



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

István Heckl^a, Ferenc Friedler^{a,*}, L.T. Fan^b

^a Department of Computer Science and Systems Technology, University of Pannonia, Egyetem u. 10, Veszprém 8200, Hungary

^b Department of Chemical Engineering, Kansas State University, Manhattan, KS 66506, USA

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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.

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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.

Separation networks and processes are ubiquitous throughout the chemical and allied industries (Amale & Lucia, 2008; Huang, Ramaswamy, Tschirner, & Ramarao, 2008; King, 1980; Takoungsakdakun & Pongstabodee, 2007). The energy demands and consequently the operating costs of separation tasks tend not only to be inordinately high but also to be capital intensive. Naturally, it is highly desirable that the structures of separation networks be optimized (Biegler, Grossmann, & Westerberg, 1997; Wang, Li, Hu, & Wang, 2008).

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 (Tahmassebi, 1986).

The methods for SNS problems are usually classified according to the search techniques for solution; they can be heuristic, evolutionary, or algorithmic. The main advantages of the heuristic methods are that these methods are applicable to industrial-scale problems, yield acceptable solutions with dispatch compared to the other methods, and are capable of taking into accounts various problem specific constraints. On the other hand, the heuristic methods frequently require extensive manual effort for solution, and yet cannot assure its optimality. In theory, the algorithmic methods render it possible to attain the optimal solution; nevertheless, they usually require excessive computational effort. A problem of any relevant size often cannot be solved fully with these methods; as a result, simplified models are, more often than not, adopted. The evolutionary methods are situated between the heuristic and algorithmic methods in terms of computational effort required and quality of solution attained.

The essence of heuristic methods is to obtain an acceptable solution structure through a sequence of decisions on the basis of engineering knowledge systematically acquired through experience. A heuristic method has been introduced by Gomez and Seader (1976) for estimating the costs of different structures; the method is capable of reducing the search space for identifying the optimal solutions. An optimization method enhanced by pinch technology, which is essentially heuristic in nature, has been presented by Fonyó, Mészáros, Rév, and Kaszás (1985) to implement energy integration.

An evolutionary method initiates a search at a plausible initial structure and reaches the optimal or, at least, near-optimal structure by sequentially improving it. A two-stage evolutionary method has been demonstrated by Muraki and Hayakawa (1984)

* Corresponding author. Tel.: +36 88 424483; fax: +36 88 428275.

E-mail addresses: Heckl@dcs.vein.hu (I. Heckl), Friedler@dcs.vein.hu (F. Friedler), fan@ksu.edu (L.T. Fan).

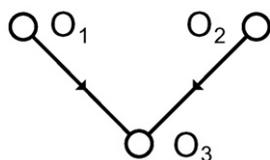


Fig. 1. Conventional graph representation of a process network.

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 give rise to systematic computational approaches to the solution of SNS problems. The synthesis of separation networks has been implemented by Floudas (1987) 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 conventional NLP algorithm. Another method has been introduced by Quesada and Grossmann (1995) 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 proposed approach is also algorithmic. Its main advantage is that it is based on the rigorous super-structure, thereby assuring the optimality of the solution (Kovács, Ercsey, Friedler, & Fan, 2000), and it can take into account separators of different families, e.g., separators based on rectification and extraction (Heckl, Kovács, Friedler, Fan, & Liu, 2007).

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 cannot 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.

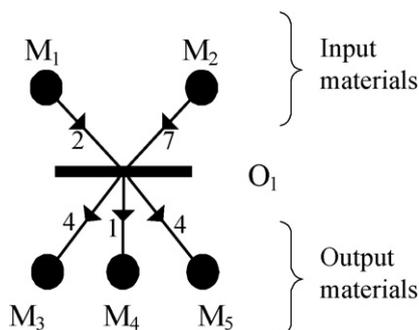


Fig. 2. Graphical representation of an operating unit.

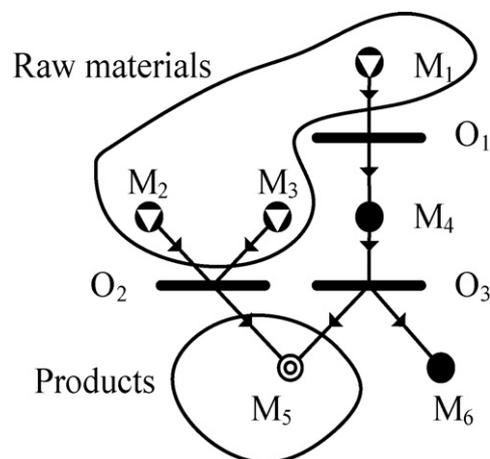


Fig. 3. PNS network involving three operating units and six materials.

2. P-graph-based methodology

Friedler, Tarjan, Huang, and Fan (1992) have proposed the P-graph (process graph) framework for PNS problems. This framework has three fundamental cornerstones: the representation of process networks with P-graphs; five axioms underlying the combinatorially feasible process networks, i.e., solution structures; and effective algorithms derived from the first two cornerstones.

The conventional graph representation of a process network is ambiguous; consequently, it is unfit for creating rigorous algorithms. For example, the nodes represent the operating units and the arcs indicate the material flows between them in Fig. 1, which gives rise to two possible interpretations. First, two different materials are produced separately, one by operating unit O_1 and the other by operating unit O_2 . Moreover, it is necessary to feed both of them to operating unit O_3 . Second, one material is produced by both operating units O_1 and O_2 . This material is subsequently fed to operating unit O_3 .

In the P-graph-based methodology, a process network comprises two types of nodes, the nodes for materials and those for operating units. The arcs between these nodes signify that a material is input to or output from an operating unit. 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

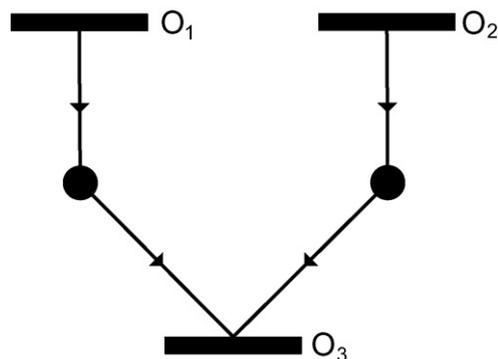


Fig. 4. PNS network involving three operating units and two materials.

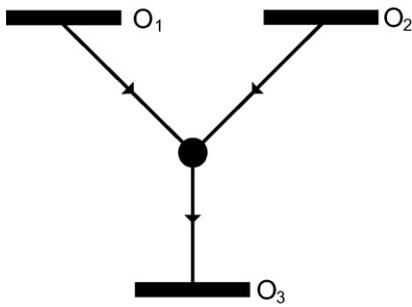


Fig. 5. PNS network involving three operating units and one material.

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.

Fig. 2 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 two units of M_1 and seven units of M_2 into four units of M_3 , one unit of M_4 , and four units of M_5 .

Fig. 3 represents a process network featuring operating units O_1 , O_2 , and O_3 , and materials M_1, M_2, \dots, 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.

The P-graph representation renders it possible to discern the two different meanings of Fig. 1. First, two different materials are produced separately, one by operating unit O_1 and the other by operating unit O_2 . Moreover, both materials are fed to operating unit O_3 ; see Fig. 4. Second, one material is produced by both operating units O_1 and O_2 , and this material is subsequently fed to operating unit O_3 ; see Fig. 5.

Five axioms have been identified to describe the properties of a combinatorially feasible network. These are the following: (a)

every demand is represented in the structure; (b) a material represented in the structure is a resource if and only if it is not an output from any operating unit represented in the structure; (c) every operating unit represented in the structure is defined in the synthesis problem; (d) any operating unit represented in the structure has at least one directed path leading to a product; and (e) a material belongs to the structure, it must be an input to or output from at least one operating unit represented in the structure.

These axioms have given rise to various algorithms including the maximum structure generator, MSG (Friedler, Tarjan, Huang, & Fan, 1993), the solution structure generator, SSG (Friedler et al., 1992), and the optimal structure generator algorithm, ABB (Friedler, Varga, & Fan, 1995), which is based on an accelerated branch-and-bound strategy.

The maximal structure of a process synthesis problem comprises all the combinatorially feasible structures capable of yielding the specified products from the specified raw materials. Certainly, the optimal network or structure is among these feasible structures. The implementation of this algorithm on a computer involves four major phases.

In the first phase, synthesis problem (P, R, O) is formulated by inputting set M of all plausible materials, set P of the final products, set R of the raw materials, and set O of all plausible candidate operating units. Note that set M contains not only all the intermediate materials associated with the operating units in set O but also the final products in set P and the raw materials in set R .

In the second phase, an initial, or input, structure of the network is constructed by merging all the common material nodes.

In the third phase, the materials and operating units, which should not belong to the maximal structure are eliminated stepwisely and layer by layer, starting from the deepest layer, i.e., raw-material end, of the input structure by assessing alternatively the nodes in a material layer with those in the succeeding oper-

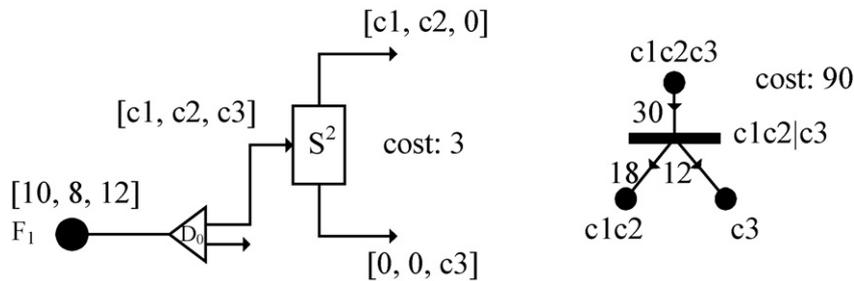


Fig. 6. Representation of a separator and the corresponding operating unit.

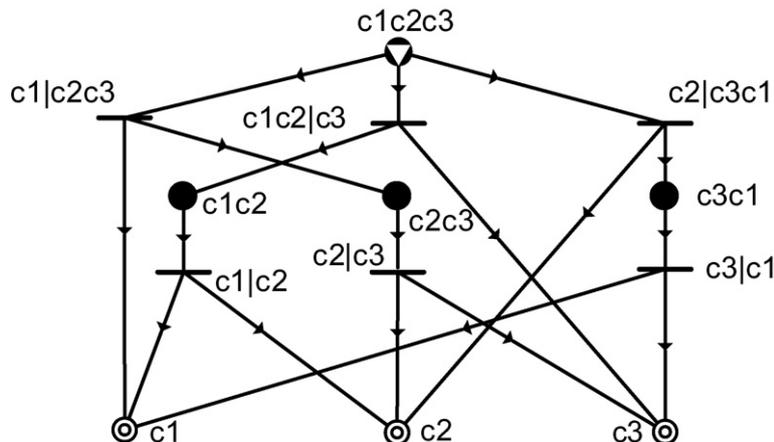


Fig. 7. Maximal structure of a pure product problem.

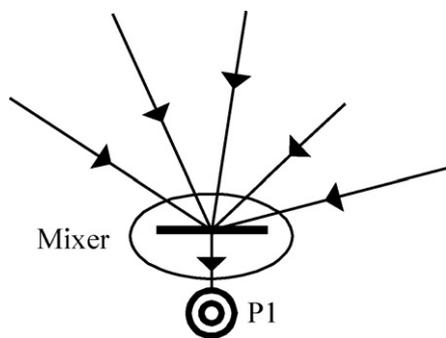


Fig. 8. Unsuitable P-graph representation of a mixer; a mixer cannot be uniquely represented by a single operating unit.

ating unit layer to ascertain that each intermediate material node has a producer and each operating unit node has its corresponding inputs. Naturally, the elimination of one node often leads to the elimination of other nodes linked to it.

In the fourth and final phase, the nodes are linked, again stepwisely and layer by layer, starting from the shallowest end, i.e., final-product end, of the remaining input structure by assessing the participation of the linked nodes in the production of one of the products. The unlinked nodes are excluded from the maximal structure.

Algorithm SSG generates all the solution structures, i.e., all combinatorially feasible flowsheets, capable of producing every desired product. The inputs to algorithm SSG includes the products in set P , the raw materials in set R , and all materials in set M containing all other pertinent materials, e.g., intermediate materials and byproducts, besides the materials in sets P and R . The inputs also include $\Delta[M]$, which is a set whose elements are pairs, each consisting of material x and mapping $\Delta(x)$, signifying all operating units that yield x , for each x in set M , i.e., $\Delta[M] = \{(x, \Delta(x)) | x \in M\}$. Moreover, the raw materials cannot be generated by any operating unit; thus, $\Delta(x) = \emptyset$ for every $x \in R$. Decision mapping $\delta[m]$, where m is an active set, is defined as $\{(x, \delta(x)) | x \in m\}$ where $\delta(x) \subseteq \Delta(x)$. $\delta[m]$ corresponds to a P-graph where each $x \in m$ material is produced by $\delta(x)$. With all the inputs in place, algorithm SSG is executed recursively by systematically and combinatorially selecting a series of active sets and carrying out decision mappings $\delta[m]$. The procedure is terminated when all the active sets are exhausted.

Any of the general branch-and-bound methods is inefficient in solving the MIP model of process synthesis: it gives rise to an unduly large number of free variables. These methods do not exploit the structural features of the process system. This deficiency is magnified when the model is based on the conventional super-structure containing all possible networks, the majority of which tends to be combinatorially infeasible and thus redundant for any sizeable process.

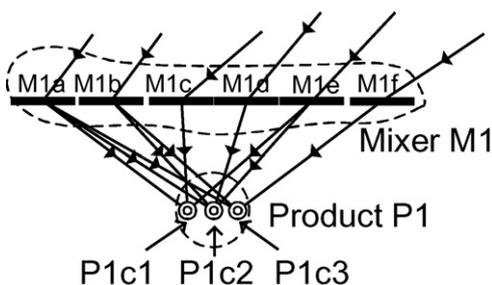


Fig. 9. Representation of a mixer and a multi-component product in the P-graph framework; one sub-operating unit is assigned to each of the potential inputs to the mixer.

Table 1

Component flowrates of the feed and the products.

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

In contrast, algorithm ABB judiciously exploits the structural features of the process to be synthesized, which manifest themselves in the maximal structure consisting of only combinatorially feasible networks, or flowsheets. The procedure is initiated at the final, or desired, product and proceeds upward through the maximal structure towards the raw materials, i.e., feeds. At each branching step, a decision is made about which operating unit or units should produce a given material. Algorithm ABB examines if the selection of an operating unit requires an additional operating unit to be selected. This is the case if the latter is the only one yielding a material necessary as the input to the former.

The P-graph-based methodology has demonstrated its efficacy in many areas such as emission reduction (Klemeš & Pierucci, 2008), optimal retrofit design for a steam-supply system (Halasz, Nagy, Ivicz, Friedler, & Fan, 2002), and downstream processes for biochemical production (Liu, Fan, Seib, Friedler, & Bertok, 2004). Our aim is to extend the P-graph-based methodology to SNS.

3. SNS problems with pure products

General SNS problems cannot 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. (2007) and Heckl, Friedler, and Fan (2009) 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 P-graph-based 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 unit node representing each separator.

The symbol for a material signifies its components, e.g., material c1c2 contains components c1 and c2, and the symbol for an operating unit signifies the nature of separation, e.g., operating unit c1c2|c3 separates c1c2 from c3. 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. 6. 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

Table 2

Available separators.

Separators	S ¹	S ²
Components to be separated	c1 c2, c3	c1, c2 c3
Total cost coefficients (\$/kg)	4	2

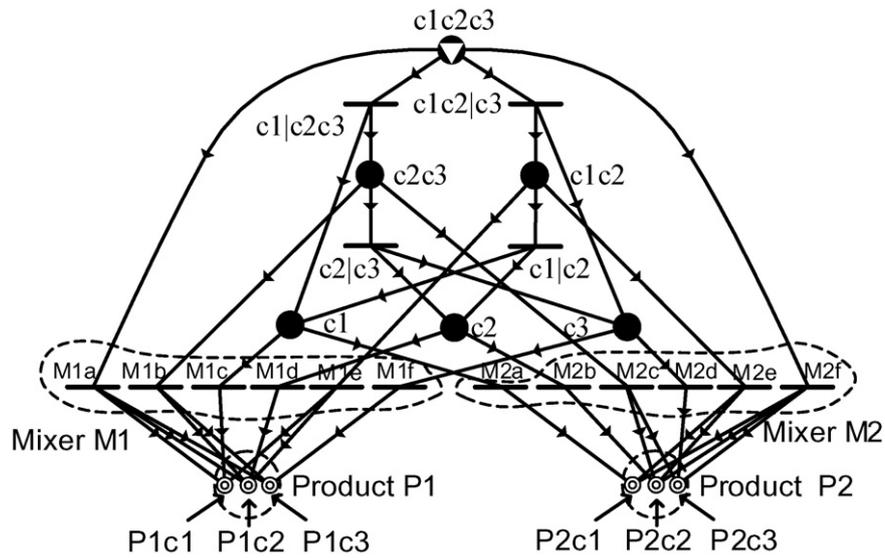


Fig. 10. Maximal structure of the example in Section 6.

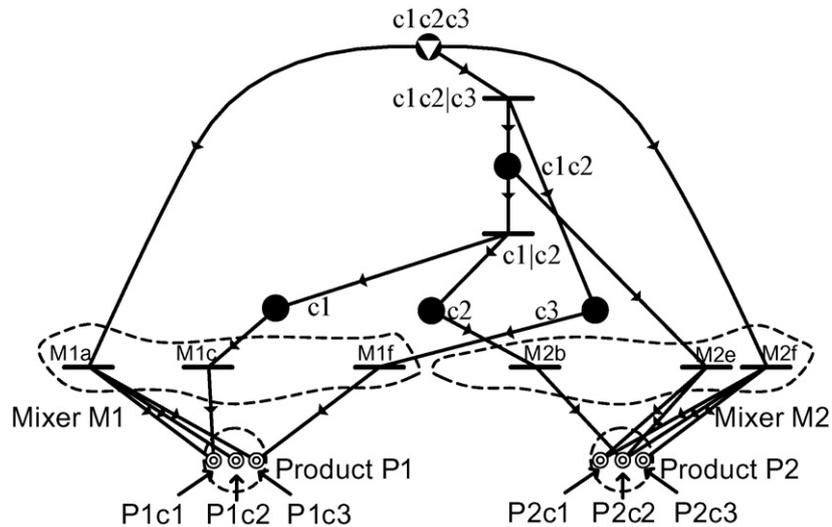


Fig. 11. Optimal network of the example in Section 6 with PNS notation.

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. Fig. 7 shows the maximal structure of a three-components, single-feed, pure-product problem. It is worth noting that simple, or purely physical, splitting and merging of material streams without inducing the transformation of materials are not explicitly indicated by operating units in the P-graph representation.

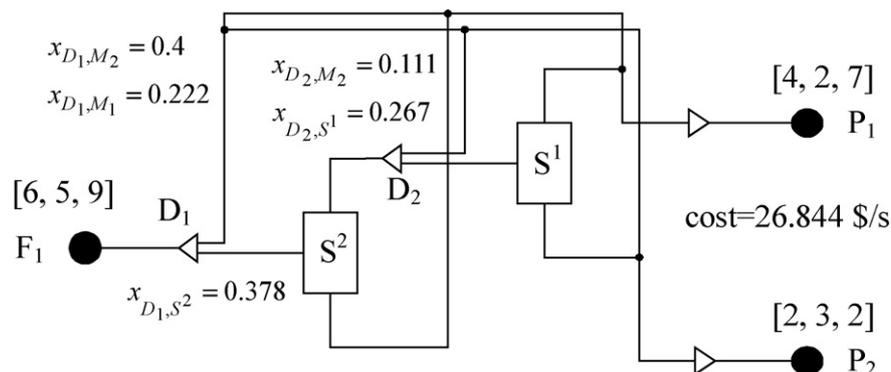


Fig. 12. Optimal network of the example in Section 6 with SNS notation.

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 (Heckl et al., 2009): these methods are potentially capable of leading to substantial energy savings (King, 1980). For instance, if the relative volatilities of two components are close to each other, it is reasonable to perform this separation by a method other than rectification, e.g., extraction. The transformation of a separator based on relative volatility, solubility, or any other property can be performed similarly.

5. SNS problems with multi-component products

The inclusion of multi-component products requires the explicit representation of the mixers in the maximal structure. Unfortunately, a mixer cannot be uniquely represented by a single operating unit as defined in the P-graph framework. In this framework, an operating unit, e.g., a reactor, normally requires all its inputs to function. In contrast, however, even if some of the potential inputs to a mixer are missing, it is still capable to mix the remaining inputs; see Fig. 8.

Fig. 9 depicts a mixer represented, for convenience, by multiple hypothetical operating units termed sub-operating units, each of which is assigned to a potential input to the mixer. Each of these sub-operating units has a single input and one or more outputs. Moreover, the number of such outputs is equal to the number of components in its input. Furthermore, the product, i.e., product P1, is represented, again for convenience, by three hypothetical materials termed sub-materials, one for each of the components in it in this illustration.

Fig. 10 depicts the maximal structure of a separation network, which involves one feed stream and two product streams. On this figure, mixers M1 and M2 are represented by sub-operating units M1a through M1f and sub-operating units M2a through M2f, respectively. Products P1 and P2 are represented by sub-materials P1c1, P1c2, and P1c3 and sub-materials P2c1, P2c2, and P2c3, respectively. The sub-operating units of each mixer and the sub-materials of each product are circled by dashed lines for lumping.

In Fig. 10, sub-operating unit M1a signifies that one of the inputs to mixer M1 is the feed to the entire network. Naturally, the feed contains all three components, and thus, sub-operating unit M1a is linked to sub-materials P1c1, P1c2, and P1c3. The inputs to sub-operating units M1b and M1e are materials c2c3 and c1c2, respectively. Thus, sub-operating unit M1b is linked to sub-materials P1c2 and P1c3; and sub-operating unit M1e to sub-materials P1c1 and P1c2. The inputs to sub-operating units M1c, M1d, and M1f correspond to materials c1, c2, and c3, respectively. Consequently, sub-operating unit M1c is linked only to sub-material P1c1; sub-operating unit M1d to sub-material P1c2; and sub-operating unit M1f to sub-material P1c3. Obviously, the representation of mixer M2 by sub-operating units can be visualized similarly. The number of links between mixer M1 and product P1 appears to exceed one; in reality, however, they collectively constitute a single link. For example, sub-operating M1b has two outputs but both are part of the single link between mixer M1 and product P1. Thus, sub-operating M1b performs neither splitting nor separation.

6. Example

Let us consider an example involving one feed stream containing three components and two product streams of mixed components.

The feed and the product streams are specified in Table 1, and the available separators are listed in Table 2. As indicated previously, the separation problem, termed SNS-LIN is to be solved here with the P-graph-based methodology (Heckl et al., 2007). This is an important separation problem featuring simple and sharp separators with proportional cost functions. Specifically, each separator has a single inlet and two outlets; each component of the inlet appears only in one of the outlets; and the cost of a separator can be calculated as the product of the flowrate of its inlet and its total cost coefficient. The total cost coefficient of a separator comprises both the operating and annualized investment costs. The cost of the separation network is the sum of the costs of its separators. Sections 3, 4, and 5 detail the conversion of SNS problems of this class into PNS problems.

Fig. 10, presented in the preceding section for illustration, exhibits the maximal structure generated for this example by algorithm MSG. It features four potential separators, 18 operating units and 12 materials. The solution time is 0.21 s on a PC (Athlon 2 GHz, 2GB RAM). Figs. 11 and 12 display the optimal network determined by algorithm ABB, the former represented by the PNS notation, and the latter, by the SNS notation. The optimal network involves two separators and two mixers. Fig. 11 shows that mixer M1 is represented by sub-operating units M1a, M1c, and M1f. Consequently, mixer M1 has three inputs; the same holds for mixer M2.

The SNS notation gives rise to essentially a pictorial representation of the separation network, which is easier to comprehend or visualize than the network represented by the PNS notation, which yields a compact and abstract representation. Nevertheless, as the structure of the separation network becomes increasingly large, the complexity of its representation will magnify exponentially. This complexity is substantially circumvented by resorting to the PNS notation. The solution of this example reveals that the P-graph-based methodology is indeed versatile to handle certain classes of SNS problems. For instance, it is capable of handling multiple separator families and of generating the near-optimal solutions in ranked order.

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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