

SYSTEMATIC SYNTHESIS OF SLOPPY MULTICOMPONENT SEPARATION SEQUENCES

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(ABSTRACT)

An important process-design problem in multicomponent separations is separation sequencing, which is concerned with the selection of the best method and sequence for a separation system. Essentially all of the published work on this subject has been limited to high-recovery or sharp separations, in which each component to be separated appears in one and only one product stream. In industrial practice, however, it is often useful to permit components that are being separated to appear in two or more product streams. This type of separation results in products that have overlapping components and is called nonsharp or sloppy separations. The present work proposes and demonstrates a simple and practical approach to the systematic synthesis of sloppy multicomponent separation sequences.

The task of synthesizing sloppy multicomponent separation sequences is inherently more complicated than that of synthesizing sharp separation sequences as identification of infeasible splits and stream splitting, and transformation of infeasible product sets into equivalent feasible product sets are examples of some difficult tasks involved. A successful synthesis strategy calls for the development of an effective and flexible framework for representing the synthesis problem and for analyzing the feasibility of component splits. In this thesis, we propose a "component assignment diagram (CAD)" for problem representation. It is shown that the use of a CAD allows the design engineer to consider many alternative solutions (or sequences) and eliminate all infeasible component splits. Further, a "separation specification table (SST)" is proposed for feasibility analysis. In particular, the use of an SST provides a means to : (i) properly define and specify key and nonkey components; (ii) quickly identify feasible and infeasible splits; (iii) effectively deal with fuel products with unmatched compo-

nent specifications; and (iv) systematically consider sloppy separations with multiple split points.

One difficult problem arising from the design of multicomponent distillation columns for sloppy separations is to appropriately specify the distributions of non-key components in both overhead and bottoms products. Despite the importance of these specifications, there is very little information available on this subject in the literature. This thesis reports the results from a comparative study of rigorous simulation and shortcut modeling of multicomponent distillation columns for sloppy separations. One objective was to obtain improved quantitative understanding and practical design insights into the characteristics of nonkey distributions through a shortcut modeling based upon the Fenske equation.

One method proposed in this work for synthesizing sloppy multicomponent products is a heuristic method that involves a two-phase approach. The first phase is concerned with the feasibility analysis of splits pertinent to a CAD with the aid of an SST. The second phase is to specify systematically a subsequent split by applying heuristics, an activity that involves the sequential application of several "rank-ordered" heuristics.

A unifying approach is proposed and demonstrated for the synthesis of sloppy multicomponent product sets. Its objective is to generate equally good initial separation schemes, featuring as many as three characteristically different sequences, including all-sharp, all-sloppy, and both sharp and sloppy (i.e., mixed separation).

The proposed methods have been applied to a number of industrial separation problems. The results show that the new methods offer an extremely useful means for design engineers to generate a number of good initial sequences for obtaining sloppy multicomponent product sets prior to the ultimate separator optimization and heat integration.

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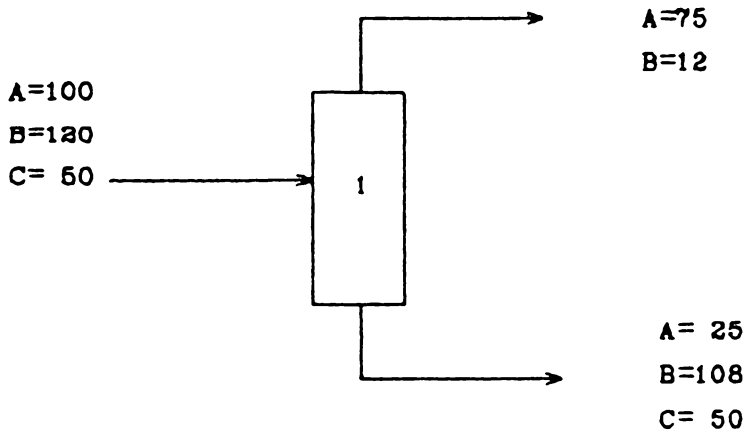
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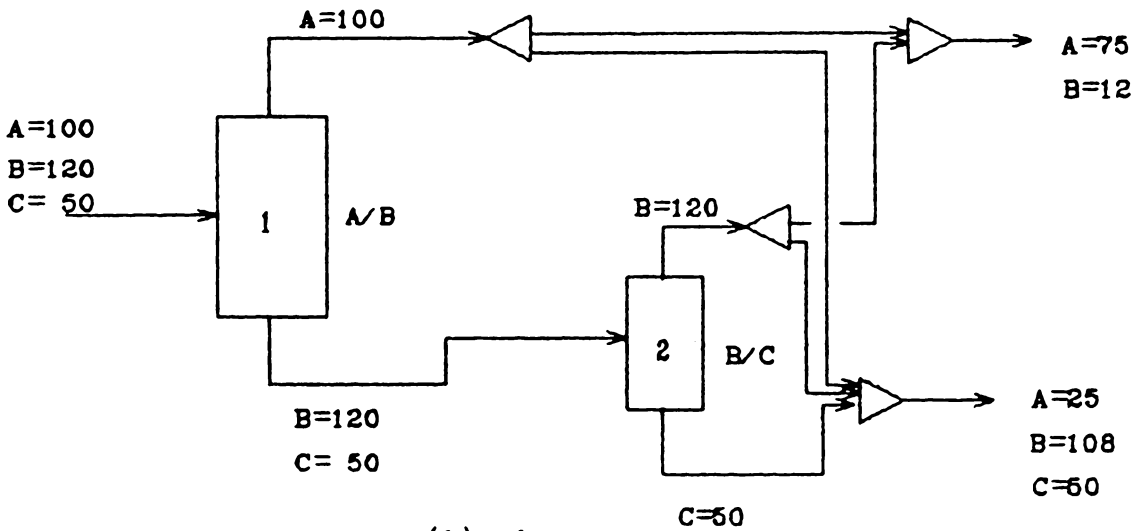
# CHAPTER 1 INTRODUCTION AND SCOPE

Process synthesis is a science that is concerned primarily with the identification of plausible process structure arrangements and economically favorable unit interconnections. Synthesis of separation system is an important application in the field of process synthesis, among many other applications such as heat-exchanger network synthesis, reactor network synthesis, etc. (see, for example, Hendry, 1973; Hlavacek, 1978; Fair, 1980; Nishida et al., 1981). Numerous researchers have looked for ways to synthesize separation systems that feature an enormous number of possible alternatives. However, in the past, most of the research studies in the area of separation sequence synthesis have focused on sharp separations, aiming at obtaining pure product streams. The importance of synthesis problems containing sloppy multicomponent product sets, in which overlapping species are allowed, was recently addressed by several investigators (see, for example, Westerberg, 1985; Lu and Motard, 1985). The economic incentive for employing sloppy separations can be understood by examining the two alternative schemes in Figure 1 on page 2, noting that one more fractionating column is needed for the sharp sequence, and that both columns are sharp for that sequence.

A typical chemical process usually comprises a reaction system and a separation system. A separation system generally involves reactant recovery, product separation, and waste and by-product separations. As was pointed out by Douglas (1985), the problem of flowsheet synthesis can be posed as an optimization problem in which the reaction conversion is a key



(a) sloppy



(b) sharp

◁: Splitter

▷: Blender

Figure 1. Comparison of Sharp and Sloppy Separations

parameter for the optimum flowsheet. Further, there is an economic trade-off between high reactor costs and significant selectivity losses associated with high conversions, which are balanced against large separation costs at low conversions. This implies that purifying unconverted reactants to a high level prior to recycling them back to the reactor system may not be necessary. In other words, sharp products (defined below) may not be required for many processes, while sloppy products (defined below) may be sufficient. Consequently, a need for synthesizing the above product sets can be justified.

To avoid any confusion that may arise hereafter, we need to define the terms *sharp* and *sloppy products* here. A common approach to the design of multicomponent distillation columns is to assume that each component to be separated appears in one and only one product stream. This type of separation yields products with nonoverlapping components (i.e., components not simultaneously appearing in both product streams of a distillation column) and is called a high-recovery or sharp separation. The product streams are then termed sharp products. In the case of sloppy product sets, components are allowed to appear in two or more product streams.

In most previous studies, the problem of separation synthesis was presented as a minimization problem in which a feed stream of known flow rate, composition, temperature, and pressure was given. The goal was to synthesize a sequence that would separate the feed into specified products at a minimum cost.

In effect, one was not only concerned with the structure of separation systems, but also operating and design variables of separators involved. It is evident that this is a rather complicated problem.

The objective of this work is to synthesize sequences for separating a multicomponent feeds into product streams having overlapping components, with an emphasis placed on the incorporation of sloppy separators. A number of good initial sequences are generated. The

proposed method does not pinpoint the optimal sequence. However, the total cost for sequences synthesized by this method are close to the minimum cost, in line with the argument of Douglas et al. (1985) that the synthesis of a separation system is coupled with the problem of process flow specifications. There may exist strong interactions between the separation system and other parts of the process. Therefore, an optimal separation system does not necessarily lead to an overall profitable process.

The following assumptions are made in this work : (1) the relative volatility is assumed constant and is independent of composition, (2) only conventional, single-feed, two-product columns are considered (see, however, Section 8.3 for a two-feed problem), and (3) the entire analysis is confined to ideal systems (i.e., systems with no azeotropes).

In Chapter 2, a number of previous studies in the literature related to the synthesis of separation sequences are reviewed. A novel representation, i.e., component assignment diagram (CAD), for the synthesis problem is given in Chapter 3, along with descriptions of its use. In Chapter 4, the feasibility of sloppy-separation synthesis is analyzed in depth. Heuristics are introduced and discussed in Chapter 5. The proposed rank-ordered heuristics upon which the heuristic sloppy-separation synthesis method is based are also presented. Industrial examples are given in Chapter 6 to demonstrate the synthesis technique in a step-by-step fashion. A thorough analysis of product sets is described in Chapter 7. A unifying framework for systematic synthesis of sloppy multicomponent product sets is also given. Finally, conclusions, significance, and recommendations are detailed in Chapter 8.



## CHAPTER 2 LITERATURE REVIEW

In this Chapter, the literature on multicomponent separation synthesis is discussed. Almost all of the methods used are reviewed here, except for heuristic and evolutionary methods, which are introduced in Chapter 5. The majority of research studies in this area focused on synthesizing sharp products.

The subject of synthesis of sloppy multicomponent products is fairly new. Despite its importance, very few papers and theses have addressed the subject. They will also be reviewed.

### ***2.1 Synthesis of Sharp Multicomponent Products***

To solve the problem of synthesis of sharp products, one can first arrange the components in a mixture to be separated in some ranked lists (Hendry and Hughes, 1972) of proper physical properties or separation factors, e.g., relative volatility, boiling point, etc. With this list of components in the order of their property ranking, one is then able to easily identify feasible sharp separations among existing components to achieve the overall separation goal.

In a ranked list, components above a certain property value can be separated from components beneath it. Using this list-splitting operation, all the alternative separation configurations can be generated. For example, consider the problem of a four-component mixture of A, B, C, and D in an order of descending volatility into pure-component products. One can come up with five possible sequences as shown in Figure 2 on page 7.

In fact, the number of theoretically possible alternative separation sequences with one separation method (e.g., distillation) can be obtained by the following generalized expression (Thompson and King, 1972).

$$S_C = \frac{[2(C - 1)]!}{C!(C - 1)!} \quad [2.0 - 1]$$

where

S = the number of possible separation configurations

C = the number of components in the feed

The numbers of possible sequences for a wide range of multicomponent feeds are tabulated in Table 1 on page 8. If one were to evaluate each alternative sequence for a given separation problem to obtain some economically plausible sequences, it would be an increasingly frustrating task as the number of components in the system increases. Consequently, there is a need to develop creative methods to solve this synthesis problem. Voluminous literature is available on the subject of synthesis of separation sequences for multicomponent mixtures. The variety of synthesis methods reported thus far in the literature can be broadly classified into four categories : (1) algorithmic methods, (2) quantitative shortcut methods, (3) heuristic methods, and (4) evolutionary methods. With the exception of the last two methods, which

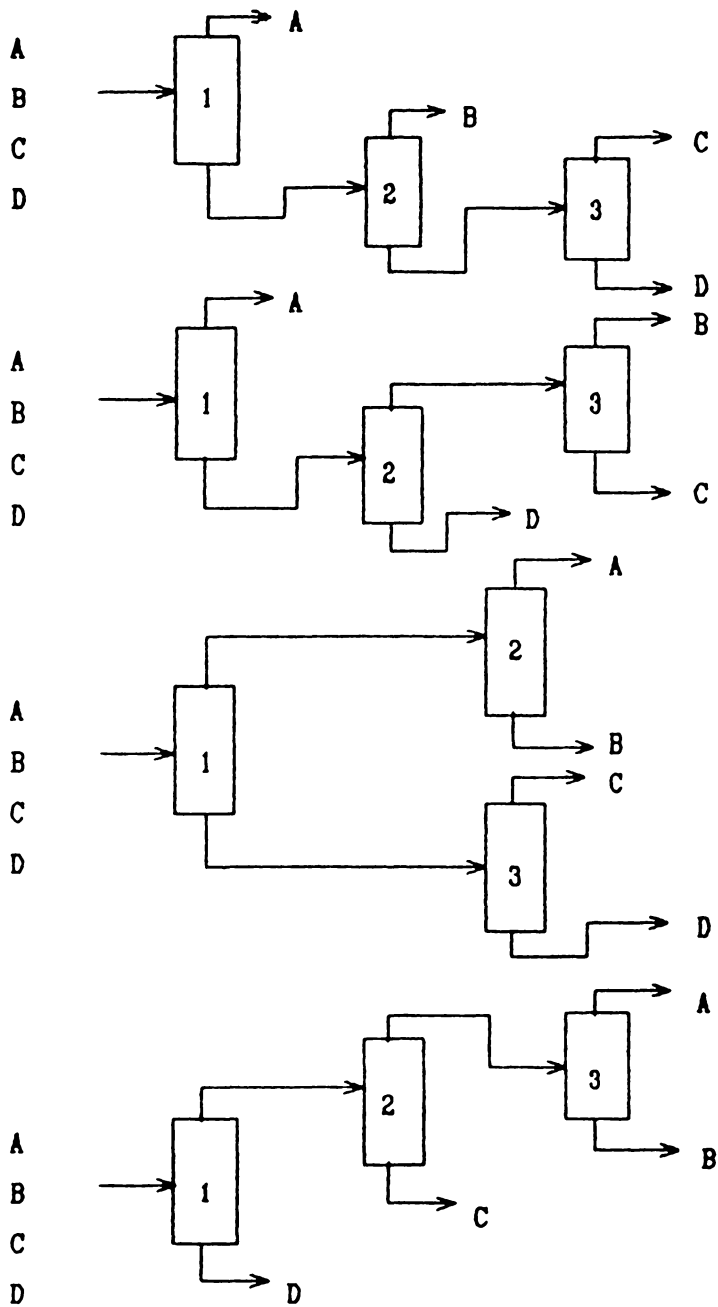


Figure 2. Possible Sharp Sequences of a Four-Component Feed

will be introduced in the beginning of Chapter 5, we will devote the remaining parts of the section to the first two methods.

**Table 1. Numbers of Possible Sharp Sequences for Various Feeds**

C ( No. of Components)	$S_c$ (Theoretical No. of Sharp Sequences)
2	1
3	2
4	5
5	14
6	42
7	132
8	429
9	1430
10	4862

### 2.1.1 Algorithmic Methods

All the methods to be introduced involve the use of different optimization techniques in the realm of mathematical programming. Most of the algorithmic methods discussed here are, in principle, based on an evaluation of all possible separation configurations by using rigorous search algorithms in a systematic manner to solve the complex combinatorial problem.

Henry and Hughes (1972) first used a branch of mathematical programming techniques, i.e., dynamic programming, in conjunction with a list-processing operation to conduct a search for the optimal sequence. In this method, focus is placed on separation subproblems that constitute each possible separation sequence. Initially, one searches for the optimal configuration at the lowest level of separation subproblems consisting of only two products (or components). One level after another, in a backward fashion, the search continues for three-product, and four-product subproblems, and so forth, until a point is reached where the entire product set is synthesized.

It should be noticed that the principle of optimality, upon which the dynamic programming method is based, requires that information feedback is prohibited. In other words, decisions made in early subproblems should not be affected by later decisions. This method requires substantial amounts of computation time for evaluating all possible separators, the main drawback of the method.

Taking heat integration into account, Rathore et al. (1974a, 1974b) also utilize the dynamic programming technique to synthesize the optimal separation sequence. For the purpose of analyzing the feasibility of heat integration of isobaric sequences of sharp distillation columns, they propose five rules of thumb.

Westerberg and Stephanopoulos (1975), in another study, use a branch-and-bound strategy for obtaining the optimal separation configuration. The underlying concept is as follows.

The goal is to minimize an objective function (e.g., sequence cost). Assume that an upper bound on the optimal value of the objective function is available. This is usually the value of the objective function for the best feasible solution identified so far. The first step is to partition the set of all feasible solutions into several subsets. For example, subsets for the initial partition of all feasible separations of a five-component sequencing problem involving A, B, C, D, and E arranged in an order of decreasing volatility are splits A/BCDE, AB/CDE, ABC/DE,

and ABCD/E. For each subset, a lower bound is obtained for the value of the objective function of the solutions within the subset. Those subsets whose lower bounds exceed the current upper bound on the objective function value are then excluded from further consideration. One of the remaining subsets, for example, the one with the smallest lower bound, is then partitioned further into several subsets. Their lower bounds are obtained in turn and used as before to exclude some of these subsets from being considered again. From all the remaining subsets, another one is selected for further partitioning and so on. This process is repeated over and over again until a feasible solution is found such that the corresponding value of the objective function is no greater than the lower bound for any subset. Such a feasible solution must be optimal. In some sense, the search is performed in the forward direction, contrary to the dynamic programming approach.

Rodrigo and Seader (1975) adopt a scheme called ordered-branch search, which is essentially a variation of the branch-and-bound technique, to identify the optimal sequence. At the beginning, the search strategy takes a view of "best-first" at all levels of the decision stage, then goes back to the last decision node and picks a slightly inferior alternative. During the search, the current minimum objective function is stored. The synthesis step is terminated during the course of synthesizing a complete sequence, if the accumulating objective function exceeds the current minimum. The method is claimed to be more computationally efficient than the dynamic programming approach.

Apart from the difficulty associated with their implementation, all the preceding algorithmic methods share one significant weakness, that is, the steep rise in the size of the solution space (or sharp increase in the number of decision variables) as the number of products increases will become unmanageable, even though theoretically an optimality with respect to the chosen objective function may be reached.

## 2.1.2 Quantitative Shortcut Methods

Malone et al. (1985) recently proposed a different approach to the column-sequencing problem, based on shortcut design techniques. An approximate cost expression of a distillation column (Marquez, 1982), given in equation (2.1-1), was linearized around a base case to give equation (2.1-2).

$$\text{TAC} = C_0 N^{0.82} V^{0.53} + C_1 V^{0.65} + C_2 V \quad [2.1 - 1]$$

where

TAC = total annualized capital cost of a column, \$/yr

$C_0, C_1, C_2$  = cost coefficients

N = the number of trays in a column

V = internal vapor flow rate, mole/hr

$$\text{TAC} = \text{TAC}_0 + K_1 \dot{N} + K_2 V \quad [2.1 - 2]$$

Malone et al. assumed that the actual reflux ratio would equal 1.2 times minimum reflux ratio. By using material balance relationships, they expressed V by

$$V = (1.2 R_{\min} + 1) D \quad [2.1 - 3]$$

Recognizing the crucial role of  $R_{\min}$  in the design of a distillation column, Glinos and Malone (1983) in a separate study investigated the dependence of minimum reflux ratio on relative volatility and feed composition. Approximate equations for the minimum reflux at saturated feed conditions were derived using shortcut methods. For instance, the minimum reflux for the sharp A/BC split was given as

$$R_{\min} = \frac{\alpha_B(X_A + X_B)}{fX_A(\alpha_A - \alpha_B)} + \frac{X_C}{fX_A(\alpha_A - 1)} \quad [2.1 - 4]$$

where

$x_A, x_B, x_C$  = mole fraction of component A, B, and C in the feed, respectively

$\alpha_A, \alpha_B$  = relative volatility of component A and B, respectively, with respect to component C

$f$  = empirical correction factor =  $1 + 1/(100x_B)$

A ternary-feed separation-sequencing problem was analyzed in which only two possible sequences exist, i.e., (I) first split between keys A/B, followed by split B/C, and (II) first split between keys B/C, followed by split A/B. The cost difference between these two sequences was defined as :

$$\Delta = TAC_I - TAC_{II} \quad [2.1 - 5]$$

Using equation (2.1-2),  $\Delta$  can be rewritten as



$$\Delta = K_1\{N_{I,AB} - N_{II,AB} + N_{I,BC} - N_{II,BC}\} + K_2\{V_{I,AB} - V_{II,AB} + V_{I,BC} - V_{II,BC}\} \quad [2.1 - 6]$$

Further assumptions were made : (1)  $N = 2N_{\min}$ , and (2) the cost coefficients of each column for the linear cost model were roughly the same. Finally, the cost difference  $\Delta$  (eqn. [2.1-6]), used as a sequencing criterion was developed as a function of feed composition and relative volatility. These assumptions were not always valid. Conditions which favored certain sequences were demonstrated successfully for ternary feeds. The weakness of the work lies in the fact that the method is not capable of generating good starting configurations, and there are generally too many sequences to compare as the number of components in the system increases.

## ***2.2 Synthesis of Sloppy Multicomponent Products***

Compared with the methods examined in section 2.1, the purpose of methods to be reviewed in this section centers around synthesis techniques concerned with sloppy product sets in which components are permitted to appear in two or more product streams. In other words, the products to be treated contain overlapping components. Because of the nature of the problem, synthesis strategies are more complicated than their counterparts for sharp product sets. As a consequence, very limited literature work has been devoted to this subject to date.

The work reported in the literature can be broadly subdivided into two groups according to the degree of sharpness used in separation : (1) nonsharp-separation synthesis methods,

and (2) all-sharp separation synthesis methods. Specifically, methods in the latter group consider sharp separation as the only means to achieve separation requirements, while sloppy separations are included in separation sequences for the former methods, which we will discuss in detail.

## 2.2.1 Nonsharp-Separation Synthesis Methods

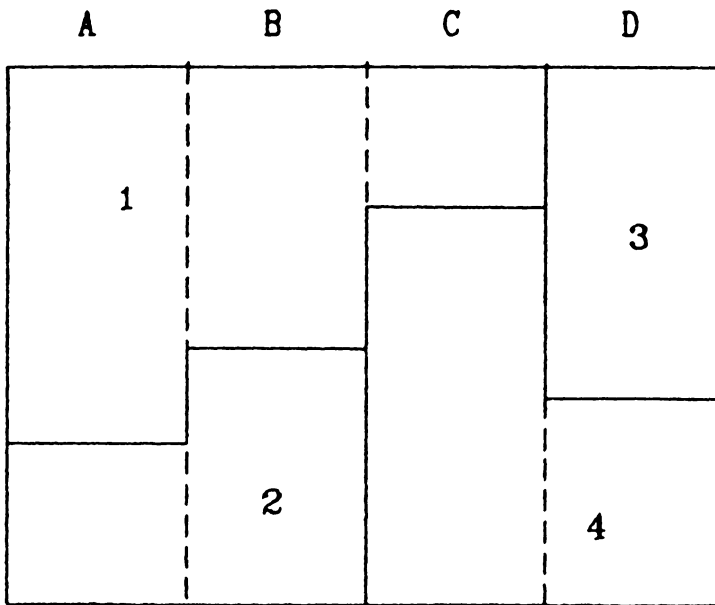
A synthesis method specifically designed for sloppy separations was first developed by Nath (1977). The method provides a way to synthesize an "optimal" sloppy multicomponent separation sequence starting from a material allocation diagram (MAD), as shown in Figure 3 on page 16 which has four components -- A, B, C, and D -- and four product streams -- 1, 2, 3, and 4 -- in the system. In the MAD, each component is represented by a fixed-height rectangle with its width being proportional to the concentration of the component. Two neighboring species are separated by a dotted vertical line. It can also be seen from the figure that each of product streams 1, 2, 3, and 4 is bounded by solid lines (or boundaries). Since the locations of product streams can be somewhat randomly assigned, confusion often arises. Several on-diagram manipulations are frequently required to modify the topology of the MAD at hand before final workable MAD's containing desirable splits come into existence. Examples of such manipulations include (1) aligning, an operation making adjacent species of a product stream of uniform height; (2) centering, an operation making a product stream fill the entire height, and having its boundaries being as far as possible; and (3) off-centering, an operation making a product stream fill the entire height, and having one of its boundaries coincide with the left-most or right-most boundary of the MAD (see Figure 8 on page 32 in

Chapter 3). To ensure that an economical sloppy split be selected, Nath created a coefficient of difficulty of separation (CDS) (see equation [5.2] in Chapter 5) to carry out the selection process.

The work of Nath was very preliminary. He only analyzed a single example problem, which revealed the complexity exhibited by more general problems (see Chapter 7). In addition, he presented only one "optimal" separation sequence for the example problem without considering to other potentially good alternative sequences. Most importantly, feasibility aspects involved with sloppy separations were completely ignored.

In another attempt, Bamopoulos (1984) also tried to incorporate sloppy separations, along with sharp separations, in the synthesis of sloppy product streams. However, sloppy splits included in his work were restricted to binary feeds. Therefore, problems associated with non-key distribution for components adjacent to key components were deliberately avoided. The synthesis approach consisted of many tedious steps based on the use of a component recovery matrix, in which each element  $r_{ij}$  represented the recovery of component  $i$  in product  $j$ , to generate possible sequences.

Tedder (1984) used a totally different approach to study the synthesis of sloppy product sets. He chose the technique of dynamic programming, which has demonstrated little success in applying to the synthesis of sharp product sets, coupled with the use of some heuristics to reduce the search space in order to solve a refinery light-ends fractionation problem. The example problem contained many sloppy splits. Tedder assumed that each sloppy split was feasible and distributed non-keys were allowed to be present in fuel product streams. Non-conventional distillation columns were taken into consideration in his work. Because of the nature of the solution scheme, the method can be considered as a combined heuristic-algorithmic synthesis method.



**(a) Material Allocation Diagram (MAD)**

product streams	(component flow rate)			
	A	B	C	D
1	15.0	12.5	5.0	-
2	10.0	12.5	-	-
3	-	-	-	15.0
4	-	-	20.0	10.0

**(b) Corresponding Desired Product Set**

Figure 3. Material Allocation Diagram proposed by Nath (1977): (The width of each species rectangle is proportional to its concentration. The vertical scale shows quantities of flows.)

In order to accommodate nonsharp separations in synthesizing sloppy products, Muraki and Hayakawa (1987) developed new ways to manipulate the MAD (Nath, 1977). After putting the problem into the form of non-linear programming, they applied an optimization technique called the complex method, coupled with the use of MAD, to solve for the optimal flowsheet. Even though degrees of separation sloppiness were taken as key design variables, the potentially undesirable distribution of non-key components which may severely restrict the synthesis problem in properly specifying process flows, had been completely ignored. As a consequence, optimization results of the work could be misleading.

## **2.2.2 All-Sharp Separation Synthesis Methods**

Realizing that the crux of synthesizing sloppy product sets using non-sharp splits lies in the fact that the recovery of non-key components cannot be arbitrarily specified, which was apparently neglected by most investigators one way or another, Sophos (1981) took a completely different path to perform the separation task : only sharp separations were employed in sequences he presented.

To make use of the MAD, which was originally proposed by Nath, to create all-sharp separation sequences, he also developed some on-diagram operations. A procedure was given in his study with regard to the use of the MAD and its operations.

Muraki and Hayakawa (1985) and Muraki et al. (1986) also extended the work of Nath, and they again utilized and modified the MAD to develop sequences with the same key assumptions as Sophos, namely separators must be sharp. By using a much simplified objective function, instead of detailed costing as shown below, they searched for the sequence with the best performance of their objective function in an evolutionary approach.

$$\text{objective function} = \sum_i (L_i D_i)^{0.6} \quad [2.2 - 1]$$

where

$L_i$  = separation mass load of  $i$ th separator

$D_i$  = difficulty of  $i$ th separator

The synthesis problem using all-sharp separations was recently studied by Floudas (1987) who formulated the problem in the form of mathematical programming. A so-called superstructure, which embedded all alternative all-sharp separation configurations, was utilized to aid the formulation of the mathematical programming problem. The same objective function as equation (2.2-1) was employed throughout the examples he presented except for one example case, in which the separation mass load was used.

# CHAPTER 3 PROBLEM REPRESENTATION OF SLOPPY SEPARATIONS

In an effort to solve the sloppy multicomponent separation sequencing problem, a simple representation is first sought which allows one to effectively analyze the complex nature of the synthesis problem. A Component Assignment Diagram (CAD) is proposed that clearly elucidates the difficult synthesis task.

In this chapter, methods concerning the formation of a CAD and the arrangement of product sets on a CAD are first described, followed by the classification of possible splits in the context of a CAD. Then the use of a Separation Specification Table (SST) is introduced. At the end of this chapter, advantages of using this novel representation by CAD and SST are stressed from a comparative and pragmatic point of view.

## ***3.1 Component Assignment Diagram (CAD)***

As one would expect, the synthesis of sloppy separations is inherently much more difficult than the synthesis of sharp separations. For instance, in the case of sharp separation syn-

thesis, each split is well defined. That is, splitting of key components is fixed for all separations. This is not true for the sloppy separation synthesis, in which various degrees of component splits are possible. Furthermore, the likelihood of having stream bypass, infeasible splits, etc. needs to be efficiently identified and resolved. To that end, a Component Assignment Diagram is developed to facilitate the feasibility analysis and stream handling, which will be covered in detail in Chapter 4.

For a separation problem of interest, we are usually given desired component flow rates for each product stream, which are specified by design engineers.

In constructing a CAD to represent a given synthesis problem, all components are first placed from left to right, in an order of decreasing separation factor or relative volatility, as shown in Figure 4 on page 21. Product lines (PL) are horizontal lines in the CAD that partition each individual product, whereas vertical component lines (CL) in the CAD represent the component distribution in each product. The length of each segment of CL (in-between two adjacent PL's) should somewhat stand for the relative amount of a component in a specific product stream. It also reflects the relative amount of the same component in different product streams (if any). The flow-rate (moles/hr) information is indicated next to each product. Also, a full line, connected by two adjacent PL's, implies that a component associated with the line is the most plentiful component. In the product stream bounded by the two PL's, there must be at least one full component line. Furthermore, for convenience, one can write down the flow rate of each product on the left-hand side of a CAD, as well as all current possible splits on the right-hand side.



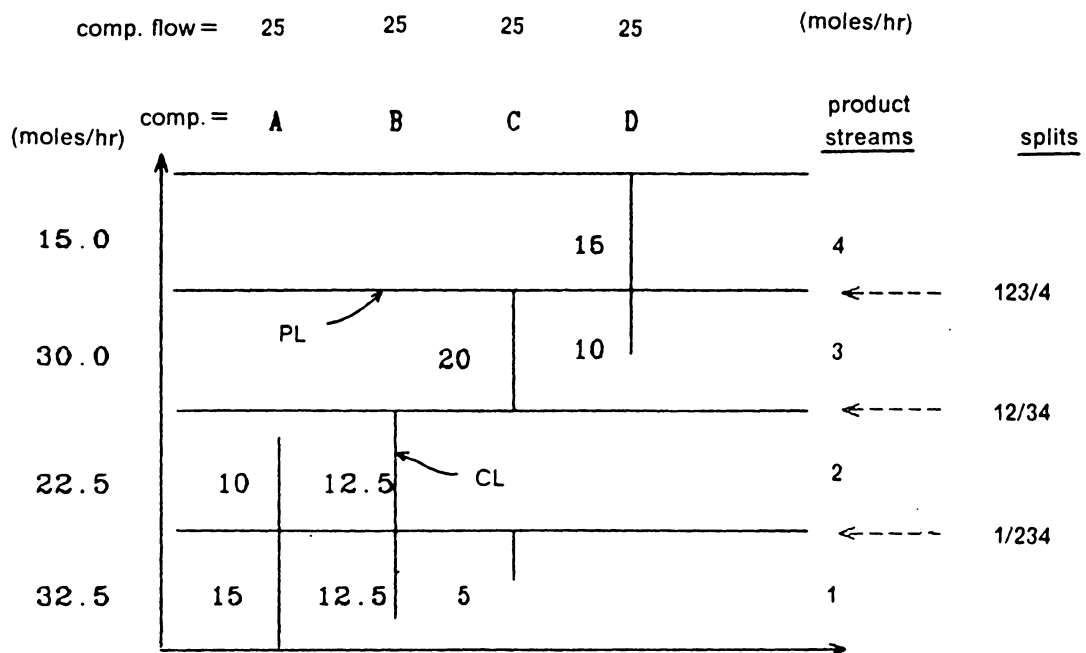


Figure 4. Component Assignment Diagram (CAD)

## 3.2 Arrangement of Product Sets

For any two products in a CAD, the product with the more volatile component(s) or more plentiful of the most volatile component is placed at a position lower than the others. This simply means that if component  $i$  is the most volatile species in two neighboring products, then those products are to be arranged in a CAD such that

$$n_{i,k} \geq n_{i,k+1} \quad [3.2 - 1]$$

where

$n$  = the component molar flow rate

$i$  = the most volatile component in two adjacent product streams on a CAD

$k$  = product stream number reflecting the position of a certain product on a CAD, counting from bottom to top

If two products have an equal amount of the most volatile component (in both products), one should pay attention to the next volatile component to decide which product is more volatile.

Again taking Figure 4 on page 21 as an example, let us start with the most volatile component, A (which exists in product streams 1 and 2), and since  $n_{A,1} > n_{A,2}$ , we can assume product stream 1 is more volatile than product stream 2. In general, this is true only when both product streams are feasible; see Chapter 4 for a detailed discussion of feasible products. We place product stream 1 in the CAD at a position lower than product stream 2. Now that we have taken care of the positions of product streams 1 and 2, we will next focus our attention on product streams 2 and 3. Figure 4 on page 21 shows that the most volatile

component existing in product stream 2 is component A; whereas component C, which is less volatile than component A, is the most volatile component in product stream 3. It is evident that product stream 2 is more volatile than product stream 3. Since product stream 2 is already in place, we will therefore put product stream 3 above product stream 2 to show the relative magnitude of the product volatility. In a similar manner, the remaining product stream, 4, can be arranged in a CAD.

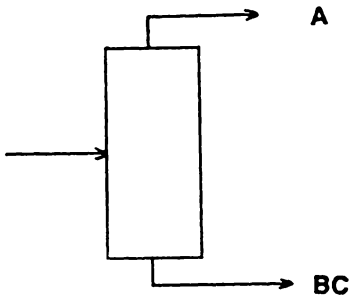
### ***3.3 Possible Splits***

Essentially two types of split can be found in a CAD. In Figure 5 on page 24, they are classified as : 1) sharp splits (or separations), and 2) sloppy splits (or separations). In order to distinguish the splits, we designate a point linking two adjacent segments of a CL as a split point (SP). It becomes apparent that when no line crosses the product line (PL) dividing two product streams (i.e., no split point), the splits are sharp (S). By contrast, in the case of sloppy splits, there is at least one split point. In this work, the fractional recovery ratio of distillate to bottoms product flow rates ( $d/b$ ) for sharp splits is set to be (0.98/0.02) or (0.02/0.98) for light-key (LK) and heavy-key (HK) components, respectively.

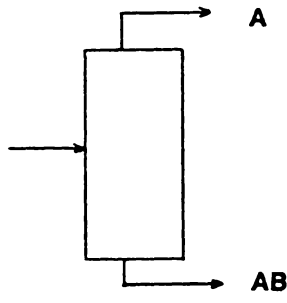
As shown in parts (b1) and (b2) of Figure 5 on page 24, sloppy splits with only one split point are termed single-split-point (SSP) sloppy splits. For sloppy splits with more than one split point, however, they are termed multiple-split-point (MSP) sloppy splits. Typical examples are given in parts (b3) and (b4) of Figure 5 on page 24 .



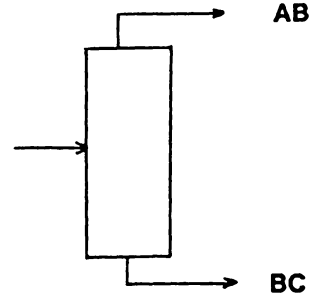
(continued)



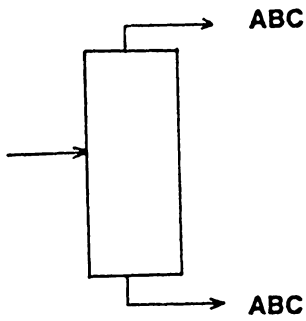
(a) sharp separation



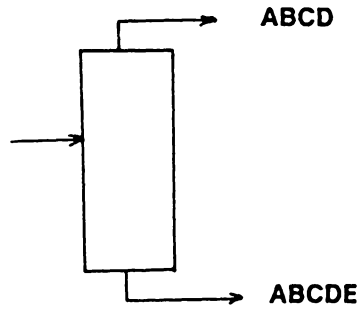
(b1) sloppy separation (SSP)



(b2) sloppy separation (SSP)



(b3) sloppy separation (MSP)



(b4) sloppy separation (MSP)

(b) Schematic Analogs of Separations in Part (a)

In this work, the sloppy separation can also be subdivided into two groups : (1) semi-sharp (SS), and (2) non-sharp (NS). One measure for differentiating SS and NS is by computing the ratio of distillate and bottoms flow rates, i.e.,  $d/b$ , for LK and HK. They are categorized in the following fashion :

**semi-sharp (SS) :**

$$1.204 \leq \log\left[\left(\frac{d}{b}\right)_{LK} \left(\frac{b}{d}\right)_{HK}\right] < 3.380 \quad [3.3 - 1]$$

where

$$3.380 = \log\left[\left(\frac{0.98}{0.02}\right)_{LK} \left(\frac{0.98}{0.02}\right)_{HK}\right]$$

**non-sharp (NS) :**

$$\log\left[\left(\frac{d}{b}\right)_{LK} \left(\frac{b}{d}\right)_{HK}\right] < 1.204 \quad [3.3 - 2]$$

where

$$1.204 = \log\left[\left(\frac{0.80}{0.20}\right)_{LK} \left(\frac{0.80}{0.20}\right)_{HK}\right]$$

Furthermore, we call certain semi-sharp splits as pseudo-sharp splits (PS) if their key-component splitting ratios satisfy the following relationships :

$$\left(\frac{d}{b}\right)_{LK} \sim 19 \text{ to } 49 \quad [3.3 - 3]$$

$\nearrow \frac{98}{4}$        $\frac{98}{2}$   
 $\searrow$

where

$$19 = \frac{0.95}{0.05} \text{ and } 49 = \frac{0.98}{0.02}$$

$$\left(\frac{d}{b}\right)_{HK} \sim 0.0204 \text{ to } 0.0526 \quad [3.3 - 4]$$

where

$$0.0204 = \frac{0.02}{0.98} \text{ and } 0.0526 = \frac{0.05}{0.95}$$

These splits can alternatively be expressed in a compact form :

$$2.558 < \log\left[\left(\frac{d}{b}\right)_{LK} \left(\frac{b}{d}\right)_{HK}\right] < 3.380 \quad [3.3 - 5]$$

### **3.4 Separation Specification Table (SST) :**

In order to examine the feasibility of splits, which will be discussed in detail in the next Chapter, a Separation Specification Table (SST) is developed in support of a CAD. An example is shown in Figure 6 on page 28. As it will become apparent, this table greatly facilitates the synthesis of separation sequences.

Essentially, an SST contains information such as the ratios of split fraction of component in the distillate to that in the bottoms, separation factor, choices of the light key (LK) and the heavy key (HK), and types of separation.

It should be noted that certain entries of (d/b) ratios are underlined in the SST of Figure 6 on page 28. Specifically, a solid horizontal line denotes an infeasible product split specification (see the next Chapter for details), while a dashed horizontal line denotes an assumed value. Double solid horizontal lines denote values calculated by using the Fenske equation (explained also in the next Chapter). In addition, a dashed vertical line designates

Separation	ovhd./btm.	LK/HK	$\Delta^\circ\text{C}$	$\frac{d}{b} \Big _{LLK1}$	$\frac{d}{b} \Big _{LK}$	$\frac{d}{b} \Big _{HK}$	$\frac{d}{b} \Big _{HHK1}$
SS(MSP)	1/2	A/B	30.2		<u>0.974</u>	<u>0.026</u>	<u>0.203</u>
					<u>0.026</u>	<u>0.974</u>	<u>0.797</u>
SS(SSP)	2/3	B/C	11.3	<u>0.98</u>	<u>0.90</u>	<u>0.02</u>	
				<u>0.02</u>	<u>0.10</u>	<u>0.98</u>	
SS(MSP)	3/4	C/D	28.3	<u>0.80</u>	<u>0.88</u>	<u>0.05</u>	<u>0.25</u>
				<u>0.20</u>	<u>0.12</u>	<u>0.95</u>	<u>0.75</u>
NS(MSP)	4/5	D/E	8.2	<u>0.90</u>	<u>0.60</u>	<u>0.30</u>	<u>0.17</u>
				<u>0.10</u>	<u>0.40</u>	<u>0.70</u>	<u>0.83</u>

Figure 6. Example of Separation Specification Table (SST): solid horizontal lines denote infeasible product splits; dashed horizontal lines denote assumed values; Double solid horizontal lines denote values calculated by using the Fenske equation; dashed vertical lines designate boundaries between LK and HK.



the boundary between LK and HK, with the component to the left of this line being the LK, and the one to the right being the HK.

## 3.5 Discussion

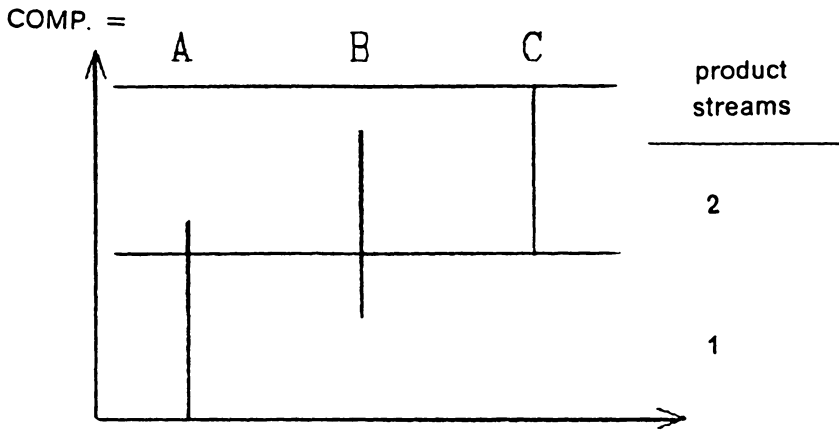
Like other process-synthesis problems such as the synthesis of heat-exchanger network, a successful sloppy-separation synthesis strategy must be established on a framework (or problem representation structure) that is flexible enough to encompass a fair number of alternative solutions (or sequences), and yet explicit enough to eliminate infeasible ones.

Compared with the Material Allocation Diagram (MAD) introduced by Nath (1977), the problem representation presented in this chapter offers the following advantages:

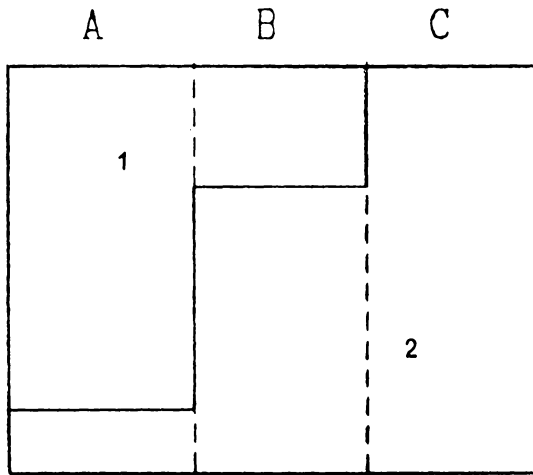
1. Characteristics of various types of sharp and sloppy split are more clearly stated in a quantitative sense.

For example, in defining a non-sharp split such as the one pictured in part (a) of Figure 7 on page 31, all it takes to characterize this type of split is to check equation (2.3-2) and use a CAD. Note that equation (2.3-2) gives the criterion for a non-sharp split based on a logarithmic term that indicates the quantitative effect of sloppiness of key components on the minimum number of ideal stages,  $N_{min}$ . By contrast, the proper representation of the same split in an MAD, such as that shown in part (b) of Figure 7 on page 31 depends a great deal on the topology of the MAD. The latter also lacks a quantitative basis as in a CAD.

2. The proposed problem representation is free of many cumbersome manipulations frequently required to make an MAD more recognizable.



(a) CAD



(b) MAD

Figure 7. Different Problem Representations of Non-sharp Splits: (a) CAD ; (b) MAD

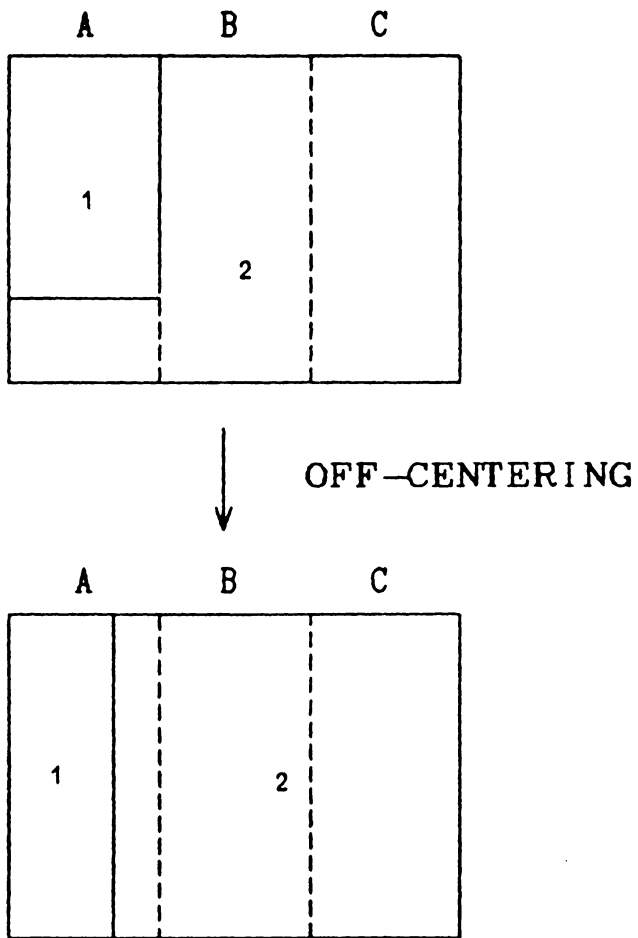


Figure 8. Off-Centering Operation on MAD

Diagrammatical manipulations an MAD such as off-centering (see Figure 8 on page 32 ) are not straightforward to apply and often cause unnecessary confusion.

3. In terms of the multitude of the sloppy splits being treated, this work is more inclusive.

Multiple-split-point (MSP) sloppy splits, as illustrated in parts (b3) and (b4) of Figure 5 on page 24 and section 4.3, have never been explored by other investigators. The present study incorporates them into the solution domain. In addition, the feasibility of such splits is studied (see the next chapter).

# **CHAPTER 4 FEASIBILITY ANALYSIS OF SLOPPY SEPARATIONS**

The purpose of the present study is to synthesize multicomponent sloppy product sets with the emphasis on incorporating sloppy splits. This is the major difference between our work and the studies by the majority of other investigators, who adopted the approach of employing sharp separations only. However, using sloppy separations has inevitably complicated the synthesis process in the sense that a feasibility analysis must be conducted.

Since not all splits in a component assignment diagram (CAD) are feasible, it becomes necessary to look for a basis to sort them out. This will be treated first in Chapter 4. In the section that follows, the technique of using stream bypassing is described. Next, rules concerning the selection of light and heavy key components are given. They differ from the conventional way of selecting keys for sharp separations. Product split specifications are discussed in Section 4.4 . Finally, transformation techniques needed to convert CADs containing infeasible splits into equivalent feasible product sets are presented.

## 4.1 Infeasible Splits

In order to analyze the characteristic of a chosen split, one should analyze the feasibility of the split. Prior to this analysis, one needs to : (a) calculate the ratio the  $i$ th component flow rate in the distillate  $d_i$  to that in the bottoms  $b_i$  for all components that exist in both distillate and bottoms products; and (b) set  $d_i + b_i = 1$  . Consider, for example, an  $n$ -component feedstock (say, components 1,2,3,..., and  $n$ , in order of decreasing relative volatilities). The splits associated with these components are said to be feasible provided that

$$d_1 > d_2 > d_3 > \dots > d_n \quad [4.1 - 1]$$

or

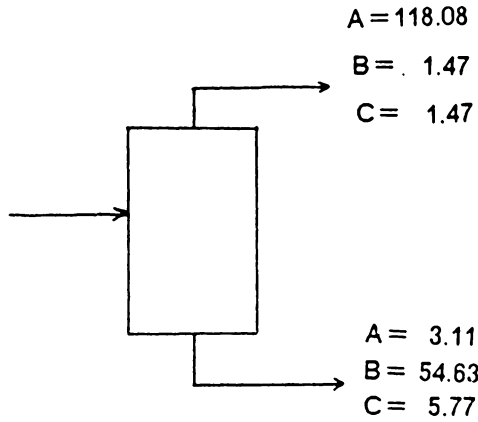
$$b_1 < b_2 < b_3 < \dots < b_n \quad [4.1 - 2]$$

To verify equation (4.1-1), one should first examine the well-known Fenske equation (Fenske, 1932), in which the minimum number of ideal stages,  $N_{\text{MIN}}$  and the logarithm of the relative volatility between light and heavy key components,  $\log \alpha_{\text{LK,HK}}$  are both positive. Thus,

$$\log \left[ \left( \frac{d}{b} \right)_{\text{LK}} \left( \frac{b}{d} \right)_{\text{HK}} \right] > 0 \quad [4.1 - 3]$$

Replace  $b_{\text{LK}}$  and  $b_{\text{HK}}$  by  $(1 - d_{\text{LK}})$  and  $(1 - d_{\text{HK}})$ , respectively to yield

$$d_{\text{LK}} (1 - d_{\text{HK}}) > (1 - d_{\text{LK}}) d_{\text{HK}} \quad \text{or} \quad d_{\text{LK}} > d_{\text{HK}} \quad [4.1 - 4]$$



(a) An Infeasible Fractionation

	A	B	C	product streams	(moles/hr)
				2	( 63.51)
	3.11	54.63	5.77		
	118.08	1.47	1.47	1	( 121.02)

$$\left(\frac{d}{b}\right)_A = \frac{118.08}{3.11} = \left(\frac{0.9743}{0.0257}\right) \quad \left(\frac{d}{b}\right)_B = \frac{1.47}{54.63} = \left(\frac{0.0262}{0.9738}\right) \quad \left(\frac{d}{b}\right)_C = \frac{1.47}{5.77} = \left(\frac{0.2030}{0.7970}\right)$$

(b) Corresponding CAD Showing an Infeasible Split

Figure 9. A Portion of a CAD Representing an Infeasible Split:  $(d_B < d_C$  and  $b_B > b_C$ ).



Since a component with a smaller flow rate can be considered as LK and that with a higher flow rate as HK, we see that equation (4.1-4) is equivalent to the general expression (4.1-1).

Shown in Figure 9 on page 36 are two product streams in a CAD. The more volatile product, A, is the distillate if a fractionation of a feedstock composed of a mixture of products A and B is performed so as to make a cut between products A and B. The less volatile product B is the bottoms stream. From the figure, one can easily conclude that the split in Figure 9 on page 36 is infeasible since  $d_B < d_C$  and  $b_B > b_C$  which violate the criterion given in eq. (4.1-1) and eq. (4.1-2), respectively.

## ***4.2 Possibility of Bypassing***

How does one identify the possibility of bypassing? If product streams contain the same components as those in the feed streams, then bypassing can be performed on the feed to reduce the mass load of downstream separation operations.

Despite the fact that a larger bypass can result in a lower mass load for a downstream fractionation unit, it also leads to the use of a sharper separation, which requires higher capital and operating costs. An economic trade-off is therefore involved with the amount of bypass chosen. An optimum bypass can be obtained through rigorous optimization techniques.

An optimum bypass is our concern here. For the purpose of creating initial sequences, bypassing corresponds to 90 percent of the least plentiful component (in terms of percentage) in the "all-component" inclusive product (note that this component should be present in more than one product stream).

COMP. =	A	B	C	product streams
	10-a	12-b	5-c	2
	15	8		1

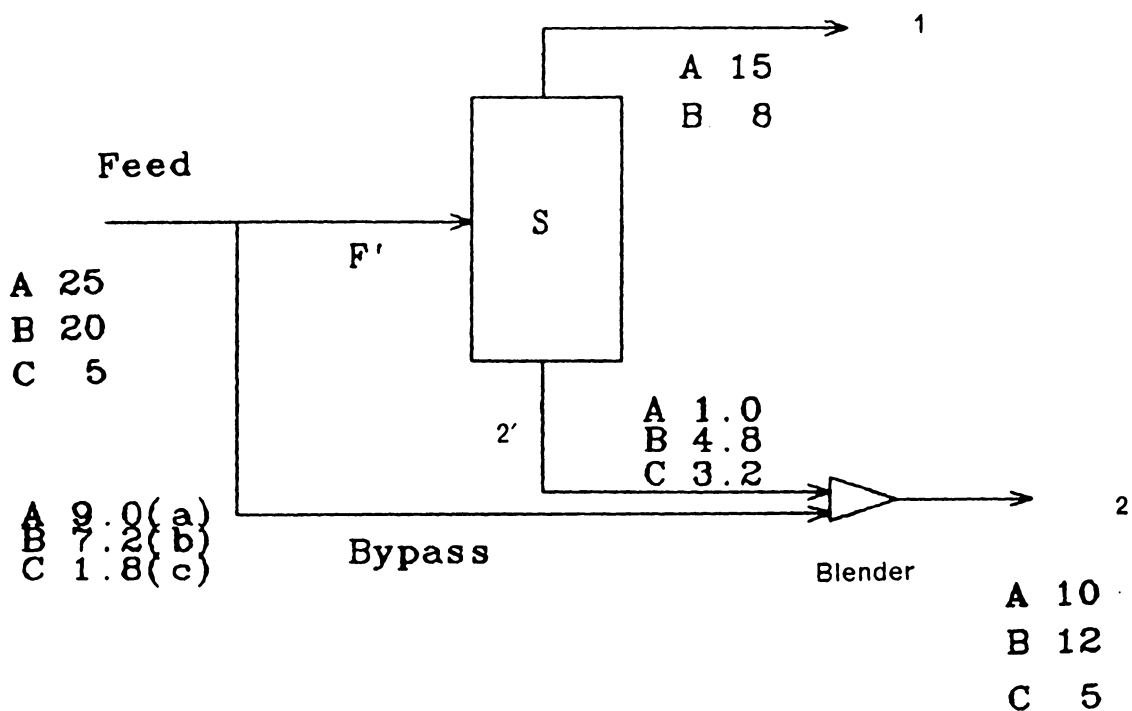


Figure 10. An Illustration of Bypass

A representative bypassing situation is illustrated in Figure 10 on page 38, where a CAD is given for a desired product set, together with a schematic flowsheet resulting from bypassing. In this example, product stream 2 corresponds to the "all-component" inclusive product since it contains the same components as those in the feed stream (i.e., the mixture of product streams 1 and 2). Also, component A is the least plentiful component in product 2 that distributes itself in both products. Therefore, a bypassing basis can be set such that :

90% of A in product stream 2 bypasses the fractionation tower S

$$= 90\% \cdot (10 \text{ moles/hr})$$

$$= 9 \text{ (moles/hr)}$$

Since compositions of the feed, stream F', and bypass stream are identical,

$$\text{mole \% A} = \frac{25}{25 + 20 + 5} = \frac{a}{a + b + c} = \frac{25 - a}{(25 - a) + (20 - b) + (5 - c)} \quad [4.2 - 1]$$

$$\text{mole \% B} = \frac{20}{25 + 20 + 5} = \frac{b}{a + b + c} \quad [4.2 - 2]$$

Solving for b and c, one finds

$$b = 7.2, c = 1.8$$

Thus, material flows of the system can be determined. They are shown in Figure 10 on page 38 .

## 4.3 Choice of Light and Heavy Key (LK and HK)

### Components

The conventional way to define light and heavy key components is valid for sharp separations. Key components are commonly described by the statement (Coulson et al., 1980) "light key (LK) is the lightest component appearing in the bottoms and heavy key (HK) is the heaviest component in the distillate". When dealing with sloppy separations, this definition is not adequate to identify key components. For example, by applying the definition to the split in part (a) of Figure 11 on page 42, one ends up with C=LK and C=HK. Consequently, a set of rules for properly identifying key components for sloppy separations is required.

#### Rule 1:

*Most splits have a distinctive discontinuity of the ratio (d/b).*

e.g.

$$\text{component} = \quad A \quad B \quad C \quad D$$

$$\left(\frac{d}{b}\right) = \frac{0.99}{0.01} \quad \frac{0.975}{0.025} \quad \frac{0.025}{0.975} \quad \frac{0.01}{0.99}$$

Here, we observe a discontinuity of (d/b) between components 2 and 3, since  $d_A > b_A$  and  $d_B > b_B$ , while for components C and D,  $d_C < b_C$  and  $d_D < b_D$ . Thus, a vertical dashed discontinuity line can be drawn between components B and C. Two components immediately adjacent to that line whose distribution ratios are

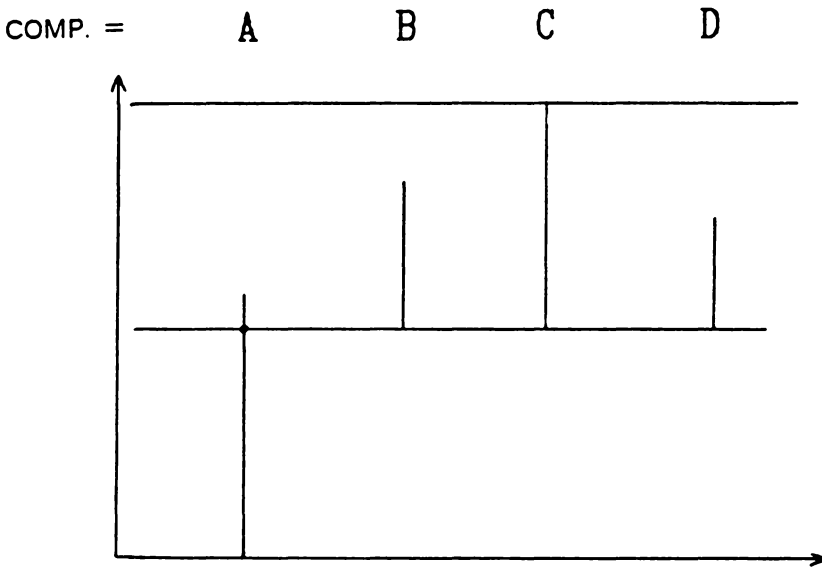
within the range of the pseudo-sharp splits defined by equations (3.3-3) to (3.3-5) are treated as key components (LK = B and HK = C, in this case).

**Rule 2:**

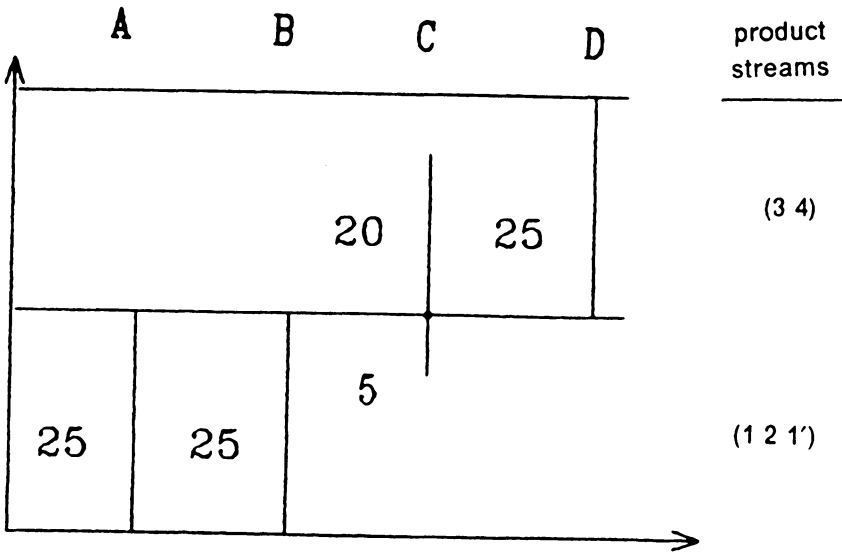
*For a single-split-point (SSP) sloppy separation whose split point (in a CAD) corresponds to the most volatile or least volatile component in association with that split, keys are the distributed component and its neighboring component. For other types of single-split-point (SSP) sloppy separations, there exist several possible choices of LK/HK.*

The former split given in the rule is shown in part (a) of Figure 11 on page 42. From the rule, one finds that keys are A (LK), and B (HK). In what follows, we will discuss the possibilities of having several choices of LK/HK for splits in the latter group.

Consider, for example, split 1 2 1' / 3 4 to be used in Example 1 of Chapter 6, which has been redrawn in part (b) of Figure 11 on page 42, as an illustration. In this case, possible candidates of LK/HK are - B/C, C/D, and B/D. These possibilities are subjected to testing by the Fenske equation. Specifically, on a plot of  $\log(d/b)$  vs.  $\log \alpha$ , one draws a straight line passing through the data points that correspond to the proposed key components and compares the difference between the resulting non-key distributions and the desired non-key distributions. In the present study, it is assumed that the desired distribution ratio  $(d/b)$ 's of nondistributed components are prescribed to be no less than (0.98/0.02) for lighter-than-light-key components (LLK), and no greater than (0.02/0.98) for heavier-than-heavy-key components (HHK).



(a) A Single-Split-Point (SSP) Sloppy Split Whose Split Point Corresponds to the Most Volatile Component



(b) A Single-Split-Point (SSP) Sloppy Split Whose Split Point Does Not Correspond to the Most or Least Volatile Component Example 1 of Chapter 6.

Figure 11. Portions of CAD Representing Single-Split-Point (SSP) Sloppy Separations

COMPONENT DISTRIBUTIONS OF  
SLOPPY DISTILLATION SEPARATION  
FROM RIGOROUS SIMULATIONS

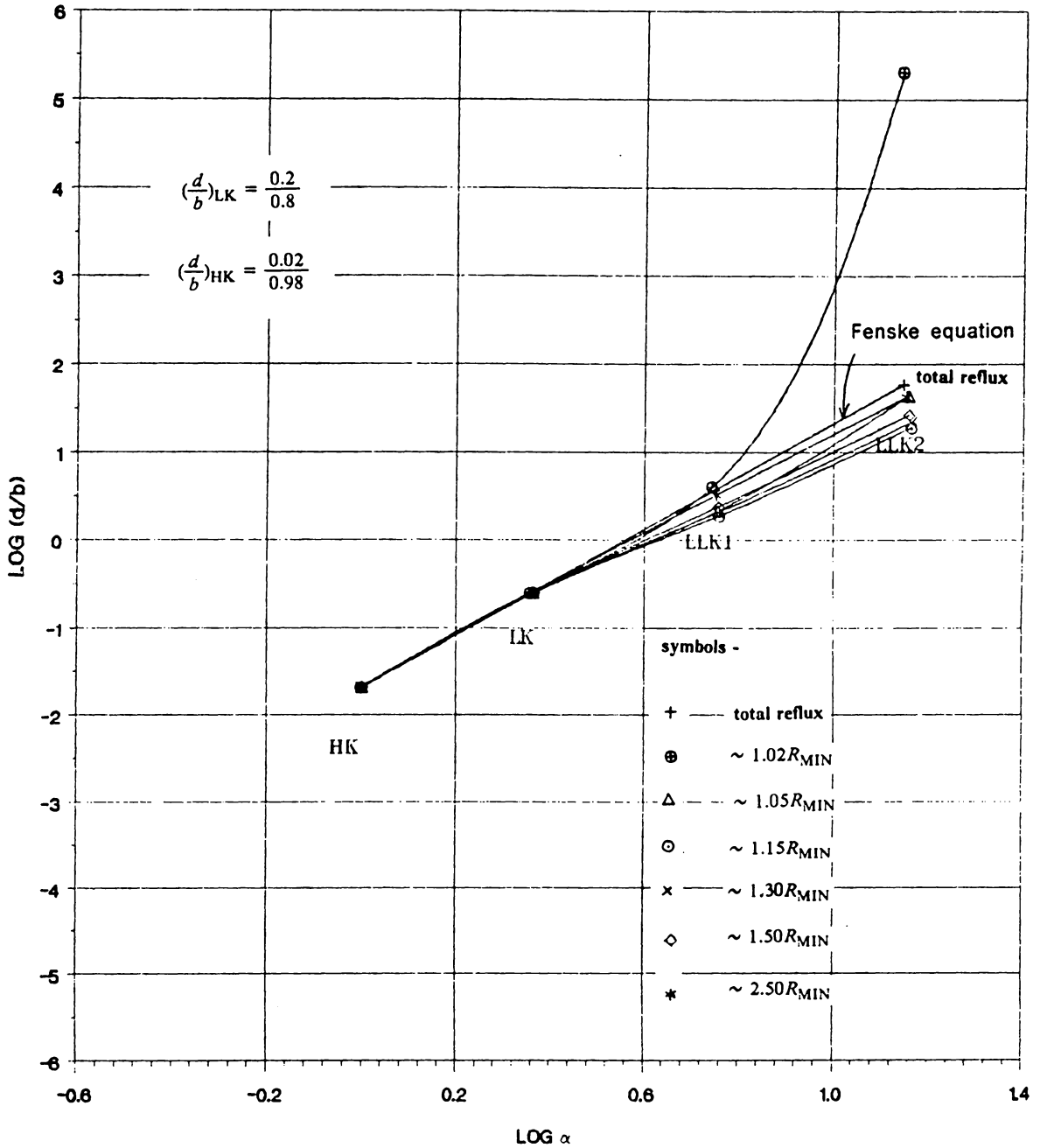


Figure 12. Component Distributions of SSP Sloppy Separation: Example 1 of Chapter 6

**COMPONENT DISTRIBUTIONS OF  
SLOPPY SEPARATION  
FROM RIGOROUS SIMULATIONS**

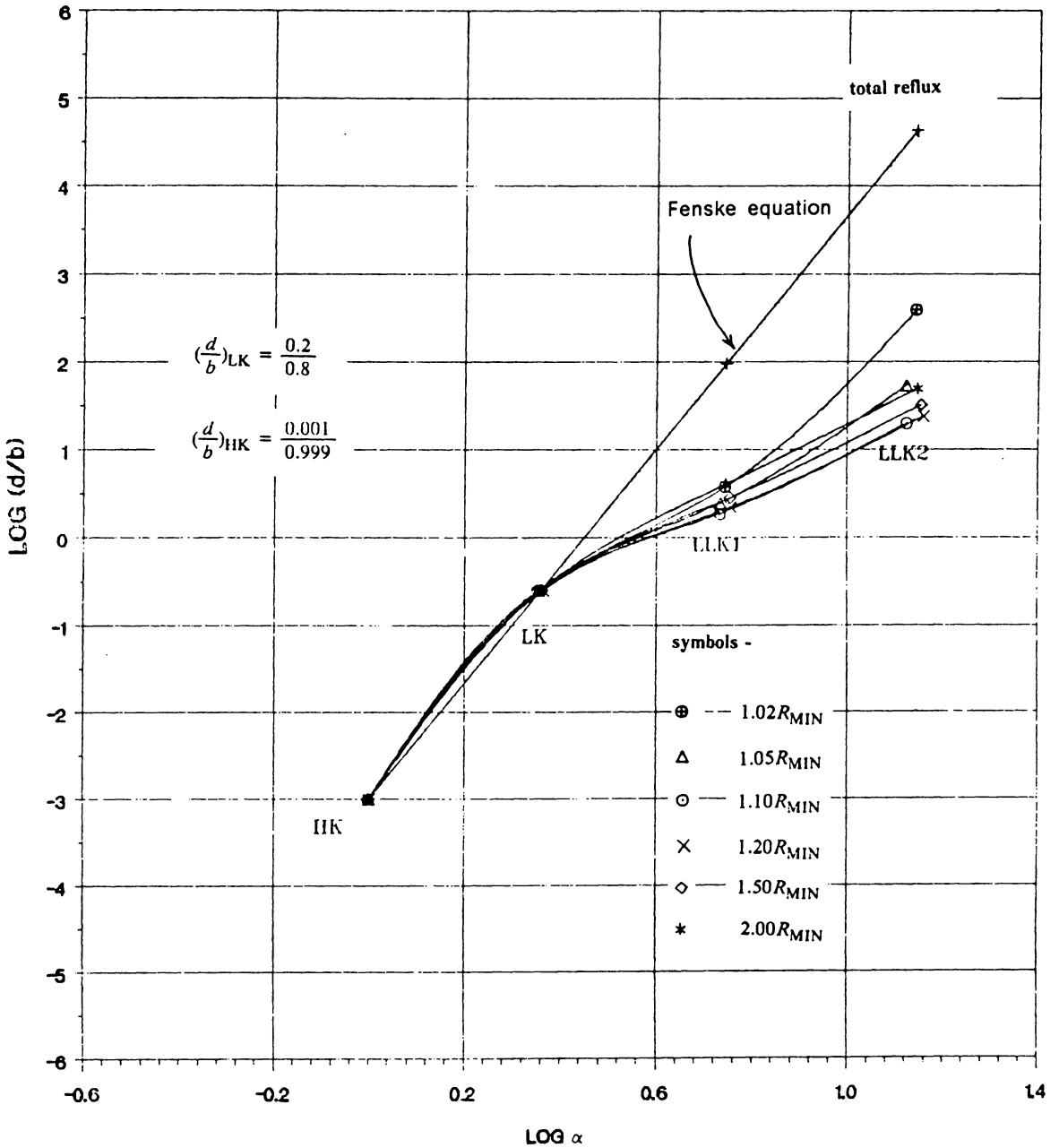


Figure 13. Component Distributions of SSP Sloppy Separation: Example 1 of Chapter 6



Figure 12 on page 43 and Figure 13 on page 44 show that the distribution ratio (d/b) of LLK1 (i.e., component B) for the case of LK/HK = C/D predicted by the Fenske equation gives misleading information when the recovery basis of sharp-heavy key (i.e., a heavy key that is sharp) jumps from (d/b) = (0.02/0.98) to (0.001/0.999) , compared with actual non-key distributions from rigorous plate-to-plate simulation results. In Figure 13 on page 44, the distributions of non-keys at various reflux ratios are far off the distribution predicted by the Fenske equation. While the distributions of non-keys in Figure 12 on page 43 agree favorably with that given by the Fenske equation. One may find that the recovery ratio of LLK2 at 1.02  $R_{MIN}$  is well above the predicted value. However, this case can be ignored by the fact that it is an extreme case ( $\sim R_{MIN}$ ) for which an uneconomical large number of equilibrium stages is required, and that accordingly it cannot reflect the normal operating condition. (note : the justification and procedure of rigorous distillation simulation are detailed in Appendix A.) LK/HK set C/D must be removed from the list of the choice of LK/HK on the ground that rigorous simulation results demonstrate that LLK1 is distributed unavoidably and undesirably.

In summary, for the purpose of examining non-key distributions, (d/b) = (0.98/0.02) or (0.02/0.98) will be used henceforth as the distribution ratios for LK and HK, respectively.

**Rule 3:**

*For multiple-split-point (MSP) sloppy separations, component distributions resulting from different sets of LK/HK should also be examined by the Fenske equation.*

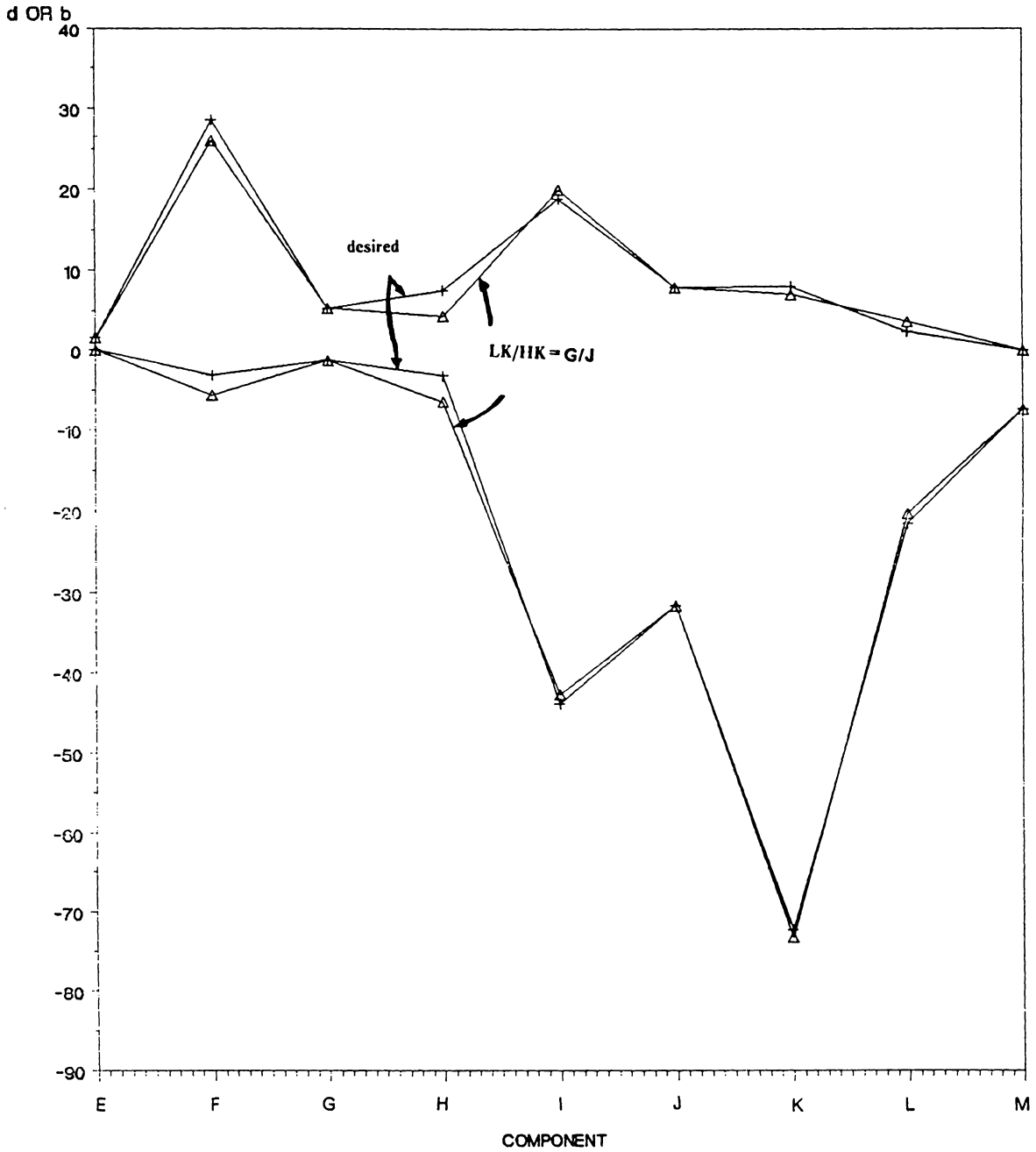
split	$\frac{evhd}{btm}$	LK/HK	$\frac{d}{b} _6$	$\frac{d}{b} _6$	$\frac{d}{b} _7$	$\frac{d}{b} _8$	$\frac{d}{b} _8$	$\frac{d}{b} _{10}$	$\frac{d}{b} _{11}$
desired	6/7		$\frac{0.999}{0.001}$	$\frac{0.9}{0.1}$	$\frac{0.8}{0.2}$	$\frac{0.7}{0.3}$	$\frac{0.3}{0.7}$	$\frac{0.2}{0.8}$	$\frac{0.1}{0.9}$
shortcut	6/7	H/I		$\frac{0.9998}{0.0002}$	$\frac{0.9998}{0.0004}$	$\frac{0.7}{0.3}$	$\frac{0.3}{0.7}$	$\frac{0.031}{0.969}$	$\frac{0.0007}{0.9993}$
shortcut	6/7	G/J	$\frac{0.978}{0.024}$	$\frac{0.82}{0.18}$	$\frac{0.8}{0.2}$	$\frac{0.4}{0.6}$	$\frac{0.318}{0.682}$	$\frac{0.2}{0.8}$	$\frac{0.087}{0.913}$
shortcut	6/7	F/K	$\frac{0.99}{0.01}$	$\frac{0.9}{0.1}$	$\frac{0.88}{0.14}$	$\frac{0.48}{0.54}$	$\frac{0.377}{0.623}$	$\frac{0.258}{0.742}$	$\frac{0.1}{0.9}$

Table 2. Separation Specification Table for a Split in Example 2 of Chapter 6

Figure 14. COMPONENT DISTRIBUTIONS  
 IN RELATION TO CHOICES OF LK AND HK  
 DESIRED VS. LK=G HK=J  
 d = distillate flow (+) b = bottoms flow (-)

COMP. FLOWS

Example 2 of Chapter 6



Take split 6/7 in Example 2 of Chapter 6 as an example. As shown in Table 2 on page 46, choices of LK and HK such as H/I and F/K for that split generate larger deviations in mass flows from the desired separation than that of LK/HK = G/J (see Figure 14 on page 47) Consequently, components G and J will be chosen as LK and HK, respectively.

Comp.	$\alpha$	Feed (mole/hr)	Top (mole/hr)	Bottoms (mole/hr)
A	7.00	20.0	20.0	-
B	5.80	35.0	35.0	-
C1	3.97	280.0	-	-
C2	3.80	76.0	343.5(C1,C2)	12.5(C1,C2)
D1	2.18	350.0	68.9(D1,D2,D3)	504.1(D1,D2,D3)
D2	2.02	125.0	-	-
D3	1.89	98.0	-	-
E	0.35	60.0	-	60.0

It is worthwhile to mention that it is possible to have products with special purity specifications such as the one shown above. In the table, the values of relative volatilities of several near-key components are so close to (within 30%) those of "apparent" keys (i.e., LK-C2, HK-D1) that product requirements with combined yield rates for these components, including keys, are likely to be used.

Under these circumstances, we employ the concept of "lumped-keys" to specify the desired separation. Specifically, by using the procedure described below (modified and improved from Hengstebeck, 1976), we find the relative volatilities of the lumped-keys:

1. Assume that at normal operating conditions, the distributions of all components contained in the lumped-keys can be predicted by the Fenske equation. Thus, the relationships between the fractional recoveries and relative volatilities of components can be expressed by the following equation :

$$\log\left(\frac{d_i}{f_i - d_i}\right) = N_{\min} (\log\alpha_i) + l \quad [4.3 - 1]$$

where

$f$  = feed rate, mole/hr

$l$  = constant

2. Note that there are two key unknowns in the above equation (i.e.,  $N_{\min}$  and  $l$ ). One solves for them by imposing the following two conditions : (a) the sum of flow rates of components included in the lumped-light key meets the specified value, and (b) the sum of flow rates of components included in the lumped-heavy key meets the specified value :

$$\sum_{l_{pk}=1}^{n_{lk}} d_{l_{pk}} = 343.5 \quad [4.3 - 2]$$

$$\sum_{l_{phk}=1}^{n_{hk}} d_{l_{phk}} = 68.9 \quad [4.3 - 3]$$

where

$l_{plk}$  = component grouped by the lumped-light key

$l_{phk}$  = component grouped by the lumped-heavy key

$n_{lk}$  = number of components constituting the lumped-light key

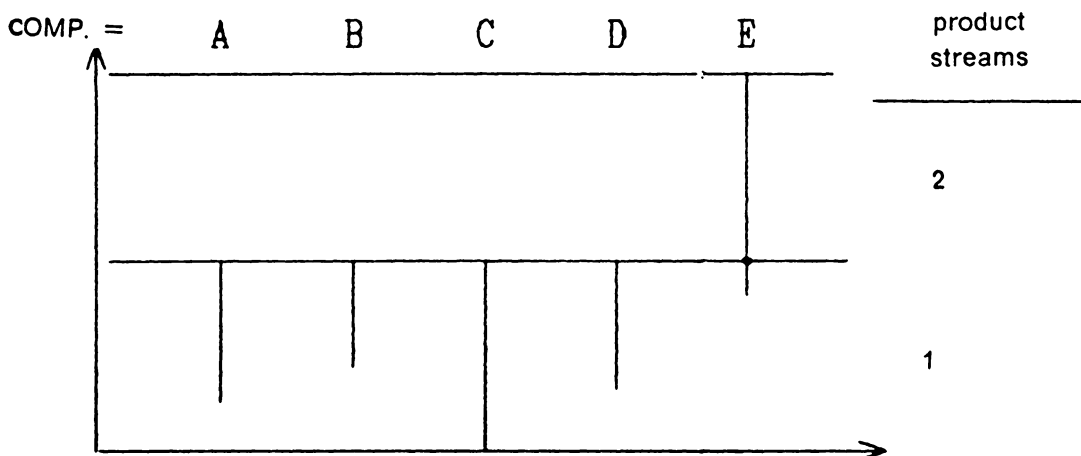
$n_{hk}$  = number of components constituting the lumped-heavy key

3. Substituting the recovery ratios of lumped-keys into equation (4.3-1), we obtain the relative volatilities of lumped-keys. In this example, it can be found that  $N_{min} = 8.5460$ ,  $l = -3.6385$ , and  $\alpha_{LK,HK} = 1.86$ . The relative volatilities of the lumped-light key and lumped-heavy key are, in effect, the characteristics (i.e., difficulty of the split from a physical property standpoint) of this particular split.

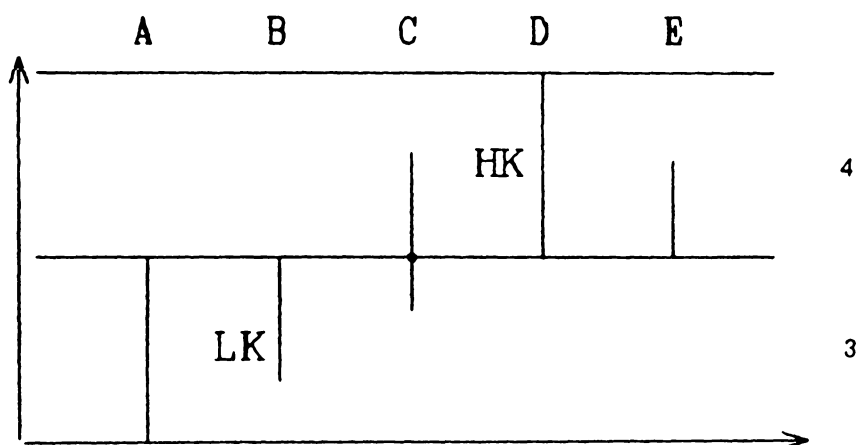
## 4.4 Product Split Specifications

We now discuss several types of SSP, some of which are always feasible, whereas others are only feasible for specific problems. For example, the sloppy split shown in part (a) of Figure 15 on page 52 is always feasible, since we can always specify the distribution ratio  $(d/b)$  of component D (LK), which is set to be  $(d/b)_{LK} = 0.98/0.02$ , and that of component E (HK) without worrying about whether non-key components (or LLK in this case) are distributed. By contrast, for sloppy splits such as the one shown in part (b) of Figure 15 on page 52, it is important to consider the feasibility of the split. Assume that components B and D are chosen as LK and HK, respectively. The distribution ratio  $(d/b)$  of intermediate component C is rather sensitive to the change of the operating reflux ratio of the distillation column. Therefore, we rule out this choice of LK and HK except for a rare situation in which only a negligibly small amount of intermediate component exists in the products. Other pairs of LK and HK, such as B (LK) / C (HK) and C (LK) / D (HK), are used instead (refer to section 4.3 for the choice of LK and HK).

King (1980) summarized the findings of Stupin and Lockhart (1968) and plotted  $\log(d/b)_i$  vs.  $\log \alpha_i$  (see Figure 16 on page 53). As King described, the distribution of components behaved in such a way that at reflux ratios ranging from  $1.2 R_{\min}$  to  $1.5 R_{\min}$ , the component distribution curves approximated the distribution at  $R_{\infty}$ . Furthermore, at reflux ratios lower than  $1.2 R_{\min}$ , those curves had a tendency to approach the distribution curve at  $R_{\min}$ . However, it should be emphasized here that the plot is good for cases where both keys are pseudo-sharp.



(a) A CAD - always feasible



(b) A CAD - not always feasible

Figure 15. CAD's for Different Types of SSP



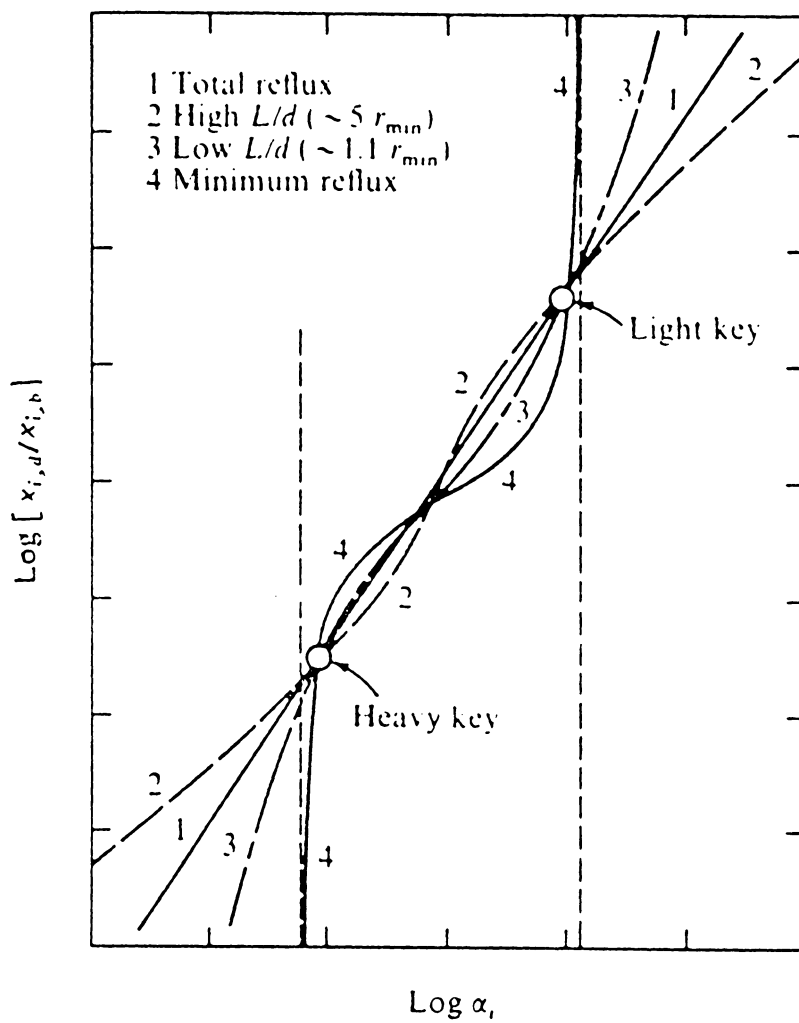


Figure 16. Distribution of Components at Various Reflux Ratios (King, 1980)

By close inspection of Figure 16 on page 53, one finds that at common operating reflux conditions (i.e.,  $R < 1.5R_{\min}$ ),

- for LLK :

$$\left(\frac{d}{b}\right)_{LLK} > \left(\frac{d}{b}\right)_{LLK, LB} \quad [4.4 - 1]$$

where

LB = a lower bound predicted by the Fenske eqn.

if the desired condition is - LLK to be non-distributed, i.e.,

$$\left(\frac{d}{b}\right)_{LLK} > \left(\frac{0.98}{0.02}\right) \quad [4.4 - 2]$$

Hence, the Fenske equation provides us with a lower bound for  $(d/b)_{LLK}$ ; that is, if  $(d/b)_{LLK, LB} > (0.98/0.02)$ , component LLK is said to be non-distributed.

- for HHK :

$$\left(\frac{d}{b}\right)_{HHK} < \left(\frac{d}{b}\right)_{HHK, UB} \quad [4.4 - 3]$$

or

$$\left(\frac{b}{d}\right)_{HHK} > \left(\frac{b}{d}\right)_{HHK, UB} \quad [4.4 - 4]$$

where

UB = an upper bound predicted by the Fenske eqn.

if the desired condition is - HHK to be non-distributed, i.e.,

$$\left(\frac{b}{d}\right)_{HHK} > \left(\frac{0.98}{0.02}\right) \quad [4.4 - 5]$$

Likewise, the Fenske equation provides us with an upper bound for  $(d/b)_{HHK}$  (i.e., if  $(d/b)_{HHK,UB} < (0.02/0.98)$ , component HHK is said to be non-distributed).

Oftentimes, unmatched non-key distributions are encountered. In most instances, those unmatched distributions can nevertheless be accepted because many products associated with those splits are fuels. However, the emphasis should be placed on the economic gain or loss as a result of the unmatched product streams. This means that the unmatched products may have been upgraded or downgraded. Consequently, the economic gain or loss is often to be investigated for the case considered above. Using these arguments, we are in a position to deal with the afore-mentioned splits without any difficulty.

Additionally, since prior knowledge of relative volatilities is involved in evaluating approximate values of non-key distributions for a specific separation through the Fenske equation, one can do it by first using the conventional way to establish the column operating pressure for that split (see Figure 17 on page 56) , followed by making a bubble-point calculation for feed compositions at the column pressure to obtain the feed temperature, and finally computing the relative volatility for each component at the feed condition.

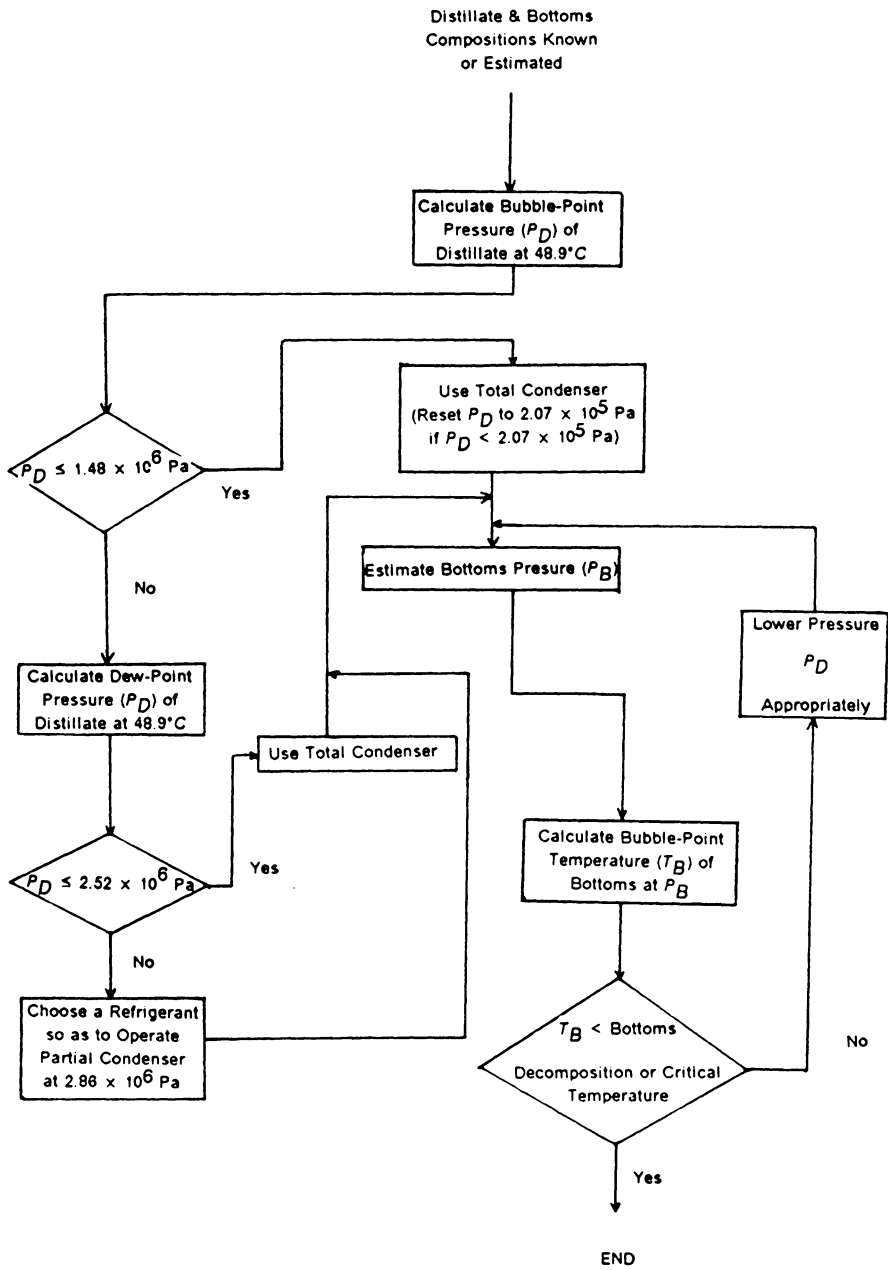


Figure 17. Scheme for Distillation Column Pressure Selection (Henley and Seader, 1981)

COMPONENT DISTRIBUTIONS OF  
SLOPPY DISTILLATION SEPARATION  
FROM RIGOROUS SIMULATIONS

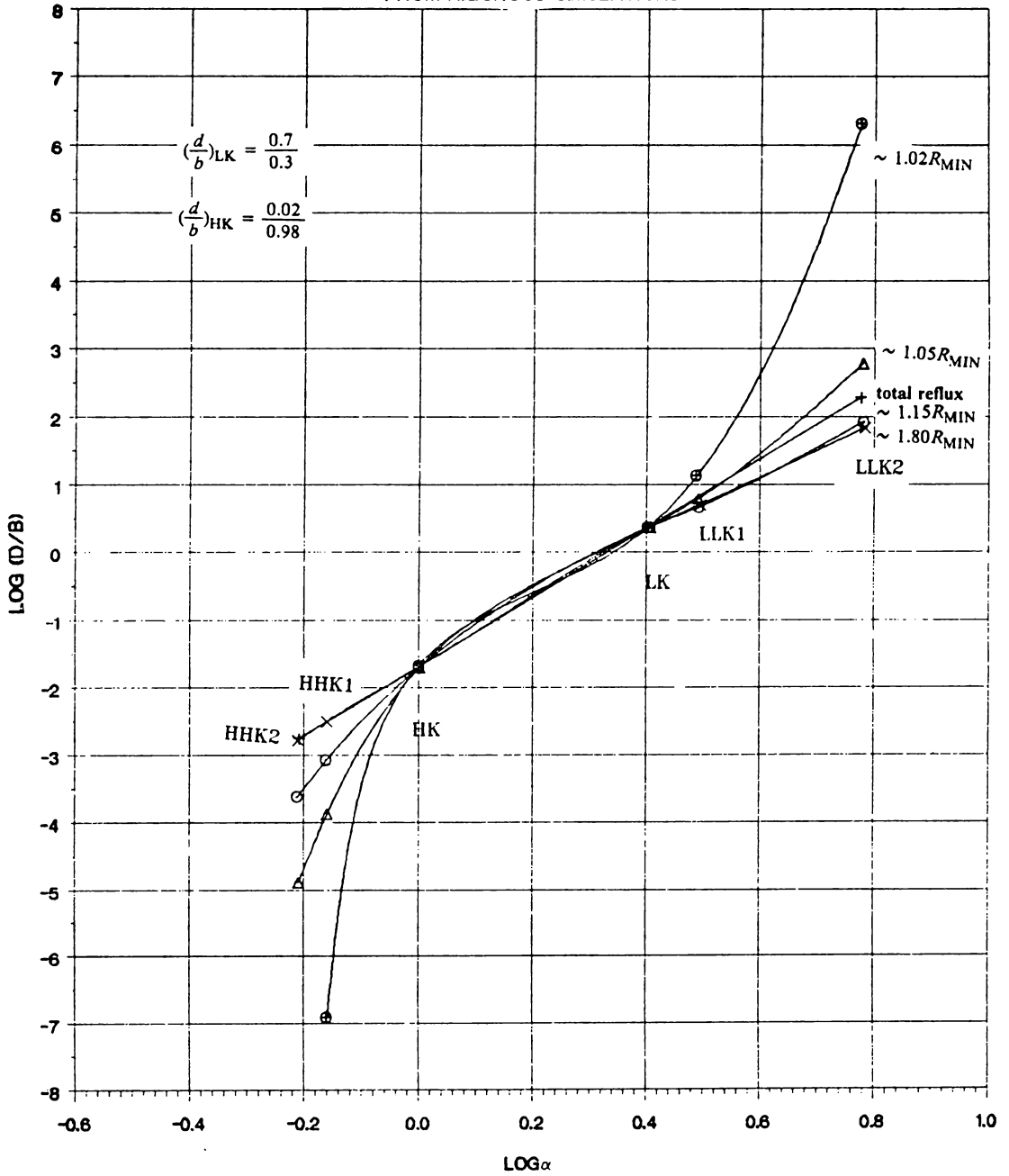


Figure 18. Component Distributions of Semi-Sharp Distillation (SSP)

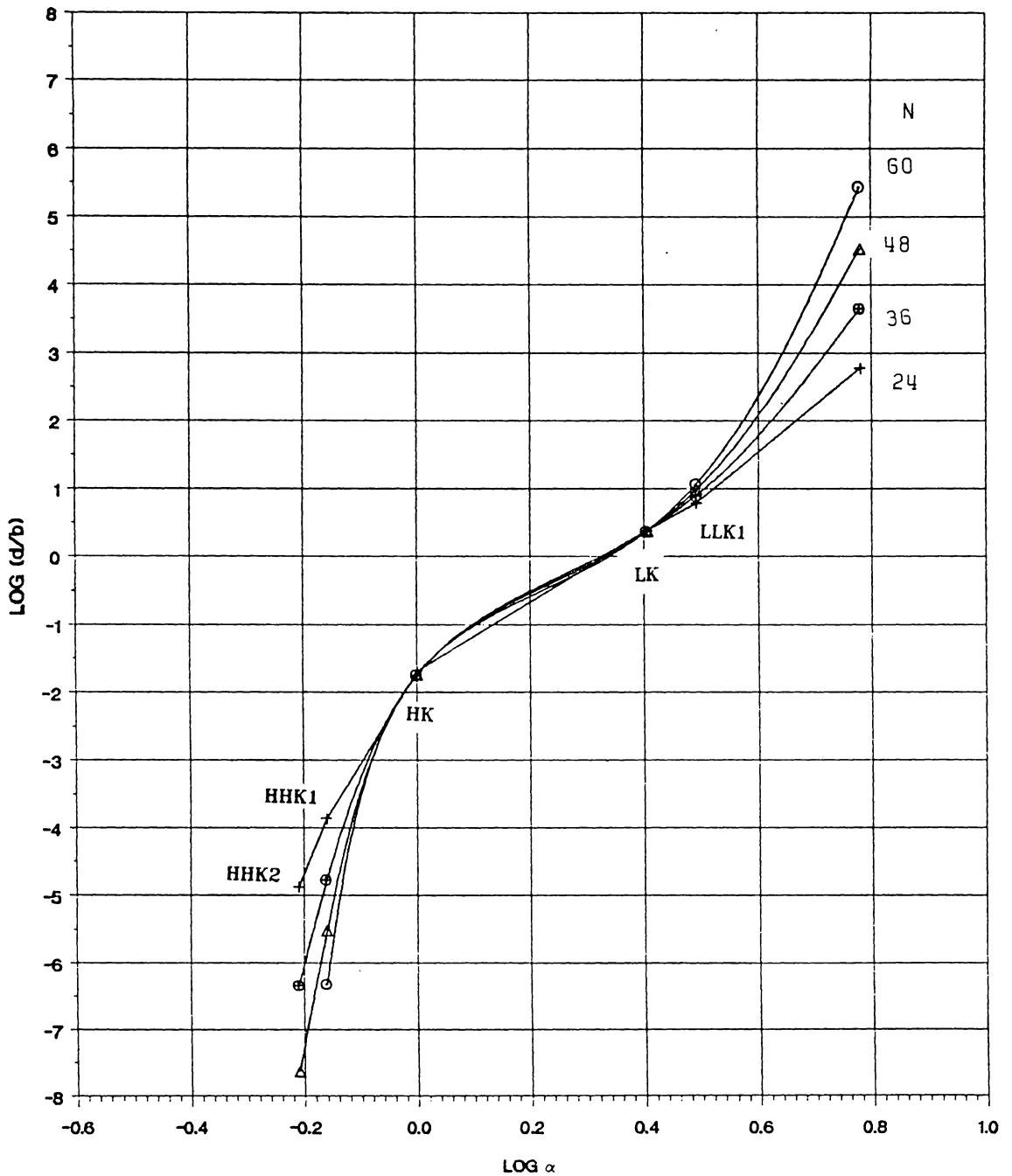


Figure 19. Effect of the Number of Ideal stages  $N$  on Non-Key Distributions at Constant Operating Reflux Ratio  $R$ :  $R = 0.815$ , (D/B) of LK =  $0.7/0.3$ , (D/B) of HK =  $0.02/0.98$ .

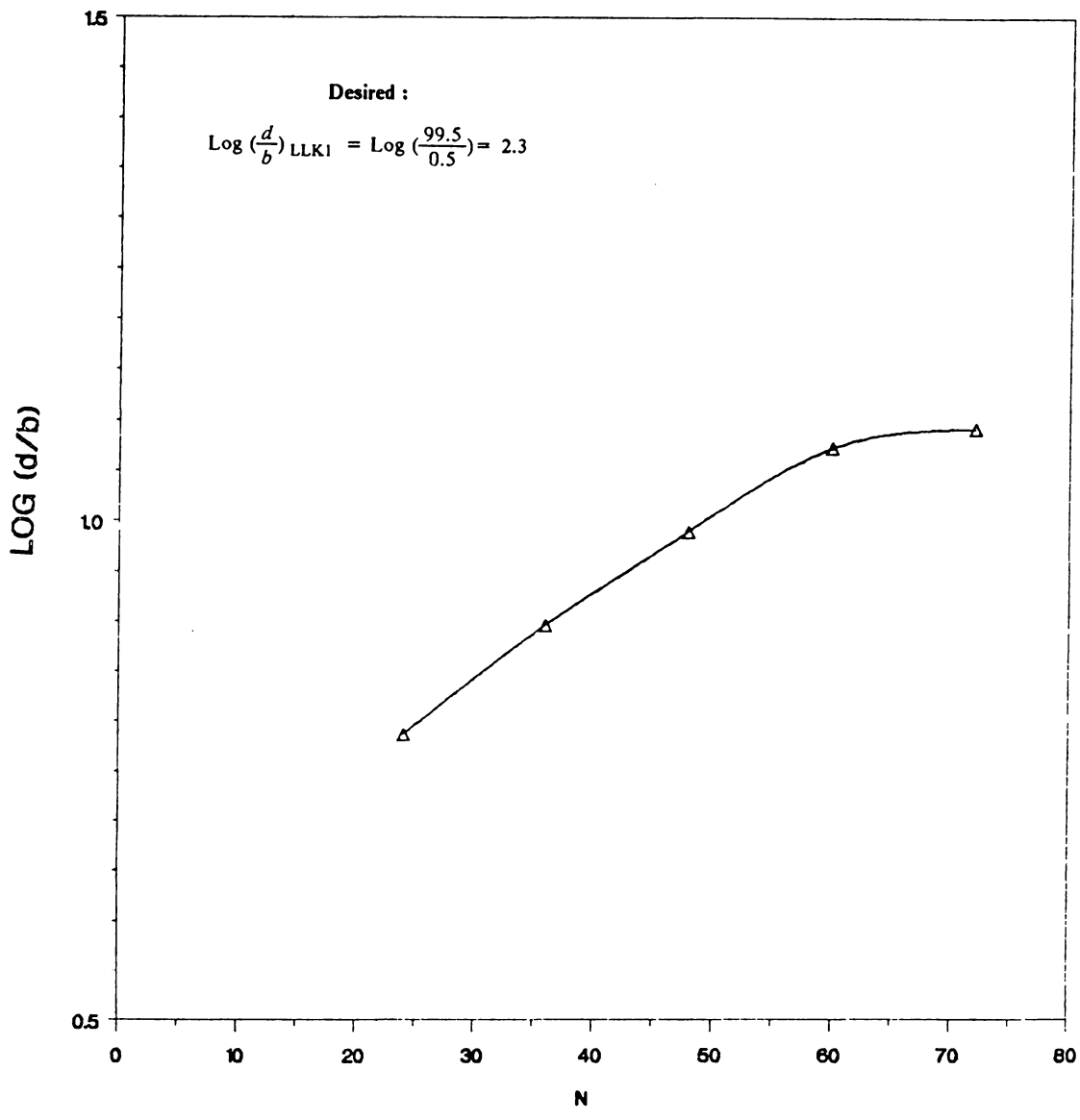


Figure 20. Effect of the Number of Ideal Stages N on the Distribution of Non-key Component

Rigorous plate-to-plate simulations using a commercial computer-aided design package, DESIGN II (ChemShare Corporation, 1985), have been conducted to show how the non-key component distributions behave. In a typical semi-sharp separation as shown in Figure 18 on page 57 (  $(d/b)_{LK} = 0.7/0.3$  ,  $(d/b)_{HK} = 0.02/0.98$  ) , one finds that LLK1 is distributed over a wide range of normal operating reflux ratios of 1.05 - 1.79 times  $R_{min}$  . (Incidentally, it is also noted that in this case where distributed nonkeys exist, an operating reflux ratio fixed at 1.1 - 1.3 times the minimum reflux ratio, as assumed in many previous investigations [e.g., Muraki and Hayakawa, 1987; Malone, et al., 1985], may not be valid.) To eliminate this, the number of theoretical stages has been increased at a constant reflux ratio ( $R = 0.815$ ). As can be seen in Figure 19 on page 58 and Figure 20 on page 59, component LLK1 becomes less distributed as  $N$  increases. However, there seems to exist a maximum amount of LLK1 to be recovered in the distillate beyond which it cannot be reached.

This clearly suggests that a large number of ideal stages is necessary when distributed non-key components are undesirable, resulting in an extra cost. In addition, the sensitivity of the reflux ratio to the non-key distribution will inevitably give rise to operational problems. It is for this reason that certain splits like the above are to be abandoned when the likelihood of having distributed non-keys is observed after applying the Fenske equation (total reflux situation). However, this consideration is not essential for fuel products which will eventually be blended together for burning, and thus allow for the existence of unmatched non-key distributions (see Example 2 of Chapter 6).



## ***4.5 Transformation from Infeasible Product Sets into Equivalent Feasible Product Sets***

Basically there are a number of ways of transforming infeasible product sets into equivalent feasible product sets. In this section, we will present several examples along with some pertinent rules.

Initially, to convert infeasible product sets into feasible product sets, our primary concern is how to classify acceptable feasible sloppy splits, rather than by their quantitative differences (see eqns. (3.3-1) and (3.3-2) ). Two kinds of sloppy splits, single-split-point (SSP) and multiple-split-point (MSP), as described in Section 3.3, will be employed in the transformation.

Since we have delineated the difference between SSP and MSP in Section 3.3, several cases are exemplified below to show how infeasible splits can be converted into equivalent feasible splits by using SSP or MSP.

***Case A Infeasible MSP sloppy product sets reduced to feasible product sets by incorporating mainly SSP sloppy splits :***

As shown in Example 1 in Figure 21 on page 62 , the original CAD contains an infeasible split. Since SSP splits will be used throughout, we must first remove the envelope in part (a) of Figure 21 on page 62 and leave A1 and B1 as qualified feasible SSP products. In the mean time, the products in the envelope are properly placed in the CAD to form fictitious product streams 1'' and 2''. Note in the final SST, it contains

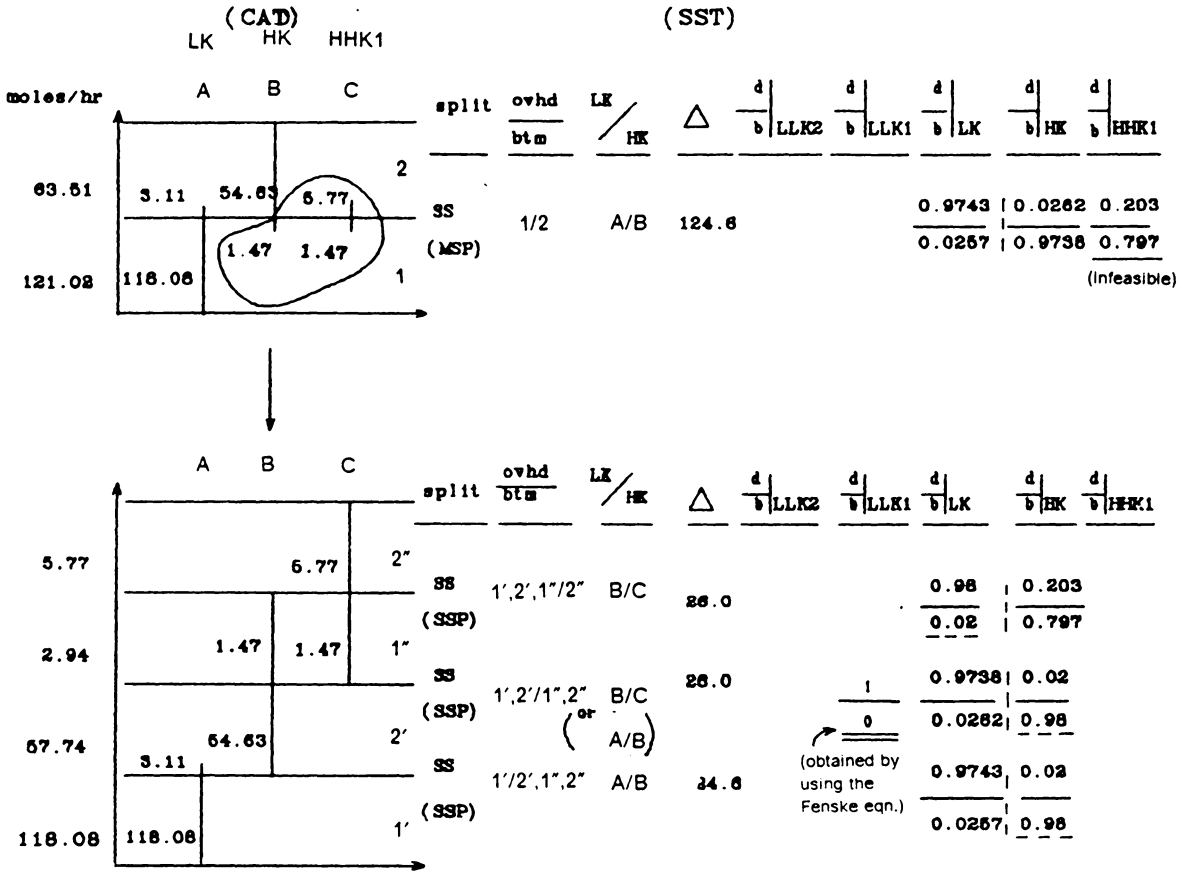


Figure 21. CAD and SST of a Split Before and After Transformation: Example 1 ( $K_A = 7.30, K_B = 3.25, K_C = 2.58$ , at  $P = 50$  psia,  $T = 175^\circ\text{F}$ , where  $K$ 's are vapor-liquid equilibrium ratios).

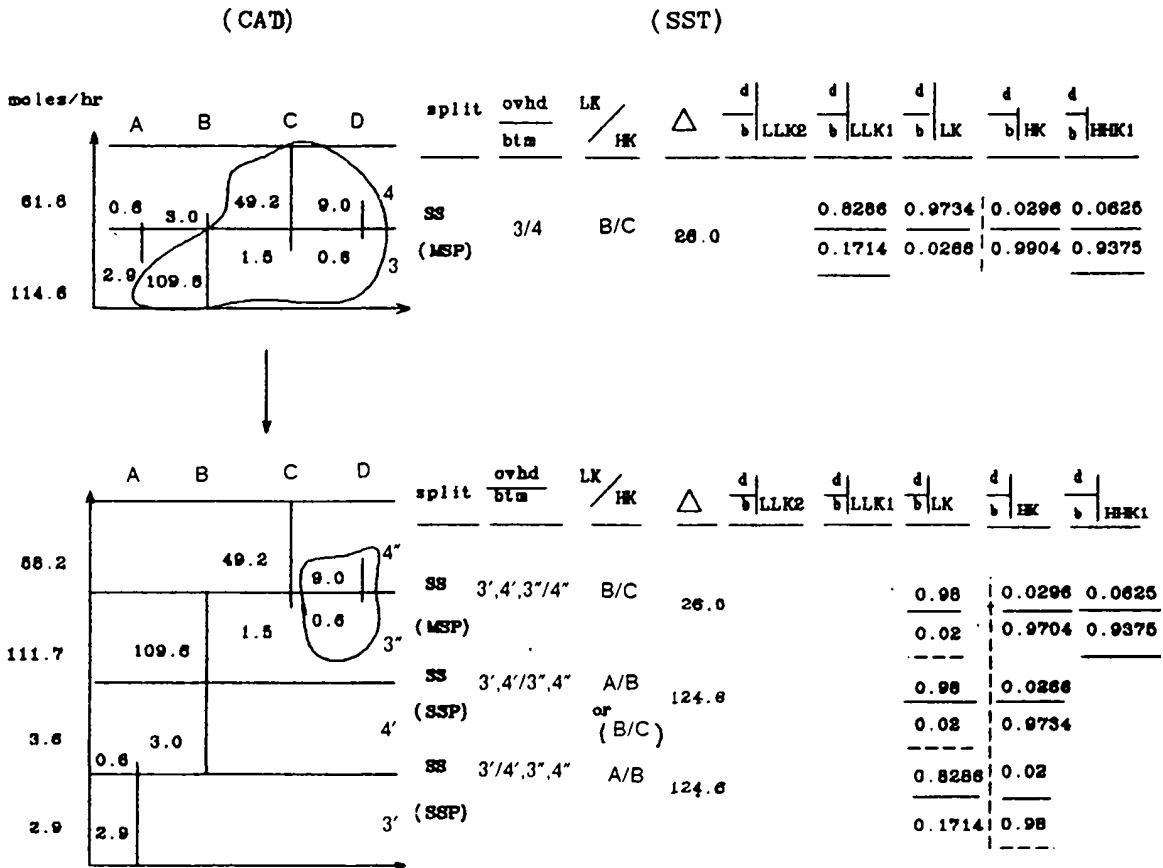
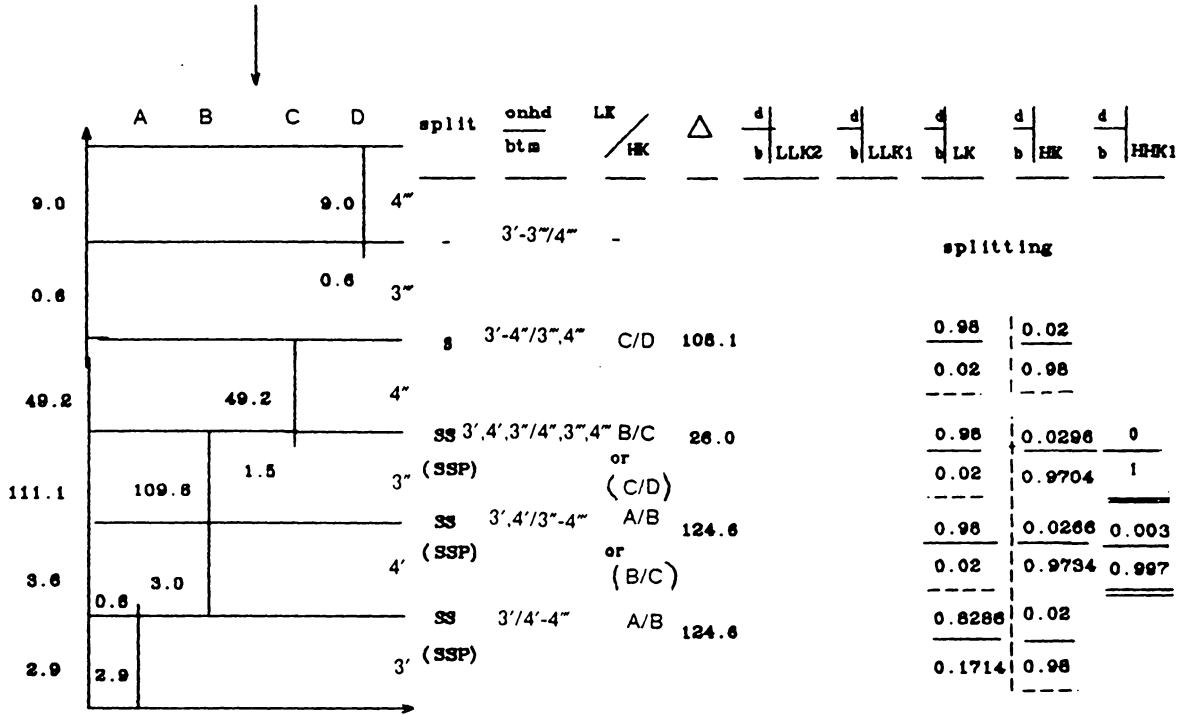


Figure 22. CAD and SST of a Split Before and After Transformation: Example 2 ( $K_A = 7.30, K_B = 3.25, K_C = 2.58, K_D = 1.24$  at  $P = 50$  psia,  $T = 175^\circ$  F., where  $K$ 's are vapor-liquid equilibrium ratios).

(continued)



three semi-sharp (SS) splits. A similar case can be found in Example 2 (see Figure 22 on page 63). It should also be noted the original CAD's in Examples 1 and 2 are only members of their CAD families where more than three and four components exist, respectively. Accordingly, we will not concern ourselves with bypassing at this point. The same thing happens in Examples 3 and 4 as well (see Figure 23 on page 66 and Figure 24 on page 67) If it turns out, however, that portions of CAD have same components as their CAD families presently under consideration, then the possibility of bypassing should be explored.

**Case B** *Infeasible MSP sloppy product sets reduced to feasible product sets by incorporating mainly MSP sloppy splits :*

As opposed to the preceding case, MSP sloppy splits will be used instead to transform infeasible product sets. As a result, they may lead to some purity contamination. Thus in this case, an economic analysis concerning product purity should be conducted,

As shown in Figure 23 on page 66 , the split for component C in the original CAD is infeasible. Let components A and B be, respectively, LK and HK. One can use the Fenske equation to estimate the cut for component C. For the remaining quantity of component C, we will create a fictitious product stream 1' to accommodate that. In Example 3 (Figure 23 on page 66), two SS separations are employed. As for example 4 (see Figure 24 on page 67), it will be left for the reader to see how the original CAD is evolved into the final CAD.

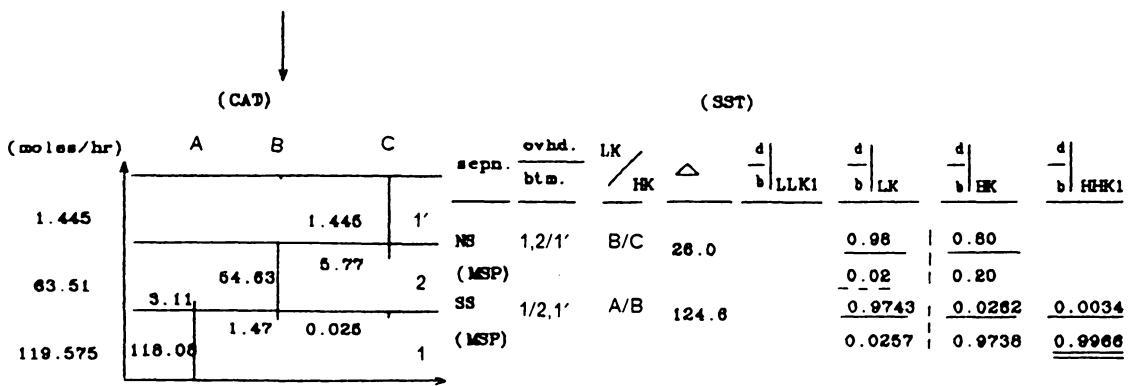
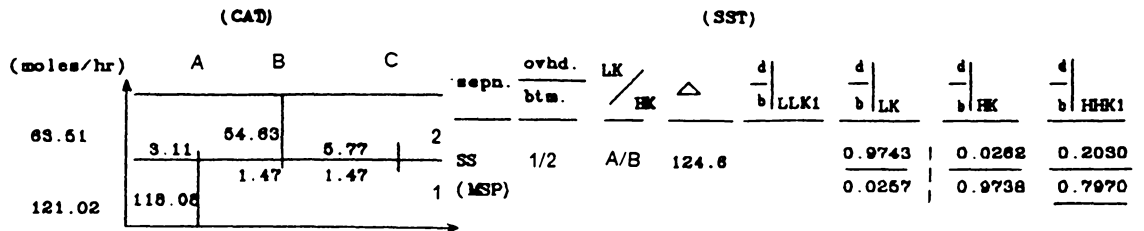


Figure 23. CAD and SST of a Split Before and After Transformation: Example 3 ( $K_A = 7.30, K_B = 3.25, K_C = 2.58$ , at  $P = 50$  psia,  $T = 175^\circ\text{F}$ , where  $K$ 's are vapor-liquid equilibrium ratios).

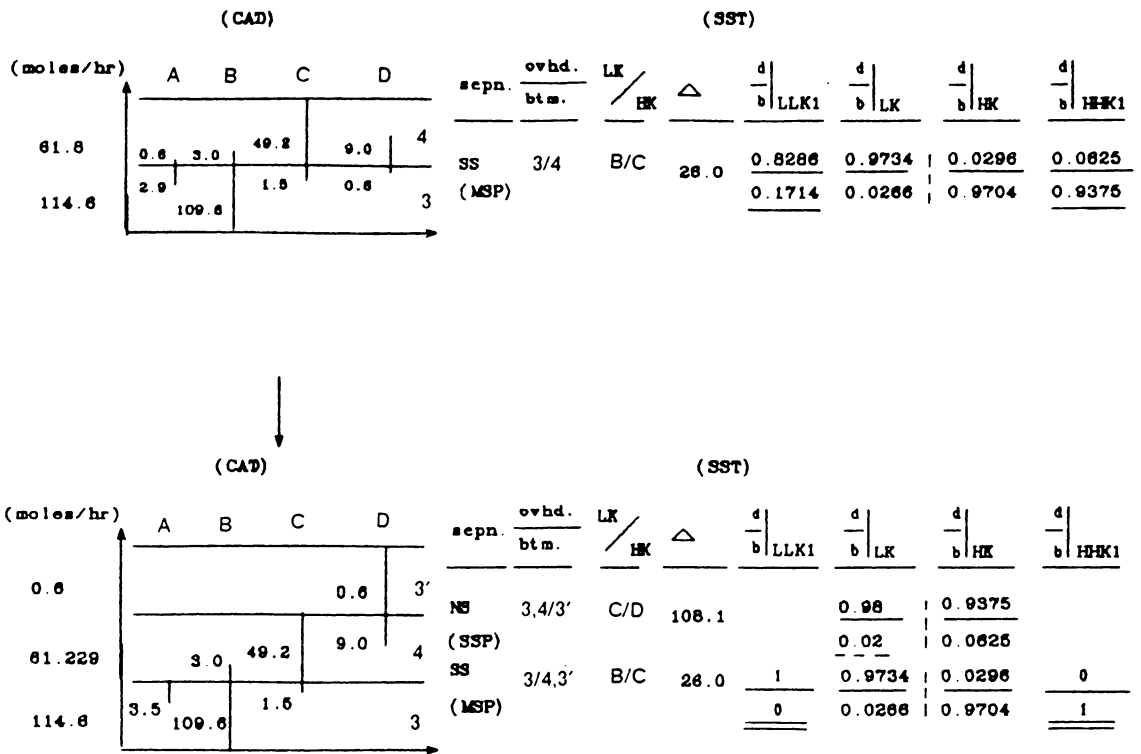
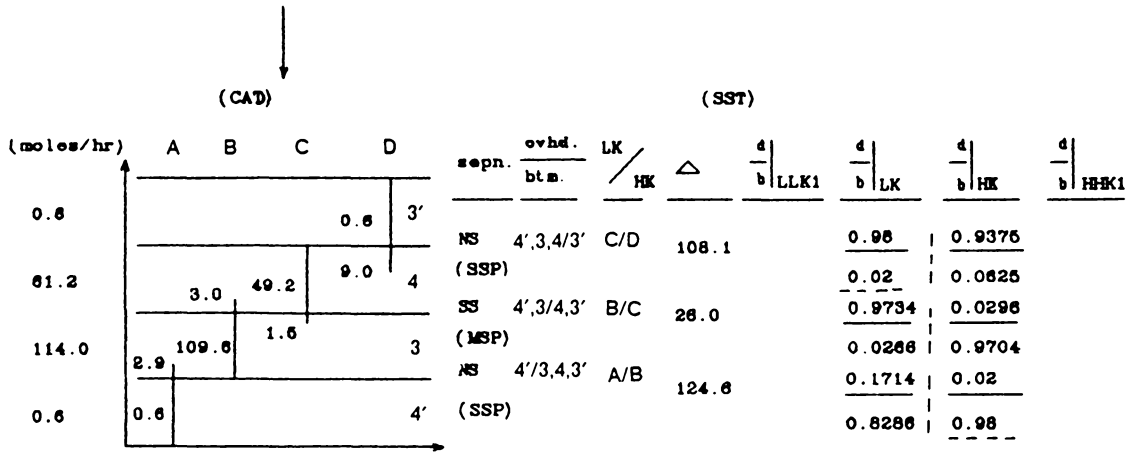


Figure 24. CAD and SST of a Split Before and After Transformation: Example 4 ( $K_A = 7.30, K_B = 3.25, K_C = 2.58, K_D = 1.24$  at  $P = 50$  psia,  $T = 175^\circ\text{F}$ , where  $K$ 's are vapor-liquid equilibrium ratios).

(continued)





Finally, it should be stressed that the transformation usually is not unique. Consequently, one needs to consider the following rules 1 and 2 when choosing a transformation for later use.

**Rule 1 :**

The smaller number of fictitious products, the fewer separators are needed.

**Rule 2:**

The following separations are preferred in a decreasing order :

NS (nonsharp) > SS (semisharp) > S (sharp)

## 4.6 Summary

In the first phase of synthesizing sloppy distillation sequences, one will have to go through the feasibility analysis which is, however, not needed for sharp separation synthesis. In this Chapter, we have examined all aspects surrounding the issue of separation feasibility. In particular, when a CAD at hand is being analyzed with respect to feasibility, the questions that arise for discussion are as follows :

(a) Is there an infeasible split in the CAD? If so, how does one get around it?

(b) Is there a way to reduce the load of separation?

(c) What are the two components (i.e., key components) that will determine the degree of a separation?

(d) Can one ascertain that problems associated with non-key distributions are resolved appropriately for cases in which distributed non-keys are undesirable?

The foregoing sections have individually addressed those problems, and the analysis leading to justifiable conclusions and recommendations is detailed. As a result, one can utilize the findings in this Chapter to come up with a modified or an equivalent CAD containing candidate "feasible" splits which will become the starting point in the second phase of synthesis process, as presented in the next Chapter.

# CHAPTER 5 HEURISTIC SYNTHESIS OF SLOPPY SEPARATIONS

As mentioned previously, the present work involves a two-step heuristic synthesis method. After feasible candidate splits have been identified using the techniques given in the last Chapter (i.e., step of feasibility analysis), one proceeds to the heuristic-synthesis step in which an actual split is proposed to be incorporated in the separation sequence by applying rank-ordered heuristics.

Presented in this Chapter are an overview of numerous heuristic techniques including combined heuristic and evolutionary methods (i.e., derivatives of original heuristic method) reported in the literature, a comparison of the above approaches, a detailed description of the heuristic rules for sloppy separations embodied in the synthesis step, as well as a discussion of merits offered by the proposed heuristic method.

## 5.1 Previous Heuristic Methods for Sharp Separations

The first investigation on the sequencing of multicomponent distillation separations dates back in 1947 by Lockhart, who discovered that the economics of column configurations were dependent upon the composition of the feed mixture. Two heuristics aimed at obtaining optimum sequences were developed as a result of his pioneering study : (i) favor the direct sequence (i.e., the sequence separates components one by one in an order of decreasing volatility), if the lightest product is present in large quantities; and (ii) favor the inverted sequence (i.e., the sequence in which components are split one by one in an order of increasing volatility). The system he analyzed was a three-component natural-gas purification unit.

Later on, Harbert (1957) presented two heuristic rules whose derivations were based on the assumption that the energy needed for achieving individual separations would dominate the column economics. The heuristics he proposed were : (i) favor smallest amounts of mass separation load for difficult splits; and (ii) favor more nearly equimolar separations (or 50/50 splits) of the feed between the distillate and bottoms products.

In another work, Heaven (1969) reported two heuristics evolved from a large number of case studies, in addition to two heuristics similar to those previously suggested by Harbert. One of Heaven's heuristics states that "separations where the relative volatility of the key components is close to unity should be performed in the absence of nonkeys", which is found to be in line with the first heuristic proposed by Harbert, favoring the direct sequence. The other heuristic by Heaven states that separations involving high recovery fractions should be reserved until late in a sequence.

With a more realistic costing function obtained by common shortcut techniques, Nishimura and Hiraizumi (1971) were able to compare the costs of different configuration

patterns of distillation columns and concluded their investigation with two heuristics - remove the most plentiful component first, and favor the direct sequence.

In an attempt to evaluate alternative sequences, Power (1971) proposed assigning weighting factors to heuristics. The alternative sequences with the highest accumulated, weighted values would then be favored.

Recognizing that most of the previous work was directed towards identifying or validating specific heuristic rules for certain circumstances, Tedder (1975) in his thesis listed nearly all heuristics including those of some importance and yet being ignored, and classified all of them into four categories :

1. Species Heuristics (based on the property differences between species) :

S1 - Perform the difficult separations last.

S2 - Separations where the relative volatilities of the key components are close to unity should be performed in the absence of non-key components.

S3 - Remove corrosive components early.

2. Design Heuristics (related to certain configuration being favored) :

D1 - Favor the direct sequence.

D2 - The next separator that is incorporated into a sequence should always be the cheapest.

D3 - Favor processes generating the least number of products.

D4 - Select a sequence that will remove the most desirable or valuable species as a distillate.

D5 - Protect the most valuable product by removing it from the process as quickly as possible.

3. Composition Heuristics (involving the effects of feed and product compositions on separation costs) :

C1 - Remove the most plentiful components first.

C2 - The direct sequence is preferred when the lightest product is present in large amounts.

C3 - The inverted sequence is preferred when the heaviest product is present in large amounts.

C4 - Favor equimolar splits of overhead and bottoms products.

C5 - Favor the direct sequence whenever equimolar amounts are present in the feed, and the relative volatilities are both the same.

C6 - High-recovery separations should be saved until last.

C7 - Reduce the separation load by stream splitting or blending whenever possible.

C8 - Differences involving stream compositions tend to dominate their economics. Select the separation tasks first.

4. State Heuristics (concerning operating states of columns) :

T1 - Avoid excursions in temperature and pressure, but aim high rather than low.

Instead of using simple two-product distillation columns, Tedder and Rudd (1978) explored new ways in obtaining optimum distillation sequences for ternary-feed mixture separation problems. A number of complex column configurations (e.g., fractionators with multiple feeds, sidedraws, sidestream strippers, etc.) were looked into in their work, as shown in Figure 25 on page 76 .

After examining a large number of case studies for very restricted three-component separation systems, they proposed many empirical heuristics (typical ones can be found in Figure 26 on page 77) based on feed compositions and a parameter called Ease of Separation Index (ESI), defined as follows:

$$ESI = \frac{\alpha_{AB}}{\alpha_{BC}} = \frac{\frac{k_A}{k_B}}{\frac{k_B}{k_C}} \quad [5.1]$$

where

A, B, and C = components in order of decreasing volatility

A new branch of heuristic approach called heuristic-evolutionary method was developed (Seader and Westerberg, 1977; Nath and Motard, 1981) which involved the use of heuristics, together with evolutionary procedures of different nature. First, an initial separation sequence is generated by using heuristics. Evolutionary rules are then applied to the initial sequence to come up with other alternate sequences. In each evolutionary step, substantial amounts of design and costing computation will be invested for the sequence produced, so that a better sequence can be synthesized. Specific heuristics and evolutionary rules suggested by the above workers are listed as follows.

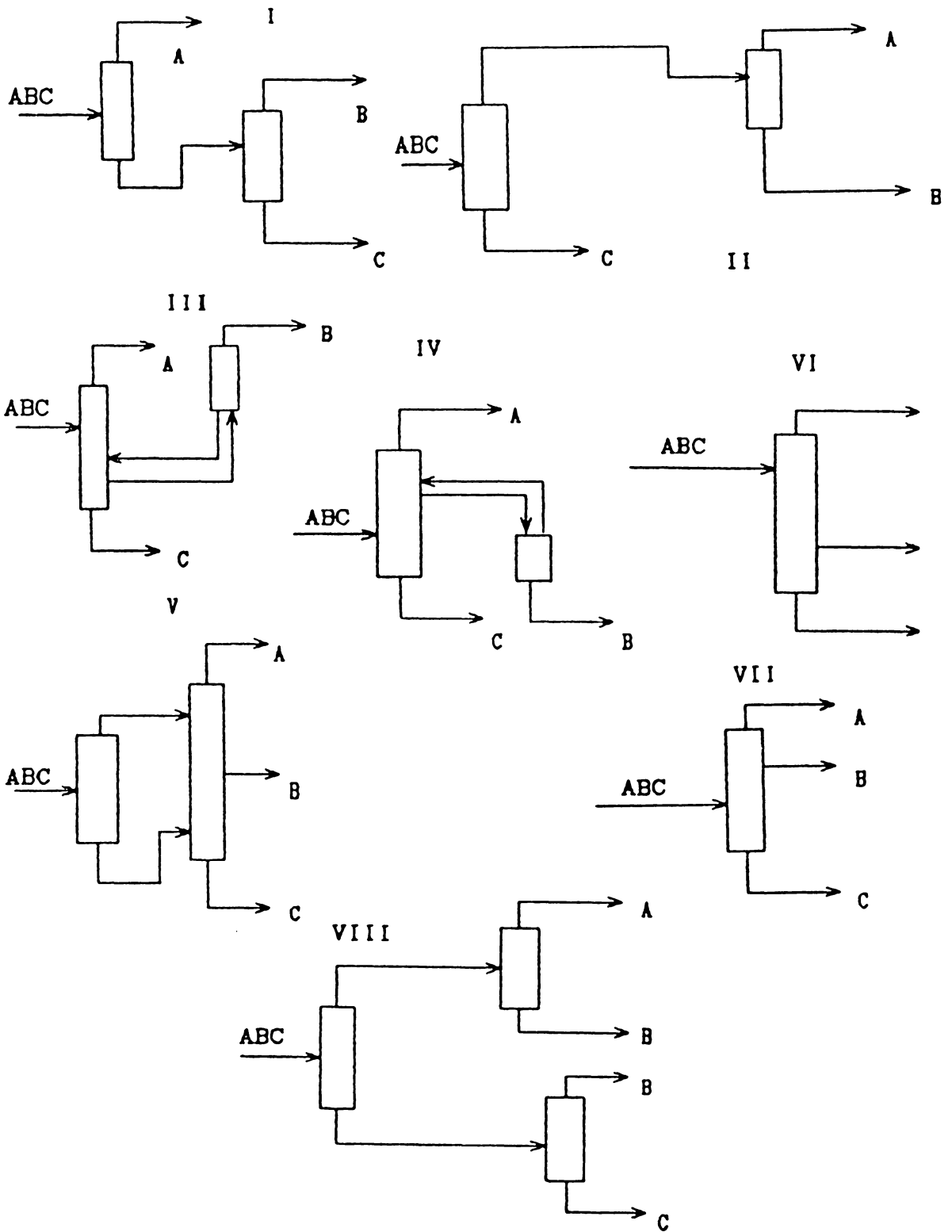
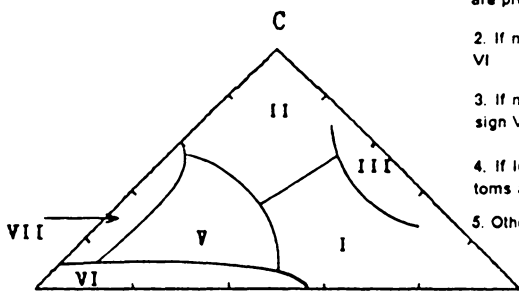


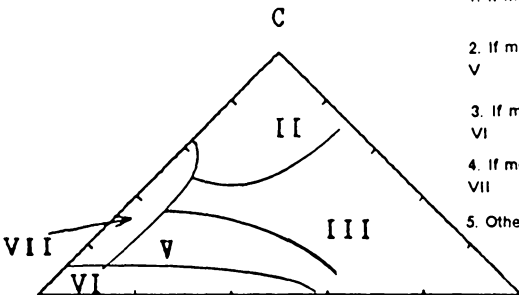
Figure 25. Complex Column Configurations (Tedder and Rudd, 1978)





B Expected regions of optimality for  $ESI < 1.6$  A

1. If 40 to 80% is middle product and nearly equal amounts of overhead and bottoms are present, then favor design V
2. If more than 50% is middle product and less than 5% is bottoms, then favor design VI
3. If more than 50% is middle product and less than 5% is overheads, then favor design VII
4. If less than 15% is middle product and nearly equal amounts of overhead and bottoms are present, then favor design III
5. Otherwise, favor design I or II, whichever removes the most plentiful component first



B Expected regions of optimality for  $ESI \geq 1.6$  A

1. If more than 50% is bottoms product, then favor design II
2. If more than 50% is middle product and from 5 to 20% is bottoms, then favor design V
3. If more than 50% is middle product and less than 5% is bottoms, then favor design VI
4. If more than 50% is middle product and less than 5% is overheads then favor design VII
5. Otherwise, favor design III

Figure 26. Complex Column Heuristics (Tedder and Rudd, 1978): Refer to Figure 25 for Numbering of Column Configurations.

- **Combined Heuristic-Evolutionary Method (Seader and Westerberg, 1977) :**

- \* *Heuristics -*

- (1) favor ordinary distillation

- (2) avoid vacuum and refrigeration

- (3) perform easy separations first

- (4) remove most plentiful component first

- (5) favor direct sequence

- (6) remove mass separating agent (MSA) first

- (7) favor smallest product set

- \* *Evolutionary Rules -*

- (1) change the separation method for a given separation task

- (2) given a separation sequence, move a given separation task to the upstream in the sequence

- **Combined Heuristic-Evolutionary Method (Nath and Motard, 1981) :**

- \* *Heuristics -*

- (1) favor the smallest product set

- (2) favor ordinary distillation

(3) easiest separation should be done first

(4) a separation method using an MSA cannot be used to isolate another MSA

(5) a separation method with  $\alpha_{LK,HK} < \alpha_{\min}$  is not acceptable

(6) operating pressure should be close to ambient

(7) set split fractions of the keys to prespecified values

(8) set operating reflux ratios equal to 1.3 times the minimum reflux ratio for each column

\* *Evolutionary Rules* -

(1) challenge heuristic 1

(2) examine the neighboring separation sequences if [a]- their CDS<sup>+</sup> values are within .10% of each other; and [b]- refrigeration is required to condensate the reflux

(3) challenge heuristic 2

(4) examine neighboring separations to decide if the removal of MSA should be delayed

(5) challenge heuristic 3 if [a]-  $R_{\min}$  of the immediate successor  $\gg R_{\min}$  of the unit under consideration; or [b]- the cost of the immediate successor  $\gg$  the cost of the unit under consideration.

---

<sup>+</sup> : coefficient of difficulty of separation is defined as :

$$CDS = \left[ \log \frac{\frac{sp_{LK}}{1 - sp_{LK}} \frac{sp_{HK}}{1 - sp_{HK}}}{\log \alpha_{LK-HK}} \right] \frac{D}{D + B} \left( 1 + \left| \frac{D - B}{D + B} \right| \right) \quad [5.2]$$

where

sp = split fraction

Based on the above evolutionary rules, one sees that essentially two different evolutionary schemes are adopted in these methods - i.e., (i) global evolution (Nath and Motard, 1981); and (ii) local evolution (Seader and Westerberg, 1977). In the former case, all downstream structure is discarded and will be replaced by a new sequence obtained by applying the evolutionary rules. This follows because the evolutionary rules actually challenge the heuristic rules upon which first initial sequences are built. In the case of local evolution only, upstream splits will be altered, and the evolutions are localized in part of the initial sequence.

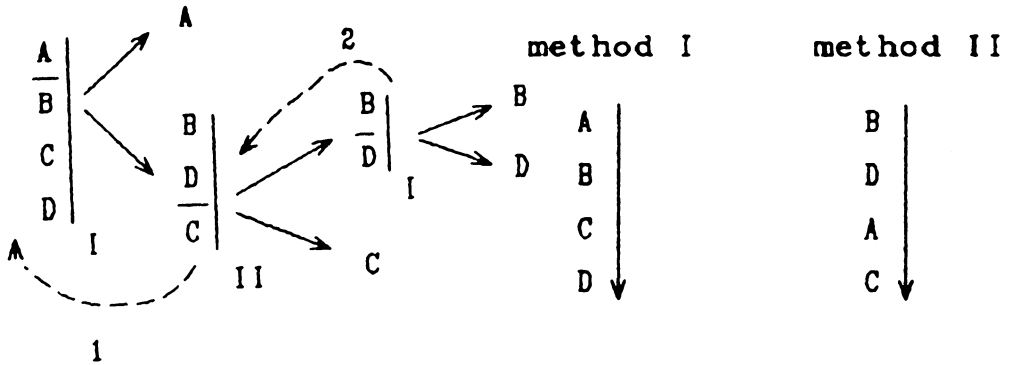
To briefly explain how the evolutionary rules work, two examples are given in Figure 27 on page 81 and Figure 28 on page 82, which respectively illustrate evolutionary rules 1 and 2 of Seader and Westerberg (1977).

**Table 3. Classification of Heuristics (Nadgir and Liu, 1983)**

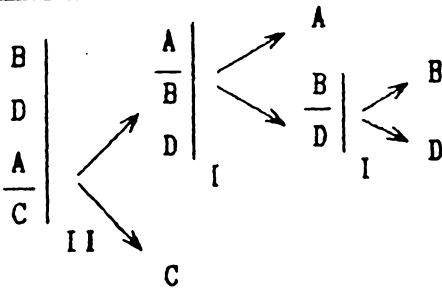
Heuristic Type	Descriptions
M1a (Method)	favor ordinary distillation
M1b	remove MSA first
M1c	remove MSA properly
M2	avoid vacuum distillation and refrigeration
S1 (Species)	remove corrosive and hazardous components first
S2	perform difficult splits last
C1 (Composition)	remove most plentiful component first
C2	favor 50/50 split
D1 (Design)	favor smallest product set
D2	direct sequence rule

original

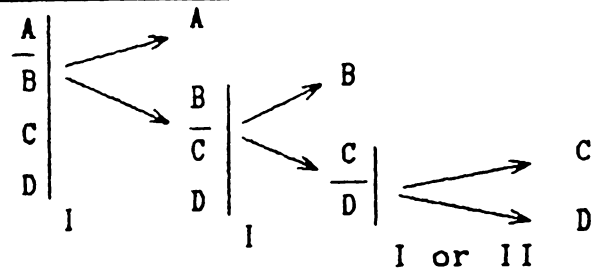
ranked property lists :



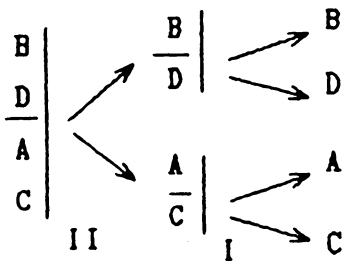
evolution 1



evolution 2



evolution 1'



evolution 2'

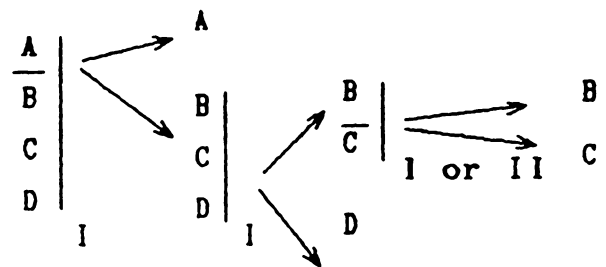
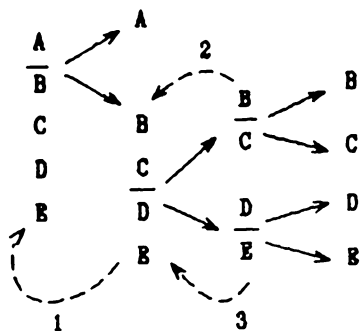
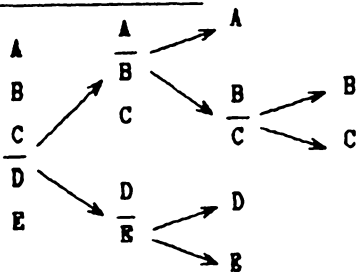


Figure 27. Alternate Sequences Produced by Evolutionary Rule 1 (Seader & Westerberg)

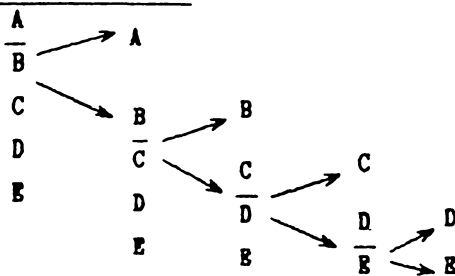
original



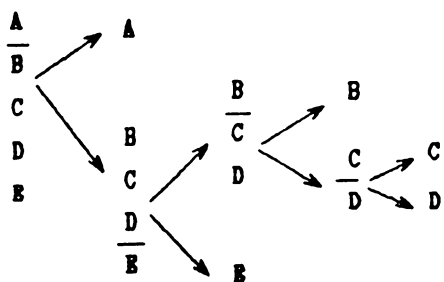
evolution 1 :



evolution 3 :



evolution 2 :



evolution 2 + 3 :

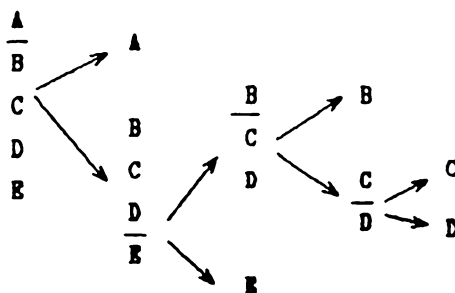


Figure 28. Alternate Sequences Produced by Evolutionary Rule 2 (Seader & Westerberg)

Eventually, it remained for Nadgir and Liu (1983) to succinctly clarify the redundancy existing in the previously reported heuristics. For a simple two-product separation sequencing problem, they essentially divided heuristics into four groups, three of which were the same as the classification adopted by Tedder (i.e., design, species, and composition heuristics); they also defined a new group - method heuristics in place of state heuristics. Specifically, method heuristics comprised of several rules of thumbs favoring certain separation methods. Table 3 on page 80 lists their classification of heuristics. Elaborate discussion of certain important heuristics is given in the next section.

Up to this point, we have already reviewed most of the work pertaining to heuristic methods for sharp separations. In closing the section, a summary of the available heuristic methods is given in Table 4 on page 84.

**Table 4. Comparison of Heuristic Methods for Sharp Separations**

HEURISTIC METHODS	SYSTEM	HEURISTICS RULES	EVOLUTIONAR APPROACH (# RULES)	FEATURES AND OTHER REMARKS
A. CONVENTIONAL HEURISTIC				order insensitive
Lockhart (1947)	ternary	2	none	case studies
Harbert (1957)	ternary	2	none	assumed heat required dictates economics; case studies
Heaven (1969)	3- and 5-component	4	none	detailed costing; case studies
Nishimura & Hiraizumi (1971)	general	2	none	mathematical verification of specific heuristics
Tedder & Rudd (1978)	ternary	a number of quantitative ones	none	complex columns considered; heuristics correlated with feed compositions and ESI (equation (5.1) )
B. HEURISTIC-EVOLUTIONARY:				order-sensitive heuristics
Seader and Westerberg (1977)	general	7	local evolution (2)	drawback of tremendous amount of calculations



(continued)

HEURISTIC METHODS	SYSTEM	HEURISTICS RULES	EVOLUTIONAR APPROACH(# RULES)	FEATURES AND OTHER REMARKS
Nath and Motard (1981)	general	8	global evolution (5)	same drawback as above, but even more severe
C. WEIGHTED HEURISTIC:				numerical values given to alternate sequences by heuristics
Power (1971)	general	5	none	less promising due to limited success
D. RANK-ORDERED HEURISTIC:				rank-ordered, purely heuristic methods
Nadgir and Liu (1983)	general	7	none	most computationally efficient and effective method; tested against virtually all previous case studies with great success

## ***5.2 The Proposed Heuristic Method for Sloppy Separations***

In the past, process-synthesis strategies involving the use of heuristics were often criticized for their shortcomings resulting from conflicting heuristic rules. If one takes two heuristics - "difficult separation last", and "remove the most plentiful component first", for instance, one would find that they may sometimes end up with contradictory separation schemes - e.g., confusion may arise when one of the difficult separation products contains the most plentiful component.

Among all previously published heuristic methods for sharp separations, no work fully responded to the need of developing a purely heuristic method made up of a general set of coherent heuristics that can accommodate virtually all separation problems. Instead, most work was concerned with verifying certain heuristics for very restricted systems (or subproblems).

In the work of Nadgir and Liu (1983), this problem has been addressed and resolved, and their method for sharp separations is adopted and modified in the current study to deal with sloppy separations. The main thrust of this method is that heuristics are proposed in a hierarchical (or rank-ordered) fashion such that conflicts among the heuristics are eliminated. The success of the method in dealing with synthesis problems of sharp separation has been clearly demonstrated in their work.

Since the focus herein is on synthesis of sloppy product sets, attempts have been made to tailor the above method to suit our current need. In what follows, the heuristics being employed in this study are described in detail.

***M1 : Favor ordinary distillation and remove mass separating agent first.***

It is advisable not to use other indirect separation means such as extractive distillation. More often than not, a solvent or mass separating agent (MSA) from outside the system will be needed, thereby increasing the possibility of product contamination (by MSA). However, using extractive distillation will lead to higher equipment costs and additional make-up solvent expenses. Obviously, all of these make extractive distillation an unfavorable separation method.

For mixtures with close-boiling key components (i.e., the relative volatility of key components  $\alpha_{LK,HK} < 1.10$ ), however, using other available alternative methods to do the separation will be inevitable. In the event that an MSA is used, it will usually be removed immediately after the unit into which it is introduced in order to prevent products contamination. However, this second part of heuristic may be challenged when two or more difficult splits exist in the system. As shown in Figure 29 on page 88 (Nath and Motard, 1981), the strategy of removing the MSA early is unlikely to be viable, since in sequence a, two splits are difficult, both requiring the use of the MSA; higher equipment costs will result if MSA is stripped early.

***M2 : Avoid vacuum distillation and refrigeration.***

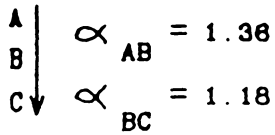
A low-temperature refrigeration system is known for its high cost to run. As with refrigeration, vacuum operation is expensive too. Thus, it is best not to run the separation system at such extreme conditions (i.e., low temperature and pressure).

***S1 : Remove corrosive and hazardous products first.***

For safety and economic reasons (associated with high material costs of process equipment), corrosive and hazardous products are best removed early.

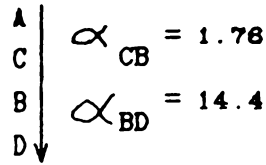
property list I

ordinary distillation



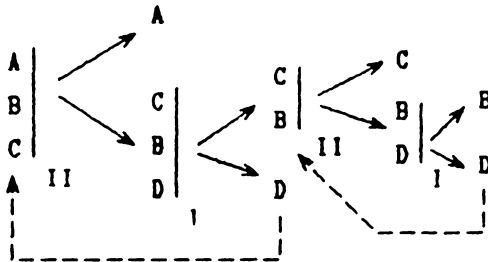
property list II

extractive distillation



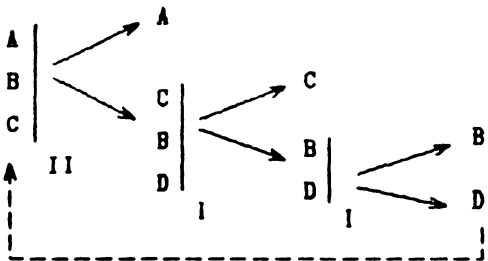
D=solvent

sequence a : total annual cost = \$214,675/yr



remove MSA  
early

sequence b : total annual cost = \$158,699/yr



delayed removal  
of MSA

Figure 29. Comparison of Sequences Based on Heuristic M1: (Nath and Motard, 1981).

**S2 : Difficult splits should be performed lastly.**

As a widely used rule-of-thumb, difficult separations ought to be done when non-key components are absent (King, 1980). Hence, difficult splits are best saved for last.

**C1 : Remove the most plentiful product first; readily removable splits are preferred over non-readily removable ones.**

Take a separation problem shown in Figure 30 on page 90 as an example. Product streams 1, 2, 3, and 4 are in the order of decreasing volatility. For simplicity, let product stream 1 be the most plentiful product, and the flow rate of each product stream be equal to D. One sees that as the flow rate of product stream 1 increases, sequences a and b will stand out because of their less overall separation loads.

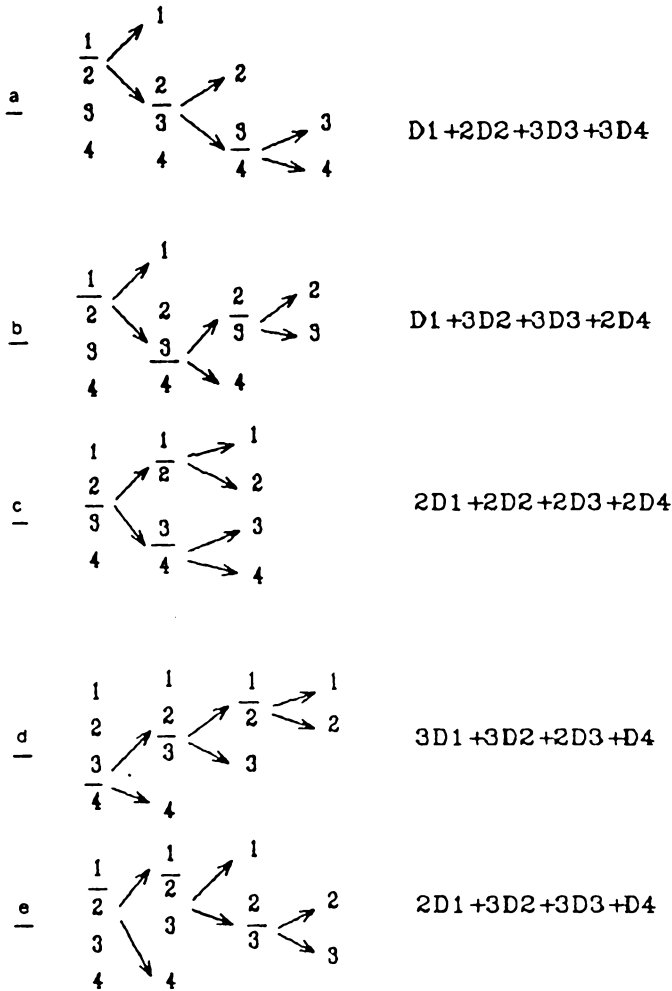
**C2 : Perform the split with the largest value of CES (i.e., favor 50/50 split).**

For sharp separations (Rudd et al., 1973), it can also be observed from Figure 30 on page 90 that sequence 3 (equimolar split in each separator) is favored (letting  $D_1 = D_2 = D_3 = D_4 = D_5$ , total separation load equals  $9D, 9D, 8D, 9D,$  and  $9D$ , respectively for sequences a, b, c, d, and e). In the case of non-sharp separations, however, we propose a parameter called the coefficient of ease of separation (CES), as defined in equation [5.3], which will help us locate a split that combines the features of equimolar division, reasonable separation factor or relative volatility, and large sloppiness of the cut in key components. Note that the effect of split sloppiness on the ease of separation is expressed in logarithmic form, mimicking the effect of sloppiness of cut on the minimum number of ideal equilibrium stages (according to the Fenske equation).

$$CES = f \times \Delta \times \frac{1}{\log\left[\left(\frac{d}{b}\right)_{LK} \left(\frac{b}{d}\right)_{HK}\right]} \quad [5.3]$$

Seq.

total mass load



total separation loads ( $D2=D3=D4=D5$ ) :

seq.	a	b	c	d	e
$D1=2D$	10D	10D	10D	10D	11D
$D1=3D$	11D	11D	12D	13D	13D
$D1=4D$	12D	12D	14D	16D	15D

Figure 30. A Separation Problem Illustrating Heuristics C1 and C2.

where

$f = D/B$  or  $B/D$ , whichever is smaller than or equal to unity

$\Delta = \Delta T$  (in °C)  $\times 1.8$  or  $(\alpha - 1) \times 100$

**C3 : If two or more splits have approximately the same magnitude of CES, then take a split leading to a maximum amount of bypass (or stream splitting) in the subsequent sequence.**

Suppose that all preceding heuristics (M1 through C2) cannot distinguish one split from the others, the only way to resolve this situation is by "looking-ahead" - i.e., to identify a possibility of stream splitting, leading to a future mass reduction in separation load.

Since the heuristics presented above are given in a ranked order and are applied in a sequential manner, the heuristic with a higher rank can override the one with a lower rank. However, it may happen occasionally that certain heuristics are not applicable, then lower-ranked heuristics can subsequently be employed.

## 5.3 Discussion

Finally in this Chapter, to emphasize the importance of the proposed heuristic approach in synthesizing separation sequences and to fully appreciate the value of each individual technique, we start by first subdividing the literature research work to date on heuristic methods into four categories :

1. **Conventional Heuristic Methods** : Most early heuristic methods fall into this category.

Specifically, the methods under this division were either evolved from case studies for

systems containing small numbers of products (i.e., experience gained from studying effects of certain variables such as feed compositions on sequence economics) or derived from non-rigorous mathematical validation (e.g., by making simplifying assumptions and approximations). Regardless of the means used, heuristic methods of this kind suffer the drawback of being inflexible - since they have only dealt with a part of the whole problem. In reality, problems encountered may challenge two or more heuristics available all at the same time. For example, a likely scenario would be that a separation problem can be treated by different heuristics (e.g., heuristics of "perform easy separations first" and "remove most plentiful product first"), but there does not exist a preference order or a weighting factor to decide which heuristic will outweigh the other.

2. **Heuristic-Evolutionary Methods** : It may appear that these methods offer an advantage of successive improvement. However, one should be aware of not only the costly computational efforts they require, but also the implication associated with the penalty of employing a bad choice of initial sequences (as a result of applying improper heuristics) as a starting point for evolution. Furthermore, these methods by no means guarantee achieving sequence optimality.
3. **Weighted Heuristic Methods** : It should be noted that the method itself does not provide guidelines as to how to synthesize initial sequences; rather, it only gives a means to compare different sequences. The success of this approach is very limited.
4. **Rank-Ordered, Purely Heuristic Methods** : One must understand the motivations behind this approach lie in the following facts:

In the first place, by using the heuristic method, one is able to generate good initial sequences which will have to go through operating state optimization (e.g., by varying state variables such as the feed condition of each column, column pressures,



etc.) as well as to perform heat-integration analysis before any final scheme emerges. Therefore, initial separation sequences with guaranteed optimality is not necessary.

Secondly, although many heuristics were inferred by examining column economics of varying separation systems containing small numbers of components, it is generally accepted that adequately developed heuristics can be indiscriminately applied to separation problems under question regardless of the size of the problems. Thus, by all accounts, the present heuristic approach can offer the most effective way in reducing the search space wherein the multitude of all possible alternatives will be too formidable to cope with as the number of products increases. In fact, this situation will even become more severe for our problem in which sloppy split and stream splitting are both allowed.

# CHAPTER 6 ILLUSTRATIVE EXAMPLES

In this Chapter, two typical separation problems are presented to demonstrate how the synthesis method described in Chapters 3 to 5 can be applied to generate initial sequences for obtaining sloppy multicomponent product sets.

For clarity, the synthesis method involving problem representation as well as feasibility analysis and heuristic synthesis is illustrated in a step-by-step manner. Costing results of proposed sequences are also reported.

## *6.1 Example Problem 1*

The first example problem, taken from Nath (1977), is concerned with the separation of a feed mixture consisting of four components (n-butane, n-pentane, n-hexane, and n-heptane) into four products. Specific data for separation requirement are given below. The initial Component Assignment Diagram (CAD) for this example is constructed in Figure 4 on page 21. Also, the Separation Specification Table (SST) corresponding to possible first splits is given in Table 5 on page 96. Next, the SST that corresponds to possible final splits is shown in Table 6 on page 96.

One can see in Table 6 on page 96 that there is an infeasible last-split candidate, for which certain transformations described in Section 4.5 may have to be applied during the

course of synthesis. Suppose we will only use the candidates in Figure 4 on page 21 as first splits, a decision tree can then be drawn (see Figure 31 on page 97).

Product Streams	Desired (component mole fraction)				(flow rate)
	A	B	C	D	moles/hr
1	0.4615	0.3846	0.1539	-	32.5
2	0.4444	0.5556	-	-	22.5
3	-	-	0.6667	0.3333	30.0
4	-	-	-	1.0000	15.0

Feed : 37.8 ° C, 1.0333 kg/ $m^2$ , 100 moles/hr

Component	Component Name	Mole Fraction
A	n-butane	0.25
B	n-pentane	0.25
C	n-hexane	0.25
D	n-heptane	0.25

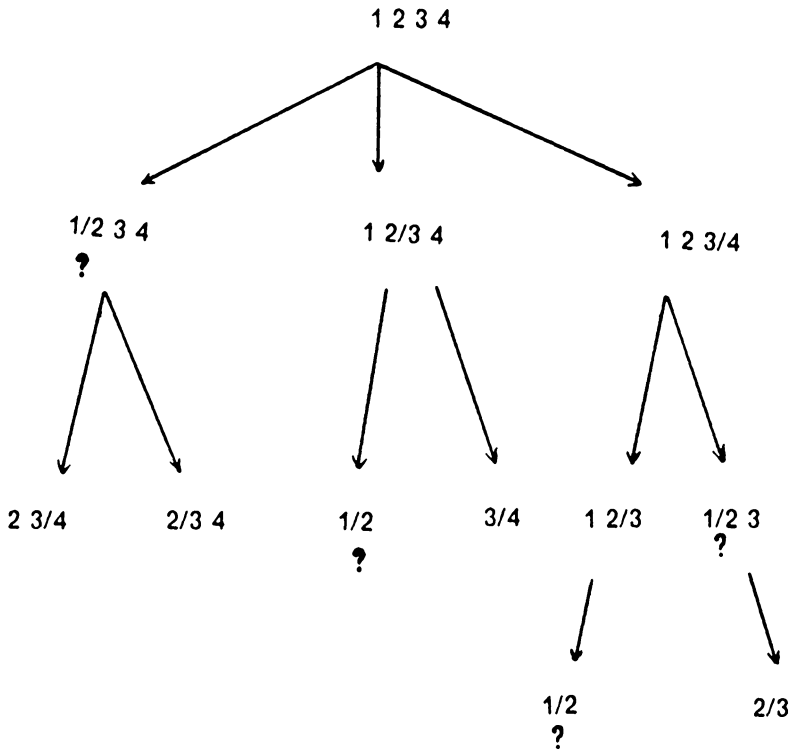
Available Separation Method : Ordinary Distillation

Table 5. SST for Possible First Splits

Separation	ovhd/btm	LK/HK	$\Delta^\circ C$	$\frac{d}{b} LLK2$	$\frac{d}{b} LLK1$	$\frac{d}{b} LK$	$\frac{d}{b} HK$	$\frac{d}{b} HHK1$	$\frac{d}{b} HHK2$
NS(MSP)	1/2 3 4	A/B	36.6			0.6	0.5	0.2	0.02
						0.4	0.5	0.8	0.98
NS(MSP)	"	B/C	32.7		0.6	0.5	0.2	0.02	
					0.4	0.5	0.8	0.98	
SS(SSP)	1 2/3 4	B/C	32.7			0.98	0.2	0.02	
						0.02	0.8	0.98	
NS(SSP)	"	C/D	29.7			0.2	0.02		
						0.8	0.98		
SS(SSP)	1 2 3/4	C/D	29.7			0.98	0.4		
						0.02	0.8		

Table 6. SST for Possible Final Splits

Separation	ovhd/btm	LK/HK	$\Delta^\circ C$	$\frac{d}{b} LLK2$	$\frac{d}{b} LLK1$	$\frac{d}{b} LK$	$\frac{d}{b} HK$	$\frac{d}{b} HHK1$	$\frac{d}{b} HHK2$
Infeasible	1/2	A/B	36.6			0.6	0.5	0.98	
						0.4	0.5	0.02	
S	2/3	B/C	32.7			0.98	0.02		
						0.02	0.98		
SS(SSP)	3/4	C/D	29.7			0.98	0.4		
						0.02	0.6		



**Figure 31. Decision Tree for Example 1:** (The Question Mark in the Tree represents an infeasible split involving 1/2)

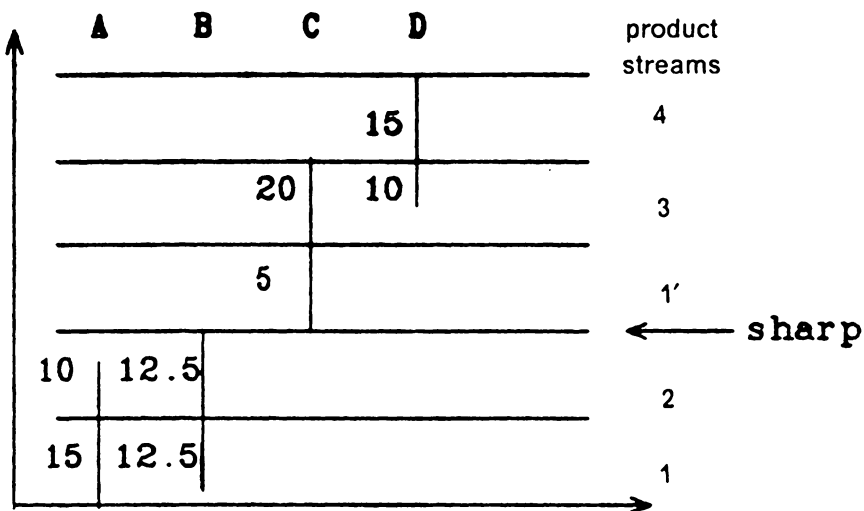


Figure 32. Abandoned Transformation of the CAD in Example 1

Although one can apply transformation techniques to infeasible splits such as  $1/2$ ,  $1\ 2/3$ , and  $1/2\ 3$ , transformation will take place at the beginning of the solution that follows. This is because if component C in product 1 were to be removed, it would give rise to a sharp separation as depicted in Figure 32 on page 98.

However, if components B and C in product 1 are removed instead, the CAD then becomes the CAD shown in Figure 33 on page 99. What should be noted in this figure is that each split in the CAD is sloppy, which is a highly desirable case. The SST corresponding to the CAD (Figure 33 on page 99) is given in Table 7 on page 100. Next applying the heuristics to the splits in Table 7 on page 100 gives :

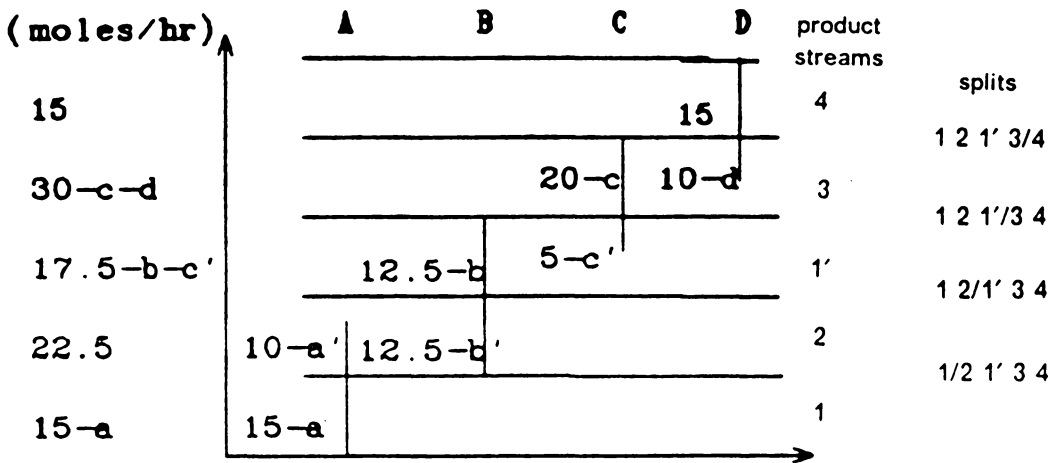


Figure 34. Proposed Transformation of the CAD in Example 1

Table 7. SST for the First Splits in the CAD

(Note : several splits are abandoned due to undesirably distributed non-keys)

Separation	ovhd/btm	LK/HK	$\Delta$ °C	$\frac{d}{b}$   LLK2	$\frac{d}{b}$   LLK1	$\frac{d}{b}$   LK	$\frac{d}{b}$   HK	$\frac{d}{b}$   HHK1	$\frac{d}{b}$   HHK2	CES
SS(SSP)	1/2 1' 3 4	A/B	36.6			0.6   0.02				6.22
						0.4   0.98				
SS(SSP)	1 2/1' 3 4	A/B	36.6			0.98   0.5	0.02			23.36
						0.02   0.5	0.98			
8	"	A/C	69.3			0.98   0.02	$\frac{d}{b}$		= $\frac{0.30}{\text{INTER}}$	abandoned
						0.02   0.98	$\frac{d}{b}$		= $\frac{0.70}{\text{INTER}}$	
SS(SSP)	"	B/C	32.7		0.98	0.5   0.02				20.91
					0.02	0.5   0.98				
SS(SSP)	1 2 1'/3 4	B/C	32.7			0.98   0.2	0.002			21.02
						0.02   0.8	0.998			
3	"	B/D	62.4			0.98   0.02	$\frac{d}{b}$		= $\frac{0.301}{\text{INTER}}$	abandoned
						0.02   0.98	$\frac{d}{b}$		= $\frac{0.699}{\text{INTER}}$	
NS(SSP)	"	C/D	29.7		0.786	0.2   0.02				abandoned
					0.214	0.8   0.98				
SS(SSP)	1 2 1' 3/4	C/D	29.7			0.98   0.4				5.05
						0.02   0.6				

M1: Separation factors ( $\Delta$ 's) are large enough to use ordinary distillation.

M2: To avoid vacuum and refrigeration, high pressure is preferred to operate a De-nC4 column (since n.b.p. of nC4 = 17.1°C).



S1: Not applicable.

S2: All boiling point differences appear to be large, so no difficult separation exists.

C1: The most plentiful product is product 3, so our first choice will be either 1 2 1' 3 4 or 1 2 1' 3/4.

C2: CES's for each split (given in Table 7 on page 100) are computed as follows :

split 1/2 1' 3 4 -

$$\text{LK/HK} = \text{A/B}, \text{CES} = \frac{15}{85} (65.8) \frac{1}{\log\left[\left(\frac{0.6}{0.4}\right)\left(\frac{0.98}{0.02}\right)\right]} = 6.22 \quad [6.1 - 1]$$

split 1 2/1' 3 4 -

$$\text{LK/HK} = \text{A/B}, \text{CES} = \frac{37.5}{62.5} (65.8) \frac{1}{\log\left[\left(\frac{0.98}{0.02}\right)\left(\frac{0.5}{0.5}\right)\right]} = 23.36 \quad [6.1 - 2]$$

$$\text{LK/HK} = \text{B/C}, \text{CES} = \frac{37.5}{62.5} (58.9) \frac{1}{\log\left[\left(\frac{0.5}{0.5}\right)\left(\frac{0.98}{0.02}\right)\right]} = 20.91 \quad [6.1 - 3]$$

split 1 2 1' 3 4 -

$$\text{LK/HK} = \text{B/C}, \text{CES} = \frac{45}{55} (58.9) \frac{1}{\log\left[\left(\frac{0.98}{0.02}\right)\left(\frac{0.8}{0.2}\right)\right]} = 21.02 \quad [6.1 - 4]$$

$$LK/HK = C/D, CES = \frac{45}{55} (53.4) \frac{1}{\log\left[\left(\frac{0.2}{0.8}\right)\left(\frac{0.98}{0.02}\right)\right]} = 40.15 \quad [6.1 - 5]$$

split 1 2 1' 3/4 -

$$LK/HK = C/D, CES = \frac{15}{85} (53.4) \frac{1}{\log\left[\left(\frac{0.98}{0.02}\right)\left(\frac{0.6}{0.4}\right)\right]} = 5.05 \quad [6.1 - 6]$$

C3: Not applicable.

---> Thus, split 1 2 1' 3/4 (LK/HK = B/C) is preferred. Note that the same split with a different set of LK/HK = C/D is abandoned since LLK - B is distributed. In what follows, we will perform the feasibility analysis for both products of the first split.

- Feasibility Analysis for the bottoms product (3 4) : bypassing is possible (refer to Figure 33 on page 99)

Basis = bypassing 90% of D in product stream 3

i.e.,

$$d = 90\% \cdot 10 = 9 \text{ (moles/hr) ... amount of D bypassed}$$

since

$$Z_C = \frac{20}{20 + 25} = \frac{20 - c}{(20 - c) + (25 - 9)} \quad [6.1 - 7]$$

Solving for  $c$  (amount of C bypassed) gives,

$$c = 7.2 \text{ (moles/hr)}$$

- Feasibility Analysis for the top product (1 2 1') : there are two possibilities for subsequent separations; i.e., 1 2/1' and 1/2 1'. But we observe that from the original CAD (Figure 4 on page 21), a bypass is possible for the combined overhead stream 1 2 (equivalent to 1 2 1' in Figure 33 on page 99). We can make the following calculations by referring to Figure 4 on page 21 and Figure 33 on page 99 :

Basis = bypassing 90% of B in product stream 1

i.e.,

$$b = 90\% \cdot 12.5 = 11.25 \text{ (moles/hr) ... amount of B bypassed}$$

since

$$Z_A = \frac{25}{25 + 25 + 5} = \frac{25 - a}{(25 - a) + (25 - 11.25) + (5 - c')} \quad [6.1 - 8]$$

$$Z_C = \frac{5}{25 + 25 + 5} = \frac{5 - c'}{(25 - a) + (25 - 11.25) + (5 - c')} \quad [6.1 - 9]$$

Solving for  $a$  and  $c'$  gives,

$$a = 11.25 \text{ (moles/hr) ; } c' = 2.25 \text{ (moles/hr)}$$

Again, the heuristics can be employed to resolve the next split (see also Table 8 on page 105) :

M1: Separation factors ( $\Delta$ 's) are large enough to use ordinary distillation.

M2: Use high pressure to avoid refrigeration.

S1: Not applicable.

S2: Not applicable.

C1: Remove product 2 first (since it is most plentiful) ---> either 1/2 1' or 1 2/1'.

C2: The computed CES's for each split are given in Table 8 on page 105. One finds that the values of the CESs are relative close.

C3: By inspecting the CAD shown in Figure 33 on page 99, one can identify a bypass. This bypass leaves products 1 and 2 to be separated near the end, instead of products 1' and 2. Therefore, split 1 2/1' is chosen here.

We then calculate new component flow rates after bypassing (still referring to Figure 33<sup>4</sup> on page 99) :

Basis = amount of A bypassed

i.e.,

$$a' = 90\% \cdot 10 = 9 \text{ (moles/hr)}$$

since

$$Z_A = \frac{(25 - a)}{(25 - a) + 12.5} = \frac{25 - a - a'}{(25 - a - a') + (12.5 - b')} \quad [6.1 - 10]$$

Solving for b' gives,

Table 8. SST for Splits in the CAD

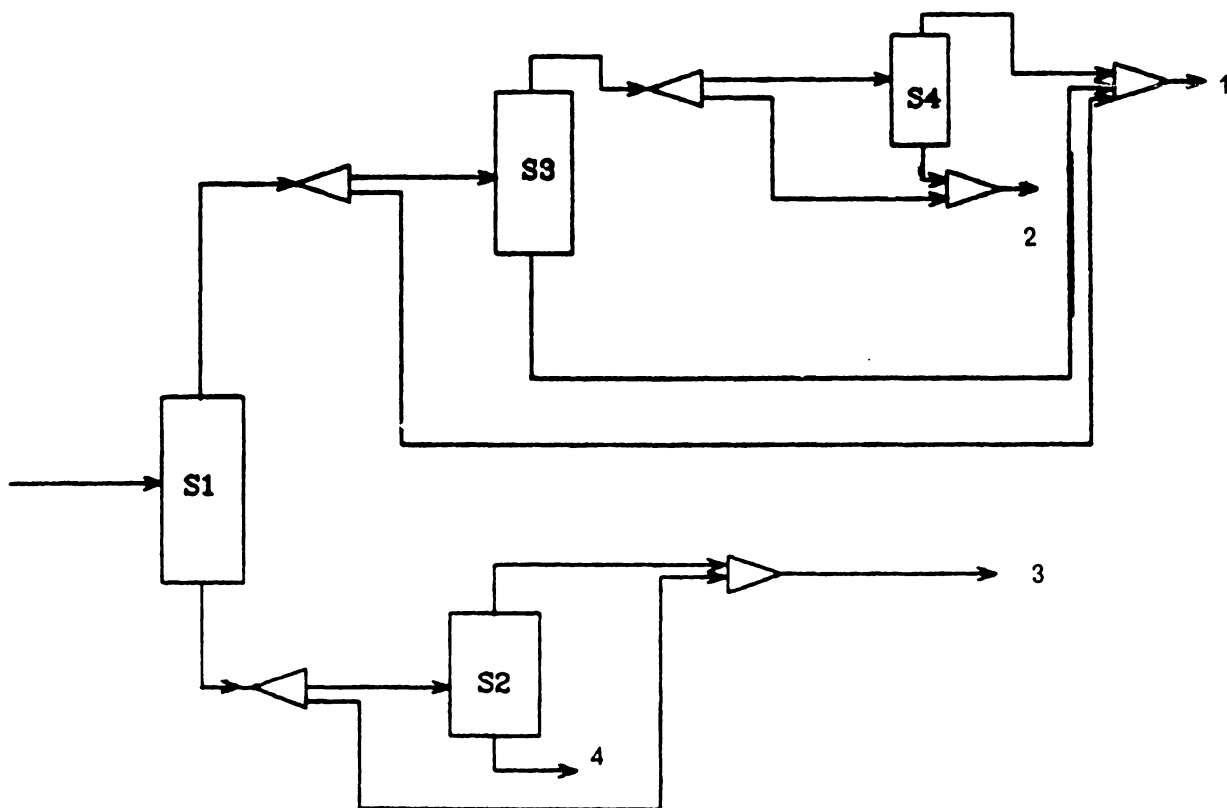
Separation	ovhd/btm	LK/HK	$\Delta^\circ\text{C}$	$\frac{d}{b} _{LLK2}$	$\frac{d}{b} _{LLK1}$	$\frac{d}{b} _{LK}$	$\frac{d}{b} _{HK}$	$\frac{d}{b} _{HHK1}$	$\frac{d}{b} _{HHC2}$	CES
NS(MSP)	1,2/1'	A/B	36.6			$\frac{0.98}{0.02}$	$\frac{0.009}{0.091}$	$\frac{0.6814}{0.3186}$		abandoned
SS(SSP)	"	B/C	32.7	$\frac{0.9996}{0.0008}$		$\frac{0.909}{0.091}$	$\frac{0.02}{0.98}$			3.84
S	"	A/C	69.3			$\frac{0.98}{0.02}$	$\frac{0.02}{0.98}$	$\frac{d}{b}$	$\frac{d}{b} \text{ INTER} = \frac{0.30}{0.70}$	abandoned
SS(SSP)	1/2,1'	A/B	36.6			$\frac{0.2727}{0.7273}$	$\frac{0.02}{0.98}$			7.36

---


$$b' = 8.18 \text{ (moles/hr)}$$

Putting these all together, one can sketch the complete flowsheet (*sequence a*), as shown in Figure 34 on page 106.

Another sequence (*sequence b*) can also be synthesized, if one chooses split 1 2/1' 3 4, which has the largest value of CES among several options for the initial split (see Table 7 on page 100).



Separator	LK	HK	$\frac{d}{b} \Big _{LK}$	$\frac{d}{b} \Big _{HK}$
S1	B	C	$\frac{0.98}{0.02}$	$\frac{0.2}{0.8}$
S2	C	D	$\frac{0.98}{0.02}$	$\frac{0.0625}{0.9375}$
S3	B	C	$\frac{0.909}{0.091}$	$\frac{0.02}{0.98}$
S4	A	B	$\frac{0.7825}{0.2105}$	$\frac{0.02}{0.98}$

Figure 35. The Flowsheet of Proposed Sequence a (Example 1)

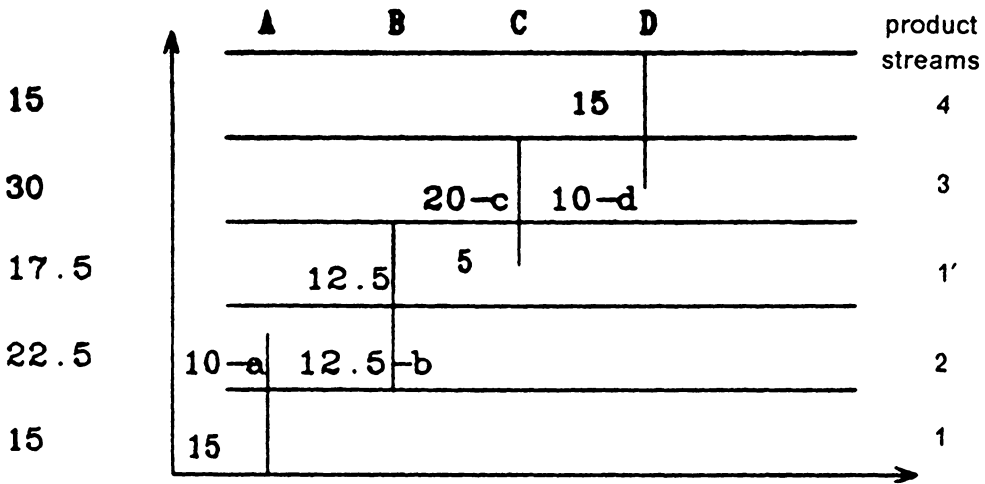


Figure 35. CAD Used for Synthesis of Sequence b

Thus, after the initial split 1 2/1' 3 4 has been selected, one performs the feasibility analysis on splits 1 2 and 1' 3 4. A new CAD (see Figure 35) is created to aid in the following analysis.

- Feasibility Analysis for the overhead product 1 2 : Bypassing can be done as follows.

Basis = bypassing 90% of A in product stream 2

i.e.,

$$a = 90\% \cdot 10 = 9 \text{ (moles/hr)}$$

since

$$Z_A = \frac{25}{25 + 12.5} = \frac{25 - a}{(25 - a) + (12.5 - b)} \quad [6.1 - 11]$$

Solving for C (amount of C bypassed) gives,

$$b = 4.5 \text{ (moles/hr)}$$

Table 9. First SST for Sequence b in Example 1

Separation	ovhd/btm	LK/HK	$\Delta^\circ C$	$\frac{d}{b} \Big _{LLK1}$	$\frac{d}{b} \Big _{LK}$	$\frac{d}{b} \Big _{HK}$	$\frac{d}{b} \Big _{HHK1}$	CBS
SS(SSP)	1'3 4	B/C	32.7		$\frac{0.98}{0.02}$	$\frac{0.2}{0.8}$	$\frac{0.02}{0.98}$	10.00
NS(SSP)	"	C/D	29.7	$\frac{0.7858}{0.2144}$	$\frac{0.2}{0.8}$	$\frac{0.02}{0.98}$		abandoned
S	"	B/D	62.4		$\frac{0.98}{0.02}$	$\frac{0.02}{0.98}$	$\frac{d}{b} \Big _{INTER} = \frac{0.29}{0.71}$	abandoned
SS(SSP)	1' 3/4	C/D	29.7		$\frac{0.98}{0.02}$	$\frac{0.40}{0.60}$		9.04

- Feasibility Analysis for the bottoms product 1' 3 4 : Bypassing is not applicable at this point. Before we proceed to the heuristic-synthesis step, we develop an SST for possible splits (see the Table above).

Then, heuristics can be applied in the following manner :

M1: Separation factors (  $\Delta$ 's ) are large enough to use ordinary distillation.

M2: Not applicable.

S1: Not applicable.

S2: Not applicable.



C1: Remove product stream 3 first. Either split 1'3 4 or split 1' 3/4 will be chosen.

C2: From the computed values of CES's in Table 9 on page 108, split 1'3 4 with the largest CES value is preferred.

Next, for the bottoms product of split (3 4), bypassing calculations are performed as follows :

Basis = bypassing 90% of D in product stream 3

i.e.,

$$d = 90\% \cdot 10 = 9 \text{ (moles/hr)}$$

since

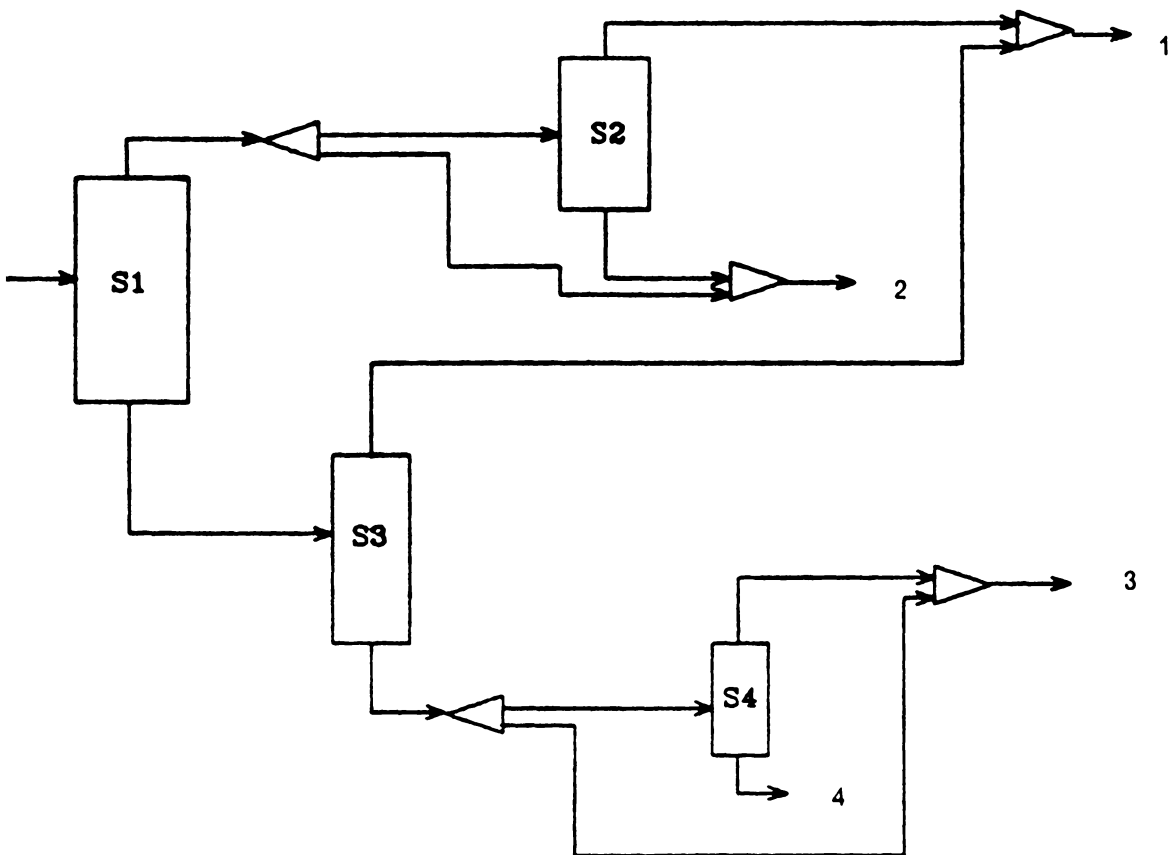
$$Z_D = \frac{25}{25 + 20} = \frac{25 - d}{(25 - d) + (20 - c)} \quad [6.1.11]$$

Solving for c (amount of C bypassed) gives,

$$c = 7.2 \text{ (moles/hr)}$$

The final flowsheet of **sequence b** is given in Figure 36 on page 110.

Among all possible initial splits, split 1/2 1' 3 4 has the next lower CES value (see Table 7 on page 100) than splits 1 2 1'3 4 (Column S1 in Sequence a) and 1 2/1' 3 4 (Column S1 in Sequence b). Starting from this split, the subsequent separation scheme can be constructed.



Separator	LK	HK	$\frac{d}{b} \Big _{LK}$	$\frac{d}{b} \Big _{HK}$
S1	A	B	$\frac{0.98}{0.02}$	$\frac{0.5}{0.5}$
S2	A	B	$\frac{0.9375}{0.0625}$	$\frac{0.02}{0.98}$
S3	B	C	$\frac{0.98}{0.02}$	$\frac{0.2}{0.8}$
S4	C	D	$\frac{0.98}{0.02}$	$\frac{0.0625}{0.9375}$

Figure 37. The Flowsheet of Proposed Sequence b (Example 1)

Table 10. SST for Synthesis of Sequence c in Example 1

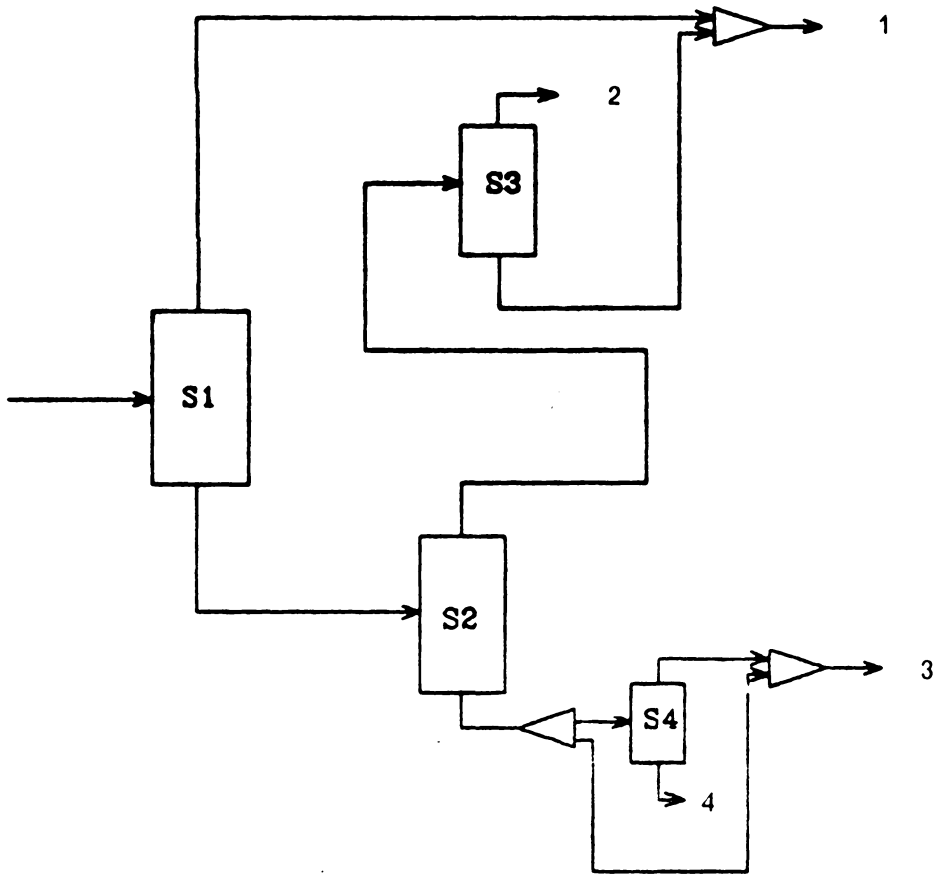
Separation	ovhd/btm	LK/HK	$\Delta^\circ C$	$\frac{d}{b} _{LLK2}$	$\frac{d}{b} _{LLK1}$	$\frac{d}{b} _{LK}$	$\frac{d}{b} _{HK}$	$\frac{d}{b} _{HHK1}$	$\frac{d}{b} _{HHK2}$	CES
SS(SSP)	2 1' 3/4	C/D	29.7			$\frac{0.98}{0.02} $	$\frac{0.4}{0.6}$			6.13
BS(SSP)	2 1' 3 4	B/C	32.7			$\frac{0.98}{0.02} $	$\frac{0.2}{0.6}$	$\frac{0.0018}{0.9982}$		22.84
S	"	B/D	62.4			$\frac{0.98}{0.02} $	$\frac{0.02}{0.98}$	$\frac{d}{b}$	$\frac{0.295}{INTER}$	abandoned
NS(SSP)	"	C/D	29.7		$\frac{0.79}{0.21}$	$\frac{0.2}{0.8}$	$\frac{0.02}{0.98}$			43.62

First, splits 2 1' 3/4 and 2 1' 3 4 will stand out after making use of heuristic C1. However, by comparing their CES values (see Table 10), 2 1' 3 4 is chosen and the rest is obvious.

The flowsheet of this sequence (*sequence c*) is given in Figure 37 on page 112.

### Sensitivity of CES Ranking to Relative Volatility Values

In this section, we will use Example 1 to study the sensitivity of the ranking of CES to relative volatility values. Basically in our work, CES can be evaluated by using the difference in normal boiling point or separation factor  $\Delta$ . Of course, the most accurate way to calculate CES which would reflect the real ease of separation is through using relative volatilities of components taken at actual feed conditions.



Separator	LK	HK	$\frac{d}{b}$   LK	$\frac{d}{b}$   HK
S1	A	B	$\frac{0.6}{0.4}$	$\frac{0.02}{0.98}$
S2	B	C	$\frac{0.98}{0.02}$	$\frac{0.2}{0.8}$
S3	B	C	$\frac{0.5}{0.5}$	$\frac{0.02}{0.98}$
S4	C	D	$\frac{0.98}{0.02}$	$\frac{0.0625}{0.9375}$

Figure 38. The Flowsheet of Proposed Sequence c (Example 1)

**Table 11. Comparison of CES's for the Initial Splits in Example 1**

split	LK/HK	P(psia)	T(°F)	$K_A$	$K_B$	$K_C$	$K_D$	CES <sup>I</sup>	rank	CES <sup>II</sup>	rank
1/2 1' 3 4	A/B	67.6	197.8	2.46	1.00	0.47	0.21	6.22	4	13.82	5
1 2/1' 3 4	A/B	52.0	177.0	2.55	0.98	0.44	0.19	23.36	1	56.86	1
1 2/1' 3 4	B/C	52.0	177.0	2.55	0.98	0.44	0.19	20.91	3	43.57	3
1 2 1'/3 4	B/C	40.9	158.9	2.70	0.98	0.42	0.17	21.02	2	47.59	2
1 2 1' 3/4	C/D	30.0	137.0	2.80	0.98	0.38	0.15	5.05	5	14.50	4

Taking all the splits in Table 7 on page 100, Table 8 on page 105, and Table 9 on page 108 as examples, some observations can be made (see Table 11 on page 113, Table 12, and Table 13); that is, two different ways of determining CES (superscripts I and II represent CES values obtained through normal-boiling-point difference, and through relative volatility, respectively) would generally result in the same ranking orders. One should, however, be aware that for whatever CES measure is used, rank should be treated the same only when CES values (evaluated through normal-boiling-point difference) of two different splits are small, say, less than 10, and within 20 percent or within 10 percent when CES's are large. In other words, it is more accurate to evaluate CES's using the normal-boiling-difference if their values are relatively large.

**Table 12. Comparison of CES's for Candidate Separations of Split (1 2 1') in Example 1**

split	LK/HK	P(psia)	T(°C)	$K_A$	$K_B$	$K_C$	CES'	rank	CES''	rank
1/2 1'	A/B	67.0	91.6	1.80	0.70	0.295	7.36	1	17.59	1
1 2/1'	B/C	45.4	71.1	1.65	0.58	0.225	3.34	2	8.92	2

**Table 13. Comparison of CES's for Candidate Separations of Split (1' 3 4) in Example 1**

split	LK/HK	P(psia)	T(°C)	$K_B$	$K_C$	$K_D$	CES'	rank	CES''	rank
1/3 4	B/C	30.0	110.6	2.238	0.950	0.427	10.00	1	23.00	1
1 3/4	C/D	30.0	110.6	2.238	0.950	0.427	9.04	2	20.72	2

## 6.2 Example Problem 2

### 6.2.1 Case A

An example problem involving the fractionation of thirteen refinery light-end components into seven product streams (Tedder, 1984) is given herein, which is a modified version of Case B (Watkins, 1979). The original data are given below. Also, product specifications have been converted to the form of CAD shown in Figure 38 on page 117.

Components	Product Flow Rates						
	1	2	3	4	5	6	7
A. C <sub>3</sub>	118.08	3.11					
B. i-C <sub>4</sub>	1.47	54.63	2.88	0.60			
C. n-C <sub>4</sub>	1.47	5.77	109.60	2.99			
D. i-C <sub>5</sub>			1.50	49.20	8.68	0.58	
E. n-C <sub>5</sub>			0.63	9.08	51.43	1.55	
F. cyclC <sub>5</sub>					0.81	28.53	3.17
G. 22DMB					0.07	5.25	1.31

H. 23DMB	0.05	7.53	3.23
I. 2MEP		18.82	43.90
J.3MEP		7.92	31.69
K.n-C <sub>6</sub>		8.02	72.31
L.C <sub>6</sub> H <sub>6</sub>		2.39	21.52
M.C <sub>7</sub> <sup>+</sup>			7.37

---

- **Feasibility Analysis** - The Separation Specification Tables for all possible first splits and final splits are given in Table 14 on page 118 and Table 15 on page 119, respectively, in which one can find some questionable splits associated with distributed non-keys. However, since most products are treated as fuels and are blended together later for burning, we would not be concerned about that (i.e., assume that all splits are feasible).

- **Heuristic Synthesis** -

M1: Separation factors are large enough to use ordinary distillation.

M2: Refrigeration operated at high pressure is needed to distill off species of very low boiling point.

S1: Not applicable.

S2: Perform difficult separation later - i.e., avoid split 1234/567 with the smallest  $\Delta$  (see Table 14 on page 118).



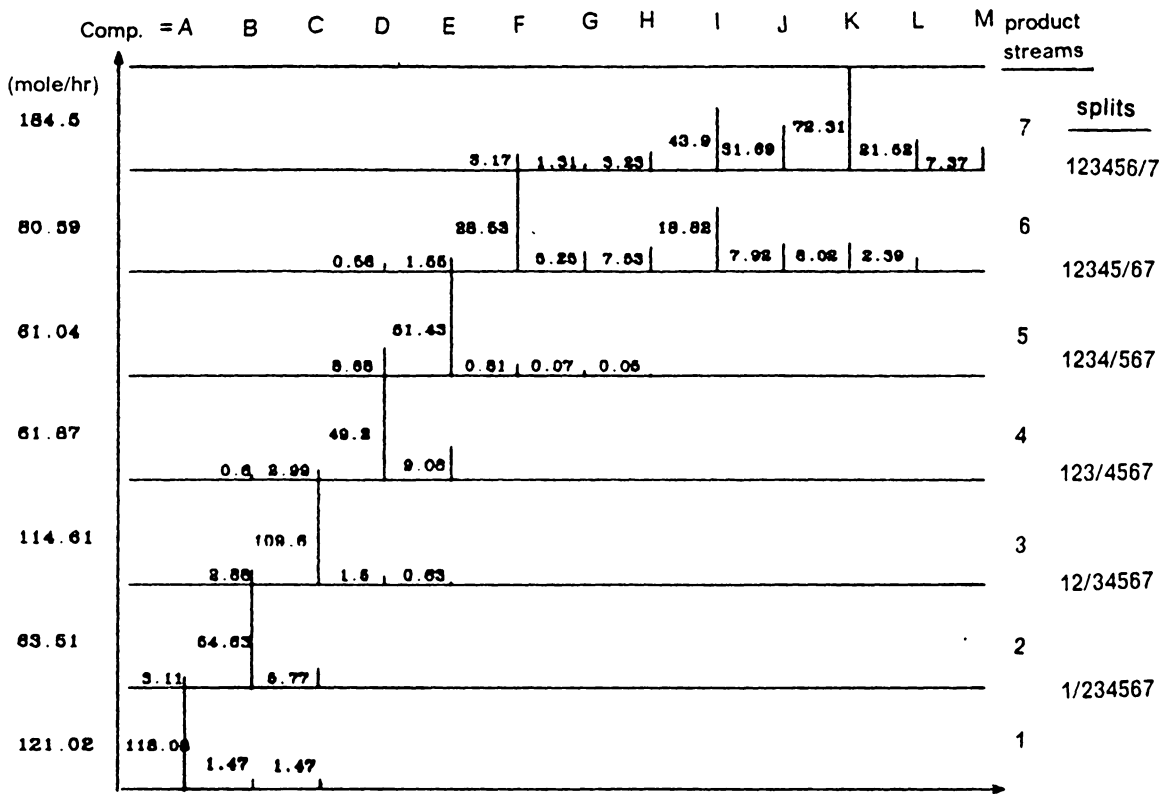


Figure 38. CAD of Example 2A

Table 14. SST for the First Splits in Example 2A

CES	Separation	ovhd/btm	LK/HK	$\Delta^\circ\text{C}$	$\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$							
					LLK3	LLK2	LLK1	LK	HK	HK1	HK2	HK3
3.675	SS(MSP)	1/234567	A/B	30.2				0.974	0.025	0.013		
								0.026	0.976	0.988		
3.114	SS(MSP)	12/34567	B/C	11.3				0.948	0.08			
								0.068	0.94			
12.367	SS(MSP)	123/4567	C/D	28.3			0.99	0.975	0.025	0.01		
							0.01	0.026	0.976	0.99		
9.079	SS(MSP)	1234/567	D/E	8.2				0.846	0.156			
								0.166	0.846			
9.660	SS(MSP)	12345/67	E/F	13.2			0.99	0.975	0.025	0.01	0.005	
							0.01	0.026	0.976	0.99	0.995	
7.440	SS(MSP)	123456/7	G/J	13.6	0.9	0.8	0.701	0.3	0.2	0.1	0.1	
					0.1	0.2	0.299	0.7	0.8	0.9	0.9	
							(comp. G)			(comp. J)		

C1: Not applicable.

C2: Split 123/4567 has the largest CES (see the above table).

C3: Not applicable.

----> Thus, the first split is 123/4567.

Table 15. SST for the Last Splits in Example 2A

Separation	ovhd/btm	LK/RK	$\Delta$ °C	$\frac{d}{b}$ LLLS	$\frac{d}{b}$ LLK2	$\frac{d}{b}$ LLK1	$\frac{d}{b}$ LK	$\frac{d}{b}$ RK	$\frac{d}{b}$ RKK1	$\frac{d}{b}$ RKK2	$\frac{d}{b}$ RKK3
SS(MSP)	1/2	A/B	30.2				0.974	0.026	0.803		
							0.026	0.974	0.797		
SS(MSP)	2/3	B/C	11.3				0.950	0.050			
							0.050	0.950			
SS(MSP)	3/4	C/D	28.9			0.830	0.973	0.030	0.060		
						0.170	0.027	0.970	0.940		
SS(MSP)	4/5	D/E	8.8				0.850	0.150			
							0.150	0.850			
SS(MSP)	5/6	E/F	13.2			0.935	0.971	0.028	0.018	0.007	
						0.065	0.029	0.972	0.987	0.993	
SS(MSP)	6/7	G/J	13.6	0.999	0.900	0.800	0.700	0.300	0.200	0.100	0.100
				0.001	0.100	0.200	0.300	0.700	0.800	0.900	0.900

Table 16. SST for Split (123)

CES	Separation	ovhd/btm	LE/HK	$\Delta^\circ\text{C}$	$\frac{d}{b} _{LLK3}$	$\frac{d}{b} _{LLK2}$	$\frac{d}{b} _{LLK1}$	$\frac{d}{b} _{LK}$	$\frac{d}{b} _{HK}$	$\frac{d}{b} _{HSK1}$	$\frac{d}{b} _{HSK2}$
11.66	SS(MSP)	1/2 3	A/B	30.2				0.9745	0.0249	0.0126	
								0.0267	0.9751	0.9874	
6.13	SS(MSP)	1 2/3	B/C	11.3				0.9618	0.0382		
								0.0486	0.9580		

For split (123), the top product of the first column, the Separation Specification Table is given in Table 16.

- **Heuristic Synthesis** - for downstream separation of split (123)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult split 12/3 later.

C1: Not applicable.

C2: CES values have been computed and given in Table 16.

C3: Not applicable.

----> The choice is split 1/23.

For split (4567), the corresponding SST is given in Table 17 on page 122.

- **Heuristic Synthesis** - for downstream separation of split (4567)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Not applicable since separation factors are relatively close.

C1: Remove product stream 7 (relatively plentiful product flow) first.

C2: Computed CES's are given in Table 17 on page 122.

C3: Not applicable.

----> Split 456/7 will be chosen as the next separation.

Table 17. SST for Split (4567)

CES	Separation	ovhd/btm	LK/HK	$\Delta^\circ\text{C}$	$\frac{d}{N_{LLKS}}$	$\frac{d}{N_{LLKS}}$	$\frac{d}{N_{LLK1}}$	$\frac{d}{N_{LK}}$	$\frac{d}{N_{HK}}$	$\frac{d}{N_{HK1}}$	$\frac{d}{N_{HK2}}$	$\frac{d}{N_{HK3}}$
1.88	SS(MSP)	4/567	D/E	8.8				0.8416	0.1463			
								0.1584	0.8537			
9.45	SS(MSP)	45/67	E/F	13.2			0.9901	0.9750	0.0249	0.0106		
							0.0099	0.0250	0.9751	0.9894		
18.27	SS(MSP)	456/7	G/J	13.6			0.9025	0.8024	0.7012	0.3001	0.1999	0.0998
							0.0975	0.1976	0.2988	0.6999	0.8001	0.9002

Table 18. SST for Split (456)

CES	Separation	ovhd/btm	LK/HK	$\Delta^\circ\text{C}$	$\frac{d}{N_{LLKS}}$	$\frac{d}{N_{LLKS}}$	$\frac{d}{N_{LLK1}}$	$\frac{d}{N_{LK}}$	$\frac{d}{N_{HK}}$	$\frac{d}{N_{HK1}}$	$\frac{d}{N_{HK2}}$	$\frac{d}{N_{HK3}}$
4.33	SS(MSP)	4/56	D/E	8.2				0.842	0.148			
								0.158	0.854			
4.96	SS(MSP)	45/6	E/F	13.2			0.99	0.975	0.025	0.013	0.007	
							0.01	0.025	0.975	0.987	0.993	

For split (456), the corresponding SST is given in Table 18.

- **Heuristic Synthesis** - for downstream separation of split (456)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Boiling point differences for two splits are relatively close.

C1: Product flow rates are close too.

C2: Only small difference between the CES of split 4/56 and that of split 45/6 is observed.

C3: Not applicable.

---> Let's choose 45/6 as the next split, but it should be noted that both 4/56 and 45/6 are almost equally good. The simplified flowsheet of this sequence (**sequence a**) is depicted in Figure 39 on page 124.

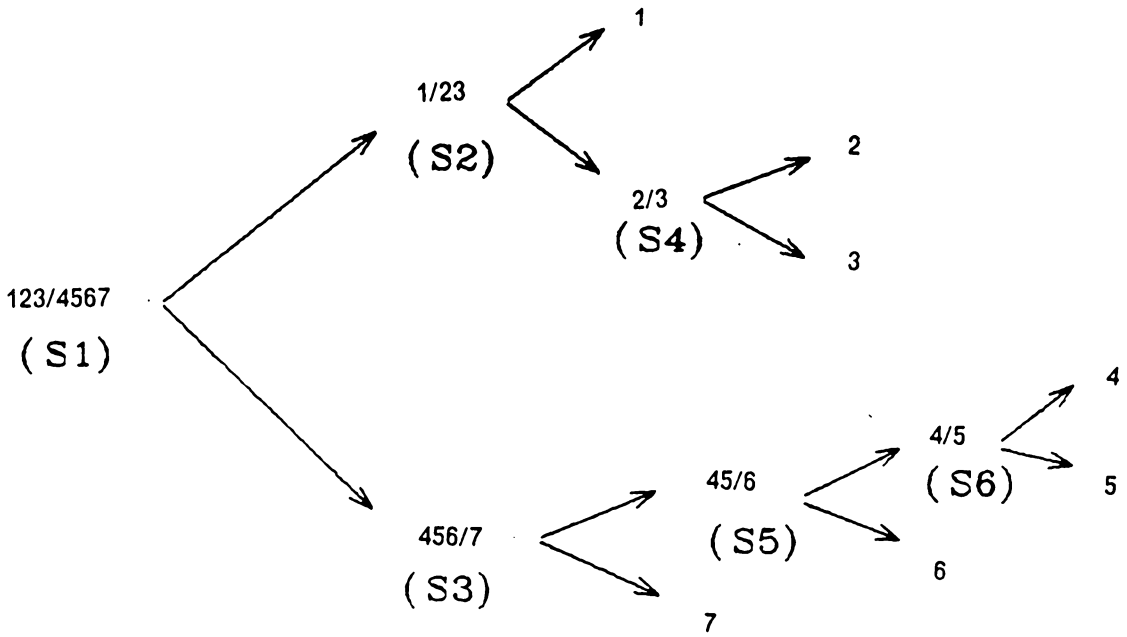
The **second sequence** will be synthesized as follows.

- **Heuristic Synthesis** - for the initial separation of the feed stream (1234567)

M1-C1: See the first initial sequence.

C2: By excluding split 1234/567 which does not satisfy the constraint imposed by heuristic S2 and also split 123/4567 which has already been used in Sequence a, one will pick split 123456/7 having the second largest CES.

C3: Not applicable.



Separator	LK	HK	$\frac{d}{b} \Big _{LK}$	$\frac{d}{b} \Big _{HK}$
S1	C	D	$\frac{0.975}{0.025}$	$\frac{0.025}{0.975}$
S2	A	B	$\frac{0.9743}{0.0257}$	$\frac{0.0249}{0.9751}$
S3	G	J	$\frac{0.8024}{0.1976}$	$\frac{0.1999}{0.8001}$
S4	B	C	$\frac{0.95}{0.05}$	$\frac{0.05}{0.95}$
S5	E	F	$\frac{0.975}{0.025}$	$\frac{0.028}{0.972}$
S6	D	E	$\frac{0.850}{0.150}$	$\frac{0.150}{0.850}$

Figure 40. Simplified Flowsheet of Proposed Sequence a (Example 2A)



Table 19. SST for Split (123456)

CES	Separation	ovhd/btm	LE/HK	$\Delta^\circ\text{C}$	$\frac{d}{d_{LLK3}}$	$\frac{d}{d_{LLK2}}$	$\frac{d}{d_{LLK1}}$	$\frac{d}{d_{LK}}$	$\frac{d}{d_{HK}}$	$\frac{d}{d_{HEK1}}$	$\frac{d}{d_{HEK2}}$
6.46	SS(MSP)	1/23456	A/B	30.2				$\frac{0.974}{0.026}$	$\frac{0.026}{0.974}$	$\frac{0.012}{0.988}$	
4.92	SS(MSP)	12/3456	B/C	11.3				$\frac{0.942}{0.058}$	$\frac{0.06}{0.94}$		
10.90	SS(MSP)	123/456	C/D	28.3			$\frac{0.99}{0.01}$	$\frac{0.976}{0.024}$	$\frac{0.026}{0.974}$	$\frac{0.01}{0.99}$	
3.93	SS(MSP)	1234/56	D/E	6.2				$\frac{0.846}{0.154}$	$\frac{0.156}{0.844}$		
1.44	SS(MSP)	12345/6	E/F	13.2			$\frac{0.99}{0.01}$	$\frac{0.976}{0.024}$	$\frac{0.026}{0.974}$	$\frac{0.013}{0.987}$	$\frac{0.007}{0.993}$

For split (123456) , the SST is given in Table 19 on page 125.

- **Heuristic Synthesis** - for downstream separation of split (123456)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult split 1234/56 later.

C1. Product stream 1 should be removed first.

C2: Split 123/456 has the largest CES value.

C3: Not applicable.

---> Even though split 123/456 has the largest CES of 10.9, split 1/23456 is chosen because C1 overrides C2.

For the bottoms product of the preceding split, (23456), the SST is given in Table 20 on page 127. Next, the heuristic-synthesis step is invoked to decide the following separation task.

- **Heuristic Synthesis** - for downstream separation of split (23456)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult split 234/56 later.

C1: Not applicable.

C2: Split 23/456 has the largest CES value.

C3: Not applicable.

---> Let's choose 45/6 as the next split, but one should realize split 45/6 and split 4/56 are almost equally good. At this point, the whole separation scheme can be synthesized, as shown in Figure 40 on page 128.

The **third sequence** will be synthesized as follows. By examining all the remaining first-split candidates (see Table 14 on page 118), one finds that CES values of all the splits tend to

Table 20. SST for Split (23456)

CES	Separation	ovhd/btm	LK/HK	$\Delta$ °C	$\frac{d}{d_{LLK3}}$	$\frac{d}{d_{LLK2}}$	$\frac{d}{d_{LLK1}}$	$\frac{d}{d_{LK}}$	$\frac{d}{d_{HK}}$	$\frac{d}{d_{HK1}}$	$\frac{d}{d_{HK2}}$
1.84	SS(MSP)	2/3456	B/C	11.3				<u>0.940</u>	<u>0.049</u>		
								0.060	0.951		
14.08	SS(MSP)	23/456	C/D	28.9				<u>0.990</u>	<u>0.976</u>	<u>0.026</u>	<u>0.010</u>
								0.010	0.025	0.975	0.990
6.92	SS(MSP)	234/56	D/E	8.8				<u>0.946</u>	<u>0.155</u>		
								0.164	0.846		
2.03	SS(MSP)	2345/6	E/F	13.2				<u>0.990</u>	<u>0.976</u>	<u>0.028</u>	<u>0.013</u>
								0.010	0.025	0.978	0.987
										<u>0.007</u>	<u>0.993</u>

be low except that of split (1234/567). Since the negative factor (i.e., heuristic S2) against the split (1234/567) is a relative measure ( $\Delta < 20^\circ F$ ) and there is no other competitive alternative in terms of CES values, it is clear that split (1234/567) may be considered.

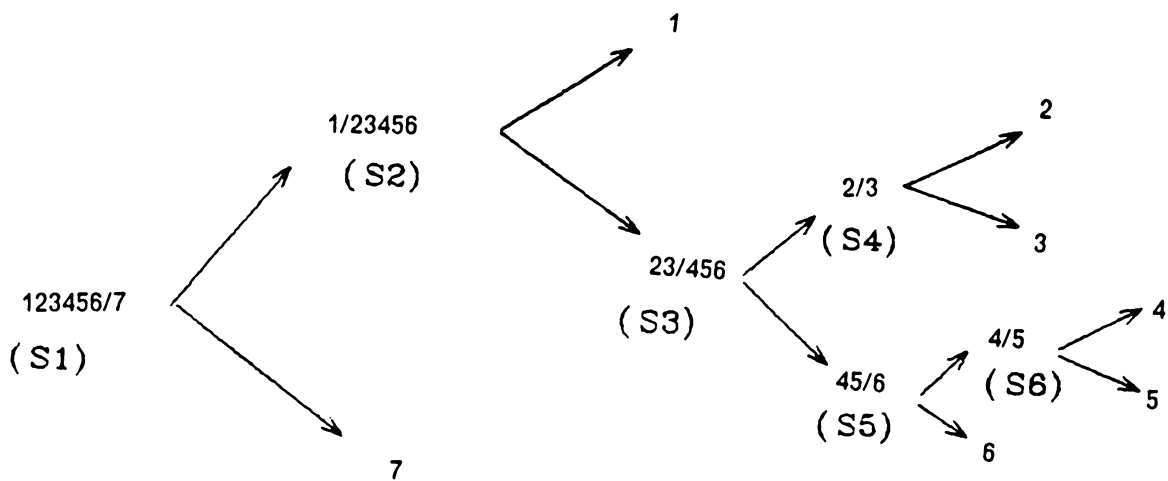
We will proceed to carry on the heuristic synthesis without transformation of the product set (note that there is an unlikely component split existing in split 123/4 - that is, component E), knowing that the present step is based on the fact that all products are treated as fuels.

- **Heuristic Synthesis** - for downstream separation of split (1234)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult separation - 12/34 later.



Separator	LK	HK	$\frac{d}{b} \Big _{LK}$	$\frac{d}{b} \Big _{HK}$
S1	G	J	$\frac{0.8}{0.2}$	$\frac{0.2}{0.8}$
S2	A	B	$\frac{0.974}{0.026}$	$\frac{0.025}{0.975}$
S3	C	D	$\frac{0.9750}{0.0250}$	$\frac{0.025}{0.975}$
S4	B	C	$\frac{0.95}{0.05}$	$\frac{0.05}{0.95}$
S5	E	F	$\frac{0.975}{0.025}$	$\frac{0.028}{0.972}$
S6	D	E	$\frac{0.85}{0.15}$	$\frac{0.15}{0.85}$

Figure 41. Simplified Flowsheet of Proposed Sequence b (Example 2A)

Table 21. SST for Split (1234)

CES	Separation	ovhd/btm	LK/HK	$\Delta^{\circ}C$	$\frac{d}{W_{LLKCS}}$	$\frac{d}{W_{LLKCB}}$	$\frac{d}{W_{LLKCI}}$	$\frac{d}{W_{LK}}$	$\frac{d}{W_{HK}}$	$\frac{d}{W_{HKCI}}$
0.07	SS(MSP)	1/234	A/B	30.2				0.974	0.025	0.018
								0.026	0.975	0.988
0.11	SS(MSP)	12/34	B/C	11.3				0.942	0.050	
								0.058	0.940	
3.40	SS(MSP)	123/4	C/D	28.3			0.990	0.975	0.030	0.085
							0.010	0.025	0.970	0.935

C1: Not applicable.

C2: Referring to Table 21, splits 1/234 and 12/34 have close values of CES.

Table 22. SST for Split (234)

CES	Separation	ovhd/btm	LK/HK	$\Delta^{\circ}C$	$\frac{d}{W_{LLKS}}$	$\frac{d}{W_{LLKCB}}$	$\frac{d}{W_{LLKCI}}$	$\frac{d}{W_{LK}}$	$\frac{d}{W_{HK}}$	$\frac{d}{W_{HKCI}}$
2.06	SS(MSP)	2/34	B/C	11.3				0.940	0.049	
								0.050	0.951	
5.71	SS(MSP)	23/4	C/D	28.3			0.975	0.950	0.065	
							0.025	0.970	0.935	

C3: Although future bypassing is possible for split 12/34, we will still pick 1/234 as the next split simply because S2 overrides C2 and C3.

Table 23. SST for Split (567)

CES	Separation	ovhd/btm	LI/HK	$\Delta$ °C	$\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$								
					$\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$								
1.76	SS(MSP)	5/67	E/F	13.2									
10.48	SS(MSP)	56/7	G/J	13.6	0.995	0.902	0.802	0.701	0.300	0.200	0.100	0.100	0.100
					0.005	0.098	0.198	0.299	0.700	0.800	0.900	0.900	0.900

The SST for split (234) is given in Table 22 on page 129. As explained earlier, we will ignore the infeasibility associated with split 23/4.

- **Heuristic Synthesis** - for downstream separation of split (234)

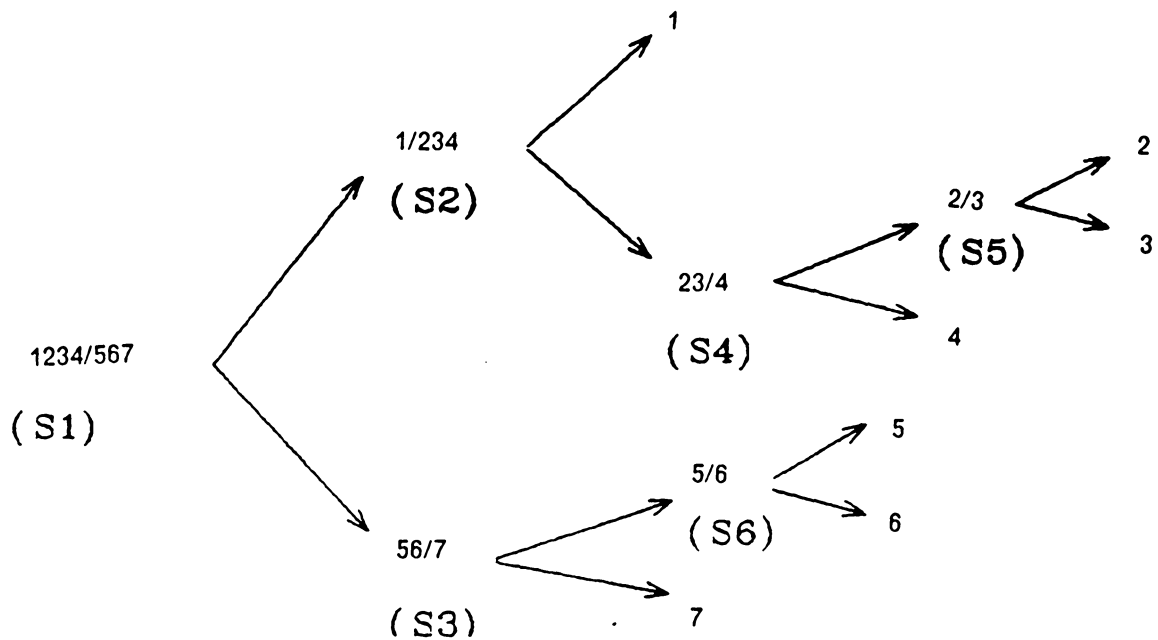
M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult separation 2/34 later.

C1: Not applicable.

C2: Split 23/4 has the largest CES.



Separator	LK	HK	$\frac{d}{b}  _{LK}$	$\frac{d}{b}  _{HK}$
S1	D	E	$\frac{0.845}{0.155}$	$\frac{0.155}{0.845}$
S2	A	B	$\frac{0.974}{0.026}$	$\frac{0.025}{0.975}$
S3	G	J	$\frac{0.802}{0.198}$	$\frac{0.20}{0.80}$
S4	C	D	$\frac{0.975}{0.025}$	$\frac{0.030}{0.970}$
S5	B	C	$\frac{0.95}{0.05}$	$\frac{0.05}{0.95}$
S6	E	F	$\frac{0.971}{0.029}$	$\frac{0.028}{0.972}$

Figure 42. Simplified Flowsheet of Proposed Sequence c (Example 2A)

----> So split 23/4 is chosen.

SST is given For split (567), we will still ignore any infeasibility of splits. The SST is given in Table 23 on page 130. The heuristic-synthesis step is described below.

**Heuristic Synthesis** - for downstream separation of split (567)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Not applicable.

C1: Remove the most plentiful product 7 first.

----> Split 56/7 is chosen as the next split. Summarizing the above analysis, the final flowsheet can be given (i.e., **sequence c**, see Figure 41 on page 131).



## 6.2.2 Case B

This example, taken from Wakins' book (1979), is essentially the same as Example 2A except that two additional products (0 and 8) and one extra component ( $C_2H_6$ ) are included. For simplicity, all product stream data have been converted into the CAD shown in Figure 42 on page 134.

Here we present the SST for the first splits (see Table 24 on page 135); however, it should be noted that the SST looks similar to Table 14 on page 118 but with some minor changes.

**Heuristic Synthesis** - for the initial separation of feed (012345678)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult separation 01234/5678 later.

C1: Remove product stream 8 first. Therefore, split 01234567/8 is preferred because 8 is readily separable. Note that this split has the largest CES value among all the first split candidates.

For bottoms product (01234567), the possible subsequent candidate splits are listed in Table 25 on page 136, along with their feasibility analysis.

- **Heuristic Synthesis** - for downstream separation of split (01234567)

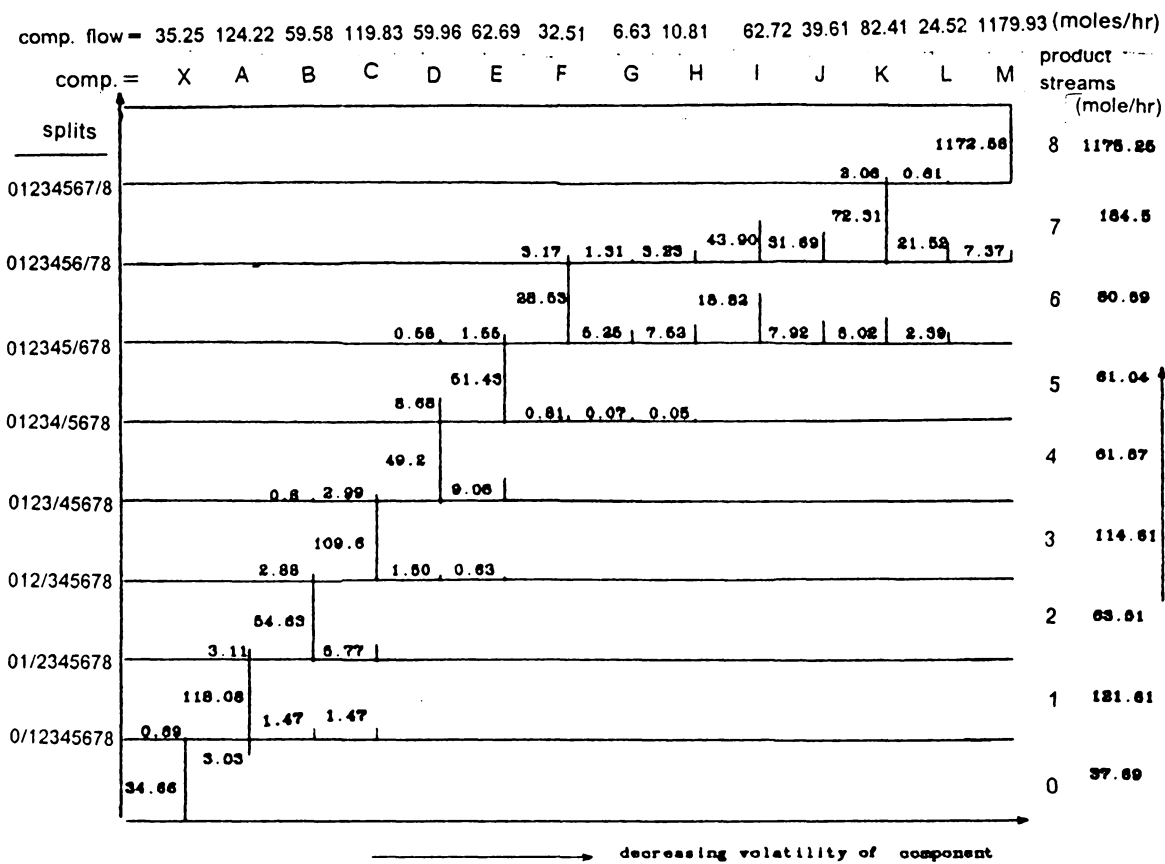


Figure 42. Component Assignment Diagram for Example 2B

Table 24. SST for the First Splits in Example 2B

CES	Separation	ovhd/bcm	LK/HK	$\Delta^{\circ}C$	$\frac{d}{W_{LLK0}}$	$\frac{d}{W_{LLK2}}$	$\frac{d}{W_{LLK1}}$	$\frac{d}{W_{LK}}$	$\frac{d}{b_{HK}}$	$\frac{d}{W_{HK1}}$	$\frac{d}{b_{HK2}}$	$\frac{d}{b_{HK3}}$
0.532	SS(MSP)	01/2345678	X/A	46.5				$\frac{0.976}{0.026}$	$\frac{0.026}{0.976}$			
1.572	SS(MSP)	01/2345678	A/B	30.2				$\frac{0.976}{0.026}$	$\frac{0.026}{0.974}$	$\frac{0.010}{0.090}$		
1.126	.	012/345678	B/C									same as 12/34567 in Table 14
3.459	.	0123/45678	C/D									same as 123/4567 in Table 14
2.572	.	01234/5678	D/E									same as 1234/567 in Table 14
2.380	.	012345/678	E/F									same as 12345/67 in Table 14
6.061	.	0123456/78	G/J									same as 123456/7 in Table 14
28.180	SS(MSP)	01234567/8	L/M	96.6				$\frac{0.976}{0.026}$	$\frac{0.976}{0.026}$	$\frac{0.006}{0.994}$		

Table 25. SST for Split (01234567)

CES	Separation	ovhd/btm	LK/HK	$\Delta$ °C	$\frac{d}{D_{LLK}}$	$\frac{d}{D_{LLEK}}$	$\frac{d}{D_{LLK1}}$	$\frac{d}{D_{LK}}$	$\frac{d}{D_{HK}}$	$\frac{d}{D_{HK1}}$	$\frac{d}{D_{HEK1}}$	$\frac{d}{D_{HEK2}}$
1.44	SS(MSP)	0/1234567	X/A	46.5				$\frac{0.976}{0.020}$	$\frac{0.026}{0.976}$			
4.64	SS(MSP)	01/234567	A/B	30.2				$\frac{0.976}{0.020}$	$\frac{0.026}{0.974}$	$\frac{0.010}{0.990}$		
3.78	.	012/34567	B/C	11.2								same as 12/34567 in Table 14
13.94	.	0123/4567	C/D	28.3								same as 123/4567 in Table 14
8.21	.	01234/567	D/E	8.2								same as 1234/567 in Table 14
4.29	.	012345/67	E/F	13.2								same as 12345/67 in Table 14
6.91	.	0123456/7	G/J	13.6								same as 123456/7 in Table 14

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult separation 01234/567 later.

C1: Not applicable.

C2: Split 0123/4567 has the largest CES.

----> Hence, the second split is 0123/4567.

- **Heuristic Synthesis** - for split (0123)

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult separation 012/3 later.

C1: Not applicable.

C2: Split 01/23 has the largest CES.

----> Split 01/23 will be employed.

Subsequent separation tasks for split (4567) will be 456/7, 45/6, and 4/5, in that order, as demonstrated in sequence a of case A, Example 2. In summary, the flowsheet of **sequence a** can be depicted in Figure 43 on page 139.

If we use other heuristics ranked lower than C1 as in the first sequence, a different first split will evolve as follows :

- **Heuristic Synthesis** - (for split 012345678)

Table 26. SST for Split (0123)

CES	Separation	ovhd/btm	LK/HK	$\Delta$ °C	$\frac{d}{W_{LLK2}}$	$\frac{d}{W_{LLK1}}$	$\frac{d}{W_{LK}}$	$\frac{d}{W_{HK}}$	$\frac{d}{W_{HK1}}$
9.31	88(MBP)	0/123	X/A	46.5			0.975	0.025	
							0.025	0.975	
16.97	88(MBP)	01/23	A/B	30.2			0.975	0.025	0.010
							0.025	0.974	0.990
4.21	88(MBP)	012/3	B/C	11.3			0.951	0.050	
							0.049	0.941	

C2: Among all first split candidates, except for (01234567/8) which is the first split synthesized in the first sequence, split 0123456/78 has the largest CES.

----> Thus, split 0123456/78 is done first. (See Table 24 on page 135.)

- **Heuristic Synthesis** - for split (0123456)

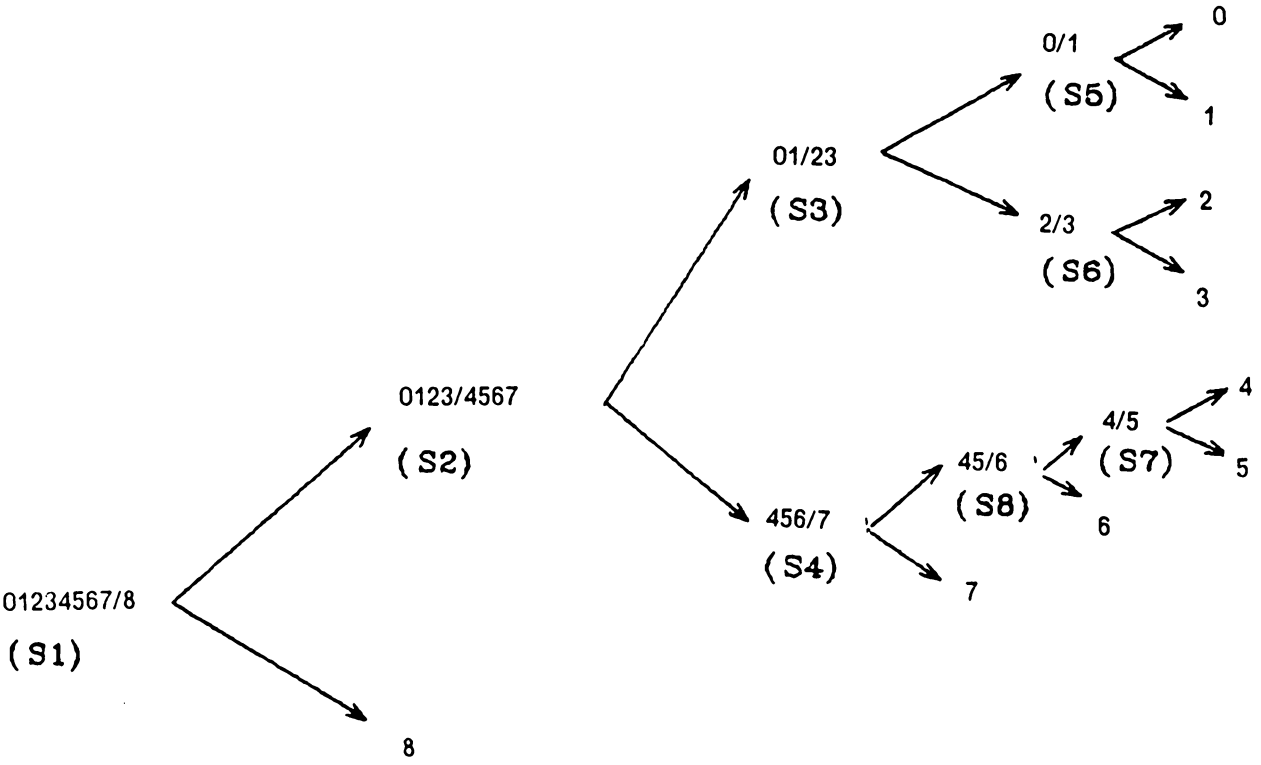
M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult separation, 01234/56 later.

C1: Not applicable.

C2: Split 0123/456 has the largest CES. (See Table 27 on page 140.)



Separator	LK	HK	$\frac{d}{b}   LK$	$\frac{d}{b}   HK$
S1	L	M	$\frac{0.975}{0.025}$	$\frac{0.006}{0.994}$
S2	C	D	$\frac{0.975}{0.025}$	$\frac{0.025}{0.975}$
S3	A	B	$\frac{0.975}{0.025}$	$\frac{0.026}{0.974}$
S4	G	J	$\frac{0.802}{0.198}$	$\frac{0.200}{0.800}$
S5	X	A	$\frac{0.975}{0.025}$	$\frac{0.025}{0.975}$
S6	B	C	$\frac{0.95}{0.05}$	$\frac{0.05}{0.95}$
S7	D	E	$\frac{0.85}{0.15}$	$\frac{0.15}{0.85}$
S8	E	F	$\frac{0.975}{0.025}$	$\frac{0.028}{0.972}$

Figure 43. Simplified Flowsheet of Proposed Sequence a (Example 2B)

Table 27. SST for Split (0123456)

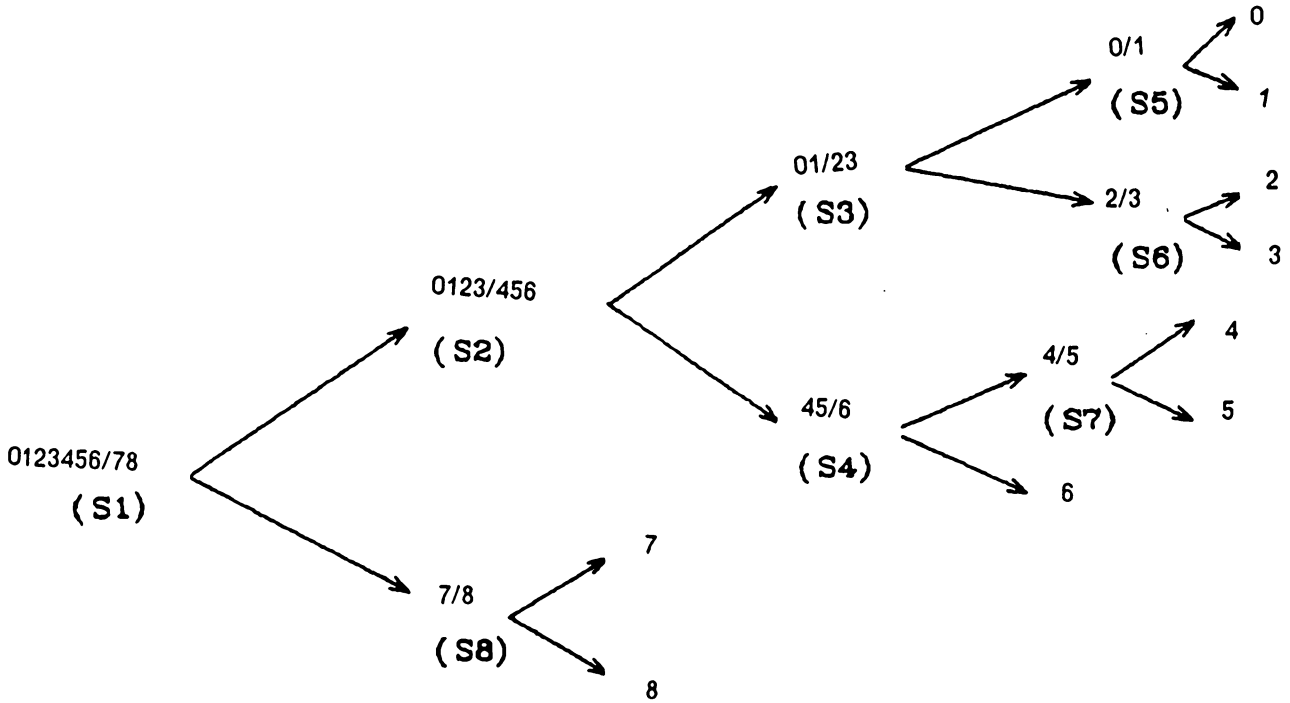
CRS	Separation	ovhd/btm	LK/HK	$\Delta^\circ C$	$\frac{d}{b} \frac{1}{LLK3}$	$\frac{d}{b} \frac{1}{LLK2}$	$\frac{d}{b} \frac{1}{LLK1}$	$\frac{d}{b} \frac{1}{LK}$	$\frac{d}{b} \frac{1}{HK}$	$\frac{d}{b} \frac{1}{HK1}$	$\frac{d}{b} \frac{1}{HK2}$
1.97	SS(MSP)	0/123456	X/A	48.5				$\frac{0.975}{0.025}$	$\frac{0.025}{0.975}$		
7.16	SS(MSP)	01/23456	A/B	30.2				$\frac{0.975}{0.025}$	$\frac{0.026}{0.974}$	$\frac{0.010}{0.990}$	
6.94	SS(MSP)	012/3456	B/C	11.3				$\frac{0.942}{0.058}$	$\frac{0.080}{0.940}$		
9.66	SS(MSP)	0123/456	C/D	28.3			$\frac{0.990}{0.010}$	$\frac{0.975}{0.025}$	$\frac{0.026}{0.975}$	$\frac{0.010}{0.990}$	
3.66	SS(MSP)	01234/56	D/E	8.2				$\frac{0.845}{0.155}$	$\frac{0.155}{0.855}$		
1.32	SS(MSP)	012345/6	E/F	13.2			$\frac{0.990}{0.010}$	$\frac{0.975}{0.025}$	$\frac{0.028}{0.972}$	$\frac{0.013}{0.987}$	$\frac{0.007}{0.993}$

----> Split 0123/456 is therefore chosen.

For splits (0123) and (456), subsequent separations 01/23 and 45/6 are used, as described in sequence a (case B), and sequence a (case A), respectively. Then, the flowsheet for the **second sequence** can be finalized (see Figure 44 on page 141).

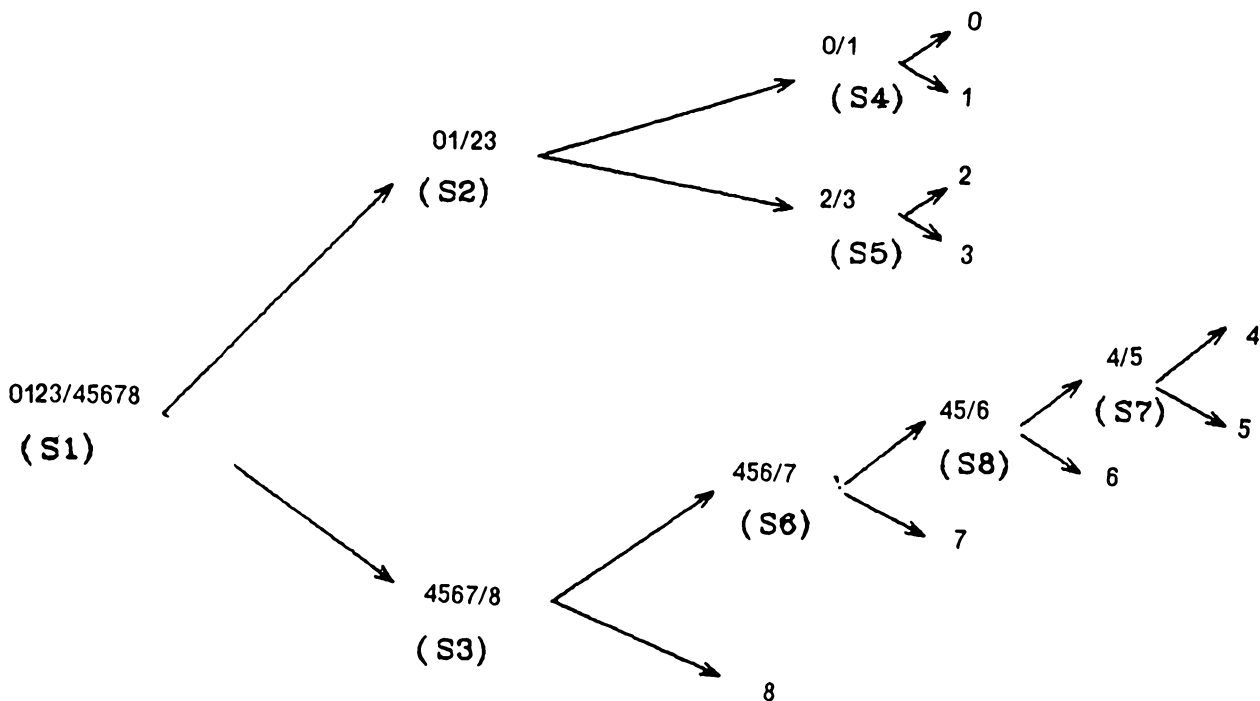
As in the synthesis of the first split of the second sequence, the following split, 0123/45678, which has the third largest CES value (see Table 24 on page 135), is chosen. For overhead





Separator	LK	HK	$\frac{d}{b}   LK$	$\frac{d}{b}   HK$
S1	G	J	$\frac{0.80}{0.20}$	$\frac{0.20}{0.80}$
S2	C	D	$\frac{0.975}{0.025}$	$\frac{0.025}{0.975}$
S3	A	B	$\frac{0.975}{0.025}$	$\frac{0.025}{0.974}$
S4	E	F	$\frac{0.975}{0.025}$	$\frac{0.025}{0.972}$
S5	X	A	$\frac{0.975}{0.025}$	$\frac{0.025}{0.975}$
S6	B	C	$\frac{0.95}{0.05}$	$\frac{0.05}{0.95}$
S7	D	E	$\frac{0.850}{0.150}$	$\frac{0.150}{0.850}$
S8	L	M	$\frac{0.972}{0.028}$	$\frac{0.028}{0.994}$

Figure 44. Simplified Flowsheet of Proposed Sequence b (Example 2B)



Separator	LK	HK	$\frac{d}{b}   \text{LK}$	$\frac{d}{b}   \text{HK}$
S1	C	D	$\frac{0.976}{0.025}$	$\frac{0.025}{0.975}$
S2	A	B	$\frac{0.975}{0.025}$	$\frac{0.028}{0.974}$
S3	L	M	$\frac{0.975}{0.025}$	$\frac{0.008}{0.994}$
S4	X	A	$\frac{0.975}{0.025}$	$\frac{0.025}{0.975}$
S5	B	C	$\frac{0.950}{0.050}$	$\frac{0.050}{0.950}$
S6	G	J	$\frac{0.802}{0.198}$	$\frac{0.200}{0.800}$
S7	D	E	$\frac{0.850}{0.150}$	$\frac{0.150}{0.850}$
S8	E	F	$\frac{0.975}{0.025}$	$\frac{0.028}{0.972}$

Figure 45. Simplified Flowsheet of Proposed Sequence c (Example 2B)

stream (0123), the downstream separation structure can be found in sequence a. **Heuristic-synthesis step**, however, will again be invoked for the bottoms product (45678).

M1&M2: Use ordinary distillation with refrigeration at high pressure.

S1: Not applicable.

S2: Perform difficult separations 4/5678, 45/678, and 456/78 later (see Table 28 on page 144).

C1: Split 4567/8 is preferred over the other splits because of its large CES value (see Table 28 on page 144).

----> Split 4567/8 is done next. Further separation tasks for (4567) can be found in sequence a. The above analysis will eventually lead to the flowsheet of **sequence c** shown in Figure 45 on page 142.

### **6.3 Discussion of the Results of Examples 1 and 2**

After rigorous flowsheet simulations by commercial package DESIGN II and detailed equipment costing (see Appendices A and B for details), costs (first quarter, 1987) for the proposed sequences of each example problem are listed in Table 29 on page 146, Table 30 on page 146, and Table 31 on page 146.

Table 28. SST for Split (45678)

CES	Separation	ovhd/btm	LE/RK	$\Delta^\circ C$	$\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$   $\frac{d}{b}$	LLK3	LLK2	LLK1	LK	RK	HK1	HK2	HK3	
0.41	SS(MSP)	4/5678	D/E	8.2					0.999	0.842	0.146	0.001		
									0.001	0.158	0.854	0.999		
0.64	SS(MSP)	45/678	E/F	13.2					0.990	0.975	0.025	0.010	0.005	
									0.010	0.025	0.975	0.990	0.995	
3.03	SS(MSP)	456/78	G/J	13.6					0.900	0.800	0.700	0.300	0.200	0.100
									0.100	0.200	0.300	0.700	0.800	0.900
15.06	SS(MSP)	4567/8	L/M	96.6					0.975	0.975	0.005			
									0.025	0.025	0.994			

One notes that the cost differences in the examples are small. It can be seen that the final ranking of the sequences in Example 1 is not in the same order of the proposed sequences (order for sequences b and c is reversed). In fact, we can attribute it to the fact that various degrees of sloppiness of separation and different extents of bypassing are individually encountered. Nevertheless, these sequences will be fairly good initial sequences at the preliminary stage before energy integration can be performed.

In Example 2A, the final ranking is found to be comparable with the proposed order in a favorable manner. However, there is discrepancy between the ranking order of sequences a and b given herein and that presented by Tedder (1984) in which the order was reversed. This can be explained by the way column pressures being differently established.

From the reported costs of Example 2B, it reveals that the best sequence is the second sequence. Considering the fact that the costs of sequences a and b are higher than the best sequence by only 3.1 percent and 3.8 percent, respectively, one concludes that these sequences are all good initial sequences. Most importantly, when comparing the costs of three sequences obtained by the present work (\$7,780,000 to \$8,079,000/yr) and that of the sequence (\$ 9,257,200/yr) given by Watkins (1979), significant saving results from our proposed sequences.

**Table 29. Sequence Costs for Example 1 (in \$1,000/yr, 1st quarter, 1987)**

---

separator	S1	S2	S3	S4	total
sequence a	1330	649	434	70	2483
sequence b	1033	227	687	650	2597
sequence c	464	1095	290	649	2498

---

**Table 30. Sequence Costs for Example 2A (in \$1,000/yr, 1st quarter, 1987)**

---

separator	S1	S2	S3	S4	S5	S6	total
sequence a	594	191	370	292	320	262	2029
sequence b	784	338	268	292	320	262	2264
sequence c	971	260	321	229	292	228	2301

---

**Table 31. Sequence Costs for Example 2B (in \$1,000/yr, 1st quarter, 1987)**

---

separator	S1	S2	S3	S4	S5	S6	S7	S8	total
sequence a	5599	861	225	370	92	292	262	320	8021
sequence b	5202	537	225	320	92	292	262	850	7780
sequence c	3816	225	2702	92	292	370	262	320	8079

---

# **CHAPTER 7 A UNIFYING FRAMEWORK FOR SYSTEMATIC SYNTHESIS OF SLOPPY MULTICOMPONENT PRODUCT SETS**

The sloppy product set, that is, a set of products having some product streams that contain same components (overlapping components) to be separated, is closely examined in this Chapter. Based on numbers of components and product streams, product sets are classified and analyzed. The pseudo-rank of a matrix with its rows consisting of product stream vectors is shown to be an important characteristic property of a product set during the course of synthesizing sloppy product sets. Its use has been explored and presented. A unifying framework incorporating the use of both sloppy and sharp separations is proposed so as to deal with all kinds of situations involving the synthesis of sloppy product sets.

## 7.1 Basis for the Classification of Product Sets

Letting  $C$  be the number of components and  $P$  be the number of products in the separation system, virtually all product sets can be categorized into three groups :

1.  $C > P$
2.  $C = P$
3.  $C < P$

By using the idea of component recovery matrix (Bamopoulos,1984), one can represent  $P$  product streams in general separation systems as vectors,  $V_{(1)} \dots , V_{(P)}$ . Denoting components of the vector  $V_{(j)}$  by  $f_{1j} , \dots , f_{nj} \dots , f_{cj}$  , where  $f_{nj}$  represents the flow rate of component  $n$  in product stream  $j$ , we can then make the following claim about those vectors, that is :

**$P$  vectors  $V_{(1)}, \dots , V_{(P)}$  will be linearly independent if the matrix ( $P$  by  $C$ ) with row vectors  $V_{(1)}, \dots , V_{(P)}$  has a rank  $P$ ; they are linearly dependent provided that the rank is less than  $P$ .**

A matrix is said to have a rank  $r$  if it contains one  $r$ -rowed square submatrix having a nonzero determinant, while the determinant of any square submatrix with  $r + 1$  or more rows, possibly contained in this matrix, is zero. It is also clear that the rank of the matrix should satisfy

$$r \leq \min (C,P)$$

[7.1 – 1]



In the case that  $r$  is less than  $P$ , there are, of course,  $r$  linear independent product streams. For the remaining  $(P-r)$  product stream vectors, they can be expressed in terms of those  $r$  product stream vectors. However, it should be noted that coefficients which give the linear dependence between those  $r$  product stream vectors and each individual  $(P-r)$  product stream vectors may not be practical (i.e., some of them may be negative numbers). Hence, before any further analysis can be performed, one should first ensure the non-negativity of the coefficients.

Also, we define a term called pseudo-rank  $r'$ , for which the following expression holds :

$$r \leq r' \leq \min (C,P) \quad [7.1 - 2]$$

where

$r'$  = pseudo-rank of the product matrix, being equal to the rank of the matrix plus the number of dependent product streams which cannot be linearly expressed as a function of  $r$  independent product vectors by positive coefficients

---

	(component distribution)				
Component =	A	B	C	D	total flow (moles/hr)
Product 1	0.2	0.1	0.1	0.1	12.0
Product 2	0.1	0.2	0.0	0.1	12.2
Product 3	0.5	0.2	0.1	0.4	32.6
Product 4	0.0	0.3	0.5	0.3	34.0
Product 5	0.2	0.2	0.3	0.1	19.2

---

The above product specifications are taken from Muraki et al. (1986) as an illustration.

One sees that in this problem  $P=5$  and  $C=4$ .

In a vector form, the five product streams can be given as follows.

$$V1 = (2.0,3.2,2.0,4.8)$$

$$V2 = (1.0,6.4,0.0,4.8)$$

$$V3 = (5.0,6.4,2.0,19.2)$$

$$V4 = (0.0,9.6,10.0,14.4)$$

$$V5 = (2.0,6.4,6.0,4.8)$$

The order of the largest nonzero determinant contained in the matrix that consists of those product streams is found to be four. One can also derive the following relationship to describe the linear dependence of  $V5$  on the other vectors, if one chooses  $V1$ ,  $V2$ ,  $V3$ , and  $V4$  as the independent vectors.

$$V5 = (2.25)V1 + (0)V2 + (-0.5)V3 + (0.25)V4$$

The pseudo-rank in this example case will be five. If one were to, however, find only positive coefficients on the right-hand side of the above equation, the original set of products would be achieved using the new set of product streams containing only dependent product streams.

## 7.2 A Unifying Framework for Synthesizing Sloppy

### *Multicomponent Product Sets*

By using the argument presented in the last section, one can first simplify product sets of interest before any synthesis scheme commences. In the following, we will partition the problem of multicomponent-product separation synthesis into a number of subproblems by considering the implication of the analysis given in section 7.1 in relation to the global synthesis framework. Specific synthesis strategies are suggested for a variety of product sets. Here, we will first present an alternative solution to Example 1 of Chapter 6.

#### 7.2.1 Mixed-Separation Synthesis Method

Now, let us first take a second look at Example 1 given in the last Chapter. One immediately finds that  $P=4$ ,  $C=4$ , and  $r'=4$ . Suppose that one desires to utilize the least number of separators to perform the separation task. The constraint for this particular case can be set such that

$$S_{\min} = \min(C, P) - 1 \quad [7.2 - 1]$$

where

$S_{\min}$  = minimum number of separators

$P$  = number of product streams

$C$  = number of components

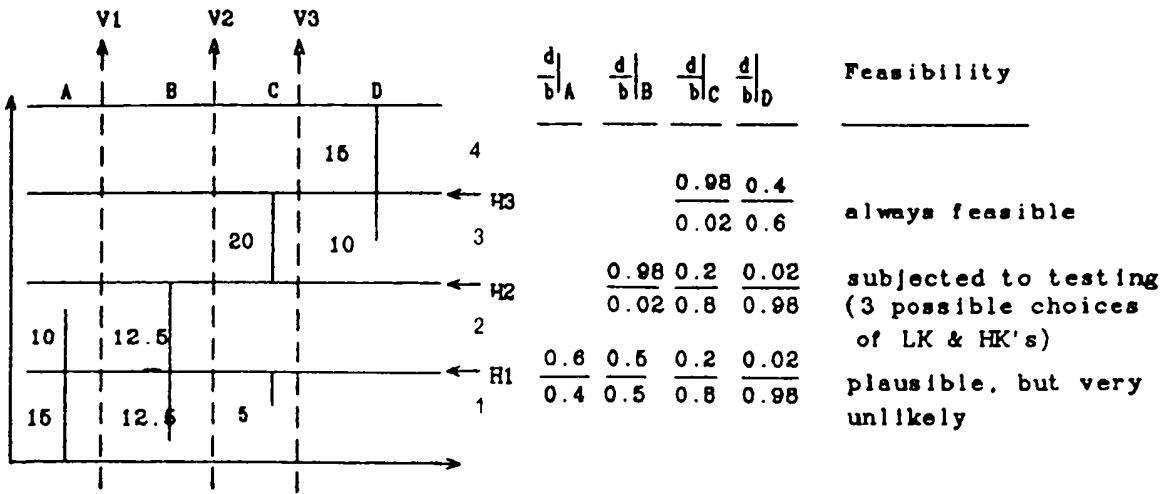
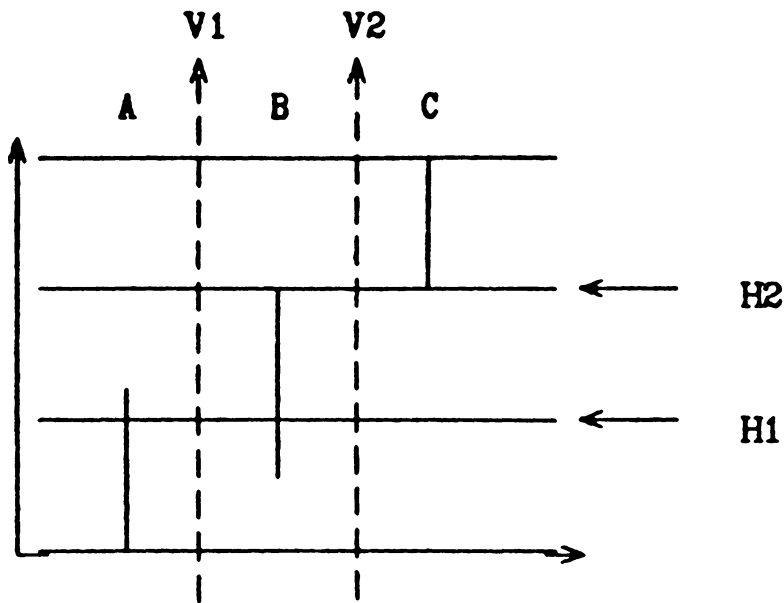
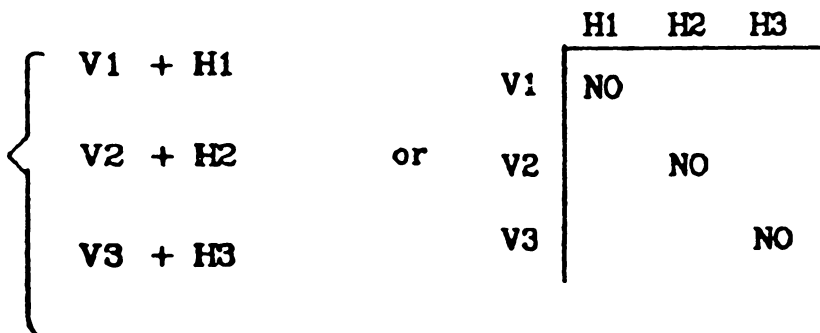


Figure 46. Modified CAD and SST for Example 1



(a) A CAD Showing Vertical and Horizontal Operations



(b) Combinations of Operations to be Avoided

Figure 47. Vertical and Horizontal Operations on a CAD

In what follows, we will use the same example (Example 1) to show how to achieve the desired product set, given the above constraint. To facilitate our further analysis, a CAD is given in Figure 46 on page 152 for the problem, along with an SST. Two types of split lines are shown in the figure - Vertical Split Line which is created to separate components, and Horizontal Split Lines for separating products. In this example, all possible sequences corresponding to  $S_{\min} = 3$  will be enumerated. Prior to that, the following considerations are given :

1. As can be seen in the example shown in part (a) of Figure 47 on page 153, the type of separation delineated by Horizontal Split Line - H2 is the same as that by Vertical Split Line - V2. In other words, Horizontal Split Lines may represent sharp as well as non-sharp separations, whereas Vertical Split Lines always represent sharp separations.

2. Since we are searching for three-separator sequences, the following combinations are provided in a decreasing order of desirability -

3 separators :

H-H-H (most desirable, but it does not work out this way in this example)

V-H-H

V-V-H

V-V-V (least desirable; all sharp separators)

3. One should pay attention to avoid using the same LK/HK for different separators. Specifically, one needs to avoid the combinations of separators given in part (b) of Figure 47 on page 153. Further, it goes without saying that each separator is forbidden to be used twice.

4. In view of the fact that sharp and sloppy separations are both considered here, the bypassing rule for this method will generally follow the rule that was given in Section 4.4 except that the bypassing basis will be varied from 90% to 100% so as to avoid problems arising from an undesirable distribution of nonkeys.

### **Alternative Solution to Example 1**

To demonstrate the use of Vertical Split Lines, the problem of separation synthesis can be treated differently in that one can, with relative freedom, use sharp separations during the synthesis task in order not to violate the constraint of minimum number of separators.

In the following, we will present this method by using *Horizontal and Vertical Split Lines* to manipulate the CAD of Example 1.

\*Starting with *Horizontal Split Lines* yields -

- H1 ---> plausible, but unlikely due to the specified distribution of component C
- H2 ---> (part 1) The CAD containing product streams 1 and 2 (part 1) is given as follows

:

	A	B	C	
10	12.5			2
15	12.5	5		1

The CAD after bypassing 12.5 moles/hr of A, 12.5 moles/hr of B, and 2.5 moles/hr of C to product stream 1 is shown in part (a) of Figure 48 on page 157.

---> needs at least 2 more separators

(part 2) Remaining product streams are 3 and 4 (see Figure 46 on page 152) ---> after bypassing, two operations are plausible, i.e., H3 and V3; but using H3 is apparently more favorable since it is a sloppier split.

(Note that in this solution, more than three separators are needed.)

- H3 ---> The CAD containing products 1, 2, and 3 is shown in part (b) of Figure 48 on page 157:

There are four options at this point :

(i). ---> first perform operation H2 which is subjected to feasibility testing --->

The CAD containing product streams 1 and 2 and the corresponding SST are shown below :

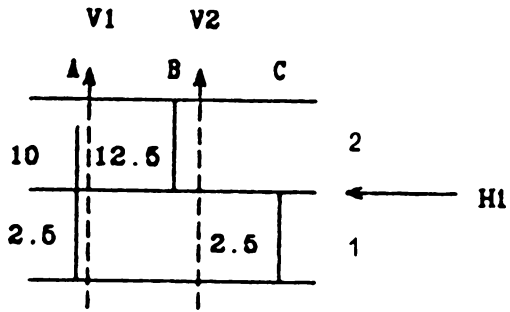
A	B	C	
10	12.5		2
15	12.5	5	1

← H1

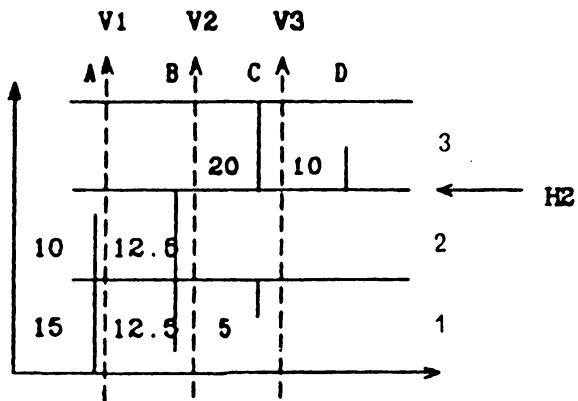
$\frac{d}{b} A$	$\frac{d}{b} B$	$\frac{d}{b} C$
0.6	0.5	0.98
0.4	0.5	0.02

The CAD after bypassing 12.5 moles/hr of A and 12.5 moles/hr of B to product stream 1 will be identical to the one in part (a) of Figure 48 on page 157.





(a) CAD After Bypassing



(b) CAD After Operation V2

Figure 48. CAD of Example 1 After Operations

---> needs at least two more separators to achieve the remaining separation requirement.

(In this option, it should be noticed that again more than three separators are used and H1 is subjected to testing for feasibility.)

(ii). ---> first perform operation V1 ---> the CAD containing the remaining components B, C, and D and the corresponding SST are given below :

B	C	D		$\frac{d}{b} B$	$\frac{d}{b} C$	$\frac{d}{b} D$
20	10		3	0.98	0.2	0.02
12.5			2	0.02	0.8	0.98
12.5	5		1	0.5	0.2	0.02
				0.5	0.8	0.98

(This option will require four separators since at least two more separators are needed.)

(iii). ---> first perform operation V2 ---> CAD is divided into two parts (see part (b) of Figure 48 on page 157)

Part 1 contains components A, and B ---> two options after bypassing

---> H1 (more favorable due to its sloppiness)

---> V1 (less favorable than the above)

Part 2 contains components C, and D ---> two options after bypassing

---> H2 (more favorable due to its sloppiness)

---> V3 (less favorable than the above)

(This option requires also four separators.)

*(iv)*. ---> V3 ...

(This option will obviously need at least four separators.)

\* Alternatively, operations can be done by starting with Vertical Split Lines -

- V1 ---> Remaining components are B,C, and D (see Figure 46 on page 152) :

there are several options at this point :

**a.** try V-H-H --> the only possibility left : V1 + H2 + H3.

**b.** try V-V-H -

*(i)* V1 + V2 ---> Remaining components are C and D ---> bypass 10 moles/hr of C and 10 moles/hr of D to product stream 3 ---> must perform operation V3 to achieve the specified product set.

(This option will use three separators, i.e., V1-V2-V3.)

*(ii)* V1 + V3 ---> Remaining components are B and C ---> bypass 5 moles/hr of B and 5 moles/hr of C to product stream 1 ---> must perform V2 to achieve the separation requirement.

(This option again uses three sharp separators, i.e., V1-V3-V2.)

- V2 ---> Dividing into two parts (1 and 2) :

a. part 1 contains components A and B (see Figure 46 on page 152) : H1 is preferred over V1 due to the sloppiness of the former split.

b. part 2 contains components C and D (see Figure 46 on page 152) :

there are two options at this point :

(i) try V-H-H --> the only possibility : V2 + H1 (used in part 1) + H3 ---> bypass 10 moles/hr of C and 10 moles/hr of D to product stream 3 ---> H3 (= V3)

(This option can be represented by V2 - V3.)

(ii) try V-V-H - \ H1

V2 + V1 (used in part 1) ---> remaining components are C and D ---> bypass 10 moles/hr of C and 10 moles/hr of D to product stream 3 ---> V3 (= H3)

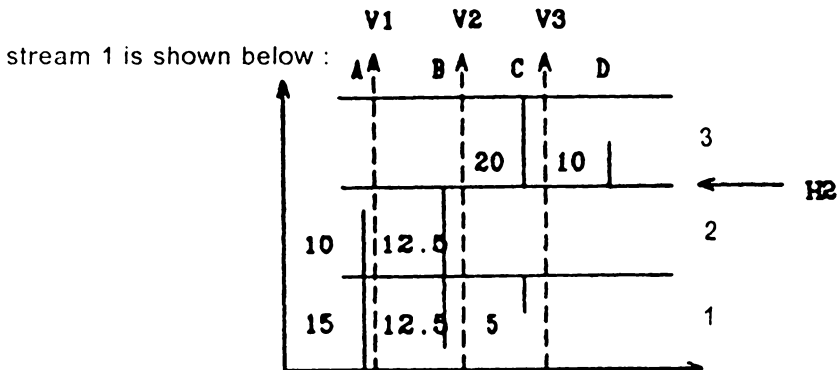
(This option will use three sharp separators V2 - V1.)

\ V3

- V3 ---> Remaining components are A,B, and C :

there are several options at this point :

a. try V-H-H --> the only possibility left : V3 (used already) + H1 + H2 ---> CAD after bypassing 5 moles/hr of A, 5 moles/hr of B, and 5 moles/hr of C to product stream 1 is shown below :



(i) ---> H1 will be the second split ---> V2 (or H2)

(This will lead to the sequence of V3-H1-V2 with H1 subjected to feasibility testing.)

(ii) ---> H2 (or V2) will be the second split ---> H1

b. try V-V-H - ---> after bypassing 5 moles/hr of A, 5 moles/hr of B, and 5 moles/hr of C to product stream 1 ---> V2 (=H2) ---> H1.

(This option will give the sequence of V3-V2-H1.)

c. try V-V-V --> after bypassing 5 moles/hr of A, 5 moles/hr of B, and 5 moles/hr of C to product stream 1 :

(i) V3-V1-V2 (all sharp)

(ii) or V3-V2-V1 (all sharp)

In summary, the above sequences that use three separators are listed as follows :

1. V2 - V3 (one non-sharp separator; rest are sharp)  
    `  
    H1
2. V3-V2-H1 (one non-sharp separator; rest are sharp)
3. V3-H1-V2 (one non-sharp separator subjected to feasibility testing; rest are sharp)
4. V1-V2-V3 (all sharp)
5. V1-V3-V2 (all sharp)
6. V2 - V1 (all sharp)  
    `  
    V3
7. V3-V1-V2 (all sharp)

8. V3-V2-V1 (all sharp)

## 7.2.2 Synthesis Strategies for Various Product Sets

What one has gained from the preceding section is that the separation requirements in Example 1 can be achieved using one less separation ( $S=3$ ) than the sequences proposed in section 6.1. In fact, it can be understood that one can always attain the separation goal by performing (C-1) sharp separations. It, however, does not mean that there is no need to pursue alternative solutions in the manner described in section 6.1 due to the fact that all the separations given therein are sloppy. Therefore, to set the tone for the remaining parts of this section, one ought to realize that the intent of the analysis given herein is to give a somewhat different but more general perspective view about synthesizing sloppy product sets. In this context, we will propose a unifying approach to the systematic synthesis of multicomponent sloppy product sets.

### *Product Set of the Type $P = C = r'$*

In the present case, up to this point, we have already shown two different paths in solving this type of separation problems (i.e., solution of Example 1 given in Chapter 6, and an alternative solution given in section 7.2.1). The first proposed approach was demonstrated in the last chapter (heuristic sloppy-separation synthesis method), which favors the use of sloppy separators. The other technique presented in the preceding sections gives different sequences and will be called mixed-separation synthesis method. In addition, other sharp-

separation synthesis techniques, such as the methods proposed by Muraki et al.(1986) and Floudas (1987) should also be taken into consideration, since those methods use only sharp separators. Note that using sharp separators will result in sequences with the least number of separators. Three characteristically different kinds of separation sequences, generated by the above-mentioned methods can become good initial separation candidates.

### ***Product Set of the Type $r' < P = C$***

Synthesis strategies for problems falling into this group are the same as those for the group of  $P < C$ . The reason for it is that both groups have one thing in common, that is,  $r' < C$ . Synthesis strategies for this class of product sets are detailed in the next group.

### ***Product Set of the Type $P < C$ .***

Examples 2a ( $P=7$ ,  $C=13$ , and  $r=r'=7$ ) and 2b ( $P=9$ ,  $C=14$ , and  $r=r'=9$ ) are typical examples of this type. It can be shown that  $r$  is no greater than  $P$  in this particular case and knowing the relation that  $r$  is also no larger than  $r'$ , one can arrive at the following :

$$r' < C \quad [7.2 - 2]$$

In view of this, it may be worthwhile to incorporate sloppy splits during the course of synthesizing multicomponent product sets, since there is a chance that using sharp separations alone would result in too many separators. Nonetheless, a sharp-separation synthesis

scheme may have to be used if  $r'$  product streams constitute an infeasible product set which may lead to too many fictitious product streams after transformation. The example shown below, taken from Floudas (1987), will demonstrate this point.

(Component Flow Rates)					
Component =	A	B	C	D	moles/hr
Feed	15	20	10	15	60
Product 1	5	10	4	10	29
Product 2	10	10	6	5	31

$D_i$ , Difficulty of  $i$ th separation (sharp) between two components :

$$D_{AB} \text{ (or } D_1) = 2.5$$

$$D_{BC} \text{ (or } D_2) = 3.0$$

$$D_{CD} \text{ (or } D_3) = 1.5$$

$$\text{objective function} = \sum_i (L_i D_i)^{0.6} \quad [7.2 - 3]$$

where

$$L_i = \text{separation mass load of } i\text{th separator}$$

Shown in Figure 49 on page 165 are the CAD for this example problem after converting the given data, and the CAD consisting of transformed product streams, along with their corresponding SST's. As can be seen from the transformed CAD, the sloppy-separation synthe-



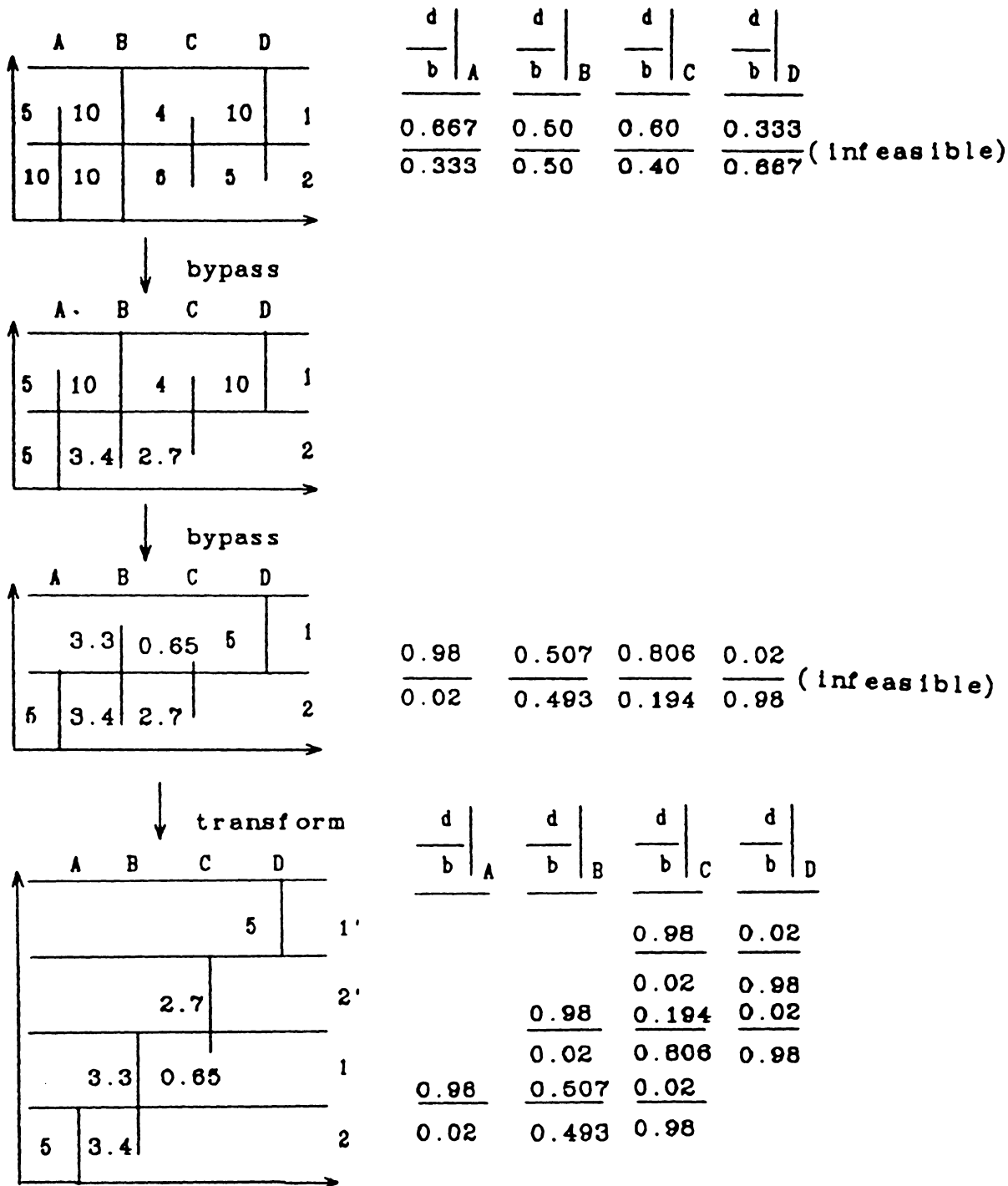


Figure 49. CADs and SSTs Before and After Transformation

sis method will proceed provided that the splits on the CAD exempt from the consideration involving distributed non-keys.

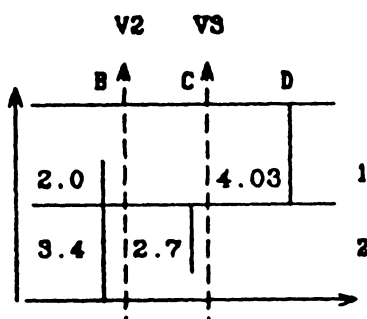
This may ultimately lead to a number of good initial sequences that include sloppy splits. Three separators would be required to perform the task. However, if one starts with sharp-separation synthesis scheme, one will end with three (= C-1) sharp separators. Hence, both schemes would have to be considered.

Alternatively, if one applies the mixed-separation synthesis method to the present example, then the search steps can be followed below. First, the CAD after bypassing for the same problem is given in Figure 50 on page 167.

1. Starting from H :

It fails because of the infeasibility of split 1/2.

2. Starting from V1 : After bypassing 1.3 moles/hr of B, 0.65 moles/hr of C, and 0.97 moles/hr of D, the CAD containing Components B, C, and D is shown below :



Option (i) ---> perform operation V2 ---> then do operation V3 for the remaining CAD that includes components C and D

Option (ii) ---> perform V3 and then bypass 3.4 moles/hr of B and 1.7 moles/hr of C to yield the CAD given below ---> the last step is to perform V2

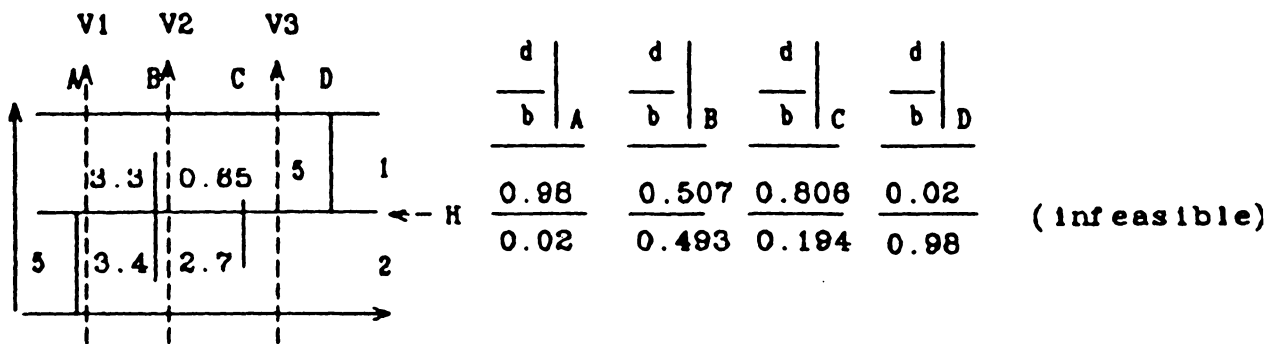
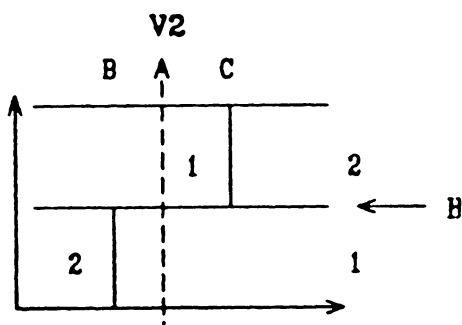
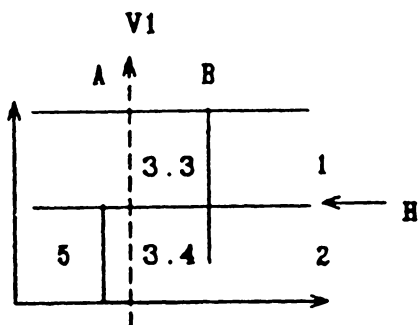


Figure 50. CAD and SST Used in Mixed-Separation Synthesis Method



3. Starting from V2 : The CAD will be divided into two parts -

---> (part 1) The CAD containing components A and B is shown below. After bypassing 2.535 moles/hr of A and 3.4 moles/hr of B, one is left with V1 to carry out the required separation.



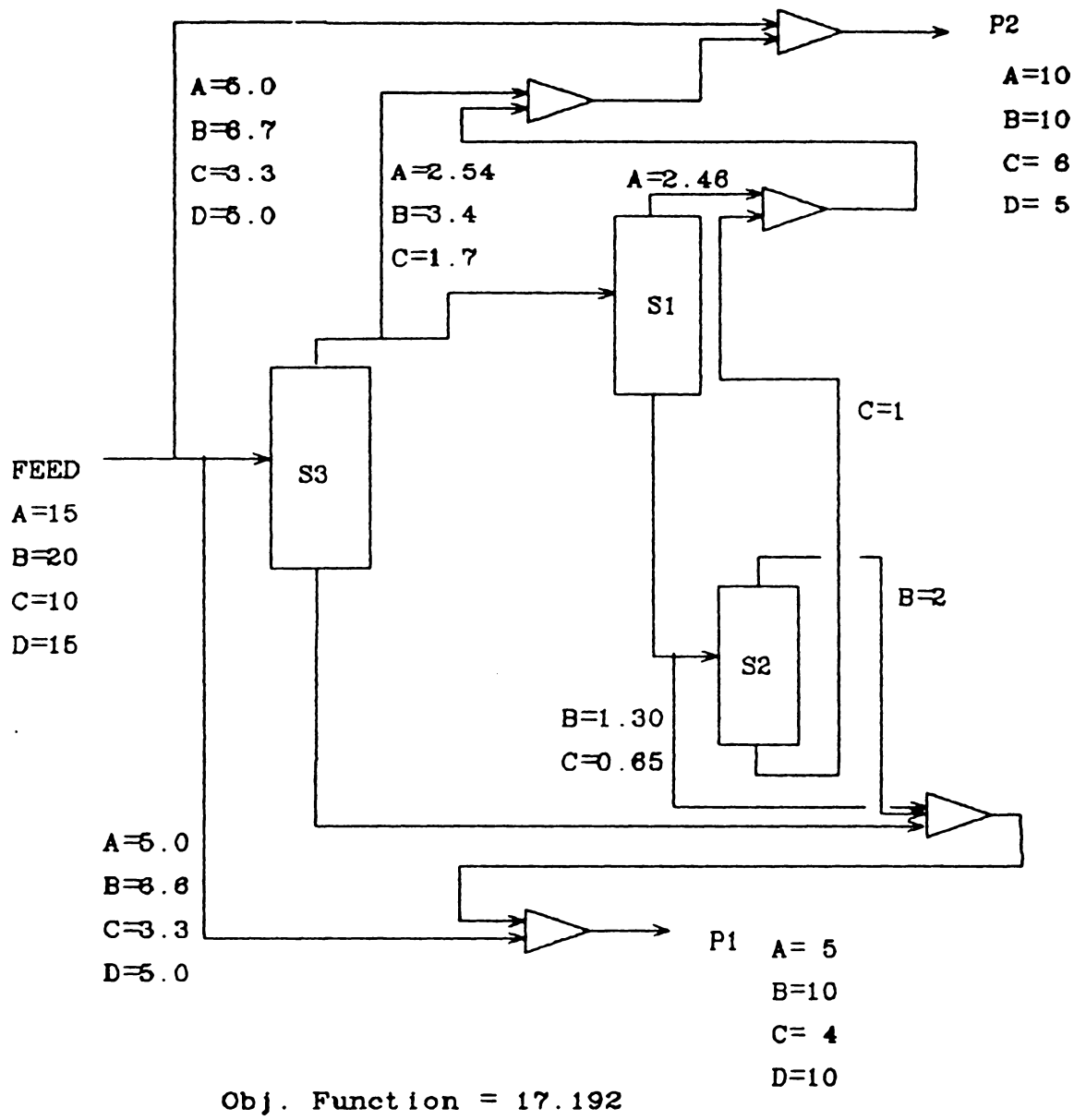
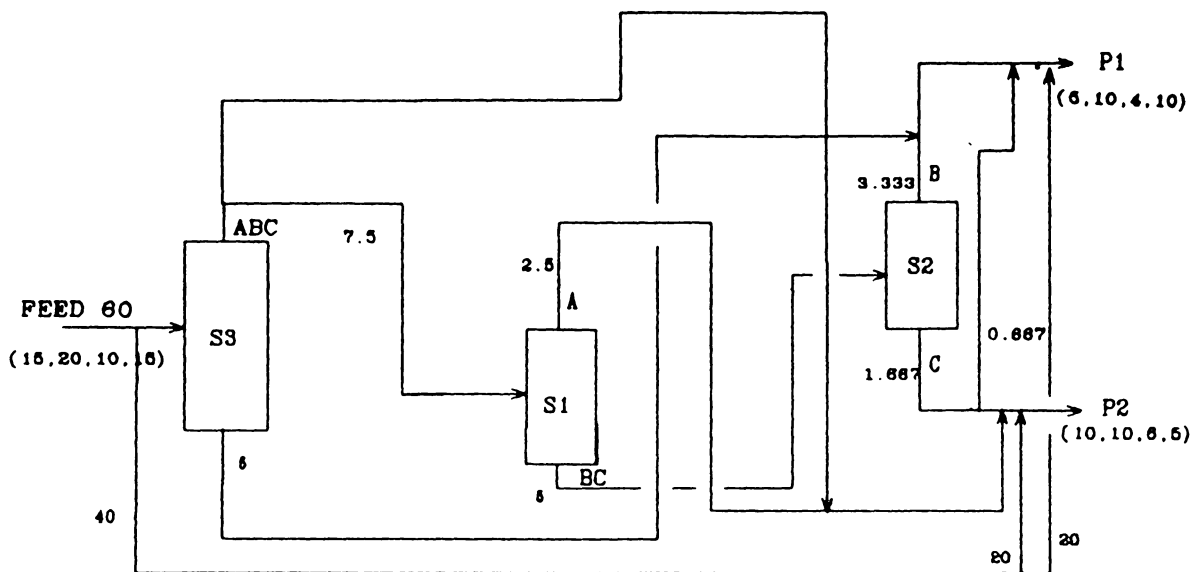


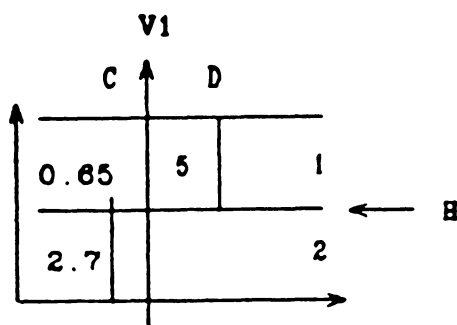
Figure 51. Flowsheet of Proposed Sequence (V3-V1-V2)



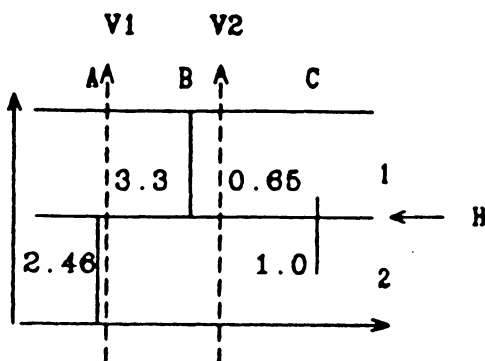
Obj. Function = 18.578

Figure 52. The Optimal Flowsheet of Floudas (1987)

---> (part 2) The CAD containing components C and D is shown below. Again, first bypass 0.65 moles/hr of C and 0.97 moles/hr of D. ---> the remaining part of CAD is synthesized by using V1.



4. Starting from V3 : After bypassing 2.537 moles/hr of A, 3.4 moles/hr of B, and 1.7 moles/hr of C, the remaining CAD containing components A, B, and C becomes -



Option (i) ---> perform operation V1 first, and then bypass 1.3 moles/hr of B and 0.65

moles/hr of C ---> final split will be V2

(Figure 51 on page 168 shows the complete flowsheet for option (i).)

Option (ii) ---> perform operation V2 first ---> do operation V1

Unlike Example 1 of Section 6.1, applying the mixed-separation method to synthesize this example problem does not lead to any sequences involving sloppy splits. However, it is striking to note that the optimal sequence (optimum with respect to the objective function given by Floudas (1987), see equation [7.2-3] ) using only sharp separators can be obtained by employing this method without making much computational effort, which is desired by the method of Floudas (1987). The optimal all-sharp separation configuration follows the sequence of V3-V1-V2. In fact, We have already shown the optimal sequence can be worked out by the above technique.

What is more striking is that this sequence is even better than one given by Floudas (see Figure 52 on page 169) in terms of his objective function, equation [7.2-3].

To sum up, the synthesis of this type of product sets ( $P < C$ ) may conditionally call for the use of all the methods mentioned above.

### ***Product Set of the Type $P > C$***

Product sets within this can be further divided into three subgroups :

a.  $r' = C$  -

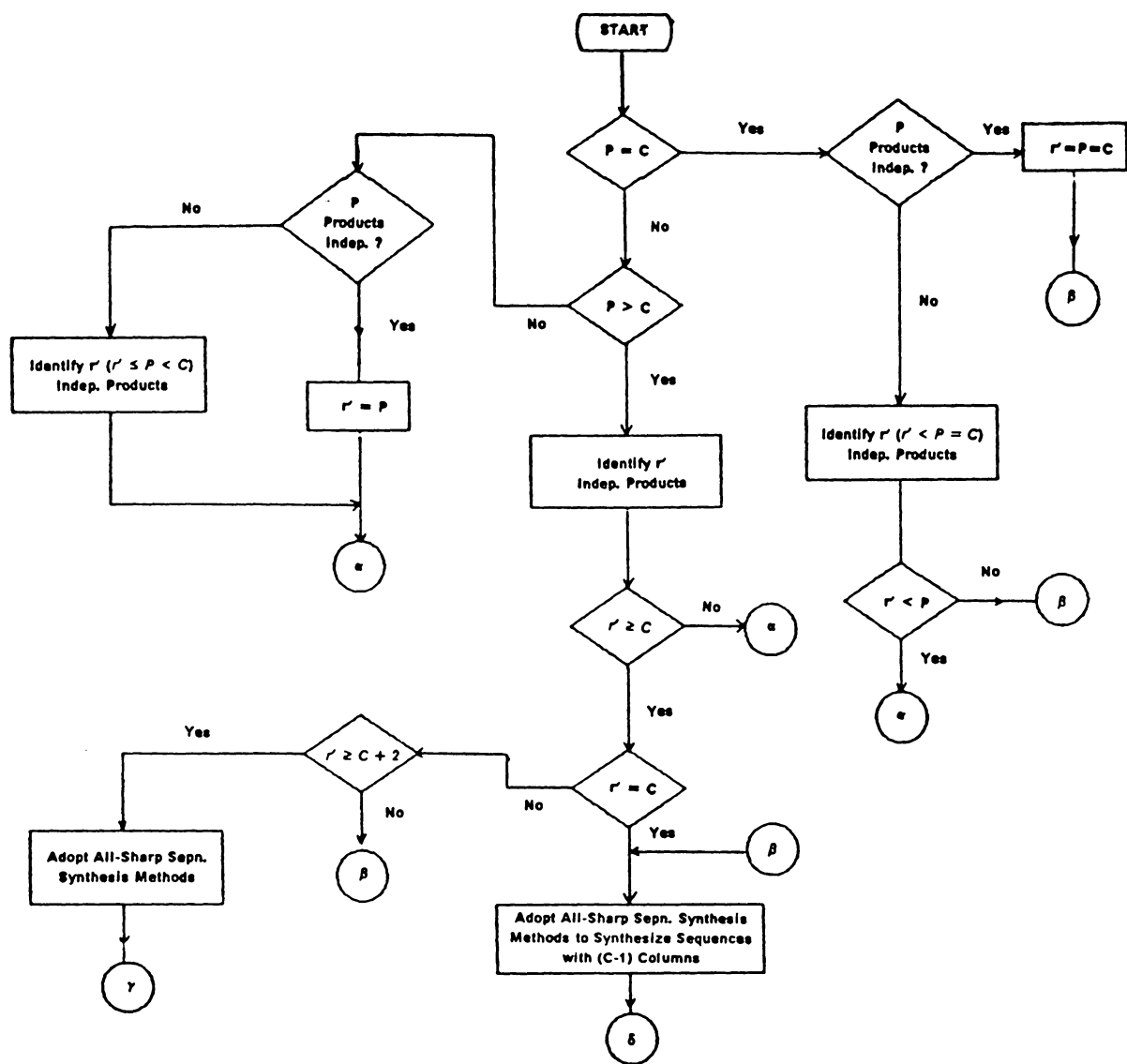
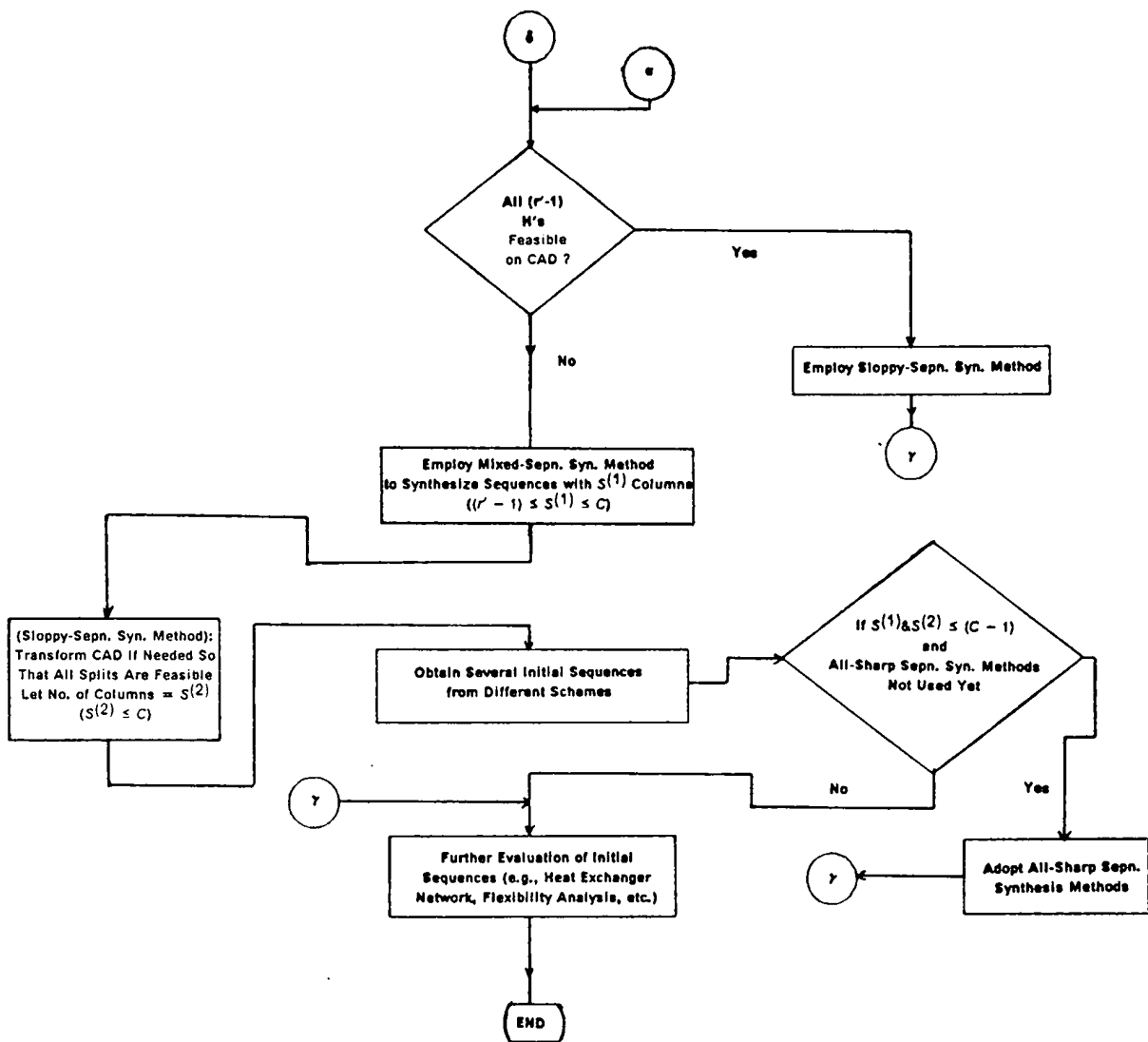


Figure 53. Flowchart of the Unifying Scheme for Synthesizing Multicomponent Sloppy Product Sets





For this type of product set, the synthesis scheme is essentially the same as that for the product sets under the heading of  $P = C = r'$ . This can be easily followed because the original product streams in this subgroup have been reduced to a new product set with  $C$  (or  $r'$ ) product streams made up of  $C$  components.

**b.  $P \geq r' > C$  –**

To rationalize the synthesis scheme for this type of product sets, one must know our overall strategy is to consider possible sequences incorporating sloppy splits having at most one more column than other competing all-sharp separation sequences since the former sequences are as economically appealing as the latter ones. As a result, it is still worthwhile to employ sloppy-separation synthesis techniques for product sets whose  $r'$  values equal to  $C + 1$ . For product sets with higher  $r'$  values, however, one should use the sharp-separation synthesis methods.

**c.  $P > C > r'$  –**

Recall that earlier in the product group  $P < C$ , one obtained the relationship  $r' < C$ . Apparently, the present product set bears close resemblance with it and, therefore, their synthesis scheme should be identical.

## 7.3 Summary

In this Chapter, we have thoroughly analyzed sloppy multicomponent product sets. Essentially, all possible sloppy product sets are categorized according to their values

of numbers of product streams and system components, and the pseudo-rank of product stream matrix. For different classes of product sets, synthesis schemes have been suggested individually to develop sequences that are all-sloppy, all-sharp, and both sharp and sloppy.

A new approach called mixed-separation method, which still relies on the use of CAD (with the addition of vertical split lines) and SST, has been introduced. For solving many separation problems, the effectiveness of the heuristic synthesis method as well as the mixed-separation synthesis is demonstrated.

Finally, in order to summarize the scheme in solving different types of separation problems given in Section 7.2.2, a flowchart is presented in Figure 53 on page 172.

# CHAPTER 8 CONCLUSIONS, SIGNIFICANCE, AND RECOMMENDATIONS

## 8.1 Conclusions

A novel problem representation - component assignment diagram (CAD) for conveniently synthesizing sloppy product sets has been developed. This representation is somewhat similar to the use of temperature-interval diagram, an on-diagram-oriented method widely used in heat-exchanger network synthesis.

Based on the component assignment diagram, one can visualize the synthesis problem itself more clearly and solve the problem creatively. Needless to say, the task of synthesizing sloppy product sets is by far more difficult than that of synthesizing sharp product sets in that such things are not easy to manifest as identifications of infeasible splits and stream splitting, transformation of infeasible product sets into equivalent feasible product sets, and so forth.

All the above have been successfully treated in the Chapter of feasibility analysis, with the aid of a "separation specification table (SST) " which proves to be an extremely useful tool to : (i) properly define and specify key and non-key components; (ii) quickly identify feasible

and infeasible splits; (iii) effectively deal with fuel products with unmatched component specifications; and (iv) systematically consider sloppy separations with multiple split points.

In fact, feasibility aspects of sloppy splits are in many ways like those of heat integration. For example, the analysis of split feasibility corresponds to the analysis of heat-exchange feasibility (minimum approach-temperature constraint), and the transformation of infeasible splits into equivalent feasible splits is analogous to the use of stream splitting to avoid the minimum-approach-temperature violation.

Sufficient information has been extracted from a comparative study of rigorous simulation and shortcut modeling of multicomponent distillation columns for sloppy separations. Specifically, quantitative criteria and limitations for applying the Fenske equation in estimating non-key distributions have been clearly identified. As a result, one can directly apply the findings presented to properly utilize the shortcut design technique during the course of synthesizing sloppy splits. Most notably, unlike sloppy-separation synthesis, this kind of situation will not be encountered in the synthesis of sequences using only sharp separators.

In principle, the heuristic synthesis method proposed in this work involves a two-step approach - one is concerned with the analysis of separation feasibility pertinent to a CAD, which seeks a way to interpret and modify a CAD at hand from a feasibility standpoint; the other is concerned with the procedure to resolve a subsequent split by applying heuristics.

As tested by examples, this method offers a simple and practical way for design engineers to generate a number of good initial sequences for obtaining sloppy multicomponent product sets prior to the ultimate detailed design optimization. It will definitely save tremendous amount of time for doing exhaustive search for good separation sequences from innumerable possible structures.

A unifying framework has been developed specifically for the synthesis of sloppy product sets and it is useful to direct the right pathway to generate equally good initial separation

**Table 32. Comparison of Various Methods for the Synthesis of Sloppy Multicomponent Products**

INVESTIGATOR	NATH (1977)	SOPHOS (1981)	MURAKI ET AL. (1986)
Consideration of sloppy splits	yes	no	no
Feasibility of sloppy splits	not considered	not considered	not considered
Quantitative criteria for feasible sloppy split	not given	not given	not given
Means for ranking sequences other than costing	by coefficient of difficulty of separation only (equation 5.2)	by mass load	by an objective function (eq. 2.2-1)
Remarks	Material allocation diagram is employed to synthesize sloppy products. Only an "optimum" sequence is developed. No near optimum sequences are given	All candidates of "optimum" sequences are developed. However, only sharp separators are used. A modified material allocation diagram is used	Evolutionary search is used to improve the objective function for each sequence, whose mass flows are assigned by a modified material allocation diagram

(continued)

INVESTIGATOR	BAMOPOULOS (1984)	TEDDER (1984)	FLOUDAS (1987)
Consideration of sloppy splits	yes	yes	no
Feasibility of sloppy splits	considered	not considered	not considered
Quantitative criteria for feasible sloppy split	not given	not given	not given
Means for ranking sequences other than costing	costing only	costing only	by an objective function (eq. 2.2-1)
Remarks	Sloppy separations are used in combination with sharp separations. Severe restrictions on the use of types of sloppy separations	Complex columns are treated in the combined heuristic-dynamic programming method	All sharp configurations are embedded in the so-called superstructure. Optimum is obtained by a mathematical programming method

(continued)

INVESTIGATOR	MURAKI AND HAYAKAWA (1987)	THIS WORK
Consideration of sloppy splits	yes	yes
Feasibility of sloppy splits	not considered	considered
Quantitative criteria for feasible sloppy split	not given	given
Means for ranking sequences other than costing	costing only	by rank-ordered heuristics
Remarks	An optimization technique is used to solve for the best sequence. Problems associated with undesirable non-key distributions are not taken into account	New problem representation - component assignment diagram is presented. Sloppy splits are broadly utilized. A unifying scheme is given for the general problem



schemes featuring possibly three characteristically different sequences - i.e., all-sharp, all-sloppy, and both sharp and sloppy (i.e., mixed separation).

## 8.2 Significance

Separation-system synthesis, which is one of the most important problems in process synthesis concerning the selection of the best method and flowsheet, has been thoroughly investigated in this work.

Essentially all of the published work on this subject has been limited to high-recovery or sharp separations, in which each component to be separated appears in one and only one product stream. In industrial practice, however, it is often useful to permit components to be separated to appear in two or more products. This type of separation results in products with overlapping components and is called nonsharp or sloppy separations. The present work proposes and demonstrates a simple and practical approach to the systematic synthesis of sloppy multicomponent separation sequences.

Employing component assignment diagram (CAD) to solve the synthesis problem is a unique approach in that not only different kinds of splits can be well represented and treated, but also the complex synthesis problem can be more clearly elucidated.

Criteria and limits developed from rigorous simulation, when compared with the short-cut modeling, provide valuable insights for the consideration of feasibility of sloppy splits which have been completely ignored by previous workers.

Also, for the first time, the problem of synthesizing multicomponent sloppy product sets has been critically analyzed by using a unifying synthesis framework, thereby allowing design

engineers to consider developing good initial flowsheets of separation system with different types of separators.

A summary on the comparison of a number of synthesis methods is given in Table 32 on page 178. From the comparison, it is evident that this study is truly unique in many ways and, suffice it to say, significant progress has been made in the area of separation synthesis.

### **8.3 Recommendations**

Insofar as the future work is concerned, undoubtedly, one of directions should be heading toward the use of complex columns, since it is sometimes advantageous to utilize complex columns than simple one-feed, two-product columns to handle some particular types of product sets.

One should be aware of the fact that thermodynamically speaking, it is not advisable to use excessive splittings and blendings. Thus, an important question is to decide how one comes up with an economically profitable set of product streams for a given separation task that is also thermodynamically acceptable. This question is, however, yet to be addressed.

At the design stage, flexibility is also an important issue that design engineers must face. Specifically, flexibility is concerned with the process adjustability with respect to variations in product specifications, product demand, and process operating conditions, etc. Criteria that enable design engineers to determine the "best" separation system not only in terms of process economics but system flexibility as well are desirable.

In this work, we have dealt with separation problems having only one feed stream, which have been a major focus of most literature work. It is not impossible, however, for industrial processes to have two or even more sources of feed for separation. Here, we will present

some preliminary ideas about solving problems of this kind. The following problem is taken from Mahalec and Motard (1977) and Floudas (1987).

Component =	(component distribution)			flow rate
	A	B	C	(moles/hr)
Product 1	0.5		0.5	200
Product 2	0.417	0.417	0.167	1200
Product 3	0.091	0.909		1100
Feed 1	0.168	0.833		1200
Feed 2	0.385	0.385	0.231	1300

By our way of problem representation, this problem can be visualized in Figure 54 on page 185. After bypassing portions of feed 1 (100 mole/hr of A and 500 moles/hr of B) and feed 2 (333 moles/hr of A, 333 moles/hr of B, and 200 moles/hr of C), the modified separation problem can be seen in Figure 55 on page 186, in which feeds 1' and 2' represent, respectively, the remaining portions of feeds 1 and 2, and products 2', and 3' are the remaining products of products 2 and 3, respectively. By performing vertical split operations V1 on feed 1' (to isolate product 3') and V2 on feed 2' (to isolate product 2'), one is able to easily synthesize the whole product set. The flowsheet is given in Figure 56 on page 187. This solution turns out to be the "optimal" sequence in terms of separation mass load. Some guidelines can be drawn from this example. First, it is best to avoid mixing of feeds with different compositions in order to reduce the separation mass load. Following this line of reasoning, the feeds in the example problem have been treated individually. Secondly, split operations should take place so as to isolate component(s) that immediately forms products or part of

products. In this example, one identifies a portion of feed 2' ( $A = 170$ ,  $B = 170$ ) which is exactly the desired product 2'. Therefore, even though bypassing is effective for feed 1' to give a part of product 2', vertical split operation V2 will be performed instead. As can be seen in the proposed sequence, all splits are sharp.

However, if this matching does not exceed one component, then one can start constructing the structure of separation. Take the case in Figure 57 on page 188 for an example. One can first construct a column (S2) for splitting feed II, and in the mean time construct another column (S1) for splitting feed I (see Figure 58 on page 189). These two columns correspond to V2 and V1, respectively, on the CAD. Since the overhead product of column S2 does not directly lead to any desirable product, this stream will go back to column S1 for further separation. Essentially, the flowsheet consists of two columns with two feed streams individually fed into one of the two columns. Because initial feeds are not mixed together before separation, significant reduction in the mass load can be achieved. Future work is needed to include sloppy splits into the synthesis scheme for multiple-feed separation problems.

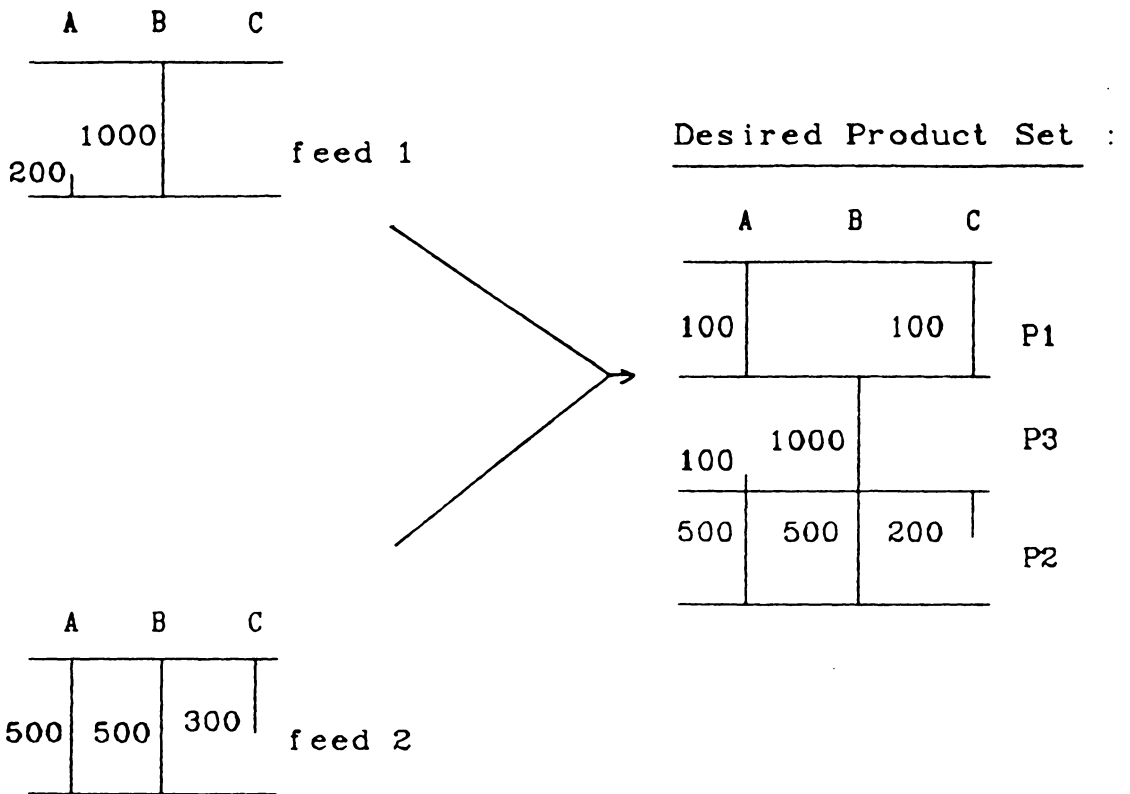


Figure 54. CADs of a Two-Feed Separation Problem

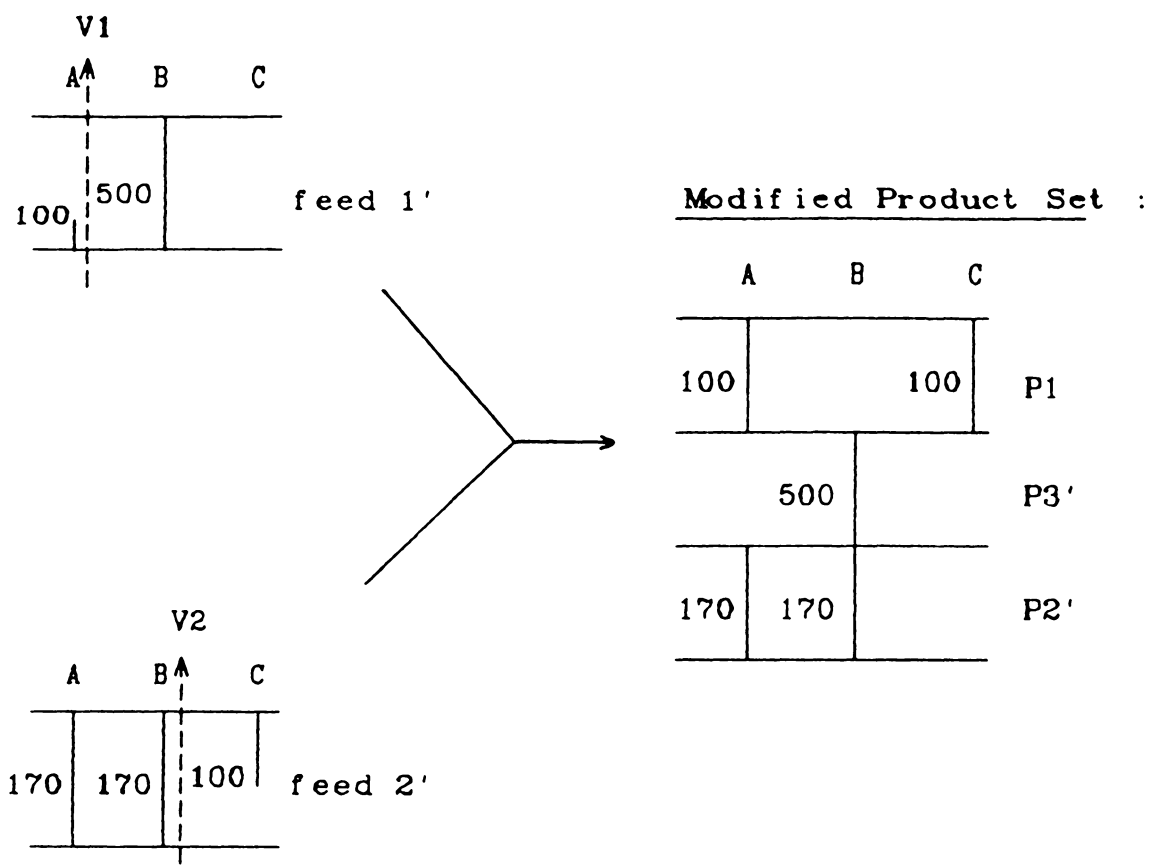


Figure 55. CADs of a Two-Feed Separation Problem After Bypassing

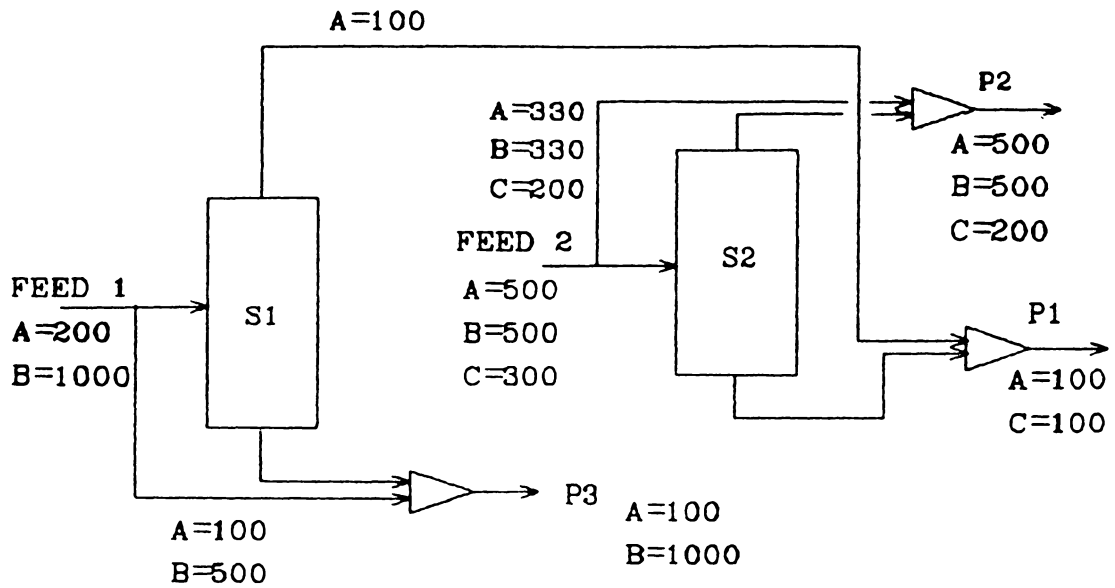


Figure 56. The Proposed Flowsheet of the Two-Feed Separation Problem

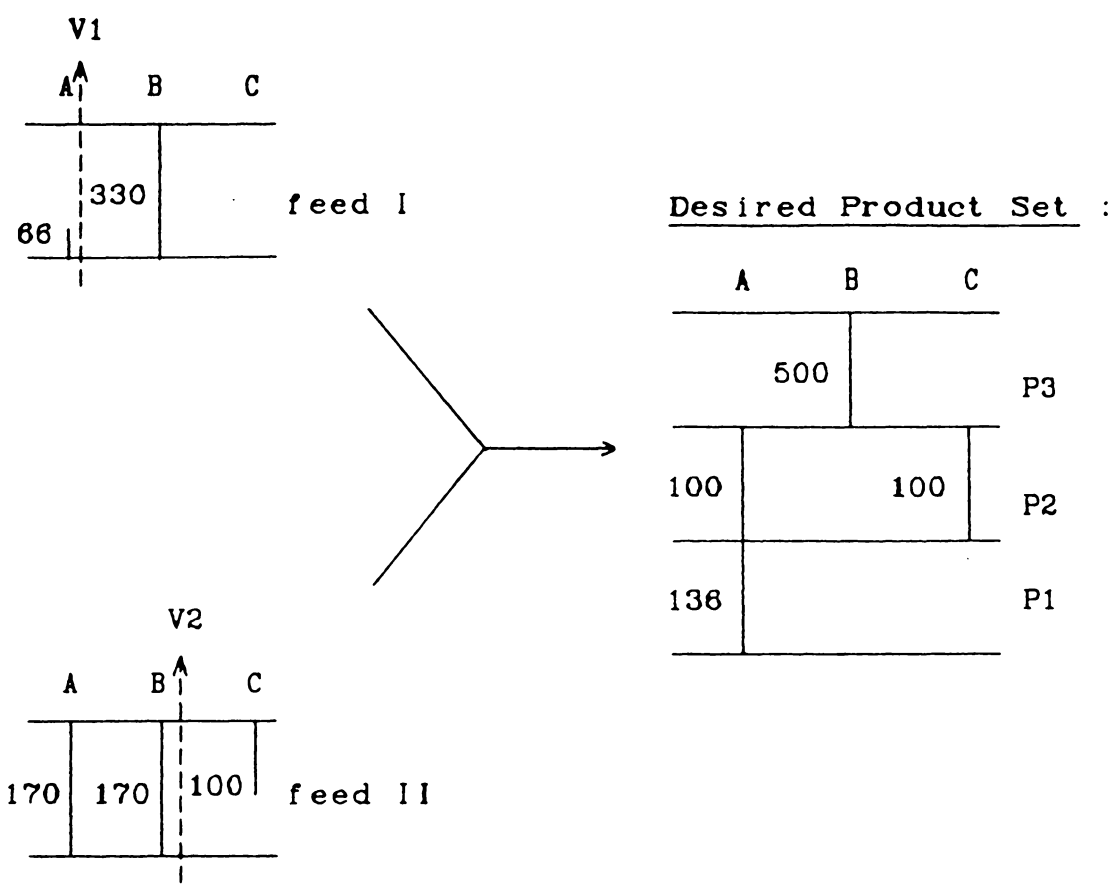


Figure 57. CADs of a Two-Feed Separation Problem



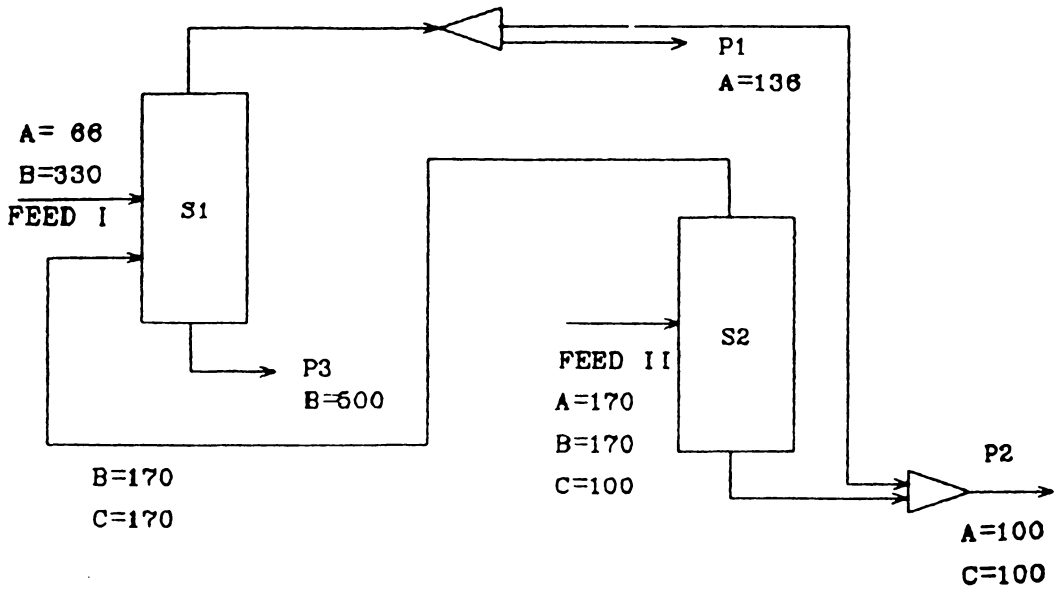


Figure 58. The Proposed Flowsheet of the Two-Feed Separation Problem

# NOMENCLATURE

## **NOTATION**

<b>b</b>	= component molar flow rate in the bottoms product, mole/hr
<b>B</b>	= molar flow rate of the bottoms product, mole/hr
<b>C</b>	= number of components
<b>CES</b>	= coefficient of ease of separation defined in eqn. (5.3)
<b>d</b>	= component molar rate in the overhead product, mole/hr
<b>D</b>	= molar flow rate of the overhead product, mole/hr
<b>f</b>	= $D/B$ or $B/D$ , whichever is smaller than or equal to unity
<b>HHK</b>	= a collective term for components heavier than HK, i.e., heavy components
<b>HHK1-3</b>	= heavy components whose volatilities are in a descending order
<b>HK</b>	= heavy key component
<b><math>K_i</math></b>	= vapor-liquid equilibrium ratio of component $i$
<b>LK</b>	= light key component
<b>LLK</b>	= a collective term for components lighter than LK, i.e., light components
<b>LLK1-3</b>	= light components whose volatilities are in an ascending order

- $N$  = number of equilibrium stages
- $n_{i,j}$  = molar flow rate of component  $i$  in product  $j$ , mole/hr
- $N_{MIN}$  = minimum number of equilibrium stages
- $P$  = number of product streams
- $P_C$  = column pressure, Pa
- $Q_C$  = condenser duty, J/hr
- $Q_R$  = reboiler duty, J/hr
- $R$  = reflux ratio
- $R_{MIN}$  = minimum reflux ratio
- $R_{\infty}$  = total reflux condition
- $r$  = rank of the product matrix
- $r'$  = pseudo-rank of the product matrix
- $S$  = number of separators in a sequence
- $S_{MIN}$  = minimum number of separators

$x_{D,i}$  = mole fraction of component  $i$  in the distillate

$x_{F,i}$  = mole fraction of component  $i$  in the feed

$Z_i$  = mole fraction of component  $i$  in the feed before and after bypassing

### **GREEK LETTERS**

$\alpha_{LK,HK}$  = relative volatility of LK with respect to that of HK

$\alpha_i$  = relative volatility of component  $i$  with reference to that of HK

### **SYMBOLS**

$\Delta$  =  $\Delta T$  (normal-boiling-point difference, °C)  $\times 1.8$  or  $(\alpha - 1) \times 100$

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# Appendix A. JUSTIFICATION OF RIGOROUS DISTILLATION AND ITS PROCEDURE

In ordinary cases (high-recovery columns), short-cut methods can adequately provide valuable information for designing and in turn costing a column. Specifically, the minimum reflux ratio, and minimum number of stages can be obtained by employing Underwood (1946) equations and Fenske (1932) equation, respectively.

Once these two key design variables are known, an empirical correlation established by Gilliland (1940) between actual number of stages and reflux ratio can be used. Then, column optimization can be easily executed. Unfortunately, this scheme may fall apart for the case of sloppy separations. Underwood equations are not capable of giving good approximation of the minimum reflux ratio. This follows in part because, unlike high-recovery cases, fractional recoveries of distributed non-keys are not readily accessible for sloppy separations. In addition, Underwood equations are based on two underlying assumptions, i.e., constant molal overflows and constant relative volatilities. In reality, the former assumption, valid when molar heats of vaporization of all column mixtures are constant, may sometimes be a source of large error in predicting the minimum reflux ratio. For the purpose of properly evaluating column costs which requires sufficiently accurate values of reflux ratios, it is imperative that rigorous simulations be conducted.

Despite the fact that in relatively sharp separations, the distribution of non-key components can be estimated by the Fenske equation, actual distribution of non-keys can only be revealed by rigorous plate-to-plate calculations, if not by experimental means, in a tedious trial-and-error fashion. Accordingly, in order to substantiate the limits and criteria that shortcut methods possess, one would have to rely on rigorous simulation.

To appreciate the considerable amount of calculations involved, the concept of rigorous distillation simulation will be briefly described as follows.

In the first place, one needs to define the term degrees of freedom (DOF) which is the number of independent variables to be specified for designing multicomponent equilibrium-stage processes such as a fractionator. For a typical  $N$ -stage single-feed (containing  $C$  components) column equipped with a total condenser and a partial reboiler, shown in Figure 59 on page 200, there are  $2NC + 5N + 6C + 7$  variables (e.g., interstage liquid mole fractions, temperatures, pressures, etc.) and  $2NC + 5N + 5C + 1$  independent relationships (e.g., phase equilibrium relationships for liquid and vapor streams leaving the same stage, component material balances, enthalpy balances, etc.) relating these variables. Hence, the resulting number of degrees of freedom is  $C + 6$ .

The following are some examples of degrees of freedom which can be specified in designing a distillation column.

Case A	Case B
feed composition	feed composition
feed rate	feed rate
column pressure	column pressure
feed enthalpy	feed enthalpy

number of stages	recovery of light key
reflux ratio	recovery of heavy key
feed-plate location	reflux ratio
recovery of light key	optimum feed location

---

Needless to say, there are more combinations of choices of degrees of freedom. For practical reasons, the examples listed above are the most common cases. It should be noted that the first four variables are always required to be set.

Case A is often referred to as the rating (or analysis) case in which the number of stages as well as feed location are both fixed. The variable - number of stages is not to be specified in Case B (design case) , it will be calculated instead. With different variables specified in the preceding two cases, schemes for solving the following system equations will be handled differently.

#### A. Component material balance equations :

$$v_{i,s} + l_{i,s} - v_{i,s-1} - l_{i,s+1} = f_{i,s} \quad [A - 1]$$

$$i = 1, \dots, C ; s = 1, \dots, N$$

where

$$l_{i,s} = L_s x_{i,s} = \text{liquid flow of component } i \text{ leaving plate } s$$

$$v_{i,s} = V_s y_{i,s} = \text{vapor flow of component } i \text{ leaving plate } s$$

$$f_{i,s} = F_s z_{i,s} = \text{flow of component } i \text{ of the feed on plate } s$$

#### B. Phase equilibrium equations :

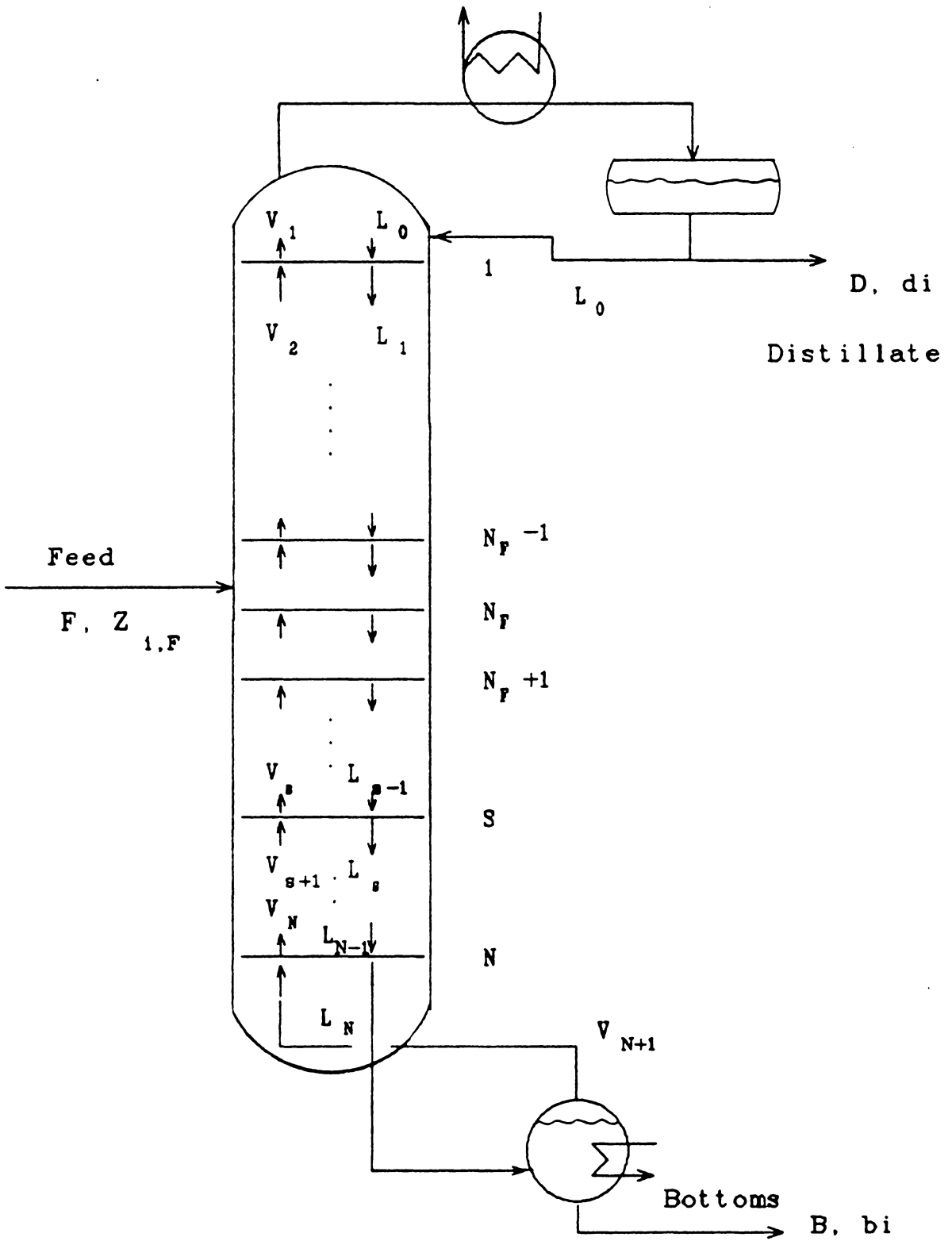


Figure 59. Schematic of a Distillation Column

$$K_{i,s} = \frac{y_{i,s}}{x_{i,s}} \quad [A - 2]$$

$$i = 1, \dots, C ; s = 1, \dots, N$$

where

$K_{i,s}$  = equilibrium ratio of component  $i$  on plate  $s$

### C. Energy balance equations :

$$V_s H'_s + L_s H_s - V_{s-1} H'_{s-1} + L_{s+1} H_{s+1} - F_s H_{fs} = q_s \quad [A - 3]$$

$$s = 1, \dots, N$$

where

$H_s$  = molal enthalpy of liquid mixture leaving plate  $s$

$H'_s$  = molal enthalpy of vapor mixture leaving plate  $s$

$H_{fs}$  = molal enthalpy of feed mixture on plate  $s$

$q_s$  = heat supplied on plate  $s$

### D. Mole fraction summation equations :

$$\sum_i x_{i,s} = 1, \sum_i y_{i,s} = 1 \quad [A - 4]$$

It is shown that there are four groups of equations involved in the stagewise calculations. Also, it is well known that  $H$ ,  $H'$ , and  $K$  are functions of temperature, pressure, and composition. Together, they form the system equations that are highly nonlinear, making them rather difficult to solve.

Lewis-Matheson method, among many other methods, was primarily developed for solving the equilibrium-stage calculation problem with known values for variables prescribed in Case B. Here, however, we will not dwell on the method since it oftentimes runs into convergence problem. For our purposes, the specified variables being chosen to carry out rigorous simulation are the same as in Case A. The algorithm is as follows. Initially, it starts with an assumed temperature profile which may be a linear profile between given estimates of overhead and bottoms temperatures. Knowing the stage temperatures, one can then perform stage-to-stage calculations in an iterative manner. Specifically, one will have to solve the foregoing system equations to evaluate component mole fractions on each plate. In order to obtain an improved temperature profile for the next iteration, bubble-point calculations are performed. Iterations will continue until the temperature profile is converged. The iterative stage-to-stage calculations are extremely tedious and use of computer can be justified.

The procedure used for obtaining actual column flow information is described as follows.

1. Find column operating pressure by using the scheme given in Chapter 4 (Figure 17 on page 56).
2. Specify feed composition, flow rate, pressure (assume the same as the column pressure which is constant throughout the column), and thermal condition (saturated liquid).
3. Fix fractional recoveries of light and heavy keys. Assume that a total condenser is used.
4. Use the short-cut techniques to find initial estimates of  $N_{\text{MIN}}$  and  $R_{\text{MIN}}$ , and a set of R and N values by the Fenske equation, Underwood equations, and Gilliland correlation, respectively. An equipment module from the available commercial simulation package

DESIGN II (ChemShare Corp., 1985, PP.4.18.1-4) called SHO has been used to do the computations.

5. Obtain estimates of overhead and bottoms temperatures through the above computations.

6. Set up the input data file which includes column pressure, number of plates, feed-plate location, estimates of temperatures of top and bottoms products, recoveries of LK and HK, and an assumed value of distillate flow rate, and run a rigorous plate-to-plate simulation program called DIS (ChemShare Corp., 1985, PP.4.4F.1-8).

7. Appropriately adjust reflux ratio and rerun the rigorous simulation program until the output recoveries of keys match the specified values.

## Appendix B. DISTILLATION COSTING DATA

Column - (Rathore et al., 1974)

column diameter (m) :

$$D_c = 1.7057 \sqrt{\frac{(1 + R)DT}{VP}} \quad [B - 1]$$

column height (m) :

$$H_c = 0.61 \frac{N}{\eta} + 4.27 \quad [B - 2]$$

where

D = distillate flow rate (mole/hr)

N = number of theoretical stages

P = column pressure (Pa)

R = reflux ratio

$\eta$  = average stage efficiency = 0.8



T = dew point of the vapor at the column top (K)

V = average vapor velocity (m) = 25.31 (1/P)\*\*0.5

Total installed column cost (Peters and Timmerhaus, 1980) :

$$\text{\$COL} = 4263.67 D_c^{1.1292} H_c \frac{803.7(\text{CE index, 1987})}{599.4(\text{CE index, 1979})} \quad [B - 3]$$

**Reboiler - (Guthrie, 1969)**

Assume U (overall heat-transfer coefficient) = 13232 J/hr m<sup>2</sup>

Total installed cost :

$$\text{\$RINS} = 1613.52 A^{0.65} \frac{803.7(\text{CE index, 1987})}{274.0(\text{CE index, 1969})} \quad [B - 4]$$

Reboiler operating cost :

$$\text{\$ROP} = (8500 \frac{\text{hr}}{\text{yr}}) C_{u,s} Q_R + 0.02(\text{\$RINS}) \quad [B - 5]$$

**Condenser - (Guthrie, 1969)**

Assume U (overall heat-transfer coefficient) = 10782 J/hr m<sup>2</sup>

Total installed cost :

$$\text{\$CINS} = 1613.52A^{0.65} \frac{803.7(\text{CE index, 1987})}{274.0(\text{CE index, 1969})} \quad [B - 6]$$

Condenser operating cost :

$$\text{\$COP} = \left(8500 \frac{\text{hr}}{\text{yr}}\right) C_{u,c} Q_R + 0.02(\text{\$CINS}) \quad [B - 7]$$

**Utility costs -**

utility	available temp. (°C)	pressure (Pa)	cost (\\$/10 <sup>9</sup> J)
steam	115.0	68932	5.414
steam	130.6	275728	7.396
steam	185.6	1033980	10.036
steam	231.1	2757280	13.294
steam	281.1	6445142	16.610
cooling water	35.0		0.145
propylene	4.4		2.765
propylene	-17.8		7.261
freon	-106.7		9.479

**Total Annual Cost -**

(costing basis for column optimization, project life of 10 yrs. is assumed)

$$\text{\$TAC} = \text{\$ROP} + \text{\$COP} + \frac{\text{\$COL} + \text{\$RINS} + \text{\$CINS}}{10} \quad [B - 8]$$

## **Appendix C. SIMULATION RESULTS OF EXAMPLE**

**1**

Sequence	1		1		1	
Column	S1		S2		S3	
$N$ (no. of plates)	20		36		28	
$N_F$ (feed-plate no.)	6		14		22	
$R$ (reflux ratio)	0.374		1.679		0.452	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	50.00	0.00	0.00	0.00	27.50	0.00
B	49.00	1.00	0.64	0.00	24.72	2.49
C	10.00	40.00	25.09	0.51	0.11	5.39
D	0.07	49.33	2.00	29.95	0.00	0.03
$P_C \times 10^{-5}$ (Pa)	2.818		2.068		3.132	
$Q_R \times 10^{-9}$ (J/hr)	1.821		0.865		0.745	
$-Q_C \times 10^{-9}$ (J/hr)	1.616		0.843		0.758	

Note 1: To ensure that the size of each column falls in the range of cost correlation, feed rates are increased by a factor of two.

Note 2:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 3:  $P_C$  denotes the column operating pressure.

Sequence	1		2		2	
Column	S4		S1		S2	
$N$ (no. of plates)	23		18		31	
$N_F$ (feed-plate no.)	17		14		21	
$R$ (reflux ratio)	1.184		0.698		0.971	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	1.50	2.00	49.00	1.00	29.40	1.96
B	0.17	8.30	25.00	25.00	0.32	15.68
C	0.00	0.20	1.40	48.60	0.00	0.69
D	0.00	0.00	0.00	50.00	0.00	0.02
$P_C \times 10^{-5}$ (Pa)	4.789		3.584		4.671	
$Q_R \times 10^{-9}$ (J/hr)	0.140		1.412		0.492	
$-Q_C \times 10^{-9}$ (J/hr)	0.144		1.250		0.497	

Note 1: To ensure that the size of each column falls in the range of cost correlation, feed rates are increased by a factor of two.

Note 2:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 3:  $P_C$  denotes the column operating pressure.

Sequence	2		2		3	
Column	S3		S4		S1	
$N$ (no. of plates)	26		25		20	
$N_F$ (feed-plate no.)	6		10		14	
$R$ (reflux ratio)	1.313		1.813		1.520	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	1.00	0.00	0.00	0.00	30.00	20.00
B	24.50	0.50	0.32	0.00	1.00	49.00
C	9.78	39.14	24.54	0.50	0.00	50.00
D	0.26	49.71	2.00	29.93	0.00	50.00
$P_C \times 10^{-5}$ (Pa)	2.068		2.068		4.789	
$Q_R \times 10^{-9}$ (J/hr)	0.923		0.879		0.811	
$-Q_C \times 10^{-9}$ (J/hr)	0.918		0.858		0.796	

Note 1: To ensure that the size of each column falls in the range of cost correlation, feed rates are increased by a factor of two.

Note 2:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 3:  $P_C$  denotes the column operating pressure.

Sequence	3		3		3	
Column	S2		S3		S4	
$N$ (no. of plates)	31		12		36	
$N_F$ (feed-plate no.)	9		10		14	
$R$ (reflux ratio)	0.570		0.546		1.679	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	20.00	0.00	19.27	0.73	0.00	0.00
B	48.02	0.98	24.01	24.01	0.64	0.00
C	10.00	39.98	0.20	9.78	25.09	0.51
D	0.09	49.90	0.00	0.09	2.00	29.95
$P_C \times 10^{-5}$ (Pa)	2.153		2.883		2.068	
$Q_R \times 10^{-9}$ (J/hr)	1.477		0.662		0.865	
$-Q_C \times 10^{-9}$ (J/hr)	1.359		0.683		0.843	

Note 1: To ensure that the size of each column falls in the range of cost correlation, feed rates are increased by a factor of two.

Note 2:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 3:  $P_C$  denotes the column operating pressure.

## **Appendix D. SIMULATION RESULTS OF EXAMPLE**

**2A**



Sequence	1		1		1	
Column	S1		S2		S3	
$N$ (no. of plates)	38		55		28	
$N_F$ (feed-plate no.)	20		29		12	
$R$ (reflux ratio)	1.35		2.64		1.30	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	121.19	0.00	118.08	3.11	0.00	0.00
B	59.42	0.16	1.48	57.94	0.16	0.00
C	116.83	3.00	0.89	115.94	3.00	0.00
D	1.50	58.46	0.00	1.50	58.46	0.00
E	0.07	62.62	0.00	0.07	62.62	0.00
F	0.00	32.51	0.00	0.00	28.26	4.25
G	0.00	6.63	0.00	0.00	5.32	1.31
H	0.00	10.81	0.00	0.00	3.93	6.88
I	0.00	62.72	0.00	0.00	18.23	44.49
J	0.00	39.61	0.00	0.00	7.92	31.69
K	0.00	80.33	0.00	0.00	6.72	73.61
L	0.00	23.91	0.00	0.00	4.70	19.21
M	0.00	7.37	0.00	0.00	0.00	7.37
$P_C \times 10^{-5}$ (Pa)	10.86		18.96		2.07	
$Q_R \times 10^{-9}$ (J/hr)	6.33		2.44		5.15	
$-Q_C \times 10^{-9}$ (J/hr)	5.26		2.38		5.03	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	1		1		1	
Column	S4		S5		S6	
$N$ (no. of plates)	78		75		53	
$N_F$ (feed-plate no.)	34		41		27	
$R$ (reflux ratio)	9.30		3.08		6.11	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	3.11	0.00	0.00	0.00	0.00	0.00
B	55.04	2.90	0.16	0.00	0.16	0.00
C	5.12	110.82	3.00	0.00	3.00	0.00
D	0.00	1.50	58.46	0.00	49.69	8.77
E	0.00	0.07	61.05	1.57	9.16	51.89
F	0.00	0.00	0.79	27.47	0.00	0.79
G	0.00	0.00	0.02	5.30	0.00	0.02
H	0.00	0.00	0.00	7.58	0.00	0.00
I	0.00	0.00	0.00	18.82	0.00	0.00
J	0.00	0.00	0.00	7.92	0.00	0.00
K	0.00	0.00	0.00	8.02	0.00	0.00
L	0.00	0.00	0.00	2.39	0.00	0.00
M	0.00	0.00	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	7.77		2.12		2.35	
$Q_R \times 10^{-9}$ (J/hr)	4.79		5.21		4.40	
$-Q_C \times 10^{-9}$ (J/hr)	4.85		5.17		4.46	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	2		2		2	
Column	S1		S2		S3	
$N$ (no. of plates)	39		57		44	
$N_F$ (feed-plate no.)	18		28		24	
$R$ (reflux ratio)	0.52		3.75		1.43	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	121.19	0.00	118.04	3.15	3.15	0.00
B	59.58	0.00	1.48	58.09	58.04	0.05
C	119.83	0.00	0.01	119.82	116.82	3.00
D	59.96	0.00	0.00	59.96	1.50	58.46
E	62.65	0.04	0.00	62.69	0.39	62.30
F	29.36	3.15	0.00	32.51	0.00	32.51
G	5.29	1.34	0.00	6.63	0.00	6.63
H	3.59	7.22	0.00	7.58	0.00	7.58
I	17.78	44.94	0.00	18.82	0.00	18.82
J	8.00	31.61	0.00	0.61	0.00	0.61
K	9.48	70.85	0.00	0.01	0.00	0.01
L	5.25	18.66	0.00	2.12	0.00	2.12
M	0.00	7.37	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	6.95		18.95		6.22	
$Q_R \times 10^{-9}$ (J/hr)	8.40		3.45		3.52	
$-Q_C \times 10^{-9}$ (J/hr)	7.85		3.12		3.46	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	2		2		2	
Column	S4		S5		S6	
$N$ (no. of plates)	78		75		53	
$N_F$ (feed-plate no.)	34		41		27	
$R$ (reflux ratio)	9.30		3.08		6.11	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	3.15	0.00	0.00	0.00	0.00	0.00
B	55.14	2.90	0.05	0.00	0.05	0.00
C	5.84	110.98	3.00	0.00	3.00	0.00
D	0.00	1.50	58.46	0.00	49.69	8.77
E	0.00	0.39	60.74	1.56	9.25	51.80
F	0.00	0.00	0.81	28.52	0.00	0.80
G	0.00	0.00	0.00	5.30	0.00	0.02
H	0.00	0.00	0.00	7.58	0.00	0.00
I	0.00	0.00	0.00	18.82	0.00	0.00
J	0.00	0.00	0.00	7.92	0.00	0.00
K	0.00	0.00	0.00	8.02	0.00	0.00
L	0.00	0.00	0.00	2.39	0.00	0.00
M	0.00	0.00	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	7.77		2.12		2.35	
$Q_R \times 10^{-9}$ (J/hr)	4.79		5.21		4.40	
$-Q_C \times 10^{-9}$ (J/hr)	4.85		5.17		4.46	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	3		3		3	
Column	S1		S2		S3	
$N$ (no. of plates)	71		56		28	
$N_F$ (feed-plate no.)	36		29		12	
$R$ (reflux ratio)	2.04		2.89		1.98	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	121.19	0.00	118.04	3.15	0.00	0.00
B	59.58	0.00	1.49	58.09	0.00	0.00
C	119.83	0.00	0.10	119.73	0.00	0.00
D	50.67	9.29	0.00	50.67	9.29	0.00
E	9.72	52.97	0.00	9.72	52.88	0.09
F	0.01	32.50	0.00	0.01	27.75	4.75
G	0.00	6.63	0.00	0.00	5.32	1.32
H	0.00	10.81	0.00	0.00	4.25	6.56
I	0.00	62.72	0.00	0.00	19.39	43.33
J	0.00	39.61	0.00	0.00	7.92	31.69
K	0.00	80.33	0.00	0.00	6.63	73.70
L	0.00	23.91	0.00	0.00	4.41	19.50
M	0.00	7.37	0.00	0.00	0.00	7.37
$P_C \times 10^{-5}$ (Pa)	9.22		18.95		2.07	
$Q_R \times 10^{-9}$ (J/hr)	10.22		2.62		4.40	
$-Q_C \times 10^{-9}$ (J/hr)	9.25		2.50		4.52	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	3		3		3	
Column	S4		S5		S6	
$N$ (no. of plates)	43		78		73	
$N_F$ (feed-plate no.)	25		34		39	
$R$ (reflux ratio)	1.10		9.30		4.69	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
A	3.15	0.00	3.15	0.00	0.00	0.00
B	58.08	0.01	55.06	3.02	0.00	0.00
C	116.64	3.09	5.83	110.81	0.00	0.00
D	1.52	49.15	0.02	1.50	9.29	0.00
E	0.01	9.71	0.00	0.01	51.44	1.44
F	0.00	0.01	0.00	0.00	0.78	26.97
G	0.00	0.00	0.00	0.00	0.00	5.32
H	0.00	0.00	0.00	0.00	0.00	4.25
I	0.00	0.00	0.00	0.00	0.00	19.39
J	0.00	0.00	0.00	0.00	0.00	7.92
K	0.00	0.00	0.00	0.00	0.00	6.63
L	0.00	0.00	0.00	0.00	0.00	4.41
M	0.00	0.00	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	6.23		7.77		2.07	
$Q_R \times 10^{-9}$ (J/hr)	3.00		4.79		3.56	
$-Q_C \times 10^{-9}$ (J/hr)	3.03		4.85		3.62	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

## **Appendix E. SIMULATION RESULTS OF EXAMPLE**

### **2B**

Sequence	1		1		1	
Column	S1		S2		S3	
$N$ (no. of plates)	55		58		30	
$N_F$ (feed-plate no.)	24		31		16	
$R$ (reflux ratio)	0.24		1.26		1.34	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
X	35.55	0.00	35.55	0.00	35.55	0.00
A	124.22	0.00	124.22	0.00	121.11	3.11
B	59.58	0.00	59.54	0.03	1.60	57.94
C	119.53	0.00	116.52	2.99	0.03	116.49
D	59.96	0.00	1.50	58.36	0.00	1.50
E	62.69	0.00	0.02	62.52	0.00	0.26
F	32.51	0.00	0.00	32.30	0.00	0.02
G	6.63	0.00	0.00	6.60	0.00	0.00
H	10.81	0.00	0.00	10.69	0.00	0.00
I	62.72	0.00	0.00	61.95	0.00	0.00
J	39.61	0.00	0.00	38.97	0.00	0.00
K	82.39	0.00	0.00	80.39	0.00	0.00
L	23.91	0.61	0.00	23.91	0.00	0.00
M	7.35	1172.60	0.00	7.37	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	6.41		15.03		28.70	
$Q_R \times 10^{-9}$ (J/hr)	38.72		7.11		2.71	
$-Q_C \times 10^{-9}$ (J/hr)	11.08		5.59		2.56	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.



Sequence	1		1		1	
Column	S4		S5		S6	
$N$ (no. of plates)	28		27		78	
$N_F$ (feed-plate no.)	12		11		34	
$R$ (reflux ratio)	1.30		2.56		9.30	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
X	0.00	0.00	34.66	0.89	0.00	0.00
A	0.00	0.00	2.95	118.16	3.10	0.00
B	0.03	0.00	0.01	1.48	55.04	2.90
C	2.99	0.00	0.00	0.19	5.51	110.82
D	58.36	0.00	0.00	0.00	0.00	1.50
E	62.52	0.00	0.00	0.00	0.00	0.26
F	28.05	4.25	0.00	0.00	0.00	0.02
G	5.32	1.31	0.00	0.00	0.00	0.00
H	3.81	6.88	0.00	0.00	0.00	0.00
I	17.46	44.49	0.00	0.00	0.00	0.00
J	7.28	31.69	0.00	0.00	0.00	0.00
K	6.78	73.61	0.00	0.00	0.00	0.00
L	4.70	19.21	0.00	0.00	0.00	0.00
M	0.00	7.37	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	2.07		15.38		7.77	
$Q_R \times 10^{-9}$ (J/hr)	5.15		0.72		4.79	
$-Q_C \times 10^{-9}$ (J/hr)	5.03		0.70		4.85	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	1		1		2	
Column	S7		S8		S1	
$N$ (no. of plates)	53		75		45	
$N_F$ (feed-plate no.)	27		41		17	
$R$ (reflux ratio)	6.11		3.08		1.17	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
X	0.00	0.00	0.00	0.00	35.55	0.00
A	0.00	0.00	0.00	0.00	124.22	0.00
B	0.03	0.00	0.03	0.00	59.58	0.00
C	2.99	0.00	2.99	0.00	119.53	0.00
D	49.61	8.75	58.36	0.00	59.58	0.38
E	8.73	51.78	60.51	1.55	61.60	1.09
F	0.00	0.78	0.78	27.26	22.72	9.79
G	0.00	0.02	0.02	5.30	5.30	1.33
H	0.00	0.00	0.00	3.81	3.94	6.87
I	0.00	0.00	0.00	17.46	19.92	42.80
J	0.00	0.00	0.00	7.28	7.92	31.69
K	0.00	0.00	0.00	6.78	9.05	73.34
L	0.00	0.00	0.00	4.70	3.37	21.15
M	0.00	0.00	0.00	0.00	0.05	1179.90
$P_C \times 10^{-5}$ (Pa)	2.35		2.12		9.99	
$Q_R \times 10^{-9}$ (J/hr)	4.40		5.21		36.02	
$-Q_C \times 10^{-9}$ (J/hr)	4.46		5.17		11.29	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	2		2		2	
Column	S2		S3		S4	
$N$ (no. of plates)	42		30		75	
$N_F$ (feed-plate no.)	24		16		41	
$R$ (reflux ratio)	1.05		1.34		3.08	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
X	35.55	0.00	35.55	0.00	0.00	0.00
A	124.22	0.00	121.11	3.11	0.00	0.00
B	59.41	0.17	1.47	57.94	0.17	0.00
C	116.54	3.00	0.05	116.49	3.00	0.00
D	1.49	57.98	0.00	1.49	57.98	0.00
E	0.11	61.14	0.00	0.11	60.51	1.55
F	0.00	27.48	0.00	0.00	0.82	28.52
G	0.00	5.30	0.00	0.00	0.02	5.30
H	0.00	4.34	0.00	0.00	0.00	4.34
I	0.00	20.74	0.00	0.00	0.00	20.74
J	0.00	7.92	0.00	0.00	0.00	7.92
K	0.00	7.10	0.00	0.00	0.00	7.10
L	0.00	5.42	0.00	0.00	0.00	5.42
M	0.00	0.00	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	15.02		28.70		2.12	
$Q_R \times 10^{-9}$ (J/hr)	5.68		2.71		5.21	
$-Q_C \times 10^{-9}$ (J/hr)	5.08		2.56		5.17	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	2		2		2	
Column	S5		S6		S7	
$N$ (no. of plates)	27		78		53	
$N_F$ (feed-plate no.)	11		34		27	
$R$ (reflux ratio)	2.56		9.30		6.11	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
X	34.66	0.89	0.00	0.00	0.00	0.00
A	2.95	118.16	3.11	0.00	0.00	0.00
B	0.00	1.47	55.04	2.90	0.17	0.00
C	0.00	0.05	5.67	110.82	3.00	0.00
D	0.00	0.00	0.00	1.49	49.23	8.75
E	0.00	0.00	0.00	0.11	8.73	51.78
F	0.00	0.00	0.00	0.02	0.00	0.82
G	0.00	0.00	0.00	0.00	0.00	0.02
H	0.00	0.00	0.00	0.00	0.00	0.00
I	0.00	0.00	0.00	0.00	0.00	0.00
J	0.00	0.00	0.00	0.00	0.00	0.00
K	0.00	0.00	0.00	0.00	0.00	0.00
L	0.00	0.00	0.00	0.00	0.00	0.00
M	0.00	0.00	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	15.38		7.77		2.35	
$Q_R \times 10^{-9}$ (J/hr)	0.72		4.79		4.40	
$-Q_C \times 10^{-9}$ (J/hr)	0.70		4.85		4.46	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	2		3		3	
Column	S8		S1		S2	
$N$ (no. of plates)	60		40		30	
$N_F$ (feed-plate no.)	15		19		16	
$R$ (reflux ratio)	14.90		1.80		1.34	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
X	0.00	0.00	35.55	0.00	35.55	0.00
A	0.00	0.00	124.22	0.00	121.11	3.11
B	0.00	0.00	59.33	0.25	1.39	57.94
C	0.00	0.00	116.54	2.99	0.05	116.49
D	0.38	0.00	1.50	58.46	0.00	1.50
E	1.09	0.00	0.21	62.48	0.00	0.21
F	2.18	0.99	0.01	32.50	0.00	0.01
G	1.05	0.26	0.00	6.63	0.00	0.00
H	1.41	1.82	0.00	10.81	0.00	0.00
I	14.00	28.80	0.00	62.72	0.00	0.00
J	6.33	25.36	0.00	39.61	0.00	0.00
K	3.36	69.98	0.00	82.39	0.00	0.00
L	1.67	19.48	0.00	24.52	0.00	0.00
M	0.00	1179.90	0.00	1179.90	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	2.07		13.10		28.70	
$Q_R \times 10^{-9}$ (J/hr)	6.88		26.43		2.71	
$-Q_C \times 10^{-9}$ (J/hr)	5.94		7.19		2.56	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	3		3		3	
Column	S3		S4		S5	
$N$ (no. of plates)	42		27		78	
$N_F$ (feed-plate no.)	17		11		34	
$R$ (reflux ratio)	0.58		2.56		9.30	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
X	0.00	0.00	34.66	0.89	0.00	0.00
A	0.00	0.00	2.95	118.16	3.11	0.00
B	0.25	0.00	0.00	1.39	55.04	2.90
C	2.99	0.00	0.00	0.05	5.67	110.82
D	58.46	0.00	0.00	0.00	0.00	1.50
E	62.48	0.00	0.00	0.00	0.00	0.21
F	32.50	0.00	0.00	0.00	0.00	0.01
G	6.63	0.00	0.00	0.00	0.00	0.00
H	10.81	0.00	0.00	0.00	0.00	0.00
I	62.72	0.00	0.00	0.00	0.00	0.00
J	39.61	0.00	0.00	0.00	0.00	0.00
K	82.25	0.14	0.00	0.00	0.00	0.00
L	24.05	0.47	0.00	0.00	0.00	0.00
M	7.37	1172.58	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	2.07		15.38		7.77	
$Q_R \times 10^{-9}$ (J/hr)	18.64		0.72		4.79	
$-Q_C \times 10^{-9}$ (J/hr)	6.88		0.70		4.85	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

Sequence	3		3		3	
Column	S6		S7		S8	
$N$ (no. of plates)	28		53		75	
$N_F$ (feed-plate no.)	12		27		41	
$R$ (reflux ratio)	1.30		6.11		3.08	
Comp. Flow(mole/hr)	Distillate	Bottoms	Distillate	Bottoms	Distillate	Bottoms
X	0.00	0.00	0.00	0.00	0.00	0.00
A	0.00	0.00	0.00	0.00	0.00	0.00
B	0.25	0.00	0.25	0.00	0.25	0.00
C	2.99	0.00	2.99	0.00	2.99	0.00
D	58.46	0.00	49.71	8.75	58.46	0.00
E	62.48	0.00	9.15	51.78	60.93	1.55
F	28.25	4.25	0.00	0.79	0.79	27.46
G	5.32	1.31	0.00	0.02	0.02	5.30
H	3.93	6.88	0.00	0.00	0.00	3.93
I	18.23	44.49	0.00	0.00	0.00	18.23
J	7.92	31.69	0.00	0.00	0.00	7.92
K	8.64	73.61	0.00	0.00	0.00	8.64
L	4.84	19.21	0.00	0.00	0.00	4.84
M	0.00	7.37	0.00	0.00	0.00	0.00
$P_C \times 10^{-5}$ (Pa)	2.07		2.35		2.12	
$Q_R \times 10^{-9}$ (J/hr)	5.15		4.40		5.21	
$-Q_C \times 10^{-9}$ (J/hr)	5.03		4.46		5.17	

Note 1:  $Q_R$  and  $Q_C$  denote the heat duty of reboiler and condenser, respectively.

Note 2:  $P_C$  denotes the column operating pressure.

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