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Algorithmic synthesis of an optimal separation network comprising separators of different classes

I. Heckl[a], Z. Kovács[a,b], F. Friedler[a,*], L.T. Fan[c], J. Liu[c]

[a] *Department of Computer Science, University of Pannonia, Veszprém, Hungary*
[b] *Department of Computer Science, University of Szeged, Szeged, Hungary*
[c] *Department of Chemical Engineering, Kansas State University, Manhattan, KS 66506, USA*

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Abstract

A novel class of separation-network synthesis (SNS) problems is examined, where the separators in the separation network can be affected by various separation methods subject to different constraints imposed on the product specifications. Such a class of SNS problems has been rapidly gaining importance for chemical processing in general and biochemical processing in particular. The available methods for SNS are not intended to address these problems; therefore, an efficient method is proposed here to amend this situation. The method composes algorithmically the necessary mathematical model of the super-structure on which the determination of an optimal separation network is based. The resultant mathematical model is linear, thus the proposed method renders it possible to generate the optimal solution without fail. The solution might serve as the lower bound for a separation network with a non-linear cost function. The uniqueness and efficacy of the proposed method are amply demonstrated by two examples of different complexities.

Keywords: Process synthesis; Separation; Super-structure; Mathematical; Modeling; Optimization

1. Introduction

The separation-network synthesis (SNS) is a major branch in the field of process synthesis. Its significance is obvious: separation processes and networks are ubiquitous throughout the chemical and allied industries where a sequence of separation tasks must be performed to produce the desired products. The energy demands of separation tasks are usually inordinately high; moreover, separators are often capital intensive. Thus, optimizing separation networks tends to substantially reduce the cost of production.

A separation network comprises separators, mixers, and dividers through which multi-component streams flow while being processed. The streams are distinguished according to their locations in the network; they can be the feed, intermediate and product streams. Various combinations of the separators, mixers, and dividers give rise to a multitude of networks, which differ from one another according to their intended purposes. The aim of a SNS problem is to configure a separation network for generating the desired products from the given feeds under the constraints imposed. A typical example is the crude oil separation in which a countless number of products are manufactured.

The known SNS methods almost always suppose that the available separators are of the same class. Some of these methods do not even specify the class of separators; they assume that only a single class of separators is available. For example, some methods solve a problem comprising exclusively rectifiers or a problem comprising exclusively extractors. Our aim is to develop a procedure that generates the optimal structure comprising both the rectifiers and extractors. Such a procedure might significantly reduce the cost, which is to be elaborated in the current work.

Numerous methods are available in the literature for solving various SNS problems. These methods can be categorized in terms of the configurations of initial structures, the mathematical-programming models adopted, the search techniques for solution, the cost functions of the models of the separators, and the reliabilities of the results. Nevertheless, the methods are mainly classified according to the search tech-

* Corresponding author. Tel.: +36 88 424483; fax: +36 88 428275.
E-mail address: friedler@dcs.vein.hu (F. Friedler).

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niques for solution; they can be heuristic, evolutionary, or algorithmic.

The essence of heuristic methods is to obtain a good solution structure through a sequence of decisions on the basis of engineering knowledge systematically acquired through experience. A heuristic method has been introduced in Ref. [1] for estimating the costs of different structures; the method renders it possible to reduce the search space for identifying at least near-optimal solutions. An optimization method enhanced by pinch technology, which is essentially heuristic in nature, has been presented in Ref. [2] to implement energy integration. A heuristic method has been proposed in Ref. [3] to take into account the energy consumption for the separation of three-component feeds.

An evolutionary method initiates the search from a plausible initial structure and reaches the optimal or near-optimal structure by sequentially improving it. A two-stage evolutionary method has been demonstrated in Ref. [4] for creating multi-component products. In the first stage, the optimal separation sequence is determined; in the second stage, the flow rates of streams through the optimal sequence are optimized.

Algorithmic methods provide systematic computational approaches to the solution of SNS problems. The synthesis of separation networks has been implemented in Ref. [5] for generating multi-component products in which only sharp separators are considered. A super-structure of the process network is proposed and the resultant model is solved with a standard NLP algorithm. A new method has been introduced in Ref. [6] to determine the global optimum of SNS problems with linear cost functions. A reformulation-linearization technique is applied to overcome the difficulties due to the presence of bilinear terms in the mathematical model. The notion of the rigorous super-structure has been presented in Ref. [7] for dealing with the same problem. Moreover, a novel algorithm for its generation has also been proposed. Consequently, this method is algorithmic in each of its steps.

The present work proposes a methodology for solving SNS problems involving various classes of candidate separators that perform separations effected by different mechanisms. Such mechanisms are naturally based on different physical or chemical properties of components in the mixture to be separated, e.g., volatility, solubility, permeability, absorptability and density. The incorporation of various classes of separators effected by different mechanisms or physical properties enlarges the search space, thereby increasing the possibility of generating a separation network far superior to that comprising a single class of separators. The current contribution introduces a novel algorithmic method for generating the super-structure and the associated mathematical-programming model for a class of SNS problems, which can be stated as follows.

Determine the cost-optimal separation network for transforming the compositions of n-component feed streams to obtain at most n-component product streams with a given set of simple and sharp separators based on various separation methods effected by different mechanisms. Any separator's cost is regarded as a linear function of its mass load. Note that it is not always necessary to define the products in terms of their exact compositions; instead, we can specify the products by various constraints imposed on their components, e.g., the sum of the components and the ratios of the components.

2. Features of separation networks

A separation network can be characterized by several key features. Some are attributable to the streams, and components in them to be separated, and others pertain to the devices performing the separation in the network.

2.1. Components, component orders, and streams

A stream is specified by a vector, termed stream vector, whose elements are the flow rates of the stream's components. The flow rates are usually ordered according to the property on which the separation is based. For example, if the separation is based on volatility, the first element of the stream vector is the amount of the most volatile component in the stream while the last element is the amount of the least volatile component. Suppose that the order of the elements in a stream vector is A, B, and C based on relative volatilities. Then, the vector $[8.0, 4.0, 3.0]^T$ kg/s implies that the flow rate of component A is 8.0 kg/s; that of component B, 4.0 kg/s; that of component C, 3.0 kg/s.

Situations often arise in which the separation of a stream can be carried out with various separators, based on separation methods effected by different mechanisms; this gives rise to their respective component orders. The component order of the stream vector must be given unambiguously to facilitate the representation of the corresponding stream.

Separation effected by the difference in relative volatility has long been ubiquitous in practice. Nevertheless, the implementation of methods of separation effected by the differences in other properties has been steadily gaining popularity in recent years because of their potential for leading to substantially energy saving and profound simplification in designing separation networks. For instance, the separation of a mixture comprising propylene (component A), propane (component B), and propadiene (component C) into its components can be carried out by three different classes of methods including distillation, extractive distillation with polar solvent, and extraction, see Ref. [8]. The component orders in the stream vectors are A, B, and C for the first method; B, A and C for the second method; C, A, and B for the third method.

For a separation network consisting of separators based on a single method of separation, none of the stream vectors can contain a null element, i.e., gap, unless some of the components are absent from one or more feed streams. According to the definition, a simple and sharp separator converts its input stream in such a way that the stream vector of the top output stream contains only those components from the first component through the light key component in the stream vector, and the bottom output stream contains those components from the heavy key component through the last component. This conversion is termed a cut between the light and heavy key components. Naturally, this transformation will not introduce a gap into any of the stream vectors of the output streams; see Fig. 1.

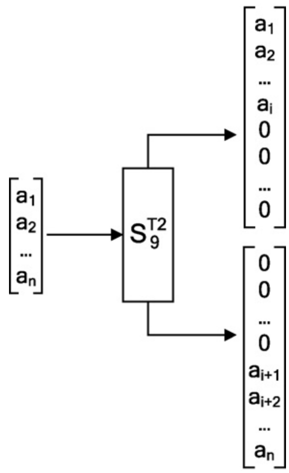

Fig. 1. Graphical representation of the separator.

If separators based on different separation methods can be incorporated into a separation network, then a gap can occur in the associated stream vectors. Suppose that a separator based on extraction, which is effected by the differences among the components' solubilities in terms of their distribution coefficients, is implemented; the component order in the stream vector of its feed stream comprise B, A, and C; a cut is made between B and A. Obviously, no-gap exists in the stream vectors of output streams from the top and bottom of the extractor based on the component order for the extraction: each separator class by itself preserves the 'no-gap' property according to its own component order in the stream vector. A gap, however, appears in the component order in the stream vector of one of the output streams in terms of components' other properties effecting separation, e.g., relative volatilities; see Fig. 2. Such an apparent gap becomes a reality if this output stream is fed to a separator based on these relative volatilities. We can exploit gaps in the component orders of streams to facilitate separation: in general, the greater the difference between the magnitudes of the property on which the separation is based, the easier the separation between two successive components; a gap in the stream vector magnifies the difference. In other words, the cost of separation can be reduced in separating A and C without the presence of B.

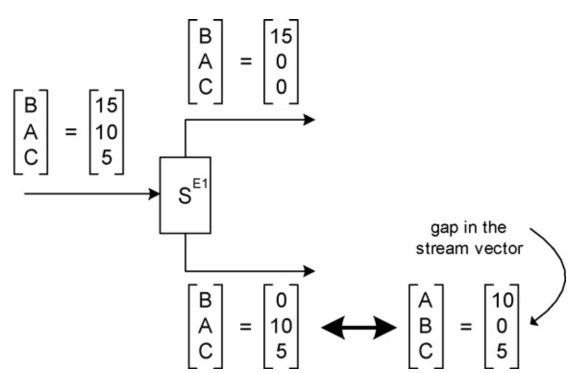

Fig. 2. Gap generated by switching the methods of separation effected by one property to another.

2.2. Separators

A separation is always carried out by exploiting the difference in the magnitude of one of the properties of the components in mixtures or solutions. In petroleum processing, the components are most frequently separated on the basis of the difference in their relative volatilities.

A simple and sharp separator partitions the components in the input stream into two output streams so that each component appears only in one of the output streams; see Fig. 1. Naturally, n components in the feed stream may give rise to $(n-1)$ separations.

Suppose that it is possible to construct a separation network with separators based on different separation methods. Also suppose that k varieties of properties can be identified in an n-component system, which can be exploited to effect the separation. This leads to a maximum of $k(n-1)$ separations. As such, each separator can be described by the mechanism effecting the separation and the location of cut in the stream vector based on this mechanism. It is increasingly popular to incorporate separators based on different separation methods into separation networks. This can be attributed to the fact that it is often exceedingly difficult, if not impossible, to separate mixtures, such as fine chemicals, pharmaceuticals and biochemicals, by a single separation method. If the separation between components not adjacent to each other is possible, additional separators can be incorporated into the system; apparently, little has been done in this regard.

The set of separators based on a single method of separation is termed a separator class; for example, the set of separators based on relative volatility constitutes a separator class. A separator type is a member of a separator class. It is defined by the components, which can be present in its input streams, and by its overall cost coefficient. In designating separators, the type and class to which any separator belongs is clearly indicated. For instance, in S_9^{R2}, superscript R2 stands for the separator type, where letter R refers to the separator class, rectification in this case, and subscript 9 specifies a separator in the separation network, which distinguishes among separators of the same type.

In the current work, the cost of a separator is calculated as the product of the flow rate of the input to the separator and the overall cost coefficient of this specific separator, which is given in the problem definition. In general, the overall cost coefficient signifies the cost of separating a stream with a unit flow rate (1 kg/s) with a specific separator. Obviously, it depends on various parameters affecting the separator's performance. For simplicity, however, no effort is made to explore the effects of such parameters in the current work.

The current work adopts a simple separator model based on sharp separation. In practice, sharp separation is impossible, and the cost function of a separator depends not only on the flow rate of its input stream but also on various other factors, such as purity of the products and extent of recovery. The sharp separation is an over-simplification for the majority of separators. Nevertheless, the performance of the separators can be approximated by the simple sharp-separation model under many circumstances, especially for preliminary design in general and process-network synthesis in particular, see Refs. [5–7]. The solution based on the simple sharp-separation model might serve as the lower bound in an algorithm involving a non-linear cost function or as an initial point of a design that takes into account additional details, including non-linearity and non-sharp separation.

Our understanding is that the cost of a separation network is more strongly influenced by its structure than by the performance of individual separators. The importance of the structure is clearly revealed in Ref. [7] where it is demonstrated that the cost of the structure resultant from an incomplete super-structure can exceed as much as 30% the cost of the optimal structure, based on the same separator model as used in the current work. This implies that it is of the utmost importance to establish the complete, or rigorous, supers-structure even with the simple separation model. Naturally, the resultant super-structure needs to be evolved to the one with a realistic model.

2.3. Mixers and dividers

These devices are for routing streams; their costs are regarded negligible in the current work. A mixer blends two or more input streams, thereby increasing the amounts of the components in the resultant stream.

A divider physically or mechanically splits one input stream. Thus, the component ratios in all the resultant output streams remain identical to those of the input stream.

3. Generation of the rigorous super-structure

The algorithmic solution of any SNS problem involves two major steps, the generation of the mathematical model that defines the problem and its solution. The former can be divided into two main parts, the construction of the network's structural model and the generation of the linear or non-linear mathematical-programming model with the aid of the structural model. Thus, if the mathematical model is based on an inadequate structural model, it would be uncertain that the optimal solution of the original problem could be obtained.

Most, if not all, of the available algorithmic methods assume the existence of a structural model, referred to as the super-structure, and proceed to determine the corresponding optimal solution. Nevertheless, it has seldom been proved rigorously whether this super-structure indeed contains the optimal structure under all circumstances. To amend this defect, the term, rigorous super-structure, as introduced in Ref. [7] is adopted throughout this work. The definition of the rigorous super-structure can be found in Appendix B. The demonstration program is available to generate the rigorous super-structure and its solution for the given class of problems at http://www.dcs.vein.hu/capo/demo/sns/heckl2006.

The class of SNS problems considered in the current work is the generalization of those addressed in Ref. [7]. The major difference is that the former takes into account separators effected by various separation mechanisms whereas the latter does not. None of the available methods for algorithmic SNS have dealt with such a generalization, although its practical importance is obvious as indicated in the preceding section.

The structural property of the optimal networks pertinent to the generation of the rigorous super-structure is (see Ref. [7] for proof):

> "Each instance of the class of SNS problems of interest gives rise to an acyclic optimal network in which mixers are attached only to the output streams."

The proof of this property does not demand that the separators be based only on a single separation method. The proof, therefore, is valid without amendment as long as the cost of a separator is proportional to its mass load. The significance of the statement is that it specifies the positions of the mixers in the rigorous super-structure, thereby greatly reducing the number of configurations to be explored. In the remaining part for the generation of the rigorous super-structure, all possible separator layouts are included in such a way that desired separation occurs on every stream.

The algorithm for generating the rigorous super-structure, as outlined in the following, creates a loopless optimal network where mixers are assigned only to the product streams. According to the aforementioned statements, such an optimal network always exists. The stepwise generation of the rigorous super-structure is illustrated in Fig. 3(a)–(d). Step 1 creates one divider for and links to each feed stream, and step 2 creates one mixer for and links to each product stream; see Fig. 3(a). Step 3 selects an unexplored divider and creates a separator for each possible cut and a bypass to each mixer created in step 2, both of which are connected to the selected divider; step 4 generates a divider for each of the outlets from the separators created in step 3, see Fig. 3(b); hereafter, steps 3 and 4 are iterated until the complete super-structure is generated; see Fig. 3(c) and (d). It is worth noting that the creation of a bypass between an outlet of any divider and the inlet of a mixer is possible only when every component in the former appears in the product stream from the latter.

The procedural details of step 3 are what differentiate the algorithm in Ref. [7] from the current algorithm. It is relatively simple to determine the possible cuts in the former, because a stream containing n components gives rise to $n-1$ cuts and thus $n-1$ possible separations. In contrast, the number of separations also depends on the number of available separator classes in the latter. The effectiveness of each separator type must be evaluated for any given stream. Two conditions should be satisfied; none of the components in the stream is forbidden for the separator type of concern, and at least one component from the inlet stream appears in both outlet streams of this separator type. Moreover, in constructing the super-structure, it is probable that various separators based on different separation methods linked to a single divider yield identical output streams from a given inlet. Obviously, only the least-cost separator should be retained in the super-structure under this situation which does not arise if all the separators are based on a single separation method.

4. Mathematical model

Even when all the cost functions are linear, the mathematical model of a SNS problem is non-linear unless it is based on the proposed super-structure. Formulating the mathematical

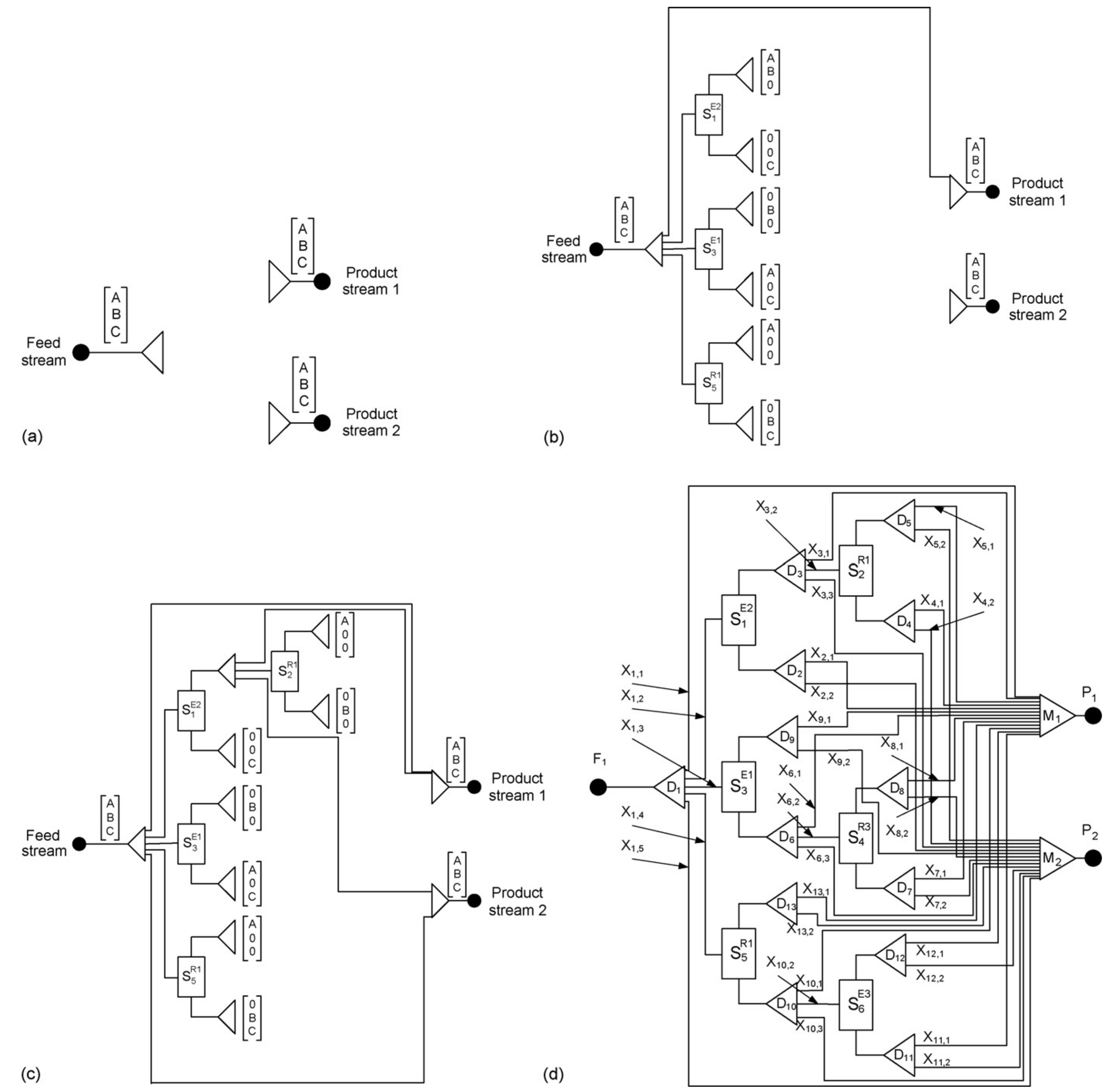

Fig. 3. (a) Generation of the rigorous super-structure for the first example: step 1 for creating a divider to each feed stream, and step 2 for generating a mixer to each product stream. (b) Generation of the rigorous super-structure for the first example: steps 3 and 4; iteration 1. (c) Generation of the rigorous super-structure for the first example: steps 3 and 4; iteration 2. (d) Generation of the rigorous super-structure for the first example: steps 3 and 4 resulting in the super-structure; iteration 13.

model in terms of the compositions and total flow rates introduces non-convex terms in the equations of the separators and mixers; see Ref. [6], while formulating the mathematical model in terms of the component flow rates and splitting ratios makes the equations of the dividers non-convex; see Ref. [5]. One of the main advantages of the proposed method is that mathematical-programming model remains linear as long as the cost function is defined to be linear, as will be made obvious in what follows.

Let *F* be the index set for the feeds; *P*, the index set for the products; *D*, the index set for the dividers; *M*, the index set for the mixers; *S*, the index set for the separators; *A*, the set of arcs (connections). Variable x_{ij} represents the fraction of the rate, or amount, of the feed stream in the network in outlet *j* from divider *i*; therefore, this variable can be conveniently termed, “feed-allocation ratio”, in analogy to the conventionally defined splitting ratio. In fact, for the divider of the feed stream to the network, the feed-allocation ratio and the corresponding splitting ratio are identical. In general, however, the former differs clearly from the latter: for any given divider, the sum of the splitting ratios of its outlets is always unity; in contrast, the sum of the

Table 1
Input data for the first example

Components	Relative volatility	Distribution coefficient	Amount in the feed	Amount in product 1	Amount in product 2
A	1.7	1.2	10	8	2
B	1.02	0.8	15	2	13
C	1	52	5	4	1

feed-allocation ratios of its outlets is equal to the feed-allocation ratio of its inlet.

It is worth noting that the feed-allocation ratio is defined such that its value for any output stream from a divider propagates unaltered to the top and bottom outlets of the separator succeeding the divider. The output stream from either of these outlets serves as the input stream to the divider, which follows. The flow rate or amount of an arbitrary component c in the outlet j from divider i can be computed from three parameters. These parameters are the feed-allocation ratio of this stream, the feed rate or amount of component c in the feed to the network, and delta function δ_{ki}^{c} expressing the presence or absence of component c in the given stream from the kth feed to the network.

The definition of the feed-allocation ratio renders it possible to formulate the mathematical model of the problem as the linear-programming model as follows:

Minimize:

$$\sum_{s\in S}\left(g_s\sum_{\{i:(i,s)\in A\}}\left(x_{is}\sum_{c=1}^{n}\sum_{k\in F}\delta_{ki}^{c}f_k^{c}\right)\right) \quad (1)$$

subject to

$$0\le x_{ij}\quad \forall(i,j)\in A,\ \text{where}\ i\in D \quad (2)$$

$$\sum_{\{j:(i,j)\in A\}}x_{ij}=1\quad \forall i\in D,\ \text{where}\ \exists k\in F\ \text{such that}\ (k,i)\in A \quad (3)$$

$$\sum_{\{j:(i,j)\in A\}}x_{ij}=x_{si}\quad \forall(s,i)\in A,\ \text{where}\ i\in D \quad (4)$$

$$p_q^{c}=\sum_{\{(i,m):(i,m)\in A,(m,q)\in A\}}\left(x_{im}\sum_{k\in F}\delta_{ki}^{c}f_k^{c}\right)$$
$$\forall q\in P\ \text{and}\ c=1,2,\ldots,n \quad (5)$$

$$\delta_{ki}^{c}=\begin{cases}1 & \text{when a path exists between feed } k \text{ and divider } i \text{ both of which contain component } c\\ 0 & \text{otherwise}\end{cases}, \quad (6)$$

$$k\in F,\quad q\in P,\quad i\in D,\quad m\in M,\quad s\in S,\quad j\in M\cup S$$

In the objective function, expression (1), g_s denotes the overall cost coefficient by which the mass load is multiplied in the cost function for separators s, i.e., the cost per unit mass load through separator s; f_k^{c} is the rate of flow, or amount of component c in feed k. Constraint (2) is a natural assumption indicating that x_{ij}, cannot be negative; constraint (3) expresses the mass balance around the dividers assigned to the feed streams; constraint (4) expresses the mass balance around the remaining dividers; constraint (5) results from the mass balance around the product streams, where p_q^{c} signifies the amount of component c in product stream q; (6) indicates the presence or absence of the connections between the operating units.

The proposed model renders it possible to define a product without specifying the exact amounts of components in it. We can prescribe only the ratios of the components, the upper and lower bounds of the amounts of the components, or the minimum or maximum amount of the product. The model's capability is limited only by the requirement that all such constraints be linear as well.

The model appears to be the first of its kind to systematically take into account separators based on different separation methods in SNS. Thus, the current model differs from the model introduced in Ref. [7] even though both are linear. Naturally, the former model is a special case of the current one.

The solution of the linear-programming model yields the optimal structure. Nevertheless, we should examine if two or more separation devices of the same kind in the optimal structure can be merged. Merging of such separators does not affect the structure's cost because of the linearity of the cost function as defined by the model. Two or more separators can be merged if and only if they belong to the same type so that the difficulties of the separations are identical; the dividers for the top output streams of such separators are connected to the same mixer; the dividers for the bottom streams of these separators are also connected to the same mixer, and splitting ratios of the corresponding dividers are identical.

5. Examples

In the first example two multi-component product streams are to be produced from a three-component feed stream. The separation can be carried out by resorting to two separation methods, i.e., rectification (distillation) and extraction. These two different separation methods are needed because the relative volatilities of B and C are close to each other, thus making the separation of the two components with only rectification exceedingly expensive. The solvent for the extraction is selected so as to reduce the cost of separating components B and C.

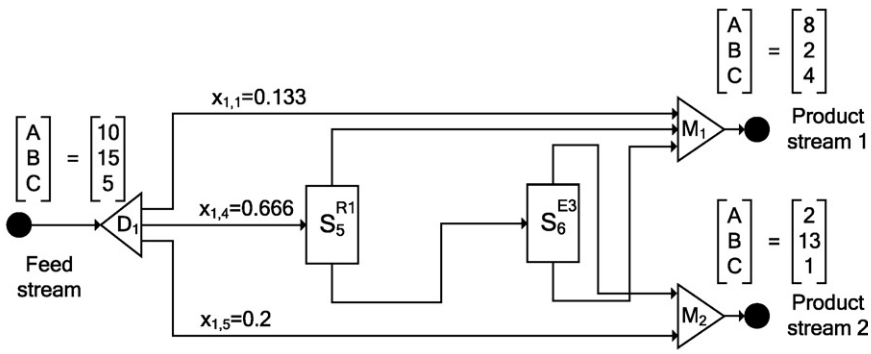

Fig. 4. Optimal structure incorporating both rectifiers and extractors for the first example (cost: 86.7 $/s).

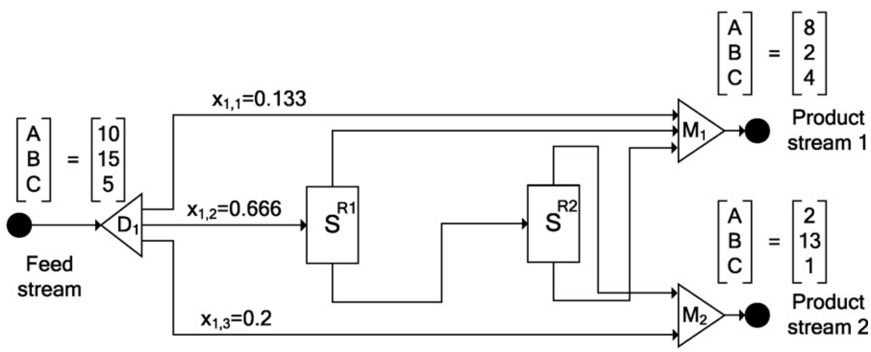

Fig. 5. Optimal structure incorporating only the rectifiers for the first example (cost: 186.7 $/s).

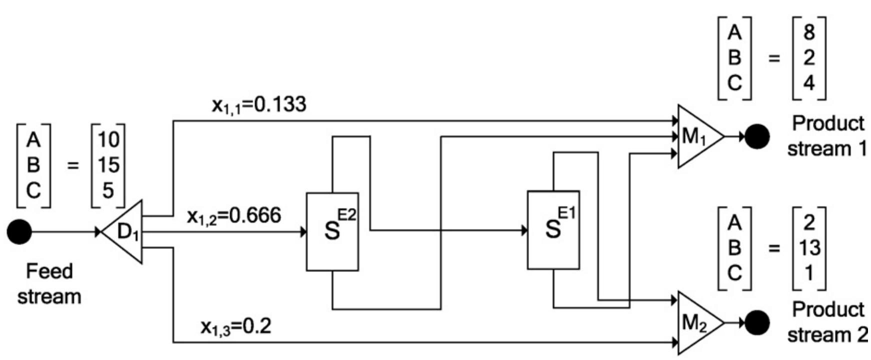

Fig. 6. Optimal structure incorporating only the extractors for the first example (cost: 613.3 $/s).

Table 1 contains the parameter values of the properties and amounts of the components in the feed stream and the product streams; Table 2 lists the data pertaining to the available separators, in which S^R and S^E refer to the rectification and extraction, respectively. Table 2 also lists six overall cost coefficients for the six possible separators.

It is worth noting that only three separators are created for the initial divider although four cuts are possible in the superstructure shown in Fig. 3(d), when there are three components and two separation methods: S^{R2} and S^{E2} perform the same separation task although they are based on different separation methods, and thus, only the less expensive needs to be included

Table 2
Data pertaining to the available separator types for the first example

Separator designation	Inlet components	Top-product components	Bottom-product components	Overall cost coefficients, g_s
S^{R1}	A, B, C	A	B, C	2
S^{R2}	A, B, C	A, B	C	11
S^{R3}	A, C	A	C	1.7
S^{E1}	B, A, C	B	A, C	32
S^{E2}	B, A, C	B, A	C	4
S^{E3}	B, C	B	C	3.5

Table 3
Data pertaining to the available separator types for the second example

Separator designation	Top-product components	Bottom-product components	Overall cost coefficient, g_s
S^{R1}	A	B, C, D, E, F, G	1.5
S^{R2}	A, B	C, D, E, F, G	3
S^{R3}	A, B, C	D, E, F, G	2
S^{R4}	A, B, C, D	E, F, G	2.5
S^{R5}	A, B, C, D, E	F, G	4
S^{R6}	A, B, C, D, E, F	G	4
S^{E1}	D	F, C, A, G, B, E	4.5
S^{E2}	D, F	C, A, G, B, E	1
S^{E3}	D, F, C	A, G, B, E	2.5
S^{E4}	D, F, C, A	A, G, B, E	3.5
S^{E5}	D, F, C, A, G	B, E	1.75
S^{E6}	D, F, C, A, G, B	E	4.5
S^{K1}	A, E, C, D	G, B, F	6.6

in the super-structure. If both separators are included, the solution time increases without yielding a superior solution. It is also worth noting that the gaps in the stream vector can be exploited through the super-structure. For example, only components B and C are present at divider 10, thereby giving rise to a gap according to extraction and rendering it advantageous to install S^{E3} instead of S^{E1} or S^{E2}. Naturally, the cost of S^{E3} is less than that of either S^{E1} or S^{E2}. Appendix C contains the mathematical-programming model and its solution for the first example.

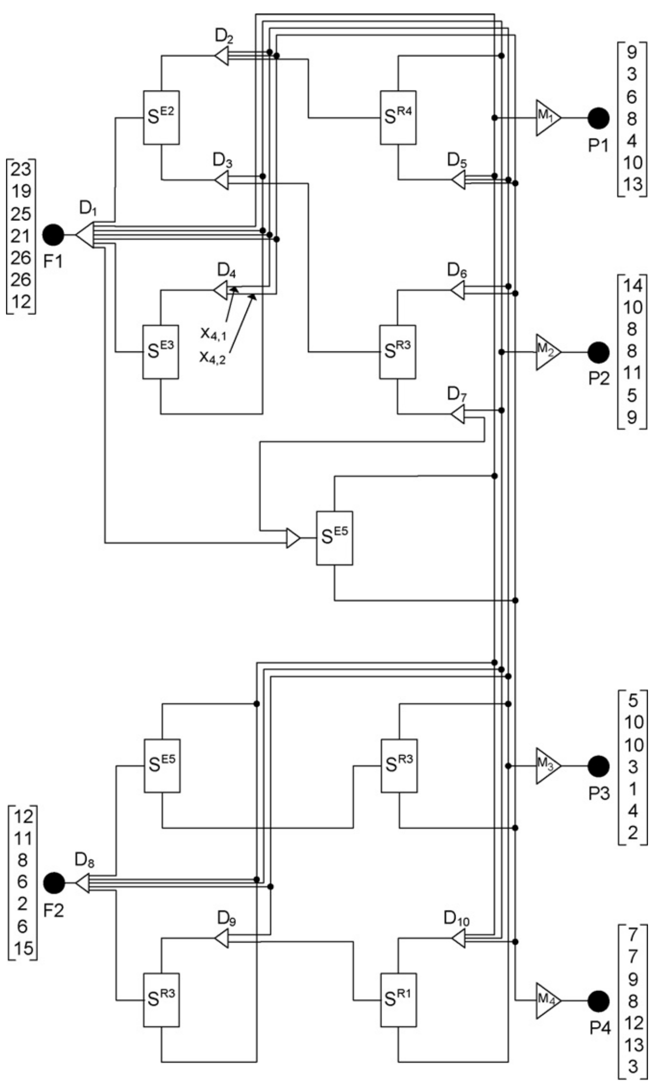

Fig. 7. Optimal structure incorporating both rectifiers and extractors for the second example (cost: 261.1 $/s).

The optimal structure of the first example has been generated in 0.22 s on a PC (Athlon 2 GHz) according to the proposed algorithm. The resultant structure is illustrated in Fig. 4, where $x_{1,1}$, $x_{1,4}$, and $x_{1,5}$ denote the feed-allocation ratios, which are the same as the corresponding splitting ratio for the divider created for the feed stream. The corresponding cost of the separation network is 86.7 $/s. If only either the rectifiers (distillation columns) or extractors are available, the cost of the optimal network is 186.7 or 613.3 $/s, respectively; see Figs. 5 and 6. Obviously, each of these costs far exceeds 86.7 $/s.

The second example features seven components, two feeds and four product streams, and 13 possible separators, involving 3 different separation methods (see Table 3). Fig. 7 illustrates the resultant optimal structure of the separation network, which has been generated in 24 s on a PC (Athlon 2 GHz). Table 4 lists the corresponding feed-allocation ratios. The cost of the optimal structure is 261.1 $/s compared to 442.1 and 358.6 $/s corresponding to the separation networks comprising solely rectifiers

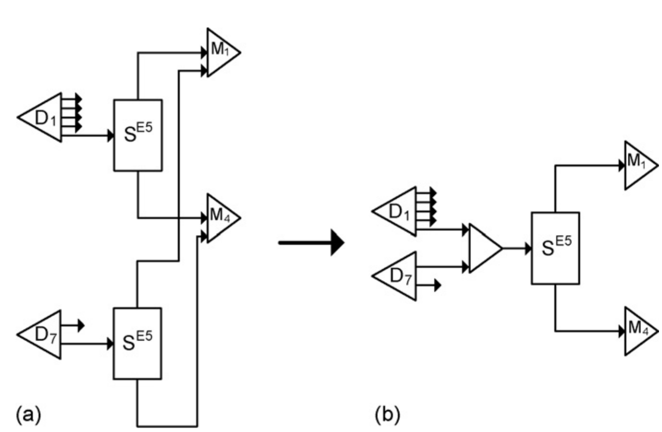

Fig. 8. Merging two separators.

Table 4
Designations and values of the feed-allocation ratios for Fig. 7

Designation	Value
$x_{1,1}$	0.252
$x_{1,2}$	0.108
$x_{1,3}$	0.128
$x_{1,4}$	0.030
$x_{1,5}$	0.250
$x_{1,6}$	0.134
$x_{1,7}$	0.098
$x_{2,1}$	0.037
$x_{2,2}$	0.042
$x_{2,3}$	0.173
$x_{3,1}$	0.103
$x_{3,2}$	0.149
$x_{4,1}$	0.045
$x_{4,2}$	0.089
$x_{5,1}$	0.037
$x_{5,2}$	0.017
$x_{5,3}$	0.119
$x_{6,1}$	0.128
$x_{6,2}$	0.021
$x_{7,1}$	0.037
$x_{7,2}$	0.112
$x_{8,1}$	0.020
$x_{8,2}$	0.086
$x_{8,3}$	0.279
$x_{8,4}$	0.109
$x_{8,5}$	0.506
$x_{9,1}$	0.004
$x_{9,2}$	0.502
$x_{10,1}$	0.249
$x_{10,2}$	0.188
$x_{10,3}$	0.065

Note: the first index indicates the divider number, the second the outlet number (numbered from top to bottom)—for example $x_{4,2}$ is the feed-allocation ratio of the second output from D_4.

and extractors, respectively. It is worth noting that Fig. 7 is the transformed optimal structure generated by appropriately merging the suitable separators of the original optimal structure. Specifically, the original optimal structure contains the part depicted in Fig. 8(a), in which the two separators are linked to the same mixers. These separators are of the same type, and neither of their outputs is divided, and thus, they can be merged; the result is shown in Fig. 8(b). This transformation does not change the cost of the network.

The solver and the two examples together with other examples are available for downloading from web page http://www.dcs.vein.hu/capo/demo/sns/heckl2006.

6. Concluding remarks

A systematic procedure is proposed constructing the rigorous super-structure for a novel class of separation-network synthesis problems involving various classes of separators based on different separation methods. The rigorous super-structure renders it possible to develop an efficient method to optimally synthesize such a class of separation networks. The efficacy of the proposed method is amply demonstrated with two examples.

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Appendix A. Nomenclature

Sets

A	arcs
C	components
D	dividers
F	feeds
M	mixers
P	products
S	separators

Parameters

f_k^c	flow rate of component c in feed stream k (kg/s)
g_s	overall cost coefficient for separator s ($/kg)
p_q^c	flow rate of component c in product stream k (kg/s)
δ_{ki}^c	symbol indicating the existence of a path between $k \in F$ and $i \in D$ in the super-structure containing $c \in C$ (Boolean)

Variables

a_{ij}	flow rate of the jth component in the ith input of a mixer (kg/s)
a_j	flow rate of the jth component in the output of a mixer (kg/s)
b_{ij}	flow rate of the jth component in the ith output of a divider (kg/s)
b_j	flow rate of the jth component in the input of a divider (kg/s)
x_{ij}	feed-allocation ratio, $i \in D, j \in M \cup S$
λ_i	splitting ratio of the ith output of a divider

Appendix B. Definition of the rigorous super-structure

Let a set of operating units and their mathematical models be given. Moreover, a systematic procedure is presumed to exist to generate a valid mathematical-programming model for a network of the given operating units. Then, this network is deemed to be the rigorous super-structure for a class of separation-network synthesis (SNS) problems if the optimality of the resultant solution cannot be improved for any instance of this class of problems by any other network of operating units and model generation procedure.

Appendix C. Details of the first example

The rigorous super-structure has been constructed according to the procedure illustrated in Fig. 3(a)–(d) from the six separators given in Table 2. Fig. 3(d) depicts the resultant super-structure. This super-structure together with the information provided in Tables 2 and 3 make it possible to formulate a linear-programming problem according to expressions from (1)–(6) in the text. In the model, the feed-allocation ratios are designated based on the number of dividers and the number of outlets (counting from the top to the bottom). For example $x_{6,3}$ is assigned to the third outlet of divider 6; as can be seen in Fig. 3(d). Moreover, the same figure indicates that

$$F = \{F_1\}, \qquad P = \{P_1, P_2\},$$

$$D = \{D_1, D_2, D_3, D_4, D_5, D_6, D_7, D_8, D_9, D_{10}, D_{11}, D_{12}, D_{13}\}, \qquad M = \{M_1, M_2\},$$

$$S = \{S_1, S_2, S_3, S_4, S_5, S_6\},$$

$$A = \{(F_1, D_1), (D_1, M_1), (D_1, S_1), (D_1, S_3), (D_1, S_5), (D_1, M_2), (S_1, D_3), (S_1, D_2), (S_3, D_9), (S_3, D_6), (S_5, D_{13}), (S_5, D_{10}), (D_3, M_1), (D_3, S_2), (D_3, M_2), (D_2, M_1), (D_2, M_2), (D_9, M_1), (D_9, M_2), (D_6, M_1), (D_6, S_4), (D_6, M_2), (D_{13}, M_1), (D_{13}, M_2), (D_{10}, M_1), (D_{10}, S_6), (D_{10}, M_2), (S_2, D_5), (S_2, D_4), (S_4, D_8), (S_4, D_7), (S_6, D_{12}), (S_6, D_{11}), (D_5, M_1), (D_5, M_2), (D_4, M_1), (D_4, M_2), (D_8, M_1), (D_8, M_2), (D_7, M_1), (D_7, M_2), (D_{12}, M_1), (D_{12}, M_2), (D_{11}, M_1), (D_{11}, M_2), (M_1, P_1), (M_2, P_2)\}$$

The resultant linear-programming model is given below.

Minimize:

$$4(10 + 15 + 5)x_{1,2} + 2(10 + 15)x_{3,2} + 32(10 + 15 + 5)x_{1,3} + 1.7(10 + 5)x_{6,2} + 2(10 + 15 + 5)x_{1,4} + 3.5(15 + 5)x_{10,2} \quad \text{(C1)}$$

subject to

$$x_{i,j} \geq 0 \quad \text{for all feed-allocation ratios} \quad \text{(C2)}$$

$$x_{1,1} + x_{1,2} + x_{1,3} + x_{1,4} + x_{1,5} = 1 \quad \text{(C3)}$$

$$x_{2,1} + x_{2,2} = x_{1,2} \quad \text{(C4.2)}$$

$$x_{3,1} + x_{3,2} + x_{3,3} = x_{1,2} \quad \text{(C4.3)}$$

$$x_{4,1} + x_{4,2} = x_{3,2} \quad \text{(C4.4)}$$

$$x_{5,1} + x_{5,2} = x_{3,2} \quad \text{(C4.5)}$$

$$x_{6,1} + x_{6,2} + x_{6,2} = x_{1,3} \quad \text{(C4.6)}$$

$$x_{7,1} + x_{7,2} = x_{6,2} \quad \text{(C4.7)}$$

$$x_{8,1} + x_{8,2} = x_{6,2} \quad \text{(C4.8)}$$

$$x_{9,1} + x_{9,2} = x_{1,3} \quad \text{(C4.9)}$$

$$x_{10,1} + x_{10,2} + x_{10,2} = x_{1,4} \quad \text{(C4.10)}$$

$$x_{11,1} + x_{11,2} = x_{10,2} \quad \text{(C4.11)}$$

$$x_{12,1} + x_{12,2} = x_{10,2} \quad \text{(C4.12)}$$

$$x_{13,1} + x_{13,2} = x_{1,4} \quad \text{(C4.13)}$$

$$8 = 10(x_{1,1} + x_{3,1} + x_{5,1} + x_{6,1} + x_{8,1} + x_{13,1}) \quad \text{(C5.1.1)}$$

$$2 = 15(x_{1,1} + x_{3,1} + x_{4,1} + x_{9,1} + x_{10,1} + x_{12,1}) \quad \text{(C5.1.2)}$$

$$4 = 5(x_{1,1} + x_{2,1} + x_{6,1} + x_{7,1} + x_{10,1} + x_{11,1}) \quad \text{(C5.1.3)}$$

$$2 = 10(x_{5,2} + x_{3,3} + x_{8,2} + x_{6,3} + x_{13,2} + x_{1,5}) \quad \text{(C5.2.1)}$$

$$13 = 15(x_{4,2} + x_{3,3} + x_{9,2} + x_{12,2} + x_{10,3} + x_{1,5}) \quad \text{(C5.2.2)}$$

$$1 = 5(x_{2,2} + x_{7,3} + x_{6,3} + x_{11,2} + x_{10,3} + x_{1,5}) \quad \text{(C5.2.3)}$$

Note that Eqs. (C4.*i*), $i = 2, 3, \ldots, 13$, is the mass-balance equation around divider i in terms of the feed-allocation ratios, and Eqs. (C5.*i.j*), $i = 1, 2$; $j = 1–3$, is the mass-balance equation for component j, which is one of components A, B, and C in product i, i.e., product P_1 or P_2.

The optimal solution of the linear-programming model is

$$x_{1,1} = 0.133, \quad x_{1,4} = x_{10,2} = x_{11,1} = x_{12,2} = x_{13,1} = 0.666, \quad x_{1,5} = 0.2$$

The values of all other variables are 0, and the corresponding value of the overall cost function is 86.7 \$/s. The optimal structure obtained is given in Fig. 4 in the text.

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