Separation Vector Formulation for the Synthesis of Multicomponent Separation Sequences

Yuen-Koh Kao
Dept. of Chemical Engineering, University of Cincinnati, Cincinnati, OH 45221

A new separation system representation uses stream separation vectors in the separation space. The characteristics of a separation sequence are clarified by its separation base vectors that form the sequence basis and those of a separation system by the geometrical properties of separation vectors. The optimal flowsheet of each sequence under separation vector formulation can be obtained as the solution of a linearly-constrained optimization problem. A set of simple rules determines the minimum separation loads of any sharp separation sequence by inspection. A modified cost measure, which combines the separation cost with the savings due to stream bypass, can be used to select the optimal sequence without the overall cost analysis.

The optimal separation sequence is obtained first by identifying the best sequence configuration according to modified cost measures and then by finding the actual costs of maximum-bypass and its neighboring sequence configurations. For the nonlinear objective function, the exact optimal flowsheet is determined by solving a linearly-constrained optimization problem. Since this procedure is a linearly-constrained optimization problem, the mathematical programming solution is not likely to lead to a local minimum.

Introduction

Chemical processes invariably involve a number of separation tasks, which constitute a significant fraction of the overall process cost. The significant economic factor of separation tasks in the overall capital and operating costs has led to extensive research on the design of optimal separation processes and sequencing.

The number of possible sequences increases dramatically with the number of components to be separated. To reduce the number of separation sequences that needs to be considered, most of the works on the synthesis of optimum sequences are restricted to systems consisting exclusively of simple, sharp separators. Even under the restrictions that the sequence consists of only simple sharp separators and pure products, the number of possible sequences increases exponentially with the number of components. For an N-component mixture, there are $[2(N-1)]!/[N!(N-1)!]$ possible sequences (Thompson and King, 1972). Without these restrictions, the number of possible sequences is even higher (Chen et al., 1991). Obviously, some simplification is needed so that it is not necessary to evaluate all possible sequences. Many methods have been proposed to assemble an optimal or a near optimal sequence without examining all possible sequences.

Methods for identifying the optimal separation sequence can be classified into three categories:

(1) Heuristic based on rules of thumb evolving from long periods of engineering experience.

(2) Evolutionary based on the evolutionary improvement from a preliminary separation sequence.

(3) Algorithmic based on various methods of mathematical programming.

Heuristic rules, such as those listed by Nishida et al. (1981) and more recently by Nadgir and Liu (1983), are not precise and frequently contradict each other. For example:

- *Remove the most plentiful component first* contradicts *Remove the lightest component first*, unless the most abundant component is the most volatile component.
- *Make the easier separation first and the most difficult last* contradicts the result that an indirect sequence becomes the better choice when either the volatilities of the two most volatile components are close and much higher than those of the remaining components, or when the volatilities of the two less volatile components are close.
- *Favor a 50-50 split* can only be safely used if the ratio of the heaviest and the lightest components is large.

One approach to resolve the contradictory heuristics is to evaluate a separation sequence by some kind of quantitative measure, such as the coefficient of difficulty of separations (Nath and Motard, 1981; Lu and Motard, 1982), which is an intuitive combination of heuristic. Another intuitive measure is based on the commonly-used six-tenth rule for equipment cost correlation:

$$\text{Objective Function} = \sum_{i=1}^{n-1} (L_i D_i)^{0.6} \tag{1}$$

for the separation of an n-component mixture, where L_i and D_i are the separation mass load and the cost index of separation of the i-th simple separator, respectively. Malone et al. (1985) proposed the total annualized cost (TAC), which is a function of the number of trays, N, and the vapor rate, V,

$$\text{TAC} = C_0 N^{0.8} V^{0.5} + C_1 V^{0.65} + C_2 V \tag{2}$$

as the basis to determine the optimal sequence.

The problem of optimal separation sequence synthesis is further complicated by the introduction of justifiable options of stream splitting and blending that require little energy, but can offer considerable improvement in process economics. Muraki et al. (1984) and Muraki and Hayakawa (1986) employed the material allocation diagram originally proposed by Nath (1977) in an evolutionary procedure to obtain the optimal sequence consisting of only sharp separators that include these options. In their later work, this approach was extended to sequences including nonsharp separators (Muraki and Hayakawa, 1988). The evolutionary procedure requires a trial-and-error process and the resulting design may not be optimal.

Floudas (1987) questioned the ability of Muraki et al.'s approach to handle multiple feed streams with stream splitting and blending. He developed an algorithmic procedure using a superstructure encompassing all possible sequences of separators, blenders and dividers. A realistic and practical optimal separation sequence can be obtained by formulating and solving this superstructure as a mixed-integer, nonlinear programming problem that minimizes an objective cost function such as Eq. 1. This method was later applied to the synthesis of distillation sequences (Floudas and Anastasiadis, 1988). Stream splitting and blending play an important role in minimizing the total cost of the optimal separation sequence.

Due to the nonconvexity of the synthesis problem, the optimal separation sequence obtained with a superstructure-based approach may not be globally optimal. Wehe and Westerberg (1987) developed a different algorithm for the synthesis of an optimal sequence consisting of sharp separators with bypass and mixers. Due to the nonlinearity in this formulation, the minimum cost sequence is determined indirectly by first establishing a lower bound by relaxing the nonlinear constraints, followed by the determination of the upper bounds of the most promising separation sequences that include the constraints. The global optimum is considered to be achieved if these two bounds of the optimal sequence are within a tolerably small range.

We have developed an entirely new concept for the synthesis of multicomponent separation sequences. This concept is to represent a separation sequence in *separation* space. Each stream of the sequence is represented by a stream *separation vector*. In terms of separation vectors, all conceivable operators of a separation sequence, such as stream splitting, mixing, and bypassing, have their own definitive representations. When the inner structure of a separation sequence is depicted in separation space, a lucid picture of the sequence emerges.

In the following, we will first present a brief exposition on the separation space geometry and its properties, illustrated by examples of how a separation sequence is represented in the separation space. A new synthesis procedure will be formulated on the basis of separation vector representation. Savings in the cost of a separation task come from two sources: minimizing the amount of material to be separated and arranging these separation tasks in an optimal sequence. A geometrical examination of sharp separation sequence synthesis will lead to a set of simple rules that can determine the minimum separation loads of any sharp separation sequences by inspection. A modified cost measure will be introduced that can guide the search of the optimal separation sequence without exhaustive enumerating of all possible sequences. Three example problems will be used to illustrate the new synthesis procedure.

Separation Space Geometry

Traditionally, a separation system is represented by its stream compositions (x_{ir} being the fraction of component i in product stream r) and sizes (θ_r being the fraction of feed recovered in product stream r, commonly called the "cut"). The separation of an n-component feed stream of composition x_{if} into m product streams is represented in terms of mole (or mass) fractions by the following equation:

$$x_{if} = \sum_{r=1}^{m} x_{ir}\theta_r, \quad i = 1, \ldots, n-1 \tag{3}$$

This representation is not linear with respect to the system variables, x_{ir} and θ_r. Consequently, one has to rely on the *Lever Arm Rule* to visualize this nonlinear representation. For example, Figure 1 depicts geometrically, in terms of stream composition, the separation of a three-component feed mixture into two product streams:

$$\begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \end{pmatrix} = \theta \begin{pmatrix} 0.5294 \\ 0.3529 \\ 0.0667 \end{pmatrix} + (1-\theta) \begin{pmatrix} 0.0769 \\ 0.3077 \\ 0.6154 \end{pmatrix} \tag{4}$$

by three stream composition points. The sizes of the two product streams cannot be readily visualized but must be determined by the Lever Arm Rule, which states that "the ratio of the two product sizes is the inverse ratio of the lengths of the lines connecting the feed mole fraction to the mole fractions of each product, in order" (King, 1980).

$$\frac{\theta}{1-\theta} = \frac{|OA|}{|OB|} \tag{5}$$

This leads to the result of $\theta = 0.5667$. In the cases of separating a feed into more than two products, the stream sizes must be obtained by repeated application of the Lever Arm Rule.

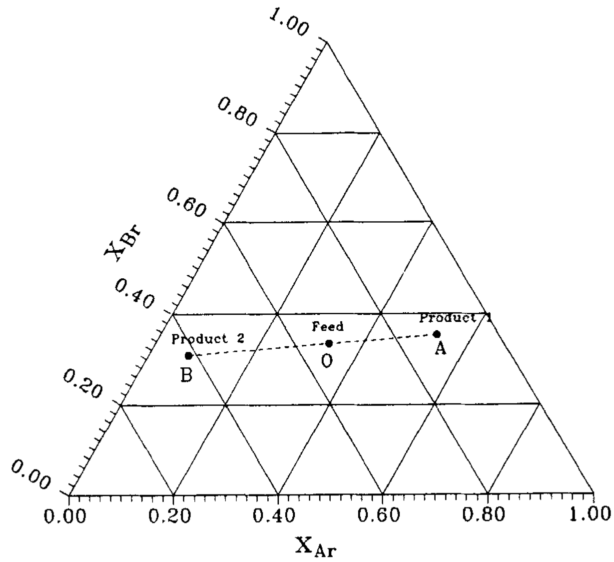

Figure 1. Stream composition space representation of three-component two-stream separation system.

Each stream is represented by stream composition point, O: feed stream, A and B: product streams.

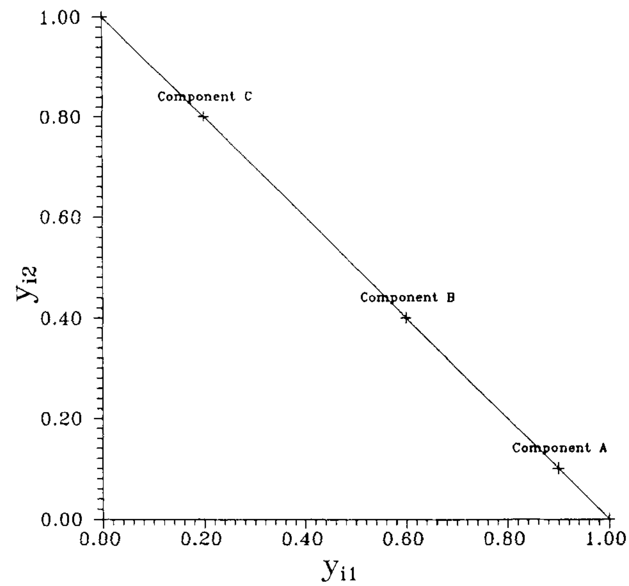

Figure 2. Component segregation space representation of a three-component two-stream separation system.

Each component is represented by component segregation point.

The feed composition dependency of Eq. 3 can be eliminated by normalizing the composition of a component with respect to its feed composition. A different variable, the segregation fraction, $y_{ir} = x_{ir}\theta_r/x_{if}$, can be formed by combining the cut with the normalized compositions of each stream. Physically, y_{ir} is the fraction of component i in the feed recovered in product stream r. Thus, an equivalent separation representation of Eq. 3 in terms of the segregation fraction variables is:

$$1 = \sum_{r=1}^{m} y_{ir}, \quad i = 1, \ldots, n \tag{6}$$

The following is the equivalent representation of the same example shown in Figure 1 in terms of the three component segregation fractions:

$$\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.9 \\ 0.6 \\ 0.2 \end{pmatrix} + \begin{pmatrix} 0.1 \\ 0.4 \\ 0.8 \end{pmatrix} \tag{7}$$

This representation is shown in Figure 2 by three component segregation points in the one-dimensional manifold: the straight line: $y_{i1} + y_{i2} = 1$.

This representation provides measures of the individual component distributions, obliterating the feed composition dependency. Consequently, it is seldom used except in separation sequence synthesis, such as the material allocation diagram representation (Nath, 1977; Muraki and Hayakawa, 1984). The complete characterization of a separation system requires the knowledge of the stream sizes (cut), which is related to feed composition by the following equation:

$$\theta_r = \sum_{i=1}^{n} y_{ir} x_{if} \tag{8}$$

The full potential of the segregation fraction representation can be realized by the introduction of the following separation vector representation. The crux of the new approach is to represent each stream by a *separation vector*. There are $n-1$ independent separations for an n-component separation system. The separation between component i and $i+1$ of stream r can be represented by the difference of the segregation fractions of component i and component $i+1$ of that stream:

$$z_{ir} = y_{ir} - y_{i+1r} \tag{9}$$

The quantities, $\{z_{ir}, i = 1, \ldots, n-1\}$, together form the separation vector:

$$z_r = (z_{1r}, \ldots, z_{n-1r})' \tag{10}$$

of stream r. The vector is capable of providing a clear picture of the separation sequence. *By representing streams by their separation vectors*, the act of separation is represented by the following formula that simply states: *the sum of separation of the vectors of the separated streams equals the separation vector of the feed stream*:

$$z_f = \sum_{r=1}^{m} z_r \tag{11}$$

This new representation unifies the composition representation, Eq. 3, and the segregation fraction representation, Eq. 6. A simple picture of separation emerges from the separation vector representation. Figure 3 shows the same example when the two streams are represented by their separation vectors:

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0.3 \\ 0.4 \end{pmatrix} + \begin{pmatrix} -0.3 \\ -0.4 \end{pmatrix} \tag{12}$$

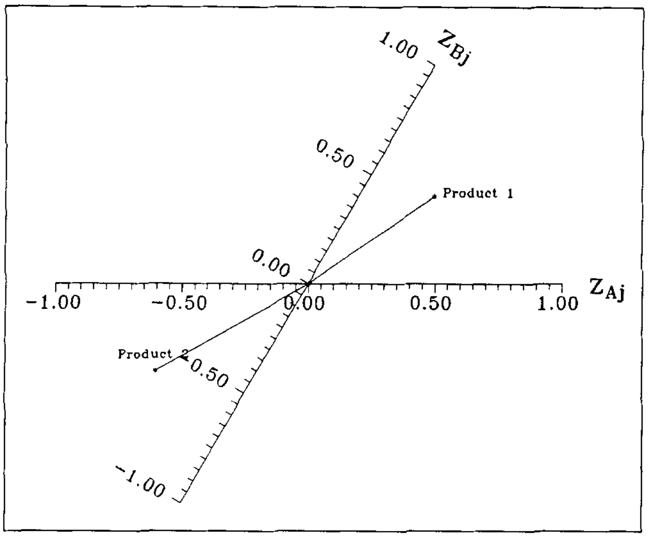

Figure 3. Separation vector representation of a three-component two-stream separation system.

The sum of the two stream separation vectors equals the null feed vector.

Separation measures

The potential of a universal separation index to advance the analysis of separation processes was well articulated by Rony (1972). This new representation has led to the development of a series of separation indices. These new indices have the desirable universal property as indicated in Rony's initial proposition:

- The index is independent of the starting and the final compositions.
- The index is not dependent on how the separation system is labeled (that is, how the stream and component indices are assigned).
- The index is a normalized quantity so that an index of unity means a perfect separation and zero means no separation.
- The formulation of the index is independent of the physical process.

In the following, we will provide a short description of the single-stream separation index which will be used in this article. For a complete description of other separation indices, readers are referred to an earlier article (Kao, 1992).

The separation vector, z_r, embodies both the separation direction and the size of a separated stream in a separable format:

$$z_{ir} = \left(\frac{x_{i,r}}{x_{i,f}} - \frac{x_{i+1,r}}{x_{i+1,f}}\right) \times \theta_r \tag{13}$$

The separation vector is the product of a composition element and a stream size element. The composition element, $\{(x_{i,r}/x_{i,f}) - (x_{i+1,r}/x_{i+1,f})\}$, defines the separation direction; the size of the vector, θ_r, the fraction of feed going to stream r defines the quantity of separation. Separation systems of any configuration can be characterized geometrically by their separation vectors. In order to do so, a metric tensor for the *separation vector manifold* must be defined. This metric tensor can be obtained as the *contragradient* transformation of the stream composition metric tensor with respect to the $z \rightarrow y$ affine transformation defined by Eq. 9. Consequently, the properties of a separation system remain unchanged when it is represented in the separation vector manifold. For an n-component system, the metric tensor is:

$$g_{ij} = \frac{i(n-j)}{n}, \quad \text{for } i \leq j: \quad \text{and } g_{ij} = g_{ji}, \quad \text{for } i > j, \quad i, j = 1, \ldots, n-1 \tag{14}$$

The derivation of the metric tensor can be found in the Appendix.

Equipped with this metric tensor, it is possible to thoroughly characterize any separation system by its separation vectors. The composition difference between two streams can be measured by the *angle* formed by the two stream vectors. The length of the vector can be used to define a single-stream separation index:

$$\eta_r = \sqrt{\sum_{i=1}^{n-1} \sum_{j=1}^{n-1} g_{ij} z_{ir} z_{jr}} \tag{15}$$

The single-stream separation index provides the composite separation measure of a product stream with respect to the feed stream. It accounts for both the fractions of every component recovered in all streams and the separation of the components within a stream. From this point forward, the "single-stream separation index" will be referred to simply as the separation index.

For example, the separation indices of two product streams separated from a three-component feed, as shown in Figure 2, according to the two vectors of Eq. 12 computed by the formula Eq. 15, are identical 0.4967 *irrespective of the initial feed composition*. For a three-component system, the single stream index can be rearranged in terms of segregation fractions as the following equation:

$$\eta_r^2 = 2/3(z_{1r}^2 + z_{1r}z_{2r} + z_{2r}^2) = 1/3[(y_{1r} - y_{2r})^2 + (y_{2r} - y_{3r})^2 + (y_{3r} - y_{1r})^2] \tag{16}$$

Thus, the separation index of a stream that completely recovers either one or two components of a three-component feed is $\sqrt{2/3}$. If a normalized index is desired, the value computed by Eq. 15 can be normalized with respect to the total separation index.

The compositional change of a separated stream can be measured by an index that eliminates the stream size factor and reflects only the composition change. This is the *purification* index, which measures the purity of a separated stream:

$$\pi_r = \eta_r / \theta_r \tag{17}$$

The separation indices of two streams separated from a *single* feed stream are always identical. The degrees of purification of the two streams are generally different, except for the special case of an even split.

For the example of separating a feed containing equal amounts of three components (Figures 1 to 3), the purification indices of the two streams are:

$$(\pi_1 \quad \pi_2) = [\eta_1/\theta \quad \eta_2/(1-\theta)] = (0.8764 \quad 1.1462) \tag{18}$$

This means that the purity of stream 2 is higher than that of stream 1. On the other hand, if the feed compositions of three components are 0.1, 0.3 and 0.6, and the three components are also segregated between two streams as shown in Figure 2, then the cut of the first stream computed by Eq. 8 is 0.39. The purification indices of the two streams are 1.2736 and 0.8143, respectively. This means that the purity of stream 1 is higher than that of stream 2.

An *overall purification index* can be defined to measure the degree of purification of separating a feed stream into two streams by the geometric means of the two stream purification indices:

$$\pi = \frac{\eta}{\sqrt{\theta(1-\theta)}} \tag{19}$$

This index measures the difficulty of separating a feed into two separated streams. Comparing the overall purification indices of the two different feed cases, it is obvious that the first case ($\pi = 1.0023$) is an easier separation than the second case ($\pi = 1.0184$).

The most efficient separation of a feed into two streams, if the costs of separation into different compositions are identical, is when the feed is equally distributed in the two streams. Using the equal-composition feed case as an example, the same products can be produced by bypassing 2/15 of the feed while the remaining feed is separated, as shown in the following equation:

$$\begin{pmatrix}1\\1\\1\end{pmatrix} = \begin{pmatrix}2/15\\2/15\\2/15\end{pmatrix} + \begin{pmatrix}23/30\\14/30\\2/30\end{pmatrix} + \begin{pmatrix}0.1\\0.4\\0.8\end{pmatrix} \tag{20}$$

The first product can be produced by blending the bypass stream with one of the separated streams. The above bypass does not alter the directions of two separation vectors, except their sizes are enlarged by 15/13. The separation index is now 0.5731 and the purification indices of both separated streams are 1.1462. However, since only 13/15 of the feed is subjected to separation, the overall purification index of the balanced separation is 0.9934, which is less than that of the unbalanced separation of 1.0023. Thus, *the easiest separation is the separation with the lowest overall purification index.*

Separation space visualization of separation sequences

In the separation space, the separation of a stream into two product streams can be represented by the decomposition of the feed vector into two product vectors. The division of a stream into several streams of identical composition can be represented by partitioning that stream separation vector into segments proportional to the sizes of divided streams. The mixing of several streams into one stream can be represented by the summation of the separation vectors of those streams. Thus, a separation sequence can be uniquely represented in separation space by separation vectors. The geometrical structure of separation space provides astute perspectives on the synthesis of a separation sequence.

For a three-component separation system with the components labeled in the order by which they can be separated (such as in the order of decreasing volatilities for ordinary distillation), a feasible sharp separation between component 1 and component 2 can be represented by a top stream separation vector on the positive z_1 axis and a bottom stream vector *of the same magnitude* on the negative z_1 axis. Similarly, a feasible sharp separation between component 2 and component 3 can be represented by a top stream separation vector on the positive z_2 axis and a bottom stream vector *of the same magnitude* on the negative z_2 axis. A feasible sloppy separation can be represented by a pair of diametrically-opposed, equal-magnitude vectors in the first (for the top stream) and the third (for the bottom stream) quadrant of the separation space. For example, if a feed mixture consisting of 5 moles of A, 3 moles of B, and 2 moles of C is separated to produce three products: Product 1 (4.5 A, 0.5 B and 0.1 C), Product 2 (0.4 A, 2 B and 0.8 C), and Product 3 (0.1 A, 0.5 B and 1.1 C), the separation task can be represented in terms of composition variables (Eq. 3):

$$\begin{pmatrix}0.5\\0.3\\0.2\end{pmatrix} = \begin{pmatrix}0.8824\\0.0980\\0.0200\end{pmatrix}0.51 + \begin{pmatrix}0.1250\\0.6250\\0.2500\end{pmatrix}0.32 + \begin{pmatrix}0.0588\\0.2941\\0.6471\end{pmatrix}0.17 \tag{21}$$

or the following separation vector formulation (Eq. 6):

$$\begin{pmatrix}0\\0\end{pmatrix} = \begin{pmatrix}0.7333\\0.1167\end{pmatrix} + \begin{pmatrix}-0.5867\\0.2667\end{pmatrix} + \begin{pmatrix}-0.1467\\-0.3833\end{pmatrix} \tag{22}$$

The products are represented by three separation vectors: $\vec{OA}$, $\vec{OC}$ and $\vec{OD}$ in Figure 4. The products can be produced in a sequence that consists of two sloppy separations: the first product is produced directly as the top stream of a sloppy separation of the feed. The bottom stream from the first separation (which is represented by the vector, $\vec{OB}$) is then separated in a second sloppy separator to produce the other two products. This sequence can be geometrically portrayed by the vector decomposition as shown in Figure 4: Feed $\vec{O}$, a null vector, is separated into $\vec{OA}$ (Product 1) and $\vec{OB}$; $\vec{OB}$ is then separated into $\vec{OC}$ (Product 2) and $\vec{OD}$ (Product 3).

A more complex nonsharp separation sequence, such as the sequence of Bamopoulos et al. (1988) to produce a set of five products as listed in Table 1, can also be explicitly visualized in the separation space, as shown in Figure 5. The five product separation vectors:

$$(z_1, z_2, z_3, z_4, z_5) = \begin{pmatrix}-0.2 & 0.3 & 0.1 & 0.2 & -0.4\\ 0.1 & -0.1 & -0.3 & 0.0 & 0.3\end{pmatrix} \tag{23}$$

are represented by solid arrow vectors. The separated streams are shown by open arrow vectors. The first sharp A/BC split

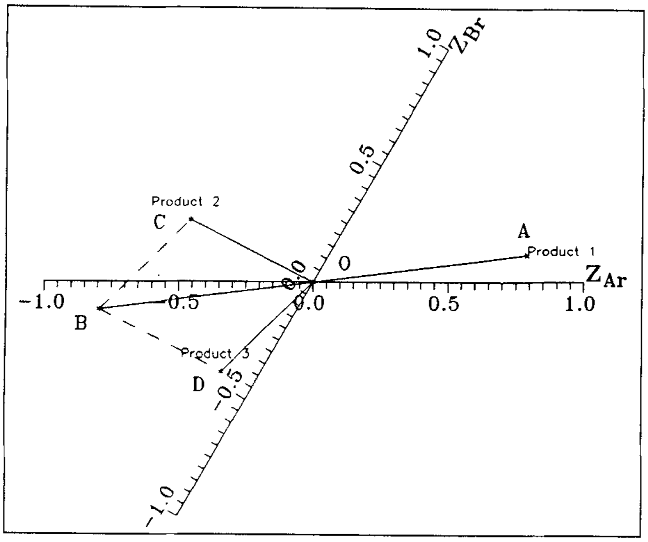

Figure 4. Separation vector representation of a three-component three-stream separation system of Eq. 21.

Each stream is represented by a separation vector.

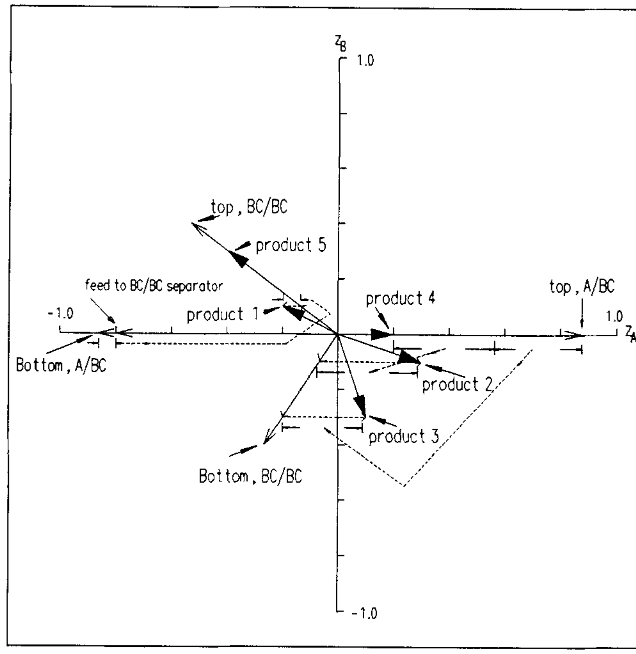

Figure 5. Separation space decomposition of a five-product separation sequence.

For clarity, separation space oblique coordinate is changed to orthogonal one. This change does not affect basic separation operations, such as stream splitting, separation and blending of several streams.

(separator S1) separates 13/15 of the feed and produces two streams: the top stream (top, A/BC) and the bottom stream (bottom, A/BC). The bottom stream is split into two parts: 1/13 of the bottom stream bypasses and the remaining fraction is fed to a second sloppy BC/BC separator. The top stream vector (top BC/BC) of the second separator (S2) is oriented in the direction of Product 5. The five products are produced by blending proper fractions of the streams emerging from the two separators and the bypassed feed. Product 1 is produced by blending 1/4 of the top stream from S2 and 1/13 of the bottom stream from S1. Product 2 is produced by blending 11/26 of the top stream from S1 and 1/4 of the bottom stream from S2. Product 3 is produced by blending 3/4 of the bottom stream from S2 and 9/26 of the top stream from S1. Product 4 is produced directly from 3/13 of the top stream of S1. Product 5 is produced directly from 3/4 of the top stream from S2. The balance of Product 1 and Product 3 are made up by proper fractions of the feed. The separation sequence is shown in Figure 6. The division and blending operations can be identified in the separation space by segmenting the stream vectors and the summing of the proper set of stream vectors to produce the product set, respectively.

Synthesis of Separation Sequences with Separation Vectors

The optimal separation sequence can be obtained, in general, as the solution of a mixed-integer (of the sequencing) nonlinear

Table 1. Three-Component Five-Product Separation Problem

Comp.	Product 1	2	3	4	5
A	0.1	0.4	0.3	0.2	0.0
B	0.3	0.1	0.2	0.0	0.4
C	0.2	0.2	0.5	0.0	0.1

(the objective function) programming problem. For each sequence considered, the optimization problem is subject to only linear constraints. Overall, the procedure consists of the following two steps:

(*1*) *Integer Programming Problem.* Select a sequence and thereby fix the separation vector basis of the sequence, which represents the directions of streams emerging from the separators of the sequence.

(*2*) *Nonlinear Programming Problem.* Determine the best flow sheet that will produce the products at the minimal cost.

Exhaustively repeating the above steps for all possible sequences will identify the best sequence with the least cost. An exhaustive search can be prevented by combining the two steps into a mixed-integer mathematical-programming (MIMP) problem, such as the superstructure formulation of Floudas (1987). It should be noted that if the nonlinear programming problem is nonconvex, then neither the exhaustive search nor the MIMP superstructure approach will necessarily find the global minimum.

The separation sequence that produces a set of products can be explicitly resolved in terms of separation vectors. The vectorial directions of the streams emerging from the separators in a given sequence are fixed *a priori* by their respective base vectors. The product vectors, which represent product separation specifications, must be constructed from the set of sequence base vectors. This construction determines the mass loads of each separator and the division and the blending of the separated streams from these separators to meet the separation specifications of these products. The remaining bulk of a product is filled by blending a certain fraction of the feed that bypasses all separators. The best sequence will be the one that incurs the least cost.

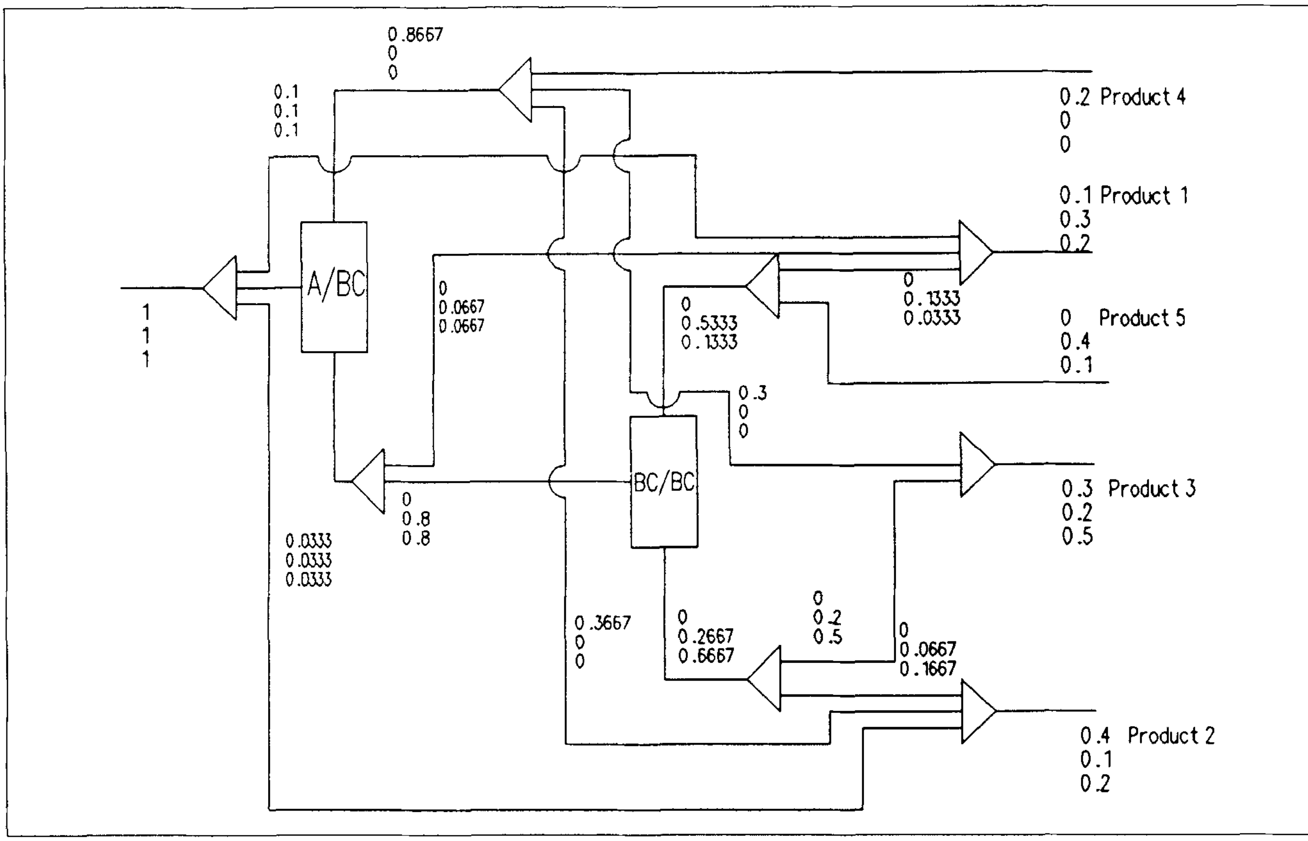

Figure 6. Five-product separation sequence.

Optimization problem formulation with separation vectors

The sequencing aspect of the optimization problem can be methodically dealt with by representing each sequence by a set of separation base vectors. Each base vector represents the direction of a stream emerging from one of the separators in the sequence. The sharp separation between the component pair, i and $i+1$ ($S_{i/i+1}$) of the feed stream, represented by a null vector, generates two nonzero elements, one for the top stream vector:

$$z_i^+ = 1$$

and one for the bottom stream vector:

$$z_i^- = -1$$

They are the only nonzero elements of the top and the bottom stream vectors, respectively.

In general, the sharp separation of a stream produces (a) a top stream vector that contains all feed vector elements above the separation boundary and a " + 1" element at the separation boundary and (b) a bottom stream vector that contains all elements of the feed vector below the separation boundary plus a "−1" at the separation boundary.

The following is a five-component example:

- B/C separation of the original feed:

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

- A/B separation of a feed, which was the top product of above B/C separation:

$$\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

- D/E separation of a feed, which was the bottom product of above B/C separation:

$$\begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}$$

- C/D separation of a feed, which was the top product of the above D/E separation of a feed:

$$\begin{pmatrix} 0 \\ -1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ -1 \\ 1 \end{pmatrix}$$

These four separations form a sharp separation sequence: $S_{B/C} \rightarrow \{S_{A/B}, S_{D/E} \rightarrow S_{C/D}\}$. This sequence can be represented by the following separation sequence base vectors:

$$S = \begin{matrix} & s_1 & s_2 & s_3 & s_4 & s_5 & s_6 & s_7 & s_8 \\ A/B & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ B/C & 1 & -1 & 0 & 1 & -1 & 0 & -1 & 0 \\ C/D & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ D/E & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 1 \end{matrix} \quad (24)$$

Each vector represents a stream from a separator of the sequence.

The separation sequence base vectors can be used to formulate the optimization problem of a sharp separation sequence. Each product is represented by a product separation vector, p_j. A set of n_p products is represented by the product separation matrix $(p_{i,r})$, where $p_{i,r}$ represents separation i (that is, the separation between component i and $i+1$) of product r. The separation direction of the stream k emerging from one of the separators is represented by the k-th column of the separation sequence basis matrix $\{s_{i,k},\ i=1, \ldots, n-1\}$. Each product is produced by the blending of the separated streams emerging from the separators of the sequence. Thus,

$$p_{i,r} = \sum_{k=1}^{n_k} m_{r,k} s_{i,k} \quad (25)$$

where $m_{r,k}$ is the normalized size of stream k for product r. The total amount of stream k required for all products is $\Sigma_{r=1}^{n_p} m_{r,k}$. Since the total amount available of any stream cannot be greater than 1, the $m_{r,k}$s are subjected to the following constraint:

$$0 \leq \sum_{r=1}^{n_p} m_{r,k} \leq 1 \quad (26)$$

The normalized separation load of separator $S_{i/i+1}$, which must meet the $i/i+1$ separation requirements of all products, is computed by the following formula:

$$l_i = \sum_k s_{i,k}^{+} \sum_{r=1}^{n_p} m_{r,k} = \sum_k s_{i,k}^{-} \sum_{r=1}^{n_p} m_{r,k} \quad (27)$$

where the superscripts + and − represent, respectively, the positive and negative components of separation base vectors. The above formulation provides the framework upon which an optimal separation sequence can be determined.

Assuming that the cost of separation i is $C_i(L_i, D_i)$, where L_i is the actual size of the feed stream (mass load) to separator $S_{i/i+1}$ with D_i as the cost index, then the objective function to be minimized is the overall separation cost:

$$J = \sum_{i=1}^{n-1} C_i(L_i, D_i) \quad (28)$$

The optimal separation sequence is the set of $m_{j,k}$ that minimizes the objective function subjected to the linear constraints: Eq. 25 and Eq. 26.

Maximum-Bypass Sharp-Separation Sequences

When the product set is given, then each separation has a minimum load. The normalized loads of separators in a given sequence can be determined by an examination of the product separation vectors. The minimum normalized load of separation i, $(l_i)_{\min}$, equals the magnitude of the sum of the i-th elements of all product vectors of the same sign.

$$(l_i)_{\min} = \sum_{r=1}^{n_p} p_{i,r}^{+} = -\sum_{r=1}^{n_p} p_{i,r}^{-} \quad (29)$$

where the superscript indicates the sign of the element. If the sum of all minimum separation loads is less than one, then these products can be produced by separators in a parallel arrangement. Otherwise, some or all separators must be arranged in a sequence in order to meet the product separation requirement. Even for cases when the total minimum separation load is less than one, certain sequential arrangements can reduce the total separation load if the signs of separation vector elements of some individual products are not identical.

A separation sequence that minimizes the amounts of separations for producing a set of products is a maximum-bypass sequence. These sequences minimize the total separation load or, equivalently, maximize the sizes of bypass streams, and the products should be derived as much as possible from these bypass streams. Properties related to maximum-bypass sequences can be compiled in the process of constructing a maximum-bypass, sharp-separation sequence geometrically. These properties can be summarized in a set of rules that can construct maximum-bypass sequences by inspection.

Geometrical construction of maximum-bypass sharp-separation flowsheet

A maximum-bypass sequence can be constructed geometrically with the separation vector representation. Each separator should produce the minimal amount of separated streams that meet the product separation specifications and provide a feed stream (or feed streams, if the sequence branches from that point on) for the subsequent separator(s). The load of each separator is minimized if products are made up, whenever possible, of streams that bypass all subsequent separators. Since the last separator of a sequence has no bypass stream, the flowsheet should therefore be constructed by working backward from the end(s) of the separation sequence.

We will use the following problem of producing from a five-component feed two products (1R2P) to demonstrate the construction procedure. The problem is represented by the following two separation vectors:

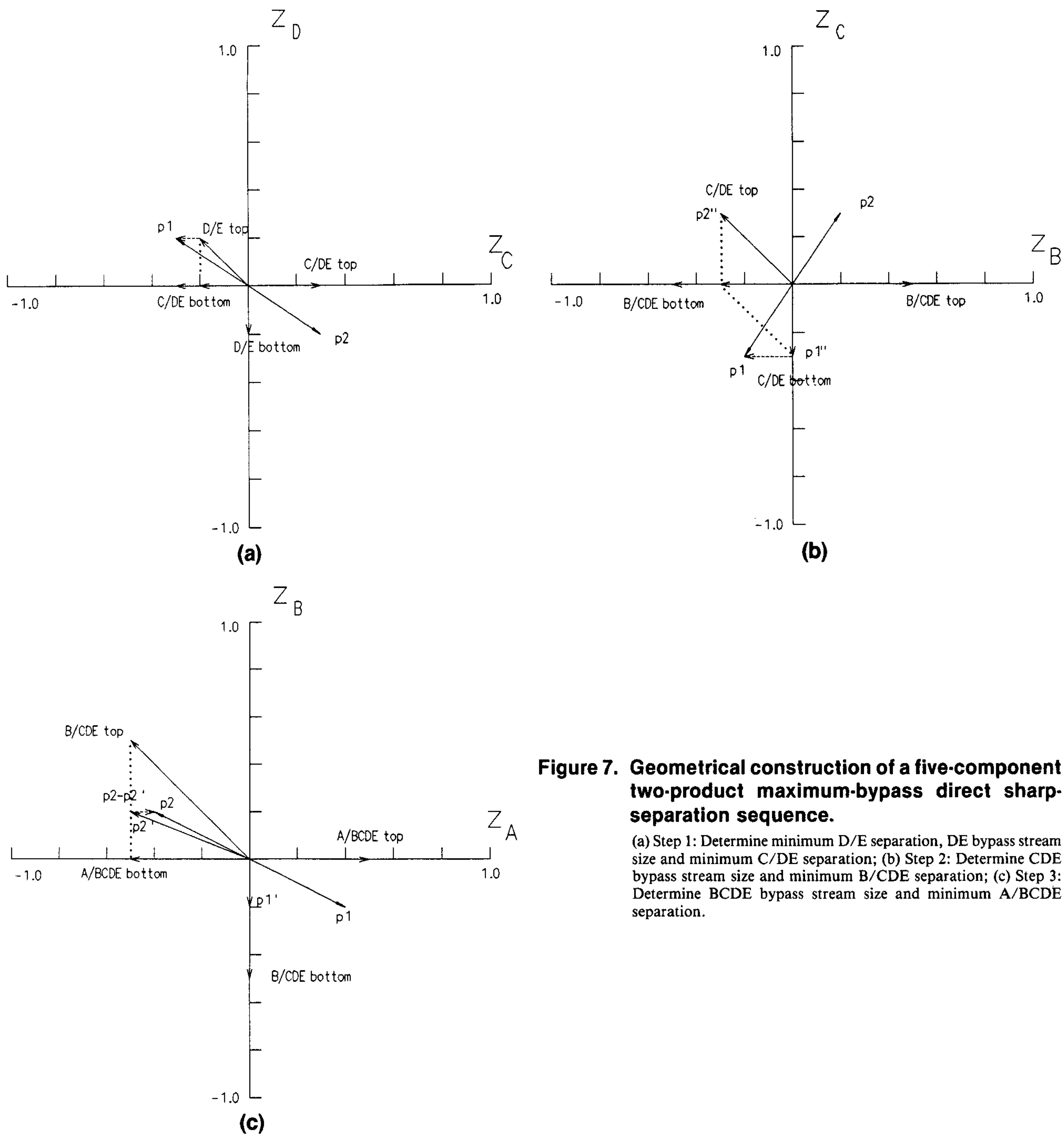

Figure 7. Geometrical construction of a five-component two-product maximum-bypass direct sharp-separation sequence.

(a) Step 1: Determine minimum D/E separation, DE bypass stream size and minimum C/DE separation; (b) Step 2: Determine CDE bypass stream size and minimum B/CDE separation; (c) Step 3: Determine BCDE bypass stream size and minimum A/BCDE separation.

$$(p_1 \quad p_2) = \begin{pmatrix} 0.4 & -0.4 \\ -0.2 & 0.2 \\ -0.3 & 0.3 \\ 0.2 & -0.2 \end{pmatrix} \tag{30}$$

These two product vectors, which are shown in three two-dimensional plots in Figure 7a to 7c as solid-arrow vectors, will be produced by a direct sequence.

An examination of the two product vectors in Figure 7a reveals that their z_D separation requirements can be met by two open-arrow vectors, labeled D/E top and D/E bottom. These two vectors represent the last D/E separator separating 0.2 of DE (D and E in the original feed proportion) to produce 0.2 of D and 0.2 of E of the original feed. Furthermore, the C/D separation requirement of Product 1 can be met by a dashed vector of size 0.1 in the negative z_C direction. This vector represents 0.1 DE that bypasses the D/E separator. This amount, in addition to 0.2 of DE as the feed to the D/E separator, must be produced by the C/DE separator. Therefore, a total of 0.3 DE must be produced by the C/DE separator. At this stage of construction, the separated streams of

D/E and C/DE separators are combined for the two products as follows:

$$p_1'' = \begin{pmatrix} 0 \\ 0 \\ -0.2 \\ 0.2 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ -0.1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -0.3 \\ 0.2 \end{pmatrix} \quad (31)$$

$$p_2'' = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -0.2 \end{pmatrix} + \begin{pmatrix} 0 \\ -0.3 \\ 0.3 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -0.3 \\ 0.3 \\ -0.2 \end{pmatrix} \quad (32)$$

These two vectors meet the D/E and the C/D separation requirements of both products. It is apparent that, *in a direct sequence, only those products whose vector elements are negative may need additional separation for bypass streams.*

The above two vectors are plotted in Figure 7b. For the reason stated above, Product 1 may need additional separation in the negative z_B direction because $p_{C,1}$ is negative. This amount is the difference $(p_1 - p_1'')$, represented by the dashed vector. Thus, an additional 0.2 separation in the negative z_B direction is needed to meet the B/C separation requirement of Product 1. This requirement will be met by the bottom stream produced by the preceding B/CDE separator. The B/CDE separator load is, therefore, 0.5. At this stage, the available separated streams are combined for the two products as follows:

$$p_1' = \begin{pmatrix} 0 \\ 0 \\ -0.3 \\ 0.2 \end{pmatrix} + \begin{pmatrix} 0 \\ -0.2 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -0.2 \\ -0.3 \\ 0.2 \end{pmatrix} \quad (33)$$

$$p_2' = \begin{pmatrix} 0 \\ -0.3 \\ 0.3 \\ -0.2 \end{pmatrix} + \begin{pmatrix} -0.5 \\ 0.5 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -0.5 \\ 0.2 \\ 0.3 \\ -0.2 \end{pmatrix} \quad (34)$$

These two vectors satisfy the B/C, C/D and D/E separation requirements of both products.

Again, the above two vectors are plotted in Figure 7c. A bypass stream may be needed for Product 2, since the first element of p_2 is negative. The vector $(p_2 - p_2')$ is in the positive z_A direction. Therefore, no BCDE bypass stream is needed. The load of A/BCDE separator is also 0.5. The vector $(p_2 - p_2')$ will be obtained by using a fraction of the top stream of the A/BCDE separator. The two products are produced from the separated streams as follows:

$$p_1 = \begin{pmatrix} 0 \\ -0.2 \\ -0.3 \\ 0.2 \end{pmatrix} + \begin{pmatrix} 0.4 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0.4 \\ -0.2 \\ -0.3 \\ 0.2 \end{pmatrix} \quad (35)$$

$$p_2 = \begin{pmatrix} -0.5 \\ 0.2 \\ 0.3 \\ -0.2 \end{pmatrix} + \begin{pmatrix} 0.1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -0.4 \\ 0.2 \\ 0.3 \\ -0.2 \end{pmatrix} \quad (36)$$

The same construction procedure can be used for the inverted sequence by defining the separation vector after rearranging the five components from E to A. An alternate approach is to look for bypass streams in the *positive* direction, that is, only those products whose vector elements are positive may need bypass streams. For example, the inverted (DCBA) sequence (ABCD/E→ABC/D→AB/C→A/B) consists of the following eight base vectors:

$$(s_1, s_2, \ldots, s_8) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 1 & 0 \\ 0 & 0 & -1 & 1 & 1 & 0 & 0 & 0 \\ -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (37)$$

The product separation requirements of the last A/B separation can only be met by the last A/B separator that produces two streams in the direction of s_7 and s_8. The product separation requirements in the positive directions of the other separation can be satisfied by both the bypass stream and the separated stream. For example, positive B/C separation requirements can come from two sources: the AB stream that bypasses the A/B separator, s_7 and the B stream produced by the A/B separator, s_6.

Furthermore, the geometrical construction procedure is equally applicable to sequences that produce more than two products (1RmP problem), with the exception that more than one product may need extra separation loads. The following example derived from Muraki et al. (1988) will be used to demonstrate the geometrical construction of maximum-bypass sharp-separation sequences. Five products with the segregation fractions given by the following matrix:

$$y_{i,r} = \begin{pmatrix} 0.20 & 0.10 & 0.45 & 0.05 & 0.20 \\ 0.10 & 0.20 & 0.20 & 0.30 & 0.20 \\ 0.10 & 0.05 & 0.10 & 0.45 & 0.30 \\ 0.10 & 0.10 & 0.40 & 0.30 & 0.10 \\ 0.05 & 0.15 & 0.25 & 0.35 & 0.20 \end{pmatrix} \quad (38)$$

will be produced from a five-component (labeled A to E) feed by an inverted separation sequence. The five products are represented by five separation vectors:

$$(p_1, \ldots, p_5) = \begin{pmatrix} 0.10 & -0.10 & 0.25 & -0.25 & 0.00 \\ 0.00 & 0.15 & 0.10 & -0.15 & -0.10 \\ 0.00 & -0.05 & -0.30 & 0.15 & 0.20 \\ 0.05 & -0.05 & 0.15 & -0.05 & -0.10 \end{pmatrix} \quad (39)$$

which are shown as solid-arrow vectors in three two-dimensional plots in Figure 8a to 8c. These five product vectors must

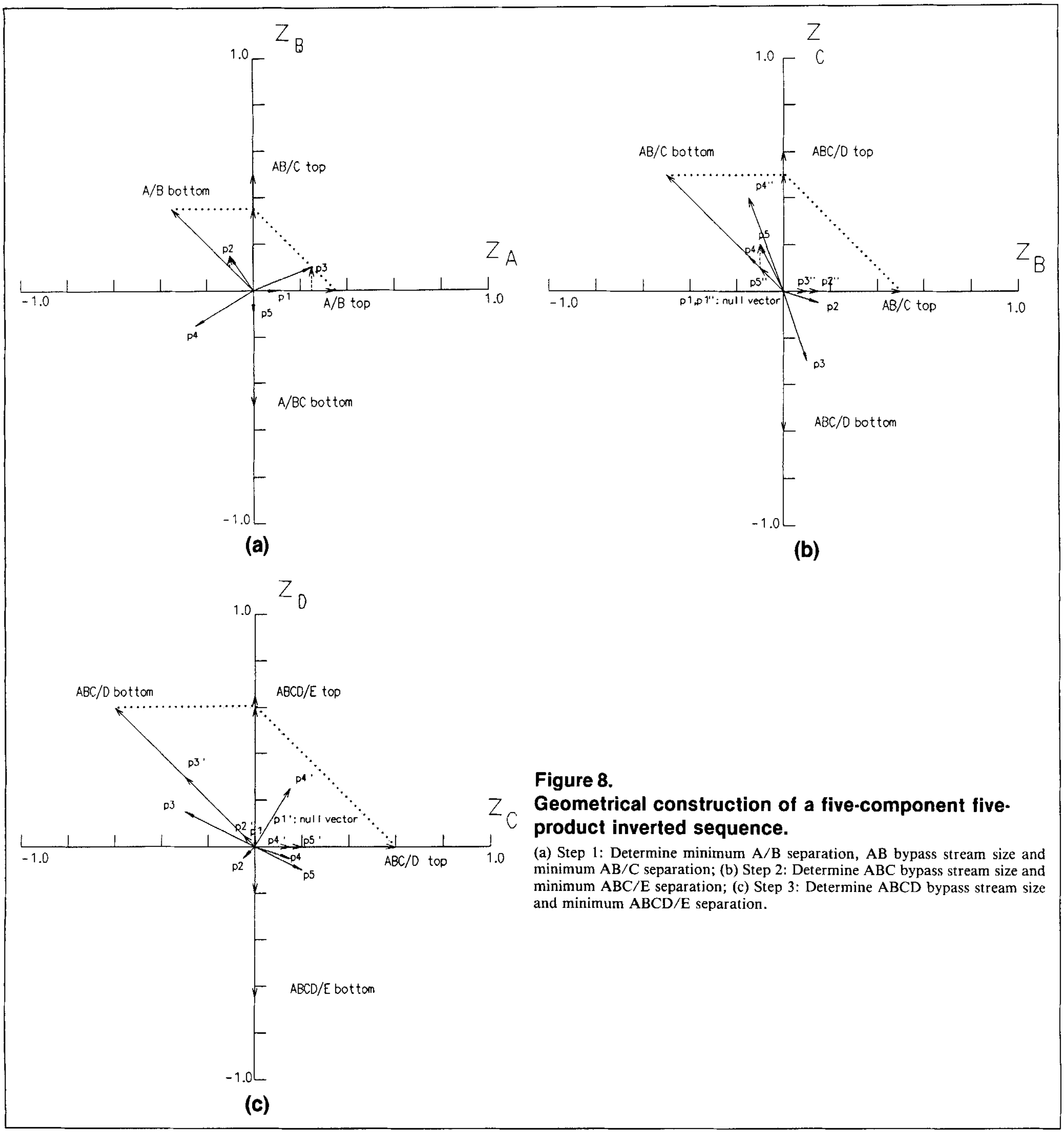

Figure 8.
Geometrical construction of a five-component five-product inverted sequence.

(a) Step 1: Determine minimum A/B separation, AB bypass stream size and minimum AB/C separation; (b) Step 2: Determine ABC bypass stream size and minimum ABC/E separation; (c) Step 3: Determine ABCD bypass stream size and minimum ABCD/E separation.

be constructed by certain combinations of vectors that represent streams emerging from the four separators.

The minimum separation loads for the product set according to Eq. 29 are:

$$[(l_A)_{\min}, \ldots, (l_D)_{\min}] = (0.35 \quad 0.25 \quad 0.35 \quad 0.20) \tag{40}$$

The maximum-bypass flowsheet is constructed from the end of the sequence and working backwards. The A/B separation requirements of all products can only be obtained from streams produced by the last A/B separator. The A/B separation load is the minimum separation load $(l_A)_{\min} = 0.35$. Thus, the last A/B separation produces two streams in the direction of s_7 and s_8 as shown by the two vectors, A/B top and A/B bottom, respectively, in Figure 8a.

The feed stream for the A/B separator (0.35 AB) originates from the top stream of the preceding AB/C separator. In addition, Product 2 and Product 3 require additional separation loads in the *positive* z_B direction in the amount of 0.05 and 0.1, respectively. These are shown in Figure 8a by two dashed vectors. Thus, the load of AB/C separator is 0.5, which is separated into the following two streams, AB/C top and

AB/C bottom. These two streams are represented by open-arrow vectors in Figure 8a and Figure 8b.

The feed stream for the AB/C separator originates from the top stream of the preceding ABC/D separator. Furthermore, it can be seen from Figure 8b that Product 5 requires an additional 0.1 separation in the *positive* z_C direction, represented by the dashed vector. Thus, the ABC/D separator load is 0.6, which is separated into two streams represented in Figure 8b and Figure 8c by two vectors, ABC/D top and ABC/D bottom, respectively.

Following similar geometrical construction procedure in Figure 8c, Product 1 needs an additional 0.05 separation in the *positive* z_D direction. Thus, 0.65 of the feed must be separated in the first ABCD/E separator.

Rules for computing separation loads of maximum-bypass sequences

If the components are arranged in the order by which they are removed, the construction procedure for the direct sequence can be used for any sequence configuration. This is admissible because the separation vector is *invariant* in the sense that different separation vectors obtained from the same product segregation fractions under different component arrangements are equivalent. Instead of rearranging the components and determining the minimum separation loads of a separation sequence geometrically, we have deduced a set of simple rules that can accomplish this task algebraically without the relabeling procedure. These rules are presented in the following paragraphs.

The procedure always starts at the end of a sequence and works backwards. The first rule determines the minimum separation load of the separator at the end (or ends, if the sequence evolves into several branches) of a sequence.

- *Rule 1.* The separation load(s) of a separator at the end of a sequence equals its minimum separation load(s).

$$l_i = (l_i)_{\min} \tag{41}$$

Other separators must produce, in addition to providing feed stream(s) for the subsequent separator(s), extra separation that may be required for meeting their own product separation requirements. Based on the geometrical construction procedure, only certain pertinent products may need extra separation. These pertinent products are determined by the sign of product vector elements relative to the sequence configuration. For the case of separation k (sharp separation between component k and $k+1$) followed by separation i (sharp separation between component i and $i+1$), there are two distinct situations:

- If k is a heavier separation than i, $k>i$ (such as in an inverted sequence), extra separation loads in the positive direction may be needed. A product, p_r, whose k-th vector element, $p_{k,r}$, is positive, is a pertinent product.
- If k is a lighter separation than i, $k<i$ (such as in a direct sequence), extra separation loads in the negative direction may be needed. A product, p_r, whose kth vector element, $p_{k,r}$, is negative, is a pertinent product.

Furthermore, the extra load of separation k of a pertinent product r, $el_{k,r}$, is determined by the set of separation vector elements, $\{p_{s,r}, s=k, \ldots, l\}$, consisting of certain vector elements of the pertinent product r from the current separation k to the last separation of the sequence. Again, there are two distinct situations:

- If $p_{s,r}$'s have at most one sign change, the set consists of all vector elements from the current to the last separations of the sequence.
- If $p_{s,r}$'s have more than one sign change, then the set consists only of those product separation vector elements, $\{p_{s,r}, s=k, \ldots, l\}$, in the direction from k to i, where $p_{l,r}$ is the last element of the first group of separation vector elements of the same sign but different from that of $p_{k,r}$.

The following set of rules determines the extra load of separation k:

Rule 2. There are three distinct situations:

(1) If the signs of $p_{s,r}$s are the same, then the extra load for product r is:

$$el_{k,r} = |p_{k,r}| \tag{42}$$

(2) If $(\Sigma_{s=k}^{l} p_{s,r})p_{k,r} < 0$, then no extra load is needed for product r:

$$el_{k,r} = 0 \tag{43}$$

(3) If $(\Sigma_{s=k}^{l} p_{s,r})p_{k,r} > 0$, then the extra load for product r is:

$$el_{k,r} = \left| \sum_{s=k}^{l} p_{s,r} \right| \tag{44}$$

The total extra load for separation k followed by separation i is the sum of the extra loads of all pertinent products:

$$el_k = \sum_r el_{k,r} \tag{45}$$

The load for separation k is

$$l_k = l_i + el_k \tag{46}$$

The first situation of Rule 2 implies that when some groups of consecutive separation vector elements of *all* products are of the same sign, the total separation load of these separations will be smaller if these separators are in a parallel arrangement. For example, if the product separation vectors are the following matrix:

$$(p_{i,r}) = \begin{pmatrix} + & - & - & - & + \\ + & + & - & + & - \\ + & + & - & + & - \\ - & + & + & + & - \end{pmatrix}$$

the second and the third elements of all product separation vectors have the same sign. According to the first situation, the total separation load of these two separators in series is always greater than the total load of the two separators in parallel.

- *Rule 3.* If the signs of a group of consecutive product vector elements of all products are the same, then these separations, when possible, should be conducted concurrently. In applying Rules 2 to the current situation, the roles of single product separation vector elements are replaced by the sums of these individual groups of elements.

Rule 4 determines the load of the first separation.

• *Rule 4.* The normalized load of the first separator, l_s, is uniquely determined by the minimum segregation fractions of the products. This load for the first separator of a sequence is:

$$l_s = 1 - \sum_{r=1}^{n_p} \min_{i=1,n} y_{i,r} \quad (47)$$

This rule is not needed except for sequences consisting of multiple branches. Furthermore, it can be used to verify the maximum-bypass sequence constructed by the first two rules.

Illustrations

The construction of maximum-bypass sequences according to the above rules is illustrated by the following three examples.

Example 1. This is the second example used by Floudas (1987) of producing two products from a four-component feed:

$$\begin{array}{ccc} \text{Feed} & \text{Product 1} & \text{Product 2} \end{array}$$
$$\begin{pmatrix} 15 & 5 & 10 \\ 20 & 10 & 10 \\ 10 & 4 & 6 \\ 15 & 10 & 5 \end{pmatrix}$$

The segregation fractions, $y_{i,r}$, and the separation vectors of the two products, $p_{i,r}$, are:

$$(y_{i,r}) = \begin{pmatrix} 1/3 & 2/3 \\ 1/2 & 1/2 \\ 2/5 & 3/5 \\ 2/3 & 1/3 \end{pmatrix}, \quad (p_{i,r}) = \begin{pmatrix} -1/6 & 1/6 \\ 1/10 & -1/10 \\ -4/15 & 4/15 \end{pmatrix}$$

These products can be produced by three parallel separators because the sum of their minimum separation loads is 16/30, which is less than one. Therefore, the products can be produced by separating a total of 16/30 of the feed in three separators. Specifically, the separations are 1/6 of the feed by an A/BCD separator, 1/10 by an AB/CD separator and 4/15 by an ABC/D separator. The total separation load is 32.

Since the signs of separation vector elements of either product are not identical, certain serial arrangements of the three separators will reduce the total separation load.

An examination of $y_{i,r}$'s determines that 2/3 of the feed can bypass all separators (1/3 for Product 1 and 1/3 for Product 2). Therefore, the feed to the first separator is always 1/3 of the feed (Rule 4).

Using the direct sequence as an example, the normalized load of the last $S_{C/D}$ separator is $l_C = 4/15$ (Rule 1). The extra load of the preceding B/CD separation is in the negative direction, which indicates that Product 2 may need extra load ($p_{B,2} < 0$). No extra load is needed because $(p_{C,2} + p_{B,2})p_{B,2} < 0$ (Rule 2, Situation 2), and $l_B = l_C = 4/15$. Product 1 may need extra A/BCD separation load because $p_{A,1} < 0$. The amount of extra load is decided by $p_{A,1}$ and $p_{B,1}$ only since there are two sign changes from A to C. Since $(p_{B,1} + p_{A,1})p_{A,1} > 0$, an extra load $el_A = 1/15$ is needed according to Rule 2, Situation 3. The normalized load of A/BCD separation is 1/3, which agrees with the load determined earlier by Rule 4.

Using the CAB ($S_{C/D} \rightarrow S_{A/B} \rightarrow S_{B/C}$) sequence as another example, the load of the last B/C separation is 1/10 (Rule 1). The extra load for the second A/BC separation is in the negative direction. Product 1 may need extra load. According to Rule 2, Situation 3, $el_A = 1/15$ and $l_A = 1/6$. The extra load of the first ABC/D separation is in the positive direction. An extra load of $el_C = |p_{C,2} + p_{B,2}| = 1/6$ is needed for Product 2 (Rule 2, Situation 3) and $l_C = 1/3$.

The separation normalized loads of the five possible sequences can be determined following the rules of construction. The results are listed below:

Sequence	Normalize Load	Actual Load	Total Load
$S_{A/B} \rightarrow S_{B/C} \rightarrow S_{C/D}$	1/3, 4/15, 4/15	20, 12, 6.67	38.67
$S_{A/B} \rightarrow S_{C/D} \rightarrow S_{B/C}$	1/3, 4/15, 1/10	20, 12, 3	35.00
$S_{B/C} \rightarrow \{S_{A/B}, S_{C/D}\}$	1/3, 1/6, 4/15	20, 5.83, 6.67	32.50
$S_{C/D} \rightarrow S_{A/B} \rightarrow S_{B/C}$	1/3, 1/6, 1/10	20, 7.5, 3	30.5
$S_{C/D} \rightarrow S_{B/C} \rightarrow S_{A/B}$	1/3, 1/6, 1/6	20, 7.5, 5.83	33.33

The actual separation loads depend on the feed composition. The maximum-bypass sequence is the $S_{C/D} \rightarrow S_{A/B} \rightarrow S_{B/C}$ sequence. The total separation load of this sequence is 30.5, which is less than the total load of three parallel separators.

Example 2. The example was used originally by Muraki and Hayakawa (1986) to demonstrate their evolutionary synthesis procedure using the material allocation diagram. This example was later used in (Floudas, 1987) to demonstrate the superstructure-based mixed-integer nonlinear programming synthesis technique.

The synthesis problem is given by the following matrix:

$$\begin{array}{ccc} \text{Feed} & \text{Product 1} & \text{Product 2} \end{array}$$
$$\begin{pmatrix} 10 & 2 & 8 \\ 8 & 2.4 & 5.6 \\ 20 & 16 & 4 \\ 16 & 8 & 8 \\ 10 & 1 & 9 \end{pmatrix}$$

The segregation fractions, y_{ir}, and the separation vector elements, p_{ir}, of the two products are:

$$(y_{i,r}) = \begin{pmatrix} 0.2 & 0.8 \\ 0.3 & 0.7 \\ 0.8 & 0.2 \\ 0.5 & 0.5 \\ 0.1 & 0.9 \end{pmatrix} \quad (p_{i,r}) = \begin{pmatrix} -0.1 & 0.1 \\ -0.5 & 0.5 \\ 0.3 & -0.3 \\ 0.4 & -0.4 \end{pmatrix}$$

For the DCAB ($S_{D/E} \rightarrow S_{C/D} \rightarrow S_{A/B} \rightarrow S_{B/C}$) sequence, the maximum-bypass flowsheet can be determined as follows: The last B/C separation load is $l_{B,1} = 0.5$ (Rule 1). The A/BC separation load is $l_{A,1} = 0.6$ because the signs of $p_{A,1}$ and $p_{B,1}$ are identical and $el_A = |p_{A,1}|$ (Rule 2, Situation 1). The ABC/D separation load is also 0.6 because $(\Sigma_{s=C}^{A} p_{s,1})p_{C,1} < 0$ (Rule 2, Situation 2). The first ABCD/E separation load is 0.7 because $(\Sigma_{s=D}^{A} p_{s,1})p_{D,1} > 0$ and $el_D = |\Sigma_{s=D}^{A} p_{s,1}| = 0.1$ (Rule 2, Situation 3, also Rule 4).

Table 2. Separation Loads of Maximum-Bypass Two-Product Sequences*

Sequence	A/B	B/C	C/D	D/E	Total Load
ABCD	0.7 (44.8)	0.7 (37.8)	0.7 (32.2)	0.4 (10.4)	125.2
ABDC	0.7 (44.8)	0.7 (37.8)	0.3 (10.8)	0.7 (32.2)	125.6
ACBD	0.7 (44.8)	0.5 (14.0)	0.7 (32.4)	0.4 (10.4)	101.6
ADBC	0.7 (44.8)	0.5 (22.0)	0.3 (10.8)	0.7 (37.8)	115.4
ADCB	0.7 (44.8)	0.5 (14.0)	0.5 (22.0)	0.7 (37.8)	118.6
BACD	0.1 (1.8)	0.7 (44.8)	0.7 (32.2)	0.4 (37.8)	88.6
BADC	0.1 (1.8)	0.7 (44.8)	0.3 (10.8)	0.7 (10.4)	89.2
CDAB	0.6 (22.8)	0.5 (9.0)	0.7 (44.8)	0.4 (11.2)	87.8
CDBA	0.1 (1.8)	0.6 (22.8)	0.7 (44.8)	0.4 (11.2)	80.6
DABC	0.6 (32.4)	0.5 (22.0)	0.3 (10.8)	0.7 (44.8)	110.0
DACB	0.6 (32.4)	0.5 (14.0)	0.5 (22.0)	0.7 (44.8)	113.2
DBCA	0.1 (1.8)	0.6 (32.4)	0.3 (10.8)	0.7 (44.8)	89.6
DCAB	0.6 (22.8)	0.5 (14.0)	0.6 (32.4)	0.7 (44.8)	114.0
DCBA	0.1 (1.8)	0.6 (22.8)	0.6 (32.4)	0.7 (44.82)	101.8

*Actual size in parenthesis.

For the ADBC sequence, the last C/D separation load $l_{C,1}=0.3$ (Rule 1). The B/CD separation load $l_{B,1}=0.5$ (Rule 2, Situation 3). The BCD/E separation load is 0.7 (Rule 2, Situation 3). The A/BCDE separation load is also 0.7 because $(\Sigma_{s=A}^{D} p_{s,1})p_{A,1}<0$ (Rule 2, Situation 2, also Rule 4).

The separation loads of the fourteen maximum-bypass sequences can be readily obtained according to Rules 1 to 3. These are listed in Table 2. The CDBA sequence separation load of 80.6 is the lowest.

The signs of $p_{A,1}$ and $p_{B,1}$ are negative, and the signs of $p_{C,1}$ and $p_{D,1}$ are positive. According to Rule 3, A/B and B/C separations should be conducted in parallel as should C/D and D/E separations. A natural choice of the first-stage separators is 0.3 of ABC/DE and 0.4 of ABCD/E, since the magnitude of the sum of these two vector elements is 0.7, which is greater than that of the other two, A/BCDE and AB/CDE, which is 0.6 (Rule 3, Rule 2, Situation 2). Consequently, 0.1 of BCDE can bypass the second-stage separators. Thus, the total separation load, consisting of 0.7 of the original feed, 0.2 of ABCD and 0.4 of ABC, is 72.4, which is considerably less than that of the best serial CDBA sequence of 80.6.

The reason for the significant reduction in separation load can be explained by a closer examination of the dual function of a separator: to produce the required product separation and to provide feed streams for the subsequent separation. For example, the two first-stage parallel separators separating 0.3 of the feed into two streams:

$$0.3\begin{pmatrix}0\\0\\1\\0\end{pmatrix} \text{ and } 0.3\begin{pmatrix}0\\0\\-1\\0\end{pmatrix} \text{ by ABC/DE}$$

and 0.4 of the feed into two streams:

$$0.4\begin{pmatrix}0\\0\\0\\1\end{pmatrix} \text{ and } 0.4\begin{pmatrix}0\\0\\0\\-1\end{pmatrix} \text{ by ABCD/E}$$

a total of 0.7 of the feed is subjected to these two separations which meet the required C/D and D/E separations. On the other hand, with the two separators in a sequential arrangement, the first separator must also process 0.7 of the feed:

$$0.7\begin{pmatrix}0\\0\\1\\0\end{pmatrix} \text{ and } 0.7\begin{pmatrix}0\\0\\-1\\0\end{pmatrix} \text{ by ABC/DE}$$

In addition, 4/7 of the bottom stream must undergo the D/E separation in order to meet the D/E separation requirement.

The other choice of the first-stage separators, A/BCDE and AB/CDE also resulted in considerably smaller total separation load. The total separation load of the two first-stage separators is 0.6 of the feed, 0.1 A/BCDE and 0.5 AB/CDE. The bottom streams of the two separators does not provide enough feed stream for the subsequent C/D and D/E separators (0.3 C/D and 0.4 D/E). An additional 0.1 of the original feed is needed to be separated in the second-stage separators in order to meet the C/D and D/E separation requirement of the two products. The total separation load, consisting of 0.7 of the original feed and 0.1 of BCDE and 0.5 of CDE, is 73.2.

The construction rules cannot readily determine individual minimum separation loads of sequences that include parallel configurations. An alternate procedure to obtain maximum-bypass sharp sequence flowsheets is obtained by solving a linear programming problem that minimizes the total separation load

$$J=\sum_{i=1}^{n} l_i \tag{48}$$

using the same separation vector optimization problem formulation presented earlier. The separation sequence base matrix must be expanded to include the parallel separator configuration. For example, the separation base vectors of the first parallel sequence are expanded from eight to ten:

$$(s_1\ \ldots,\ s_{10}) = \begin{pmatrix}1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0\\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & -1\\ 0 & 1 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & -1 & 1 & 0\end{pmatrix} \tag{49}$$

Table 3. Definition of Example 3

Comp.	Feed	Product 1	2	3	4
A	32	7	10	5	10
B	16	8	3	5	0
C	20	3	5	6	6
D	25	9	5	7	4
E	24	8	4	3	9

The pair of base vectors, s_5 (top) and s_6 (bottom), represent two streams of ABC/DE separation, and the pair, s_7 (top) and s_8 (bottom) represent the two streams of ABC/DE separation. The set of three base vectors, s_1 (top), s_2+s_9 (bottom), represents the A/B separator separating a feed stream that blends certain fractions of the top streams (s_5 and s_7) of the two first-stage separations. The set of three base vectors, s_3 (top), s_4+s_{10} (bottom), represents the B/C separator separating another feed stream also derived from the top streams of the two first-stage separators.

Example 3. The construction of 1RmP maximum-bypass sharp separation sequences according to the above set of rules is illustrated by an example of producing four products from a five-component feed taken from the literature (Wehe and Westerberg, 1987). The problem statement is summarized in Table 3. The product segregation fractions are listed in Table 4. The separation vectors of the four products of separations are tabulated in Table 5.

An examination of the sign distribution of the product separation matrix in Table 5 rules out the possibility of parallel arrangements according to Rule 3 since none of the consecutive separation vector elements of all products are of the same sign. The minimum separation loads determined by Eq. 29 are also listed in Table 5. The normalized load of the first separator of any sequence according to Rule 4 is always 0.5583.

In the following, the direct sequence is used as an example to illustrate the construction of 1RmP maximum-bypass sequences.

- The load to the last $S_{D/E}$ separator is 0.2150, the minimum separation requirement (Rule 1). Normalized loads for remaining separators of a sequence can be determined by Rule 2.
- The extra load for separators in the direct sequence is in the negative direction. For the C/DE separation, the extra load is determined by the C/D and D/E elements of the product separation vectors in the following tabulation:

C/D	$p_{C,r}$	−0.2100	0.0500	0.0200	0.1400
D/E	$p_{D,r}$	0.0267	0.0333	0.1550	−0.2150
extra load	$el_{C,r}$	0.1833			

Only Product 1 needs extra load, since $p_{C,1}<0$ and $(p_{C,1}+p_{D,1})p_{C,1}>0$. The amount of extra load computed by Eq. 44 is $el_{C,1}=|0.0267-0.2100|=0.1833$ (Rule 2, Situation 3). Therefore, the total C/DE separation load is $l_C=0.2150+0.1833=0.3983$ (Eq. 46).

Table 4. Segregation Fractions of Example 3

$y_{i,j}$	Product j			
A	0.2188	0.3125	0.1563	0.3125
B	0.5000	0.1875	0.3125	0.0000
C	0.1500	0.2500	0.3000	0.3000
D	0.3600	0.2000	0.2800	0.1600
E	0.3333	0.1667	0.1250	0.3750

Table 5. Product Separation Vectors and Difficulty Indices of Example 3

$p_{i,r}$	Product r				D_i	$(l_i)_{min}$
A/B	−0.2813	0.1250	−0.1563	0.3125	0.5	0.4375
B/C	0.3500	−0.0625	0.0125	−0.3000	1.0	0.3625
C/D	−0.2100	0.0500	0.0200	0.1400	0.4	0.2100
D/E	0.0267	0.0333	0.1550	−0.2150	0.6	0.2150

- For the B/CDE separation load, one needs to examine $\{p_{s,r},\ s=B,\ C,\ D\}$, since the next C/DE separation is not the last separation of the sequence:

B/C	$p_{B,r}$	0.3500	−0.0625	0.0125	−0.3000
C/D	$p_{C,r}$	−0.2100	0.0500	0.0200	0.1400
D/E	$p_{D,r}$	0.0267	0.0333	0.1550	−0.2150
extra load	$el_{B,r}$		0.0000		0.1600
Rule			2.2		2.3

Product 2 and 4 may need extra separation loads because their product vector elements are negative. For Product 2, one needs to consider all three components since there is only one sign change from B to D. According to Rule 2, Situation 2, no extra load is needed because $(\Sigma_{i=D}^{B}p_{i,2})p_{B,2}<0$. For Product 4, one needs to consider only $p_{B,4}$ and $p_{C,4}$ since there are two sign changes from B to D. The amount of extra load according to Rule 2, Situation 3 is $el_{B,4}=0.16$. The B/CDE separation load is 0.5583.

- For the A/BCDE separation load, one needs to examine $\{p_{s,r},\ s=A,\ B,\ C,\ D\}$, for the same reason stated above for B/CDE separation.

A/B	$p_{A,r}$	−0.2813	0.1250	−0.1563	0.3125
B/C	$p_{B,r}$	0.3500	−0.0625	0.0125	−0.3000
C/D	$p_{C,r}$	−0.2100	0.0500	0.0200	0.1400
D/E	$p_{D,r}$	0.0267	0.0333	0.1550	−0.2150
extra load	$el_{A,r}$	0.0000		0.0000	
Rule		2.2		2.2	

Only products 1 and 3 may need extra separation because their A/B vector elements are negative. Since $(p_{A,1}+p_{B,1})<0$ and $(\Sigma_{i=D}^{A}p_{i,3})p_{A,3}<0$, no additional A/BCDE separation is needed for either product. The A/BCDE separation load is also 0.5583.

The following summarizes the loads of the maximum-bypass ADBC sequence:

- The last C/D separation load according to Rule 1 is $l_C=(l_C)_{min}=0.2100$.
- For the remaining separation loads of the sequence (underlined are the pertinent products):

A/B	$p_{A,r}$	$\underline{-0.2813}$	0.1250	$\underline{-0.1563}$	0.3125
B/C	$p_{B,r}$	0.3500	$\underline{-0.0625}$	0.0125	$\underline{-0.3000}$
C/D	$p_{C,r}$	−0.2100	0.0500	0.0200	0.1400
D/E	$p_{D,r}$	$\underline{0.0267}$	$\underline{0.0333}$	$\underline{0.1550}$	−0.2150
extra load	$el_{B,r}$		0.0125		0.1600
Rule			2.3		2.3
		$el_B=0.1725$		$l_B=0.3825$	

Table 6. Separation Loads of Maximum Bypass Sequences*

Sequence	A/B	B/C	C/D	D/E	Total Load
ABCD	0.5583 (65.32)	0.5583 (47.46)	0.3983 (27.48)	0.2150 (10.54)	150.80
ABDC	0.5583 (65.32)	0.5583 (47.46)	0.2100 (9.45)	0.3983 (27.48)	149.71
ACBD	0.5583 (65.32)	0.3625 (13.05)	0.5583 (47.46)	0.2150 (10.54)	136.47
ADBC	0.5583 (65.32)	0.3825 (23.33)	0.2100 (9.45)	0.5583 (47.46)	145.56
ADCB	0.5583 (65.32)	0.3625 (13.05)	0.3825 (23.33)	0.5583 (47.46)	149.16
BACD	0.4375 (21.00)	0.5583 (65.32)	0.3983 (27.48)	0.2150 (10.54)	124.34
BADC	0.4375 (21.00)	0.5583 (65.32)	0.2100 (9.45)	0.3983 (27.48)	123.25
CDAB	0.5062 (34.43)	0.3625 (13.05)	0.5583 (65.43)	0.2150 (10.54)	123.45
CDBA	0.4375 (21.00)	0.5062 (34.43)	0.5583 (65.32)	0.2150 (10.54)	131.29
DABC	0.5062 (47.08)	0.3825 (23.33)	0.2100 (9.45)	0.5583 (65.32)	145.18
DACB	0.5062 (47.08)	0.3625 (13.05)	0.3825 (23.33)	0.5583 (65.32)	148.78
DBCA	0.4375 (21.00)	0.5062 (47.09)	0.2100 (9.45)	0.5583 (65.32)	142.86
DCAB	0.5062 (34.43)	0.3625 (13.05)	0.5062 (47.09)	0.5583 (65.32)	159.89
DCBA	0.4375 (21.00)	0.5062 (34.43)	0.5062 (47.09)	0.5583 (65.32)	167.84

*Actual size in parenthesis.

extra load	$el_{D,r}$	0.0000	0.0208	0.1550
Rule		2.2	2.3	2.1
	$el_D = 0.1758$			$l_D = 0.5583$
extra load	$el_{A,r}$	0.0000		0.0000
Rule		2.2		2.2
	$el_A = 0.0000$			$l_A = 0.5583$

• The first A/BCDE separation load agrees with the value obtained by Rule 4.

The separation loads of the 14 maximum-bypass sequences are summarized in Table 6. The total separation loads of the BACD, BADC and CDAB sequences, whose total loads are 124.34, 123.24 and 123.45, respectively, are the lowest among all maximum-bypass sequences.

Optimal Sharp Sequence Synthesis with Modified Cost Measure

If all separation costs are equal, then the best sequence would be the one that bypasses the most and separates the least amount of the process streams. Usually, costs of different separations vary and the maximum-bypass sequence with the lowest total separation load is not always the optimal sequence. One has to select from among all maximum-bypass sequences the sequence that costs the least.

The precise knowledge of the normalized minimum loads of separators of any sequence can be used to choose the optimal sequence by evaluating the costs of all possible maximum-bypass sequences. A more practical selection procedure should not require an exhaustive enumeration of all possible sequences. We have discovered a better approach in place of the exhaustive enumeration procedure. This procedure selects the best sequence with the help of a modified cost measure that combines the separation costs and savings due to bypass into a single quantity.

Modified cost

For separations of equal cost, it is obvious that one should always choose the easiest, least pure separation. From another perspective, without precise knowledge of what the next separation may be, the best decision is to do an even split. Such a split will ensure the maximum reduction in subsequent separation loads irrespective of what the next separation may be.

The purification index can be combined with the cost forming a single measure that accounts for both the separation cost and the saving due to the reduction of subsequent separation loads. For the sharp separation between component i and component $i+1$ of a feed stream at a cost of D_i into two product streams, this modified cost measure is:

$$D_i' = (\text{cost of separation } i)\pi = \frac{D_i}{\sqrt{\theta_i(1-\theta_i)}} \tag{50}$$

where θ_i is the cut and D_i is the separation cost of separation i. The modified cost merges two predominant heuristics: *do the easiest separation first* and *prefer even split* into a single measure.

Synthesis procedure

It is proposed that among all possible separations, one should always choose the separation that *incurs the lowest modified cost*. The arrangement of separations into an optimal sequence should proceed in the direction of the sequence, since the separation loads decrease in the direction of the sequence.

The synthesis procedure is based on a modified cost table that lists all possible separations. The optimal sequence is determined by following an evolutionary search procedure:

(1) Select the separation of the original feed with the lowest modified cost to be the first separation. Among all possible separations of each stream produced by the first separation, select the one with the lowest cost as the second separation. Continue the selection process until all subsequent separations have been identified. The actual cost of the sequence is then evaluated according to its minimum separation loads.

(2) Identify a neighboring sequence by selecting the first separation to be the one with the second lowest modified cost. Subsequent separations are selected to be those with the lowest modified costs among their respective possible separations. This is a *breadth-first* search.

(3) Identify another neighboring sequence by selecting the second separation, that follows the lowest-cost first separation, to be the separation with the second lowest modified cost among all possible second separations. Subsequent separations are selected to be those with the lowest modified costs. This is a *depth-first* search.

(4) Evaluate the costs of the two neighboring sequences. If the costs of both sequences are higher than the sequence identified in step 1, the search ends.

(5) If a neighboring sequence has a lower cost, repeat the depth-first and the breadth-first searches of steps 2 to 4. Continue the search procedure until the optimal sequence is found.

The above synthesis procedure is illustrated by continuing the Example 3 in the previous section.

Example 3 (continued). The difficulty indices of separations are tabulated in Table 5. The cost function is linear. In addition to the fixed total cost of 23 for the four separators, the cost of each separation is proportional to its mass load and its difficulty indices, D_i:

$$J = 23 + \sum_{i=1}^{n} D_i L_i \tag{51}$$

It was determined earlier based on the sign distribution of the product separation matrix that only sequential separator arrangements should be used. The selection of the best sequence can be obtained by an inspection of the modified cost measures: $D_i/\sqrt{\theta_i(1-\theta_i)}$. The following is a tabulation of the modified costs of all possible separations and their feed sizes:

- For the feed (feed size = 1):

A/BCDE	AB/CDE	ABC/DE	ABCD/E
1.1217	2.0330	0.8108	1.4860

- Four components:

Feed size	0.7949	Feed size	0.7265
A/BCD	1.0525	B/CDE	2.5582
AB/CD	2.0010	BC/DE	0.8095
ABC/D	0.9002	BCD/E	1.3329

- Three components:

Feed size	0.5812	Feed size	0.5214	Feed size	0.5897
A/BC	1.0017	B/CD	2.2732	C/DE	0.8816
AB/C	2.1947	BC/D	0.8133	CD/E	1.2598

- Two components:

Feed size	0.4103	Feed size	0.3077	Feed size	0.3846	Feed size	0.4188
A/B	1.0607	B/C	2.0125	C/D	0.8050	D/E	1.2002

Of all separations of the feed, the first separation should be ABC/DE because this separation has the lowest modified cost. The subsequent separations are determined in an analogous manner. The best sequence is CDAB ($S_{C/D} \rightarrow \{\{S_{A/B} \rightarrow S_{B/C}\}, S_{D/E}\}$). The cost of processing a unit of feed according to the separation loads listed in Table 6 is 0.5360, excluding the fixed cost. Two neighboring sequences are identified. One sequence starts with the A/BCDE separation, which is the second lowest in modified cost, to be followed by separations with the lowest modified cost. This sequence is ACBD ($S_{A/B} \rightarrow S_{C/D} \rightarrow \{S_{B/C} \cdot S_{D/E}\}$) with a unit cost (excluding fixed cost) of 0.6069. Another sequence replaces the second separation of the first sequence with the next to the lowest in modified cost to be followed by separations with the lowest modified cost. This sequence is CDAB ($S_{C/D} \rightarrow \{\{S_{B/C} \rightarrow S_{A/B}\}, S_{D/E}\}$) with a unit cost of 0.6614. Clearly, the first CABD sequence is the best.

The flowsheet of CABD sequence is identical to that of the maximum-bypass sequence. The flowsheet can also be obtained by solving the linear programming problem with the following set of base vectors:

$$(s_1 s_2, \ldots, s_8) = \begin{pmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix} \tag{52}$$

The amount of separated stream k needed to produce product r, $m_{r,k}$ is determined by GAMS to be:

$$m_{r,k} = \begin{pmatrix} 0.069 & 0 & 0.350 & 0 & 0 & 0.183 & 0.027 & 0 \\ 0.125 & 0 & 0 & 0.062 & 0.021 & 0 & 0.033 & 0 \\ 0 & 0.144 & 0.012 & 0 & 0.031 & 0 & 0.155 & 0 \\ 0.312 & 0 & 0 & 0.300 & 0 & 0.160 & 0 & 0.215 \end{pmatrix} \tag{53}$$

The normalized separation duties of the four separators are:

$$l_A = 0.5062, \quad l_B = 0.3625, \quad l_C = 0.5583, \quad l_D = 0.2150 \tag{54}$$

The mass loads to the four separators are 65.32 to $S_{C/D}$, 34.43 to $S_{A/B}$, 13.05 to $S_{B/C}$, and 10.54 to $S_{D/E}$. The objective function value is 85.71 which is very close to 85.65, the only value reported by Wehe and Westerberg (1987) as the upper bound of the same sequence.

The objective function values of all maximum-bypass sequences were evaluated with GAMS, and the results are listed in Table 7 for comparison. The CABD sequence is superior to any of the other sequences. The modified cost not only can correctly select the best sequence but also correctly identify the neighboring sequences of the best sequence.

Limitations

The synthesis procedure does not account for a number of design options, such as mixing of intermediate process streams and recycle. The improvement resulting from increasing the degrees of freedom in design, in general, is small. Additional design options can be included in the same separation vector

Table 7. Separation Costs of Maximum Bypass Sequences

Sequence	Objective Function
ABCD	120.43
ABDC	123.38
ACBD	94.01
ADBC	111.24
ADCB	106.51
BACD	116.14
BADC	119.09
CDAB	85.71
CDBA	100.38
DABC	112.85
DACB	108.12
DBAC	123.56
DCAB	111.29
DCBA	129.96

formulation of the optimization problem. The option of internal blending of process streams as a feed to a subsequent separator can be included by expanding the separation basis. For example, the internal blending option can be included for the best CABD sequence by expanding the number of base vectors from 8 (Eq. 52) to 9:

$$(s_1 s_2, \ldots, s_8, s_9) = \begin{pmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \end{pmatrix} \quad (55)$$

The additional base vector s_9 accounts for the option of blending the bottom BC stream emerging from $S_{A/B}(s_2)$ with the top ABC stream of $S_{C/D}(s_5)$ as the feed to $S_{B/C}$. The B/C separator produces a bottom stream (s_4) and a top stream consisting of a certain combination of s_3 of s_9. A different flowsheet is obtained by solving the optimization problem with the expanded separation basis:

$$m_{r,k} = \begin{pmatrix} 0 & 0 & 0.281 & 0 & 0 & 0.183 & 0.027 & 0 & 0.069 \\ 0.125 & 0 & 0 & 0.062 & 0.021 & 0 & 0.033 & 0 & 0 \\ 0 & 0.144 & 0.012 & 0 & 0.031 & 0 & 0.155 & 0 & 0 \\ 0.312 & 0 & 0 & 0.300 & 0 & 0.160 & 0 & 0.215 & 0 \end{pmatrix} \quad (56)$$

The internal blending option reduces the mass load to $S_{A/B}$ from 34.43 ($\Sigma_r m_{r,1} = 0.506$ of ABC according to Eq. 53) to 29.72 ($\Sigma_r m_{r,1} = 0.437$ of ABC according to Eq. 56). At the same time, the mass load of $S_{B/C}$ is increased from 13.05 ($\Sigma_r m_{r,3} = 0.362$ of BC according to Eq. 53) to 15.24 by blending 0.069 ($= \Sigma_r m_{r,9}$ according to Eq. 56) of ABC from $S_{C/D}$ and 0.293 ($= \Sigma_r m_{r,3}$ according to Eq. 56) of BC from $S_{A/B}$. The objective function value is reduced from 85.71 to 85.57, a savings of less than 1%.

Conclusions

A new concept of representing separation by separation vectors in the separation space is developed. All operators in a separation sequence, that is, the separation of a stream and the division and the combination of streams, have their respective vectorial representations. The maximum-bypass sequences of a separation problem are easily obtained with the new representation. A set of simple rules has been developed that can be used to determine the separation loads of any maximum-bypass sequences by inspection.

Every sequence is represented by a unique set of separation base vectors that forms the separation basis of the sequence. The product set is constructed from these base vectors. This representation leads to a more efficient mathematical programming formulation for the synthesis of optimal multicomponent separation sequences. The optimal flowsheet of a given sequence is readily obtainable as the solution of an optimization problem that minimizes the cost subject to a set of *linear* constraints.

A modified cost that combines the cost factor with the savings of stream bypass is introduced. This cost measure can be used as a guide to select the best sequence without an exhaustive evaluation of the costs of all possible sequences. A simple procedure consisting of two steps: the identification of a best sequence followed by a brief examination of its neighboring sequences will determine the optimal sequence.

Three examples taken from the literature were used to illustrate the new synthesis procedure. Optimal sequences can be identified by inspection with the new procedure, in contrast to previous more complicated synthesis methods that require sophisticated mathematical programming methods.

Acknowledgment

The author wishes to acknowledge Professor Amy Ciric for many helpful discussions, especially on the use of GAMS software. Financial support from the National Science Foundation is gratefully acknowledged.

Notation

C_i = cost coefficient, or cost function of separator i
D_i' = modified cost of separation i
$el_{i,r}$ = extra load of separation i for product r
el_i = total extra load of separation i
f_i = normalized feed stream size for separation i
l_i = normalized mass load of separator i
m = number of streams
n = number of components
n_k = number of separation base vectors
p_r = separation vector of product r
$p_{i,r}$ = extent separation between components i and $i+1$ of Product r
s_k = k-th separation basis of a sequence
$s_{i,k}$ = extent of separation between components i and $i+1$ of the kth separation basis of a sequence
$x_{i,r}$ = mole (or mass) fraction of component i in stream r
$z_{i,r}$ = extent of separation between components i and $i+1$ in stream r

Greek letters

η_r = separation index of stream r
π = overall purification index
π_r = purification index of stream r

Literature Cited

Bamopoulos, G., R. Nath, and R. L. Motard, "Heuristic Synthesis of Nonsharp Separation Sequences," *AIChE J.*, **34**, 763 (1988).

Brooke, A., D. Kendrick, and A. Meeraus, *GAMS, A User's Guide*, The Scientific Press, Redwood City, CA (1988).

Chen, Y.-M., Y. W. Huang, and L. T. Fan, "An Approximating Formula for Evaluating the Number of Possible Schemes of 1FmP Separation Problems," *Sep. Technol.*, **1**, 222 (1991).

Floudas, C. A., "Separation Synthesis of Multicomponent Feed Streams into Multicomponent Product Streams," *AIChE J.*, **33**, 540 (1987).

Floudas, C. A., and S. H. Anastasiadis, "Synthesis of Distillation Sequences with Several Multicomponent Feed and Product Streams," *Chem. Eng. Sci.*, **43**, 2407 (1988).

Kao, Y. K., "Separation Vector: A New Method to Represent and Measure Separation," *Chem. Eng. Comm.*, **118**, 279 (1992).

King, C. J., *Separation Processes*, McGraw-Hill, New York, p. 90 (1980).

Lu, M. D., and R. L. Motard, "A Strategy for the Synthesis of Separation Sequence," *AIChE Symp. Ser.*, No. 74 (1982).

Malone, M. F., K. Glinos, F. E. Marquez, and J. M. Douglass, "Simple, Analytical Criteria for the Sequencing of Distillation Columns," *AIChE J.*, **31**, 683 (1985).

Muraki, M., and T. Hayakawa, "Separation Process Synthesis for Multicomponent Products," *J. Chem. Eng. Jpn.*, **17**, 533 (1984).

Muraki, M., K. Kataoka, and T. Hayakawa, "Evolutionary Synthesis of a Multicomponent Multiproduct Separation Process," *Chem. Eng. Sci.*, **41**, 1843 (1986).

Muraki, M., and T. Hayakawa, "Synthesis of a Multicomponent Multiproduct Separation Process with Nonsharp Separators," *Chem. Eng. Sci.*, **43**, 259 (1988).

Nadgir, V. M., and Y. A. Liu, "Studies in Chemical Process Design and Synthesis: V. A Simple Heuristic Method for Systematic Synthesis of Initial Sequences for Multicomponent Separations," *AIChE J.*, **29**, 926 (1983).

Nath, R., "Studies in the Synthesis of Separation Sequences," PhD Diss., Univ. of Houston (1977).

Nath, R., and R. L. Motard, "Evolutionary Synthesis of Separation Process," *AIChE J.*, **27**, 578 (1981).

Nishida, N., G. Stephanopoulos, and A. W. Westerberg, "A Review of Process Synthesis," *AIChE J.*, **27**, 321 (1981).

Rony, P. R., "The Extent of Separation: On the Unification or the Field of Chemical Separations," *AIChE Symp. Ser.* No. 120, pp. 68 and 89 (1972).

Thompson, R. W., and C. J. King, "Systematic Synthesis of Separation Schemes," *AIChE J.*, **18**, 941 (1972).

Wehe, R. R., and A. W. Westerberg, "An Algorithmic Procedure for the Synthesis of Distillation Sequences with Bypass," *Comput. Chem. Eng.*, **11**, 619 (1987).

Appendix: General Formula of Transformation from y_{ir} to z_{ir}

For the general case of n-component mixture, the transformation y_r to z_r is defined by the following equation:

$$\begin{pmatrix} 1 & -1 & 0 & 0 & \cdots & \cdots \\ 0 & 1 & -1 & 0 & \cdots & \cdots \\ 0 & 0 & 1 & -1 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \ddots & \cdots \\ -1 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_{1r} \\ y_{2r} \\ y_{3r} \\ \vdots \\ y_{nr} \end{pmatrix} = \begin{pmatrix} z_{1r} \\ z_{2r} \\ z_{3r} \\ \vdots \\ z_{nr} \end{pmatrix} \tag{57}$$

Since only $(n-1)$ of the z_{ir}s are independent, z_{nr} can be eliminated to yield the following equation:

$$\begin{pmatrix} 1 & -1 & 0 & 0 & \cdots & \cdots \\ 0 & 1 & -1 & 0 & \cdots & \cdots \\ 0 & 0 & 1 & -1 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \ddots & \cdots \\ 1 & 1 & 1 & 1 & \cdots & 2 \end{pmatrix} \begin{pmatrix} y_{1r} \\ y_{2r} \\ y_{3r} \\ \vdots \\ y_{n-1,r} \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \Sigma_{i=1}^{n} y_{ir} \end{pmatrix} = \begin{pmatrix} z_{1r} \\ z_{2r} \\ z_{3r} \\ \vdots \\ z_{n-1,r} \end{pmatrix} \tag{58}$$

or in matrix notation:

$$A y_r - b_r = z_r \tag{59}$$

The matrix A represents the transformation from y_r to z_r. The invariance of this transformation is maintained by requiring the metric tensor of the z-coordinate system to change contragradiently with the above transformation of variables. The metric tensor is thus transformed from the y-manifold to the z-manifold, according to the following equation:

$$g_{z_{ij}} = \sum_{k=1}^{n-1} \sum_{l=1}^{n-1} b^{ki} b^{lj} g_{kl} \tag{60}$$

where b^{ij}'s are the entries of A^{-1}, the contragradient transformation of A. For simplicity, let the new metric tensor also be designated by g_{ij}:

$$g_{ij} = \frac{i(n-j)}{n}, \quad \text{for } i \leq j; \quad g_{ij} = g_{ji}, \quad \text{for } i > j \tag{61}$$

The invariance of the above transformation is confirmed by the fact that the distance between two streams, y_r and y_s,

$$\sigma(y_r - y_s) = \sqrt{\sum_{i=1}^{n-1} \sum_{j=1}^{n-1} g_{y_{ij}} (y_{ir} - y_{is})(y_{jr} - y_{js})} \tag{62}$$

can also be computed by the length of the vector, $\Sigma_{q=r}^{s-1} z_q$:

$$\sigma(y_r - y_s) = \sqrt{\sum_{i=1}^{n-1} \sum_{j=1}^{n-1} g_{z_{ij}} \left(\sum_{q=r}^{s-1} z_{iq}\right) \left(\sum_{q=r}^{s-1} z_{jq}\right)} \tag{63}$$

which remains unchanged after the transformation.

Manuscript received May 4, 1993, and revision received Feb. 14, 1994.