left[\frac{\frac{(\ell_{B2}-v_{B2})_{MK}}{B}}{}\right]$$

The parameters $Y^{\wedge}_{-4}$ and Y_{5-6} are assumed equal 1 or given by expressions which can readily be derived by a similar treatment to that shown before. Of course, the largest R_m is the minimum value of that operating parameter.

On the other hand, a component with a volatility Of_k such that $Of_{MK} < or_k < or_{LK}$ distributes itself between the products D and P. Its split is predicted from

$$\left(\frac{x_k}{{}^{v}x_{MK}}\right)_{UP_{3-4}} = \left(\frac{x_k}{x_{MK}}\right)_{LP_{3-4}}$$

which leads to

$$d_k = \frac{\rho_k}{1+\rho_k}(v_{T1}-\ell_{T1})_k$$

where

$$\rho_k = \frac{(\alpha_k-\alpha_{MK})(\alpha_{LK}-\alpha_{MK})(R_m-\sigma_3)}{\alpha_{MK}(\alpha_{LK}-\alpha_k)[\frac{(v_{T1}-\ell_{T1})_{MK}}{D}]}$$

In the same way, components with volatilities between those of MK and HK split between the products P and B. Such pplits can be determined from

$$\left(\frac{x_m}{x_{HK}}\right)_{UP_{5,6}} = \left(\frac{x_m}{x_{HK}}\right)_{LP_{5,6}} , \qquad 1 < \alpha_m < \alpha_m$$

It should be noted that one of the fractionators either (3,4) or (5,6) (that one with smaller R_m), at limiting flow conditions, operates normally and not at pinched conditions. Therefore, the use of the above equations to predict the splits of distributed components among the products in such a case yields poorer results.

V. Discussion of the Proposed Method

Several examples are included in the Appendix to show the performance of the method for a wide variety of situations. Thus, in examples 1.1.1/2 neither distributed components nor lights/heavies with close volatilities to the keys are contained in the feed to a conventional distillation column. In such cases, the value of R_m is found in a straightforward manner with good accuracy.

Lights/heavies with close volatilities to the keys or in large amounts are considered in examples 1.2.1/2 to check the results given by the equations proposed to predict the parameter Y. Here, the method not only provides satisfactory R_m-values but also converges in one or two iterations. Example I,3.1 adds another complication to the problem; it also includes two distributed components so as to verify the performance of the equations enabling us to determine their split at limiting flow conditions. The comparison of the results with those found by Underwood (1948) for this example shows a satisfactory agreement.

Although the proposed technique tends to give R_m-values a little lower than the real ones, it is still very reliable because of the normal shape of the cost-versus-reflux curve. Stupin and Lockhart (1971) found the same pattern in Petlyuk's thermally coupled distillation system.

Finally, the performances of conventional and thermally coupled distillation schemes are compared through two examples III.1/2, using the amount of liquid to be vaporized in the reboilers as the criterion for comparison. In both cases, the thermally coupled schemes prove to be better than the conventional ones, especially Petlyuk's, leading to savings which amount to around 35%.

Example III.1 was also studied by Stupin and Lockhart (1971) to make the same kind of comparison for Petlyuk's thermally coupled system. They found R_m equal to 1.50 and the amount of liquid to be vaporized in the reboiler equal 0.885, when the degreeSof recovery of the keys are 90%. For complete separations, this method predicts for those parameters, 1.97 and 0.99, respectively. We believe an error exists in the earlier calculations.

Appendix

(I) Limiting flow conditions in conventional distillation columns.

(I.I) Examples in which the reduction of lights and/or heavies to negligible amounts is not a difficult task:

(1.1.1) Example proposed by C.J. King (1971):

Components	f_i	"l	d_i	b_i
C_1	26	18.65	26	-
C_2	9	4.75	9	-
C_3(LK)	25	1.92	25	-
n-C_4(HK)	17	1.00	-	17
n-C_5	11	0.46	-	11
n-C_6	12	0.23	-	12
	100		60	40

Thermal condition of the feed: $q = 0.33$

Since the keys are adjacent in volatility, no distributed component is present in the feed. Furthermore, the ratios (an≤%/&TV) and (^/^pj are
LJ US. UK L3
greater than 2 so that the analytical expressions for R_m can be used to find its value. From equations (11), (21) and (25), one can determine o o and U), respectively.

$a_D = 0.5173$

$a_B = 0.5894$

U) = 0.4016

which when replaced in equations (28) and (29), gives:

$\Delta_1 = 1.0269$

$\Delta_2 = 0.004$

Finally, the substitution of Aj and A_2 into equation (27) gives

R_m - 1.03

which shows a good agreement with the R_m-value provided by Underwood's method (R_m =1.07).

(1.1.2) Feed - Bubble point liquid (q = 1):

Components	f_i	°$_i$	*$_i$	b_i
1	10	9.0	10	-
2	30	5.2	30	-
3 (LK)	20	1.7	20	-
4 (HK)	15	1.0	-	15
5	20	0.4	-	20
6	5	0.3	-	5
			60	40

Results:

With the proposed method: R_m =0.83

With Underwood's method: R_m =0.86

(1.2) Examples in which the reduction of lights and/or heavies to negligible amounts is a rather difficult task:

(1.2.1) Example proposed by C#J. King (1971):

Components	f_i	tt$_i$	t$_i$	b_i
A	5	3	5	-
B	10	2.1	10	-
C (LK)	30	2	30	-
D (HK)	50	1	-	50
E	5	0.8	-	5
			45	55

Thermal state of the feed: $q = 1$

Since the volatilities of components B and E are close to those of the keys, one can expect pinch points moving away from the feed plate and a Y-value greater than 1. This value can be estimated with equation (35). Assuming first $Y = 1$, we predict

$$R_m = 1.825$$

which leads through equations (1) and (35) to the following Y-value:

$$Y = 1.61$$

New evaluations of $A_{\tilde{z}}$ by equation (32) and R_m until convergence (3 iterations), finally gives

$$R_m = 2.04$$

$$Y = 1.54$$

Underwood's method provides an R_m-value equal to 2.03.

(1.2.2) Feed - Dew point vapor ($q = 0$)

Components	£i	!i	d_i	b_i
A	5	5	5	-
B	15	2.65	15	-
C (LK)	20	2	20	-
D (HK)	25	1	-	25
E	35	0.80	-	35
			40	60

Following the computation scheme described in the previous example, we obtain in 3 iterations

$$R_m = 3.16 \qquad (Y = 1,75)$$

against R^ - 3.24 given by Underwood's method.

(I.3) An example with distributed components (taken from A. Underwood (1948)): $(q = 0)$

Components	f_i	α_i	d_i	b_i
1	20	3	20	-
2 (LK)	15	2.5	15	-
3	15	2	?	?
4	15	1.5	?	?
5 (HK)	15	1	-	15
6	20	0.50	-	20

According to the criterion given before, the reduction of component 1 to negligible amounts can be considered as difficult and Ψ should be estimated by equation (36). The algorithm, quite similar to that applied to previous examples, also includes the estimation of each distributed component split between the products by equation (38). The final results are found when convergence in the values of $(d/b)_k$ have been achieved in 5 iterations. They are:

Methods	R_m	d_3	d_4	D
Underwood	2.54	12.72	9.16	56.88
Proposed method $(\Psi=1.57)$	2.48	13.05	9.38	57.43

(II) Expressions for determining limiting flow conditions in a distillation system with a side-stream enriching section (for sharp separations) - Figure 6

$$(R_m)_1 = \frac{(\Delta_1)_{1-2}}{2} + \left\{\left[\frac{(\Delta_1)_{1-2}}{2}\right]^2 + (\Delta_2)_{1-2}\right\}^{\frac{1}{2}}$$

where

$$(\Delta_1)_{1-2} = \sigma_1 + (P/D)\sigma_2 - q(F/D)$$

$$<Vl\text{-}2 = (P/D)[\omega_{1-2} + \sigma_1(q\frac{F}{P} - \sigma_2)]$$

$$j \neq MK \quad j \quad MK$$

$$\sigma_2 = \mathbf{I}_{i \neq LK} \frac{\alpha_{LK}[(B/P)(x_i)_B + (x_i)_P]}{\alpha_{LK} - \alpha_i}$$

$$\omega_{1-2} = \frac{\alpha_{LK}\alpha_{MK}(x_{LK})_D(x_{MK})_P}{(\alpha_{LK} - \alpha_{MK})^2}$$

and

$$(R'_m)_4 = \frac{(\Delta_1)_{3-4}}{2} + \left\{\left[\frac{(\Delta_1)_{3-4}}{2}\right]^2 + (\Delta_2)_{3-4}\right\}^{\frac{1}{2}}$$

where

$$(\Delta_1)_{3-4} = [(R_m)_1 + 1](D/B) + \sigma_4 + (P/B)\sigma_3 - (1-q)(F/B)$$

$$(A2>3\text{-}4 = (P/B)\{ ' \circ 3_{3-4} + \sigma_4[(1-q)(F/P) - \sigma_3 - ((R_m)_1 + 1)(D/P)]\}$$

$$\sigma_3 = A \; \frac{\alpha_j(x_j)_P}{O.-1}$$

$$4 = \sum_{i \neq MK} \frac{\alpha_i(x_i)_B}{\alpha_{MK} - \alpha_i}$$

$$\omega_{3-4} = \frac{\alpha_{MK}(x_{MK})_P(x_{HK})_B}{(\alpha_{MK} - 1)^2}$$

and

$$(R_m)_2 = [(R'J\wedge\wedge + l](B/P) - (R_m)_1(D/P) - q(F/P)$$

When distributed components are present in the feed, use the following equations to predict their splits among the products:

$$d_j = \frac{\rho_j}{1+\rho_j} f_j$$

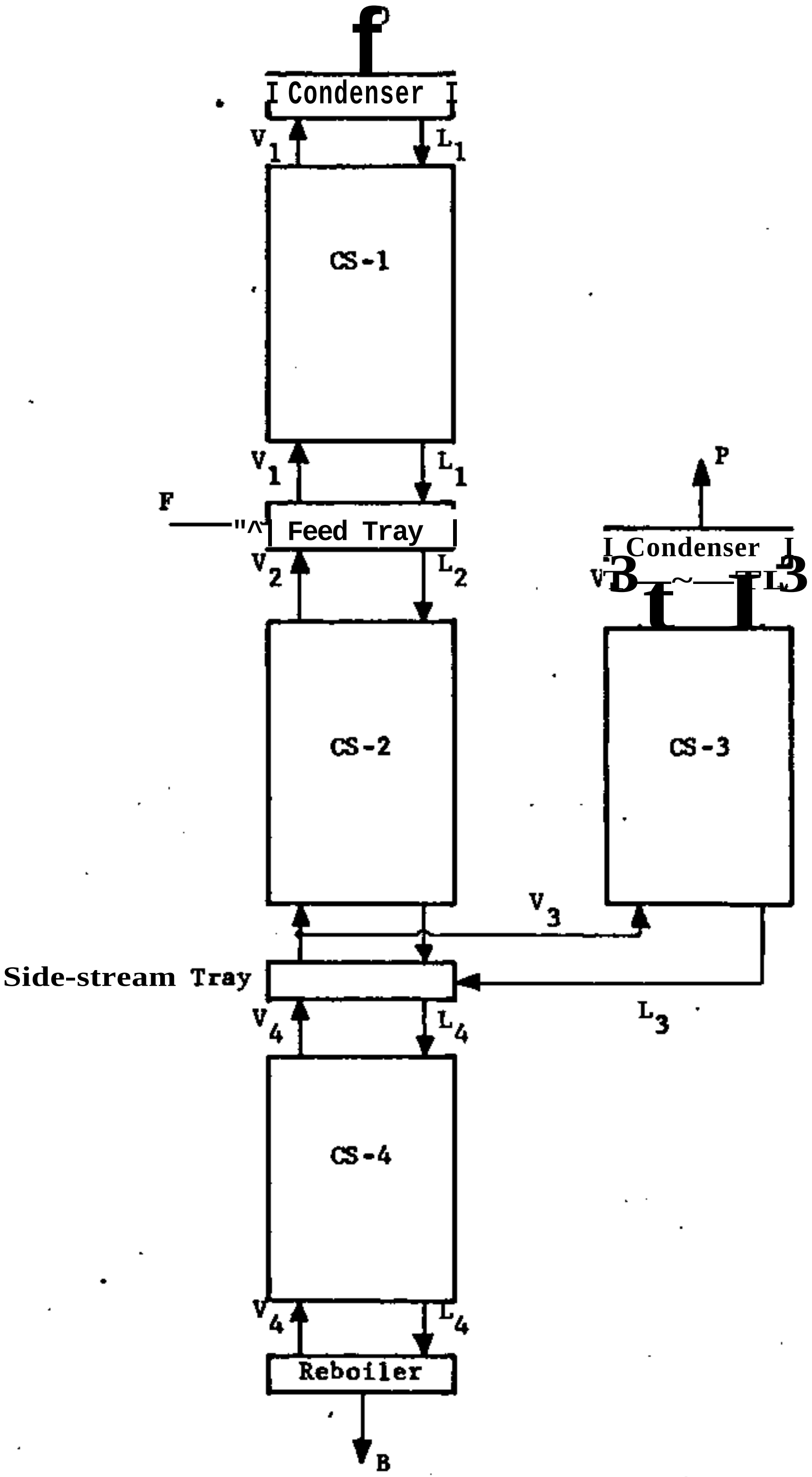

Figure 6: Distillation System with a Side-stream Rectifying Section

where

$$\rho_j = \frac{(\alpha_{LK}-\alpha_{MK})(\alpha_j-\alpha_{MK})(D/P)[(R_m)_1-\sigma_1]}{\alpha_{MK}(\alpha_{LK}-\alpha_j)(X_{MK})_P}$$

for any jth-distributed component with a volatility α_j such that $\alpha_{MK} < \alpha_j < \alpha_{LK}$ which splits between the products D and P. On the other hand

$$1+\rho_i \quad {}^{\wedge}i$$

where

$$\rho_i = \frac{(\alpha_{MK}-1)(\alpha_i-1)\left\{[(R_m)_3+1]-\sigma_3(P/B)\right\}}{(\alpha_{MK}-\alpha_i)(X_{HK})_B}$$

for any ith-distributed component with α_i such that $\alpha_{HK} < \alpha_i < \alpha_{MK}$ which splits between the products B and P.

(III) Limiting flow conditions in thermally coupled distillation schemes.

(III.1) Comparison of the conventional and thermally coupled distillation scheme performances through the example proposed by Stupin and Lockhart (1971):

Components	f_i	α_i	d_i	b_i	p_i
A (LK)	0.333	9	0.333	-	-
B (MK)	0.334	3	-	-	0.334
C (HK)	0.373	1	-	0.333	—

Feed: Bubble-point liquid (q = 1)

The results are shown in Table 1.

(III.2) Comparison of the conventional and thermally coupled distillation scheme performances through the example given by C.J. King (1971):

Components	$\overset{f}{II}$	$\tilde{I}t$	${}^{o}i$	${}^{D}i$	${}^{F}i$
C_x	26	18.65	26	-	-
C_2	9	4.75	9	-	-
C_3 (LK)	25	1.92	25	-	-
n-C_4 (MK)	17	1.00	-	-	17
n-C_5 (HK)	11	0.46	-	11	-
n-C_6	12	0.23	-	12	-
			60	23	17

Thermal state of the feed: $q = 0.33$

The results are shown in Table 2.

References

1. Colburn, A.P., Trans. Amer. Inst. Chem. Engrs., 2I»^{805} (1941).
2. Gilliland, E.R., Ind. Eng. Chem., 32(8), 1102 (1940).
3. King, C.I., "Separation Processes^{11}, McGraw-Hill Co., (1971).
4. Petlyuk, F.B., V.M. Platonov and D.M. Slavinskii, Int. Chem. Eng., 5^ 505 (1965).
5. Stupin, W.I. and F.I. Lockhart, 64th Annual AIChE Meeting, San Francisco (1971).
6. Tedder, D.W. and D.F. Rudd, AIChE Journal, 24, 303 (1978).
7. Underwood, A.I., I. Inst. Pet., 3£, 598 (1946).
8. Underwood, A.I., Chem. Eng. Progr., 44, 603 (1948).

Table 1; Comparison of conventional and thermally coupled distillation schemes in Example (EII.l)

Distillation System	Values of the independent parameters describing internal flows at limiting conditions	Limiting vapor rate generated bfr reboiler(s)
Reverse conventional distillation scheme	1st column: $R_m=0.47$; $R^1{}_m=2.93$ 2nd column: $R_m=1.00$; $R^1{}_m=2.00$	1.64
Direct conventional distillation scheme	1st column: $R_m=1.03$; $R^f{}_m=1.02$ 2nd column: $R_m=1.00$; $R^?{}_m=2.00$	1.34
Distillation system with a side-stream enriching section	$(R_m)_1=1.03$; $(R'_m)_4=3.76$ $(R_m)_3=0.73$	1.25
Distillation system with a side-stream stripping section	$(R_m)_1=2.76$*' <$R^f{}_m$>$4^{=2'93}$ $(R'_m)_2=0.83$	1.25
Petlyuk's thermally coupled distillation system	$R_m=1.97$; $R^1{}_m=2.97$ 00^,-0.375	0.99

Table 2: Comparison of conventional and thermally coupled distillation schemes in Example (III.2)

Distillation system	Values of independent operating parameters describing internal flows at limiting conditions	Limiting vapor rate generated by reboiler(s)
Reverse conventional scheme	1st column: $R_m=1.02$; $R^{\wedge}-1.35$ 2nd column: $R_m=1.72$; $R^1{}_m=2.01$	100.22
Direct conventional scheme	1st column: $R_m=0.44$; $R^f{}_m=1.90$ 2nd column: $R_m=0.71$; $R^f{}_m=6.03$	146.25
Distillation system with a side-stream enriching section	$(R_m)_1=1.03$; $(R'_m)_4=3.93$ $(R_m)_3=1.08$	90.39
Distillation system with a side-stream stripping section	$(R_m)_1=1.45$; $(R'_m)_4=1.90$ $(R'_m)_2=2.15$	80.19
Petlyuk's thermally coupled distillation scheme	$R_m=1.19$; $R'_m=2.80$ $(RX_L)_m=0.524$	64.34

Nomenclature

b : Molal flowrate of a component in the bottom product of a distillation system, mole/h

B : Molal flowrate of the bottom product, mole/h

d : Molal flowrate of a component in the top product of a distillation system, mole/h

D : Molal flowrate of the top product, mole/h

f : Molal flowrate of a component in the feed to a distillation system, mole/h

F : Molal flowrate of the feed, mole/h

K_i: Equilibrium constant of component i, dimensionless

L : Molal liquid flowrate in a column section of a distillation system. For a conventional distillation column, it denotes molal liquid rate in the rectifying section, mole/h

L': Molal liquid flowrate in the exhausting section of a standard distillation column, mole/h

p : Molal flowrate of a component in the intermediate product of a distillation system, mole/h

P : Molal flow-rate of the intermediate product, mole/h

q : Thermal condition parameter for the feed, dimensionless

R : Liquid reflux ratio in a rectifying section, dimensionless

R': Vapor reflux ratio in an exhausting section, dimensionless

V : Molal vapor flowrate in a column section of a distillation system. For a standard distillation system it means molal vapor rate in the rectifying section, mole/h

V': Molal vapor flowrate in the exhausting section of a standard distillation column, mole/h

x : Liquid mole fraction, dimensionless

X_L: Operating parameter in Petlyuk's thermally coupled distillation system, defined by equation (54), dimensionless

X_v: Operating parameter in Petlyuk's distillation system, defined by equation (54), dimensionless

y : Vapor mole fraction, dimensionless

Greek Letters:

α : Relative volatility of a component with regard to the heavy key, dimensionless

ϵ : Ratio between heavy key K-values at the upper pinch and the feed trays, respectively; dimensionless

ϵ': Ratio between heavy key K-values at the feed and lower pinch trays, respectively; dimensionless

Y : Ratio between the key mole fractions at both pinch zones of a pair of column sections, dimensionless

Y : Degree of recovery of a key component in one of the distillation system products, dimensionless

Subscripts:

B : Refers to the bottom product
8R: Refers to the bottom tray of a rectifying section
D : Refers to the top product
f^4: Refers to the feed tray
HK: Refers to the heavy key
i : Refers to component i
j : Refers to component j
LK: Refers to the light key
LP: Refers to lower pinch zone
m : Refers to limiting flow conditions
MK: Refers to the middle key
P : Refers to the middle product
TX: Refers to the top tray of the exhausting section
UP: Refers to the upper pinch zone