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PARAMETRIC STUDY OF SEPARATION NETWORK SYNTHESIS: EXTREME PROPERTIES OF OPTIMAL STRUCTURES

Z. Kovacs[1,4], F. Friedler[1,2,3], and L. T. Fan[2]

[1]Department of Computer Science, University of Veszprém, Veszprém, Hungary

[2]Department of Chemical Engineering, Kansas State University, Manhattan, KS 66506, U.S.A.

[3]Department of Systems Engineering, Research Institute of Chemical Engineering, Hungarian Academy of Sciences, H-8201 Veszprém, Pf. 125, Hungary

[4]Department of Computer Science, JGYTF, Szeged, Hungary

ABSTRACT

Optimal separation sequencing or network synthesis (SNS) has been carried out either by a heuristic or mathematical programming method. The former gives rise only to those networks that can be deduced from its heuristic rules, and the latter, only to those networks whose structures are the substructures of the super-structure. If the set of heuristic rules or super-structure is incomplete, a substantial fraction of structures that can be optimal may very likely be excluded from consideration. Our study of various SNS problems involving sharp separators, dividers, and mixers encompasses a wide variety of problems yielding pure or multicomponent product streams from single or multiple feed streams. The counter examples generated indicate that basic structural components, such as recycling or redundancy in separators, may not necessarily render the separation network structures non-optimal. The available methods, however, tend to exclude these basic structural components a priori.

The present work parametrically examines hypothetical and real SNS problems to determine under which circumstances recycling or redundancy may be involved in optimal separation structures, and under what situations bypasses should not be maximized in such structures. These results are useful in improving the available synthesis techniques.

KEYWORDS

Separation network synthesis; super-structure; parametric study.

INTRODUCTION

Unexpected optimal structures have been generated recently in some separation network synthesis (SNS) problems (Kovacs *et al.*, 1993a) illustrating that the mathematical foundation of SNS is not sufficiently well developed. It is highly desirable, therefore, that the structural features of optimal separation networks be explored. Since SNS is an extremely difficult problem, its rigorous mathematical description should be developed first for a simple class of SNS problems before proceeding to complex classes of problems.

Correspondence concerning this paper should be addressed to F. Friedler, Department of Computer Science, University of Veszprém, Veszprém, Egyetem u. 10, 8201, Hungary; E-mail: friedler@almos.vein.hu.

The present work considers SNS problems comprising separators, mixers, and dividers for separating single or multiple multicomponent feed streams into single or multicomponent product streams. The conditions assumed are as follows (Floudas, 1987):The components in a stream forming a ranked list are arranged in the descending order of a certain chemical or physical property on which the separation is based. Moreover, the order in this list remains invariant and is unaffected by elimination of any component from the stream. When two sublists are generated from the list due to separation, any component in the higher-ranked sublist will stay higher than any component in the lower-ranked sublist. The cost of an individual separator is calculated as a non-negative, monotone, strictly concave function depending on the massload of this separator. The cost of a separation system is the sum of the costs of its separators.

Non-conventional structures, such as networks containing recycling loops or redundant separators, are usually excluded from consideration in synthesizing separation networks of the class mentioned in the preceding paragraph. Nevertheless, it has been illustrated by examples that for such separation networks to be optimal, recycling loops need be included in them under certain situations (Kovacs *et al.*, 1993a). The present work conducts a parametric study of various classes of separation networks to ascertain if this is generally the case in SNS.

REPRESENTATION OF SEPARATION NETWORKS

It is crucial that an appropriate technique be selected for representing the structure of a process in any process synthesis problem because it may affect the validity of the result. In the present work, the directed bipartite graph, i.e., P-graph, representation developed for total flowsheet synthesis (Friedler *et al.*, 1992b) has been adapted for SNS; it is termed sP-graph. Since it is a bipartite graph, the sP-graph has two disjoint sets of vertices, and no two vertices from the same set are adjacent.

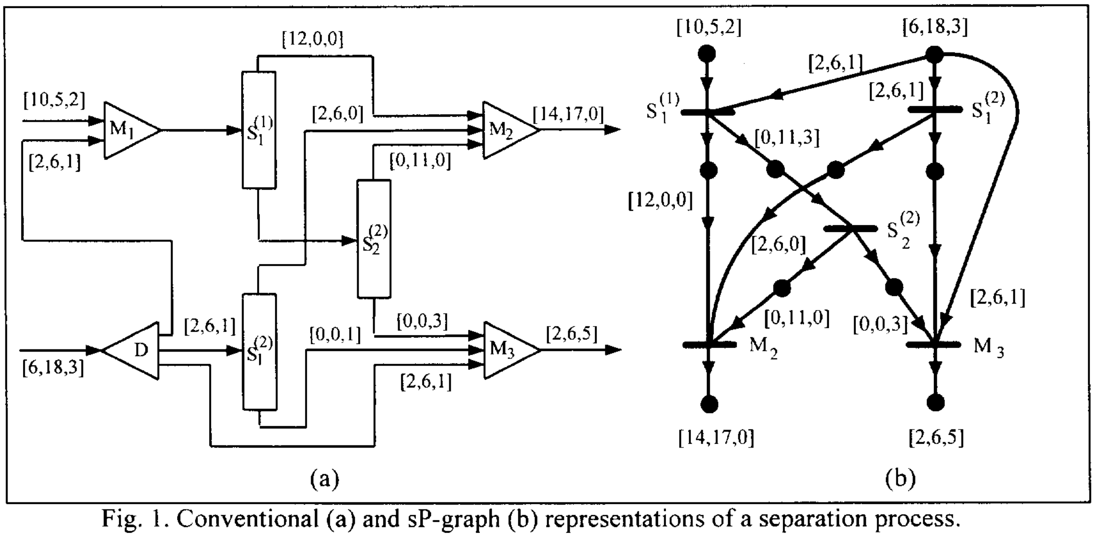

Fig. 1. Conventional (a) and sP-graph (b) representations of a separation process.

Materials and operating units are represented by vertices of different types in an sP-graph. Specifically, the materials are represented by small circles; the operating units, by horizontal bars; and the connections among them, by the arcs of the graph. A divider does not alter the compositions of a stream, and thus, no cost is assigned to it in the SNS problems considered here; therefore, the dividers are not explicitly represented on the structure. Separators and mixers are given on the structure; however, if a separator is preceded by a mixer generating the mixture solely for feeding, the latter is regarded as the integral part of the former. This does not affect the evaluation of a separation network. Conventional and sP-graph representations of a separation network are given in Figs 1(a) and 1(b), respectively.

For a formal description, let (n, F, P, G) represent an SNS problem separating feed streams F = { F_1, F_2, . . . , F_s } of n components into product streams P = { P_1, P_2, . . . , P_m }. G is a vector function of (n-1) elements; the i-th element given by function $G_i(x)$ is the cost of separating a mixture with massload x between components i and (i+1).

Example 1. The SNS problem

(3, { [120, 1, 20], [100, 1, 200] }, { [220, 0, 0], [0, 2, 0], [0, 0, 220] }, [$x^{0.6}$, $x^{0.6}$])

is to produce three pure product streams from the two three-component feed streams, [120, 1, 20] and [100, 1, 200]. The cost function is $x^{0.6}$ for separating either between the first and second components or between the second and third components. This example is also summarized in Table 1.

Table 1. Data for Example 1.

	A		B		C
feed stream 1	120		1		20
feed stream 2	100		1		200
product stream 1	220		0		0
product stream 2	0		2		0
product stream 3	0		0		220
degree of difficulty of separation		1		1	

RECYCLING IN AN OPTIMAL STRUCTURE

With simple examples, it has been illustrated that an SNS problem with two three-component feed streams and pure product streams may include a recycling loop in the optimal structure (Friedler *et al.*, 1992a). Another example has indicated that this is also the case for a problem with multicomponent product streams (Kovacs *et al.*, 1993a).

To explore the propensity of recycling to be incorporated into an optimal network, let us consider Example 1 again.

Example 1 revisited. Figure 2 shows a solution of this example. It includes three separators where separation between the second and third components is performed twice, once in separator $S_1^{(2)}$ and once in separator $S_2^{(2)}$. Let us suppose that the ratio of the massloads of the two streams, the stream from t to $S_1^{(2)}$ and that from $S_1^{(1)}$ to t, is y. The process is a feasible solution of the problem if $0 \le y < 1$; the system contains a recycling loop only when $0 < y$. Obviously, the cost of the process can be minimized by varying y.

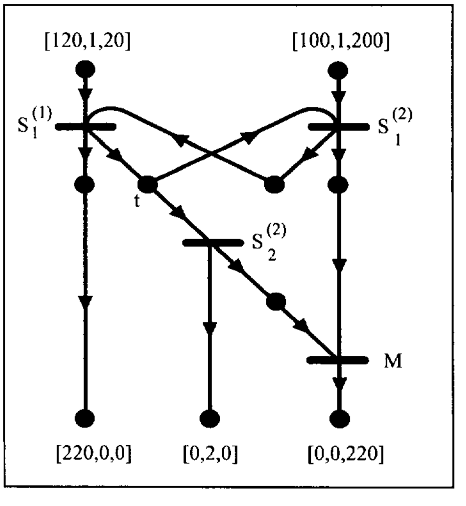

Fig. 2. Solution of Example 1 including recycling.

If recycling is disregarded, i.e., if y = 0, the cost is 64.02. Increasing the value of x increases the sizes and costs of both separators $S_1^{(2)}$ and $S_1^{(1)}$ and decreases those of separator $S_2^{(2)}$. The sum of the costs of these three separators, i.e., the overall cost of the system decreases until x reaches 0.76, and then increases (see Fig. 3). Thus, y = 0.76 is the minimal-cost solution of the configuration with the cost of 62.51. This example illustrates that inclusion of a recycling stream may reduce the cost of a simple separation process. In other words, the elimination of a recycling may increase the cost. An exhaustive comparison of this cost with those of other feasible structures reveals that it is indeed the optimal solution of the problem.

The complexity of the mathematical programming model of an SNS problem depends highly on the involvement of recycling in the solution. It is, therefore, essential to know which set of parameters induces the recycling to be included in or excluded from the optimal structure. For this purpose, the super-structure for the SNS problem of Example 1 is illustrated in Fig. 4 (Kovacs *et al.*, 1993c) and the NLP model based on this super-structure have been examined by an available global optimization method (Csendes, 1990). Every SNS problem given in set SPC1 = { (3, { [120, B, 20], [100, B, 200] }, { [220, 0, 0], [0, 2, 0], [0, 0, 220] }, $[x^b, x^b]$) : $1 \leq B \leq 5$, $0.4 \leq b \leq 0.6$ } has been found to involve recycling in the optimal structure, and every SNS problem in set SPC2 = { (3, { [120, B, 20], [100, B, 200] }, { [220, 0, 0], [0, 2, 0], [0, 0, 220] }, $[x^b, x^b]$) : $100 \leq B \leq 200$, $0.4 \leq b \leq 0.6$ } has been found to be void of recycling in the optimal structure.

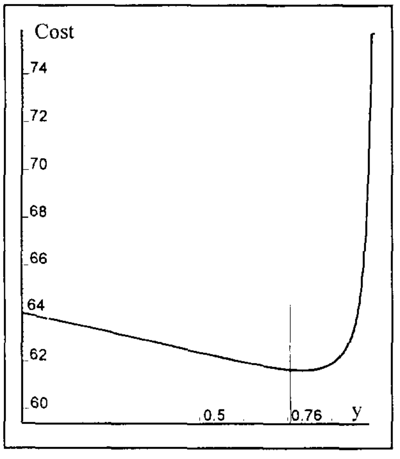

Fig. 3. Cost of the structure given in Fig. 2: It depends on the ratio of the massloads of the streams from t to $S_1^{(2)}$ and that from $S_1^{(1)}$ to t.

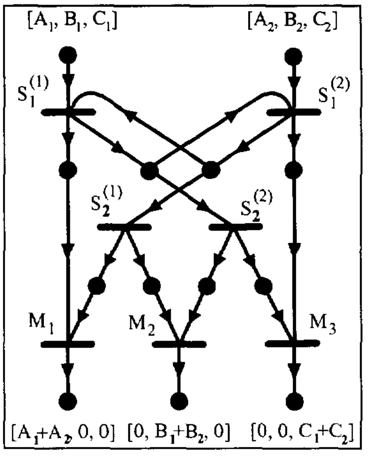

Fig. 4. Super-structure for Example 1.

Note that in these two sets of SNS problems, SPC1 and SPC2, both B and b are free parameters of a specific problem where B is the flowrate of the second component in each feed stream, and b is the power in the cost function. Both B and b must satisfy some constraints, e.g., in the set of problems SPC1, $1 \leq B \leq 5$, $0.4 \leq b \leq 0.6$. Thus, both SPC1 and SPC2 represent infinite numbers of SNS problems.

REDUNDANT SEPARATOR IN THE OPTIMAL STRUCTURE

Another peculiar property of an optimal separation network is that it may contain redundant separators (Friedler *et al.*, 1992a; Kovacs *et al.*, 1993b), i.e., the separators of the identical type may appear more than once in the structure.

Example 2. The optimal solution of SNS problem (3, { [100, 6, 15], [10, 1, 97] }, { [110, 0, 0], [0, 7, 0], [0, 0, 122] }, $[x^{0.6}, x^{0.6}]$) requires to perform separation between the first and second components twice (see Fig. 5), i.e., this structure contains redundant separators.

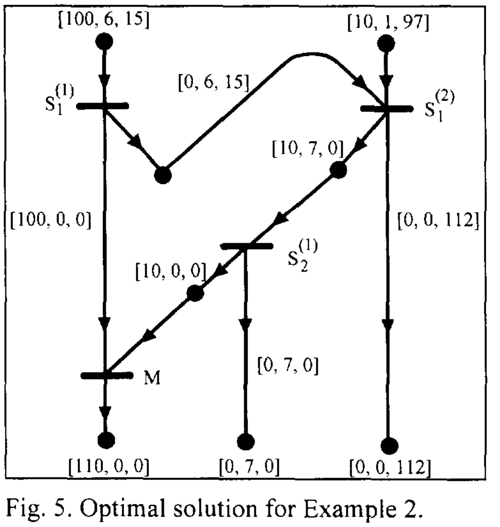

Fig. 5. Optimal solution for Example 2.

The possibility of redundancy in the optimal network greatly increases the complexity of the mathematical programming model of an SNS problem. The upper bound for the number of possible redundant separators in the optimal solution of any SNS problem has never been published, thereby indicating that the derivation of a rigorous mathematical model of this problem is extremely difficult, if not impossible. Hence, the occurrence or non-occurrence of redundancy is also an important question to be resolved.

First, let us examine the following simple SNS problem.

SP1 = (4, { [100, 100, 100, 100] }, { [100, 50, 50, 0], [0, 10, 10, 0], [0, 40, 40, 100] }, $[x^{0.6}, x^{0.6}, x^{0.6}]$)

Its optimal solution involves separation between the third and fourth components twice (Fig. 6). Note that this structure remains optimal as long as the power of the cost function is no less than 0.6 but no greater than 0.8, i.e., it is the optimal solution for the following class of SNS problems.

SPC3 = { (4, {[100, 100, 100, 100] }, { [100, 50, 50, 0], [0, 10, 10, 0], [0, 40, 40, 100] }, $[x^b, x^b, x^b]$) : $0.6 \le b \le 0.8$ }.

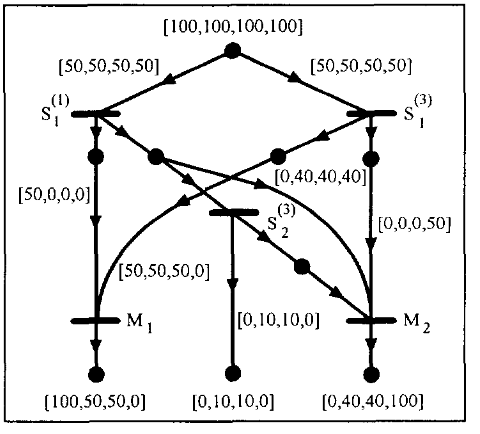

Fig. 6. Optimal solution of SP1.

Second, let us consider the following class of SNS problems.

SPC4 = { (3, { $[F_{1,1}, F_{1,2}, F_{1,3}]$, $[F_{2,1}, F_{2,2}, F_{2,3}]$ }, { $[P_{1,1}, 0, 0]$, $[0, P_{2,2}, P_{2,3}]$, $[0, P_{3,2}, P_{3,3}]$ }, $[x^{0.6}, (4x)^{0.6}]$) : $P_{1,1} = F_{1,1} + F_{2,1}$; $P_{2,2} = \alpha F_{1,2} + \beta F_{2,2}$; $P_{2,3} = \alpha F_{1,3} + \beta F_{2,3}$; $P_{3,2} = (1-\alpha)F_{1,2} + (1-\beta)F_{2,2}$; $P_{3,3} = (1-\alpha)F_{1,3} + (1-\beta) F_{2,3}$; $0 \le \alpha, \beta \le 1$ }.

An SNS problem represented in this class has two feed streams, each containing three components and three product streams. The flowrates of the components both in the feed and product streams satisfy additional constraints. Each of the three structures given in Fig. 7 is a feasible structure for any instance of the class of problems; nevertheless, the optimal structure depends on the parameters of these problems. Either the first or second structure given in Figs 7(a) and 7(b), respectively, contains two separators in different configurations; however, both perform separation between the first and second components. In contrast, two different separations are performed in the third structure.

Let us now define constants λ_1 and λ_2 as follows:

$$\lambda_1 = \max \{ z : [P_{2,2}, P_{2,3}] - z[F_{1,2} + F_{2,2}, F_{1,3} + F_{2,3}] \ge [0, 0] \}$$

$$\lambda_2 = \max \{ z : [P_{3,2}, P_{3,3}] - z[F_{1,2} + F_{2,2}, F_{1,3} + F_{2,3}] \ge [0, 0] \}$$

The domains of optimality of the three feasible structures given in Fig. 7 can be determined by comparing their costs.

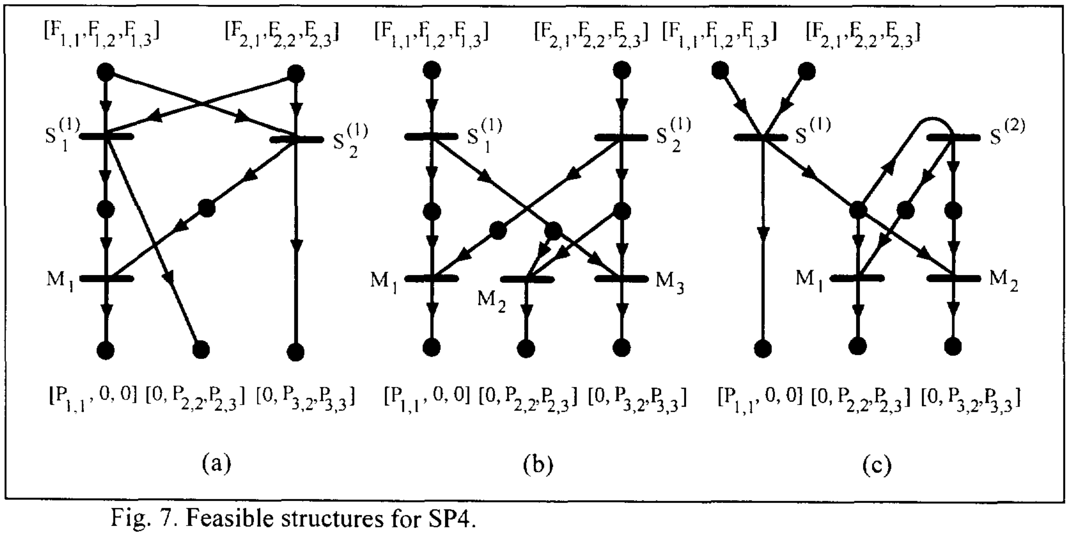

Fig. 7. Feasible structures for SP4.

(i) The structure given in Fig. 7(c) is optimal if and only if the following conditions are satisfied.

$$(4(1-(\lambda_1+\lambda_2))(F_{1,2} + F_{2,2} + F_{1,3} + F_{2,3}))^{0.6} < (F_{1,1} + F_{1,2} + F_{1,3})^{0.6} + (F_{2,1} + F_{2,2} + F_{2,3})^{0.6} - (F_{1,1} + F_{1,2} + F_{1,3} + F_{2,1} + F_{2,2} + F_{2,3})^{0.6}$$

and

$$(4(1-(\lambda_1+\lambda_2))(F_{1,2} + F_{2,2} + F_{1,3} + F_{2,3}))^{0.6} < (\alpha(F_{1,1} + F_{1,2} + F_{1,3}) + \beta(F_{2,1} + F_{2,2} + F_{2,3}))^{0.6} - ((1-\alpha)(F_{1,1} + F_{1,2} + F_{1,3}) + (1-\beta)(F_{2,1} + F_{2,2} + F_{2,3}))^{0.6} - (F_{1,1} + F_{1,2} + F_{1,3} + F_{2,1} + F_{2,2} + F_{2,3})^{0.6}$$

(ii) If condition (i) is not satisfied, then, the structure given in Fig. 7(a) is optimal if LHS < RHS; that given in Fig. 7(b) is optimal if LHS > RHS; and both structures given in Figs 7(a) and 7(b) are optimal if LHS = RHS. Note that for brevity, LHS and RHS are defined as follows:

$$\text{LHS} = \text{abs}[\,(F_{1,1} + F_{1,2} + F_{1,3}) - (F_{2,1} + F_{2,2} + F_{2,3})\,]$$

$$\text{RHS} = \text{abs}\,[\,(\alpha(F_{1,1} + F_{1,2} + F_{1,3}) + \beta(F_{2,1} + F_{2,2} + F_{2,3})) - ((1-\alpha)(F_{1,1} + F_{1,2} + F_{1,3}) + (1-\beta)(F_{2,1} + F_{2,2} + F_{2,3}))\,]$$

CONCLUDING REMARKS

A parametric study has been performed to demonstrate that the optimal configurations for various classes of SNS problems may contain unexpected structures. This occurs in sizeable domains of the free parameters of such problems.

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