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SHORTCUT METHODS FOR COMPLEX DISTILLATION COLUMNS:  
PART 2 -- NUMBER OF STAGES AND FEED TRAY LOCATION

by

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## Abstract

### Shortcut Methods for Complex Distillation Columns:

#### Part 2 ~ Number of Stages and Feed Tray Location

This paper is the second part of a two-part paper on shortcut methods for ordinary and complex columns. The shortcut method to estimate the number of stages is based on Edmister's method. The method includes a new approach which locates feed trays to minimize the total number of stages within the column.

Several example problems demonstrate the method and show, where comparisons are available, that it compares favorably with other approaches.

(I) Conventional distillation columns:

By introducing the notion of an effective absorption factor  $A_e$ , Edmister (1957) developed the following expression (see Figure 1),

$$\left(\frac{v_{BR}}{d}\right)_j = R(A_e)_j^{N_R} + \frac{-1}{1} \quad (1)$$

which relates the amounts of  $j$ th-component contained in the vapor stream coming up from the feed plate and in the top product, through variables like the reflux ratio ( $R$ ), the number of ideal stages in the rectifying section ( $N_R$ ) and the effective absorption factor  $(A_e)_j$ .

As stated in Part I, the rectifying section of a conventional distillation column serves to remove the heavy key from the vapor stream so that the fraction of the amount of heavy key in the feed present in the top product is  $(1-r_{HK})$ , where  $r_{HK}$  is the fraction of the heavy key in the feed to be recovered in the bottom product B. Equation (1) can be used as the rectifying section design equation when written for the heavy key. By rearranging equation (1), one can write

$$\left(\frac{v_{BR}}{d}\right)_{HK} = \frac{R(A_e)_{HK}^{N_R} - 1}{A_e - 1} \left(\frac{y_f}{x}\right)_{HK}$$

Using the rectifying section design specification

$$d_{HK} = (1 - r_{HK}) F_{HK}$$

and the definition of  $R$ , the ratio  $(v_M/d)_{HK}$  can be expressed as

$$\left(\frac{v_{BR}}{d}\right)_{HK} = \frac{(R+1)(D/F)}{1-r} \left(\frac{y_f}{x}\right)_{HK} \quad (3)$$

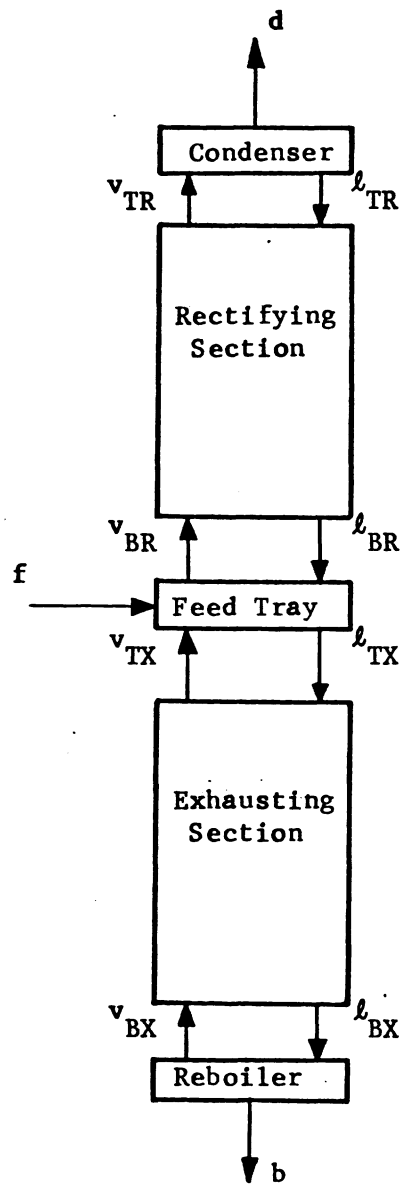


Figure 1. Conventional distillation column

where  $x_f$  is the heavy key mole fraction in the feed, while  $y_f$  is its mole fraction in the vapor leaving the feed plate. Equation (3) assumes constant molar overflow in each section of the column. Substituting (3) into (2) gives

$$n_R = \frac{\ln \left\{ \frac{1 + (A_e - 1)(R+1)(D/F)(y_f/x_f)(1-r_{HK})^{-1}}{R(A_e - 1) + A_e} \right\}_{HK}}{\ln(A_e)_{HK}} \quad (4)$$

Edmister (1957) derived an analogous equation to (1) for the exhausting section too, which is

$$\left(\frac{V}{b}\right)_j = (S_o)_j (S_e)_j^{\circ X} + \langle e \rangle^{\frac{II_X+1}{X}} \frac{-1}{1} \quad (5)$$

where  $(S_e)_j$  is the effective stripping factor for the jth-component and  $(S_o)_j$  is its stripping factor at the reboiler:

$$\langle V_j \rangle^{\frac{V'}{IT}} \langle K_j \rangle_{\text{Reb.}} \quad \langle 6 \rangle$$

As the heavy key is the design component for the rectifying section, the light key is the design component for the exhausting section. From equation (5), one can write

$$n_X = \frac{\left\{ \frac{1 + (S_e - 1)(l_{TX}/b)}{S_o(S_e - 1) + S_e} \right\}_{LK}}{\ln(S_e)_{LK}} \quad (7)$$

but

$$\left(\frac{l_{TX}}{b}\right) = \frac{(R'_m + 1)(B/F)}{(1-r_{LK})} \left(\frac{x_f}{x_F}\right)_{LK} \quad (8)$$

where  $(x_f)_{LK}$  is the light key mole fraction in the liquid coming down from the feed plate. Replacing equation (8) in (7) gives

$$n_X \left\{ \frac{1 + (S_e - 1)(R'_m + 1)(B/F)(x_f/x_F)(1-r_{LK})^{-1}}{S_o(S_e - 1) + S_e} \right\}_{LK}$$

For sharp separations between the keys, the recovery fractions  $r_{HK}$  and  $r_{LK}$  are close to 1. In such cases, design equations (4) and (9) can be simplified to eliminate either  $(y_f/x_F)_{HK}$  or  $(x_f/x_F)_{LK}$ , whose evaluation is difficult. A simple order of magnitude analysis will help us to achieve this simplification. Typical values for the variables present in equation (4) are shown in Table 1. From them it can be concluded that

$$[(A_e)_{HK} - 1] (V_{BR/d})_{HK} \gg 1$$

for sharp separations. Ignoring the term '1', equation (4) can be written

$$n_R = \frac{\ln(1-r_{HK})^{-1} - \ln\left[R + \frac{(A_e)_{HK}}{(A_e)_{HK} - 1}\right] + \ln\left[(R+1)\frac{D}{F}\right] + \ln\left(\frac{y_f}{x_F}\right)_{HK}}{\ln(A_e)_{HK}} \quad (10)$$

Characteristic values for each term in the numerator of equation (10) are shown in Table 2. For any type of separation, difficult or not, the typical value of the last term is much smaller than the other ones and may be neglected. In most cases, this simplification causes an error of less than one ideal stage.

Therefore, for sharp separations, the simplified version of Edmister's rectifying section design equation is given by

$$n_R^o = \frac{\ln\left\{\frac{(R+1)(D/F)(1-r_{HK})^{-1}}{R + \frac{A_e}{A_e - 1}}\right\}_{HK}}{\ln(A_e)_{HK}} \quad (11)$$

where  $n_R^o$  represents a good approximation to the variable  $n_R$ . In order to compute the value of  $(A_e)_{HK}$  later in this paper, an optimal criterion for feed tray location will be derived.

A similar typical value analysis can be made for the exhausting section (see Tables 1 and 2) to simplify equation (9), yielding



Table 2

Typical values for each term in the numerators of equations (10) and  
of the similar one for the exhausting section

Terms	$\ln(1-r_{HK})^{-1}$	$\ln\left[\frac{(A_e)_{HK}}{(A_e)_{HK} - 1}\right]$	$\ln\left[(R+1)\frac{D}{F}\right]$	$\ln\left(\frac{x_F}{x_F'}\right)_{HK}$
Ordinary Separations	4.60	1.61	0.22	-0.105
Difficult Separations	4.60	2.83	1.25	0.182

Terms	$\ln(1-r_{LK})^{-1}$	$\ln\left[S + \frac{S}{e} \frac{1}{e^{n-1} LK}\right]$	$\ln(R'+1)(B/F)$	$\ln(x_F/x_F')_{LK}$
Ordinary Separations	4.60	2.14	0.56	0.182
Difficult Separations	4.60	3.21	1.38	0.182

• Table 1

Characteristic values for the variables in equations (4) and (9),  
for multicomponent, sharp separations

Variables	$\langle VHK \rangle$	R	(D/F)	$(K_{fV})$	$\langle VVHK \rangle$	WHK	$r_{HK}$	(*)
Ordinary Separations	1.40	1.50	0.50	0.60	1.50	0.90	0.99	45
Difficult Separations	1.10	6.0	0.50	0.80	1.50	1.20	0.99	42

Variables	$\langle s_e \rangle_{LK}$	$R^1$	(B/F)	$(S_o)_{LK}$	$(x_F/x_F)_{LK}$	$r_{LK}$	(**)
Ordinary Separations	1.40	2.5	0.50	5	1.20	0.99	84
Difficult Separations	1.10	7.0	0.50	14	1.20	0.99	48

(\*) Characteristic values for  $[(A_e)_{HR}-1] (V_{BR}/\langle * \rangle)_{HK}$

(\*\*) Characteristic values for  $[(S_e)_{LK}] (l_{TX}/b)_{LK}$

$$n_X^o = \frac{\left\{ \frac{(R'+1)(B/F)(1-R)^{-1}}{S_{LK}} \right\} LK}{\ln(S_e)_{LK}} \quad (12)$$

Evaluation of the effective stripping and absorption factors  $(A_e)_{HK}$

and  $(S_e)_{LK}$ :

Assuming that the effective factors are functions of terminal conditions (e.i. top and bottom plates in each section), Edmister (1946) derived the following expressions:

$$A_e = \left( VD + 0.5 \right)^{-0.5} \quad (13)$$

$$S_e = \left( tS_T(S_B+1) + 0.25 \right)^{-0.5} \quad (14)$$

which result from analyzing a two theoretical plate-column. When the value of  $A_e$  (or  $S_e$ ) is close to unity, this effective factor short-cut procedure provides very accurate results even for many plates (Edmister, 1948). In the above expressions, the subscripts T and B stand for top and bottom trays in the section.

Horton and Franklin (1940) also assumed that  $A_e$  (or  $S_e$ ) is a function of the terminal conditions and proposed

$$A_e = 0.7 A_{eT} + 0.3 A_{eB} \quad (15)$$

$$S_e = 0.7 S_{eT} + 0.3 S_{eB} \quad \langle 16 \rangle$$

when  $A_e$  (or  $S_e$ ) is between 1.0 and 4.0, which is almost always the range for the values of  $(A_e)_{RR}$  and  $(S_e)_{tR}$ . As Edmister (1957) mentioned, equations (15) and (16) give essentially the same values for  $A_e$  and  $S_e$  that are found by equations (17) and (18). Equations (15) and (16) may then be used to develop an optimal feed tray location criterion. By replacing the definitions of the absorption and stripping factors in equations (15) and (16), it follows that

$$(A_{eHK})^{(R)} = \frac{(K_{BR})^{(R)}_{HK}}{(K_{BR})^{(R)}_{HK}} (A_{TR})_{HK} \quad (17)$$

$$(S_{eLK})^{(X)} = 0.70 \frac{a_{LK}^{(K_{TX})}_{HK}}{L^1/V^1} + 0.30 (S_{BX})_{LK} \quad (18)$$

where the superscripts and subscripts R and X stand for rectifying and exhausting sections, respectively. By defining the factor  $F_K$

$$K_{VHK} \quad (19)$$

both design effective factors  $(A_{eHK})^{(R)}$  and  $(S_{eLK})^{(X)}$  can be expressed in terms of  $(K_{BR})_{HK}$  by replacing equation (19) in (18)

$$\langle S_{eLK} \rangle_{UC} = 0.70 \frac{a_{LK}^{(K_{TX})}_{HK}}{L^1/V^1} + 0.30 \langle S_{BX} \rangle_{I^*} \quad \langle 20 \rangle$$

Where sharp separations are considered between two adjacent components, the compositions of the products are readily determined and so are the values of  $(A_{eHK})^{(R)}$  and  $(S_{eLK})^{(X)}$ . In this situation, they can be considered as constants, i.e. independent of the location of the feed tray.

When the sharp separation is between two non-adjacent keys with one or more distributed components, the split of the distributed components between the two final products must be estimated before evaluating  $(A_{TR})_{HK}$  and  $(S_{RX})_{LK}$ . However, even in this case, one can assume that the product compositions are a weak function of the feed tray location (within a certain span of possible locations not far from the optimal one), without making a significant error. Therefore, equations (17) and (20) show the design effective factors  $(A_{eHK})^{(R)}$  and  $(S_{eLK})^{(X)}$  as functions of the feed tray location, through the variable  $(K_{BR})_{HK}$ , assuming that the factor  $F_K$  defined by (19) to be approximately constant.

As the operating cost continues to soar, the optimal flow conditions approach the limiting ones. Moreover, the temperatures at both extreme

sections of a distillation column change rather slightly (because of the distributed components) as the reflux ratio increases from its minimal value to the optimal one. Thus, one can propose for a fast estimation of  $F^*$  the following expression:

$$r^* = \frac{(\text{t} \setminus \text{ED} - i \cdot \text{VEP} \cdot 4 - 1)^{\wedge}}{\text{TY} \cdot \text{HK}} = \frac{\text{m}}{\text{m}} \quad (21)$$

$$K \quad (K_{BR})_{HK} \quad Q_{LK} \cdot m^{R < m}$$

which holds at minimum reflux when the pinch zones occur at the trays right above and below the feed plate (see Part I).

In order to evaluate the design effective factors, we must now develop a criterion to choose  $(K_{DK})_{HK}$ .

Criterion for Optimal Feed Tray Location:

The location of the feed tray should be selected to minimize the total number of theoretical stages  $n_t$  required for a given separation, which is given by

$$n_t = t^{\wedge} + i^{\wedge} + 1 \quad (22)$$

where the last term on the R.H.S. corresponds to the feed stage. Accounting for equations (11) and (12), it follows that  $IL$  is a function of  $(K_{RR})_{HK}$  i.e. the feed tray location, through the variables  $(A)_{eHK}$  and  $(S)_{eLK}$ . Therefore, the optimality condition can be so expressed

$$\frac{dn_t}{d(K_{BR})_{HK}} = \frac{\delta n_t}{\delta (A)_{eHK}} \cdot \frac{d(A)_{eHK}^{(R)}}{d(K_{BR})_{HK}} + \frac{\delta n_t}{\delta (S)_{eLK}} \cdot \frac{d(S)_{eLK}^{(X)}}{d(K_{BR})_{HK}} = // // \cdot$$

Although  $(A)_{eNK}$  shows up in both the numerator and the denominator of equation (11), its strong influence on the value of  $n_t$  is mainly achieved through the denominator. Thus, a good approximation to  $(\delta n_t / \delta (A)_{eHK})$  is still obtained if the dependency between  $IL$  and  $(A)_{eHK}^{(R)}$  in the numerator is ignored:

$$\frac{\delta n_t}{\delta (A_e)_{HK}^{(R)}} = \frac{1}{(A_e)_{HK}^{(R)} [\ln(A_e)_{HK}^{(R)}]^2} \quad (24)$$

where  $\eta_R$  gives the value of the numerator at  $(A_e)_{HK}^{(R)} = (A_e^o)_{HK}^{(R)}$  near the sought optimal value  $e_{HK}$   $e_{nss}$ .

$$\eta_R = \ln \left[ \frac{(R+1)(D/F)(1-r_{HK})^{-1}}{R + \frac{A_e^o}{A^o - 1}} \right]_{HK} \quad (25)$$

Similarly

$$\frac{\delta n_t}{\delta (S_e)_{LK}^{(X)}} = \frac{1}{(S_e)_{LK}^{(X)} [\ln(S_e)_{LK}^{(X)}]^2} \quad (26)$$

$$\eta_X = \ln \left[ \frac{(R+1)(B/F)(1-r_{LK})^{-1}}{S_e + \frac{S_e^o}{s_{e,1}^o}} \right]_{LK} \quad (27)$$

From equations (17) and (20)

$$\frac{d(A_e)_{HK}^{(R)}}{d(K_{BR})_{HK}} = -0.70 \frac{(L/V)}{[(K_{BR})_{HK}]^2} \quad (28)$$

$$\frac{d(S_e)_{LK}^{(X)}}{d(K_{BR})_{HK}} = 0.70 \frac{\alpha_{-F}}{(L'/V')} \quad (29)$$

By substituting equations (24), (26), (28) and (29) into (23) and rearranging the optimality condition takes the following form:

$$\left\{ \frac{\ln(A_e)_{HK}^{(R)}}{\ln(S_e)_{LK}^{(X)}} \right\}^2 = \mathbf{V} \frac{1}{(A_e)_{HK}^{(R)}} \frac{\mathbf{T}}{(\frac{\alpha_{LK}^F}{K} \mathbf{Y})_{HK} \mathbf{Y}} \quad (30)$$

However, from equations (17) and (20)

$$0.70 \frac{\left(\frac{L}{V(K_{BR})_{HK}}\right)}{(A_e)^{(R)}_{HK}} = 1 - 0.30 \frac{(A_{TR})_{HK}}{(A_e)^{(R)}_{HK}} \quad (31)$$

$$0.70 \frac{(S_e)^{(X)}_{LK}}{\left(\frac{\alpha_{LK}^F (K_{BR})_{HK} V'}{L'}\right)} = 1 - 0.30 \frac{(S_{BX})_{LK}}{(S_e)^{(X)}_{LK}} \quad (32)$$

Defining

$$\Gamma = \frac{\eta_R}{\eta_X} \quad (33)$$

and replacing equations (31), (32) and (33) in (30), it follows that

$$\left\{ \frac{\ln(A_e)^{(R)}_{HK}}{\ln(S_e)^{(X)}_{LK}} \right\}^2 = \Gamma \frac{[1 - 0.30 \frac{(A_{TR})_{HK}}{(A_e)^{(R)}_{HK}}]}{[1 - 0.30 \frac{(S_{BX})_{LK}}{(S_e)^{(X)}_{LK}}]} \quad (34)$$

In most cases, the ratios  $[(A_{TR})/A_e^{(R)}]_{HK}$  and  $[(S_{BX})/(S_e)^{(X)}]_{LK}$  are not so different, especially when  $(A_{TR}/A_{BR})$  for the heavy key and  $(S_{BX}/S_{TX})$  for the light key are close. Therefore, the R.H.S. of equation (30) will usually be around 1 when similar recovery fractions for the keys are considered.

In other words, an approximate solution to equation (30) can be obtained by solving a much simpler equation:

$$\ln(A_e^0)^{(R)}_{HK} = \ln(S_e^0)^{(X)}_{LK}$$

or

$$(A_e^0)^{(R)}_{HK} = (S_e^0)^{(X)}_{LK} \quad (35)$$

where the superscript (°) means that they are approximate solutions to (30). By introducing the correction terms  $\Delta(A_e)_{HK}^{(R)}$  and  $\Delta(S_e)_{LK}^{(X)}$ , the exact solutions to (30) can be written

$$(A_e)_{HK}^{(R)} = (A_e^o)_{HK}^{(R)} + \Delta(A_e)_{HK}^{(R)} \quad (36)$$

$$(S_e)_{LK}^{(X)} = (S_e^o)_{LK}^{(X)} + \Delta(S_e)_{LK}^{(X)} \quad (37)$$

where the correction terms are usually small.

Analytical expressions for the approximate solutions  $(A_e)_{HK}^{(R)}$  and  $(S_e^o)_{LK}^{(X)}$

From substituting equations (17) and (20) into (35), it follows that

$$0.70 \frac{\alpha_{LK}^F}{\alpha_{BR}^F} + 0.30 (A_{TR})_{HK} - 0.70 \frac{\alpha_{LK}^F}{\alpha_{BR}^F} - 0.30 (S_{BX})_{LK}$$

which leads to a quadratic equation in  $(A_{TR})_{HK}$  given by

$$(K_{BR}^o)_{HK}^2 - \frac{0.428(L'/V')[(A_{TR})_{HK} - (S_{BX})_{LK}]}{\alpha_{LK}^F} (K_{BR}^o)_{HK} - \frac{(L/V)(L'/V')}{\alpha_{LK}^F} = 0$$

whose analytical solution is

$$f f S^{\wedge} H K - r + \hat{\wedge} r) + V \quad (38)$$

where

$$\Delta_1 = \frac{1}{\alpha_{LK}^F} \quad (39)$$

$$\Delta_2 = \frac{(L/V)(L'/V')}{\alpha_{LK}^F} \quad (40)$$

Finally, the approximate solutions can be evaluated by



$$(A_e^o)_{HK}^{(R)} = 0.70 \frac{(L/V)}{(K_{BR}^o)_{HK}} + 0.30 (A_{TR})_{HK} \quad (41)$$

$$(S_e)_{LK}^{(X)} = 0.70 \frac{W}{(L/V)} + 0.30 (S_{BX})_{LK} \quad (42)$$

Analytical expressions for the correction terms  $(A_e)_{TR}$  and  $\frac{\Delta(S_e)_{LK}}{e}$

Optimality condition (30) can also be written

$$G[(K_{BR})_{HK}] = [1 - 0.30 \frac{C}{V} \frac{IK}{HK}] \frac{[\ln(S_e)_{LK}^{(X)}]^2}{V} = 0 \quad (43)$$

where the error function G is equal to zero for the optimal value of the variable  $C$ . Taking into account that  $(K_{BR})_{HK} \approx i^s > *^{-n}$  most cases, a good estimation of the optimal value, we can use the first term of a Taylor series to get

$$G[(K_{BR}^*)_{HK}] = G[(K_{BR}^o)_{HK}] + \left[ \frac{dG}{d(K_{BR})_{HK}} \right]_{(K_{BR}^o)_{HK}} \Delta(K_{BR})_{HK} = 0$$

where the asterisk stands for optimal value. Therefore

$$\Delta(K_{BR})_{HK} = \frac{G[(K_{BR}^o)_{HK}]}{\left[ \frac{dG}{d(K_{BR})_{HK}} \right]_{(K_{BR}^o)_{HK}}} = (K_{BR}^*)_{HK} - (K_{BR}^o)_{HK} \quad (44)$$

By replacing equality (35) into equation (43), the following expression for  $G[(K_{BR})_{HK}]$  is derived:

$$G[(K_{BR}^o)_{HK}] = \left\{ (1-\Gamma)(A_e^o)_{HK} + 0.30 [\Gamma(A_{TR})_{HK} - (S_{BX})_{LK}] \right\} \frac{[\ln(A_e^o)_{HK}]^2}{(A_e^o)_{HK}} \quad (45)$$

On the other hand,

$$\frac{dG}{d(K_{BR})_{HK}} = \frac{\delta G}{6(A_e)^{<*>_{LK}}} \frac{d(A_e)^{(R)}_{HK}}{d(K_{BR})_{HK}} + \frac{\delta G}{>>(S_e)^{(X)}_{LK}} \cdot \frac{d(S_e)^{(X)}_{LK}}{d(K_{BR})_{HK}} \quad (46)$$

The derivatives in equation (46) can be obtained from equations (43), (17) and (20). By replacing equality (35) in them, equation (46) leads to this expression:

$$\frac{dG^0}{d(K_{BR})_{HK}} = 0.70 \left\{ \frac{(L/V)\beta_1}{[(K_{BR}^0)_{HK}]^2} + \frac{\alpha_{LK}^F K}{(L'/V')} \beta_2 \right\} \quad (47)$$

where

$$\beta_1 = 0.30 \Gamma(A_{TR})_{HK} (Z^0)^2 - 2[1-0.30 \frac{(S_{BX})_{LK}}{(A_e^0)^{(R)}_{HK}}] Z^0 \quad (48)$$

$$\beta_2 = 0.30 (S_{BX})_{LK} (Z^0)^2 - 2r[1-0.30 \frac{(S_{BX})_{LK}}{(A_e^0)^{(R)}_{HK}}] Z^0 \quad (49)$$

$$Z^0 = \frac{\ln(A_e^0)^{(R)}_{HK}}{(A_e^0)^{(R)}_{HK}} \quad (50)$$

Finally, the optimal value  $(K_{BR})_{HK}^{opt}$  can be evaluated from equation (44).

Its substitution into the equations (17) and (20) gives the sought values

for  $(A_e^*)_{HK}^{(R)}$  and  $<><*>_{LK}$ .

### Algorithm

1. Use the product compositions at minimum reflux to get the values of  $(A^*)^*$  and  $(S^*)^*$ . Then, evaluate  $F_R$  by equation (21).
2. Calculate the first approximation to the optimal design effective factors,  $(A_e^0)_{UK}$  and  $(S_e^0)_{HK}$  through equations (38), (39), (40), (41) and (42).
3. Evaluate the variables  $T_R$ ,  $T_K$ , and  $T$  by equations (25), (27) and (33), respectively.
4. Get the optimal values for the design effective factors using equations (45), (47), (48), (49), (50), (44), (17) and (20).
5. Determine the number of theoretical stages required in each column section,  $n_{\underline{L}}$  and  $n_{\underline{X}}$ , by equations (11) and (12), respectively.
6. Evaluate the total number of theoretical stages required,  $n_T$ , by means of equation (22).

### (II) Distillation system with a side-stream stripping section

Every distillation system can be regarded as comprising a set of fractionators, each of them yielding two, one or zero products. Such fractionators accomplish the task of separating two of the keys. Thus in Figure 2 the fractionator (1,2) carries out the separation (LK/MK) while (3,4) does (MK/HK). When the analysis is restricted to sharp separations, all non-recovered light key component is supposed to come out of the system in the middle product P as also does the non-recovered heavy key. In turn, the non-recovered middle key distributes between the products D and B.

The three key component recovery fractions given as design specifications are not enough to set the design of this distillation system. The number of ideal stages required in column sections 1 and 4, whose design component is MK, depends on how the non-recovered middle key distributes between the products D and B. The additional design specification can be given through the parameter  $S$ , defined by:

$$(d/f)_{MK}^{-1} - 4 \quad 0 < ? < 1 \quad (5D)$$

§ is then a design parameter whose value should be appropriately chosen.

When the volatilities  $\alpha_{MK}$  and  $\alpha_{LK}$  are relatively much closer, it is quite obvious that nearly all non-recovered middle key should go up in the product D. In other words, the parameter § should tend to unity. The other extreme case is reached when  $\alpha_{MK}$  and  $\alpha_{HK}$  are quite similar, for which § should take very small values. From these considerations, the following criterion was selected to evaluate §:

$$\xi = \frac{(\alpha_{MK}/\alpha_{HK})}{(\alpha_{LK}/\alpha_{MK}) + (\alpha_{MK}/\alpha_{HK})}$$

However, a more precise criterion should account for the effective design absorption and stripping factor values in each fractionator rather than volatility values. The next step is to develop simplified design equations for each of the column sections, especially for the new type CS-3.

Design equation for CS-3:

The goal for CS-3 is to wash the heavy key from the vapor stream. The derivation of its design equation, giving explicitly the number of ideal stages  $n_3$ , requires one to have a relationship between the internal vapor and liquid compositions at the top of CS-3, i.e. between  $(y^A - J^M)_{U \text{ HS.}}$  and  $(x_o)_{T \text{ tJ, 1J Hr}}$  (see Figure 2). Although it is an approximation, the feed tray of fractionator (1,2) can be thought of assuming the role of partial condenser for the fractionator (3,4). For such a case, Edmister (1957) derived the following design equation:

$$n_3 = \frac{1 + (R_3 + 1)(v_{B3}/v_{T3})}{\frac{V_3^{-1}}{x_{n(A), 3 > HK}}} \quad (52)$$

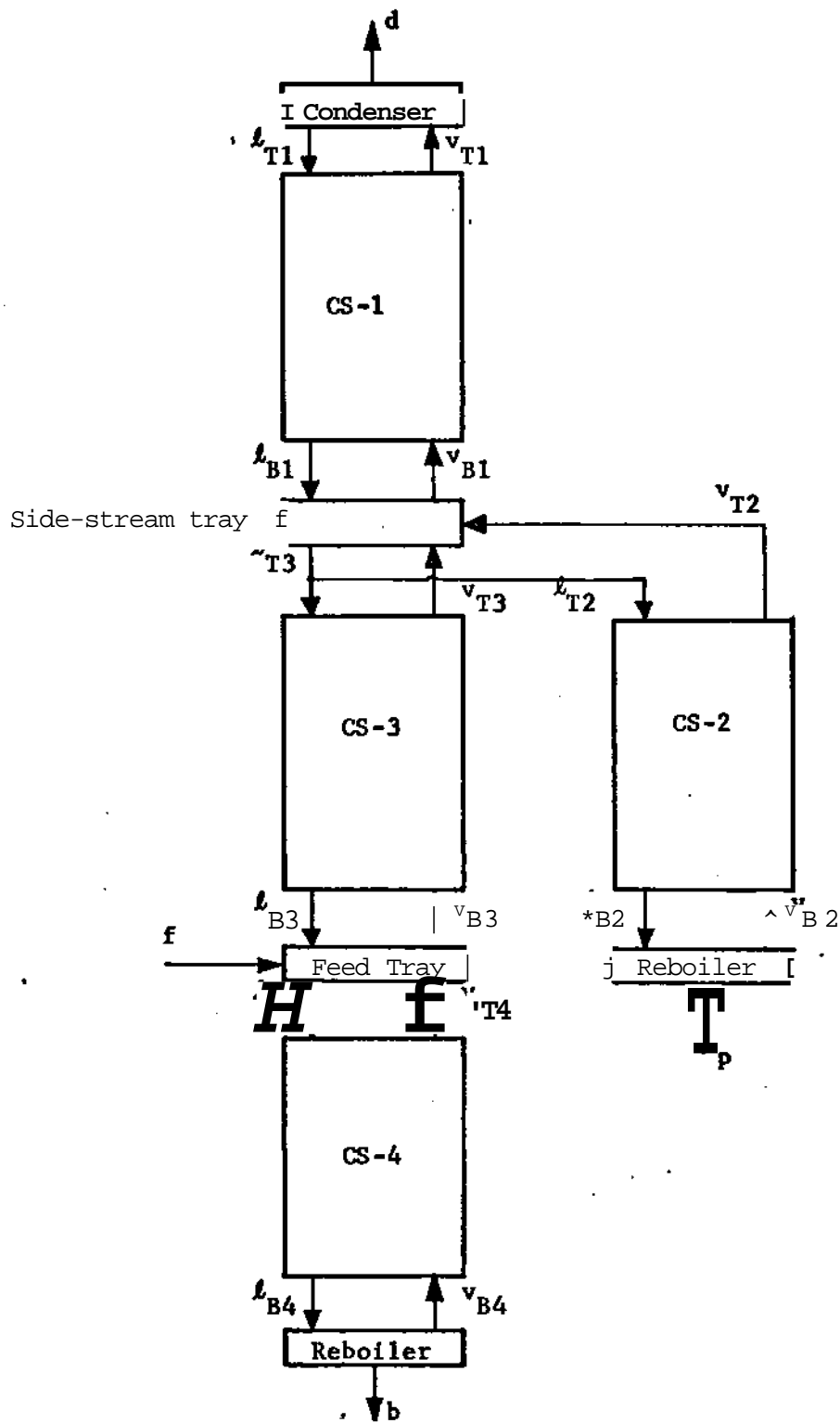


Figure 2. Distillation system with a side-stream stripping section

where

$$\langle A_{o,3} \rangle_{HK} = \frac{L_3}{Qf_3' L_3} (K_{T3})_{HK} = \frac{R_3}{(K_{T3})_{HK}}$$

Simplified versions of the column section design equations for sharp separations:

(i) CS-1<sup>f</sup>s design equation

CS-1 is a rectifying section whose design component is MK. It follows from equation (11) that

$$n_P \ll \frac{\ln \left\{ \frac{(R_1+1) \left( \frac{D}{V_1-L_1} \right) (1-r_{MK})^{-1}}{R_1} \right\}}{\ln(A_{e,1})_{MK}} \quad (53)$$

where  $R_1 = \frac{1}{D}$

and the value of  $(A_{e,1})_{MK}$  should be obtained by an additional criterion.

$(A_{e,1})_{MK}$

(ii) CS-2<sup>y</sup>s design equation

CS-2 is an exhausting section having LK as its design component.

Then, from equation (12)

$$n_2^o = \frac{\ln \left\{ \frac{P}{V_1-L_1} (1-r_{LK})^{-1} \right\}}{\ln(S_{e,2})_{LK}} \quad (54)$$

where

$$R'_2 = \frac{V_2}{P} \text{ and } (S_{o,2})_{LK} = R'_2 (K_{Reb.,2})_{LK}$$

(iii) CS-3<sup>y</sup>s design equation

$$n_3^o = \frac{\ln \left\{ \frac{(R_3+1) \left( \frac{V_3-L_3}{F} \right) (1-r_{HK})^{-1}}{A_{o,3}} \right\}}{\ln(A_{e,3})_{HK}} \quad (55)$$

(iv) CS-4's design equation

$$n_4^o = \frac{\ln \left\{ \frac{(R'_4 + 1)(B/F)(1 - r_{MK}^{1-})^{-1}}{S_{o,4} + S_{e,4}} \right\}_{MK}}{\ln(S_{e,4}^{-1})_{MK}} \quad (56)$$

where

$$R'_4 = \frac{V_4}{B}$$

Evaluation of the design effective factors:

In order to find the optimal locations of the feed trays of both fractionators (1,2) and (3,4), a similar analysis to that shown for a conventional column should be made. Equations almost equivalent to (38), (39), (40), (47), (48), (49) and (50) are obtained with small differences. Thus, for fractionator (1,2):

<u>Use</u>	<u>Instead of</u>
$(A_{e,1})_{MK}$	$(A_e)^{(R)}_{HK}$
$(S_{e,2})_{LK}$	$(S_e)^{(X)}_{LK}$
$(K_{B1})_{MK}$	$(K_{BR})_{HK}$
$(L_1/V_1)$	$(L/V)$
$(L_2/V_2)$	$(L'/V')$
$(A_{T1})_{MK}$	$(A_{TR})_{HK}$
$(S_{B2})_{LK}$	$(S_{BX})_{LK}$
$(\alpha_{LK}/\alpha_{MK})$	$\alpha_{LK}$
$(R_m)_1$	$R_m$
$(R'_m)_2$	$R'_m$

The modifications described in the table are indeed only a matter of changing nomenclature.

(III) Arbitrary thermally coupled distillation column

Because of its complexity, Petlyuk's thermally coupled distillation system shown in Figure 3 can serve to generalize the proposed design approach already applied to a conventional column and to a distillation system with a side-stream exhausting section. Design equations for column sections CS-3 and CS-6 can be readily derived from equations (11) and (12) because they are a rectifying and an exhausting section, respectively. In turn, column sections CS-1 and CS-5 can be regarded as being rectifying sections provided with partial condensers. This approximation is quite good for CS-5. Their design equations are analogous to equation (52).

Finally, column sections CS-2 and CS-4 look like exhausting sections equipped with partial reboilers, especially CS-4. Then, their design equations can be derived from equation (12).

In each case, it is important to identify the design component of the column section (which is one of the keys) before writing its design equation. When they are available for the entire distillation system, a mathematical derivation similar to that shown for a conventional column should be carried out for each of the three fractionators so as to get the optimal locations for the feed and side-stream trays.

In addition to the three key recovery fractions in each product, three more specifications should be given to set the design of a Petlyuk's distillation system. That is so because each key is involved in two consecutive separations as the design component, i.e. key HK in the separations (LK/HK) and (MK/HK) in fractionators (1,2) and (5,6), respectively. Recovery fractions for HK should be chosen in both fractionators in such a way that their product is equal to the overall recovery fraction  $r_{HK}$ . Since  $r_{HK} < 1$ , the partial recovery fractions are always greater than the overall one. This is



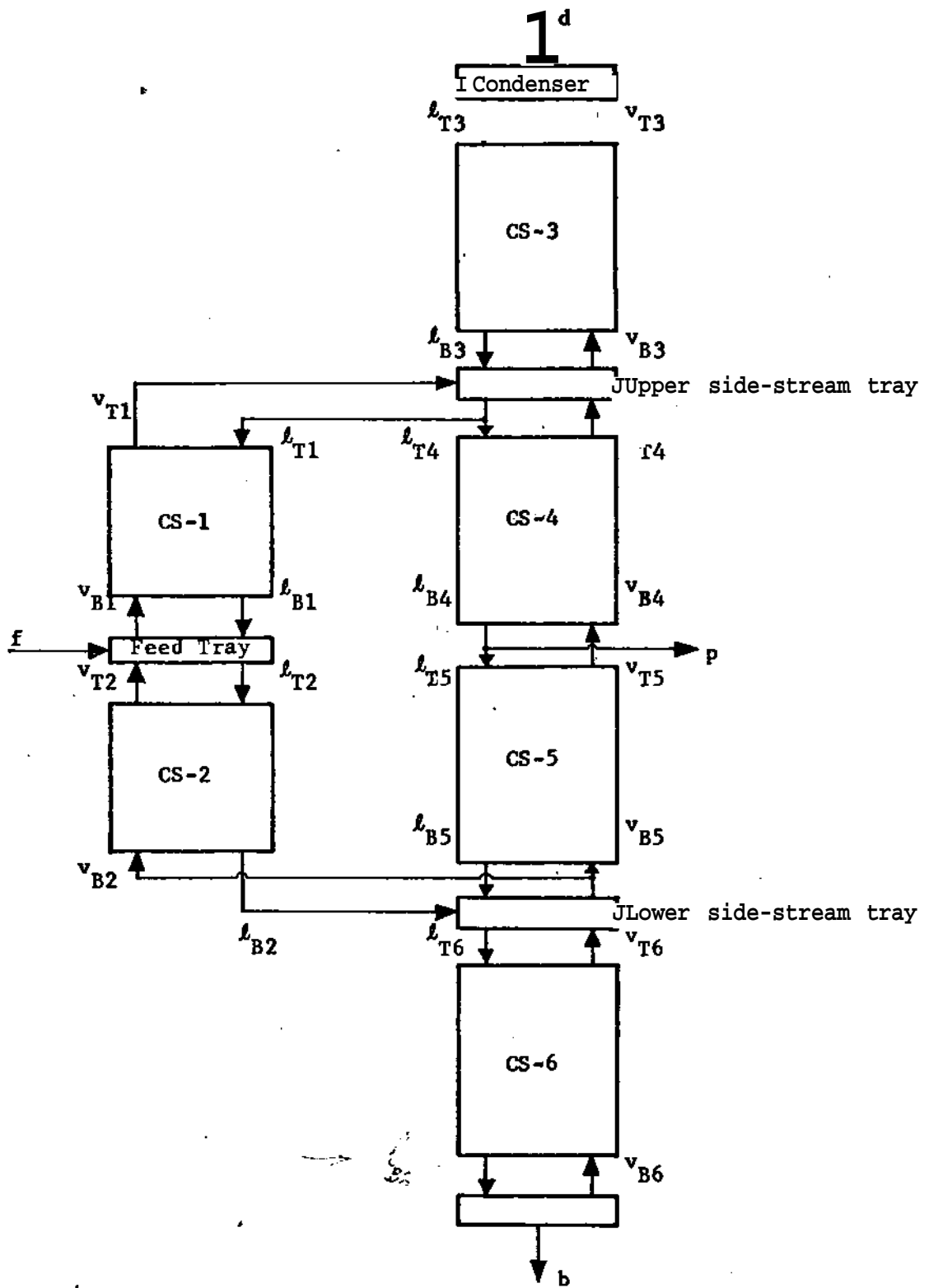


Figure 3: Petlyuk's thermally coupled distillation system

an undesirable feature of this complex unit because these recovery fractions are central to the calculation of the total number of ideal stages required for the separation. In other distillation schemes, only MK acts as the design component in two successive fractionators. As stated before, selection of the partial recovery fractions for the keys should be made accounting for the values of the design absorption and stripping factors in each fractionator. The larger the design factor is, the greater the partial recovery fraction should be. This has especially to do with Petlyuk's distillation system, where one of the fractionators is operated fairly well beyond its limiting conditions.

#### (IV) Results and discussion

In the Appendix three examples are included to illustrate the accuracy of the proposed shortcut method when applied to the design of conventional columns. Example A.I.I was solved step by step in Table 3 to clarify the way the algorithm is applied and show its simplicity. The agreement the results have with the ones provided by more rigorous techniques is satisfactory, especially where key recovery fractions are high and the operating conditions are not far from the limiting flow situation, as happens in Example A.I.I.

On the other hand, Example A.II, serves to compare the number of ideal stages required for conventional and thermally coupled schemes for a given separation. Operating parameters were chosen 1.3 times their limiting values in each case so that the comparison makes sense. Because of the symmetry of the volatilities, the partial recovery fractions were all selected equal to 0.995. For Petlyuk's distillation unit this was not a clever decision because fractionator (3,4) is operated well beyond limiting flow conditions, as shown by the values of its design effective factors,  $(A_{e,3 MK})_{opt}$  and  $(S_{e,** LK})_{opt}$ .

equal to 1.97 and 1.57, respectively. Although higher partial recovery fractions in fractionator (3,4) would lead to a smaller total number of ideal stages, Petlyuk's distillation system, at least in this example, seems to require a larger number of ideal stages than the conventional schemes, but not so much as to negate its energy saving. The other thermally coupled distillation scheme analyzed in Example A.II., a distillation system with a side-stream stripping section, seems also to be a profitable alternative leading to savings in both fixed and operating costs.

Appendix

(I) Examples related to conventional distillation columns

(1,1.) Example proposed by King (1971)

<u>Components</u>	<u>f<sub>i</sub></u>	<u>(V<sub>av.</sub></u>	<u>d<sub>i</sub></u>	<u>b<sub>i</sub></u>
c <sub>1</sub>	26	18.65	26	-
c <sub>2</sub>	9	4.75	9	-
C <sub>3</sub> (LK)	25	1.92	24.6	0.4
n-C <sub>4</sub> (HK)	17	1.00	0.3	16.7
n-C <sub>5</sub>	11	0.46	-	11
n-C <sub>6</sub>	12	0.23	-	<u>12</u>
			59.9	40.1

Other data:

$$q = 0.33; r_{LK} \ll 0.984; r_{HK} = 0.9823$$

$$R = 1.50; R^1 = 2.075$$

Table 3 shows the sequence of partial results which are obtained when applying the proposed method. Those of special interest are  $F = 1.37$  that was supposed to be around 1, and  $(K_{JK})_{HK}^{TM} = 0.559$  and  $(K_{DK}^*)_{HK}^{TM} = 0.547$  which were said to be close.

According to King (1971), Underwood's method provides the following results for this example:

$$i^{\wedge} = 7.1 \quad ; \quad i^{\wedge} = 7.2 \quad ; \quad n_{fc} = 15.3$$

while Edmister's stage-to-stage approach gives  $n_t = 16$

Table 3

Detailed illustration of the proposed method  
when applied to Example (A.I.I).

Step	From	We obtain
1	$R_{eff} = 1.03; R'_m = 1.37$ and equation (21)	$F_R = 1.78$
	$(K_{HK})_{HK} \ll \frac{\sqrt{(x)_m}}{f} \cdot \frac{1}{f} \text{ and } (A_{HK})_{HK} \cdot \frac{[m / m \dots]}{(K_{HK})_{TR}}$	$\sqrt{A_{TR}}_{HK} = z^{*19}$
3	$\frac{1}{7TT-T} - \frac{1}{7} \ll_4(x)_m \text{ and } (S_e)_{HK} = R'a_{HK}(K_{HK})_{HK}$	$(S_e)_{HK} = 6.32$
	$\frac{4}{X DA} - \frac{QV}{K} \cdot \frac{n f L}{r 1} \cdot \frac{I^2 \cdot m}{ID} \cdot \frac{V^2 J / U}{ID} \cdot \frac{A^2 I}{ID} \cdot \frac{V^2 TTr / TSV}{ID} \cdot \frac{L^2}{L 1} \cdot \frac{f^2}{X DA}$	$\frac{BV}{DA} \cdot \frac{TV}{Lix} \cdot \frac{v}{v}$
5	Equations (38), (39), (40), (41) and (42)	$(K_{BR}^O)_{HK} = 0.559; (A_e^O)_{HK}^{(R)} = 1.408$
6	Equations (25), (27) and (33)	$T = 1.37$
7	Equations (45), (47), (48), (49), (50), (44), (17) and (20)	$O^A R V = 0.547; (A_e^*)_{HK}^{(R)} = 1.125$ $(S_e^*)_{HK}^{(X)} = 1.388$
8	Equations (11), (12) and (22)	$n_{1A} = 8.07; n_{1A} = 6.25; n_{1t} = 15.32$

(1.2) Example proposed by Van Winkle (1967):

<u>Components</u>	<u>f<sub>i</sub></u>	<u>(a<sub>i</sub>)<sub>&gt;&lt;</sub></u>	<u>d<sub>i</sub></u>	<u>b<sub>i</sub></u>
i-C <sub>4</sub>	6	2.57	6	-
n-C <sub>4</sub> (LK)	17	2.04	16.81	0.19
i-C <sub>5</sub> (HK)	32	1.00	0.89	31.11
n-C <sub>5</sub>	45	0.84	-	<u>45</u>
			23.7	76.3

Other data:

$$\bar{q} = 1.0; r_{HK} = 0.972; r_{LK} = 0.1989$$

$$R = 6.20; R^1 = 2.236$$

Results:

$$\left( \frac{K_{BR}^*}{r_{i,j}} \right) = 0.817 * \left( \frac{1}{e} \right)_{i,j} = 1.279 * \left( \frac{1}{e} \right)_{i,j} - i \cdot A Q 4$$

$$i^{\wedge} = 7.17; r^{\wedge} = 9.65; n_{fc} \ll 17.82$$

According to Van Winkle (1967), the following values are obtained using Lewis-Matheson's method:

$$r^{\wedge} = 5; r^{\wedge} = 10; n_t \gg 16$$

(1.3) Example proposed by King (1971):

<u>Components</u>	<u>f<sub>i</sub></u>	<u>&lt;Vav.</u>	<u>d<sub>i</sub></u>	<u>b<sub>i</sub></u>
C <sub>3</sub> (LK)	40	2.45	39.2	0.8
n-C <sub>4</sub> (HK)	40	1.00	0.8	39.2
i-C <sub>5</sub>	10	0.49	-	10
n-C <sub>5</sub>	10	0.41	-	<u>10</u>
			40	60

Other data:

$$q = 1; r_{LK} = r_{HK} = 0.98$$

$$R = 5; R^1 = 4$$

Results:

$$(K_{BR}^*)_{LK} = 0.577; \quad (\alpha_{HK}^*)_{AV} = 1.605; \quad (S^*)_{LK}^{VA} = 1.524$$

$$i^{\wedge} = 5.81; \quad r^{\wedge} = 5.52; \quad n_t = 12.33$$

King (1971) reported that Lewis-Matheson's method leads in this case to the following results:

$$i^{\wedge} = 4 \quad ; \quad i^{\wedge} = 5 \quad ; \quad n_t = 10$$

(II) Example related to thermally coupled distillation schemes as proposed by Stupin and Lockhart (1971):

<u>Components</u>	<u>f<sub>i</sub></u>	<u>(α<sub>i</sub>)<sub>av.</sub></u>	<u>d<sub>i</sub></u>	<u>F<sub>i</sub></u>	<u>b<sub>i</sub></u>
A(LK)	0.333	9	0.3297	0.0033	-
B(MK)	0.334	3	0.00165	0.3307	0.00165
C(HK)	0.333	1	-	0.0033	0.3297

Other data:

$$r_{LK} = r_{MK} = r_{HK} = 0.99$$

Values for the operating parameters were chosen as 1.3 times their limiting values already determined in Part I. Results are shown in Table 4.

Table 4

Comparison among the number of Ideal stages required in conventional and thermally coupled distillation schemes, for the Example A.II.1

Type of distillation unit	Number of ideal stages required in each fractionator	Total number of ideal stages
Direct conventional scheme	First column: 22.20 (+ reboiler)	46.71
	Second column: 24.51 (+ reboiler)	
Reverse conventional scheme	First column: 21.07 (+ reboiler)	44.47
	Second column: 23.40 (+ reboiler)	
Distillation system with a side-stream exhausting section	Fractionator (3,4): 19.79 (+ reboiler)	40.65
	Fractionator (1,2): 20.86 (+ reboiler)	
Petlyuk's distillation system	Fractionator (1,2): 19.64	52.88
	Fractionator (3,4): 14.34	
	Fractionator (5,6): 18.90 (+ reboiler)	

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Nomenclature

A	:	Absorption factor ( $L/KV$ ), dimensionless
b	:	Molal flow-rate of a component in the bottom product, mole/h
B	:	Bottom product molal flow-rate, mole/h
d	:	Molal flow-rate of a component in the top product, mole/h
D	:	Top product molal flow-rate, mole/h
f	:	Molal flow-rate of a component in the feed, mole/h
F	:	Feed molal flow-rate, mole/h
F <sub>..</sub>	:	Parameter defined by equation (21)
G	:	Error function defined by equation (43)
K	:	Equilibrium constant, dimensionless
I	:	Molal flow-rate of a component in an internal liquid stream, mole/h
L	:	Molal flow-rate of an internal liquid stream, mole/h. Also, the liquid molal flow-rate in a conventional column rectifying section
L <sup>f</sup>	:	Liquid molal flow-rate in a conventional column exhausting section, mole/h
n	:	Number of ideal stages
p	:	Molal flow-rate of a component in the middle product, mole/h
P	:	Middle product molal flow-rate, mole/h
R	:	Liquid reflux ratio in a rectifying section, dimensionless
R <sup>f</sup>	:	Vapor reflux ratio in an exhausting section, dimensionless
S	:	Stripping factor ( $KV/L$ ), dimensionless
v	:	Molal flow-rate of a component in an internal vapor stream, mole/h
V	:	Molal flow-rate of an internal vapor stream, mole/h. Also, the vapor molal flow-rate in a conventional column rectifying section
V <sup>f</sup>	:	Vapor molal flow-rate in a conventional column exhausting section, mole/h

- x : Liquid mole fraction, dimensionless
- y : Vapor mole fraction, dimensionless
- Z : Parameter defined by equation (50)

Greek letters:

- $\alpha_f$  : Volatility of a component relative to that of the heavy key, dimensionless
- $\Delta_1, \Delta_2$ : Parameters defined by equations (39) and (40), respectively.

Subscripts:

- B : Refers to either the bottom tray of a column section or the bottom product
- BR : Refers to the bottom tray of a conventional column rectifying section
- e : Denotes an effective value
- f : Refers to the feed tray
- F : Refers to the feed
- HK : Refers to the heavy key
- j : Refers to jth-component
- LK : Refers to the light key
- m : Denotes limiting value
- MK : Refers to the middle key
- o : Denotes value defined at the reboiler of an exhausting section
- R : Refers to a rectifying section
- t : Denotes total
- T : Refers to the top tray of a column section
- X : Refers to an exhausting section

Superscripts:

- (o) : Denotes approximate value
- (R) : Refers to the rectifying section of a conventional column
- (X) : Refers to the exhausting section of a conventional column