PROCESS ENGINEERING AND DESIGN

Studies in Chemical Process Design and Synthesis. 9. A Unifying Method for the Synthesis of Multicomponent Separation Sequences with Sloppy Product Streams

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This paper presents a unifying method for the synthesis of flowsheets for multicomponent separations with sloppy product streams, in which some components being separated may simultaneously appear in two or more product streams. Our goal is to synthesize good separation sequences by using all-sharp, all-sloppy, and both sharp and sloppy separators. After introducing some basic tools and concepts for problem representation, feasibility analysis, and separation synthesis, we propose a unifying classification of all multicomponent separation-sequencing problems into four classes and suggest proper approaches to solving each class of synthesis problems. While we can apply our method with different synthesis tools such as optimization, we use six rank-ordered heuristics in a number of industrial separation problems. The resulting sequences represent good candidates for detailed flowsheet optimization. Our method can be easily applied by hand calculations by practicing engineers, and it has been implemented as an expert system using PROLOG.

1. Introduction

This work deals with the synthesis of alternative flowsheets for separating a multicomponent feed into several *sloppy* product streams, in which some components in the feed simultaneously appear in two or more product streams. As an example, Table I specifies a problem of separating a four-component mixture of light hydrocarbons (components A–D) into four sloppy product streams (products P1–P4), designated as example 1; Figure 1 illustrates three different separation sequences that give the desired product streams in example 1.

Figure 1a represents an *all-sharp sequence* S1, consisting of three sharp (S) separations in which each component being separated appears almost completely in one and only one product. Sharp separations correspond to very high recovery fractions of the light key in the overhead (denoted by d_{LK}) and of the heavy key in the bottoms (denoted by b_{HK}); that is, $0.98 \le d_{LK} \le 1.0$ and $0.98 \le b_{HK} \le 1.0$. Sequence S1 begins with a sharp split ABC/D in separator V3, followed by a sharp split AB/C in separator V2′ with a portion of the feed being bypassed around the separator to directly form a part of the overhead (denoted by a prime in V2′). The sequence ends with a sharp split A/B in separator V1″, where the double prime indicates bypassing two portions of the feed around the separator to directly form parts of both overhead and bottoms products.

Sequence S1 includes three separators ($S = 3$). This number corresponds to the apparent minimum number of separators, S_{min}, for example 1 that is specified by the following equation (Cheng and Liu, 1988, *designated hereafter as part 8*):

$$S_{min} = \min(C,P) - 1 = \min(4,4) - 1 = 4 - 1 = 3 \quad (1)$$

In the equation, C is the number of components and P is the number of products.

Figure 1b shows a four-separator, *all-sloppy sequence* SL1. This sequence consists of four sloppy (SL) or low-recovery separations, in which some components in the feed simultaneously appear in two or more products. Sequence SL1 begins with a sloppy split ABC/CD in separator H3. The overhead from H3 goes to another sloppy separator H2′(AB/BC) and then to H1′(A/AB), while the bottoms from H3 goes to H4′(CD/D). This all-sloppy sequence includes one more separator than S_{min} (=3). In this work, we are interested in the synthesis of sloppy sequences that have at most one more separator than other competing minimum-separator sequences. With less stringent component recovery fractions specified in sloppy separations, an all-sloppy sequence could cost less than a competing minimum-separator sequence.

Figure 1c depicts a four-separator, *mixed-separation sequence* MS2 that utilizes *both sloppy and sharp sepa-*

Table I. Feed and Product Specifications in Example 1[a]

desired prod streams	component flow rate, mol/h: A	B	C	D	prod flow rate, mol/h
P4	0	0	0	15	15
P3	0	0	20	10	30
P2	10	12.5	0	0	22.5
P1	15	12.5	5	0	32.5
component flow rate in feed, mol/h	25	25	25	25	100

[a] Data taken from Nath (1977). Components A, B, C, and D are, respectively, *n*-butane, *n*-pentane, *n*-hexane, and *n*-heptane with normal boiling points of −0.5, 36.1, 68.7, and 98.4 °C. For a feed mixture at 92.2 °C and 466.1 kPa, equilibrium ratios are $K_A = 2.46$, $K_B = 1.00$, $K_C = 0.47$, and $K_D = 0.21$ or the relative volatilities are $\alpha_{AB} = 2.46$, $\alpha_{BC} = 2.13$, $\alpha_{AC} = 5.23$, $\alpha_{CD} = 2.24$, and $\alpha_{BD} = 4.76$.

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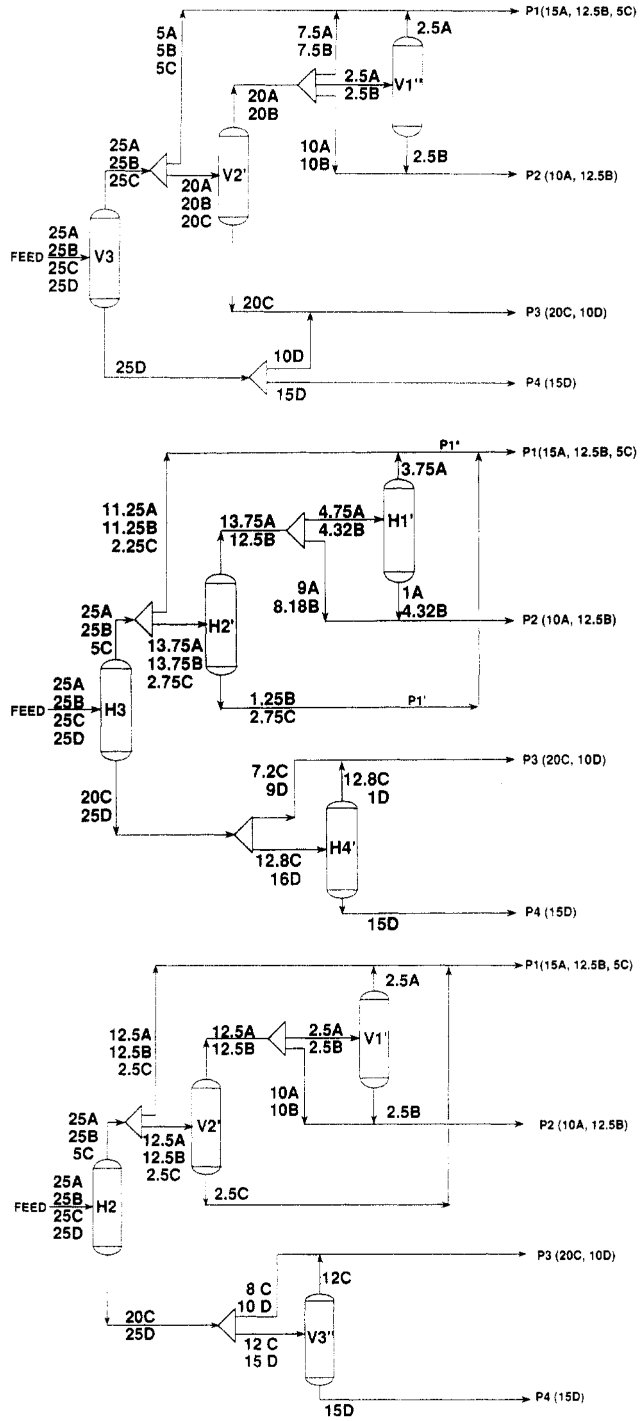

Figure 1. (a) An all-sharp, three-separator sequence for example 1: sequence S1, V3(ABC/D) - V2′(AB/C) - V1″(A/B). (b) An all-sloppy, four-separator sequence for example 1: (c) A mixed-separation sequence with four separators for example 1:

sequence SL1, H3(ABC/CD) → H2′(AB/BC) - H1′(A/AB); → H4′(CD/D)

sequence MS2, H2(ABC/CD) → V2′(AB/C) - V1′(A/B); → V3′(C/D)

rators. This sequence begins with a sloppy split ABC/CD in separator H2. The overhead from H2 goes to a sharp separator V2′(AB/C) followed by another sharp separator V1′(A/B), while the bottoms from H2 goes to a sharp separator V3′(C/D). When properly designed, a mixed-separation sequence can be competitive in cost compared to a minimum-separator, all-sharp sequence or to an all-sloppy sequence with an equal number of separators.

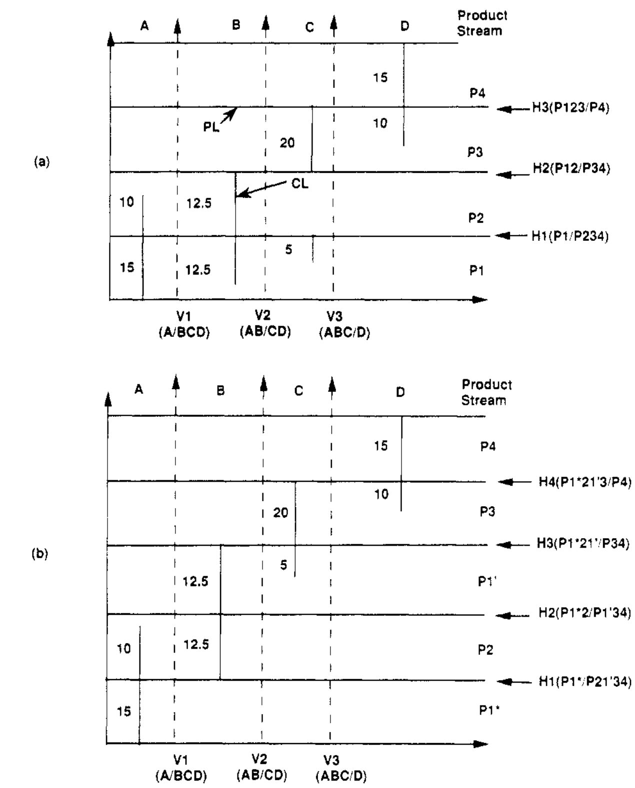

Figure 2. Component assignment diagrams (CADs) for representing example 1: (a) original product streams, (P1,P2,P3,P4); and (b) pseudoproduct streams, (P1*,P2,P1′,P3,P4), obtained by splitting product 1 into two pseudoproducts, 1* and 1′.

The objective of this work is to present a unifying method for the synthesis of multicomponent separation sequences with sloppy product streams. Our method is unifying because of its two special features: (1) it contains *a unifying classification* of all multicomponent separation-sequencing problems into four classes and suggests proper approaches to solving each class of synthesis problems; and (2) it permits the synthesis of good separation flowsheets with a minimum number or a nearly minimum number of *all three types of separations*, namely, all-sharp, all-sloppy, and mixed-separation schemes. We can implement the method with a variety of synthesis tools such as heuristics and optimization. We shall demonstrate our method in synthesizing good separation sequences for several example problems. Finally, we note that some background information on the synthesis of multicomponent separation sequences appears in the textbook by Henley and Seader (1981) and in reviews by Westerberg (1985) and Liu (1987).

2. Basic Tools and Concepts

2.1. Problem Representation. In part 8, we introduced the component assignment diagram (CAD) for representing the problem of synthesizing multicomponent separation sequences. As an illustration, Figure 2a shows a CAD for representing example 1. In the diagram, components A–D are placed from left to right in order of decreasing separation factor, such as relative volatility. Horizontal product lines (PLs), denoted by H1–H3, are used to separate one product from the other. We write down the product split corresponding to each PL on the right-hand side of a CAD. For example, H1(P1/P234) represents a split that gives an overhead of product P1 and a bottoms of P234 (=P2 + P3 + P4).

Vertical component lines (CLs) specify the component distribution in each product stream. The length of the CL

Table II. SST for First Splits in Example 1 Represented by Equation 2

separation	ovhd/btm	LK/HK	Δ, °C	$(d/b)_A$	$(d/b)_B$	$(d/b)_C$	$(d/b)_D$	CES
V1	A/BCD = 25/75	A/B	36.6	0.98/0.02[d]	0.02/0.98	0.02/0.98	0.02/0.98	3.61
V2	AB/CD = 50/50	B/C	32.6	0.98/0.02	0.98/0.02	0.02/0.98	0.02/0.98	9.67
V3	ABC/D = 75/25	C/D	29.7	0.98/0.02	0.98/0.02	0.98/0.02	0.02/0.98	2.93
H1[b]	P1/P234 = 32.5/67.5	A/B	36.6	0.6/0.4	0.5/0.5	0.416/0.584	0.02/0.98	infeasible[a]
H1	P1/P234 = 32.5/67.5	B/C	32.7	0.954/0.046	0.5/0.5	0.2/0.8	0.02/0.98	infeasible[a]
H2[b]	P12/P34 = 55/45	B/C	32.6	0.98/0.02	0.98/0.02	0.2/0.8	0.001/0.999[c]	11.7
H2	P12/P34 = 55/45	C/D	29.7	0.98/0.02	0.73/0.27	0.2/0.8	0.02/0.98	infeasible[a]
H3	P123/P4 = 85/15	C/D	29.7	0.98/0.02	0.98/0.02	0.98/0.02	0.4/0.6	2.81

[a] Infeasible product splits due to undesirable nonkey component distributions. [b] Separations with split keys, that is, H1(P1/P234) with A/C as LK/HK and H2(P12/P34) with B/D as LK/HK, are not included due to undesirable nonkey component distributions. [c] Dashed horizontal lines denote component-recovery ratios estimated by the Fenske equation. [d] Dashed vertical lines represent the partition between the LK and the HK.

represents the flow rate of a component in the specific product stream bounded by two PLs, and the numerical value of the component molar flow rate is indicated next to each CL. Vertical product lines, denoted by V1–V3, are used to separate one component from the other. For example, V1(A/BCD) represents a split that gives an overhead of component A and a bottoms of components B–D.

In this work, we simplify our problem representation by introducing a *component assignment matrix (CAM)*. Elements of this matrix correspond to component molar flow rates that are indicated next to each CL between two PLs in the CAD. Thus, the CAM for example 1 represented by Figure 2a is

$$\begin{array}{c} \\ P4 \\ P3 \\ P2 \\ P1 \\ \\ \\ \end{array}
\begin{array}{c}
\begin{array}{cccc} \;A\; & \;B\; & \;C\; & \;D\; \end{array} \\
\begin{bmatrix} 0 & 0 & 0 & 15 \\ 0 & 0 & 20 & 10 \\ 10 & 12.5 & 0 & 0 \\ 15 & 12.5 & 5 & 0 \end{bmatrix} \\
\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ \text{V1} & \text{V2} & \text{V3} \\ (\text{A/BCD}) & (\text{AB/CD}) & (\text{ABC/D}) \end{array}
\end{array}
\begin{array}{l} \\ \leftarrow \text{H3 (P123/P4)} \\ \leftarrow \text{H2 (P12/P34)} \\ \leftarrow \text{H1 (P1/P234)} \\ \\ \\ \\ \end{array} \quad (2)$$

In what follows, *we often simplify our designation of products, P1, P2, P3, ..., in a CAM by 1, 2, 3, ...* The use of the CAM for problem representation greatly facilitates the computer implementation of our synthesis method.

2.2. Feasibility Analysis. Component splits represented by vertical PLs, such as V1(A/BCD), V2(AB/CD), and V3(ABC/D) in eq 2, are *sharp* separations. These splits may not directly yield the desired sloppy product streams. For some synthesis problems, we need to blend together two or more products from different vertical component splits, V*j*'s, to obtain the desired sloppy products. Figure 1a illustrates this blending practice.

Product splits represented by horizontal PLs, namely, H1(P1/P234), H2(P12/P34), and H3(P123/P4) in eq 2, correspond to *either sloppy or sharp* separations depending on component recovery specifications. A key difference between vertical component splits V*j*'s and horizontal product splits H*i*'s is that *Vj's are always feasible but not all Hi's are technically and/or practically feasible.* The feasibility of H*i*'s depends on (1) the specification of component recovery fractions in the overhead and bottoms, d_i and b_i; (2) the choice of light-key (LK) and heavy-key (HK) components; and (3) the possibility of having significant or undesirable distributions of nonkey components in both the overhead and bottoms. In part 8, we introduced a *separation specification table (SST)* to aid in the feasibility analysis of H*i*'s. In this work, we extend the use of the SST to analyze the technical feasibility and practicality of *both* H*i*'s *and* V*j*'s. Table II gives an SST for the first splits in example 1 representation by eq 2.

An SST contains the following information: (1) type of separation, H*i*'s or V*j*'s; (2) overhead (ovhd or D) and bottoms (btm or B); (3) choice of LK and HK components; (4) separation factor between the LK and the HK; (5) calculated and estimated ratios of component recovery fraction in the overhead to that in the bottoms; and (6) coefficient of ease of separation (CES) defined by the following equation

$$\text{CES} = f\cdot\Delta\cdot\frac{1}{\log\,[(d/b)_{\text{LK}}(b/d)_{\text{HK}}]} \quad (3)$$

In this equation, f is the ratio of the molar flow rates of products, B/D or D/B, depending on which of the two ratios is smaller than or equal to unity; $\Delta = \Delta T$ = boiling-point difference between key components, or $\Delta = 100(\alpha_{\text{LK,HK}} - 1)$ with $\alpha_{\text{LK,HK}}$ being the relative volatility between the LK and the HK. The logarithmic term in the equation represents the effect of split sloppiness on the ease of separation, mimicking a similar effect on the minimum number of theoretical stages $N_{\min}$ according to the Fenske equation

$$N_{\min} = \frac{\log\,[(d/b)_{\text{LK}}(b/d)_{\text{HK}}]}{\log\,\alpha_{\text{LK,HK}}} \quad (4)$$

Part 8 described how to calculate component split ratios, (d/b)'s, listed in an SST based on given component flow rates. Let us consider an example based on eq 2. For split H1(P1/P234) with A/B as LK/HK listed in Table II, we find

$$(d/b)_{\text{LK}} = (d/b)_{\text{A}} = 15/10 \text{ (eq 2)} = 0.6/0.4 \text{ (Table II)}$$

$$(d/b)_{\text{HK}} = (d/b)_{\text{B}} = 12.5/12.5 \text{ (eq 2)} = 0.5/0.5 \text{ (Table II)}$$

$$(d/b)_{\text{HHK2}} = (d/b)_{\text{D}} = 0/25 \text{ (eq 2)} \simeq 0.02/0.98 \text{ (Table II)}$$

Here, HHK2 refers to the second heavier-than-heavy or heavy-key component, and we use a limiting ratio of 0.02/0.98 to approximate the sharp cut represented by the calculated ratio, 0/25, for component HHK2 or D.

To estimate the split ratio of a nonkey component in an SST, we take advantage of the fact tht the Fenske equation is applicable to different combinations of light and heavy components such as (LLK2, HK), (LLK1, HK), (LK, HHK1), and (LK, HHK2). Let us consider the first heavy component HHK1 or component C resulting from H1-(P1/P234) with A/B as LK/HK included in Table II. We use the relative volatilities given in Table I and first apply the Fenske equation to (LK, HK) or (A, B) to find the minimum number of theoretical stages, $N_{\min}$:

$$N_{\min} = \frac{\log\,[(d/b)_{\text{LK}}(b/d)_{\text{HK}}]}{\log\,\alpha_{\text{LK,HK}}} = \frac{\log\,[(d/b)_{\text{A}}(b/d)_{\text{B}}]}{\log\,\alpha_{\text{AB}}} = \frac{\log\,[(0.6/0.4)(0.5/0.5)]}{\log 2.46} = 0.4504$$

We then apply the equation with the calculated value of $N_{\min}$ to (LK, HHK1) or (A, C):

$$N_{\min} = 0.4504 = \frac{\log [(d/b)_{\mathrm{LK}}(b/d)_{\mathrm{HHK1}}]}{\log \alpha_{\mathrm{LK,HHK1}}} = \frac{\log [(d/b)_{\mathrm{A}}(b/d)_{\mathrm{C}}]}{\log \alpha_{\mathrm{AC}}} = \frac{\log [(0.6/0.4)(b/d)_{\mathrm{C}}]}{\log 5.23}$$

Since $d_i + b_i = 1$ for any component i, we can solve the last equation to obtain $b_C = 0.4159$ and $d_C = 0.5841$, or $(D/B)_{\mathrm{HHK1}} = (d/b)_C = 0.416/0.584$. In Table II, we use a dashed horizontal line to characterize this split ratio as an estimated value for heavy component HHK1 or component C that results from H1(P1/P234) with A/B as LK/HK. This estimated split ratio of $(d/b)_C = 0.416/0.584$ represents a significant distribution of a nonkey component C in both overhead and bottoms. As discussed in part 8, in order to avoid this undesirable distribution of nonkey components in both overhead and bottoms, the designer often needs to use a distillation column with a large number of theoretical stages, resulting in a costly design. We therefore designate H1(P1/P234) with A/B as LK/HK as *an economically or a practically infeasible split* and indicate it as "infeasible" under the CES column in Table II.

We can also apply the shortcut feasibility analysis to other H*i*'s or V*j*'s listed in Table II. For example, for H2(P12/P34) with B/C as LK/HK, we find

$$(d/b)_{\mathrm{LLK}} = (d/b)_{\mathrm{A}} = 25/0 \text{ (eq 2)} \simeq 0.98/0.02 \text{ (Table II)}$$

$$(d/b)_{\mathrm{LK}} = (d/b)_{\mathrm{B}} = 25/0 \text{ (eq 2)} \simeq 0.98/0.02 \text{ (Table II)}$$

$$(d/b)_{\mathrm{HK}} = (d/b)_{\mathrm{C}} = 5/20 \text{ (eq 2)} = 0.2/0.8 \text{ (Table II)}$$

Here, we use a limiting ratio of 0.98/0.02 to approximate the sharp cut represented by the calculated ratio, 25/0, for components A and D.

As in the case of H1(P1/P234), we can apply the Fenske equation to estimate the split ratio of nonkey component HHK1 or component D resulting from H2(P12/P34). We find $b_D \simeq 0.999$, $d_D \simeq 0.001$, and $(d/b)_D \simeq 0.001/0.999$, as indicated by a dashed horizontal line in Table II for H2(P12/P34) with B/C as LK/HK. We characterize this horizontal product split as "feasible", because (1) it does not lead to undesirable nonkey component distributions and (2) its component recovery specifications satisfy the following *feasibility conditions* developed in part 8

$$... \geq d_{\mathrm{LLK2}} \geq d_{\mathrm{LLK1}} \geq d_{\mathrm{LK}} > d_{\mathrm{HK}} \geq d_{\mathrm{HHK1}} \geq d_{\mathrm{HHK2}} > ... \tag{5}$$

or

$$... \leq b_{\mathrm{LLK2}} \leq b_{\mathrm{LLK1}} \leq b_{\mathrm{LK}} < b_{\mathrm{HK}} \leq b_{\mathrm{HHK1}} \leq b_{\mathrm{HHK2}} \leq ... \tag{6}$$

Specifically, for H2(P12/P34) with B/C as LK/HK, Table II gives

$$d_{\mathrm{LLK1}} \geq d_{\mathrm{LK}} > d_{\mathrm{HK}} > d_{\mathrm{HHK1}} \quad (0.98 = 0.98 > 0.2 > 0.001)$$

$$b_{\mathrm{LLK1}} \leq b_{\mathrm{LK}} < b_{\mathrm{HK}} < b_{\mathrm{HHK1}} \quad (0.02 = 0.02 < 0.8 < 0.999)$$

For this feasible split, we calculate the CES value listed in Table II according to eq 3, or

$$\mathrm{CES} = f \cdot \Delta \cdot \frac{1}{\log [(d/b)_{\mathrm{LK}}(b/d)_{\mathrm{HK}}]} = (45/55)(32.6)\frac{1}{\log [(0.98/0.02)(0.8/0.2)]} = 11.7$$

We should recognize that an improper choice of LK/HK may make a horizontal product split practically infeasible due to undesirable nonkey component distributions. For example, Table II shows that using a different set of LK/HK in applying the Fenske equation to H2(P12/P34) results in the following split ratios for nonkey components:

(a) B/C as LK/HK

$$(d/b)_{\mathrm{LLK1}} = (d/b)_{\mathrm{A}} = 0.98/0.02 \qquad (d/b)_{\mathrm{HHK1}} = (d/b)_{\mathrm{D}} \simeq 0.001/0.999$$

(b) C/D as LK/HK

$$(d/b)_{\mathrm{LLK2}} = (d/b)_{\mathrm{A}} = 0.98/0.02 \qquad (d/b)_{\mathrm{LLK1}} = (d/b)_{\mathrm{B}} \simeq 0.73/0.27$$

In part 8, we demonstrated that if the split ratio of a light component, LLK, predicted by the Fenske equation at total reflux is greater than or equal to a limiting ratio of 0.98/0.02, then this light component does not significantly distribute in both overhead and bottoms under common operating reflux ratios $R_D = 1.1–1.5R_{D,\min}$. This observation is also true for a heavy component, HHK, that has a split ratio not greater than a limiting ratio of 0.02/0.98. For H2(P12/P34) with B/C as LK/HK, $(d/b)_{\mathrm{LLK1}}$ and $(d/b)_{\mathrm{HHK1}}$ satisfy these limiting conditions and this split is feasible. By contrast, H2(P12/P34) with C/D as LK/HK results in a nonkey-component split ratio, $(d/b)_{\mathrm{LLK1}} \simeq 0.73/0.27 < 0.98/0.02$. Therefore, choosing C/D as LK/HK makes H2(P12/P34) infeasible.

We mention one additional item of interest that is related to the always feasible, vertical component splits V1–V3. We approximate the sharp cut of a light-key (LK) or a lighter-than-light-key (LLK) component in the overhead and bottoms by a limiting split ratio of 0.98/0.02. Likewise, we approximate the sharp cut of a heavy-key (HK) or a heavier-than-heavy-key (HHK) component by 0.02/0.98. For example, for V2(AB/CD) with B/C as LK/HK listed in Table II, we find

$$(d/b)_{\mathrm{LLK}} = (d/b)_{\mathrm{A}} = 25/0 \text{ (eq 2)} \simeq 0.98/0.02 \text{ (Table II)}$$

$$(d/b)_{\mathrm{LK}} = (d/b)_{\mathrm{B}} = 25/0 \text{ (eq 2)} \simeq 0.98/0.02 \text{ (Table II)}$$

$$(d/b)_{\mathrm{HK}} = (d/b)_{\mathrm{C}} = 0/25 \text{ (eq 2)} \simeq 0.02/0.98 \text{ (Table II)}$$

$$(d/b)_{\mathrm{HHK}} = (d/b)_{\mathrm{D}} = 0/25 \text{ (eq 2)} \simeq 0.02/0.98 \text{ (Table II)}$$

To summarize, using an SST together with the CAM provides a simple means to analyze the technical feasibility of both horizontal product splits H*i*'s and vertical component splits V*j*'s. This analysis identifies technically and/or practically infeasible splits resulting from undesirable component recovery specifications and nonkey component distributions.

2.3. Pseudoproduct Transformation and Stream Bypassing. Consider again example 1 represented by eq 2. An all-sloppy sequence for this example, such as sequence SL1, Figure 1b, may consist of the following candidates of H*i*'s: (a) first splits, P1/P234, P12/P34, P123/P4; (b) second splits, P1/P23, P12/P3, P2/P34, and P23/P4; and (c) third splits, P1/P2, P2/P3, and P3/P4. Unfortunately, not all of these H*i*'s are technically and/or practically feasible. For example, split H(P1/P2) may be represented by the following submatrix of eq 2:

$$\begin{array}{cc} & \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{array}{c} 2 \\ 1 \end{array} & \begin{bmatrix} 10 & 12.5 & 0 \\ 15 & 12.5 & 5 \end{bmatrix} \leftarrow \mathrm{H(P1/P2)} \end{array}$$

Choosing A/B as LK/HK for H(P1/P2) gives

$$(d/b)_{\mathrm{LK}} = (d/b)_{\mathrm{A}} = 15/10 = 0.6/0.4$$

$$(d/b)_{\mathrm{HK}} = (d/b)_{\mathrm{B}} = 12.5/12.5 = 0.5/0.5$$

$$(d/b)_{\mathrm{HHK1}} = (d/b)_{\mathrm{C}} = 5/0 \simeq 0.98/0.02$$

These component recovery specifications do not satisfy the feasibility conditions, eqs 5 and 6, or

$$d_{\mathrm{LK}} > d_{\mathrm{HK}} > d_{\mathrm{HHK1}} \quad (0.6 > 0.5 \not> 0.98)$$

$$b_{\mathrm{LK}} < b_{\mathrm{HK}} < b_{\mathrm{HHK1}} \quad (0.4 < 0.5 \not< 0.02)$$

Therefore, H(P1/P2) is technically infeasible; the corresponding product set, (P1/P2), represents an infeasible product set for an all-sloppy sequence for example 1.

We can convert the infeasible product set, (P1,P2), into an equivalent feasible product set (P1*,P2,P1′) by splitting part of product P1 into two pseudoproducts, P1* and P1′. Figure 2b illustrates this pseudoproduct transformation, and the corresponding CAM is

$$\begin{array}{cc} & \begin{array}{cccc} \mathrm{A} & \mathrm{B} & \mathrm{C} & \mathrm{D} \end{array} \\ \begin{array}{c} 4\\ 3\\ 1'\\ 2\\ 1^* \end{array} & \begin{bmatrix} 0 & 0 & 0 & 15\\ 0 & 0 & 20 & 10\\ 0 & 12.5 & 5 & 0\\ 10 & 12.5 & 0 & 0\\ 15 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{array}{l} \leftarrow \mathrm{H4}\\ \leftarrow \mathrm{H3}\\ \leftarrow \mathrm{H2}\\ \leftarrow \mathrm{H1} \end{array} \qquad (7)$$

$$\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ \mathrm{V1} & \mathrm{V2} & \mathrm{V3} \end{array}$$

Since all component recovery fractions corresponding to component flow rates in the equivalent product set (P1*,P2,P1′,P3,P4) satisfy eqs 5 and 6, splits H(P1*,P2), H(P2/P1′), H(P1′/P3), and H(P3/P4) are technically feasible. After carrying out these splits, we can readily obtain the desired product P1 by blending together pseudoproducts P1* and P1′.

A disadvantage of confining the sequence of separating a multicomponent mixture to using only horizontal product splits Hi's is that whenever an infeasible product split exists, stream splitting together with pseudoproduct transformation increases the number of separators by one for each pseudoproduct introduced. In the following, we first describe the concept of stream bypassing and its significance and then illustrate another approach to dealing with the problem of infeasible product splits.

In Figure 1b, we represent the all-sloppy sequence SL1 for example 1 by the following

$$\mathrm{SL1} \qquad \mathrm{H3(ABC/CD)} \begin{array}{l} \nearrow \mathrm{H2'(AB/BC)} - \mathrm{H1'(A/AB)} \\ \searrow \mathrm{H4'(CD/D)} \end{array} \qquad (8)$$

Using our standard notation for horizontal product splits, we now repreent sequence SL1 in terms of the equivalent feasible product set (P1*,P2,P1′,P3,P4) as

$$\mathrm{SL1} \qquad \mathrm{H3(P1^*21'/P34)} \begin{array}{l} \nearrow \mathrm{H2'(P1^*2/P1')} - \mathrm{P1'(P1^*/P2)} \\ \searrow \mathrm{H4'(P3/P4)} \end{array} \qquad (9)$$

We use sequence SL1 to illustrate below when stream bypassing should be used and what advantages may be gained from bypassing.

From eq 7, we write the submatrix representing the bottoms from H3(P1*21′/P34):

$$\mathrm{CAM(H3,btm)} = \begin{array}{cc} & \begin{array}{cc} \mathrm{C} & \mathrm{D} \end{array} \\ \begin{array}{c} 4\\ 3 \end{array} & \begin{bmatrix} 0 & 15\\ 20 & 10 \end{bmatrix} \end{array} \leftarrow \mathrm{H4} \qquad (10)$$

$$\begin{array}{c} \uparrow \\ \mathrm{V3} \end{array}$$

We see that product P3 contains all the components (namely, C and D) in the feed. We therefore call product P3 *an all-component-inclusive product.*

The presence of an all-component-inclusive product suggests the possibility of bypassing a portion of the feed stream around the separator to directly form a part of the product. For example, H4′(CD/D) or H4′(P3/P4) in sequence SL1 depicted in Figure 1b involves bypassing to product P3. We are limited in the amount of bypassing allowed by the material balance. Component D is the limiting component, and we can bypass at most 10 mol/h of D to P3. If we bypass 90% of that amount, i.e., 9 mol/h of D, and 7.2 mol/h of C, we get

$$\begin{array}{cc} & \begin{array}{cc} \mathrm{C} & \mathrm{D} \end{array} \\ \begin{array}{c} 4\\ 3 \end{array} & \begin{bmatrix} 0 & 15\\ 20 & 10 \end{bmatrix} \end{array} \leftarrow \mathrm{H4} \xrightarrow{-(7.2\mathrm{C},9\mathrm{D})\ \text{to P3}} \begin{array}{cc} & \begin{array}{cc} \mathrm{C} & \mathrm{D} \end{array} \\ \begin{array}{c} 4\\ 3 \end{array} & \begin{bmatrix} 0 & 15\\ 12.8 & 1 \end{bmatrix} \end{array} \leftarrow \mathrm{H4'}$$

$$\begin{array}{ccc} \uparrow & \qquad\qquad & \uparrow \\ \mathrm{V3} & & \mathrm{V3} \\ \text{H4 feed} = 45\ \text{mol/h} & & \text{H4}'\ \text{feed} = 28.8\ \text{mol/h} \end{array} \qquad (10a)$$

This bypassing reduces the feed rate from 45 mol/h (H4) to 28.8 mol/h (H4′). Stream bypassing can greatly reduce the mass load of downstream separation.

We illustrate another significance through bypassing the maximum amount, i.e., 100% of distributed component D in product P3. We bypass 10 mol/h of D together with 8 mol/h of C to get

$$\begin{array}{cc} & \begin{array}{cc} \mathrm{C} & \mathrm{D} \end{array} \\ \begin{array}{c} 4\\ 3 \end{array} & \begin{bmatrix} 0 & 15\\ 20 & 10 \end{bmatrix} \end{array} \leftarrow \mathrm{H4} \xrightarrow{-(8\mathrm{C},10\mathrm{D})\ \text{to P3}} \begin{array}{cc} & \begin{array}{cc} \mathrm{C} & \mathrm{D} \end{array} \\ \begin{array}{c} 4\\ 3 \end{array} & \begin{bmatrix} 0 & 15\\ 12 & 0 \end{bmatrix} \end{array} \leftarrow \mathrm{H4'}$$

$$\begin{array}{ccc} \uparrow & \qquad\qquad & \uparrow \\ \mathrm{V3} & & \mathrm{V3} \\ \text{H4 feed} = 45\ \text{mol/h} & & \text{H4}'\ \text{feed} = 27\ \text{mol/h} \end{array} \qquad (10b)$$

As seen, stream bypassing may convert a *sloppy* split, such as H4 ($\neq$V3) represented by eq 10, to a *sharp* one, such as H4′(=V3) specified by eq 10b. In fact, the right-hand side of eq 10b shows that both H4′(P3/P4) and V3(C/D) represent an identical sharp separation, giving component C as overhead and component D as bottoms with the following component recovery specifications:

$$(d/b)_{\mathrm{LK}} = (d/b)_{\mathrm{C}} = 12/0 \simeq 0.98/0.02$$

$$(d/b)_{\mathrm{HK}} = (d/b)_{\mathrm{D}} = 0/15 \simeq 0.02/0.98$$

Finally, stream bypassing is an effective tool to handle the problem of infeasible product splits *without* increasing the number of separators as in the case of applying stream splitting together with pseudoproduct transformation. Consider, for example, a three-component sloppy separation problem defined by Aggarwal and Floudas (1989). The CAM representing the problem is

$$\begin{array}{cc} & \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{array}{c} 2\\ 1 \end{array} & \begin{bmatrix} 20 & 70 & 80\\ 80 & 30 & 20 \end{bmatrix} \end{array} \leftarrow \mathrm{H1} \qquad (11)$$

$$\begin{array}{cc} \uparrow & \uparrow \\ \mathrm{V1} & \mathrm{V2} \end{array}$$

where components A, B, and C are propane, isobutane, and n-butane, respectively. Split H1(P1/P2) is *practically* infeasible with either A/B or B/C as LK/HK due to the undesirable nonkey component distributions. For example, when LK = A and HK = B, we find from eq 11

$$(d/b)_{\mathrm{LK}} = (d/b)_{\mathrm{A}} = 80/20 = 0.8/0.2$$

$$(d/b)_{\mathrm{HK}} = (d/b)_{\mathrm{B}} = 30/70 = 0.3/0.7$$

$$(d/b)_{\mathrm{HHK}} = (d/b)_{\mathrm{C}} = 20/80 = 0.2/0.8$$

While these component recovery specifications do satisfy the feasibility conditions, eqs 5 and 6, i.e., $d_{\mathrm{LK}} > d_{\mathrm{HK}} > d_{\mathrm{HHK}}$ (0.8 > 0.3 > 0.2) and $b_{\mathrm{LK}} < b_{\mathrm{HK}} < b_{\mathrm{HHK}}$ (0.2 < 0.7

< 0.8), there is a significant amount of nonkey component HHK or component C in the overhead with $d_{HHK} = 0.2$. The latter leads to a costly design. We therefore consider H1(P1/P2) a practically infeasible split. Applying stream splitting together with pseudoproduct transformation to H1(P1/P2) results in the need of *two* sloppy separators. In addition, eq 11 shows that products P1 and P2 can be obtained by using *two* sharp separators, V1 and V2.

Actually, the separation problem represented by eq 11 can be solved by only *one* sloppy separator. Both products P1 and P2 in eq 11 are all-component-inclusive. Thus, bypassing 100% limiting component C in product P1 and 90% limiting component A in product P2 gives

$$\begin{array}{c} \\ 2 \\ \\ 1 \end{array}\begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 20 & 70 & 80 \\ & & \\ 80 & 30 & 20 \end{bmatrix} \\ \uparrow \quad \uparrow \\ \mathrm{V1} \quad \mathrm{V2} \end{array} \leftarrow \mathrm{H1} \xrightarrow[\text{-(20A,20B,20C) to P1}]{\text{-(18A,18B,18C) to P2}}$$

H1 feed = 300 mol/h

$$\begin{array}{c} \\ 2 \\ \\ 1 \end{array}\begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 2 & 52 & 62 \\ & & \\ 60 & 10 & 0 \end{bmatrix} \\ \uparrow \quad \uparrow \\ \mathrm{V1} \quad \mathrm{V2} \end{array} \leftarrow \mathrm{H1''}$$

H1″ feed = 186 mol/h

Now the resulting horizontal split H1″(P1/P2) is feasible with the following component recovery specifications

$$(d/b)_{LK} = (d/b)_A = 60/2 = 0.968/0.032 \quad (12)$$

$$(d/b)_{HK} = (d/b)_B = 10/52 = 0.16/0.84 \quad (13)$$

$$(d/b)_{HHK} = (d/b)_C = 0/62 \simeq 0.02/0.98 \quad (14)$$

A comparison of eqs 12–14 clearly indicates of that stream bypassing can reduce both the mass load of separation and the number of separators. The fact that this separation problem requires only *one* sloppy separator, but *two* sharp separators, provides excellent incentive to systematically consider the relative merits of *both sloppy and sharp separations* in the preliminary design of multicomponent separation processes. The tools and concepts described in the preceding sections provide the simple and effective means to aid in this consideration.

2.4. Classification of Multicomponent Product Sets. To facilitate the synthesis of good initial sequences for a given separation problem, we broadly divide multicomponent product sets into four classes. Our classification involves a comparison of (a) the number of products, P; (b) the number of components, C; and (c) the rank r or pseudorank r' of the component assignment matrix.

A. Rank and Pseudorank of the CAM. The CAM is a $P \times C$ matrix with elements $\{f_{ij}\}$ representing the flow rate of the jth component in the ith product ($i = 1, 2, ..., P$; $j = 1, 2, ..., C$). This matrix may also be expressed by its product vectors $\mathbf{v}_i$ as follows:

$$\mathrm{CAM} = \begin{bmatrix} \mathbf{v}_P \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{v}_2 \\ \mathbf{v}_1 \end{bmatrix} \qquad \mathbf{v}_i = \begin{bmatrix} f_{iC} \\ \cdot \\ \cdot \\ \cdot \\ f_{i2} \\ f_{i1} \end{bmatrix}^{\mathrm{T}} = [f_{i1} \quad f_{i2} \quad \cdots \quad f_{iC}] \quad (15)$$

From the matrix theory, we know that P product vectors $\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_P$ are linearly independent if the CAM has a rank of P. This implies that the CAM contains one $P \times P$ submatrix having a nonzero determinant, and the determinant of any submatrix with $P + 1$ or more rows is zero. For example 1, the order of the largest nonzero determinant in the 4 × 4 CAM of eq 2 is four; that is, rank r of this CAM is four.

In general, rank r of a CAM is not greater than the smaller value of either the number of components C or the number of products P; that is,

$$r \leq \min\,(C,P) \quad (16)$$

When r is less than P, there are only r linearly independent product vectors, and the remaining $P - r$ product vectors can be expressed in terms of these r product vectors:

$$\mathbf{v}_k = c_{k1}\mathbf{v}_1 + c_{k2}\mathbf{v}_2 + ... + c_{kr}\mathbf{v}_r \quad (k = 1, 2, ..., P - r) \quad (17)$$

In the equation, $c_{k1}, c_{k2}, ..., c_{kr}$ are constants. If these constants are greater than zero, then $P - r$ product vectors $\mathbf{v}_k$ ($k = 1, 2, ..., P - r$) can be obtained by appropriate blending of r linearly independent product vectors, $\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_r$. This reduces the size of the original product set. When any of the constants, $c_{k1}, c_{k2}, ..., c_{kr}$, is negative, however, we cannot obtain $P - r$ product vectors $\mathbf{v}_k$ from r linearly independent product vectors, $\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_r$, without requiring an additional separator to accommodate for the negative constant c_{kj} ($j = 1, 2, ..., r$). This possibility leads us to define a pseudorank, denoted by r'. Specifically, r' is equal to the rank r of the CAM plus the number of product vectors that cannot be expressed as a linear combination of r independent product vectors by nonnegative coefficients c_{kj} ($j = 1, 2, ..., r$). This definition gives the relationship

$$r \leq r' \leq P \quad (18)$$

As an example of pseudorank, let us consider a CAM for a sloppy separation problem taken from Muraki et al. (1986):

$$\mathrm{CAM} = \begin{bmatrix} \mathbf{v}_5 \\ \mathbf{v}_4 \\ \mathbf{v}_3 \\ \mathbf{v}_2 \\ \mathbf{v}_1 \end{bmatrix} = \begin{array}{c} \begin{array}{cccc} \mathrm{A} & \mathrm{B} & \mathrm{C} & \mathrm{D} \end{array} \\ \begin{bmatrix} 2 & 6.4 & 6 & 4.8 \\ 0 & 9.6 & 10 & 14.4 \\ 5 & 6.4 & 2 & 19.2 \\ 1 & 6.4 & 0 & 4.8 \\ 2 & 3.2 & 2 & 4.8 \end{bmatrix} \end{array} \begin{array}{c} \\ \mathrm{P5} \\ \mathrm{P4} \\ \mathrm{P3} \\ \mathrm{P2} \\ \mathrm{P1} \end{array} \quad (19)$$

For this problem, we have four components ($C = 4$) and five products ($P = 5$), and the rank of CAM is four ($r = 4$). The latter implies that there are only four independent product vectors. Choosing $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$, and $\mathbf{v}_4$ as independent product vectors, we write eq 17 as

$$\mathbf{v}_5 = c_{51}\mathbf{v}_1 + c_{52}\mathbf{v}_2 + c_{53}\mathbf{v}_3 + c_{54}\mathbf{v}_4 = 2.25\mathbf{v}_1 + 0\mathbf{v}_2 + (-0.5)\mathbf{v}_3 + 0.25\mathbf{v}_4$$

Since c_{53} is negative and $\mathbf{v}_3$ is also an independent product, we find pseudorank $r' = r + 1 = 4 + 1 = 5$. Equation 18 becomes $r\ (=4) < r'\ (=5) = P\ (=5)$.

B. Classification of Product Sets (Types). On the basis of relative magnitudes of r' (pseudorank of the CAM), C (number of components), and P (number of products), we broadly divide multicomponent product sets into four classes: (a) class 1, $r' = P = C$; (b) class 2, $r' \leq P < C$; (c) class 3, $r' < P = C$; and (d) class 4, $C < P$ with class 4a, $r' = C < P$, class 4b, $C < r' = P$, and class 4c, $r' < C < P$. Figure 3 illustrates this classification, relating the pseu-

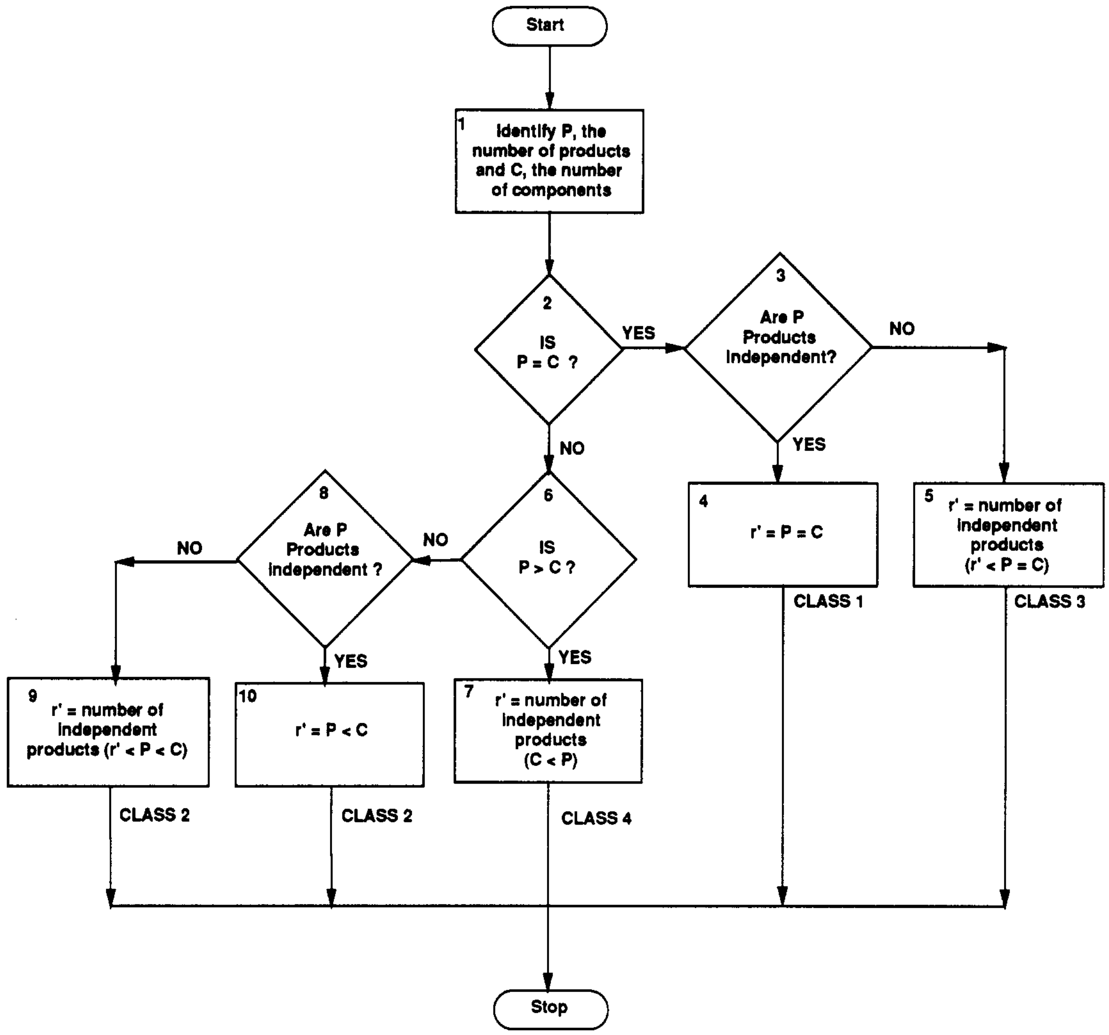

Figure 3. Classification of product types into four classes based on the pseudorank of component assignment matrix (CAM).

dorank r' to the number of independent products. Table III gives examples for each class of product sets, taken from reported studies of the synthesis of multicomponent separation sequences with sloppy product streams.

Class 3 ($r' < P = C$) in Table III refers to a separation problem that is slightly different from example 1 specified by eq 2. This modified example 1 has a CAM with $P = C = 4$ as follows:

$$\begin{array}{c} \\ \mathrm{P4} \\ \mathrm{P3} \\ \mathrm{P2} \\ \mathrm{P1} \end{array} \begin{array}{c} \begin{array}{cccc} \mathrm{A} & \mathrm{B} & \mathrm{C} & \mathrm{D} \end{array} \\ \begin{bmatrix} 25 & 25 & 25 & 10 \\ 0 & 0 & 20 & 10 \\ 10 & 12.5 & 0 & 0 \\ 15 & 12.5 & 5 & 0 \end{bmatrix} \end{array} \tag{20}$$

In this example, there are only three independent products (P1, P2, and P3); both the rank (r) and pseudorank (r') of the CAM are equal to three. Product P4 can be formed by blending together products P1–P3.

An example of class 4a ($r' = C < P$) is the multicomponent separation problem in making polymer solvent blends with controlled dielectric constants. A CAM representing this type of problem is

$$\begin{array}{c} \\ \mathrm{P4} \\ \mathrm{P3} \\ \mathrm{P2} \\ \mathrm{P1} \end{array} \begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 10 & 10 & 5 \\ 0 & 5 & 5 \\ 5 & 5 & 0 \\ 5 & 0 & 0 \end{bmatrix} \end{array} \tag{21}$$

with components A, B, and C being tetrahydrofuran, ethyl chloride, and n-hexane, respectively. For this example, we have P4 = P1 + P2 + P3 and $r' = C$ (=3) $< P$ (=4).

A minor change of eq 21 gives an example of class 4c ($r' < C < P$) in Table III:

$$\begin{array}{c} \\ \mathrm{P4} \\ \mathrm{P3} \\ \mathrm{P2} \\ \mathrm{P1} \end{array} \begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 10 & 15 & 5 \\ 5 & 10 & 5 \\ 0 & 5 & 5 \\ 5 & 5 & 0 \end{bmatrix} \end{array} \tag{22}$$

Here, we have P3 = P1 + P2, P4 = 2(P1) + P2, and r'(=2) $< C$ (=3) $< P$ (=4).

2.5. A Unifying Synthesis Method. Figure 4 shows the steps of a unifying method for the synthesis of good *all-sharp, all-sloppy, and mixed-separation sequences* that utilize a minimum number or a nearly minimum number of separators. We can implement the unifying method with a variety of synthesis tools such as heuristics and optimization. In this work, we adopt the rank-order heuristics of part 8 for horizontal product splits H*i*'s to aid in the selection of *both* H*i*'s *and* vertical component splits V*j*'s for a given separation problem represented by a CAM. Figure 5 illustrates our procedure based on the CAM and rank-ordered heuristics. The latter heuristics include the following: M1, favor ordinary distillation and remove mass-separating agent first; M2, avoid vacuum distillation and refrigeration; S1, remove corrosive and hazardous components first; S2, perform difficult separations last; C1, remove most plentiful product first; C2, favor 50/50 split.

Table III. Classification of Product Types

product type	examples of multicomponent separation-sequencing problems
class 1: $r' = P = C$	(a) separation of light hydrocarbons by ordinary distillation, example 1 ($C = 4$, $P = 4$)[a] specified in Table I; see part 8, Aggarwal and Floudas (1989), Bamapoulos et al. (1988), and Nath (1977)
	(b) example 1 ($C = 3$, $P = 3$, $F = 2$) in Floudas (1987)
	(c) example 1 ($C = 5$, $P = 5$) in Muraki and Hayakawa (1988)
class 2: $r' \le P < C$	(a) fractionation of refinery light ends, example 2A ($P = 7$, $C = 13$) of part 8; see also Tedder (1984)
	(b) fractionation in refinery saturates-gas plant, example 2B ($P = 7$, $C = 14$) of part 8; see also Watkins (1979)
	(c) examples 1 and 2 ($P = 2$, $C = 3$) in Aggarwal and Floudas (1989)
	(d) examples 2 and 3 ($P = 2$, $C = 4$) and example 4 ($P = 2$, $C = 5$) in Floudas (1987); see also Table VI
	(e) example 1 ($P = 3$, $C = 4$, $F = 2$) and examples 2 and 3 ($P = 2$, $C = 5$) in Floudas and Anastasiadis (1988)
	(f) example 1 ($P = 2$, $C = 5$) in Muraki and Hayakawa (1984, 1987)
	(g) example 2 ($P = 2$, $C = 4$) in Muraki et al. (1986)
class 3: $r' < P = C$	modified example 1, with one product capable of being formed by blending of other products; see eq 20; compare it with eq 2
class 4: $C < P$	
(4a) $r' = C < P$	multicomponent separations in making polymer solvent blends, giving solvent products of controlled dielectric constants; see eq 21
(4b) $C < r' = P$	example 1 ($C = 4$, $P = 5$) in Muraki et al. (1986); see eq 19
(4c) $r' < C < P$	similar to (4a); see eq 22

[a] The default value of F, the number of feed streams, is one.

Table IV. SST for Next Splits in Sequence S1 for Example 1 Represented by Equation 25

separation	ovhd/btm	LK/HK	Δ, °C	$(d/b)_A$	$(d/b)_B$	$(d/b)_C$	CES
V1′	A/BC = 20/40	A/B	36.6	0.98/0.02	0.02/0.98	0.02/0.98	5.41
V2′	AB/C = 40/20	B/C	32.6	0.98/0.02	0.98/0.02	0.02/0.98	4.84

Part 8 gives complete descriptions of these heuristics for choosing horizontal product splits Hi's.

3. Illustrative Examples and Discussion

3.1. "Class 1" Product Type: $r' = P = C$. Example 1, specified in Table I and by eq 2, involves the separation of a four-component mixture ($C = 4$) of hydrocarbons (nC_4–nC_7) into four sloppy product streams ($P = 4$). Both the rank (r) and pseudorank (r') of the CAM of eq 2 are four. From steps 1–4 of Figure 3, we designate sloppy products of example 1 as "class 1".

We describe the development of separation sequences for this class 1 problem in the following three subsections: (A) incorporating all-sharp sequences; (B) incorporating both sharp and sloppy (i.e., mixed-separation) sequences; and (C) incorporating all-sloppy sequences.

A. All-Sharp Separation Sequences. Step 1 of Figure 4 synthesizes all-sharp separation sequences with $C - 1$ or 3 separators for example 1. To carry our this synthesis, we apply the heuristic procedure of Figure 5 as follows.

A.1. Sequence S1.

Step 1. See eq 2.

Steps 2–4. Equation 2 reveals no all-component-inclusive product.

Step 5. See Table II, particularly for vertical component splits V1–V3, which are always feasible.

Step 6. Table II shows that normal boiling-point differences for V1–V3 are large enough to use ordinary distillation (heuristic M1). To avoid vacuum distillation and refrigeration (heuristic M2), we prefer a high-pressure operation of the debutanizer, V1(A/BCD). This follows because butane (component A) has a relatively low normal boiling point of −0.5 °C.

Steps 7 and 8. Not applicable, since there is no corrosive and hazardous component and boiling-point differences for V1–V3 are large.

Step 9. Equation 2 shows that the most plentiful product is P1 consisting of component A–C. Thus, heuristic C1 favors V3(ABC/D) with CES = 2.93 (see Table II). Although V2(AB/CD) has a larger CES of 9.67, we do not choose this split first because our heuristics are rank-ordered; i.e., heuristic C1 overrules heuristic C2.

Step 10. Split V3(ABC/D) gives the following overhead and bottoms:

$$\mathrm{CAM(V3,ovhd)} = \begin{array}{c} \\ 3 \\ 2 \\ 1 \end{array} \begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 0 & 0 & 20 \\ 10 & 12.5 & 0 \\ 15 & 12.5 & 5 \end{bmatrix} \end{array} \tag{23}$$

$$\mathrm{CAM(V3,btm)} = \begin{array}{c} \\ 4 \\ 3 \end{array} \begin{array}{c} \mathrm{D} \\ \begin{bmatrix} 15 \\ 10 \end{bmatrix} \end{array} \tag{24}$$

To further separate the overhead from V3, we apply the heuristic procedure of Figure 5 to eq 23 as follows.

Steps 2–4. Equation 23 shows that product P1 is all-component-inclusive. While it would be desirable to bypass 90–100% of the distributed components, A and B, the small flow rate of component C (5 mol/h) in P1 dictates that we can at most bypass 5 mol/h of A, 5 mol/h of B, and 5 mol/h of C to product P1. This bypass gives

$$\mathrm{CAM'(V3,ovhd)} = \begin{array}{c} \\ 3 \\ 2 \\ 1 \end{array} \begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 0 & 0 & 20 \\ 10 & 12.5 & 0 \\ 10 & 7.5 & 0 \end{bmatrix} \\ \begin{array}{cc} \uparrow & \uparrow \\ \mathrm{V1'} & \mathrm{V2'} \end{array} \end{array} \tag{25}$$

Step 5. See Table IV.

Steps 6–10. According to eq 25, the most plentiful product is P2 consisting of components A and B. Following heuristic C1, we choose V2′(AB/C) first, resulting in the following overhead:

$$\mathrm{CAM(V2',ovhd)} = \begin{array}{c} \\ 2 \\ 1 \end{array} \begin{array}{c} \begin{array}{cc} \mathrm{A} & \mathrm{B} \end{array} \\ \begin{bmatrix} 10 & 12.5 \\ 10 & 7.5 \end{bmatrix} \end{array} \tag{26}$$

The bottoms from V2′(AB/C) consists of 20 mol/h of component C going to product P3.

Further separation of the overhead from V2′, eq 26, by the heuristic procedure of Figure 5 is fairly straightforward.

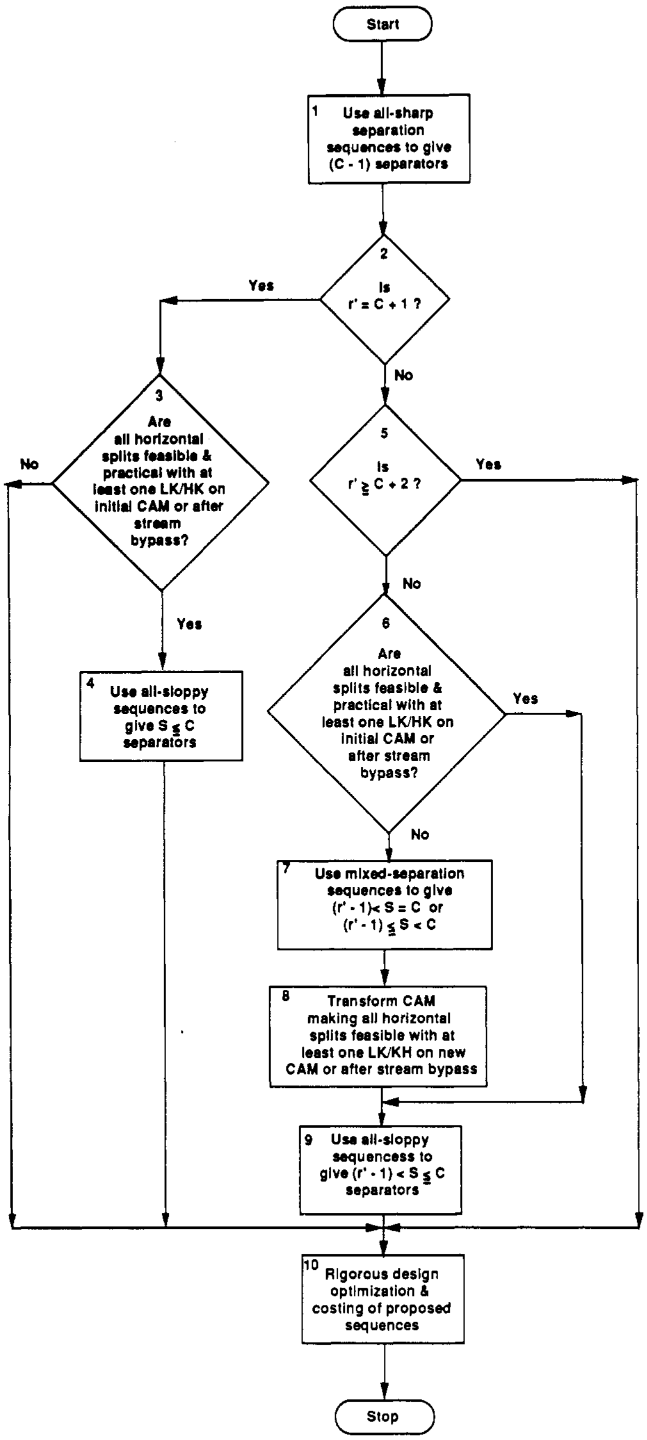

Figure 4. Unifying method for multicomponent separation sequencing with sloppy product streams. In the figure, S is the number of separators used.

We bypass 37.5% of the feed to P1 and 50% of the feed to P2, resulting in a sharp component split V1″(A/B):

$$\begin{array}{c} \\ 2 \\ 1 \end{array}\!\!\begin{array}{c} \begin{array}{cc} \text{A} & \text{B} \end{array} \\ \begin{bmatrix} 10 & 12.5 \\ 10 & 7.5 \end{bmatrix} \end{array} \xrightarrow[-(7.5\text{A},7.5\text{B})\text{ to P1}]{-(10\text{A},10\text{B})\text{ to P2}} \begin{array}{c} \\ 2 \\ 1 \end{array}\!\!\begin{array}{c} \begin{array}{cc} \text{A} & \text{B} \end{array} \\ \begin{bmatrix} 0 & 2.5 \\ 2.5 & 0 \end{bmatrix} \\ \uparrow \\ \text{V1}'' \end{array} \tag{27}$$

Equations 23–27 give the following all-sharp sequence, S1, shown in Figure 1a:

S1 V3(ABC/D) - V2′(AB/C) - V1″(A/B) (28)

A.2. Additional All-Sharp Sequences. We develop an alternative sequence by referring to eq 2 and making a minor change in the preceding synthesis of sequence S1. Specifically, we ignore heuristic C1 and follow heuristic C2. Instead of choosing V3(ABC/D) first to obtain an overhead with components A, B, and C that are present in the most plentiful product P1 as in sequence S1, we favor V2(AB/CD) with the largest CES of 9.67. From eq 2, V2(AB/CD) gives the following overhead and bottoms:

(1) overhead

$$\begin{array}{c} \text{CAM(V2,ovhd)} \\ \begin{array}{c} \\ 2 \\ 1 \end{array}\!\!\begin{array}{c} \begin{array}{cc} \text{A} & \text{B} \end{array} \\ \begin{bmatrix} 10 & 12.5 \\ 15 & 12.5 \end{bmatrix} \end{array} \\ \uparrow \\ \text{V1} \end{array} \xrightarrow[-(12.5\text{A},12.5\text{B})\text{ to P1}]{-(10\text{A},10\text{B})\text{ to P2}} \begin{array}{c} \text{CAM}''\text{(V2,ovhd)} \\ \begin{array}{c} \\ 2 \\ 1 \end{array}\!\!\begin{array}{c} \begin{array}{cc} \text{A} & \text{B} \end{array} \\ \begin{bmatrix} 0 & 2.5 \\ 2.5 & 0 \end{bmatrix} \end{array} \\ \uparrow \\ \text{V1}'' \end{array} \tag{29}$$

(2) bottoms

$$\begin{array}{c} \text{CAM(V2,btm)} \\ \begin{array}{c} \\ 4 \\ 3 \\ 2 \\ 1 \end{array}\!\!\begin{array}{c} \begin{array}{cc} \text{C} & \text{D} \end{array} \\ \begin{bmatrix} 0 & 15 \\ 20 & 10 \\ 0 & 0 \\ 5 & 0 \end{bmatrix} \end{array} \\ \uparrow \\ \text{V3} \end{array} \xrightarrow{-(10\text{C},10\text{D})\text{ to P3}} \begin{array}{c} \text{CAM}'\text{(V2,btm)} \\ \begin{array}{c} \\ 4 \\ 3 \\ 2 \\ 1 \end{array}\!\!\begin{array}{c} \begin{array}{cc} \text{C} & \text{D} \end{array} \\ \begin{bmatrix} 0 & 15 \\ 10 & 0 \\ 0 & 0 \\ 5 & 0 \end{bmatrix} \end{array} \\ \uparrow \\ \text{V3}' \end{array} \tag{30}$$

In eqs 29 and 30, we have also included the CAMs after stream bypasses according to steps 2–4 of Figure 5. Carrying out the resulting splits V1″(A/B) and V3′(C/D) gives the following all-sharp sequence, S2, shown in Figure 6a:

$$\text{S2} \qquad \text{V2(AB/CD)} \begin{array}{l} \nearrow \text{V1}''\text{(A/B)} \\ \searrow \text{V3}'\text{(C/D)} \end{array} \tag{31}$$

Further applications of the heuristic procedure of Figure 5 to eq 2 and Table II result in three more all-sharp sequences:

S3 V3(ABC/D) - V1′(A/BC) - V2(B/C) (32)

S4 V1(A/BCD) - V2(B/CD) - V3′(C/D) (33)

S5 V1(A/BCD) - V3(BC/D) - V2′(B/C) (34)

Figure 6, b–d, illustrates these sequences.

B. Mixed-Separation Sequences. We now return to Figure 4. Steps 2–7 suggest mixed-separation sequences with $r' - 1$ separators. We apply these steps to example 1 as follows.

Step 2. As noted previously, $r' = C = 4$. Thus, we find $r' \neq C + 1$ and continue with step 5.

Step 5. $r' < C + 2$.

Step 6. See Table II, noting the CES ranking of the following feasible splits:

split	LK/HK	CES
H2(P12/P34)	B/C	11.7
V2(AB/CD)	B/C	9.67
V1(A/BCD)	A/B	3.61
V3(ABC/D)	C/D	2.93
H3(P123/P4)	C/D	2.81

Step 7. To synthesize mixed-separation sequences, we use the heuristic procedure of Figure 5 as follows.

B.1. Sequence MS1.

Steps 1–8. These steps are essentially identical with those previously applied to the synthesis of sequence S1. The only difference appears in step 5, since we must now consider both horizontal product splits Hi's and vertical component splits Vj's. The feasible splits resulting from step 5 of Figure 5 are the five splits (H2, V2, V1, V3, and H3) listed above according to the CES ranking.

Step 9. Heuristic C1 favors V3(ABC/D), which gives an overhead consisting of components A–C that are present in the most plentiful product P1. We do not choose ini-

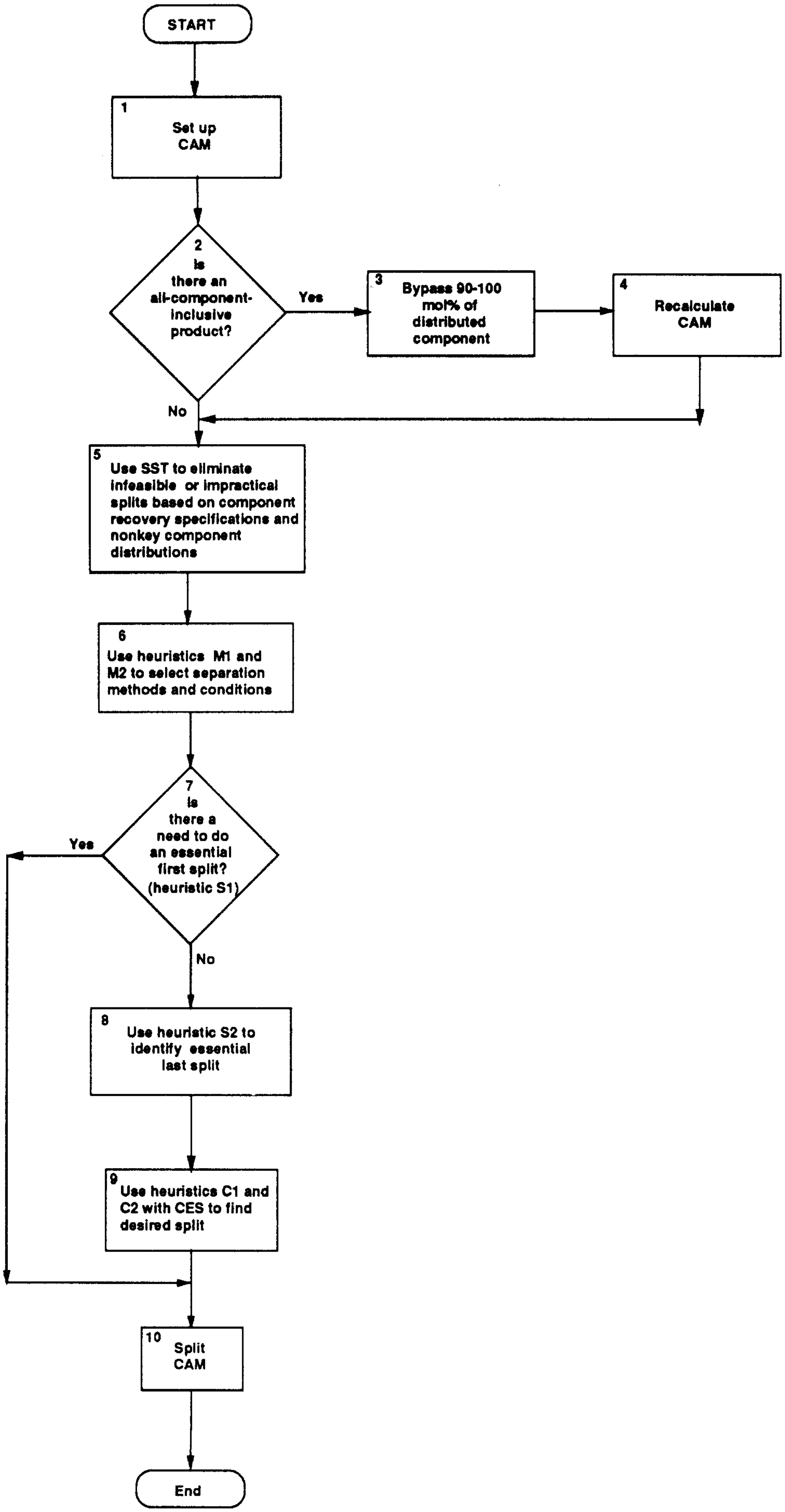

Figure 5. Heuristic procedure for choosing a horizontal product split or a vertical component split on a CAM for implementing the unifying method of Figure 4.

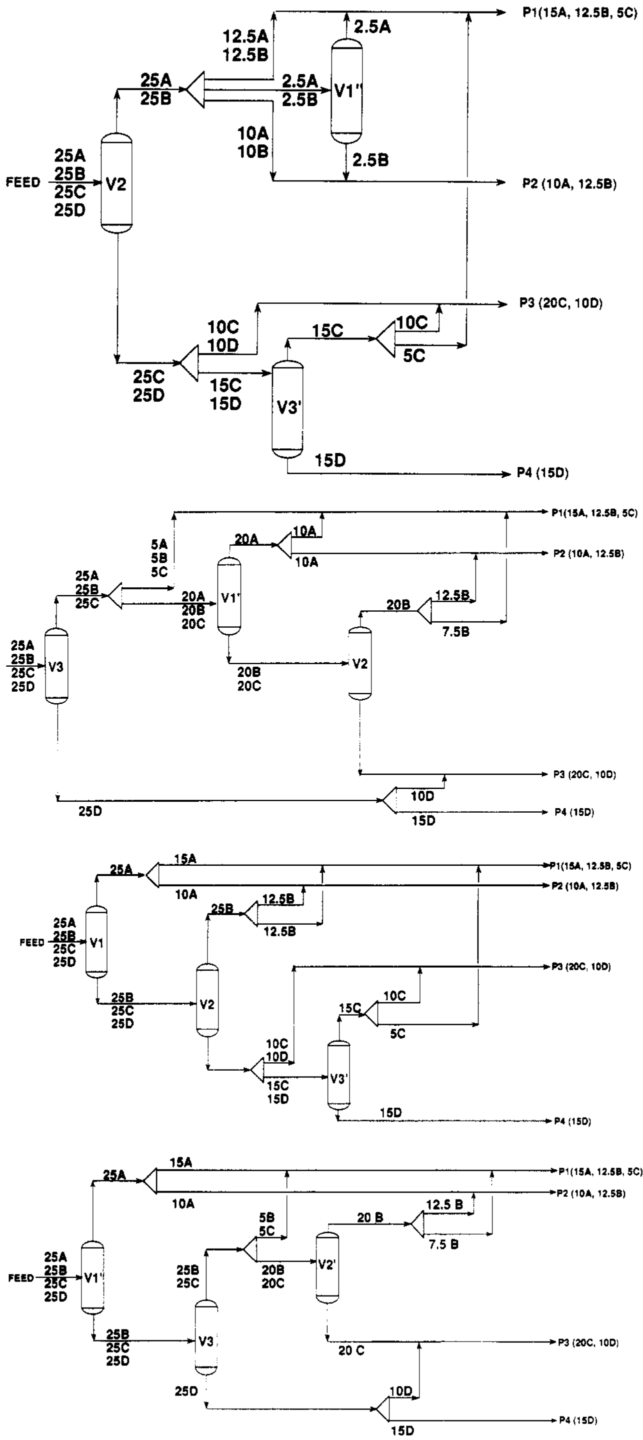

Figure 6. Additional all-sharp separation sequences with three separators for example 1:

(a) sequence S2 (=MS3), $\mathrm{V2(AB/CD)} \begin{array}{l} \nearrow \mathrm{V1''(A/B)} \\ \searrow \mathrm{V3'(C/D)} \end{array}$

(b) sequence S3 (=MS1), V3(ABC/D) – V1′(A/BC) – V2(B/C)

(c) sequence S4, V1(A/BCD) – V3(B/CD) – V3′(C/D)

(d) sequence S5, V1(A/BCD) – V3(BC/D) – V2′(B/C).

tially H2(P12/P34), V2(AB/CD), and V1(A/BCD) with larger CES values because heuristic C1 overrules heuristic C2.

Step 10. Split V3(ABC/D) gives the following overhead and bottoms: CAM (V3,ovhd) = eq 23 and CAM (V3, btm) = eq 24. We apply the heuristic procedure of Figure 5 to eq 23 to further separate the overhead from V3 as follows.

Steps 2–4. These steps are identical with those previously applied in the synthesis of sequence S1, with stream bypass resulting in an overhead represented by eq 25. We rewrite the latter equation in the form below to facilitate the subsequent considerations of both H*i*'s and V*j*'s in mixed-separation sequences.

$$\mathrm{CAM'(V3,ovhd)} = \begin{array}{c} \\ 3 \\ 2 \\ 1 \\ \\ \end{array}\begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \left[\begin{array}{ccc} 0 & 0 & 20 \\ 10 & 12.5 & 0 \\ 10 & 7.5 & 0 \end{array}\right] \\ \begin{array}{ccc} \uparrow & & \uparrow \\ \mathrm{V1'} & & \mathrm{V2'} \end{array} \end{array} \begin{array}{l} \leftarrow \mathrm{H2'} \\ \leftarrow \mathrm{H1'} \end{array} \qquad (35)$$

Step 5. See Table V.

Steps 6–10. Table V and eq 35 show that both V1′(A/BC) and H2′(P12/P3) [or H2′(ABC/C)] have the highest CES of 5.41 and are equally good according to heuristic C2. We choose V1′(A/BC) as our next separation, resulting in the following bottoms:

$$\mathrm{CAM(V1',btm)} = \begin{array}{c} \\ 3 \\ 2 \\ 1 \\ \\ \end{array}\begin{array}{c} \begin{array}{cc} \mathrm{B} & \mathrm{C} \end{array} \\ \left[\begin{array}{cc} 0 & 20 \\ 12.5 & 0 \\ 12.5 & 0 \end{array}\right] \\ \begin{array}{cc} \uparrow & \\ \mathrm{V2'} & \end{array} \end{array} \begin{array}{l} \leftarrow \mathrm{H2'} \\ \leftarrow \mathrm{H1'} \end{array} \qquad (36)$$

The overhead from V1′(A/BC) consists of 20 mol/h of component A that is to be split into two equal portions of 10 mol/h each going into products P1 and P2.

To further apply the heuristic procedure of Figure 5 to separate the bottoms from V1′, eq 36, we recognize that choosing an initial split H1′(BC/B) requires a subsequent separation H2′(B/C). By contrast, both V2′ and H2′ represent an identical, one-step sharp separation of 20 mol/h of C from 20 mol/h of B. We therefore prefer V2′(B/C) and split the resulting overhead into two portions with 7.5 and 12.5 mol/h of B going into products P1 and P2, respectively. This leads to the following sequence that is the same as the all-sharp sequence S3 shown in Figure 6b:

MS1(=S3)

$$\mathrm{V3(ABC/D) - V1'(A/BC) - V2(B/C)} \qquad (32)$$

The above example illustrates an important feature of the mixed-separation synthesis method. While the method permits the use of *both* sharp *and* sloppy separators, it may actually generate separation sequences utilizing *only* sharp splits as in sequence MS1 (=S3) or sequences incorporating *only* sloppy splits.

B.2. Additional Mixed-Separation Sequences. In the above use of the heuristic procedure of Figure 5 to synthesize sequence MS1, we favor V3(ABC/D) with CES = 2.93, over H2(P12/P34) with CES = 11.7, and thus to obtain an overhead with components A–C to form a part of the most plentiful product P1 according to heuristic C1. If we ignore heuristic C1 and follow heuristic C2, we can apply the synthesis method of Figure 5 to obtain the following mixed-separation sequence, MS2, shown in Figure 1c:

$$\mathrm{MS2} \qquad \mathrm{H2(ABC/CD)} \begin{array}{l} \nearrow \mathrm{V2'(AB/C) - V1'(A/B)} \\ \searrow \mathrm{V3'(C/D)} \end{array} \qquad (37)$$

Applications of the mixed-separation synthesis scheme may generate additional sequences. An example is that shown in Figure 6a:

$$\mathrm{MS3(=S2)} \qquad \mathrm{V2(AB/CD)} \begin{array}{l} \nearrow \mathrm{V1''(A/B)} \\ \searrow \mathrm{V3''(C/D)} \end{array} \qquad (38)$$

Table V. SST for Next Splits in Sequence MS1 for Example 1 Represented by Equation 35

separation	ovhd/btm	LK/HK	Δ, °C	$(d/b)_A$	$(d/b)_B$	$(d/b)_C$	CES
V1′	A/BC = 20/40	A/B	36.6	0.98/0.02	0.02/0.98	0.02/0.98	5.41
V2′	AB/C = 40/20	B/C	32.6	0.98/0.02	0.98/0.02	0.02/0.98	4.84
H1′	P1/P23 = 17.5/42.5	A/B	36.6	0.5/0.5	0.375/0.625	0.27/0.73	infeasible
H1′	P1/P23 = 17.5/42.5	B/C	32.7	0.961/0.039	0.375/0.625	0.02/0.98	infeasible
H2′	P12/P3 = 40/20	B/C	32.6	0.98/0.02	0.98/0.02	0.02/0.98	4.84

Table VI. Feed and Product Specifications in Example 3[a]

desired product streams	component flow rate, mol/h: A	B	C	D	product flow rate, mol/h
P2	5	10	4	10	29
P1	10	10	6	5	31
component flow rate in feed, mol/h	15	20	10	15	60

[a] Examples 2A and 2B are specified in part 8. A = propane (normal boiling point, −42.1 °C), B = isobutane (−11.7 °C), C = n-butane (−0.5 °C), and D = isopentane (27.8 °C). Difficulty of ith "sharp" separation between two key components: D_{AB} (or D_1) = 2.5, D_{BC} (or D_2) = 3.0, and D_{CD} (or D_3) = 1.5. Data taken from Floudas (1987).

C. All-Sloppy Separation Sequences. Returning to Figure 4, we see from steps 8 and 9 the need to synthesize all-sloppy sequences for example 1. We also find that the number of separators can vary from $r' - 1$ to C, that is, from 3 to 4. To carry out this synthesis, we apply the heuristic procedure of Figure 5 to eq 7. Figure 1b gives an example of the resulting sequence as represented by eq 8 or eq 9.

D. Expert System Implementation of Separation Sequencing. We have developed an interactive, rule-based expert system, called EXSEP (EXpert system for SEParation sequencing), to implement the unifying synthesis method of Figures 4 and 5 that we applied to example 1 in sections 3.1A–C. This system is written in PROLOG. Based on the problem specifications given by the user, EXSEP (1) sets up the CAM, (2) identifies any all-component-inclusive products and performs a bypass analysis, (3) develops the SST and analyzes the split feasibility, and (4) applies the rank-ordered heuristics and recommends desirable splits. The user can accept or reject the recommended split. Should the user accept the recommended split, EXSEP sets up the CAMs for the overhead and bottoms and resumes its search for the next recommended split. This process continues until the entire separation sequence is synthesized. When the user rejects the recommended split, EXSEP "backtracks" and searches for alternative splits. New split recommendations are given from which the user can choose.

EXSEP can develop three competing types of sequences, namely, all-sharp, all-sloppy, and mixed-separation sequences, for all four classes of separation-sequencing problems with sloppy product streams as categorized in Table III. EXSEP is run on a personal computer, and it is very fast, convenient, and easy to use.

3.2. "Class 2" Product Type: $r' \leq P < C$. As listed in Table III, two refinery fractionation problems solved in part 8 (example 2A with $C = 13$, $P = 7$, and $r = r' = 7$; and example 2B with $C = 14$, $P = 9$ and $r = r' = 9$) are typical examples with class 2 product type according to steps 1–10 of Figure 3. Table VI specifies example 3 introduced by Floudas (1987) with $C = 4$, $P = 2$, and $r = r' = 2$. In what follows, we illustrate the synthesis of both all-sharp and mixed-separation sequences with three separators for example 3 and then describe the application of EXSEP to example 2A.

A. All-Sharp Separation Sequences for Example 3. For example 3, step 1 of Figure 4 synthesizes all-sharp separation sequences with $C - 1$ or 3 separators. We apply the heuristic procedure of Figure 5 to carry out this synthesis.

Steps 1–4. We bypass one-third of the feed to product P1 and also one-third of the feed to product P2:

$$\begin{array}{cc} & \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{array}{c} 2 \\ 1 \end{array} & \left[\begin{array}{cccc} 5 & 10 & 4 & 10 \\ 10 & 10 & 6 & 5 \end{array}\right] \end{array} \begin{array}{l} \xrightarrow{-(5A,6.67B,3.34C,5D)\text{ to P1}} \\ \xrightarrow{-(5A,6.67B,3.34C,5D)\text{ to P2}} \end{array}$$

$$\begin{array}{cc} & \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{array}{c} 2 \\ 1 \end{array} & \left[\begin{array}{cccc} 0 & 3.33 & 0.66 & 5 \\ 5 & 3.33 & 2.66 & 0 \end{array}\right] \leftarrow \text{H1}' \\ & \begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ \text{V1}' & \text{V2}' & \text{V3}' \end{array} \end{array} \qquad (39)$$

Step 5. See Table VII. The sloppy split H1′ is infeasible; we therefore consider only sharp splits V1′–V3′.

Steps 6–10. Both V1′ and V2′ remove the most plentiful component early; we favor V1′ over V2′, since the former has a higher CES. Choosing V1′ first results in an overhead of 5 mol/h of A going to product P1 and in a bottoms represented by CAM(V1′,btm):

$$\text{CAM(V1}',\text{btm)}$$

$$\begin{array}{cc} & \begin{array}{ccc} B & C & D \end{array} \\ \begin{array}{c} 2 \\ 1 \end{array} & \left[\begin{array}{ccc} 3.33 & 0.66 & 5 \\ 3.33 & 2.66 & 0 \end{array}\right] \end{array} \xrightarrow{-(1.33B,0.66C,1D)\text{ to P2}}$$

$$\text{CAM}'\text{(V1}',\text{btm)}$$

$$\begin{array}{cc} & \begin{array}{ccc} B & C & D \end{array} \\ \begin{array}{c} 2 \\ 1 \end{array} & \left[\begin{array}{ccc} 2 & 0 & 4 \\ 3.33 & 2.66 & 0 \end{array}\right] \\ & \begin{array}{cc} \uparrow & \uparrow \\ \text{V2}' & \text{V3}' \end{array} \end{array} \qquad (40)$$

To further separate the bottoms from V1′, we apply the heuristic procedure of Figure 5 to CAM(V1′,btm). Steps 2–4 suggest bypassing 20% of the feed to product P2, giving CAM′(V1′,btm) in eq 40. Simple calculations of step 5 show that (1) V3′(BC/D) has a CES of 4.19 and (2) V2′(B/CD) has a smaller CES of 2.65, but it removes the most plentiful component, B, early. Following heuristic C1, we choose V2′(B/CD) first and then separate the resulting bottoms by V3(C/D). This gives the following all-sharp sequence:

$$\text{S1} \qquad \text{V1}''\text{(A/BCD)} - \text{V2(B/CD)} - \text{V3(C/D)} \qquad (41)$$

Table VII. SST for First Splits in Example 3 Represented by Equation 39

separation	ovhd/btm	LK/HK	Δ, °C	$(d/b)_A$	$(d/b)_B$	$(d/b)_C$	CES
H1	P1/P2 = 5/22.5	A/B or B/C	36.6 or 32.7	0.2/0.8	0.02/0.98	0.98/0.02	infeasible
V1	A/BC = 12.5/15	A/B	36.6	0.98/0.02	0.02/0.98	0.02/0.98	9.02
V2	AB/C = 25/2.5	B/C	32.7	0.98/0.02	0.98/0.02	0.02/0.98	0.97

Table VIII. CAM for Representing Example 2A

	A	B	C	D	E	F	G	H	I	J	K	L	M	
P7	0	0	0	0	0	3.17	1.31	3.23	43.9	31.7	72.31	21.52	7.37	←H6
P6	0	0	0	0.58	1.55	28.53	5.25	7.53	18.82	7.92	8.02	2.39	0	←H5
P5	0	0	0	8.68	51.43	0.81	0.07	0.05	0	0	0	0	0	←H4
P4	0	0.6	2.99	49.2	9.08	0	0	0	0	0	0	0	0	←H3
P3	0	2.88	109.6	1.5	0.63	0	0	0	0	0	0	0	0	←H2
P2	3.11	54.63	5.77	0	0	0	0	0	0	0	0	0	0	←H1
P1	118.08	1.47	1.47	0	0	0	0	0	0	0	0	0	0	
	↑ V1	↑ V2	↑ V3	↑ V4	↑ V5	↑ V6	↑ V7	↑ V8	↑ V9	↑ V10	↑ V11	↑ V12		

Similar applications of the heuristic procedure of Figure 5 give four more all-sharp sequences:

S2 V1″(A/BCD) – V3′(BC/D) – V2′(B/C) (42)

S3 V2″(AB/CD) → V1′(A/B), → V3′(C/D) (43)

S4 V3″(ABC/D) – V1′(A/BC) – V2′(B/C) (44)

S5 V3″(ABC/D) – V2′(AB/C) – V1(A/B) (45)

Figure 7a shows, for example, sequence S4. This sequence is similar to the "optimum" sequence of Figure 7b obtained by Floudas (1987) using an optimization technique to minimize the following relative cost:

$$\text{relative cost} = \sum_{i=1}^{S} (L_i D_i)^{0.6} \tag{46}$$

In the equation, S is the number of separators, L_i is the mass load of the ith separator, and D_i is the difficulty of the ith "sharp" separation between two key components (see Table VI). It is significant to note that sequence S4 of Figure 7a synthesized by our heuristic method has a lower relative cost of 17.24 when compared to that of 18.58 for the optimum sequence of Figure 7b obtained by a rigorous optimization technique. This cost improvement results from the fact that our heuristic method is able to systematically identify the dark bypass line around separator V2′(B/C) in Figure 7a, thus reducing the mass load of separation.

B. Mixed-Separation Sequences for Example 3. We apply steps 2–7 of Figure 4 to synthesize mixed-separation sequences for example 3. Step 7 suggests that the number of separators, S, can vary from $r' - 1$ to C, or from 1 to 4. We have already shown in eq 40 and Table VII that a one-separator scheme for example 3 with sloppy split H1′ is infeasible. We also note that the preceding all-sharp sequences for example 3, eqs 43–47, consist of only three separators. To ensure that our resulting mixed-separation sequences are cost-competitive, we limit our synthesis to sequences with at most three separators.

By applying the heuristic procedure of Figure 5 to the CAM of eq 40, as was done in section 3.1.B for example 1, we find the following mixed-separation sequences for example 3:

MS1 V1″(A/BCD) – V2′(B/CD) – H1′(CD/D) (47)

MS2 V1″(A/BCD) – V3′(BC/D) – H1′(B/BC) (48)

MS3 V2″(AB/CD) → H1′(AB/B), → H1′(CD/D) (49)

MS4 V3″(ABC/D) – V1′(A/BC) – H1′(B/BC) (50)

MS5 V3″(ABC/D) – V2′(AB/C) – H1′(AB/B) (51)

The last split in sequences MS1–MS5 corresponds to a sloppy separation with partial stream bypass, H1′. The word partial here reflects the fact that we do not bypass all 100% of the limiting distributed component in the feed

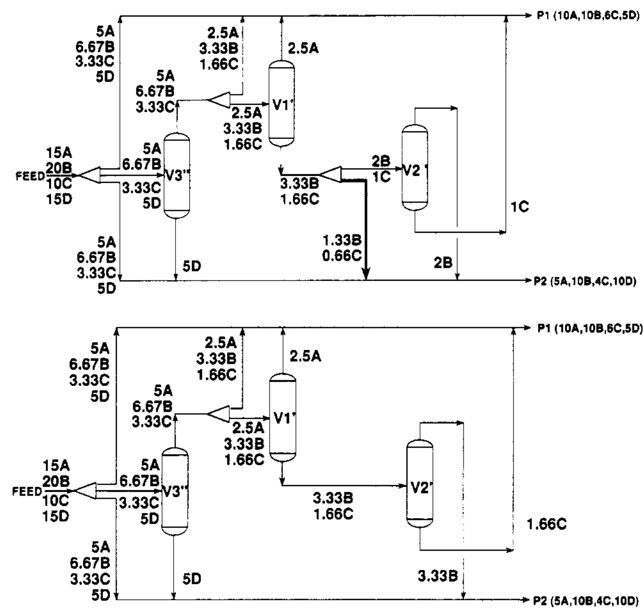

Figure 7. (a) An all-sharp separation sequence for example 3, V3″(ABC/D) – V1′(A/BC) – V2′(B/C). The darken bypass line around V2′ is not present in part b. (b) An "optimum" separation sequence for example 3 reported by Floudas (1987), V3″(ABC/D) – V1(A/BC) – V2(B/C).

to H1 to directly form part of the overhead or bottoms. Should we bypass all of the limiting distributed component, sequences MS1–MS5 reduce to all-sharp sequences S1–S5 given previously by eqs 41–45.

C. Application of EXSEP to Example 2A. Example 2A corresponds to the fractionation of 13 refinery light-end components into 7 products (Tedder, 1984). Table VIII shows the CAM for representing example 2A. The exact names for the 13 light-end components, A–M, and their normal boiling points can be found in part 8. For this example, we use the Antoine vapor-pressure equation to estimate the equilibrium ratio (K_i) for each component at the average operating temperature of 91.7 °C and operating pressure of 2758 kPa (Watkins, 1979).

We input the specifications, and EXSEP formulates the CAM shown in Table VIII. EXSEP then proceeds to different steps of our synthesis method of Figures 4 and 5. EXSEP reveals no stream bypass, completes the split feasibility analysis, and heuristically recommends an initial split H3(P123/P4567) with C/D as LK/HK (see Table VIII). EXSEP then continues to further separate the overhead of P123 (=P1 + P2 + P3) and the bottoms of P4567 (=P4 + P5 + P6 + P7). This process continues until three good initial separation sequences (depicted as sequences a–c in Figure 13 of part 8) have been synthesized.

3.3. "Class 3" Product Type: $r' < P = C$. Synthesis strategies for class 3 problems are the same as those for class 2 with $P < C$. This follows because both classes have one thing in common, that is, $r' < C$. Essentially, we look for a new product set with r' product streams, each of which consists of up to C components. The whole synthesis procedure will proceed according to the relative magnitudes of r' and C, as shown in Figure 4.

3.4. "Class 4" Product Type: $C < P$. A. "Class 4a" Product Type: $r' = C < P$. The synthesis strategy for this product type is identical with that of class 1 with $r' = P = C$. The reasoning behind this observation is that the original product streams in class 4a are reduced to a new product set with r' (or C) product streams made up of C components.

B. "Class 4b" Product Type: $C < r' = P$. For this product type, we first recognize that our synthesis strategy is to consider possible all-sloppy sequences incorporating at most one more separator than competing all-sharp sequences. Thus, we apply the all-sloppy synthesis method for product sets with r' values being equal to $C + 1$ (see Figure 4). For product sets with higher r' values, however, we should use only the all-sharp synthesis method.

C. "Class 4c" Product Type: $r' < C < P$. Recall that earlier for class 2 product type with $P < C$, we obtain the relationship $r' < C$. Therefore, class 4c product type is similar to class 2 product type, and the synthesis schemes for both types should be identical.

3.5. Two-Feed Separation Problems. In this section, we present an example to illustrate how to extend the basic tools and concepts of the preceding sections for synthesizing initial sequences for two-feed separation problems. Example 4, investigated previously by Mahalec and Motard (1977) and by Floudas (1987), may be represented by the following CAMs for feeds and products:

$$\begin{array}{c} \\ \mathrm{F1} \\ \mathrm{F2} \end{array}\begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 200 & 1000 & 0 \\ 500 & 500 & 300 \end{bmatrix} \end{array} \longrightarrow \begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 100 & 0 & 100 \\ 500 & 500 & 200 \\ 100 & 1000 & 0 \end{bmatrix} \end{array}\begin{array}{c} \\ \mathrm{P1} \\ \mathrm{P2} \\ \mathrm{P3} \end{array} \tag{52}$$

In a multiple-feed problem, we need to characterize an all-component-inclusive product *with respect to a specific feed*. Thus, product P3 is all-component-inclusive with respect to feed F1, and product P2 is all-component-inclusive with respect to feed F2.

We apply steps 1–4 of Figure 5 and bypass one-half of F1 (that is, 100 mol/h of A and 500 mol/h of B) to P3 and also two-thirds of F2 (that is, 330 mol/h of A, 330 mol/h of B, and 200 mol/h of C) to P2. Equation 52 becomes

$$\begin{array}{c} \mathrm{V1'(F1',A/B)} \\ \downarrow \\ \begin{array}{c} \mathrm{F1'} \\ \mathrm{F2'} \end{array}\begin{bmatrix} 100 & 500 & 0 \\ 170 & 170 & 100 \end{bmatrix} \\ \uparrow \\ \mathrm{V2'(F2',AB/C)} \end{array} \longrightarrow \begin{array}{c} \begin{array}{ccc} \mathrm{A} & \mathrm{B} & \mathrm{C} \end{array} \\ \begin{bmatrix} 100 & 0 & 100 \\ 170 & 170 & 0 \\ 0 & 500 & 0 \end{bmatrix} \end{array}\begin{array}{c} \\ \mathrm{P1'} \\ \mathrm{P2'} \\ \mathrm{P3'} \end{array} \tag{53}$$

By performing vertical split operation V1 on feed F1′ (to isolate product P3′) and V2 on feed F2′ (to isolate product P2′), we can easily synthesize the desired product set:

$$\begin{array}{l} \mathrm{V1'(F1',A/B)} \begin{array}{l} \nearrow \text{A to P1}' \\ \searrow \text{B to P3}' \end{array} \\ \mathrm{V2'(F2',AB/C)} \begin{array}{l} \nearrow \text{AB to P2}' \\ \searrow \text{C to P1}' \end{array} \end{array} \tag{54}$$

Figure 8 shows the resulting sequence, which represents the optimum sequence in terms of minimizing the mass load of separation (Floudas, 1987).

The solution to example 4 suggests two useful heuristics for multiple-feed separation problems: (1) avoid blending together of initial feeds with different compositions in order to reduce the mass load of separation and (2) perform sharp component splits on initial feeds early so as to isolate components that immediately form products or parts of products. Further work is needed, however, to incorporate sloppy splits into the synthesis scheme for multiple-feed separation problems.

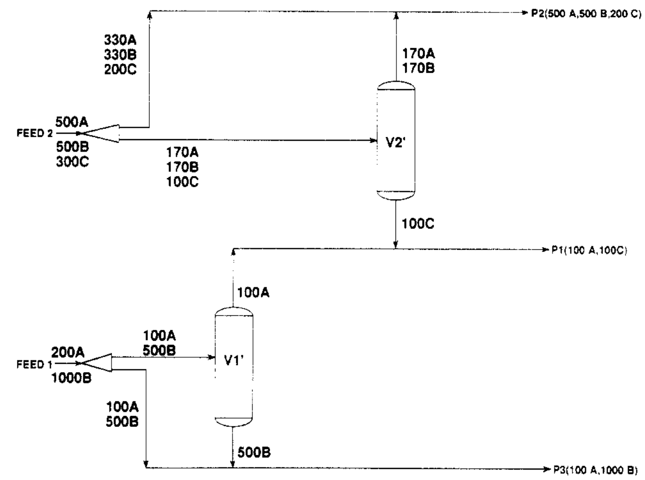

Figure 8. An all-sharp separation sequence obtained for a multiple-feed problem, example 4.

4. Conclusions

The development of simple methods for the systematic design of multicomponent separation systems with sloppy product streams is one of the most challenging problems in process design research over the past 20 years. Such separation systems find much use in the fractionations of refinery light ends and saturate gas components and in recycled reactor systems for reactant recovery and byproduct separation, where it is often unnecessary to utilize the generally more expensive, sharp separation systems with high component recoveries.

In this paper, we have presented a unifying method for the synthesis of good initial flowsheets for multicomponent separations with sloppy product streams. These flowsheets utilize a minimum number or a nearly minimum number of three types of equally good separators, namely, all-sharp, all-sloppy, and mixed-separation (i.e., both sharp and sloppy) sequences. To synthesize these competing sequences, we have introduced some simple and flexible tools for representing a given separation problem, called the component assignment matrix, and for analyzing the technical feasibility and ranking the relative ease of different separation tasks, called the separation specification table. On the basis of the rank relationship of the CAM, the number of components, and the number of products, we have proposed a unifying classification of all multicomponent separation-sequencing problems into four classes and have suggested proper approaches to solving each class of synthesis problems. We have particularly demonstrated the simplicity and effectiveness of applying six rank-ordered heuristics together with CAM, SST, and stream bypass to a number of industrial separation problems. The resulting separation sequences represent good initial flowsheets for further heat integration and separator optimization.

Of particular significance is that our synthesis method can be applied by hand calculations and can be readily used by a practicing engineer. It has also been implemented as an expert system called EXSEP using PROLOG on a personal computer. Operating interactively with a design engineer, EXSEP can easily out-pace the engineer's ability to assimilate the necessary design information and to synthesize good separation flowsheets.

Nomenclature

b_i = ith component molar flow rate in the bottoms, mol/h; or in normalized situation, ith component recovery fraction in the bottoms, dimensionless

B = molar flow rate of the bottoms, mol/h

C = number of components

CAM = component assignment matrix

CAM(Hi,btm), CAM(Hi,ovhd) = CAM for representing the bottoms and overhead resulting from horizontal product split Hi, respectively

CAM(Vj,btm), CAM(Vj,ovhd) = CAM for representing the bottoms and overhead resulting from vertical component split Vj, respectively

CES = coefficient of ease of separation defined in eq 3

d_i = ith component molar flow rate in the overhead, mol/h; or in normalized situation, ith component recovery fraction in the overhead, dimensionless

D = molar flow rate of the overhead, mol/h

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

f_{ij} = elements of the component assignment matrix representing the flow rate of the jth component in the ith product (i = 1, 2, ..., P; j = 1, 2, ..., C)

Hi = horizontal product split i (i = 1, 2, ..., P)

HHK1-3 = heavier-than-heavy-key or heavy components 1-3 whose volatilities are in a descending order

HK = heavy-key component

K_i = vapor-liquid equilibrium ratio of component i, dimensionless

LK = light-key component

LLK1-3 = lighter-than-light-key or light components 1-3 whose volatilities are in an ascending order

$N_{\min}$ = minimum number of theoretical stages

P = number of product streams, or column pressure, Pa

r = rank of the component assignment matrix

r' = pseudorank of the component assignment matrix

R_D = operating reflux ratio

$R_{D,\min}$ = minimum reflux ratio

$S_{\min}$ = apparent minimum number of separators, eq 1

SST = separation specification table

Vj = vertical component split j (j = 1, 2, ..., C)

Superscripts

$'$ = prime, indicates the CAM resulting from, or the horizontal product split Hi (vertical component split Vj) made after, bypassing a portion of the feed around the separator to directly form part of an overhead or a bottoms

$''$ = double prime, indicates the CAM resulting from, or the horizontal product split Hi (vertical component split Vj) made after, bypassing two portions of the feed around the separator to directly form parts of both overhead and bottoms

Greek Letters

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

Symbol

$\Delta = \Delta T$ (normal boiling-point difference, °C) or 100 (α − 1)

Literature Cited

Aggarwal, A.; Floudas, C. A. Synthesis of General Distillation Sequences-Nonsharp Separations. AIChE National Meeting, Houston, TX, April, 1989; Paper 32d.

Bamapoulos, G.; Nath, R.; Motard, R. L. Heuristic Synthesis of Nonsharp Separation Sequences. *AIChE J.* **1988**, *34*, 763–780.

Cheng, S. H.; Liu, Y. A. Studies in Chemical Proces Design and Synthesis. 8. A Simple Heuristic Method for the Synthesis of Initial Sequences for Sloppy Multicomponent Separations. *Ind. Eng. Chem. Res.* **1988**, *27*, 2304–2322.

Floudas, C. A. Separation Synthesis of Multicomponent Feed Streams into Multicomponent Product Streams. *AIChE J.* **1987**, *33*, 540–551.

Floudas, C. A.; Anastasiadis, S. H. Synthesis of General Distillation Sequences with Several Multicomponent Feeds and Products. *Chem. Eng. Sci.* **1988**, *43*, 2407–2419.

Henley, E. J.; Seader, J. D. *Equilibrium-Stage Separation Operations in Chemical Engineering*; Wiley: New York, 1981; pp 527–555.

Liu, Y. A. Process Synthesis: Some Simple and Practical Developments. In *Recent Developments in Chemical Process and Plant Design*; Liu, Y. A., McGee, H. A., Jr., Epperly, W. R., Eds.; Wiley: New York, 1987; pp 147–260.

Mahalec, V.; Motard, R. L. Procedures for the Initial Design of Chemical Processing Systems. *Comput. Chem. Eng.* **1977**, *1*, 57–68.

Muraki, M.; Hayakawa, T. Separation Process Synthesis for Multicomponent Products. *J. Chem. Eng. Jpn.* **1984**, *17*, 533–538.

Muraki, M.; Hayakawa, T. Multicomponent Product Separation Process Synthesis with Separation Sharpness. *J. Chem. Eng. Jpn.* **1987**, *20*, 195–198.

Muraki, M.; Hayakawa, T. Synthesis of a Multicomponent Multiproduct Separation Process with Nonsharp Separators. *Chem. Eng. Sci.* **1988**, *43*, 259–268.

Muraki, M.; Kataoka, K.; Hayakawa, T. Evolutionary Synthesis of a Multicomponent Multiproduct Separation Process. *Chem. Eng. Sci.* **1986**, *41*, 1843–1851.

Nath, R. Studies in the Synthesis of Separation Processes. Ph.D. Dissertation, University of Houston, Houston, TX, 1977.

Tedder, D. W. The Synthesis of Optimal Gas Saturates Separation System. AIChE Annual Meeting, San Francisco, CA, 1984.

Watkins, R. N. *Petroleum Refinery Distillation*, 2nd ed.; Gulf: Houston, TX, 1979; p 159.

Westerberg, A. W. The Synthesis of Distillation-Based Separation Systems. *Comput. Chem. Eng.* **1985**, *9*, 421–429.

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