Heuristic Synthesis of Nonsharp Separation Sequences

The preliminary synthesis of ordinary distillation schemes for separating a single feed into desired products is examined. Nonsharp products are emphasized, i.e., when components are desired in more than one product. Such sets lead naturally to columns with incomplete separation of the key components, including one-section columns. Stream bypassing around separators and limited stream splitting are permitted. Sequences cannot have separators with identical key components, and only limited product fragmentation is considered. A heuristic ordering of separation options, coupled with a depth-first application on a pictorial or a matrix representation of a stream, is proposed. Subsequently a best-first search identifies the few better schemes. Partial sequences are (sub)optimized heuristically. Employing the present methodology on an example problem of four components and products resulted in annual cost savings of 42%, compared to the best sequence isolating the feed components.

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Introduction

The aim of process synthesis activity is to generate a process flowsheet that achieves certain objectives, subject to constraints on available materials, energy, and equipment, and optimal with respect to an appropriate criterion of merit. The development of a process flowsheet is performed in practice by engineers drawing from their past experience and by analogy to existing similar modes of operation. Efforts toward a formal and systematic approach in the synthesis of chemical processes are less than two decades old. Relevant work was recently reviewed by Umeda (1983).

The focus of this paper is the (sub)problem of separation train synthesis, defined as follows:

> The desired products are to be isolated from a multicomponent feed stream, utilizing one or more separation types, at minimum cost

The (single) feed is specified in terms of composition, flow rate, temperature, and pressure. In addition, no solid phases present and relatively well-behaved phase equilibria are assumed (for systems containing azeotropes see Levy et al., 1983). The case of any one feed component being assigned to a unique product, and $p \leq n$, is termed here a "sharp product set." Attention will be limited to conventional distillation (for other separations see Seader and Westerberg, 1977, and Lu and Motard, 1982).

The alternative distillation configurations, consisting of simple, sharp separators (Nishida et al., 1981), can be generated from the ranked list of the feed components (Hendry and Hughes, 1972), an ordering in decreasing volatility. If the desired products contain species adjacent in relative volatility, the number of possible sequences is (Thompson and King, 1972) $[2(p-1)]!/p!(p-1)!$. The problem can be simplified by recognizing that there are only $(p-1)\,p\,(p+1)/6$ unique separators (Rathore et al., 1974), as far as material balance is concerned, that can be combined in different ways. This is the case even if not perfect separation at each column is assumed, but rather key component recoveries sufficiently sharp that only these two components appear in both column product streams. Furthermore, product specifications (in terms of purities and recoveries) can be translated, employing modifications of formulas given by Nath (1977), to process specifications (in terms of column key component recoveries). Complex fractionators (Minderman and Tedder, 1982; Doukas and Luyben, 1978) and heat-integrated sequences (Linnhoff et al., 1983) lie outside the scope of this work.

The objective of the optimal search is to discover, expending a reasonable amount of effort, the few best alternatives. The search techniques, developed for sharp product sets and not nec-

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essarily limited to distillation, are classified here as (see also Nishida et al., 1981):

- Integrated flowsheet methods (Grossmann, 1983; Eliceche and Sargent, 1981)
- Heuristic methods (Seader and Westerberg, 1977; Lu and Motard, 1982)
- Algorithmic methods (Hendry and Hughes, 1972; Westerberg and Stephanopoulos, 1975; Gomez and Seader, 1976)

A "nonsharp (sloppy) product set," the main topic of this paper, occurs when at least one component is specified to be present in more than one product. This implies that there is no ranking of products in terms of volatility, and furthermore, *there is no limitation in the number of products*. The ranked list of the components can be used to generate the sequences, isolating the feed components, with the latter subsequently mixed in the required proportions. However, such practice is wasteful in that sharper than necessary separation occurs. On the other hand, the list-splitting operation fails in the case of not nearly perfect splits of adjacent components, due to distribution of the nonkey components in both sublists (which in turn implies the same for the products).

The problem of systematically synthesizing sequences for nonsharp product sets was first addressed by Nath (1977). A graphical representation of process streams (material allocation diagram, MAD), was proposed and manipulated according to a set of rules to generate plausible networks of columns with key component recoveries not always one or zero. Hohmann et al. (1982) advanced the concept of limiting distillation sequences, which provide targets for energy consumption as well as topological limits to sequences for arbitrary product sets. Their insight is useful; however, they did not propose a systematic synthesis method.

Plausible sequences can be generated by a systematic application of the operations of distillation, stream splitting, and stream mixing on a representation of a process stream in terms of a component recovery matrix (***R*** matrix), an algebraic extension of the MAD.

The separators considered in this work were classified, in terms of key component recoveries, by Nath (1977) as: sharp (both recoveries close to one), semisharp (one recovery close to one), and nonsharp (no recovery close to one). In this work another type is proposed: three-specification (both recoveries close to one, nonadjacent keys).

Separators with at least one key recovery not close to one provide the designer with two opportunities. First, a one-section column (rectifier or stripper) or, in the extreme, a single-stage flash unit may be sufficient. Second, bypassing a fraction of the column feed to its top or bottom stream (semisharp), or a final product (nonsharp case) is possible.

Feed bypass cases are examined analytically, under the simplifying assumptions of constant relative volatility and molar overflow, and using the CHESS simulation package (Motard and Lee, 1971).

The term "stream splitting" is distinguished from feed bypassing in that all fractions require further separation. For the purposes of this work, stream splitting is limited to the case of no product fragmentation. Furthermore, no material recycle is considered.

A heuristic ordering of options, coupled with a depth-first (Nilsson, 1980) technique, is proposed for generating schemes containing up to a prespecified number of units. In a distinct second step, following the generation of alternatives, a best-first method (Nilsson, 1980) is proposed for searching for the few better schemes. Heuristic rules are employed to (sub)optimize the partially developed sequences.

For an example problem of four components and four products, significant savings (42%) were realized using the present methodology, over the best among the sequences that completely isolate (and remix) the feed components.

Product and Process Specifications

The problem of product specifications has not received attention in the literature of separation processes synthesis, with the notable exception of the work of Nath (1977) and Gawin (1975). Since its importance is crucial in the case where nonsharp separations are considered, a closer look at the subject seems in order.

Nath defined product recovery:

$$\rho_i = \sum_j d_{ji} \Big/ \sum_j f_j \qquad j \in C_i \tag{1}$$

and product purity:

$$p_i = \sum_j d_{ji} \Big/ \sum_k d_{ki} \qquad j \in C_i,\ k \in K_i \tag{2}$$

where d_{ji} is the flow rate of component j in product i (mol/time), f_j is the flow rate of component j in the feed (mol/time), C_i is the set of components specified to be present in product i, K_i is the set of components actually present in product i. Also define component recovery:

$$r_{ji} = d_{ji}/f_j \qquad j \in K_i \tag{3}$$

Next we will examine the usefulness of these definitions for the cases of sharp separations and nonsharp separations.

Sharp separations

By expressing ρ_i and p_i in terms of r_{ji}, one can show that, for sharp product sets, ρ_i and p_i are close to unity for all products i. Under some mild assumptions (Bamopoulos, 1984), it can also be shown that the number of product specifications must equal $2(p - 1)$. A reasonable choice would be to specify the recoveries and purities of the first $p - 1$ products, or the impurity levels of all products.

A component can be a column key component zero times, once (light key, LK, or heavy key, HK), or twice (LK and HK), in a sequence producing the required product set. The formulas given by Nath (1977) can be generalized to read:

$$\rho_i = \frac{\Sigma R_{j,LK} R_{j,HK} f_j}{\Sigma f_j} \qquad j \in C_i \tag{4}$$

$$p_i = \frac{\Sigma R_{j,LK} R_{j,HK} f_j}{(1 - R_{il,LK}) R_{il,HK}^{1-\delta_{il}} f_{il} + \Sigma R_{j,LK} R_{j,HK} f_j + (1 - R_{ih,HK}) R_{ih,LK}^{\delta_{ih}} f_{ih}} \qquad j \in C_i \tag{5}$$

where:

$R_{j,LK}(R_{j,HK})$ is the column recovery of component j, being a light (heavy) key, in the stream rich with it (meaningless $R_{j,LK}$ or $R_{j,HK}$ are set to 1)

$f_o, f_{n+1} \equiv 0$

$il(ih)$ denotes the light (heavy) impurity of product i

$\delta_k = 0$ if component k is a HK before it is a LK in the (sub)sequence used to produce i
$= 1$ otherwise

Product recoveries can always be met (or exceeded) by setting

$$R_{j,LK} = \rho_{i,\text{spec}} \quad \text{if} \quad R_{j,\text{HK}} = 1$$
$$R_{j,HK} = \rho_{i,\text{spec}} \quad \text{if} \quad R_{j,LK} = 1 \tag{6}$$

else

$$R_{j,LK} = R_{j,HK} = \sqrt{\rho_{i,\text{spec}}}$$

Product purities, on the other hand, depend on the column sequence.

As an example consider the separation of a ternary feed ABC into its components, represented in Figure 1. For the direct sequence:

$$p_I = \frac{R_{A,LK} \cdot f_A}{0 + R_{A,LK} \cdot f_A + (1 - R_{B,HK}) \cdot 1 \cdot f_B} \tag{7}$$

while for the inverted sequence:

$$p_I' = \frac{R_{A,LK} \cdot 1 \cdot f_A}{0 + R_{A,LK} \cdot 1 \cdot f_A + (1 - R_{B,HK})R_{B,LK}^1 \cdot f_B} \neq p_I \tag{8}$$

In general then, if $2(p - 1)$ product specifications are made, Eqs. 4 and 5 must be solved for the unknown $R_{j,LK}$ and $R_{j,HK}$, for a particular sequence. If one imposes more than $2(p - 1)$ specifications, a system of $(p - 1)$ columns will not in general be capable of satisfying these equations at equality. It may, however, be possible to satisfy those, using more columns with blending of products, or to satisfy some of them exactly and at the same time overpurify some products. On the other hand, if only p product purities are fixed, $(p - 2)$ degrees of freedom remain. If $p = n$, these can be consumed by setting $R_{j,LK} = R_{j,HK}$, or by means of a sequence cost optimization. The first choice has been almost universally adopted in the synthesis literature, occasionally with the added simplification:

$$R_{j,LK} = R_{j,HK} = \rho_{i,\text{spec}} \qquad j \text{ both } LK \text{ and } HK \tag{9}$$
(rather than $\sqrt{\rho_{i,\text{spec}}}$)

The optimization of individual column recoveries, in the design stage, was examined by Gawin (1975). It is noted that, in the operation of distillation trains, the trade-off of $R_{j,LK}$ vs. $R_{j,HK}$ (e.g., shifting separation duty between towers) is well known (Shinskey, 1977).

Nonsharp separations—component recoveries

The product purities are still close to unity, but this is not the case with the product recoveries. The set of product specifications will be represented by a component recovery matrix ($\boldsymbol{R}$ matrix), of dimensions $n \times p$. The jith element is the component recovery r_{ji} defined previously. All elements in the matrix will satisfy the constraint

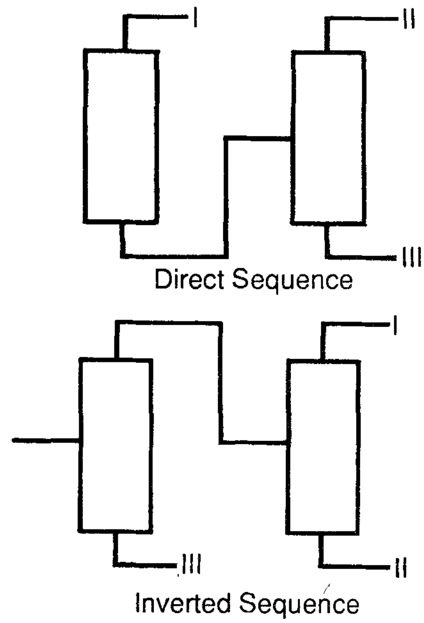


Figure 1. Configurations for A/B/C separation.

$$0 \leq r_{ji} \leq 1 \tag{10}$$

From a component material balance it follows that, for every row j,

$$\sum_i r_{ji} = 1 \tag{11}$$

There is a natural ordering of rows (components) and, by convention, the first row corresponds to the most volatile feed component. However, a meaningful ordering of columns (products) does not generally exist if $n > 2$.

Given an $\boldsymbol{R}$ matrix for a nonsharp product set, such as

	I	II	III	IV
A	0.60	0.40	—	—
B	0.50	0.50	—	—
C	0.20	—	0.80	—
D	—	—	0.40	0.60

it is not obvious what column arrangement(s) will produce the desired products. (A dash [—] in the matrix is interchangeable with a zero entry.) Little more is known other than that $(n - 1)$ sharp columns will suffice and that, in general, at least $(p - 1)$ columns are needed.

Algebraic and Geometric Representations

Operations on the component recovery matrix

The following preliminary observations can be made:

- After any operation the elements of each row are normalized to sum to unity

• If all elements of a column are equal, the product can be deleted (it just represents a fraction of the feed)

• If a column contains an internal zero entry, it is split into two, with zeros extending to opposite ends of each column (this is a consequence of the fact that products of ordinary distillation columns cannot contain components not adjacent in the volatility list)

• If a column is a linear multiple of another column, the columns represent identical compositions, and can be summed to a single product

The operations of separation and feed bypassing will be defined in the following (for simplicity, definitions in terms of matrix algebra will be avoided).

The simplest separation operation is the familiar sharp separation, where nearly perfect recovery of the (adjacent) key components in their respective streams is assumed. Also, nonkey components appear in only one product stream. Such separation is termed (Nath, 1977) sharp split and is denoted by *S LK*/*HK*.

For the example ***R*** matrix of the previous system, an *S B*/*C*, will result in:

R_1

	I	II
A	0.60	0.40
B	0.50	0.50

R_2

	I_2	III	IV
C	0.20	0.80	—
D	—	0.40	0.60

Note that zeroed-out rows and columns are eliminated for clarity and that subscripted products correspond to fragments of the initial products.

Another possibility is when a single component is split between two products. If that component is extreme in volatility, the separation can be achieved in a single column, performing what is termed a semisharp split, denoted by *SS* 1/2 or *SS* $n-1/n$, where the recovery of component $2(n-1)$ is close to 1, in its corresponding product. The recovery of component $1(n)$ is a parameter to be specified. Considering the example ***R*** matrix, an *SS C*/*D* split with $R_{D,LK} = 0.40$ will result in

R_3

	I	II	III
A	0.60	0.40	—
B	0.50	0.50	—
C	0.20	—	0.80
D	—	—	1.00

R_4

	IV
D	1.00

In practice, an *SS* $1/2$ $(n-1/n)$ split will be performed only to separate a product consisting of pure component $1(n)$.

If the component has intermediate volatility, one needs to specify the allocation of the other components. One possibility is that one product contains a specified fraction of an intermediate component and only traces of other components. Such a "heart cut" is generally not feasible with a single column. Another possibility is that one product contains a specified fraction of the intermediate key and essentially no heavier components.

In this situation, there are really three key components: the recovery of component $(j-1)$ is high in product *I*, the recovery of $(j+1)$ is low, and that of j has an intermediate value. The separation, which involves a sharp separation of two components not adjacent in volatility, is in principle achievable in a single column (a scheme is presented in Appendix A). Such a separation is termed here three-specification split and is denoted by 3*S* *LK*/*MK*/*HK*, with parameter $R_{j,MK}$, in the light product. As with *SS* splits, there are several possibilities of 3*S* splits, for instance, for the example ***R*** matrix, with $R_{C,MK} = 0.20$, we obtain

R_5

	II	I
A	0.40	0.60
B	0.50	0.50
C	—	1.00

R_6

	III	IV
C	1.00	—
D	0.40	0.60

In practice, a 3*S* split will be performed if a subset of products, say $1, 2, \ldots, i$, consists of only a subset of components, say $1, 2, \ldots, j$, and the other products $i+1, \ldots, p$ consist only of components $j, j+1, \ldots, n$.

Still another possibility is the case when two components are split between two products. For multicomponent feed streams, there are many arrangements on the ***R*** matrix, hence, no general rule can be given. For a binary feed, this separation is always achievable in a single unit and is termed nonsharp split, denoted by *NS LK*/*HK*. Parameters to be determined are $R_{A,LK}$ and $R_{B,HK}$, in the light product.

Another operation defined on the ***R*** matrix is feed bypassing to a product. If a fraction f_i of the feed is bypassed to product i, then the columns change as

$$r'_{ji} = \frac{r_{ji} - f_i}{1 - \sum_{k=1}^{p} f_k} \tag{12}$$

as can be inferred easily from a component material balance. Since $r'_{ji} \geq 0$, for all j, it follows that

$$f_{i,\max} = \min_j \, (r_{ji}) \tag{13}$$

Clearly if a product i^* does not contain all components, $f_{i^*} = 0$.

As an example consider the matrix R_1, where 50% bypassing to product *I* gives matrix R_7 (the one-column ***R*** matrix representing the bypassed fraction of feed is omitted for simplicity).

R_1

	I	II
A	0.60	0.40
B	0.50	0.50

R_7

	I′	II
A	0.20	0.80
B	—	1.00

Material allocation diagrams (MAD)

A convenient alternative representation of a nonsharp product set is the MAD (Nath, 1977). Components are represented by rectangles of fixed height and of width proportional to their concentration. The rectangles are arranged in order of decreasing volatility and are separated by dashed lines; the desired products are separated by solid lines. Such a diagram is shown in Figure 2. A MAD can typically be constructed for the restricted case of every component being assigned to at most two products, except for impurity amounts. In this case, at most one horizontal solid line appears in each component rectangle.

A MAD representation of a nonsharp product set is not always unique. Assuming that products contain only components adjacent in volatility and that a component is distributed in at most two products, all products will appear as connected

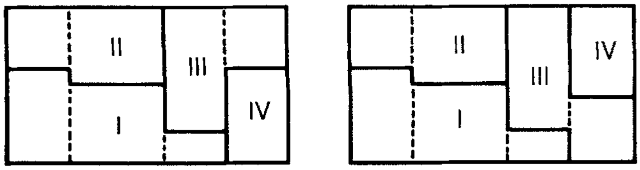


Figure 2. Material allocation diagram (MAD).

regions. Note, however, that the second MAD in Figure 2 represents the same case as the first one.

The two operations of stream splitting and distillation can be performed on the MAD as follows and as shown in Figure 3:

1. Stream splitting corresponds to a horizontal division of the MAD, with the fraction of the stream going to either product determined by the position of the horizontal line

2. Separation corresponds to superimposing a set of horizontal line segments, one in each of the component rectangles, connected by vertical line segments (possibly of zero length) that overlap with dashed lines

The case of a sharp product set corresponds to a MAD with no horizontal lines, and vertical lines extending throughout the height of the diagram. For example $A/BC/D$ is shown in Figure 4.

In Figure 5 an $S\ i-1/i$, an $SS\ 1/2$, an $3S\ i-1/i/i+1$ and an $NS\ 1/2$ split are shown.

One can identify two classes of stream splitting. The first occurs when no interior vertical solid line is broken and amounts to bypassing a specified fraction of the feed to a single product. The second class is when at least one solid line is broken, and the term "stream splitting" is reserved for this case, i.e., when both feed fractions require further separation.

Stream splitting could be beneficial in cases where at least two products go to different fractions of the feed, or the fragments of a product that is present in both fractions can be combined with other products in these fractions. Stream splitting is illustrated in Figure 6, where the separation of products I and

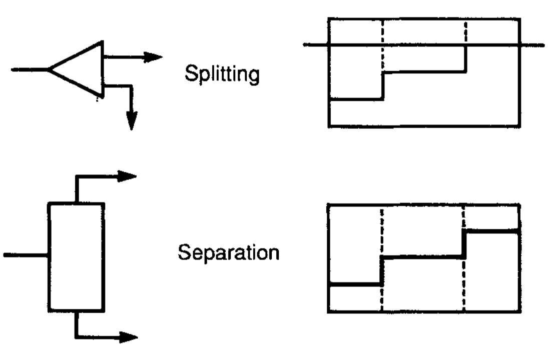


Figure 3. Operations on the MAD.

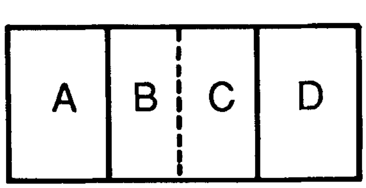


Figure 4. A/BC/D product set.

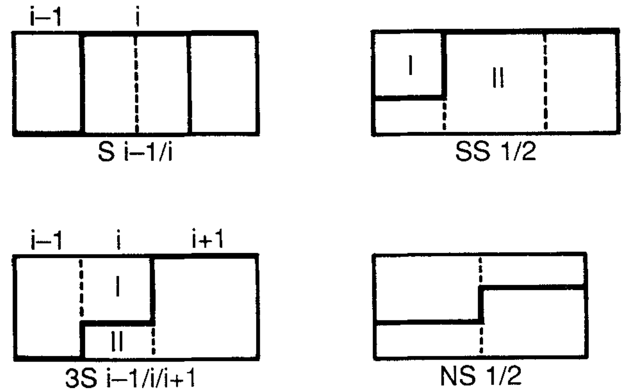


Figure 5. Separation types on the MAD.

IV from each other, as well as the merging of II_2 with I and III_2 with IV occur. Such rules restrict the growth in the number of separators, which is inherent to product splitting. It is also noted that an unambiguous determination of the two resulting $\boldsymbol{R}$ matrices is not possible, when only a split ratio of the original $\boldsymbol{R}$ matrix is specified. For the purposes of this work, stream splitting will be limited to the case when a product subset forms a fraction of the feed.

Optimal Separator Specifications

Two-section columns

In the present section the optimal flow to a single separator, when its product streams require no further processing, will be investigated (the feed flow will also determine the column key component recoveries). In following sections, one-section columns (rectifiers and strippers) and simple flash units will be considered, as well as optimal flows to separation systems.

Consider the distillation column of Figure 7 with key components A, B. If a fraction r_1 of the feed is bypassed to the top product and a fraction r_2 to the bottom, a material balance gives:

$$R_i = \frac{\rho_i - r_1}{1 - r_1 - r_2} \qquad i = A, B \tag{14}$$

From (King, 1980) the approximate distribution of the nonkey components at minimum reflux and at no bypass conditions is given by

$$\rho_i = \frac{(\alpha_i - 1)\rho_A \dfrac{z_A/x_A}{z_i/x_i} + (\alpha - \alpha_i)\dfrac{z_B/x_B}{z_i/x_i}\rho_B}{\alpha - 1}, \quad \text{if } \underline{\alpha}_o < \alpha_i < \overline{\alpha}_o$$

$$\rho_i = 0, \quad \text{if } \alpha_i \le \underline{\alpha}_o$$

$$\rho_i = 1, \quad \text{if } \alpha_i \ge \overline{\alpha}_o \tag{15}$$

At bypass conditions the volatility limits change so as to satisfy.

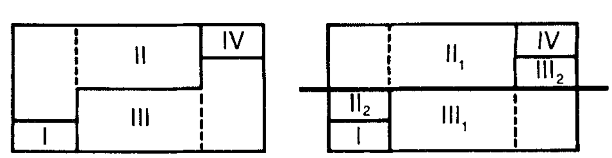


Figure 6. Feed splitting on the MAD.

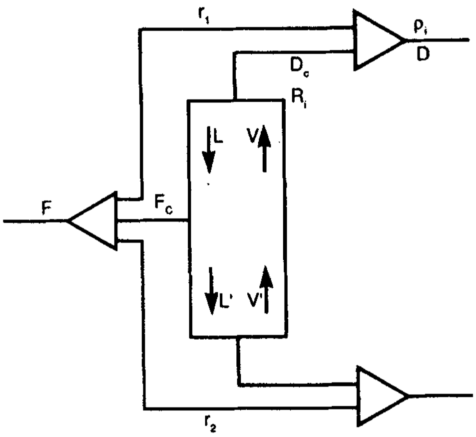


Figure 7. Column with feed bypass.

at least for $0 \le q \le 1$,

$$\underline{\alpha}_o \le \underline{\alpha} < \bar{\alpha} \le \bar{\alpha}_o \quad (16)$$

with the left (right) equality true when $r_1 = 0$ ($r_2 = 0$).

From the above the following relations can be derived, in some simple cases (see Appendix B):

$$\frac{V_{\min}}{F} - \frac{V_{\min,o}}{F} = -r_1(1 - q) \quad (17)$$

$$\frac{L_{\min}}{F} - \frac{L_{\min,o}}{F} = r_1 q \quad (18)$$

If it is further assumed that

1. The column is operated (at any bypass conditions) at a reflux rate θ times the minimum
2. The component distribution at the operating reflux is the same as at minimum reflux (true for binary feeds, as well as the multicomponent semisharp separations discussed below).

Then the following equations hold:

$$\frac{L}{F} - \frac{L_o}{F} = \theta\left(\frac{L_{\min}}{F} - \frac{L_{\min,o}}{F}\right) = \theta r_1 q \quad (19)$$

$$\frac{V}{F} - \frac{V_o}{F} = -r_1(1 - \theta q) \quad (20)$$

$$\frac{L'}{F} - \frac{L'_o}{F} = r_1 q(\theta - 1) - r_2 q \quad (21)$$

$$\frac{V'}{F} - \frac{V'_o}{F} = r_1 q(\theta - 1) + r_2(1 - q) \quad (22)$$

The energy requirements of the process can be stated as:

$$Q_C \sim \begin{cases} V \text{ for total condenser} \\ L \text{ for partial condenser} \end{cases} \quad (23)$$

$$Q_R \sim V' \quad (24)$$

We also have

$$d \sim [\max(V, V')]^{1/2} \quad (25)$$

$$N_{\min} = \ln\left[\frac{r_1 - \rho_A}{r_1 - \rho_B}\frac{r_2 - (1 - \rho_B)}{r_2 - (1 - \rho_A)}\right] \Big/ \ln \alpha \quad (26)$$

For nonsharp separations, the following conclusions can be drawn ($0 \le q \le 1$).

1. Any degree of bypassing leads generally to internal flows greater than or equal to the corresponding no bypass values. Exceptions are the vapor flow rate V, which decreases with top bypassing when the feed to the column is at least partially vapor ($q < 1/\theta$), and the liquid flow rate in the stripping section L', which decreases with bottom bypassing when the feed is at least partially liquid ($q > 0$).
2. Any degree of bypassing leads to utility requirements higher than or at best equal to those at no-bypass conditions. The only exception is a decrease of a total condenser duty, when at least partially vapor feed is bypassed to the top. (It should be noted that bypassing vapor feed to the top, when a total condenser is specified, upsets the thermal state of the desired product and additional cooling will be necessary. So the potential condenser duty advantage is eliminated.)
3. Any degree of bypassing leads to a column diameter greater than or equal to that at no-bypass conditions. An exception occurs when vapor feed is bypassed to the top and, possibly, when liquid feed is bypassed to the bottom and the diameter is determined by liquid flow.
4. Furthermore, an examination of Eq. 26 indicates that N_{min} will always increase if at least one of r_1, r_2 is not zero (column height increases).

So it is seen that under the simplifying assumptions of constant volatility and molar overflow, bypassing is in general undesirable in a binary separation. The only favorable possibility is top bypassing vapor feed (with a partial condenser), where potential savings in column diameter may offset additional expenses due to increased column height. For the typical case of an all-vapor feed ($q = 0$), the condenser or reboiler operating and capital costs are not affected by top bypassing, hence the optimal bypass occurs at the minimum column capital cost (likely at $r_1 = 0$). Test cases, using an extended version of the CHESS computer package (Motard and Lee, 1971), modified to include economic evaluation and parameter optimization, have been examined and the optimal values of r_1, r_2 have been found to be near zero.

In an SS 1/2 as in Figure 5, top bypass is inherently not possible. The pertinent equations are derived by setting $r_1 \equiv 0$. For $SS\ n - 1/n$ separations bottom bypass is not possible, hence the results are derived by setting $r_2 \equiv 0$. It is interesting, however, to examine a simulation case where unpredicted results occurred. Consider the system of Table 1, with results presented in Tables 2 and 3 (for details of cost calculation, see Appendix C).

The following observations can be made:

1. While in theory the column capital cost should increase with top bypass, there is a shallow minimum due to a drop in N, the number of stages. The latter is due to an increase in the average relative volatility, brought about by the decrease in column top temperature.
2. Although vapor flow rate V increases, the heat exchanger duty in the condenser Q_C decreases. This can be explained if heat

Table 1. Example of Top Bypass in a Full Column

Components: i = butane, hexane
F = 126.0 mol/s, saturated liquid
$z_A = 0.333$, $z_B = 0.334$, $z_C = 0.333$
$\rho_B = 0.98$, $\rho_C = 0.15$; P = 629 kPa
$R/R_{min} = 1.2$; total condenser
Utilities: steam at 779 kPa, ammonia at 274.4 K

Table 2. Effect of Top Bypass in a Full Column (Column Variables)

r_1	V mol/s	V' mol/s	α	N	Q_R kW	Q_C kW	T_{Top} K	ΔH_C kJ/mol
0.00	96.8	94.5	4.71	18	2,224	1,873	330.0	19.4
0.05	97.5	93.3	4.78	16	2,192	1,837	329.1	18.8
0.10	98.1	91.5	4.86	17	2,144	1,784	328.1	18.2
0.12	98.3	90.6	4.91	17	2,118	1,756	327.7	17.9
0.14	98.5	89.6	4.95	19	2,088	1,725	327.2	17.5

of condensation-composition dependence effects are considered. Namely, the vapor condensed becomes richer in light components, which have smaller molar heats of condensation. The decrease in Q_C results in a decrease in the condenser operating cost. However, the condenser capital cost remains constant due to a compensating effect of lower temperature driving force.

3. A change of opposite sign than expected occurred in the stripping section vapor flow rate V', which caused the reversal in the reboiler heat exchanger duty Q_R as well. This results in a small decrease in reboiler operating and capital costs.

In conclusion, an overall optimum occurs at $r_1^* = 0.12$ (overall capital minimum is at $r_1 = 0.05$), which represents an improvement of 3.6% over the base case.

The effects of deviations from the simplifying conditions of constant relative volatility and molar overflow are summarized below:

- Effect of volatilities. With top (bottom) bypass, the top (bottom) temperature decreases (increases), resulting in an increase (decrease) in relative volatilities. The latter, of course, moderates (enhances) the increase of N brought about by the increased sharpness of the separation.
- Latent heat effects. Top (bottom) bypassing in general decreases (increases) the molar heat of condensation (vaporization). These enthalpy changes compete with (compound) the changes in flows brought about by the increased sharpness of separation and reduced feed to the column.

Table 3. Effect of Top Bypass in a Full Column (Column Costs)

	Capital Cost, \$ × 1,000				Operating Cost \$/yr × 1,000			Annual Cost
r_1	Col.	Reb.	Cond.	Total	Reb.	Cond.	Total	\$/yr × 1,000
0.00	148	30	27	205	63	113	177	272
0.05	145	30	28	202	62	111	174	267
0.10	145	30	28	206	61	108	169	263
0.12	149	29	28	206	60	106	167	262
0.14	156	29	28	213	59	104	164	263

- Driving force effects. Top (bottom) bypass results in a decrease (increase) of the column top (bottom) temperature, i.e.,

$$T_R \geq T_{R,o} > T_{C,o} \geq T_C \tag{27}$$

This diminishes the available driving force for the condenser (reboiler) heat exchange, or worse, necessitates a switch to a colder (hotter), hence more expensive, medium.

In summary, bottom bypass offers no real advantage, including the "secondary" effects. Top bypass, on the other hand, offers the "primary" advantage of decreasing V (for $q < 1/\theta$). Secondary advantages are an increase in relative volatility and a decrease in the heat of condensation, while a secondary disadvantage is the possibility of using a colder refrigerant or, alternatively, a decrease in the condenser driving force.

Rectifying and stripping columns

It is possible that, for the sloppy separations considered, a one-section column will be sufficient. We have

$$L_{\min} < 0 \longrightarrow \text{stripper only} \tag{28a}$$

$$V'_{\min} < 0 \longrightarrow \text{rectifier only} \tag{28b}$$

For binary feeds and common feed vaporization fractions:

$$q = 1 \quad \text{and} \quad \alpha \geq \rho_A/\rho_B \longrightarrow \text{stripper only} \tag{28a'}$$

$$q = 0 \quad \text{and} \quad \alpha \geq (1 - \rho_B)/(1 - \rho_A) \longrightarrow \text{rectifier only} \tag{28b'}$$

A rectifier could conceivably perform an *NS* (binary) separation or an *SS* 1/2 (binary or multicomponent) separation. In the former case, feed bypass to both top and bottom streams is feasible, while in the latter only bottom bypass. In the following, only the results for a rectifier will be derived, those for a stripper following similar lines of reasoning (Bamopoulos, 1984).

Examine top bypass in a binary rectifier ($q = 0$), illustrated in Figure 8. From Eq. 14 it follows that

$$(1 - R_B)/(1 - R_A) = (1 - \rho_B)/(1 - \rho_A) \tag{29}$$

Hence, by Eq. 28b′, the rectifier will remain a rectifier.

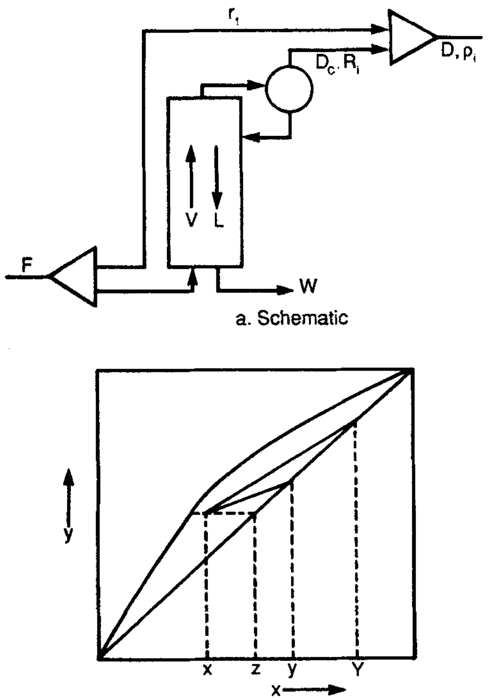
It is also obvious that

$$L = L_o = W \tag{30}$$

$$V = V_o - r_1 F = (1 - r_1)F \tag{31}$$

From a McCabe-Thiele diagram, shown in Figure 8b, it follows that N increases. Assuming a partial condenser (otherwise bypassing vapor feed to the top is unjustified), it is seen from Eq. 30 that Q_C is unaffected by bypass. There is, however, a trade-off of V (i.e., d) vs. N. This is the same with the trade-off encountered in (partially) vapor feed bypassing to top stream of a full distillation column.

The maximum reduction in V is $\rho_B F$ and this will require a rectifier with infinite stages ($Y = 1$ in Figure 8b). The optimum top bypass then corresponds to minimum column capital cost, and it can be determined via a trial-and-error procedure. However, it is likely that zero bypass is best or near best.

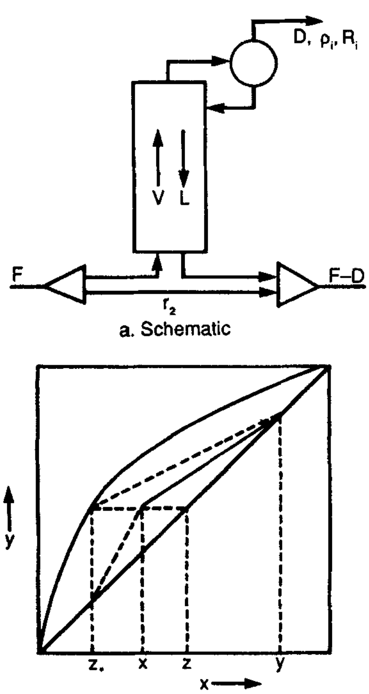


b. McCabe–Thiele Diagram

Figure 8. Top bypass in a binary rectifier.

Now consider bottom bypass in a (generally multicomponent) rectifier, Figure 9, with key components A, B. From Eq. 14 it follows that

$$\frac{1 - R_B}{1 - R_A} = \frac{(1 - \rho_B) - r_2}{(1 - \rho_A) - r_2} > \frac{1 - \rho_B}{1 - \rho_A} \tag{32}$$



b. McCabe–Thiele Diagram

Figure 9. Bottom bypass in a rectifier.

Hence, a binary rectifier will become a full column when

$$\alpha \le \frac{1 - R_B}{1 - R_A} = \frac{1 - \rho_B - r_2^*}{1 - \rho_A - r_2^*} \tag{28b''}$$

A McCabe-Thiele diagram for a binary rectifier is shown in Figure 9b. It can also be shown (Bamopoulos, 1984) that a multicomponent rectifier will eventually become a full column with bottom bypass. The following equations relate the flows when a rectifier is sufficient

$$L = L_o - r_2 F = (1 - r_2)F - D \tag{33}$$

$$V = V_o - r_2 F = (1 - r_2)F \tag{34}$$

Hence both Q_c and d decrease with increasing r_2 while N increases; i.e., a trade-off is possible.

A full column becomes more expensive as vapor feed is bypassed to the bottom (V' and N increase), hence, if a full column is better than the rectifier, it will be the one at r_2^*. At the conditions when a stripping section just becomes necessary we have

$$V_{\min} = V_o - r_2^* F; \qquad V = L + D \tag{35}$$

$$L_{\min} = L_o - r_2^* F; \qquad L = \theta L_{\min} \tag{36}$$

Depending on the value of θ chosen, L, V may or may not increase with the introduction of a stripping section. The only possibly favorable result of introducing a stripping section would be when a column could have an operating line to the right of the one for the rectifier in Figure 9b, i.e., have a lesser number of rectifying stages. It is unlikely, however, that this can compensate for increases in L, V and the introduction of a reboiler. Hence the optimum will lie in the rectifier regime.

The maximum reduction in V or L is equal to $-V'_{min,o}$. Similarly it can be shown that:

For a binary stripper, bottom bypassing offers no advantage

For a multicomponent stripper, top bypassing results in a trade-off between Q_R and d decreasing vs. N increasing

A resemblance of bottom (top) feed bypassing in a rectifier (stripper) to the classical reflux vs. stages trade-off (King, 1980), in a full column, is apparent:

- Column capital cost. In a two-section column, as R increases above its minimum value, V increases, hence d. However, N decreases rapidly so that the net effect is (up to an intermediate R value, where a minimum occurs) that the column capital cost decreases from infinity.

On the other hand, in a rectifier (stripper), as bottom (top) feed bypass increases, the vapor flow decreases linearly, while N typically increases much faster. The net result is then a capital cost increase to infinity, from its minimum at zero bypass.

- Heat exchangers cost. In a full column, with increasing reflux, the operating and capital costs of both reboiler and condenser increase from their minimum values at infinite N. In a rectifier (stripper) the condenser (reboiler) costs decrease toward their minimum values at infinite N.
- Location of optimum. In a full column the trade-off between the column and heat exchangers costs occurs at a value near R_{min}. In a one-section column, not sufficient design experience exists; however, the case of maximum flows (i.e., zero bypass) appears to be close to the optimum.

At this point a paper by Luyben (1981) should be cited. (Saturated liquid) feed bypass to the top product of a binary stripper, as well as bottom bypass in a binary two-section column, in the context of reactor recycle stream purging, were examined. In the latter case it was correctly concluded that the column heat input is independent of the fraction bypassed. In the case of a stripper, however, it is suggested to feed the separator such an amount that the reflux rate just becomes zero, in an attempt to minimize the heat input, V'. This represents an infeasible scheme, as an infinite number of stages is required.

Single-stage flash units

A binary nonsharp split (*NS A/B*) could conceivably be done in a single-stage flash unit if (assuming a separation efficiency of 100%)

$$\frac{\rho_A}{1-\rho_A}\cdot\frac{1-\rho_B}{1-\rho_A}<\alpha \tag{37}$$

It can be shown that when heating (cooling) is required for the separation, only top (bottom) bypassing is optimal, as follows:

$$r_1^* = \frac{\alpha(1-\rho_A)\rho_B - \rho_A(1-\rho_B)}{\alpha(1-\rho_A)-(1-\rho_B)} \tag{38}$$

$$r_2^* = 1 - \frac{(\alpha-1)\rho_a\rho_B}{\alpha\rho_B - \rho_A} \tag{39}$$

By increasing top (bottom) feed bypassing when heating (cooling) is required for the separation, a stripper (rectifier) will become necessary and, eventually, a two-section column. Again a trade-off is possible, similar to the one encountered in one-section columns.

Optimal Separation Systems Specifications

Binary systems

In the present section the economic impact of feed bypassing to a particular product will be analyzed. Analytical results have been obtained for binary feeds, while some generalizations and insights for multicomponent mixtures will also be presented.

When $p(>2)$ products are desired out of a binary feed, they can be ordered in decreasing volatility with $\underline{P}_1$ and $\underline{P}_p$ such that

$$\frac{r_{A1}}{r_{B1}} = \max_i\left(\frac{r_{Ai}}{r_{Bi}}\right) = M \tag{40}$$

$$\frac{r_{Ap}}{r_{Bp}} = \min_i\left(\frac{r_{Ai}}{r_{Bi}}\right) = m \tag{41}$$

where, conceivably, $m = 0$ ($M = \infty$) when pure component B (pure A) is among the products. The other products, $\underline{P}_m$, with an intermediate recovery ratio, r_{Am}/r_{Bm}, can then be expressed in terms of $\underline{P}_1$ and $\underline{P}_p$.

As an example, consider a mixture of 100 mol A and 100 mol B to be separated according to the $\boldsymbol{R}$ matrix below:

	1	2	3
A	0.3	0.6	0.1
B	0.1	0.4	0.5

Since

$$\underline{2} = \frac{13}{7}\underline{1} + \frac{3}{7}\underline{3}$$

separation scheme 1, shown in Figure 10, is possible. The above separation is the least sharp possible, in the sense of the separation factor, S

$$S = \frac{R_{LK}}{1-R_{LK}}\bigg/\frac{R_{HK}}{1-R_{HK}} \tag{42}$$

For the separation at hand, $S = M/m$. A separation less than M/m of the original mixture is not possible if products $\underline{P}_1$ and $\underline{P}_p$ are to be separated from each other in one column. The separator in Figure 10 will require the minimum number of stages. However, the scheme described has an obvious disadvantage, namely that fractions of the two products with extreme ratios r_{Ai}/r_{Bi} are mixed, hence irreversibilities occur.

An alternative scheme can be obtained if, instead of expressing $\underline{P}_m$ in terms of $\underline{P}_1$ and $\underline{P}_p$, the following rule is followed: Express products j (i) lighter (heavier) than the feed, i.e., $r_{Aj} \geq r_{Bj}$ ($r_{Ai} \leq r_{Bi}$), in terms of $\underline{F}$ and $\underline{P}_1$ ($\underline{P}_p$).

Define

$$f = \sum_j (r_{Aj} - r_{Bj}) = \sum_i (r_{Bi} - r_{Ai}) \tag{43}$$

Then the material balance can be expressed as

$$\underline{F} = \left[1 - f\left(\frac{1}{1-m} + \frac{1}{M-1}\right)\right]\cdot\underline{F} \leftarrow \text{bypassed amount}$$
$$+ \frac{f}{r_{A1}-r_{B1}}\cdot\underline{P}_1 \leftarrow \text{distillate}$$
$$+ \frac{f}{r_{Bp}-r_{Ap}}\cdot\underline{P}_p \leftarrow \text{bottoms} \tag{44}$$

For the example case, we have $m = 0.2$, $M = 3$, $f = 0.4$, and the resulting scheme 2 is shown in Figure 11.

The separation is again M/m, but this time the flow to the system is less, while mixing occurs only between "extreme" product fractions and bypassed feed. It should be noted that the scheme above cannot be obtained by feed bypassing from

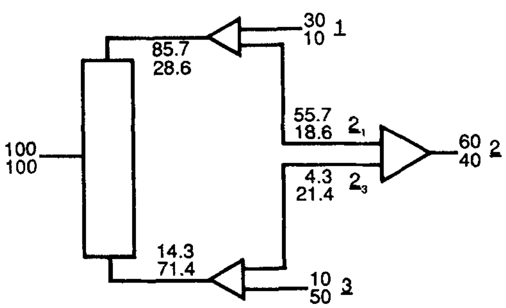


Figure 10. Scheme 1 for binary example.

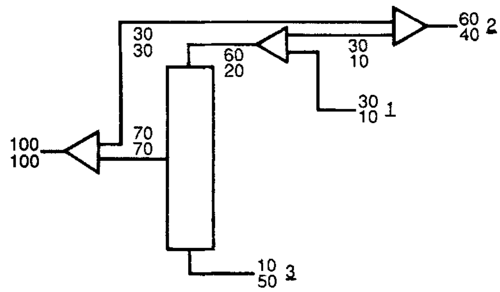


Figure 11. Scheme 2 for binary example.

scheme 1, where any amount of feed bypassing will result in an increase in the sharpness of separation.

Scheme 2 was created by bypassing fractions r_1 and r_2 of the feed, so that

$$r_1 = \sum_j \frac{Mr_{Bj} - r_{Aj}}{M - 1} \tag{45}$$

$$r_2 = \sum_i \frac{r_{Ai} - mr_{Bi}}{1 - m} \tag{46}$$

which resulted in no increase in separation. If, however, more feed is bypassed, the separation will increase. The maximum amount bypassed (resulting in a sharp A/B split) is $1 - f$, Figure 12. The then "obvious" solution of maximum bypass to each product, scheme 3, is put into the proper context as resulting from scheme 2 with maximum bypass. As has been argued in the previous section, scheme 2 (maximum flow-minimum separation) is typically preferred over scheme 3, although detailed optimization will be necessary for some cases (especially when only a rectifying or stripping section is sufficient).

Multicomponent systems

A desired product cannot, in general, be isolated from a multicomponent stream in a single column.

As an example, in the problem

		1	2	3	4	5
	A	0.1	0.4	0.3	0.2	—
R_1	B	0.3	0.1	0.2	—	0.4
	C	0.2	0.2	0.5	—	0.1

consider an $S\ A/B$ followed by an $NS\ B/C$ split. Matrix R_1 will result (second column designed as above) in scheme 1, shown in Figure 13.

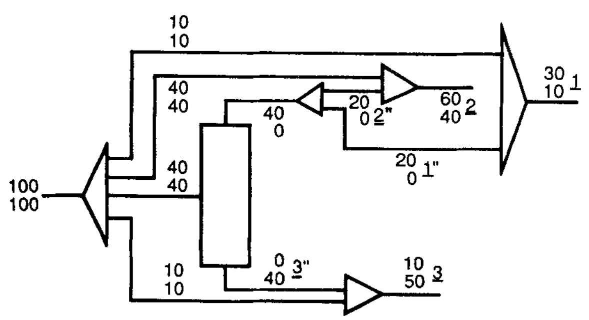


Figure 12. Scheme 3 for binary example.

One can, however, do better than that as follows: Given an $\boldsymbol{R}$ matrix, the separation of two adjacent components $j, j+1$ in a given product i is defined as

$$S_{ij} = \frac{r_{ji}}{r_{j+1,i}} \tag{47}$$

Similarly, define as minimum separation of two adjacent components $j, j+1$

$$S_j^* = \frac{\max\limits_i S_{ij}}{\min\limits_i S_{ij}} \qquad \begin{matrix} j = 1, \ldots, n-1 \\ i = 1, \ldots, p \end{matrix} \tag{48}$$

The rationale behind this definition is that if all nonkey components were separated off, S_j^* would be the minimum separation required for separating the product fragments in the fashion described previously.

The quantities S_{ij} may change, as the operations of distillation and feed bypassing (or splitting) are performed. In particular with feed bypassing:

$$\text{to product } k \neq i, \qquad S'_{ij} = S_{ij}$$

$$\text{to product } i \tag{49a}$$

$$\text{if } S_{ij} \leq 1 \qquad S'_{ij} \leq S_{ij} \qquad \text{else} \qquad S'_{ij} > S_{ij} \tag{49b}$$

The effect of feed bypassing on the cost of a separator, one immediately following the point of bypass, or a downstream unit, is as follows:

- The cost of a sharp separator decreases.
- The cost of a semisharp separator typically increases (although optimization may be necessary for one-section columns). Also, the bypassed fraction of the feed can be remixed for further processing, thus not affecting the downstream separators.
- In the case of a three-specification separator, the extent of bypassing is determined by feasibility requirements and is not subject to optimization.
- For a nonsharp (binary) separator, it has been established earlier that bypassing so that

$$\text{if } S_{ij} \leq 1 \quad S'_{ij} = \min(S_{ij})$$
$$\text{else } S'_{ij} = \max(S_{ij})$$

is beneficial, while beyond that it is typically not economical.

It follows then that bypassing fraction f_i of the feed to product

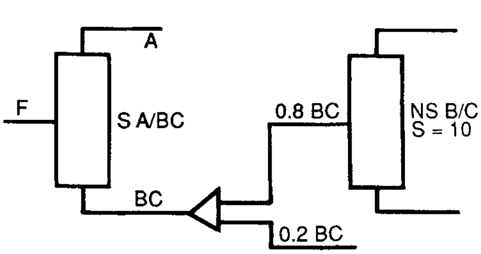


Figure 13. Scheme 1 for ternary example.

i such that

$$\min S_{ij} \le S'_{ij} = \frac{r_{ji} - f_i}{r_{j+1,i} - f_i} \le \max S_{ij} \qquad \text{for all } j \qquad (50)$$

or, equivalently, so that no S_j^* increases, is in general beneficial. Furthermore, if the extent of feed bypassing so determined, f_i, is less than $f_{i,max}$, Eq. 13, more bypass may be better. This, however, involves a cost trade-off between the separator immediately following the bypass point and the downstream ones.

For the example case (matrix R_1), we obtain

		1	2	3	4	5
S_{ij}	A	1/3	4	3/2	∞_{max}	0_{min}
	B	3/2	1/2	$2/5_{min}$	N/A	4_{max}

(∞ really means 98/2 while 0 means 2/98.) No obviously advantageous bypass to product $\underline{3}$ exists. 0.1 fraction of the feed can be bypassed to product $\underline{1}$, but only f_2 = min (0.1, 1/30) = 1/30 fraction to $\underline{2}$ (limited by S'_{2B}).

The resulting decomposition then is

$$\underline{1} = \frac{1}{10}\underline{F} + \underline{1}' \qquad \underline{2} = \frac{1}{30}\underline{F} + \underline{2}'$$

The $\boldsymbol{R}$ matrix of the processed fraction is

		1′	2′	3	4	5
	A	—	11/26	9/26	6/26	—
R_4	B	6/26	2/26	6/26	—	12/26
	C	3/26	5/26	15/26	—	3/26

An S A/B split, followed by an NS B/C split, results then in scheme 2, shown in Figure 14.

Scheme 2 represents the least one can do if an S A/B split is performed first. However, from matrix R_4 it is inferred that an additional 4/13 fraction of the reduced feed can be bypassed, resulting in an obvious decrease in the first separator cost. This action of course corresponds to feed bypass in the second separator, which is generally uneconomical. Hence, there is a possible trade-off between columns and a detailed optimization is necessary.

Synthesis Strategy

Generation of alternatives

In this section, the generation of alternatives for carrying out a nonsharp separation duty is done based on a heuristic procedure. Unlike methods developed for sharp separation problems, the search for the best alternative is not done concurrently with the generation, but in a distinct second step. This is done because the structure of the set of alternatives is not well known in advance and whole classes may be excluded at the generation stage (see rules 1 and 4, below).

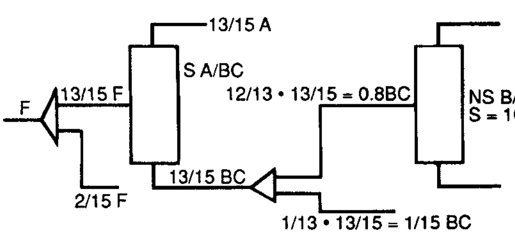


Figure 14. Scheme 2 for ternary example.

The generation of processing alternatives proceeds according to the following steps.

Step 1. Construct the $\boldsymbol{R}$ matrix representation of the problem. For sufficient characterization of a material stream, one more column is needed, which contains the component molar flows. For computational convenience, another column is added, which represents the mole fractions of the components in the stream.

The manipulations below are performed immediately, if applicable, to a newly generated $\boldsymbol{R}$ matrix.

- Delete product columns that have all elements equal and adjust other columns.
- Split product columns that contain an internal zero entry (i.e. $j \neq 1, n$) into two, with zeros extending to opposite ends of each column.

Step 2. Construct the $\boldsymbol{S}$ matrix defined previously. The following are done on the $\boldsymbol{S}$ matrix.

- If two columns are identical, delete one of them and merge the corresponding columns in the $\boldsymbol{R}$ matrix into one (one product column is a multiple of the other).
- Identify the minimum and maximum elements in each row, i.e.,

$$m_j = \min_i(S_{ij}) \qquad \text{and} \qquad M_j = \max_i(S_{ij}).$$

Step 3. Identify feed division into two or more streams undergoing processing in parallel (this may not be best under all circumstances, as it can result in many small separators).

Step 4. Identify opportunities for bypass to products. Bypass amount f_i to product i so that for all j

$$m_j \le S'_{ij} \le M_j \qquad (50)$$

and, for at least one j^*,

$$S'_{ij^*} = m_{j^*} \quad \text{or} \quad M_{j^*} \qquad (50a)$$

Update the $\boldsymbol{R}$ matrix via the formulas

$$r'_{ji} = \frac{r_{ji} - f_i}{1 - \sum_k f_k}; \quad F'_j = F_j\left(1 - \sum_k f_k\right); \quad z'_j = z_j \qquad (51)$$

(Due to conflict between symbols in Eq. 12, the component molar flow, f_j, is denoted by F_j.)

Step 5. Identify opportunities for semisharp and three-specification separations. Rearrangement of the order of columns, so that zero entries concentrate in the lower left and upper right corners of the $\boldsymbol{R}$ matrix, may be necessary.

Step 6. Perform the one separation required when the $\boldsymbol{R}$ matrix represents an elementary problem, i.e.,

- Binary feed
- Multicomponent S, SS, or $3S$ separation

Step 7. Implement the separation types, identified previously, in the following heuristic order.

- "Unavoidable" sharp separations, i.e., those with $m_j = 0$ and $M_j = \infty$
- 3S separation(s) if one of the products of the separator requires no further processing
- Other sharp separations ($m_j \neq 0$ or $M_j \neq \infty$)
- Other 3S separations
- Semisharp separations ($m_j = 0$ and $M_j \neq \infty$ or $m_j \neq 0$ and $M_j = \infty$)

Among the various restrictions imposed, the exclusion of *NS* splits for multicomponent mixtures is a key one. The intent is to remove the dependence of component splits on relative volatilities, as well as any ambiguity in defining product fragments. While the generation of alternatives if simplified, one potentially fails to take advantage of all problem-specific information.

The steps outlined above create the set of descendant nodes of a given node in the AND/OR tree (Nilsson, 1980) representing the set of alternatives, in a manner similar to the case of sharp product sets. The overall strategy employed, which makes the tree of possibilities explicit, is presented below.

Rule 1. Develop sequences that contain up to a prespecified number of units.

Sequences with more than the minimum number of units $(n - 1)$ could arise when an *SS* or 3*S* separation is performed, or when the feed stream is split into fractions undergoing processing in parallel. In order for such sequences to be considered, significantly reduced flows to separators should occur (case of parallel processing), or some columns should be one-section towers (rectifiers or strippers), or single-stage flash units.

The terminating rule can be set as

$$s \leq \text{bound} + \text{margin} \tag{52}$$

In the absence of any information, the bound is set to $(n - 1)$. When an actual sequence has been developed, the bound is set to the number of units it contains. The ordering of separation types, in step 7 of the generating procedure, is intended to aid the early identification of a tight bound (see also Rule 2, below).

The margin is set initially to zero. In a second stage, likely after the best among the available alternatives has been identified (cf. following section), the margin could be set to one.

Rule 2. The overall generation strategy proceeds in a depth-first fashion.

Rule 3. A list of generated $\boldsymbol{R}$ matrices is maintained, in order to avoid duplication.

As in the case of sharp product sets, identical material streams can be arrived at via different paths. Also, a newly generated $\boldsymbol{R}$ matrix is not further expanded if it is simply a scale-up of an existing one.

Rule 4. Do not consider sequences that contain separators (in series) which have identical key components.

This rule represents a restriction on semisharp separators, in addition to not allowing product fragmentation. The idea is to disregard sequences with separators (immediately following one another or not) forming the patterns *SS LK/HK–S LK/HK*, *SS LK/HK–SS LK/HK*. This is in accordance with the current practice in sharp product sets, where such schemes appear only in prefractionators or in heat-integrated sequences (King, 1980). Note that the rule does not exclude schemes that contain an *SS* and a 3*S* separator involving the same components.

Consider the following example

Step 1.

		1	2	3	4	f	z
R	A	0.6	0.4	—	—	400	1/4
	B	0.5	0.5	—	—	400	1/4
	C	0.2	—	0.8	—	400	1/4
	D	—	—	0.4	0.6	400	1/4

Step 2.

		1	2	3	4
S	AB	$6/5_M$	$4/5_m$	N/A	N/A
	BC	5/2	∞_M	0_m	N/A
	CD	∞_M	N/A	2	0_m

Step 3. No obvious feed splitting
Step 4. No bypass possible
Step 5. *SS* opportunity: 1, 2, 3/4; C/D $R_{D,\mathrm{Top}} = 0.4$
3*S* opportunity: 1, 2/3, 4; $B/C/D$ $R_{C,Top} = 0.2$
Step 6. Not an elementary problem
Step 7. B/C and C/D sharp splits are unavoidable. Designate (arbitrarily) B/C first.

Ordering of options, $\boldsymbol{R}$ matrix:

- *S* B/C
- *S* C/D
- No 3*S* with one product directly isolated
- *S* A/B
- 3*S* $B/C/D$ $R_{C,Top} = 0.2$
- *SS* C/D $R_{D,Top} = 0.4$

Perform B/C split. Two $\boldsymbol{R}$ matrices generated:

		1	2	f	z
R_1	A	0.6	0.4	400	1/2
	B	0.5	0.5	400	1/2

		1	3	4	f	z
R_2	C	0.2	0.8	—	400	1/2
	D	—	0.4	0.6	400	1/2

R_1 is an elementary problem, solved by an *NS* A/B split with $R_{A,Top} = 0.6$ and $R_{B,Top} = 0.5$. R_2 is again an elementary problem, i.e., bypass 0.4 fraction of the feed to product 3 and perform an *S* C/D split. The first sequence has been completed and contains three separators.

Going back to the original $\boldsymbol{R}$ matrix, the next option from step 7 is *S* C/D, creating R_3:

Step 1.

		1	2	3	f	z
R_3	A	0.6	0.4	—	400	1/3
	B	0.5	0.5	—	400	1/3
	C	0.2	—	0.8	400	1/3

Step 2.

S_3	AB	$6/5_M$	$4/5_m$	N/A
	BC	5/2	∞_M	0_m

Step 3. No feed splitting

Step 4. Up to 0.2 fraction of feed can be bypassed to product 1. It has a beneficial effect on the *S B/C* separation, but an unfavorable one on the *NS A/B* split.

Step 5. *SS* opportunity 1,2/3; *B/C* $R_{C,Top} = 0.2$

Step 6. Problem not elementary

Step 7.

- *S B/C* (unavoidable)
- No such 3*S* (see, however *S B/C* below)

R_3 matrix

- *S A/B*
- No such 3*S*
- *SS B/C* $R_{C,Top} = 0.2$

Perform *S B/C*

		1	2	*f*	*z*
	A	0.6	0.4	400	1/2
R_1	B	0.5	0.5	400	1/2

R matrix encountered before; leads to an *NS A/B* split. There exists the possibility of bypass optimization ($f_1 \leq 0.2$), as the result of trade-off between the flow to the *S AB/C* separator and the, generally unfavorable, bypass effect on the *NS A/B* separator. Second sequence completed.

Going back to the R_3 matrix, the next option is an *S A/B* split. Since the split that follows this is *S B/C*, maximum bypass is advantageous, giving R'_3. R'_3, after an *S A/B* split, gives the matrix R_4, an elementary *S B/C* separation. Third sequence completed.

		1	2	3	*f*	*z*
	A	0.5	0.5	—	320	1/3
R'_3	B	3/8	5/8	—	320	1/3
	C	—	—	1	320	1/3

		1+2	3	*f*	*z*
R_4	B	1	—	320	1/2
	C	—	1	320	1/2

Overall, five sequences containing three separators each have been identified (Bamopoulos, 1984). They contain ten unique separators, and in one of the sequences (no. 2) a nontrivial bypass optimization problem, involving two separators, exists. The alternatives are shown in Figure 15 and the problem AND/OR tree is shown in Figure 16. (The numbers on the arcs indicate the separators, in the order generated).

It can be seen from the example that the ***R*** matrix representation, and the operations performed on it, are a powerful generalization of the list-processing technique. Distillation alternatives generated bear the same characteristics as the sequences for sharp product sets:

- Sequences have separators in common, arranged in different ways
- To a first approximation, flows and compositions can be established without any separators designed

Synthesis Strategy

Evaluation of alternatives

The optimal search method employed in the present work is of the best-first type (Nilsson, 1980). In a nutshell, the method will expand the partial sequence that is the most promising (and abandon it, in favor of another, as soon as things look bad). Given that preliminary cost estimates are accurate only to ±30%, alternatives costing up to 30% more than the best one discovered are retained. While optimality of solution cost or of effort expended is of theoretical interest, in practice, assump-

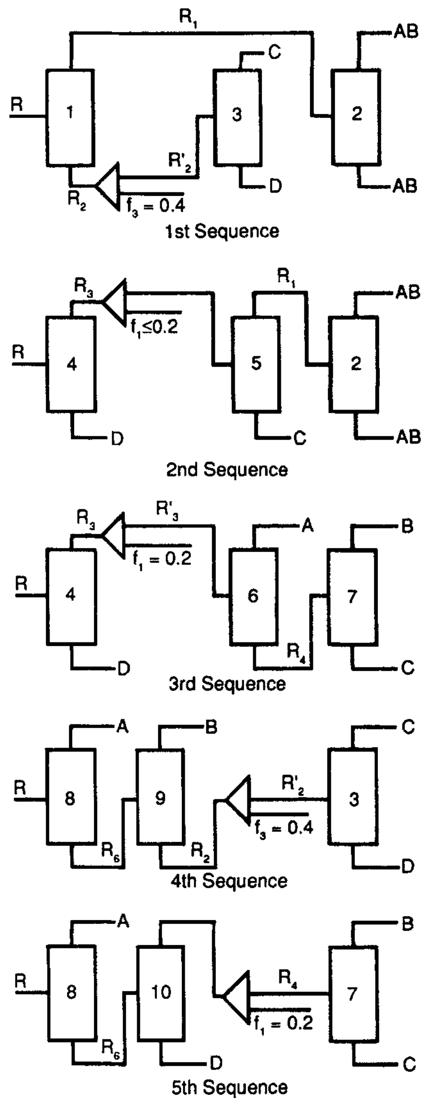


Figure 15. Set of alternatives for nonsharp example.

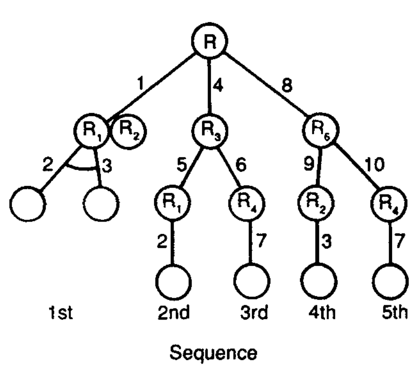


Figure 16. AND/OR tree for nonsharp example.

tions made about operating variables have a great impact on both. Hence attention will be turned to these in the following, in an attempt to obtain reasonable answers with a reasonable effort.

Depending on whether the sequence products go to storage or, alternatively, are processed downstream, some restrictions on product temperature and pressure may apply. In extreme cases these restrictions can have a significant effect on the choice of separation method, or configuration. It is, however, desirable to establish a common basis for evaluating alternatives, as well as to limit the scope of the synthesis activity to separation tasks (as opposed to heat exchange or pressure adjustment). The heuristic rules employed in the present work are shown in Table 4. Rules 1–6 apply to sharp product sets, as well, while rules 7 and 8 are specific to nonsharp product sets (Bamopoulos, 1984).

The proposed synthesis methodology was applied to a classical literature example (Heaven, 1969), involving sharp separation of light hydrocarbons. Please note that feed temperature and pressure are those chosen by Nath (1977), while other investigators have used different values. The results of the optimal search appear in Table 5.

The following points can be made:

• The cost ratio of most (no. 6) to least (no. 2) expensive sequence is 1.13, hence all separators had to be designed and all sequences fully developed.

• Other investigators have produced the same optimal sequence (Nath, 1977; Gomez and Seader, 1976), our second best, no. 11 (Rathore et al., 1974; Rodrigo and Seader, 1975), or our no. 12 sequence (Minderman and Tedder, 1982).

Consider now the example for which alternatives were generated as applied to the system of Table 6.

The separators, as they are encountered, are listed in Table 7. The search developed four out of the five sequences of Figure 15, in its attempt to locate all sequences that cost up to 30% more than the least costly one. The terminated fifth sequence can be completed to a total cost of $907,000. The five sequences, containing up to three separators, are listed in Table 8. For comparison purposes, the corresponding sequences, developed with the classical all-sharp methodology, are also listed.

It is interesting to note that the cost ratio of most to least expensive is 1.72 in the nonsharp sequences, while it is only 1.05 in the sharp sequences. Furthermore, savings of 42% are realized by employing the best nonsharp instead of the best sharp sequence.

In Appendix D, sequences containing up to four separators are generated and the optimal search repeated.

The problem-solving logic developed in this work is still preliminary, thus it has not been implemented in the form of a computer program. Manual carrying out of the steps (employing, however, the CHESS simulator [Motard and Lee, 1971]), provided useful insight and savings in calculations, but is tedious and error-prone.

Table 4. Heuristic Rules

1. Columns delivering final products (or fragments thereof) have either all total or all partial condensers.
2. Columns can operate at different pressures.
3. Columns delivering overhead products as feeds to subsequent columns should have partial condensers, unless the condenser costs of the receiving column are dominant (when a total condenser should be considered). Also, preheaters/precoolers are considered only for the first column in the sequence if the reboiler/condenser costs are dominant.
4. Feed pressure reduction has negligible cost, as well as liquid feed pumping. Vapor feed compression is not allowed.
5. Choose as column operating pressure that of its feed stream. Explore the possibility of raising (lowering) the pressure if the condenser (reboiler) costs are dominant.
6. Choose $R/R_{min} \geq 1.2$. Attempt to increase the reflux ratio if column capital costs are dominant.
7. Operating costs of a column scale linearly with feed rate F, while capital costs scale proportionally to $F^{0.62}$.

8a. The only column bypass optimization considered is in the case of top (bottom) to a stripper (rectifier). Also, bypass maximum possible to top (bottom) in a flash unit if heating (cooling) is required.

8b. Investigate bypass opportunities involving sequences of columns.

Table 5. Sequences in Order Generated for Heaven (1969) Example

No.	Sequence	Annual Cost $/yr × 1,000
1	A/BCDE, B/CDE, C/DE, D/E	2,600
2	A/BCDE, BC/DE, D/E, B/C	2,537
3	ABC/DE, D/E, A/BC, B/C	2,595
4	A/BCDE, BCD/E, BC/D, B/C	2,629
5	ABCD/E, A/BCD, BC/D, B/C	2,828
6	ABCD/E, ABC/D, A/BC, B/C	2,856
7	A/BCDE, BCD/E, B/CD, C/D	2,622
8	A/BCDE, B/CDE, CD/E, C/D	2,670
9	ABCD/E, A/BCD, B/CD, C/D	2,821
10	AB/CDE, C/DE, D/E, A/B	2,634
11	ABC/DE, D/E, AB/C, A/B	2,547
12	ABCD/E, ABC/D, AB/C, A/B	2,808
13	AB/CDE, CD/E, C/D, A/B	2,704
14	ABCD/E, AB/CD, C/D, A/B	2,776

Industrial Examples

In this section a few processing schemes from industrially significant separations are briefly described. Detailed information regarding mass balances was not available, hence the discussion will have a qualitative tone.

As a first case, consider the depropanizer column in an HF (Funk and Feldman, 1983) or sulfuric acid (Meyer et al., 1983) alkylation unit. Both flowsheets exhibit a common feature, i.e., bottom feed bypassing in the depropanizer column. This is in accordance with the results presented here, namely, $V' - V'_o = r_2 (1 - q) F$, where, for the reportedly refrigerated feed, $q > 1$, hence $V' < V'_o$.

Table 6. Nonsharp Example

Components: Butane, pentane, hexane, heptane
$F = 202$ mol/s, saturated vapor
$z_A = z_B = z_C = z_D = 0.25$
$P = 356$ kPa
Thermal state of products immaterial
For sharp splits, $R_{LK} = 0.99$, $R_{HK} = 0.01$

Table 7. Separators for Nonsharp Example

Split	Pressure, kPa Feed	Column	Feed Vapor Frac.	Venture Cost $/yr × 1,000
AB/CD	356	356	1.00	301
AB/CD	356	356	0.00	406
ABC/D	356	356	1.00	369
A/BCD	356	356	0.00	386
A/BCD	356	621	0.00	363
A/B	356	356	1.00	10
C/D*	356	356	0.00	233
C/D*	356	101	0.42	216
B/CD	356	241	0.35	257
BC/D	621	241	0.35	333
A/BC**	356	356	1.00	345
ABC/D†	356	356	1.00	428
A/BC**	356	621	0.00	217
AB/C**	356	356	1.00	231
A/B	356	356	1.00	11
AB/C	356	356	1.00	267
B/C**	621	241	0.33	198
B/C**	241	241	1.00	211

*60% of Feed
**80% of Feed
†Total Condenser

As a second example, consider the xylenes recovery process as reported by Fayon and Imperiali, (1978) and Yang and Evans (1981). Three alternative flowsheets are presented in Figure 17, about which the following points can be made:

In scheme 1, feed to the $T1$ tower is bypassed to the bottoms. According to the simplifying criterion employed by Yang and Evans, 0.5 fraction bypassed is best. Again, note that the feed is cold.

In scheme 2, feed is bypassed to the top of $T2$. It is not clear what the expected benefits in the affected towers $T2$, $T3$ are.

In scheme 3, bypass affecting three towers is performed, a combination of the encountered bottom bypass in $T1$ and top in $T2$. Yang and Evans again report that 50% fraction bypassed is best. It appears that one reason for the existing feed bypassing facilities is operational flexibility in adjusting production for different feedstock composition or product selling prices.

An example of semisharp separation followed by sharp separation is offered by the methanol recovery process (Thiagarahan et al., 1984). Two columns are used for heat-integration purposes, as shown in Figure 18. The first column is operated at higher pressure and produces an overhead stream that meets the methanol specification. Recovery, however, is low and a second column is employed to produce an essentially aqueous bottoms.

In a typical refinery or chemical complex there are several multicomponent streams that are blended to meet specifications. Blending is inherently uneconomical and it is hoped that the present work will inspire the designer to examine whether such streams originate from the same source. If, in addition, they consist of fractions having adjacent volatilities, separation that is more sharp than necessary may be recognized and better schemes envisioned.

Table 8. Sharp and Nonsharp Sequences for Example

Sequence	Cost, $/yr × 1,000 Nonsharp	Sharp
AB/CD, A/B, C/D	527	911
ABC/D, AB/C, A/B	611	949
ABC/D, A/BC, B/C	843	902
A/BCD, B/CD, C/D	836	913
A/BCD, BC/D, B/C	907	938

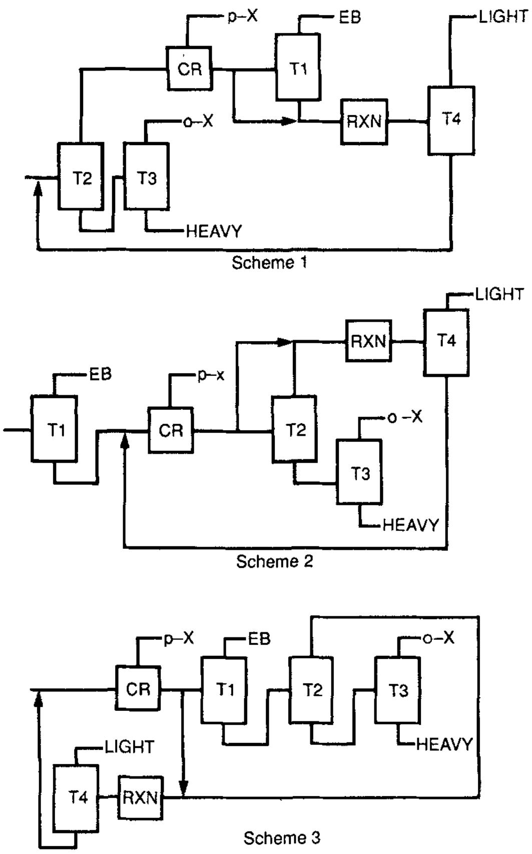


Figure 17. Xylene recovery schemes.

Conclusions

In this paper problems related to the synthesis of ordinary distillation sequences were examined. For sharp product sets, the list-processing technique (Hendry and Hughes, 1972) was combined in this work with the conversion of product specifications to column key recoveries to systematically generate simple processing alternatives. If less than $2(p - 1)$ product specifications are imposed, a train of $p - 1$ separators will have residual

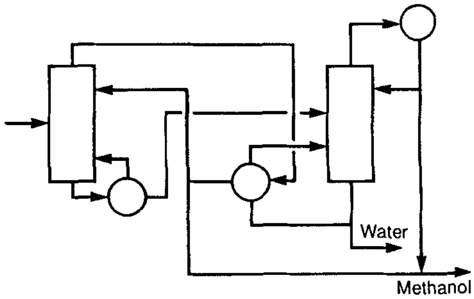


Figure 18. Methanol recovery scheme.

degrees of freedom. In this context, it is crucial that the "true" compositional targets be identified, leaving open possibilities for design optimization or operational flexibility. Plausible sequences for nonsharp product sets, the focus of this paper, are generated by a systematic application of the operations of distillation, stream splitting, and stream mixing on a representation of a process stream in terms of a component recovery matrix (**R** matrix).

Of the four separation classes considered (sharp, semisharp, nonsharp, and three-specification), the semisharp and nonsharp can occasionally be implemented with a one-section column or, in the extreme, a single-stage flash unit. Savings opportunities were identified when feed is bypassed to the top (bottom) stream of a stripping (rectifying) column, a case resembling the classical reflux vs. stages trade-off in a two-section distillation column. On the other hand, bypass in two-section columns was shown to be generally of no advantage. Feed bypassing to a final product was also investigated. Analytical results were presented for binary feeds, which can always be separated in a single unit. In the multicomponent case, trade-offs between columns in series were identified, based on the concept of minimum separation of two adjacent components defined here. The latter was found more useful than the recognition of dependence among products (Bamopoulos, 1984), i.e., when some products can be generated by mixing of others.

A heuristic ordering of options, coupled with a depth-first technique, was proposed for generating schemes containing up to a prespecified set of units. This was done because it has not been ascertained that the best sequence is among those with the minimum number of separators.

The sequences discovered by the procedures of this work, like their counterparts for sharp products sets, have separators in common, arranged in different order. Furthermore, albeit to a lesser extent, flows and compositions can be established without any separators designed. Due to the richness and the significant problem dependence of the set of alternatives, the search for the few better ones was done in a distinct second step. A best-first technique was proposed coupled with heuristic optimization of the partially developed sequences, as literature, and our own experience, indicated that the range of venture costs is narrow.

For an example problem of four components and four products, significant savings (42%) were realized using the present methodology, over the best among the sequences that completely isolate (and remix) the feed components. A few industrial schemes containing feed bypass and separators with sloppy component splits were identified, however, no detailed information enabling direct application of the results of this work was available.

The present work represents but a modest step toward the understanding of the complex domain of nonsharp separations. Some areas in which further work may be useful are highlighted below.

Design experience, for other than conventional simple, sharp separators appears to be limited. Separators with key component recoveries not close to one can sometimes be profitably employed in prefractionator or thermally-coupled schemes for sharp product sets (King, 1980). Such cases merit attention, as well as the examination of the product specifications realizable with columns employing sidestreams or multiple feeds. Sidestream columns could arise in our work by "merging" a two-section column with an immediately following one-section column. Feed bypass around a separator needs to be investigated further, with the objective of minimizing thermal and compositional irreversibilities due to stream mixing.

The restriction on other than sharp separators, namely no product fragmentation, excludes a continuum of possibilities between certain alternatives, where separation is distributed between successive columns. This area was investigated by Gawin (1975) for sharp product sets. Similar arguments point to the introduction of product fragmentation in the case of feed splitting, when heat-integrated (King, 1980) or other special alternatives (derived from the problem MAD) may be attractive. The general separation synthesis problem involving multiple feed streams could also benefit from an improved handling of feed splitting. Stream recycling within the separation train is encountered in industrial applications, and warrants a close look.

Lastly, it seems worthwhile to more closely examine how realistic problems are solved in an industrial context, where workable systems are sought (Umeda, 1983) that exhibit feed stock flexibility and resiliency to outside disturbances.

Notation

C_i = set of components specified to be present in product i
d = component flow rate in distillate, mol/time
d = column diameter
D = distillate flow rate, mol/time
f = component flow rate in feed, mol/time
f = fraction of feed bypassed
f = Eq. 4
F = feed flow rate, mol/time
HK = heavy key
HNK = heavy nonkey
i = product
j = component, product
K = recovery ratio at bypass conditions
K_i = set of components actually present in product i
L = liquid flow rate, mol/time
LK = light key
LNK = light nonkey
m = minimum ratio of component recoveries
M = maximum ratio of component recoveries
MK = middle key
n = number of components
N = number of stages
$N_R(N_S)$ = number of rectifying (stripping) stages
NS = nonsharp
p = number of products
p_i = product purity
P_i = product
$\bar{P}$ = pressure
q = feed thermal condition, =1 for saturated liquid
Q = heat exchanger duty, energy/time
r_{ji} = recovery of component j in product i
r_1 = top bypass fraction
r_2 = bottom bypass fraction
R = reflux rate
$\mathbf{R}$ = **R** matrix, component recovery matrix
R_j = component recovery at stream rich in j (sharp case) or at top stream (nonsharp case)
s = number of separators
S = sharp
S = separation factor
S_{ij} = separation of components $j, j+1$ in product i
S_j^* = minimum separation of components $j, j+1$
SS = semisharp
$3S$ = three-specification
T = temperature
V = vapor flow rate, mol/time
W = bottoms flow rate, mol/time

x = component mole fraction in liquid part of feed (two-section colummn) or in bottoms (one-section column)
y = component mole fraction in distillate stream (one-section column)
z = component mole fraction in feed
$z_*(z^*)$ = liquid (vapor) mole fraction in equilibrium with vapor (liquid) of composition z

Greek letters

α = relative volatility with respect to heavy key
$\overline{\alpha}$ = upper volatility limit
$\underline{\alpha}$ = lower volatility limit
ΔH_C = heat of condensation, energy/mol
θ = reflux ratio, actual over minimum
κ = recovery ratio at no bypass conditions
ρ = product recovery
ρ = component recovery at top stream (or product) at no bypass conditions

Subscripts

A = light key
B = heavy key
C, COL = column
C, CON = condenser
i = product, occasionally component
il = light impurity
ih = heavy impurity
j = component, occasionally product
o = no bypass conditions
R, REB = reboiler
TOT = total

Superscripts

$'$ = stripping section
$*$ = optimal

Appendix A: Realization of 3S Separations

An analysis of the degrees of freedom (King, 1980) of a conventional distillation column with fixed feed, top pressure, and reflux at its bubble point reveals that there are four free variables. In the operating problem they are usually specified as N_R, N_S, D, L (or $R = L/D$). In the design case they are specified as R_{LK}, R_{HK}, optimal feed stage location, optimal R/R_{min}. As described in the textbook by Hanson et al. (1962), it is conceivable that all four degrees of freedom are consumed by product specifications (when the feed has at least four components). Therefore, in principle, one could design a column with R_{i-1} and R_{i+1} and manipulate either the feed plate location or the amount of reflux so that the recovery R_i is also satisfied.

Another approach is taken here, under the reasonable assumption that the component distribution, at operating reflux ratios in the range 1.15 to 1.25 times the minimum, is approximately the same as under total reflux (King, 1980). The distribution can be represented as a straight line of slope equal to N in a log-log plot of K_i vs. α_i. (K_i is defined as the quantity $R_i/(1 - R_i)$.)

If the column is designed with keys $i - 1$, $i + 1$ there are two possibilities, shown in Figure 19. In the first case the key components should be i, $(i - 1)$, and overpurification of the top product in terms of $(i + 1)$ is achieved. In the second case the key components should be $(i + 1)$, i and overpurification of the bottom product, in terms of $(i - 1)$, is achieved.

Appendix B: Sketch of Derivation of Eq. 17

By applying Eq. 15 at bypass conditions (i.e., replacing ρ_i with R_i) and substituting the value for R_i from Eq. 14, it can be

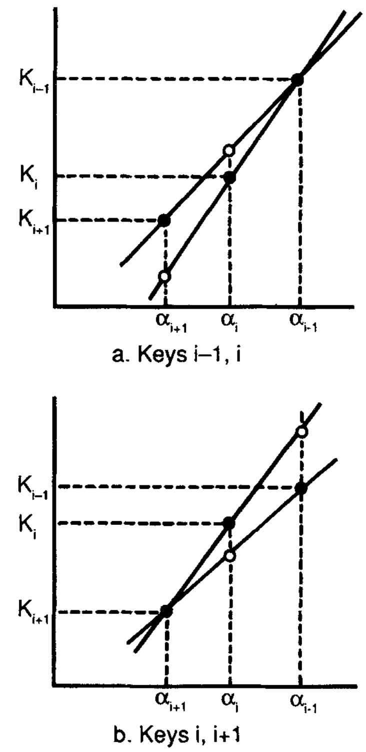


Figure 19. Realization of a 3*S* separation.

shown that Eq. 14 is valid, in general, for any component i. In other words, the following is true

$$R_i = \frac{\rho_i - r_1}{1 - r_1 - r_2}, \text{ if } \underline{\alpha} < \alpha_i < \overline{\alpha}$$
$$R_i = 0, \text{ if } \alpha_i \le \underline{\alpha} \qquad \text{(B1)}$$
$$R_i = 1, \text{ if } \alpha_i \ge \overline{\alpha}$$

The approximate value for minimum flows is given in (King, 1980) as

$$\frac{V_{min,o}}{F} = \sum_i \frac{\alpha_i \rho_i z_i}{\alpha_i - \phi} \qquad \text{(B2)}$$

where ϕ is the root, between 1 and α, of

$$\sum_i \frac{\alpha_i z_i}{\alpha_i - \phi} = 1 - q \qquad \text{(B3)}$$

By combining Eq. B2 with its version at bypass conditions, and substituting R_i from Eq. B1, the following results:

$$\frac{V_{min}}{F} - \frac{V_{min,o}}{F} = -r_1(1 - q)$$
$$- \sum_{\alpha_i \le \underline{\alpha}} \frac{\alpha_i z_i}{\alpha_i - \phi}(\rho_i - r_1) + \sum_{\overline{\alpha} \le \alpha_i} \frac{\alpha_i z_i}{\alpha_i - \phi}(1 - r_2 - \rho_i) \qquad \text{(B4)}$$

The second (third) term in the righthand side of Eq. B4 is identically zero, unless $r_i > 0$ ($r_2 > 0$) and some heavy (light) nonkeys do not appear in the distillate (bottom) product at bypass conditions.

Appendix C: Calculation of Venture Cost

The economic criterion employed is: Annual cost = Operating cost + 0.46385 (Capital cost). For details see Bamopoulos (1984). The column costing is based on papers by Miller and Kapella (1977) and Rathore et al. (1974). In short, based on an assumed overall efficiency of 0.80 and a tray spacing of 0.6 m, the column diameter, height, and shell thickness are computed. The product of these three quantities can be correlated to column body cost, and to this the tray manufacturing and installation cost are added. The reboiler and condenser costing is based on Happel and Jordan (1975). A temperature approach of 11 K is assumed and the medium is selected that just meets the minimum approach.

For the purposes of applying the heuristic rules, the total module cost is taken as the sum of three components

$$C_{TOT} = C_{COL} + C_{CON} + C_{REB}$$

and a cost component is considered dominant if it is over 50% of the total cost.

Appendix D: Remaining Alternatives for Nonsharp Example

The deferred options of the nonsharp example considered are expanded, with the limitation that the total number of separators in a sequence be less than four. Eleven new sequences are generated, bringing the total to 16 sequences. Also 16 new unique separators are added. The optimal search is repeated in the new AND/OR tree, and the following points can be made:

- Two sequences have been retained in the optimal search among schemes containing three separators, i.e., first sequence with cost $527,000 and second sequence with cost $611,000. Due to the greater complexity of four-tower sequences, it was decided to discontinue the search if the cost of a partially developed sequence exceeded the minimum cost by a smaller percentage (e.g., 20% instead of 30%).
- With the above restriction, no four-tower sequence was retained. The least costly sequence completed by the search costs 24% more than the minimum.
- Four-unit sequences do not necessarily cost more than any nonsharp three-unit sequence.
- In the course of the search, all but two separators had to be designed.

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Manuscript received Nov. 18, 1986, and revision received Jan. 29, 1988.