

## Solution of separation network synthesis problems by the P-graph methodology

István Heckl,<sup>a</sup> Ferenc Friedler,<sup>a</sup> L. T. Fan<sup>b</sup>

<sup>a</sup>*Department of Computer Science, University of Pannonia, Egyetem u. 10, Veszprém, 8200, Hungary, Istvan.Heckl@gmail.com, Friedler@dcs.vein.hu*

<sup>b</sup>*Department of Chemical Engineering, Kansas State University, Manhattan, KS 66506, USA, fan@ksu.edu*

### Abstract

The current work demonstrates that separation-network synthesis (SNS) problems can be transformed into process-network synthesis (PNS) problems: The SNS problems constitute a particular class of PNS problems. Thus, the transformed SNS problems are solvable by resorting to the P-graph methodology originally introduced for the PNS problems. The methodology has been unequivocally proven to be inordinately effective.

**Keywords:** separation-network synthesis, optimization, P-graphs, process-network synthesis, mathematical modeling

### 1. Introduction

A separation network comprises separators, dividers, mixers, and streams linking them. Depending on their locations, these streams can be categorized as feed, intermediate and product streams. To yield the desired product streams from the given feed streams, a separation network performs a sequence of separation tasks [1].

A large number of different separation networks are capable of producing the same product streams. These networks differ in the numbers of separator included and the interconnections among them, as well as in their total costs. The aim of a separation-network synthesis (SNS) problem is to identify the most favorable, i.e., optimum, network, often in terms of cost, from a multitude of alternatives. A typical example is the refining of crude oil to yield various products.

A process network creates the desired products from the specific raw materials with a given set of operating units. The objective of process-network synthesis (PNS) is also to identify the most favorable, i.e., optimum, network. The P-graph methodology is a graph theoretical approach for solving PNS problems. The P-graphs are bipartite graphs, each comprising nodes for a set of materials, a set of operating units, and arcs linking them. The materials can be the raw materials, intermediates, and products. The operating units are defined in terms of input and output materials as well as their ratios.

Apparently, SNS and PNS problems are analogous. Nevertheless, there is a fundamental difference between them: In general, the number of possible streams,

which are obviously materials, involved in any SNS is infinite, while that involved in any PNS is finite. For instance, even if only two components are involved in a separation network, a variety of streams, each with an arbitrary composition, can be generated from them by means of mixers. This fundamental difference implies that a separation network can not generally be transformed into a process network. The exceptions are separation networks in which mixers precede only the products; in any of such separation networks, the number of streams is finite.

## 2. P-graph-based methodology

Friedler et al. [2] have proposed P-graphs (process graphs) for PNS problems and have identified five axioms underlying the combinatorially feasible process networks, i.e., solution structures. These axioms have given rise to various algorithms including the maximum structure generator, MSG [3], the solution structure generator, SSG [2], and the optimal structure generator algorithm, ABB [4], which is based on an accelerated branch-and-bound strategy. The P-graph-based methodology has demonstrated its efficiency in many areas such as emission reduction [5], optimal retrofit design for a steam-supply system [6], and downstream processes for biochemical production [7]. Our aim is to extend the P-graph-based methodology to SNS.

In the P-graph-based methodology, a process network comprises two types of nodes, the nodes for materials and those for operating units. Hence, P-graphs are bipartite graphs as mentioned earlier. In the P-graph representation of a process network, the maximum available raw materials may be constrained, and the rate of manufacturing of each product must be specified. An operating unit produces its output materials if all its input materials are supplied. The input materials are consumed according to the rates given on the arcs leading to the respective operating unit. The input and output materials, and the aforementioned rates collectively define formally an operating unit. Moreover, an operating unit may have upper and lower capacities. At any material node, the sum of the outgoing flows is equal to the sum of the incoming flows, i.e., the mass balance holds.

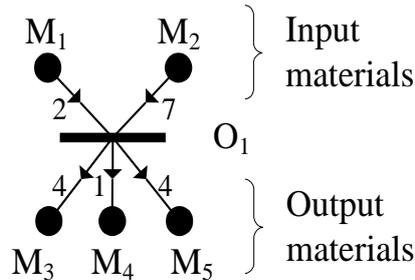


Figure 1. Graphical representation of an operating unit

Figure 1 illustrates operating unit  $O_1$ , which has two input materials,  $M_1$  and  $M_2$ , and the three output materials,  $M_3$ ,  $M_4$ , and  $M_5$ ;  $O_1$  converts 2 units of  $M_1$  and 7 units of  $M_2$  into 4 units of  $M_3$ , 1 unit of  $M_4$ , and 4 units of  $M_5$ .

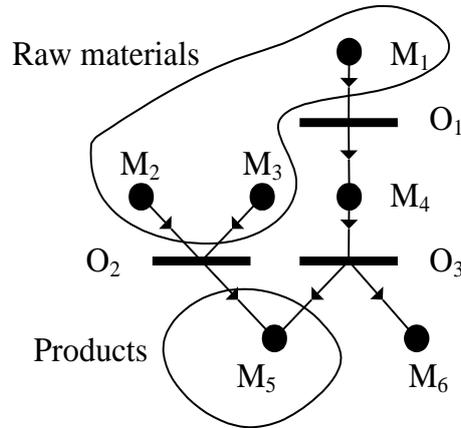


Figure 2. PNS network involving three operating units and six materials

Figure 2 represents a process network featuring operating units  $O_1$ ,  $O_2$ , and  $O_3$ , and materials  $M_1$ ,  $M_2$ , ..., and  $M_6$ , where  $M_1$ ,  $M_2$ , and  $M_3$  are the raw materials;  $M_4$ , an intermediate;  $M_5$ , the product; and  $M_6$ , a byproduct.

### 3. SNS problems with pure products

General SNS problems can not be transformed readily into PNS problems: A separation network often contains a mixer, depending on the ratio of its inputs, a mixer can yield a variety of streams, each with an arbitrary composition, and thus, the number of possible outlets is infinite. In contrast, a process network contains only a finite number of materials.

Heckl et al. [8] and Heckl et al. [9] have proposed a solution method for SNS problems, involving simple, sharp separators with proportional cost functions by applying different separation methods. The method, termed SNS-LIN, deploys a linear mathematical model, which can be solved efficiently; moreover, it invariably generates a super-structure in which mixers precede only the products. Consequently, the number of streams, i.e., materials, is finite, thereby rendering it possible to solve this type of SNS problems with the methodology developed for PNS problems.

A simplified version of SNS-LIN is addressed first where only pure products and a single separation method are considered. Initially, a material node needs to be introduced for each stream in the super-structure, which is followed by the introduction of an operating node representing each separator.

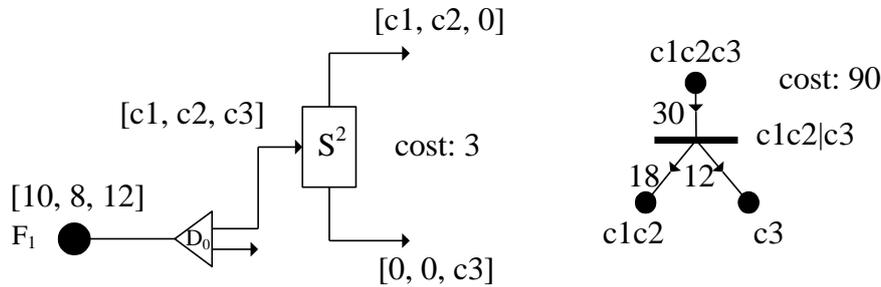


Figure 3. Representation of a separator and the corresponding operating unit

The symbol for a material signifies its components, e.g., material  $c_1c_2$  contains components  $c_1$  and  $c_2$ , and the symbol for an operating unit signifies the nature of separation, e.g., operating unit  $c_1c_2|c_3$  separates  $c_1c_2$  from  $c_3$ . The rates of flows through the arcs of the operating unit are computable from the component flow rates of the corresponding feed stream; see Fig. 3. The cost of the operating unit is calculable from the cost of the separator and the rate of the material input.

Upon defining all the materials and operating units, the maximal structure, all solution structures, and the optimal structure are determined by algorithms MSG, SSG, and ABB, respectively. Algorithm SSG generates five solution structures for a three-component problem, and algorithm ABB determines the optimal and a finite number of near optimal structures in ranked order directly from the maximal structure. The optimum value of the PNS problem and the original SNS-LIN are identical, thus ascertaining the validity of the transformation.

#### 4. SNS problems involving different separator families

Separation induced by the difference in volatility has long been ubiquitous in practice. Nevertheless, the implementation of methods of separation induced by the differences in other properties has been steadily gaining popularity in recent years [8]: These methods are potentially capable of leading to substantial energy saving [1]. The aforementioned transformation procedure and the P-graph methodology are applicable when several separation families are available.

#### 5. SNS problems with multi-component products

The inclusion of multi-component products requires the explicit representation of the mixers in the maximal structure. A single operating unit is incapable of representing a mixer: While an operating unit needs all its inputs to function, the mixer needs just one input. Figure 4 depicts a mixer as multiple operating units, each with a single input and a single output. Note that one operating unit is needed for each inlet of the mixer, and the mixer functions as long as one of its operating units functions.

#### 6. Example

Let us consider an illustrative example involving 3 components, 1 feed, 2 mixed-component product streams; see Table 1 and 2. Figures 5 and 6 show the solution structure with PNS and SNS notation respectively.

Table 1: The component flowrates of the feed and the products

	c1 (kg/s)	c2 (kg/s)	c3 (kg/s)
F <sub>1</sub>	6	5	9
P <sub>1</sub>	4	2	7
P <sub>2</sub>	2	3	2

Table 2: The available separators

Components	c1	c2	c3
Separators	S <sup>1</sup>		S <sup>2</sup>
Total cost coefficients (\$/kg)	4		2

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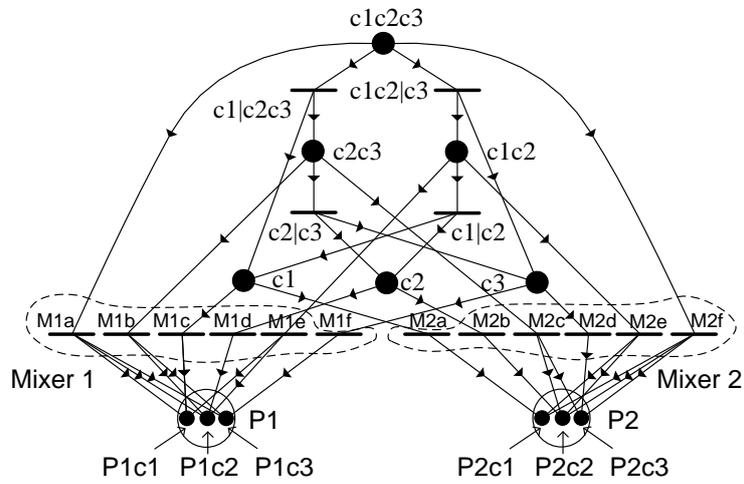


Figure 4. Maximal structure of the example

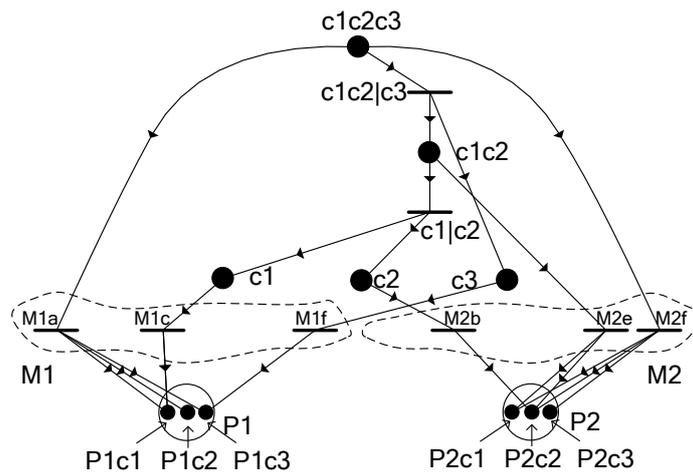


Figure 5. Solution structure of the example with PNS notation

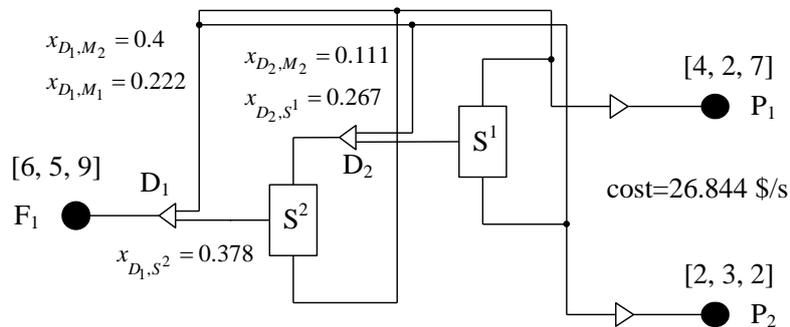


Figure 6. Solution structure of the example with SNS notation

## 7. Conclusions

A procedure is introduced to transform three classes of SNS problems into the corresponding PNS problems. The first class is the SNS problems with pure products; the second, the SNS problems involving different separator families; and the third, the SNS problems with multi-component products. The resulting PNS problems are solved by resorting to algorithm MSG for the maximal structure generation, algorithm SSG for solution structure generation, and algorithm ABB for accelerated branch-and-bound search, derived for PNS problems. The transformation involves the steps for the definition of the material for each stream in the super-structure; the specification of an operating unit for each separator in the super-structure; and the determination of the cost and other parameters of the operating units. The optimal structures obtained for the transformed PNS problems are identical to those obtained by directly solving the SNS problems, thereby indicating that the transformation is indeed valid.

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