HUNGARIAN JOURNAL
OF INDUSTRIAL CHEMISTRY
VESZPRÉM
Vol. 26. pp. 213 - 219 (1998)

REDUNDANCY IN A SEPARATION-NETWORK

Z. KOVÁCS[1,3], Z. ERCSEY[1], F. FRIEDLER[1,2*] and L. T. FAN[2]

([1] Department of Computer Science, University of Veszprém, Veszprém, Egyetem u. 10., H-8200, HUNGARY
[2] Department of Chemical Engineering, Kansas State University, Manhattan, Kansas 66506, U.S.A.
[3] Department of Computer Science, József Attila University, Szeged, HUNGARY)

Received: January 6, 1998

Separation-network synthesis (SNS) is carried out by a heuristic, algorithmic or combined method. For any separation-network, the algorithmic method may yield the optimal structure provided that a valid mathematical model of the network structure is available. In general, a mathematical model of the network structure is constructed by imposing constraints on some structural properties of optimal separation-networks, e.g., exclusion of redundant separations. The fundamental structural properties of separation-networks have been explored in the current work. The validity of the mathematical model, specifically with respect to redundancy, has been systematically studied. It is unequivocally demonstrated that redundant separators may be contained in an optimal separation-network under certain circumstances. Two definite classes of problems of separation-network synthesis have been parametrically studied extensively for illustration.

Keywords: process synthesis, separation-network, super-structure, multiple feed-streams, redundancy

Introduction

Separation-network synthesis (SNS) is carried out either heuristically or algorithmically (see, e.g., [1-12]). In spite of their effectiveness for various synthesis problems, heuristic methods often yield non-optimal solutions for some classes of SNS problems under certain circumstances. Algorithmic methods entail the construction of a "super-structure", presumed to contain the optimal structure. The algorithmic methods are generally implemented through mathematically rigorous computational procedures. They may, therefore, yield the optimal solutions for SNS problems provided that the super-structure is complete and the mathematical model is correctly constructed on the basis of this super-structure.

To configure both the potentially optimal structures as well as the super-structure is of utmost importance for algorithmic methods of process synthesis. In general, it is exceedingly difficult to generate these structures; only a limited number of papers has been published, which deal with the structure generation. To be able to accomplish this task, the fundamental structural properties of the structures must be known.

FRIEDLER et al. [13], KOVÁCS et al. [14], and KOVÁCS et al. [15] have explored unique or peculiar properties of the SNS problems, e.g., inclusion of recycling. Such unique properties need to be taken into account in generating the potentially optimal structures as well as the super-structure; nevertheless, these properties have been hardly investigated. In the current work, the completeness of the super-structures, specifically with respect to redundancy, is systematically studied; it is demonstrated that the involvement of redundancy cannot be totally avoided in synthesizing an optimal separation-network. The results are illustrated with two classes of SNS problems. In essence, this work presents some results from our continuing effort to explore the foundation of the algorithmic methods for process synthesis.

Any of the available methods including both algorithmic and heuristic methods for SNS disallows the inclusion of two or more separators performing an identical task in a network with a single feed-stream of n components, i.e., the synthesized network comprises at most $(n - 1)$ separators. Obviously, the separation of multiple feed-streams, each containing some or all of n components, can also be accomplished through a separation-network having no more than $(n - 1)$

* Author to whom correspondence should be addressed

separators without repeating any separation task. In composing a separation-network with multiple feed-streams, repeating a certain separation task is usually avoided between any pair of feed-streams and product-streams. Even when (n - 1) separators may be sufficient to construct a separation-network, the resultant network might not be optimal since the separation can also be accomplished through a network containing more than (n - 1) separators, some of which repeat one or more separation tasks, thereby contradicting a traditional heuristic rule for synthesizing nearly ideal systems. This differs from the situation in which it is economically advantageous to perform an additional separation; the product from the additional separation is eventually blended with other components from which it is separated. Nevertheless, the situation also requires an additional separation over the minimum number [2,4].

Fundamental Properties of Feasible Separation-Networks

Evidently, a stream must not be fed into any separator in an optimal separation-network where no separation occurs. Consequently, a single-component stream must not be fed into any separator. Another significant property of optimal separation-networks is stated as the theorem given below.

Theorem. Multiple feed-streams are separated into pure-product streams by a separation-network comprising simple and sharp separators, dividers, and possibly mixers. Then, every divider is in a loop of this network if the cost of the network is the sum of the costs of the separators, each of which is a monotone increasing concave function of its mass load, and if the network is optimal (see Appendix).

In the light of the fundamental properties of feasible and potentially optimal separation-networks described in the preceding two paragraphs, two classes of SNS problems are examined through extensive parametric studies. These simple problems illustrate that more than (n - 1) separators may appear in an optimal separation-network. In both classes of problems, single-component (pure) product-streams are to be generated from two multicomponent feed-streams by means of simple and sharp separators together with dividers and mixers.

Parametric Studies

The cost of a separation-network is regarded as the sum of the costs of its separators. By following the usual convention of facilitating computation and comparison, the cost of the i^{th} separator, c_i, is considered to be a concave and monotone increasing function of its mass load, e.g.,

$$c_i = (f_i \cdot D_i)^b$$

Table 1. Pertinent information on the first class of separation-network synthesis problems.

	A	B	C
Feed 1	A1	B1	C1
Feed 2	A2	B2	C2
Product 1	A1+A2	0	0
Product 2	0	B1+B2	0
Product 3	0	0	C1+C2

Note: The degree of difficulty of any separation is assumed to be 1

In this expression, f_i is the mass load through the i^{th} separator; D_i, the degree of difficulty of the i^{th} separation; and b, a constant between 0 and 1 (see, e.g., [9]). The value of b is taken to be 0.6 for the present work.

As commonly practised, the components in a stream forming a ranked list are arranged in the descending order of a certain property of any chemical species involved, e.g., relative volatility or particle size, on which the separation is based. The order in this list remains invariant when any component from the stream is eliminated by the separation. When two sublists are formed from the list by a separator, any component in the higher ranked sublist will remain higher than any component in the lower ranked sublist.

First class of problems

This class of problems involves two three-component (A,B,C) feed-streams, specifically feed1 (F1) and feed2 (F2), and three pure product-streams, each containing one of the components, A, B, and C. The pertinent information on this class of problems is listed in *Table 1*; for simplicity, the degree of difficulty of every separation is assumed to be 1, i.e., D_i is 1 for every i. We are to explore if redundant separators appear in an optimal separation-network and if a complete super-structure can be generated.

Only two types of separators are required for this class of problems; one is S1 separating components A and B, and the other is S2 separating components B and C. Because of the relative simplicity of the system of interest, all the structures satisfying the fundamental properties of feasible separation-networks described in the preceding section can be identified by exhaustively examining the appropriate combinations of S1 and S2. Specifically, as a consequence of the theorem, no feed-stream is split in an optimal structure since every feed-stream resides outside a loop. Naturally, when the feed-streams are separately connected to two individual separators identical in type, the resultant structures cannot be optimal because the cost function of each separator is concave, and thus, combining the two lowers the cost. In other words, there can be at most four separators in an optimal structure of the given class of problems: one for each of the two feed-streams, one for separating streams containing components A and B, and one for separating streams containing components B and C. The structures, each comprising four separators, in

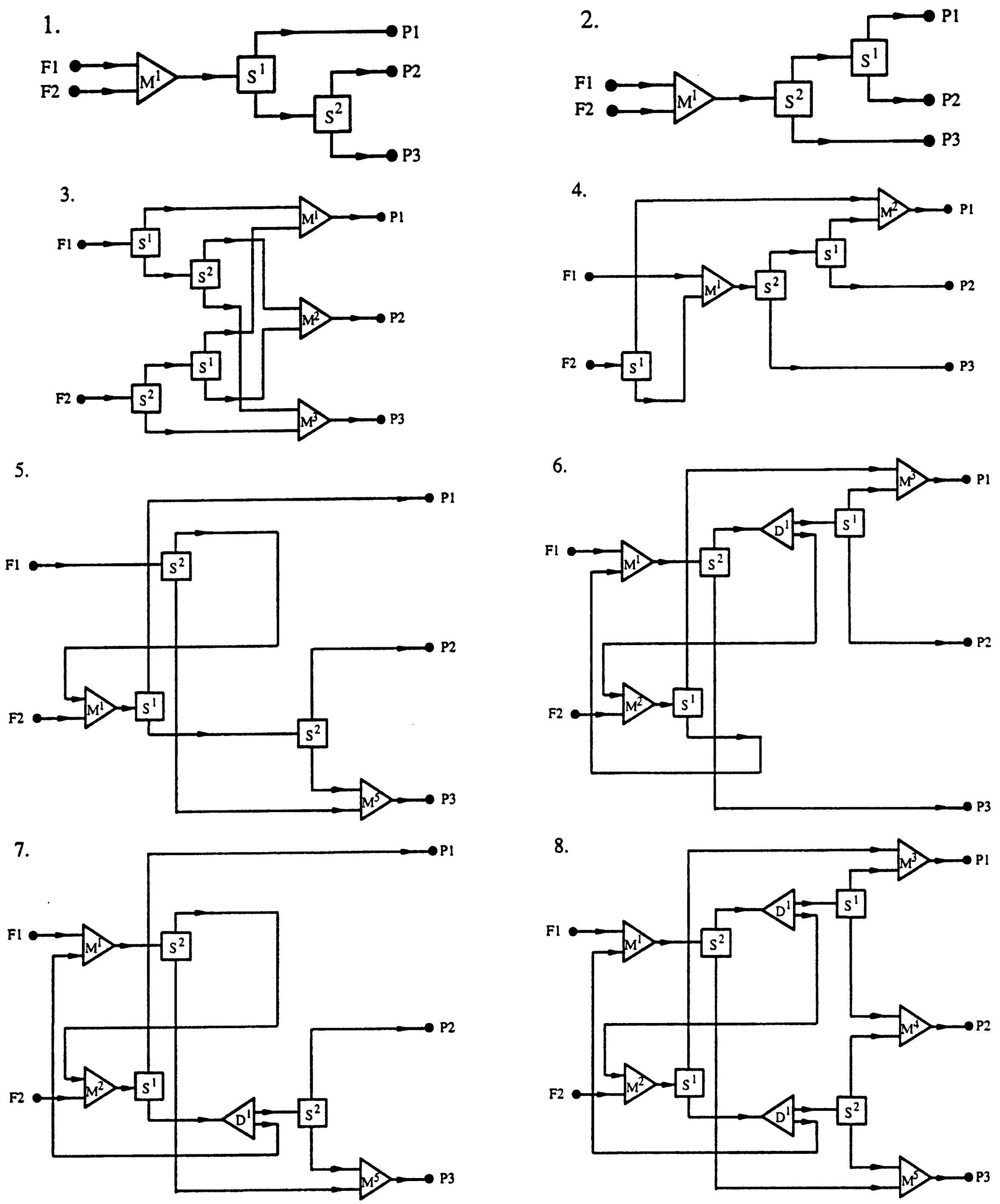

Fig.1. Feasible structures of the first class of separation-network synthesis problems.

which all the possible linkages of the streams are considered, are structures #3 and #8 in *Fig.1*. The structures containing three separators are those comprising one S1 and two S2's, which are structures #5 and #7, and those comprising two S1's and one S2, which are structures #4 and #6. The structures, each consisting of only two separators, are structures #1 and #2. It is worth noting that only these two among all the eight structures do not contain redundant separators.

Each of the eight structures is feasible in the sense that it yields the desired product-streams from any pair of three-component feed-streams. The most important question is if these feasible structures can be optimal in certain regions of the six dimensional space defined by the feed rates and compositions; hence, the structures have been parametrically studied through exhaustive trial and error by varying the feed rates and compositions and comparing the corresponding costs of all eight structures. Six out of the eight structures turn out to be indeed optimal under some feed conditions. *Table 2* lists an instance at which each structure is optimal as a numerical proof; however, structures #3 and #8 have not been found to be optimal under any circumstances even though they are feasible. Note that structures #4 through #7 contain redundant separators between a feed-stream and a product-stream. It is apparent that for an SNS problem with multiple feed-streams and pure product-streams, two or more

Table 2. Feed-streams where a specific structure is optimal in the first class of separation-network synthesis problems.

F1	F2	Optimal Structure
[130,1,100]	[100,50,30]	Structure#1
[1,50,100]	[100,1,200]	Structure#2
[5,10,100]	[200,1,100]	Structure#4
[100,1,200]	[100,10,5]	Structure#5
[1,1,100]	[200,1,100]	Structure#6
[100,1,200]	[100,2,2]	Structure#7

Table 3. Pertinent information on the second class of separation-network synthesis problems.

	A	B	C	D
Feed 1	A1	B1	C1	0
Feed 2	0	B2	C2	D2
Product 1	A1	0	0	0
Product 2	0	B1+B2	0	0
Product 3	0	0	C1+C2	0
Product 4	0	0	0	D2

Note: The degree of difficulty of any separation is assumed to be 1.

separators may perform an identical separation task between a feed-stream and a product-stream in an optimal structure even when pure product-streams are to be produced.

The optimal solution can always be deduced from a super-structure, an example of which is given in *Fig.2*, if it is constructed as the union of all the potentially optimal structures. On the contrary, it is extremely difficult, if not impossible, for heuristic methods to generate all six potentially optimal structures involving redundancy due to the fact that simple heuristic rules may be incapable of generating every potentially optimal structure even for simple problems.

Second Class of Problems

The pertinent information is given in *Table 3* on this class of SNS problems. Two three-component feed-streams, specifically feed1 (F1) (A,B,C) and feed2 (F2) (B,C,D), are to be separated into four pure product-streams, each containing one of the four components, A, B, C, and D.

All eight structures generated in the previously described exhaustive examination are given in *Fig.3*. They are feasible for any instance of the second class of SNS problems; also they are potentially optimal. *Table 4* indicates that six out of the eight feasible separation-networks can be optimal under some feed conditions; three of the six contain redundant separators. Even if structure #4 in *Fig.3* is feasible for each instance of the second class of problems, it cannot be optimal under any circumstance since structure #5 is always superior to structure #4 in terms of the cost; this can be readily

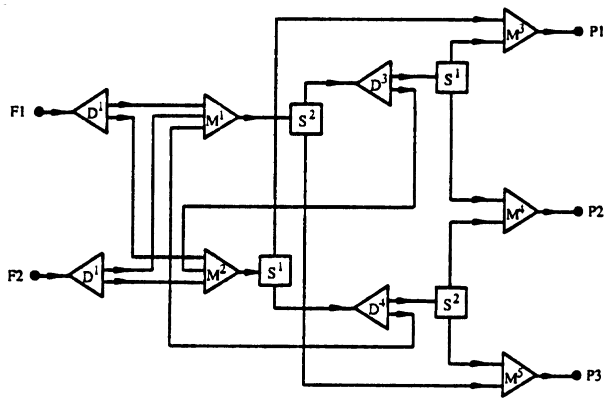

Fig.2. Super-structure of the first class of separation-network synthesis problems.

verified by means of the basic properties of concave functions, which give rise to the well-known inequality relation (see, e.g., [16]).

The super-structure given in *Fig.4* can be constructed as the union of all potentially optimal structures. The optimal solution can always be generated from this super-structure.

Conclusions

The fundamental structural properties of separation-networks have been examined for the purpose of synthesizing the complete set of potentially optimal networks. Two definitive classes of problems of separation-network synthesis have been extensively studied parametrically for illustration. Specifically, it is unequivocally demonstrated that the frequently-invoked heuristic rule or constraint on redundancy of separators may prevent the truly optimal solutions to be obtained. This heuristic rule excludes two or more separators performing an identical separation task between a feed-stream and a product-stream in a separation-network with multiple feeds. In reality, identical separation tasks may appear in an optimal network between a pair of feed-stream and product-stream; therefore, they must be allowed in establishing the super-structure for an algorithmic method or in determining a separation-network by a heuristic method. It should be cautioned, however, that a variety of practical considerations, such as piping cost, pumping energy, maintainability, and controllability, may overshadow the desirability of repeating an identical separation task in a separation-network in some situations.

Acknowledgement

This research was partially supported by the Hungarian Science Foundation Grant No. T-014212.

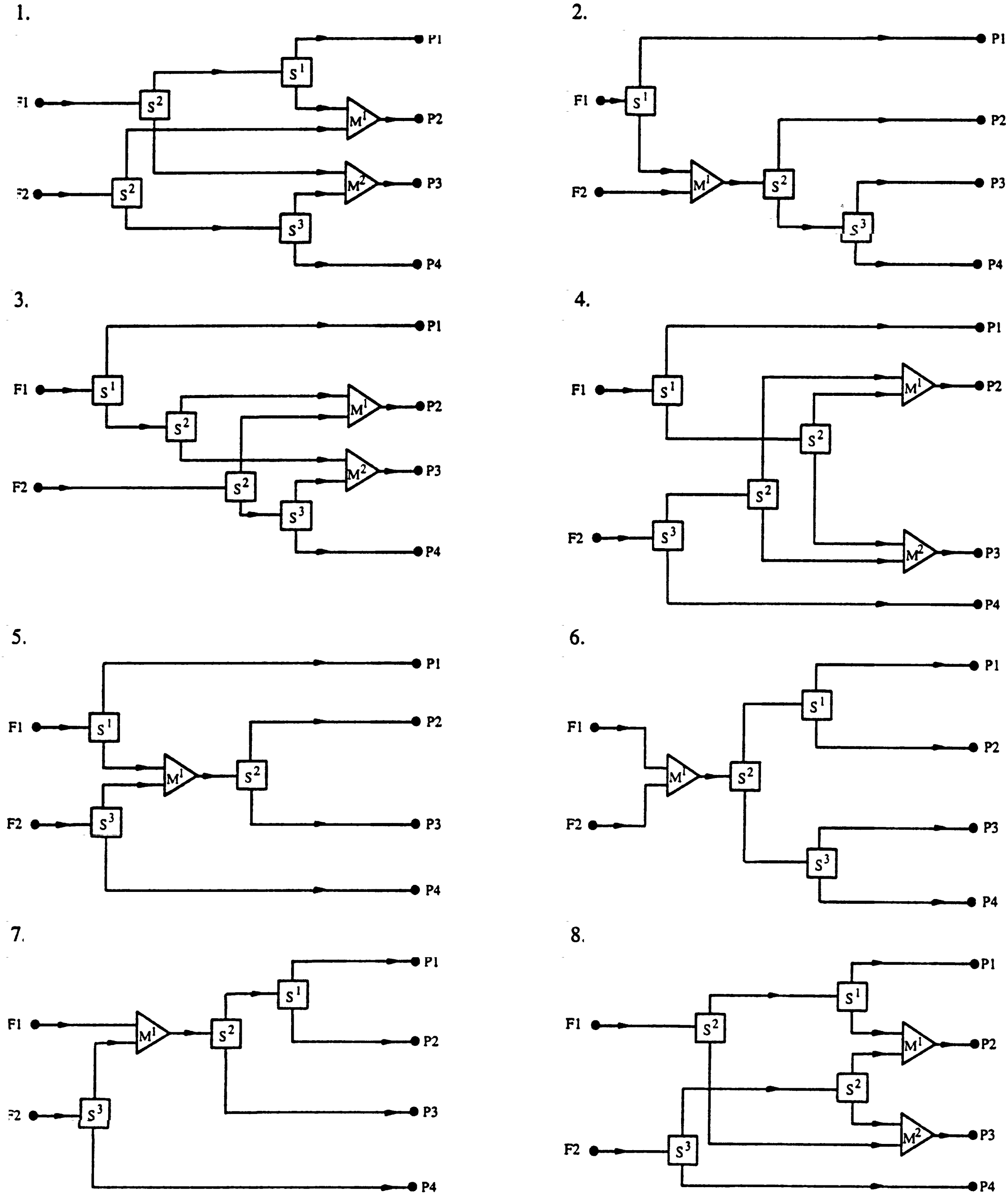

Fig.3. Feasible structures of the second class of separation-network synthesis problems.

Table 4. Feed-streams where a specific structure is optimal in the second class of separation-network synthesis problems

F1	F2	Optimal Structure
[10,10,100,0]	[0,100,10,10]	Structure#1
[150,10,1,0]	[0,110,30,10]	Structure#2
[150,10,100,0]	[0,110,30,10]	Structure#3
[100,10,70,0]	[0,20,10,10]	Structure#5
[100,10,150,0]	[0,20,10,10]	Structure#7
[10,30,110,0]	[0,100,10,150]	Structure#8

SYMBOLS

c_i	cost of the i^{th} separator
f_i	mass load through the i^{th} separator
D_i	degree of difficulty of the i^{th} separation
b	constant with a value of 0.6
A	component of the streams
B	component of the streams
C	component of the streams
D	component of the streams
F1	feed-stream 1
F2	feed-stream 2
P1	product-stream 1
P2	product-stream 2
P3	product-stream 3
P4	product-stream 4
S1	separator of type 1
S2	separator of type 2
st	original stream prior to splitting
*st*1	stream 1 after splitting

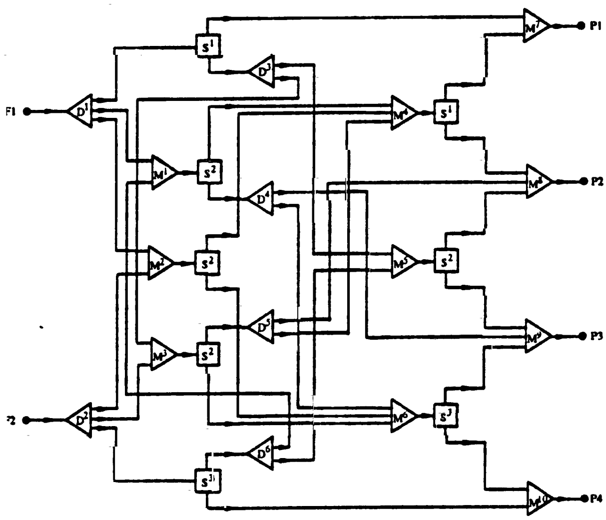

Fig.4. Super-structure of the second class of separation-network synthesis problems.

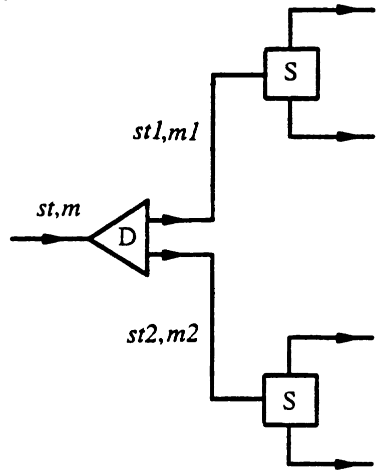

Fig.5. Stream splitting.

*st*2	stream 2 after splitting
m	mass load of stream *st*
*m*1	mass load of stream *st*1
*m*2	mass load of stream *st*2
k	real variable for changing *m*1 and *m*2

REFERENCES

1. HENDRY J.E. and HUGHES R.R.: Chem Eng. Prog., *1972*, 68(6), 71-76
2. THOMPSON R.W. and KING C.J.: AIChE J., *1972*, 18, 941-948
3. WESTERBERG A.W. and STEPHANOPOULOS G.: Chem. Eng. Sci., *1975*, 30, 963-972
4. SEADER J.D. and WESTERBERG A.W.: AIChE J., *1977*, 23, 951-954
5. NATH R. and MOTARD R.L.: AIChE J., *1981*, 27, 578-587
6. NISHIDA N., STEPHANOPOULOS G. and WESTERBERG A.W.: AIChE J., *1981*, 27, 321-351
7. FLOUDAS C.A.: AIChE J., *1987*, 33, 540-550
8. WEHE R.R. and WESTERBERG A.W.: Computers Chem. Engng., *1987*, 11, 619-627
9. FLOUDAS C.A. and ANASTASIADIS S.H.: Chem. Eng. Sci., *1988*, 43, 2407-2419
10. MOCSNY D. and GOVIND R.: Computers Chem. Engng., *1989*, 13, 839-849
11. HUANG Y.W. and FAN L.T.: „An Adaptive Heuristic Based System for Synthesis of Complex Separation Sequences," in Artificial Intelligence Applications in Process Engineering, Academic Press, San Diego, CA., pp. 311-361, 1991
12. FENG G. and FAN L.T.: Ind. Eng. Chem. Res., *1996*, 35, 1951-1958
13. FRIEDLER F., KOVÁCS Z. and FAN L.T.: „Unique separation networks for improved waste elimination," Proc. ACS Special Symposium on Hazardous-Waste Management, II, 457-460, Atlanta.(1992).
14. KOVÁCS Z., FRIEDLER F. and FAN L.T.: Computers Chem. Engng., *1995*, 19, S107-112
15. KOVÁCS Z., FRIEDLER F. and FAN L.T.: AIChE J., *1993*, 39, 1087-1089
16. MADDOX I.J.: Elements of Functional Analysis, 2nd ed., Cambridge University Press, pp.22. 1988

Appendix

Proof of the Theorem on the Dividers in an Optimal Separation-Network

Theorem. Multiple feed-streams are separated into pure-product streams by a separation-network comprising simple and sharp separators, dividers, and possibly mixers. Then, every divider is in a loop of this network if the cost of the network is the sum of the costs of the separators, each of which is a monotone increasing concave function of its mass load, and if the network is optimal.

Proof. Let us hypothesize that stream *st* with a mass load of *m* and residing outside a loop in an optimal separation-network is split into two streams, stream *st1* with a mass load of *m1* and stream *st2* with a mass load of *m2*. The resultant configuration is depicted in *Fig.5.*

Since the mass load of each stream in the optimal structure is known, the mass load through the i^{th} separator in the network, f_i, can be calculated as follows:

$$f_i = f_i^0 + f_i^1 + f_i^2$$

where f_i^1 and f_i^2 are the mass loads attributable to *m1* and *m2*, respectively, and f_i^0 is the mass load resulting from all other streams. As such, the cost function of the optimal separation-network, *cost*, can be calculated as

$$cost = \sum_i g_i\left(f_i^0 + f_i^1 + f_i^2\right) \qquad \text{(A-1)}$$

where $$g_i(x) = \left(D_i x\right)^{0.6}$$

and D_i is the degree of difficulty of the i^{th} separation.

Now let us vary the splitting ratio of stream *st* into streams *st1* and *st2* without varying the total mass load, *m*, or equivalently the sum of mass loads of the two streams. Changing the mass load of *st1*, i.e., *m1*, to

$$\left(k \cdot \frac{m1+m2}{m1}\right) \cdot m1 \text{ , } 0 \le k \le 1$$

and the mass load of *st2*, i.e., *m2*, to

$$\left((1-k) \cdot \frac{m1+m2}{m2}\right).$$

does not alter the total mass load of *st*, i.e., *m*, since

$$k \cdot \frac{m1+m2}{m1} \cdot m1 + (1-k) \cdot \frac{m1+m2}{m2} \cdot m2 = m .$$

Thus, f_i^1 is transformed to

$$k \cdot \frac{m1+m2}{m1} \cdot f_i^1 ,$$

and f_i^2 is transformed to

$$(1-k) \frac{m1+m2}{m2} \cdot f_i^2 .$$

Hence,

$$cost(k) = \sum_i g_i \left(f_i^0 + \frac{k \cdot (m1+m2)}{m1} f_i^1 + \frac{(1-k) \cdot (m1+m2)}{m2} f_i^2 \right). \qquad \text{(A - 2)}$$

It is worth noting that f_i^0 attributable to all other streams are unaffected by the change in the splitting ratio, because the mass load of *st*, i.e., *m*, is fixed. The *Eq.(A-2)* indicates that the cost of the network depends on *k*.

When $k = m1/(m1+m2)$ or $k = m1/m$, *Eq.(A-2)* reduces to *Eq.(A-1)*, i.e., the initial structure is recovered. Since the initial structure is persumed to be optimal, *cost*(*k*) is minimum at

$$0 < k = \frac{m1}{m1+m2} < 1.$$

Since function g_i is concave, i.e., its second derivative, g_i'', is negative,

$$cost(k)'' = \sum_i \left(\frac{(m1+m2)}{m1} \cdot f_i^1 - \frac{(m1+m2)}{m2} \cdot f_i^2 \right)^2 g_i'' \left(f_i^0 + \frac{k \cdot (m1+m2)}{m1} f_i^1 + \frac{(1-k) \cdot (m1+m2)}{m2} f_i^2 \right).$$

is also negative, thereby, implying that *cost*(*k*) is also concave in the interval [0,1], and consequently, its minimum is at either 0 or 1. This means that stream *st* outside a loop is not split, thus contradicting the initial hypothesis. In other words, every divider must be in a loop of any optimal separation-network with multiple feed-streams and pure product-streams.