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Exact Super-Structure for the Synthesis of Separation-Networks with Multiple Feed-Streams and Sharp Separators

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ABSTRACT

Recent insights into the nature of optimal separation-networks indicate a need to develop a rigorous technique capable of generating the optimal solution of a separation-network synthesis (SNS) problem. In principle, an SNS problem can be solved if an exact super-structure is available. Hitherto, no method has been established for generating such a super-structure when multiple feed-streams are involved. Even when a super-structure is complete, the corresponding mathematical-programming problem may not be solvable if it is unnecessarily complex. Thus, the exact super-structure should be as simple as possible.

The present paper proposes an algorithm for generating an exact super-structure for the following class of SNS problems: multiple feed-streams and multicomponent product-streams where the cost function of each separator is linear with a fixed charge. It has been proved that the super-structure generated always includes the optimal separation-network of this class of problems and that the super-structure does not include unnecessary operating units. The proposed method have been demonstrated by successfully solving several problems.

Keywords: separation-network; algorithmic approach, exact super-structure.

INTRODUCTION

Separation-network synthesis (SNS), a subfield of process synthesis, is of mathematical interest as well as of industrial significance: separation-networks are omnipresent in almost all chemical processes. Separation-networks contribute substantially to the capital cost of an overall chemical process; therefore, the development of a systematic framework and the relevant model of this framework, which yield the optimum network, is an important research issue.

It is essential for any algorithmic method of SNS to have (i) a valid model, i.e., both the rigorous super-structure and the corresponding mathematical-programming model, and (ii) a global optimization method to attain optimality.

Various unexpected optimal solutions obtained for some simple classes of SNS problems illustrate the difficulty involved in generating a valid mathematical-programming model (see, e.g., Kovács *et al.*, 1993; and Kovács *et al.*, 1998a, Kovács *et al.*, 1998b); they indicate that any mathematical-programming model obtained from an incomplete network structure may not yield the optimal solution regardless of the optimization method adopted.

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The present paper proposes a highly efficient method to resolve the dilemma, mentioned above; specifically, it focuses on the generation of the rigorous super-structure of an SNS problem for which the cost functions of the separators are linear with fixed charges. Based on this rigorous super-structure, the optimal separation-network can be generated with certainty.

PROBLEM SPECIFICATION

A set of multicomponent product-streams is to be generated from multicomponent feed-streams by a network of separators, dividers, and mixers. The models and cost functions of the operating units are as follows:

The components of the streams are in a ranked list with respect to a given separation method (Hendry and Hughes, 1972), which remains invariant over the entire separation process. This list arranges the components in decreasing order with respect to the value of the physical property on which the separation method is based; it facilitates the representation of a mixture and the identification of all possible sharp separations between the adjacent key components.

Separator S^i performs a sharp separation between components i and (i+1) of its inlet stream. In other words, if its inlet stream contains components 1 through n, then its top outlet stream contains components 1 through i, and its bottom outlet stream, components $(i+1)$ through n. The cost of an individual separator is a linear function with a fixed charge, i.e., it is assumed to be given in the form, $Cost(S_i) = a_i + b_i x_i$, where b_i signifies the degree of difficulty of the i-th separation; x_i, the mass load of separator i; and a_i, the fixed charge. The overall cost of the separation-network is the sum of the costs of individual separators in the network. In addition, the cost of the dividers and mixers in the separation-network are deemed negligible because their contribution to the overall cost is nil: they are far less costly than the separators. This type of models has been adopted by several authors, e.g., Wehe and Westerberg (1987); Floudas and Aggarwal (1990); and Quesada and Grossmann (1995).

GENERATION OF THE RIGOROUS SUPER-STRUCTURE

To initiate the super-structure generation of a SNS problem for which the cost function of an individual separator comprises the linear and fixed charges, a simplified problem without the fixed charge, i.e., the auxiliary problem, is solved first. The feed-streams and product-streams of this auxiliary problem are the same as those of the original SNS problem. This class of SNS problems has been investigated in Kovács *et al.* (1998b) where an algorithmic solution of these problems is given.

The solution of the auxiliary problem is one of the feasible solutions of the original SNS problem; however, it may not be optimal. By denoting the set of separators by H, the cost of this solution is calculated according to the original cost function as $Cost_{aux} = S_{aux} + O_{aux}$, where $S_{aux} = \sum_{i \in H} a_i$ is the sum of the fixed charges and $O_{aux} = \sum_{i \in H} b_i x_i$ is the value of the cost function of the optimal solution of the auxiliary problem. Moreover, the following inequality obviously holds between the cost of the optimal solution, $Cost_{Opt}$, and the cost of the optimal solution of the auxiliary problem, $Cost_{aux}$:

$$Cost_{aux} = S_{aux} + O_{aux} \geq S_{Opt} + O_{Opt} = Cost_{Opt} \qquad (1)$$

where S_{Opt} and O_{Opt} are the sum of fixed charges and variable charges for the optimal solution, respectively. Naturally, the definition of O_{aux} leads to O_{Opt}-$O_{aux} \geq 0$; this, in turn, yields the following inequality.

$$S_{aux} \geq S_{Opt} + (O_{Opt} - O_{aux}) \geq S_{Opt} \qquad (2)$$

In other words, S_{aux} is an upper bound of the sum of the fixed charges of the separators in the optimal solution of the original SNS problem.

A lower bound of the sum of the fixed charges for a feasible solution, S_{Need}, can be calculated as the sum of the fixed charges of those separators that must be included in any solution of the SNS problem; in general, S_{Need} can be given as the sum of the fixed charges of separators of each type. Thus, an upper limit of the number of separators of type i in a solution can be evaluated as

$$\left[\frac{S_{aux} - S_{Need}}{a_i}\right] + n_i(S_{Need}) \qquad (3)$$

where $n_i(S_{Need})$ is the minimum number of type i separators necessary for solving the SNS problem., and for any real number x, $[x]$ denotes the greatest integer less than or equal to x. The above expression represents the number of separators of type i that should be considered in the rigorous super-structure. Finally, all appropriate connections must be established between the separators.

EXAMPLES

Example 1.

This example is taken from Wehe and Westerberg (1987). In this SNS problem a three component feed-stream is to be separated into two multicomponent product-streams. The pertinent data are tabulated in Tables 1 and 2; the cost of the best known solution is 15.6.

Table 1. Feed and product streams for Example 1.

	A	B	C
F	10	10	10
P1	3	5	3
P2	7	5	7

Table 2. Cost data for Example 1.

	AB	BC
Fixed charge	3	5
Degree of difficulty	0.6	1

The optimal solution of the auxiliary SNS problem is given in Figure 1. Note that splitting ratios (Kovács *et al.*, 1998b) are assigned to the streams.

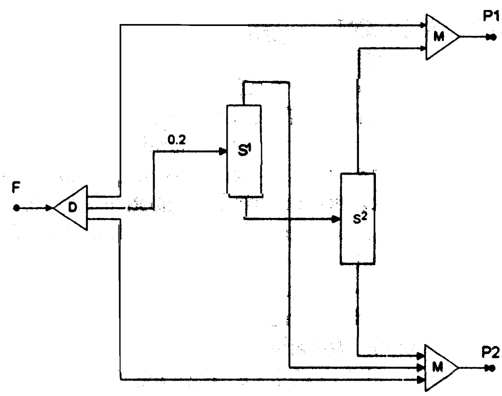

Figure 1. Optimal structure of the auxiliary SNS problem of Example 1: it is also the optimal solution of the problem.

For this example, S_{aux}=8 and S_{Need}=8 since one separator of each type is required to solve the problem. Consequently, the number of different types of separators in the rigorous super-structure is:

separator of type 1: [(8-8)/3] +1 = 1

separator of type 2: [(8-8)/5] +1 = 1

There are altogether 2 separators which must be linked every possible way to generate the rigorous super-structure which is depicted in Figure 2. The

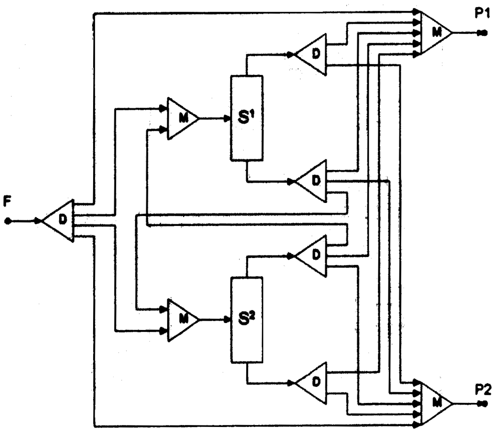

Figure 2. Rigorous super-structure of Example 1.

solution based on the super-structure generated is the same as the optimal solution of the auxiliary SNS problem, given in Figure 1, and the solution published in Wehe and Westerberg (1987).

Example 2

This example is taken from Wehe and Westerberg (1987); it is also published in Quesada and Grossmann (1995). In this SNS problem, a five-component feed-stream is to be separated into 4 multi-component product-streams. The pertinent data are tabulated in Tables 3 and 4. First, the auxiliary SNS problem is formulated and its optimal solution is determined (see Figure 3), where its cost, O_{aux}, is 62.177, while the overall cost of this network, i.e., $Cost_{aux}$ is 111.177. Moreover, S_{aux}=49 and S_{Need}=23, i.e., one separator of each type is required to solve the problem. Thus, the number of different types of separators in the rigorous super-structure is:

separator of type 1: [(49-23)/5] + 1 = 5+1 = 6
separator of type 2: [(49-23)/9] + 1 = 2+1 = 3
separator of type 3: [(49-23)/3] + 1 = 8+1 = 9
separator of type 4: [(49-23)/6] + 1 = 4+1 = 5

Table 3. Feed and product streams for Example 2.

	A	B	C	D	E
F	32	16	20	25	24
P5	7	8	3	9	8
P6	10	3	5	5	4
P7	5	5	6	7	3
P8	10	-	6	4	9

Table 4. Cost data for Example 2.

	AB	BC	CD	DE
Fixed charge	5	9	3	6
Degree of difficulty	0.5	1	0.4	0.6

There are altogether 23 separators that must be linked in every plausible way to generate the rigorous super-structure.

Example 3

This example is taken from Wehe and Westerberg (1987); it is also published in Quesada and Grossmann (1995). In this SNS problem, a four-component feed-stream is to be separated into three multicomponent product-streams. The pertinent data are tabulated in Tables 5 and 6. The optimal solution of the auxiliary SNS problem is depicted in Figure 4.

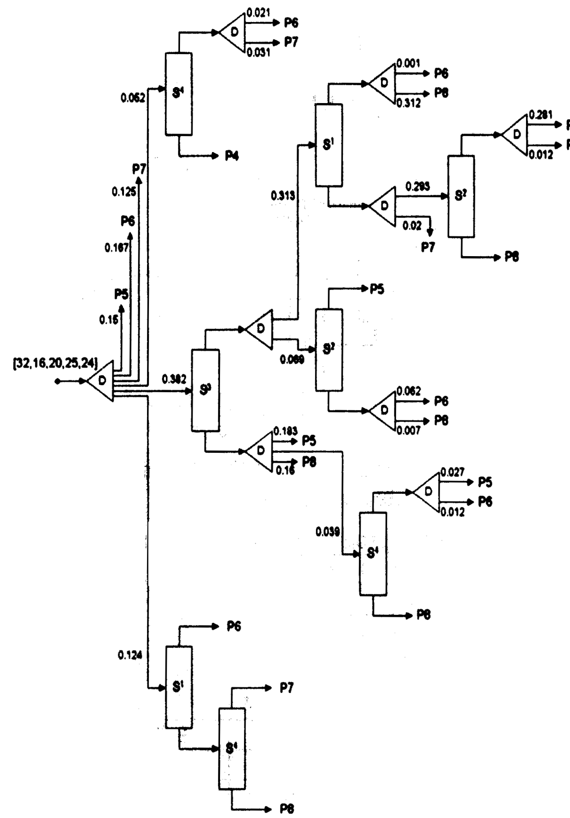

Figure 3. Optimal structure of the auxiliary SNS problem of Example 2.

Table 5. Feed and product streams for Example 3.

	A	B	C	D
F	6	8	5	9
P1	2	3	1	3
P2	1	4	1	5
P3	3	1	3	1

Table 6. Cost data for Example 3.

	AB	BC	CD
Fixed charge	5	4	6
Degree of difficulty	0.5	0.3	0.7

For this example, S_{aux}=20 and S_{Need}=15, i.e., one separator of each type is required to solve the problem. Hence, the number of different types of separators in the rigorous super-structure is:

separator of type 1: [(20-15)/5] + 1 = 2
separator of type 2: [(20-15)/4] + 1 = 2
separator of type 3: [(20-15)/6] + 1 = 1

There are altogether 5 separators that must be linked in every possible way to generate the rigorous super-structure.

Example 4.

This example is taken from Floudas and Aggarwal (1990); it is also published in Quesada and Grossmann (1995). In this SNS problem, a three-component feed-stream is to be separated into two multicomponent product-streams. The pertinent data are tabulated in Tables 7 and 8.

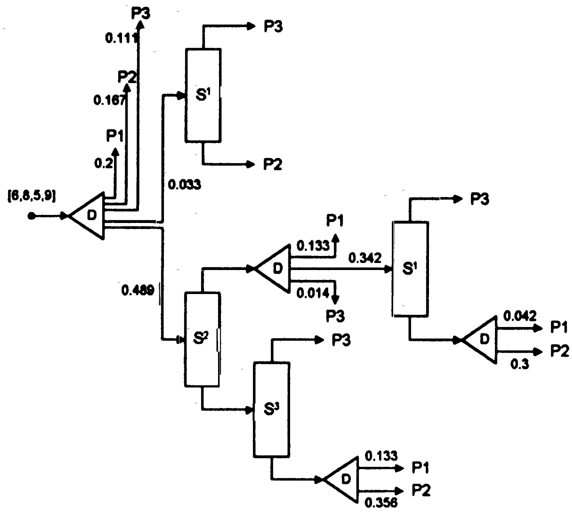

Figure 4. Optimal structure of the auxiliary SNS problem of Example 3.

Table 7. Feed and product streams for Example 4.

	A	B	C
F	100	100	100
P1	30	50	30
P2	70	50	70

Table 8. Cost data for Example 4.

	AB	BC
Fixed charge	0.2395	0.7584
Degree of difficulty	0.00432	0.01517

The optimal solution of the auxiliary SNS problem depicted in Figure 5 is identical to that of Example 1 given in Figure 1. For this example, S_{aux}=0.9979 and S_{Need}=0.9979, i.e., one separator of each type is required to solve the problem. As a result, the number of different types of separators in the rigorous super-structure is:

separator of type 1: 1

separator of type 2: 1

There are altogether 2 separators which must be linked in every possible way to generate the rigorous super-structure which is identical to that of Example 1; see Figure 6.

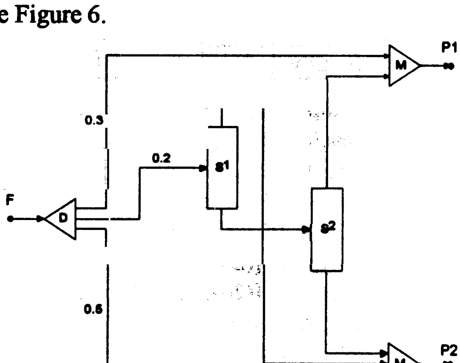

Figure 5. Optimal structure of the auxiliary SNS problem of Example 4: it is also the optimal solution of the problem.

The optimal solution of the original SNS problem can be determined on the basis of this rigorous super-structure; it is identical to that of the auxiliary SNS problem given in Figure 5. The value of the objective

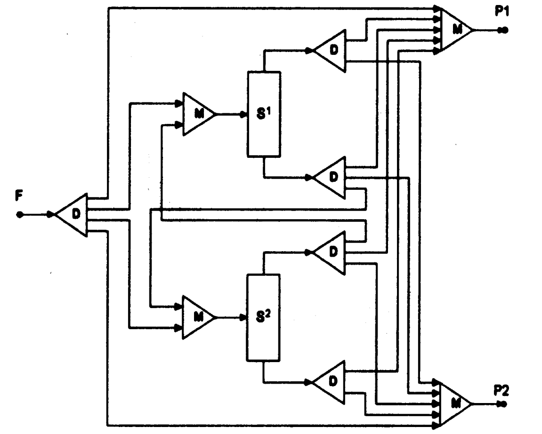

Figure 6. Rigorous super-structure of Example 4.

function is 1.864, which is identical to the best known solution (Quesada and Grossmann, 1995).

CONCLUSIONS

Algorithmic methods of SNS have been extensively investigated. Nevertheless, none of the available methods are based on the rigorous super-structures that yield with certainty the globally optimal solutions of SNS problems for which the cost function of an individual separator consists of linear and fixed charges. In the present work, a novel algorithmic method is proposed for the generation of the rigorous super-structure for such SNS problems.

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