Separation Synthesis of Multicomponent Feed Streams into Multicomponent Product Streams

The synthesis problem of separation sequences that separate several multicomponent feed streams into several desired multicomponent product streams is addressed. A superstructure is proposed for this separation problem that has embedded all the alternative separation configurations of interest. This superstructure, which has as separator units the separation tasks that are defined for each separation breakpoint, involves options for series and/or parallel sequences, as well as stream splitting, mixing, and bypassing. Formulating and solving this superstructure as a nonlinear programming problem that has as unknowns the stream interconnections, results in an optimal separation sequence. This sequence, which may involve fewer separator units than those included in the superstructure, is shown to be a realistic and practical one. The synthesis approach is illustrated with four example problems.

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Introduction

Multicomponent separation sequences are an important part of almost all chemical processing systems. As Hlavacek (1978) pointed out, such separation systems result from a need for feed preparation, product separation, product finishing, and waste treatment. Because of the significant role that separation processes play in the total capital investment and annual operating cost for a chemical plant, a great deal of interest has been generated in the development of systematic approaches that will select optimum separation sequences.

Multicomponent separation processes can be classified into the following two categories:

P1. Separation of a single multicomponent feed stream into product streams that are pure substances

P2. Separation of several multicomponent feed streams into several specified multicomponent product streams

Separation problem P1 involves product streams each of which contains a single species, and the objective of this problem is to determine an optimal separation sequence that separates a given multicomponent feed stream into pure-component product streams. Over the last two decades, various approaches have been proposed to search for the optimal separation sequence among many potential candidates. The approaches can be divided into three main groups:

1. Heuristic methods that use rules of thumb based on engineering experience and the insights in the physics and chemistry of the separation methods
2. Evolutionary strategies that attempt to identify the best separation scheme via a sequence of evolutionary improvements
3. Algorithmic approaches that utilize various optimization tools developed in the area of mathematical programming.

A very good review of the synthesis approaches for problem P1 is provided by Nishida et al. (1981).

It is interesting to note that although great attention has been directed toward solving problem P1, there has been much less systematic study of problem P2, which is the general separation problem. Rudd et al. (1973) studied the separation synthesis problem P2 in order to reduce the separation mass load in areas such as aviation and motor oil production where it is quite common to blend hydrocarbons from a variety of sources to meet octane and flash point specifications. Blending operations of this sort can result in substantial savings since species separation that might be required to upgrade the fuel source to meet specific multicomponent product requirements can be avoided. The authors developed a heuristic approach for the synthesis of multicomponent separation sequences, as part of a general strategy that synthesized alternative flowsheets in an adaptive manner. Gary and Handwerk (1984) indicated that increased operating flexibility and profits result when refinery operations produce basic intermediate streams that can be blended to produce a variety of on-specification finished products, and provided a number of applications that involve multicomponent product streams. Mahalec and Motard (1977a,b) proposed the BALTAZAR procedure for the synthesis of entire chemical processes using heuristics. In this procedure, alternative separation sequences are developed to bridge the discrepancy between the multicomponent streams encountered at certain parts of the flowsheet and potential multicomponent product streams required by design specifications. Despite the insights that are provided by these approaches, they do not appear to yield the desired quality of solution. It is apparent that due to many complications involved in problem P2 there has not been developed a synthesis approach that can tackle the problem in an efficient and rigorous manner.

Nath (1977) presented a case study of a subproblem of P2, that is the separation of a single multicomponent feed stream into two multicomponent products, which we will consider as problem P3. In this case study two structures are determined directly by the use of several heuristic rules that are case-study dependent, and it is not clear how to extend this method to cases where the number of species in a product is more than three. Muraki and Hayakawa (1984) performed an investigation of problem P3 and developed a two-stage synthesis approach. In the first stage a search for the optimal separation sequence takes place, while in the second stage optimization of the separation process by introduction of division and blending is performed. These two stages are repeated until the optimal separation process is synthesized. For the first stage, they used the evolutionary strategy (Seader and Westerberg, 1977; Stephanopoulos and Westerberg, 1976) that was developed for the synthesis of the separation sequence of one-component products. For the second stage, they developed a new evolutionary method in which the material allocation diagram (MAD) (Nath, 1977) is used to reduce the separation mass load. They took advantage of the fact that the MAD shows the separation process graphically, and obtained useful information on the possible flow rate of each species at each separation breakpoint and the feasibility of the modified separation process. Their approach, however, utilizes evolutionary strategies that may require considerable trial and error effort, and it is restricted to problem P3, which is a subproblem of P2, without making clear how it can be extended toward solving the general separation problem with several multicomponent feed streams and product streams.

In this paper, a synthesis procedure based upon a mathematical programming approach is presented for the separation of several multicomponent feed streams into several multicomponent product streams. The basic idea in the proposed synthesis approach is to derive a superstructure that has embedded all possible configurations of separation sequences and all possible options of splitting and mixing of the streams. The optimal separation sequence that can separate multiple feeds into several multicomponent products is generated by minimizing an objective function expressed in terms of the separation load and the difficulty of separation through a nonlinear programming formulation for the proposed superstructure. The effectiveness of this synthesis approach is illustrated with four example problems.

Problem Statement

The problem to be addressed in this paper can be stated as follows: Given a set of multicomponent feed streams of known conditions (i.e., composition, flow rate, temperature, pressure), synthesize a separation sequence that can separate the feed streams into several multicomponent product streams of known conditions with a minimum venture cost, which is, in general, calculated from the design data, equations, and cost data peculiar to the separation method. Thus,

$$\min_{J,D} \sum_{j} C_j(d_j) \tag{1}$$

where $j \in J$ denotes a separation unit in a feasible sequence; C_j is the total annual venture cost of separator j; J is a subset of S; S is the set of all possible separator configurations that can produce the desired products; d_j are the design variables of separator j; and D is the union of d_j.

The purpose of this study is to develop a synthesis approach that is not dependent on the separation method and the objective function of each method. To simplify the solution, the following objective function is used in this paper:

$$\min_{f_n^k} \sum_{j=1}^{NS} \left[\left(\sum_{k=1}^{NFS} f_n^k\right) \cdot D_j\right]^b \tag{2}$$

where f_n^k is the flow rate of the inlet stream to each separator unit j that corresponds to feed source k (i.e., separation mass load); D_j is the difficulty of the jth separation; NS is the number of different separation tasks; NFS is the number of multicomponent feed source streams involved; and b is a constant. Then, the separation sequence will be selected so as to minimize this objective function. The difficulty of separation task j, D_j, corresponds to the relative volatility or boiling temperature difference in the ideal case for having distillation as the separation task. If the separation method is known, it is natural to use as an objective function the one that is derived for this separation method. However, the effectiveness of the synthesis approach that is proposed in this paper is that it is not dependent on the separation method.

The basic assumptions that will be made for this synthesis problem are:

1. There exists only one separation method.
2. The physical properties of the components upon which the separation is based maintain the same order.
3. Separation is simple and involves perfect splits.
4. Heat integration among separators is not allowed.

The first assumption is desirable for process operation and process control purposes and reduces the number of separations as much as possible. The second assumption excludes possibilities of different order of the physical properties of the components. The third assumption indicates that in each separation task a single feed stream is separated into two products, which can be multicomponent, and that each component entering in the feed stream leaves in only one product. Therefore, the use of separators with multiple feeds and sidestreams as well as the use of sloppy splitters with a distribution of components in the product streams is not allowed. The fourth assumption excludes the possibility of heat-integrated separation sequences.

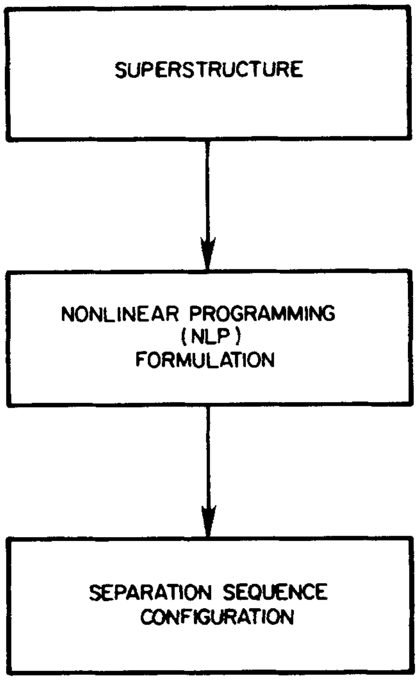

Figure 1. Outline of synthesis strategy.

Outline of Synthesis Strategy

As indicated in Figure 1, the suggested procedure for the synthesis of separation sequences for problem P2 consists of the following steps:

1. A superstructure is derived for each multicomponent feed stream that has as separators the required separation tasks according to the number of components that are involved (i.e., one separation task for each breakpoint). This superstructure contains unknown stream connections that may determine series and/or parallel arrangement, stream splitting, stream mixing, and stream bypassing. Then, the overall superstructure is considered to be the aggregate of all the feed stream superstructures.
2. The overall superstructure is formulated as a nonlinear programming (NLP) problem that has as its objective Eq. 2 and as constraints the mass balances applied to each superstructure.
3. The solution to the NLP problem of step 2 will provide the optimal separation sequence, the flow rates of the corresponding streams, and the compositions of the components for each stream.

It will be shown that many streams in the superstructure will have the tendency of being deleted, which implies that the selected optimal separation sequence is not a complicated one.

Superstructure of Separation Problem P2

The important feature of the proposed overall superstructure is that it can be partitioned into a set of superstructures that correspond to each multicomponent feed stream. Each feed stream superstructure is derived in such a way that it has embedded all configurations of interest for the separation process. Thus, alternatives on separation sequences in series, parallel, series-parallel, parallel-series, and options on feed stream splitting, mixing, and bypassing are incorporated in each multicomponent feed stream superstructure.

To demonstrate how such a superstructure can be developed, suppose that there is one multicomponent feed stream with four components, *ABCD*, and there are three separation tasks $S1$, $S2$, $S3$ at the breakpoints between A and B, B and C, C and D, respectively. The objective is to separate this feed stream into three multicomponent specified products. One can then postulate a superstructure for the feed stream as shown in Figure 2,

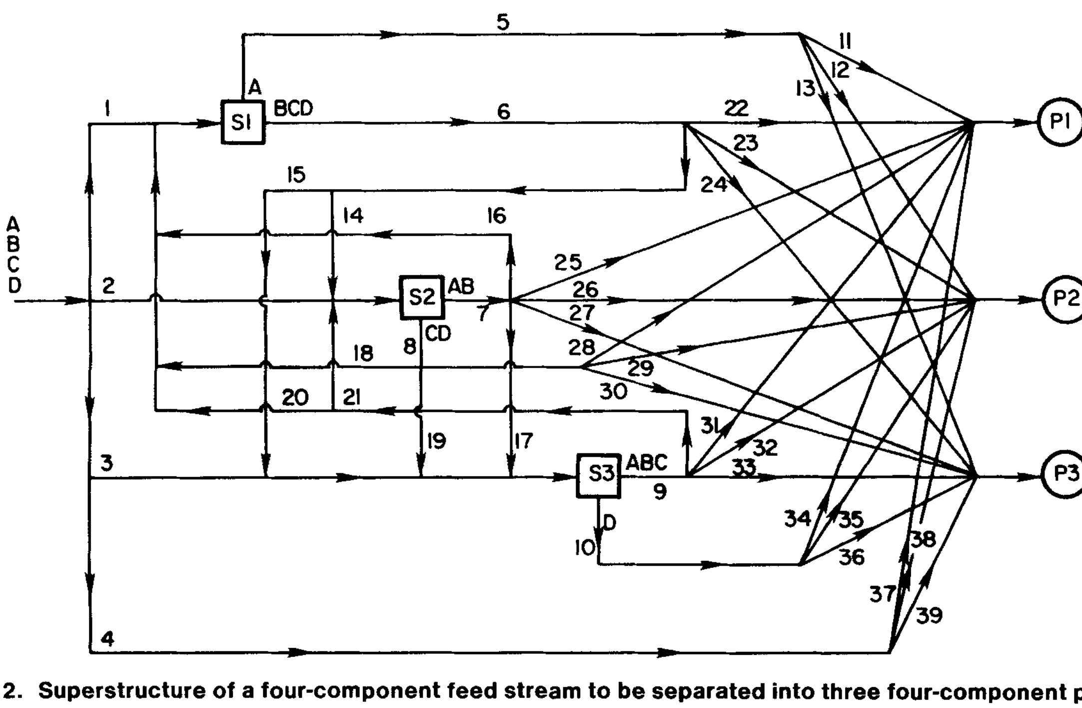

Figure 2. Superstructure of a four-component feed stream to be separated into three four-component products.

where the boxes indicate the separation tasks, and the circles the desired multicomponent products.

The basic elements in the derivation of the feed stream superstructure are the following:

1. Split the multicomponent feed stream into four streams, three of which are directed to the inlet of the separation tasks (streams 1, 2, and 3), while the fourth is considered as an overall bypass for the separation sequence (stream 4).

2. Split the outlet streams from each separation according to the following two conditions:

Condition A. If the product stream involves only one component then split that stream into 3 streams that are directed to the mixing points prior to the final multicomponent products (i.e., split stream 5 into streams 11, 12 and 13).

Condition B. If the product stream involves two or more components, split that stream into:

(a) Two streams that are mixed with the inlet streams of the other separation tasks (i.e., split stream 6 into streams 14 and 15).

(b) Three streams that are directed to the desired multicomponent products (i.e., split stream 6 into streams 22, 23 and 24).

3. Split the overall bypass stream (stream 4) into three streams directed to the desired products (streams 37, 38 and 39).

From the superstructure for the multicomponent feed stream shown in Figure 2, many serial and nonserial configurations can be verified by setting the flow rates of some of the internal streams to zero values. For instance, the following cases are some of the serial and nonserial alternatives:

- Separation sequence $S1$, $S2$, $S3$ in parallel results from setting $F14 = F15 = F16 = F17 = F18 = F19 = F20 = F21 = F4 = 0$.
- Separation sequence $S1$, $S2$, $S3$ in series results from setting $F4 = F15 = F2 = F3 = F16 = F17 = F18 = F20 = F21 = 0$.
- Separation sequence $S1$, $S2$ in parallel and then in series with $S3$ results from setting $F3 = F4 = F14 = F16 = F17 = F18 = F20 = F21 = 0$.
- Separation sequence $S1$ in series with $S2$, $S3$ in parallel and having a bypass results from setting $F2 = F3 = F16 = F17 = F18 = F19 = F20 = F21 = 0$.

Furthermore, this superstructure can easily be generalized for any number of separation tasks that is specified from the number of components of the feed stream. In particular, each multicomponent feed stream superstructure consists of:

1. An initial splitter of the feed stream
2. A splitter at each product stream of each separation task and a splitter at the overall bypass stream
3. A mixer at the inlet of each separation task
4. A mixer prior to each desired multicomponent product

It should be noted that mixing of the streams that belong to each feed stream superstructure is allowed at the mixers located prior to each separation task of the superstructure. The option of mixing the feed streams prior to any separation is not necessary to be included in the superstructure due to the fact that the objective function, Eq. 2, minimizes the summation of the inlet flow rates to each task that is determined from the separation breakpoints. As will be shown, the major advantage of the superstructure proposed in this paper is that it can be formulated as a nonlinear programming problem of managable size for extracting an optimal separation configuration of several multicomponent feed streams into several multicomponent products.

Mathematical Formulation

Having addressed the derivation of a superstructure for the separation problem P2 that has embedded all the alternative configurations of interest, a nonlinear programming formulation is presented for the optimum selection of the separation sequence.

To derive the mathematical formulation of the NLP problem, the following index sets will be defined to characterize the topology of the superstructure. First, all the feed streams will be denoted by the common index set

$$FS = \{k\} \tag{3}$$

The components will be denoted by the index set $I = \{i\}$, and the separation tasks by the index set $J = \{j\}$. The superstructure for each feed stream $k \in FS$ involves a set of streams ℓ that will be denoted by the index set $N_k = \{\ell\}$. Each of these streams ℓ, will have associated as variables the flow rate f_ℓ^k and the composition of each component i, $x_{\ell i}^k$.

The superstructure of each feed stream k involves splitters and mixers that are denoted by the index sets $S_k = \{s\}$ and $M_k = \{m\}$, respectively. The splitter $s^o \in S_k$ will represent the initial splitting point in the feed stream superstructure k. The mixers $m^f \in M_k$ will stand for the final mixers prior to each product. The relation of the sets of splitters and mixers with the internal input and output streams in the feed stream superstructure k is provided by:

$$\left.\begin{aligned} S_k^{in}(s) &= \{\ell \mid \ell \in N_k \text{ is an inlet to splitter } s\} \\ S_k^{out}(s) &= \{\ell \mid \ell \in N_k \text{ is an outlet from splitter } s\} \end{aligned}\right\} s \in S_k$$

$$\left.\begin{aligned} M_k^{in}(m) &= \{m \mid m \in N_k \text{ is an inlet to mixer } m\} \\ M_k^{out}(m) &= \{m \mid m \in N_k \text{ is an outlet from mixer } m\} \end{aligned}\right\} m \in M_k \tag{4}$$

The inlet and outlet streams of the separation units are given by:

$$\begin{aligned} SU_j &= \{n \mid n \in N_k \text{ is the inlet to separator unit } j\} \\ SU_j^{top} &= \{p \mid p \in N_k \text{ is the top product of separator unit } j\} \\ SU_j^{bot} &= \{q \mid q \in N_k \text{ is the bottom product of separator unit } j\} \end{aligned} \tag{5}$$

Also, the components of the top and bottom streams of each separation unit are given by:

$$\begin{aligned} T_j &= \{i \mid i \text{ component belongs to the top of separation } j\} \\ B_j &= \{i \mid i \text{ component belongs to the bottom of separation } j\} \end{aligned} \tag{6}$$

Having defined the index sets and variables that describe the overall superstructure for the separation problem P2, the con-

straints that apply are as follows:
Mass balances for splitters

$$\sum_{\ell \in S_k^{in}(s)} f_\ell^k - \sum_{\ell \in S_k^{out}(s)} f_\ell^k = 0 \quad s \in S_k \quad k \in FS \tag{7}$$

Mass balances for each component in mixers prior to separations

$$\sum_{\ell \in M_k^{in}(s)} f_\ell^k \cdot x_{\ell i}^k - \sum_{\ell \in M_k^{out}(m)} f_\ell^k \cdot x_{\ell i}^k = 0 \qquad m \in M_k \quad k \in FS, i \in I \tag{8}$$

Separation constraints for each component and separator j

$$f_n^k \cdot x_{n,i}^k - f_p^k x_{p,i}^k = 0 \quad i \in T_j, n \in SU_j, p \in SU_j^{top}$$
$$f_n^k \cdot x_{n,i}^k - f_q^k x_{q,i}^k = 0 \quad i \in B_j, n \in SU_j, q \in SU_j^{bot} \tag{9}$$

where f_n^k is the inlet stream flow rate, f_p^k is the top product flow rate, and f_q^k is the bottom product flow rate all in separator j.
Mass balances for each component in final mixers

$$\sum_{\ell \in M_k^{in}(m^f)} f_\ell^k \cdot x_{\ell_i}^k = C_{if} \quad m^f \in M_k, k \in FS, i \in I \tag{10}$$

where C_{if} is the desired quantity of component i in the final product f.
Specifications for flow rates

$$f_\ell^k = F_k \quad \ell \in S_k^{in}(s^\circ) \quad k \in FS \tag{11}$$

Equality of compositions for inlets and outlets of splits

$$X_{\ell i}^k = X_{pi}^k \quad \ell \in S_k^{in}(s), \quad p \in S_k^{out}(s), \qquad s \in S_k, \quad i \in T_j, \quad k \in FS$$
$$x_{\ell i}^k = x_{qi}^k \quad \ell \in S_k^{in}(s), \quad q \in S_k^{out}(s), \qquad s \in S_k, \quad i \in B_j, \quad k \in FS \tag{12}$$

Nonnegativity contraints

$$f_\ell^k \geq 0, \quad f_n^k \geq 0, \quad f_p^k \geq 0, \quad f_q^k \geq 0, \quad 1 \geq x_{\ell i}^k \geq 0 \tag{13}$$

In this way, the objective function in Eq. 2 subject to constraints in Eqs. 7 to 13 defines a nonlinear programming problem in which the variables to be optimized are the flow rates f_ℓ^k and the compositions $x_{\ell i}^k$. The numerical solution to the NLP problem can be obtained with standard algorithms. Two very good candidates of standard nonlinear programming algorithms are VMCON, which is an implementation of the Wilson-Han-Powell algorithm, and MINOS/AUGMENTED, which was developed by Murtagh and Saunders (1981) and employs a projected augmented Lagrangian algorithm. In this work, MINOS/AUGMENTED was used. The optimal solution of this NLP problem will provide automatically the separation sequence that can transform the multicomponent feed streams into the desired multicomponent products.

Remarks on the Mathematical Formulation

An important question that arises on the validity of the proposed NLP formulation is whether a practical separation configuration can result from the imposed overall superstructure. Clearly, if most of the postulated streams are not deleted (i.e., their flows set to zero), the separation configurations would be complicated and of questionable practical value. Interesting enough, however, the recycle streams that are directed toward the mixers prior to the inlet of each separation task will tend to take zero values for the flow rates, given that the mass balances in the final mixers prior to each product are satisfied. As shown in the Appendix, an increase of the flow rate of such a recycle stream results in an increase of the objective function. However, due to the minimization of the objective function, the flow rates of these recycle streams will take zero values. Hence, this proof implies that relatively simple separation sequence structures are to be expected using this approach, which is a very useful result from the practical viewpoint.

Another remark on the NLP formulation is that due to the bilinearities of flow rates and compositions present in Eqs. 8, 9, and 10, the problem is in general nonconvex. This may imply that a unique optimal solution cannot be guaranteed. Thus, the solution obtained can only be considered as a local minimum for the considered objective function. Recent work on general distillation sequences (Floudas and Anastasiadis, 1986) has shown that a very efficient initialization procedure can be developed for the nonlinear programming problem. This initialization procedure consists of solving a linear programming problem that corresponds to a selected superstructure of distillation sequences and provides very good initial points for the nonlinear programming algorithm.

The effectiveness of the proposed synthesis approach is illustrated with the following four example problems.

Example 1

This problem, taken from Mahalec and Motard (1977a), is a small problem and is selected to illustrate the synthesis approach. It consists of two multicomponent feed streams that are to be separated into three multicomponent products. The problem data are shown in Table 1. The first feed stream involves two components, A and B, while the second feed stream involves three components, A, B, and C. The first product features two components, A and C; the second product features three components, A, B, and C; and the third product features two components, A and B. For this problem all the difficulties of separation D_j are equal to one and the constant b is also equal to one.

Table 1. Data for Example 1

	Species			
	A %	B %	C %	Quantity
Feed stream 1	0.168	0.833	—	12
Feed stream 2	0.385	0.385	0.231	13
Product 1	0.5	—	0.5	2
Product 2	0.417	0.417	0.167	12
Product 3	0.091	0.909	—	11

$D_j = 1; j \in J; b = 1$

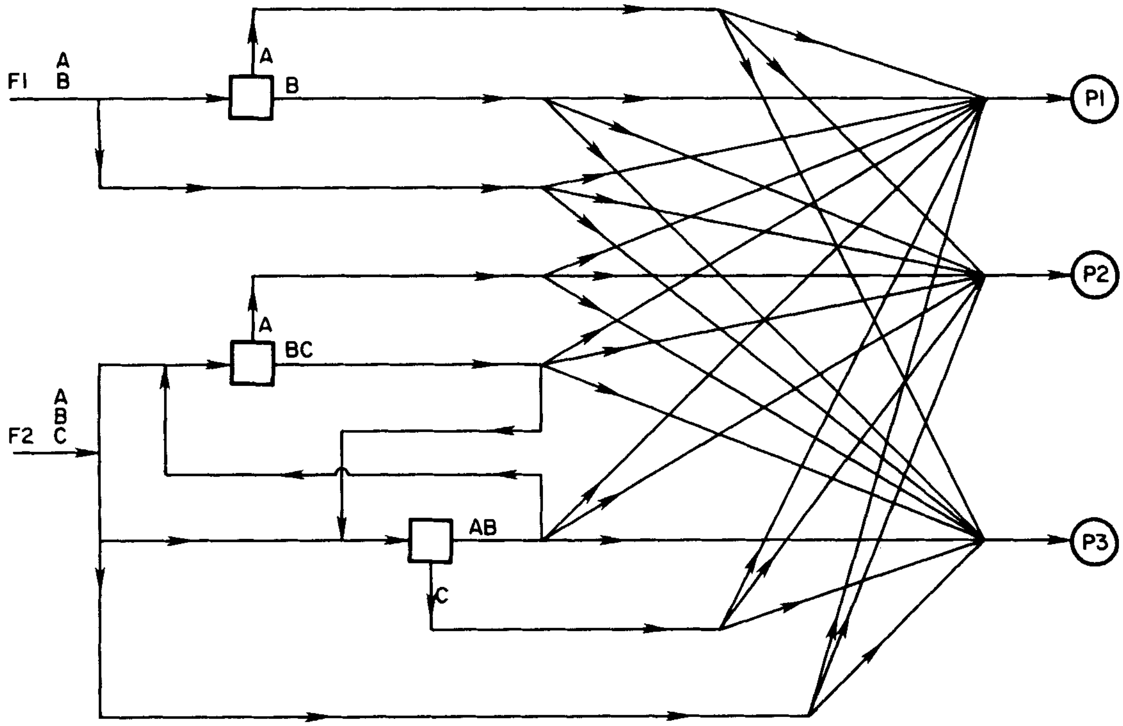

Figure 3. Superstructure of separation process for example 1.

Since there exist two separation tasks for the three-component feed stream and one separation task for the two-component feed stream, the superstructures for each multicomponent feed stream are developed according to the procedure described in a previous section and are shown in Figure 3. Having derived the overall superstructure for this separation process, mass balances are applied for each component at the splitters, mixers, and separation tasks. The resulting nonlinear programming problem involves 45 variables, 13 nonlinear constraints, and 19 linear constraints. The total CPU time (IBM 3081), for formulating the model and solving it using MINOS/AUGMENTED (Murtagh and Saunders, 1981) was 1.98 s.

The results of the optimization problem provide the separation sequence shown in Figure 4. This sequence features the minimum total separation mass load of 10.333 since in the objective function there is a minimization of the total separation mass load. Notice that there is a splitter at the first feed stream, which implies a bypass stream for the one separation task. Also,

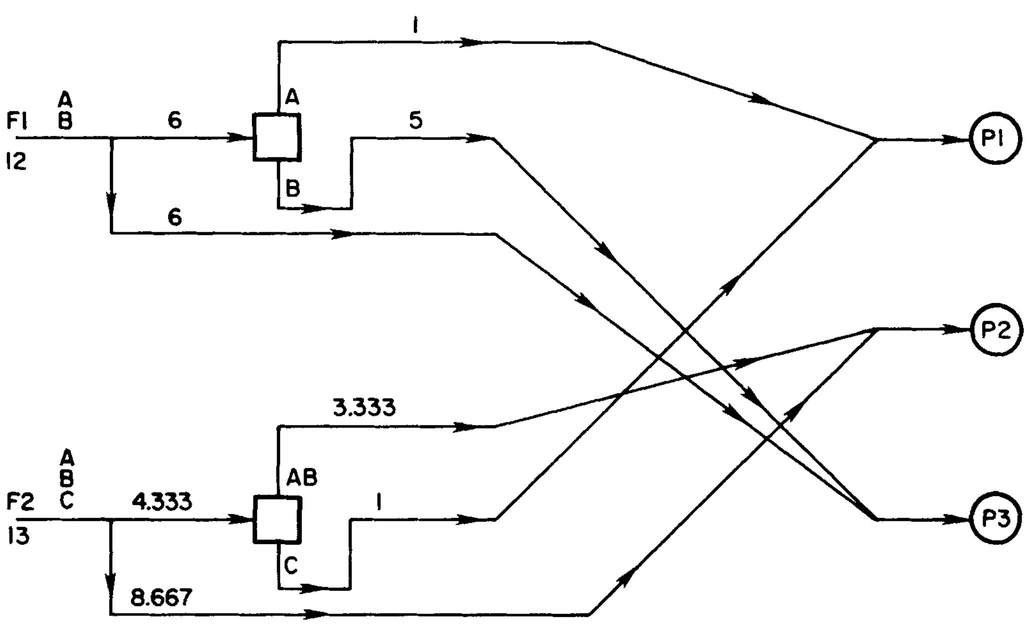

Figure 4. Optimal separation sequence for example 1.

there is an initial splitter at the second feed stream that splits the feed stream into one stream directed to one separator and one bypass stream. It is very interesting that this optimal solution does not utilize the other separation task provided in the superstructure. This is an important feature because it implies that not all of the initially considered separation tasks are required to be used and it can lead to substantial economic savings.

It should also be noted that the optimal separation sequence determined by this approach is the best sequence that Mahalec and Motard (1977a), Figure 8, found using their approach.

Example 2

This problem consists of one four-component feed stream that has to be separated into two four-component products. The problem data and the difficulties of separations D_j are shown in Table 2. For this problem the exponent b was assumed to take the value of 0.6.

In the first step, the superstructure for the single feed stream is developed using the previously described approach. This superstructure features three separation tasks since the feed stream involves four components and each separation task corresponds to a separation breakpoint of these components; it is shown in Figure 5. Formulating this superstructure as a nonlinear programming problem resulted in 33 variables, 16 nonlinear constraints, and 6 linear constraints. The total CPU time (IBM 3081) for formulating and solving this problem was 1.25 s.

Table 2. Data for Example 2

	Species A %	Species B %	Species C %	Species D %	Quantity
Feed stream	15	20	10	15	60
Product 1	5	10	4	10	29
Product 2	10	10	6	5	31

Difficulty of separation, D_j

	D_j
$S1$	2.5
$S2$	3.0
$S3$	1.5

$b = 0.6$

The results of the optimization problem provide the structure shown in Figure 6. This separation sequence features a minimum objective function of 18.578. Notice that in the optimal separation sequence shown in Figure 6, there exist three separation tasks that take place in a series sequence of $S3$-$S1$-$S2$, which is also the sequence of the lowest to the highest separation difficulty, with bypass stream at the outlet of separation task $S3$. Also, there is an initial splitter that splits the feed stream into one stream that is directed to separation $S3$ and into one overall bypass. There is also a splitter at the outlet of separation $S3$ that splits the outlet stream into one stream directed to separation $S1$ and one stream directed to the mixer prior to product $P2$.

Example 3

This example problem is a modified version of the second example; its problem data are provided in Table 3. The constant exponent b takes the value of 0.6.

Deriving and formulating the superstructure of this separation process as a nonlinear programming problem resulted in a problem of the same size as in example 2. The solution of this NLP problem provides the sequence shown in Figure 7. This sequence has a minimum objective function of 13.686. Notice that there is an initial splitter that splits the feed stream into one stream directed to separation task $S2$ and one overall bypass stream. The striking feature of this solution, however, is that it does not involve the separation task $S1$, even though this task was included in the superstructure shown in Figure 5. Therefore, as shown with this example problem, using the proposed synthe-

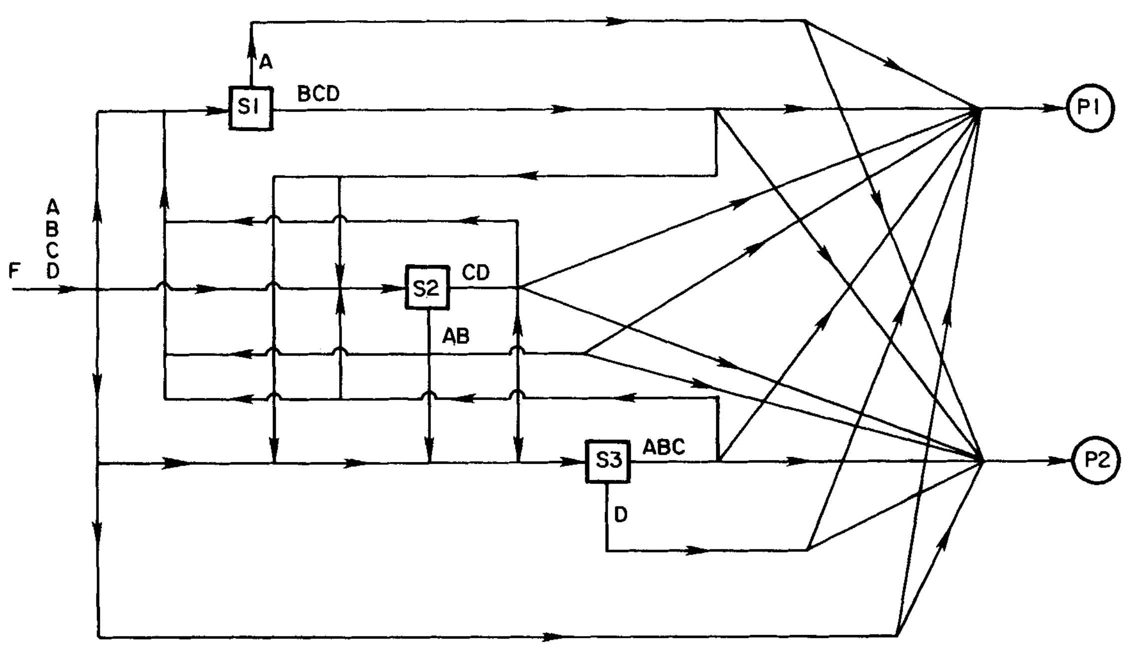

Figure 5. Superstructure of separation process for example 2.

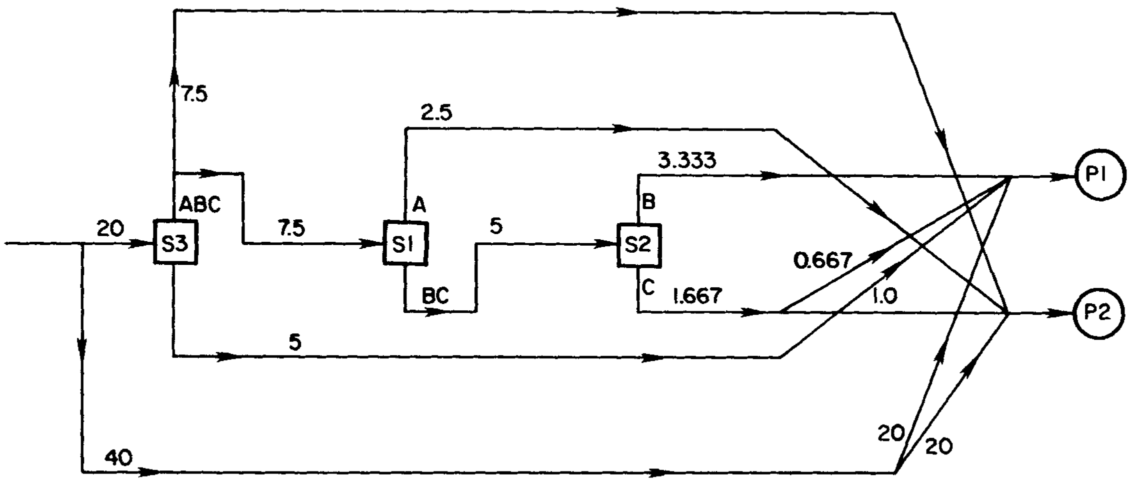

Figure 6. Optimal separation sequence for example 2.

sis approach optimal separation sequences can be identified that do not need to utilize all the separation tasks. This is a very important characteristic since it can lead to considerable economic savings.

Example 4

This problem, taken from Muraki and Hayakawa (1984), consists of a single five-component feed stream that has to be separated into two five-component product streams. The problem data and the difficulties of separations are shown in Table 4. The exponent b takes the value of 0.6.

Deriving the superstructure for this separation process as it was discussed in a previous section, and formulating it as a nonlinear programming problem resulted in 69 variables, 25 nonlinear constraints, and 22 linear constraints. The total CPU time (IBM 3081) for formulating and solving this problem was 3.8 s.

The solution of this NLP problem results in the separation

Table 3. Data for Example 3

	Species				
	A	B	C	D	Quantity
Feed stream	15	20	10	15	60
Product 1	7.5	10	4	10	31.5
Product 2	7.5	10	6	5	28.5

Difficulty of separation, D_j

	D_j
$S1$	2.5
$S2$	3.0
$S3$	1.2

$b = 0.6$

Table 4. Data for Example 4

	Species					
	A	B	C	D	E	Quantity
Feed stream	10	8	20	16	10	64
Product 1	2	2.4	16	8	1	29.4
Product 2	8	5.6	4	8	9	34.6

Difficulty of Separation D_j

	D_j
$S1$	1.2
$S2$	3.0
$S3$	2.5
$S4$	1.5

$b = 0.6$

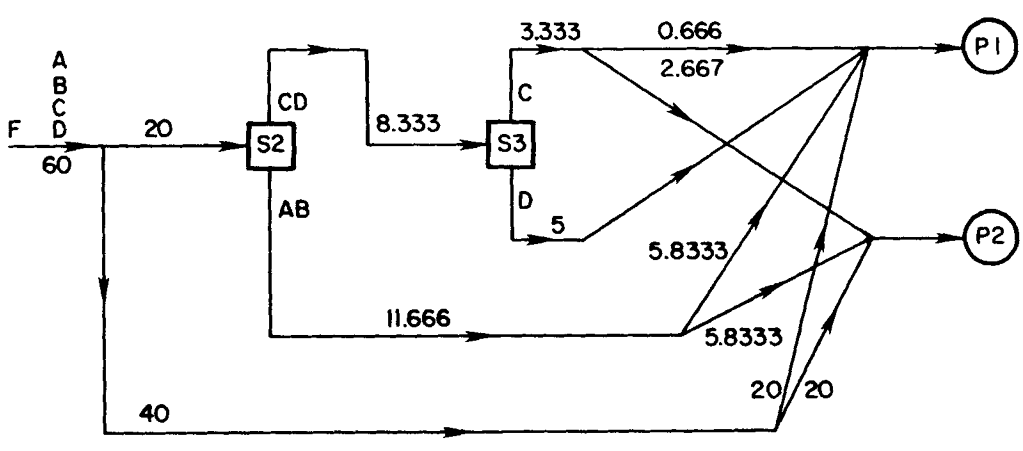

Figure 7. Optimal separation sequence for example 3.

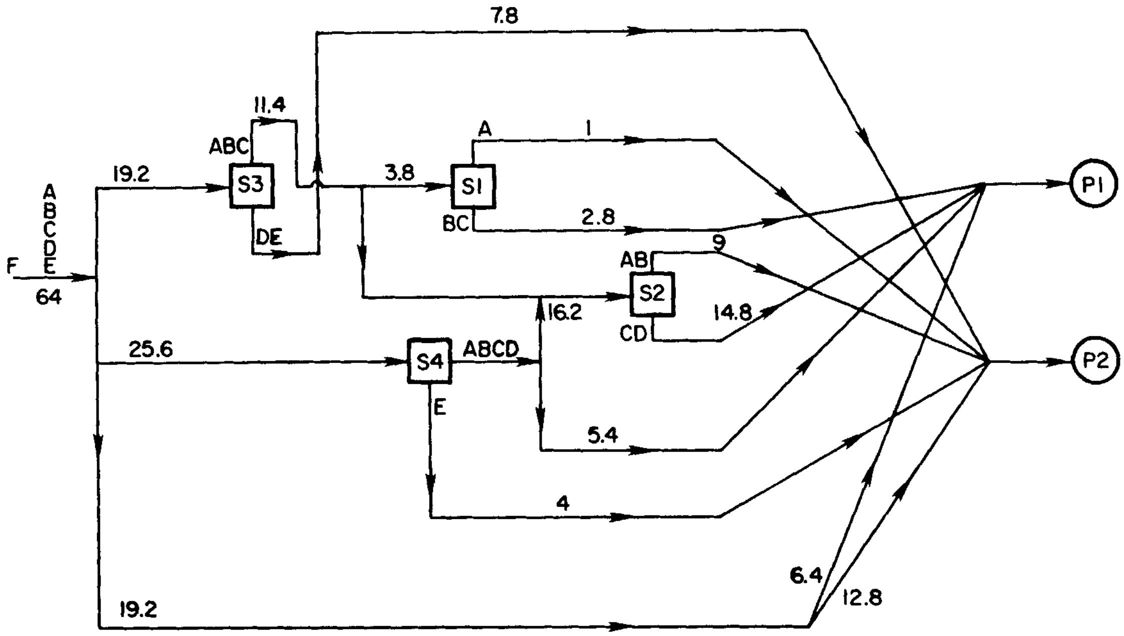

Figure 8. Optimal separation sequence for example 4.

configuration shown in Figure 8. This sequence features a minimum objective function of 34.562, which is slightly better than the best sequence of Muraki and Hayakawa (1984). Notice that there is an initial splitter of the feed stream into one bypass stream and two other streams that are directed to separation tasks $S3$ and $S4$. Also, there is a splitter at the top stream of the separation task $S4$ which splits the top stream into one stream that is directed to separation task $S2$. Also, at the splitter at the top stream of $S3$, one stream is directed to separation task $S1$ and one to separation task $S2$. In this example problem all the separation tasks are utilized at the optimum solution, which is slightly different than the one of Maraki and Hayakawa (1984). More important though, this solution is derived via an algorithmic approach in which the flow rates and compositions of the different streams are determined automatically.

Conclusions

The synthesis problem of separating several multicomponent feed streams into several multicomponent product streams has been considered. A synthesis approach has been proposed that is based upon a superstructure that has embedded alternatives for stream splitting, mixing, and bypassing. Optimizing this superstructure through a nonlinear programming formulation, separation sequences are derived that can transform several multicomponent feed streams into several desired multicomponent products.

The mathematical formulation of the superstructure features the important property that its solution can lead to practical separation configurations in which many of the implied stream connections in the proposed superstructure are reduced to zero flow rates and therefore are deleted. The significance of the approach presented in this paper is that it represents an efficient synthesis tool that is based upon mathematical programming techniques for the general separation problem P2.

The major drawback of this approach is that it is limited to finding solutions that involve sharp, noncomplex separators. These solutions, however, correspond to the least usage of sharp splits needed to produce the specified multicomponent products, and they provide very useful information on the separation tasks needed and the flow pattern. It is expected that appropriate use of that information will result in the development of a synthesis approach for general separation sequences that involve sharp and/or complex separators.

Notation

b = constant exponent
B_j = index set of components i of bottom product in separator j
C_{if} = quantity of component i in final product f
C_j = total annual venture cost of separation j
d_j = design variables of separator j
D = union of d_j
D_j = difficulty of separation j
f = index for final products
f_ℓ^k = flow rate of stream ℓ of feed stream superstructure k
f_n^k = flow rate of inlet stream to each separator j in feed stream superstructure k
f_p^k = flow rate of top product of separator j in feed stream superstructure k
f_q^k = flow rate of bottom product of separator j in feed stream superstructure k
FS = index set of feed streams
i = index for each component
I = index set of components
j = index for each separation
J = index set of separations
k = index for each feed stream superstructure
ℓ = index for streams
m = index for a mixer
M_k = index set of mixers of feed stream superstructure k
n = index for inlet streams of separation j
N_k = index set of streams that belong to feed stream superstructure k
NFS = number of multicomponent feed streams
NS = number of different separation tasks
P = index for top product of separation j
q = index for bottom product of separator j
s = index for a splitter
S = set of all separation configurations

S_k = index set of splitters of feed stream superstructure k
SU_j = index set of inlet streams to separator j
SU_j^{top} = index set of top product of separator j
SU_j^{bot} = index set of bottom product of separator j
T_j = index set of components i of top product of separator j
$X_{\ell i}^k$ = composition of component i at stream ℓ of feed stream superstructure k
X_{ni}^k = composition of component i at inlet stream of separator j in feed stream superstructure k
X_{pi}^k = composition of component i at top product of separator j in feed stream superstructure k
X_{qi}^k = composition of component i at bottom product of separator j in feed stream superstructure k

Appendix

In this appendix it will be shown that nonzero flow rates in the recycle streams of multicomponent feed stream superstructures will tend to result in an increase of the objective function. The proof will be restricted to a three-component feed stream superstructure that involves two multicomponent product streams and which is shown in Figure A1. In this figure, b_1 and b_2 stand for fractions assigned to each splitter after the two separation tasks denoted as $S1$, $S2$, and the recycle streams are indicated as F_1^R, F_2^R for separation tasks $S1$ and $S2$, respectively.

Proposition. The objective function of the NLP formulation increases monotonically with an increase of the fractions b_1 and b_2 of the flow rates of the recycle streams in the range [0, 1], given that the mass balances in the final mixers prior to the products are satisfied.

Proof. To express this statement mathematically, it has to be proved that:

$$\frac{\partial OBJ}{\partial b_1} > 0 \tag{A1}$$

$$\frac{\partial OBJ}{\partial b_2} > 0 \tag{A2}$$

for $b_1, b_2 \in [0, 1]$

For the superstructure of the three-component feed stream shown in Figure A1, the following mass balances are applied at the splitting and mixing points.

$$\left.\begin{aligned} F_0 &= F_1 + F_2 + F_3 \\ F_1 + F_2^R &= F_1^T + F_1^B \\ F_2 + F_1^R &= F_2^T + F_2^B \\ F_1^R &= b_1 F_1^B \\ F_2^R &= b_2 F_2^T \end{aligned}\right\} \tag{A3}$$

$$\left.\begin{aligned} F_1^e &= F_1 + b_2 F_2^T \\ F_2^e &= F_2 + b_1 F_1^B \end{aligned}\right\} \tag{A4}$$

where F_0 is the feed stream flow rate; F_1^T, F_1^B are the flow rates of the top and bottom, respectively, of the separation task $S1$; F_2^T, F_2^B are the flow rates of the top and bottom, respectively, of the separation task $S2$; and F_1^e, F_2^e are the inlet flow rates of separation task $S1$ and $S2$, respectively.

Solving the system of Eq. A3 for F_1^B, F_2^T the following expressions are obtained:

$$F_2^B = \frac{(F_1 - F_1^T) + b_2(F_2 - F_2^B)}{1 - b_1 b_2}$$

$$F_2^T = \frac{(F_2 - F_2^B) + b_1(F_1 - F_1^T)}{1 - b_1 b_2} \tag{A5}$$

The objective function for this superstructure will be of the following form:

$$OBJ = (F_1^e \cdot D_1)^b + (F_2^e \cdot D_2)^b \tag{A6}$$

where D_1, D_2 are the difficulties of separation for task $S1$ and $S2$, respectively, and b is a positive exponent constant.

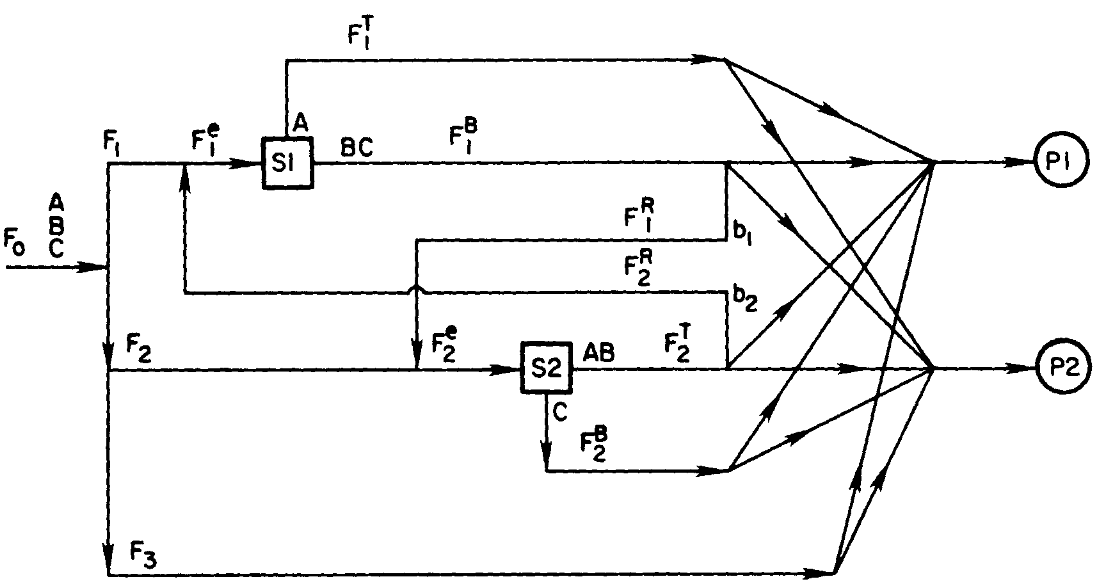

Figure A1. Superstructure of separation process in Appendix.

Then, calculating the expression given in Eq. A1 results in the following equations:

$$\frac{\partial OBJ}{\partial b_1} = b(F_1^e \cdot D_1)^{b-1} \cdot D_1 \cdot \left(\frac{\partial F_1^e}{\partial b_1}\right) + b(F_2^e \cdot D_2)^{b-1} \cdot D_2 \left(\frac{\partial F_2^e}{\partial b_1}\right) \quad (A7)$$

To show that Eq. A1 is valid, it remains to prove that

$$\left(\frac{\partial F_1^e}{\partial b_1}\right) > 0$$
$$\left(\frac{\partial F_2^e}{\partial b_1}\right) > 0$$
$$b_1, b_2 \in [0, 1]. \quad (A8)$$

But, from Eqs. A4 and A5, it is found that:

$$\frac{\partial F_1^e}{\partial b_1} = b_2 \cdot \frac{F_1^B}{1 - b_1 b_2}$$
$$\frac{\partial F_2^e}{\partial b_1} = \frac{F_1^B}{1 - b_1 b_2} \quad (A9)$$

Since $b_1, b_2 \in [0, 1]$ and F_1^B are positive, this implies that the inequalities of Eq. A8 are satisfied.

Similarily, it can be shown that $(\partial OBJ/\partial b_2) > 0$.

Therefore, given that the mass balances for each component at the final mixers prior to the products are satisfied, the flow rates of the recycle streams will tend to take zero values, which implies that they will be deleted, and simple separation sequences are to be expected.

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