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Reduced super-structure for a separation network comprising separators effected by different methods of separation

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ABSTRACT

Among separation systems, the ones comprising separators effected by different separation methods have been steadily gaining attention lately. Our earlier work has revealed that it is exceedingly complicated to optimally synthesize via super-structure any of these separation networks featuring simple and sharp separators, multiple feed and product streams, and mixed products. This complication can be substantially lessened by constituting a reduced super-structure for the network of interest. This super-structure profoundly simplifies the mathematical model and decreases the computational time required to yield the results identical to those obtained from the original super-structure.

1. Introduction

Separation-network synthesis (SNS) is one of the most important sub-disciplines of process synthesis: separation processes and networks are ubiquitous throughout the chemical and allied industries; see, e.g., King (1980), Huang, Ramaswamy, Tschirne, and Ramarao (2008), Takoungsakdakun and Pongstabodee (2007), and Amale and Lucia (2008). 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 separator networks be optimized; see, e.g., Biegler, Grossmann, and Westerberg (1997) and Wang, Li, Hu, and Wang (2008).

A separation network comprising separators, mixers, and dividers performs a sequence of separation tasks to yield the desired product streams from the given feed streams (Floudas, 1987). The multi-component streams present in the network are distinguishable according to their locations in the separation network; they can be the feed, intermediate and product streams.

Various combinations of the separators, mixers, and dividers give rise to a multitude of separation networks, which are capable of yielding the required product streams from a given multi-component feed stream or streams. The aim of SNS is to identify the structure of the most favorable separation network, often in terms of cost, from a multitude of alternatives. A typical example is the crude oil separation in which a countless number of products are manufactured (Tahmassebi, 1986).

Herein, the term, *separator family*, is defined as a set of separators that are effected by the same physical or chemical property. Any of the algorithmic methods for SNS tends to regard the available separators as belonging to a single separator family, e.g., the one effected by relative volatility. Nevertheless, separation networks, each containing separators from different separator families are becoming increasingly popular because of their immense potential for substantial cost reduction.

Thompson and King (1972) were among the firsts to synthesize separation sequences or networks. They have developed a semi-heuristic, semi-algorithmic method, which is implementable on a computer. The most significant outcome of their work is the well-known Thompson formula for determining the number of the separation networks yielding pure products. The formula indicates unequivocally that the number magnifies exponentially even for this simple class of separation-network synthesis problems.

A heuristic method has been proposed by Emtir, Rév, Mizsey, and Fonyó (1999), which takes into account the energy consumption for the separation of three-component feeds. They compared the energy demand of the integrated and coupled systems for various utilities. Demicoli and Stichlmair (2003) studied a separation network comprising complex, batch separators. They have proposed a novel operating mode for extracting efficiently the middle com-

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Nomenclature

Sets
C components
CO_a components in stream a
D dividers
F feeds
IM inner mixers
P products
PM product mixers
S separators

Parameters
$FE_{k,c}$ [kg/s] the component flowrate of component c in feed k
OC_s [$/kg] the overall cost coefficient of separator s
$PR_{k,c}$ [kg/s] the component flowrate of component c in feed k

Variables
$f_{a,c}$ [kg/s] component flowrate of component c in stream a
$x_{i,j}$ feed allocation ratio in stream (i, j)

Greek symbol
λ_a splitting ratio of stream a

Functions
first(a) the feed stream a originated from
next(a) the set of elements following a
prev(a) the set of elements preceding a
prev2(a) prev(prev(a))

ponent from a three component feed stream. In the first stage, the separator is operated in the closed operating mode with total reflux without product withdrawal. In the second stage, the complex column functions as an inverted column on the top of a regular one.

Floudas (1987) has proposed a systematic computational approach to the SNS involving a single feed stream, mixed products, and simple and sharp separators with non-linear cost function. He has solved the model resulting from the proposed super-structure of the network by resorting to a conventional NLP algorithm in GAMS. A method has been introduced by Quesada and Grossmann (1995) to determine the global optima of SNS problems with linear cost functions. The mathematical models based on the composition and component flowrates have been merged by resorting to a reformulation-linearization technique to circumvent the complexities due to the presence of bilinear terms in the model equations.

The notion of the rigorous super-structure has been presented by Kovács, Ercsey, Friedler, and Fan (2000); it contains the optimal network for every instance of the given problem. They have proposed a novel algorithm for generating the rigorous super-structure of an SNS problem involving only simple and sharp separators. The resultant mathematical model is linear, thereby giving rise to the solution without fail. More recently, Heckl, Kovács, Friedler, Fan, and Liu (2007) studied SNS involving separators of various families. They have demonstrated that the resultant novel approach can yield a solution superior to the solution obtained when SNS is carried out taking into account a single separator family. In the rigorous super-structure proposed, the product streams are invariably preceded by mixers. The mathematical model is formulated in terms of the feed allocation ratios, which render possible the solution by LP.

The algorithmic solution of any synthesis problem involves three major steps including: the construction of the network's structural model; the generation of the linear or non-linear mathematical programming model on the basis of the structural model; and the solution of the resultant model. Naturally, the larger the structural model, the more convoluted the mathematical model; and consequently, the harder and slower it is to solve it. This implies that it is imperative to construct the structural model with minimal complexity.

The current work reassesses a class of SNS problems, termed SNS-Multi for simplicity, posed by Heckl et al. (2007). Its aim is to craft a reduced super-structure for SNS-Multi that renders it possible to substantially facilitate the solution. SNS-Multi can be stated as follows: determine the cost-optimal separation network for transforming the compositions of n-component feed streams to obtain the specified product streams with a given set of simple and sharp separators where the available separators may belong to different separator families. Any separator's cost is regarded as a linear function of its mass load, and the cost of the separation network is the sum of the costs of the separators therein.

2. SNS-Multi with unreduced super-structure

The main difference between SNS-Multi (Heckl et al., 2007) and any conventional SNS is that while the former takes into account multiple separator families, the latter involves only a single separator family. Even at the dawn of SNS, Thompson and King (1972) alluded to the feasibility of applying multiple separator families. Nevertheless, it has attracted little attention. It is usually implicitly understood that SNS is performed with a single separator family. It is well known that $(n-1)$ different separations can be performed on a stream containing n components using a single separator family. $k(n-1)$ separations can be performed on such a stream applying k multiple separator families. For instance, the separation of a mixture comprising propylene (component A), propane (component B), and propadiene (component C) into its components can be carried out using three different separator families including distillation, extractive distillation with a polar solvent, and extraction (King, 1980). The component orders in the stream vectors are: A, B, and C for the first method; B, A, and C for the second method; and C, A, and B for the third method. Deploying various separator families magnifies the search space, thereby enhancing the probability of identifying a solution, which is superior to that attainable using a single separator family. For example, let us suppose that pure products are to be produced from an n-component feed stream with distillation only. If the relative volatilities of two components are close to each other, the cost of separation would be expensive. The cost can be significantly reduced by adopting another separator family.

Heckl et al. (2007) have demonstrated that any SNS-Multi problem invariably gives rise to an optimal structure in which mixers precede only the products. These mixers are termed *product mixers*. The significance of this property is that it specifies the positions of the mixers in the super-structure, thus greatly reducing the number of configurations to be explored. A stream can be linked only to separators or to product mixers, the latter linkages being termed *bypasses*. Naturally, the rigorous super-structure must contain all feasible configurations; as a result, every stream must be divided, and the outlets must be linked either to new separators or to product mixers. An additional separator is incorporated only if it is effective for separating at least one component contained in both outlets. If more than one separator produces the same streams from a given input, only the least expensive separator is included. In conventional SNS, this is not an issue: each separator would produce

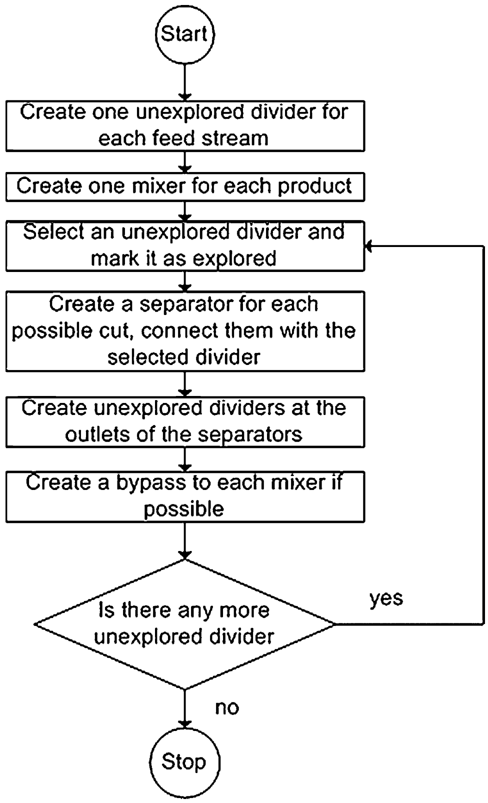

Fig. 1. Flowchart for generating the unreduced super-structure.

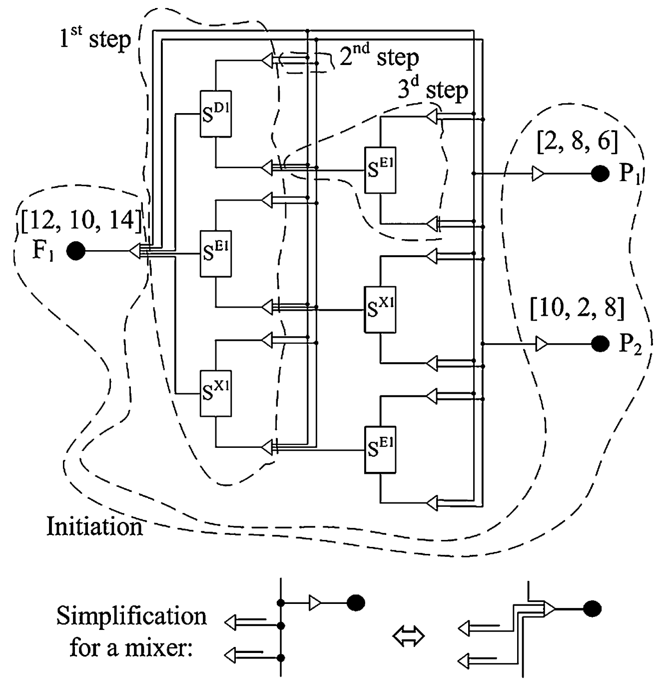

Fig. 2. Step-by-step generation of the unreduced super-structure: for clarity, every mixer in this and all other figures is simplified as illustrated.

different streams. The installation of a bypass between an outlet of any divider and the inlet of a mixer is possible only when every component in the former appears in the product stream from the latter. This strategy gives rise to the super-structure of the SNS-Multi. We term this super-structure the *unreduced super-structure* to differentiate it from the super-structure to be constructed in the current work. The flowchart for generating the unreduced super-structure is illustrated in Fig. 1, and a specific example is presented in Fig. 2.

The initiation step creates one divider for each feed stream and one mixer for each product stream with appropriate linkages. The newly created dividers are termed unexplored, thus implying that they have not yet been examined in the iteration step. The iteration step selects any of the unexplored dividers, and subsequently creates a separator for each possible cut and a bypass to each mixer, both of which are connected to the selected divider. This is immediately followed by the generation of a divider for each of the outlets from the separators created. The iteration step is repeated until all the unexplored dividers are exhausted, thereby terminating the execution of the algorithm.

The mathematical model of the unreduced super-structure is formulated in terms of the feed allocation ratio, $x_{i,j}$, introduced by Kovács et al. (2000), which specifies the fraction of the flowrate of the feed stream in stream (i, j). One feed allocation ratio is defined for each outlet of an individual divider. No additional variables need to be defined to the outlets of the separators: a separator does not induce change in the feed allocation ratio. The feed allocation ratios completely determine the network's structure, which in turn determines the compositions of each stream.

The cost of the network, comprising the costs of the separators, is minimized based on the mathematical model. The cost of an individual separator can be calculated by multiplying the flowrate of the inlet of the separator with its overall cost coefficient. The flowrate of any stream in the network can be expressed in terms of its feed allocation ratio in conjunction with the appropriate component flowrates of the corresponding feed stream. Material balances must hold for the dividers, mixers, and separators in the super-structure. One mass-balance equation is associated with each divider, and one with each component of a product; these equations are needed for the dividers and mixers. Material balances hold automatically for the separators in this super-structure because they do not affect the feed allocation ratios as mentioned earlier. Note that the equations for the dividers reveal the difference between the feed allocation ratio and the well known splitting ratio. For any given divider, the sum of the splitting ratios of its outlets is always unity; in contrast, the sum of their feed allocation ratios is equal to the feed allocation ratio of its inlet. Naturally, the feed allocation ratios are in the interval of [0, 1]. The resultant mathematical model is linear, thereby giving rise to a great advantage: any linear model can be solved efficiently and robustly. Nevertheless, the resultant super-structure magnifies exponentially with the number of components in the feed stream. The current work is intended to circumvent such a situation.

3. Simplification of separation structures

For practicality, simplification is almost always desirable as long as it does not alter the network's performance. The simplification of a separation network reduces the number of necessary separators, thereby facilitating the network's operation.

3.1. Simplification based on identical splitting ratios

As pointed out in an earlier work (Heckl et al., 2007), the optimal structure can be simplified under some situations. Specifically, two or more separators can be merged if their overall cost coefficients are identical due to the fact that: they are of the same type; the dividers for the top outlet streams of the separators are connected to the same mixer; and the dividers for the bottom outlet streams of these separators are also connected to the same mixer. Note that the

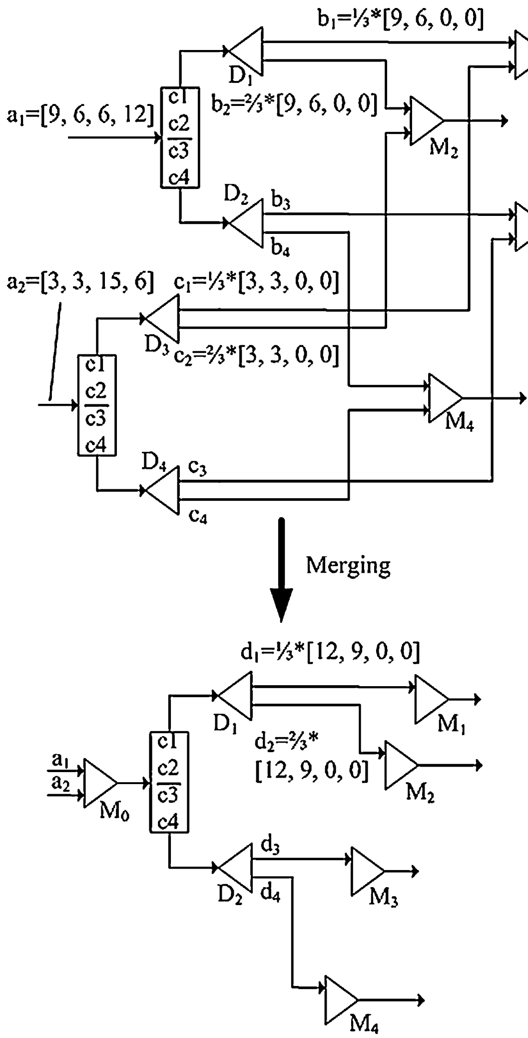

Fig. 3. Merging of separators with the identical splitting ratios.

splitting ratios of the corresponding dividers are identical. Because of the linearity of the costs of the separations, the merging of the separators affects neither the structure's cost nor the operation of the network: the streams entering and leaving the merged part of the network remain invariant.

Fig. 3 illustrates the merging. The inlet streams, a_1 and a_2, in both the unmerged and merged structures naturally must be identical. Moreover, to ensure that the outlet streams also remain identical, the following relationships must hold for d_1 and d_2.

$$b_1 + c_1 = d_1 \tag{1}$$

$$b_2 + c_2 = d_2 \tag{2}$$

Similar equations must also hold for d_3 and d_4: the material balances need to be satisfied for each outlet of a divider. Expressing the streams in terms of the component flowrates and taking into account the types of separators result in the following expressions;

$$[f_{b_1,1}, f_{b_1,2}, 0, 0] + [f_{c_1,1}, f_{c_1,2}, 0, 0] = [f_{d_1,1}, f_{d_1,2}, 0, 0] \tag{3}$$

$$[f_{b_2,1}, f_{b_2,2}, 0, 0] + [f_{c_2,1}, f_{c_2,2}, 0, 0] = [f_{d_2,1}, f_{d_2,2}, 0, 0] \tag{4}$$

where $f_{b_i,j}, f_{c_i,j}$, and $f_{d_i,j}$, $i, j = 1, 2$, are the component flowrates of the jth component in streams b_i, c_i, and d_i, respectively. The component flowrates at the outlet of a divider can be calculated from those of its inlet and from the splitting ratio of this outlet, for example, see the following equation.

$$\lambda_{b_1}[f_{a_1,1}, f_{a_1,2}] = [f_{b_1,1}, f_{b_1,2}] \tag{5}$$

Expressing the component flowrates at each outlet similarly transforms Eqs. (3) and (4), respectively, into

$$\lambda_{b_1}[f_{a_1,1}, f_{a_1,2}] + \lambda_{c_1}[f_{a_2,1}, f_{a_2,2}] = \lambda_{d_1}([f_{a_1,1}, f_{a_1,2}] + [f_{a_2,1}, f_{a_2,2}]) \tag{6}$$

$$\lambda_{b_2}[f_{a_1,1}, f_{a_1,2}] + \lambda_{c_2}[f_{a_2,1}, f_{a_2,2}] = \lambda_{d_2}([f_{a_1,1}, f_{a_1,2}] + [f_{a_2,1}, f_{a_2,2}]) \tag{7}$$

where λ_{b_i}, λ_{c_i}, and λ_{d_i}, $i = 1, 2$, are the splitting ratios of streams b_i, c_i, and d_i, respectively.

The solution of the mathematical model yields the optimal structure, for which the component flowrates and the splitting ratios are known. As a result, only the splitting ratios in the merged structure, λ_{d_1} and λ_{d_2}, are unknown. The two separators can be merged only if the system of equations, comprising Eqs. (6) and (7), has a solution. This system of equations, however, is overdefined: it has 2 variables and 4 equations, thus, rendering them solvable only in special cases. For example, the system is solvable if the splitting ratios corresponding to the same outlets are identical as expressed below.

$$\lambda_{b_1} = \lambda_{c_1} \tag{8}$$

$$\lambda_{b_2} = \lambda_{c_2} \tag{9}$$

These equations also imply that $\lambda_{b_1} = \lambda_{d_1}$ and $\lambda_{b_2} = \lambda_{d_2}$. It is worth noting that the equations similar to Eqs. (1) and (2) must hold for the divider of the bottom streams in Fig. 3. The drawback of this simplification is that it can be implemented only after the optimal structure is determined when the values of the feed allocation ratios, and consequently, the splitting ratios become known.

3.2. Simplification based on identical inlet composition

A judicious analysis reveals that the system of equations, comprising Eqs. (6) and (7), can also be solved under the condition that the compositions of the inlets of the two separators are identical, i.e.,

$$\gamma[f_{a_1,1}, f_{a_1,2}] = [f_{a_2,1}, f_{a_2,2}] \tag{10}$$

Subject to this equality, Eqs. (6) and (7) can be rewritten, respectively, as

$$\frac{\lambda_{b_1} + \gamma\lambda_{c_1}}{1+\gamma} = \lambda_{d_1} \tag{11}$$

$$\frac{\lambda_{b_2} + \gamma\lambda_{c_2}}{1+\gamma} = \lambda_{d_2} \tag{12}$$

Eqs. (11) and (12) do not demand that the separators be connected to the same mixers. The merged separator will be connected to each of such mixers to which either of the original separator is connected. Fig. 4 illustrates a simplification based on identical inlet composition. In this figure, Eq. (10) holds for the two separators with $\gamma = 2$. The divider for the top stream of the merged separator is connected to three operating units, S^1, M_1, and M_2; the corresponding splitting ratios can be calculated, respectively, as follows:

$$\lambda_{d_1} = \frac{0.3 + 2 \times 0}{1+2} = 0.1 \tag{13}$$

$$\lambda_{d_2} = \frac{0.7 + 2 \times 0.8}{1+2} = 0.7666 \tag{14}$$

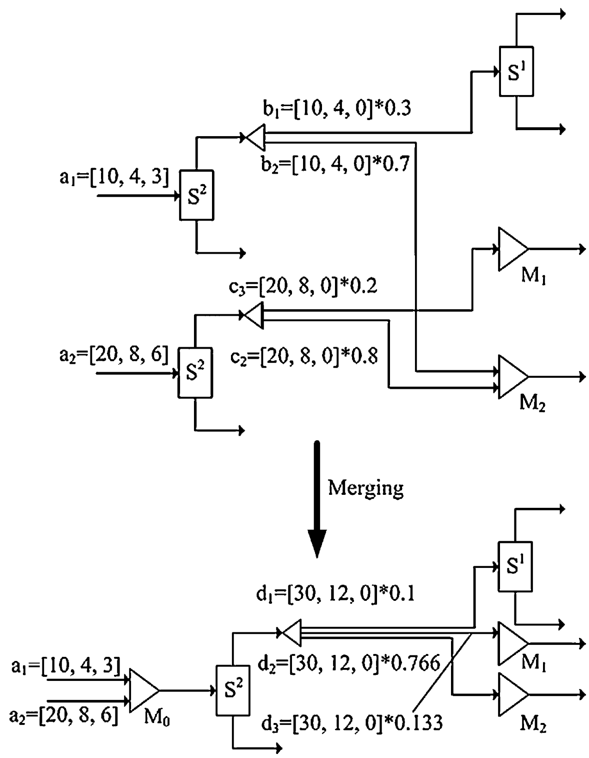

Fig. 4. Merging of separators with identical inlet composition.

$$\lambda_{d_3} = \frac{0+2\times 0.2}{1+2} = 0.1333 \quad (15)$$

4. Reduced super-structure

Simplification based on identical inlet composition is much more effective than simplification based on identical splitting ratios. While the former can be applied to both the solution structures and the super-structure, the latter is applicable only to the solution structures. Let us suppose that stream a is the inlet of separator S^i. The component flow rates of stream a can be described with the following equation;

$$f_{a,i} = \begin{cases} x_a \cdot \mathrm{FE}_{\mathrm{first}(a),c} & c \in \mathrm{CO}_a \\ 0 & c \notin \mathrm{CO}_a \end{cases} \quad (16)$$

where $\mathrm{FE}_{k,c}$ is the flowrate of component c in feed k; first(a) indicates the feed stream from which stream a originates; and CO_a is the set of components in stream a.

Let stream b the inlet of another S^i-type separator; first(a) = first(b); and $\mathrm{CO}_a = \mathrm{CO}_b$. In other words, streams a and b originate from the same feed, and thus, they contain the same components. As such, the two streams can be merged: they have the same compositions.

It is worth emphasizing that the compositions of the streams of the super-structure are known, thereby simplification based on identical inlet composition can be executed on the super-structure prior to optimization. Merging the separators reduces the size of the super-structure, thus simplifying the mathematical model and reducing the solution time. Let us focus on Fig. 5, which exhibits part of the unreduced super-structure of a separation network with a five-component feed stream. Streams a and b have the same composition, and therefore, the two S^2-type separators as well as the two S^3-type separators can be merged. The resultant simplified structure is illustrated in Fig. 6. The encircled part of this figure contains two dividers and two mixers. The compositions of streams a and

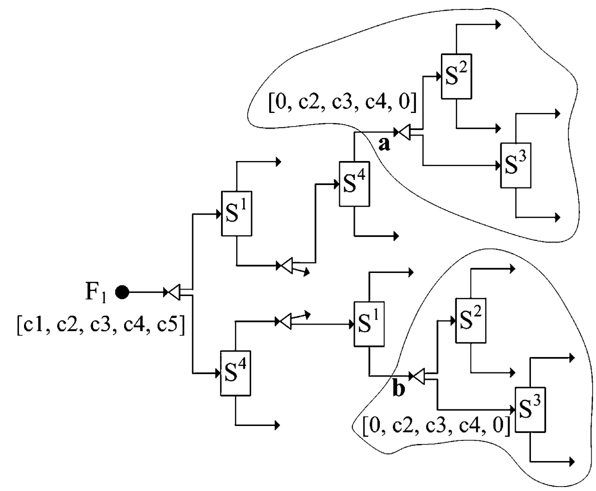

Fig. 5. Part of the super-structure before merging separators.

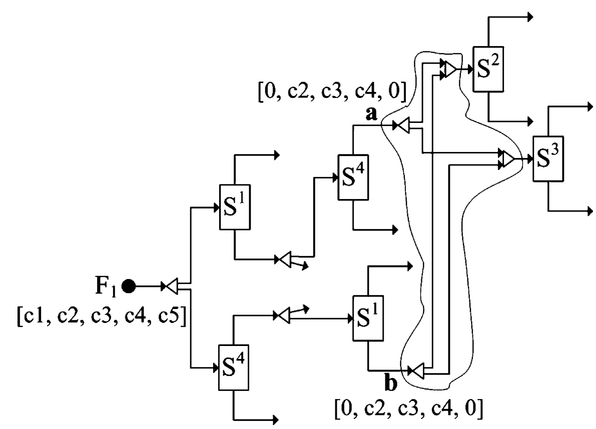

Fig. 6. Part of the super-structure after merging separators.

b are identical; as a result, it is possible to mix the streams first and divide them later; see Fig. 7. This simplification is significant: it minimizes the number of divider outlets, thus further decreasing the number of variables.

Our aim is to merge all suitable separators in the unreduced super-structure based on identical inlet composition. The resulting structure is termed the *reduced super-structure* of the SNS-Multi problem. In the unreduced super-structure the mixers always

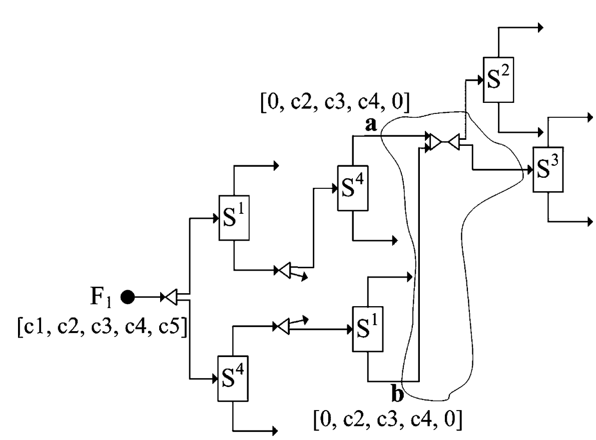

Fig. 7. Part of the super-structure after exchanging the positions of dividers and mixers.

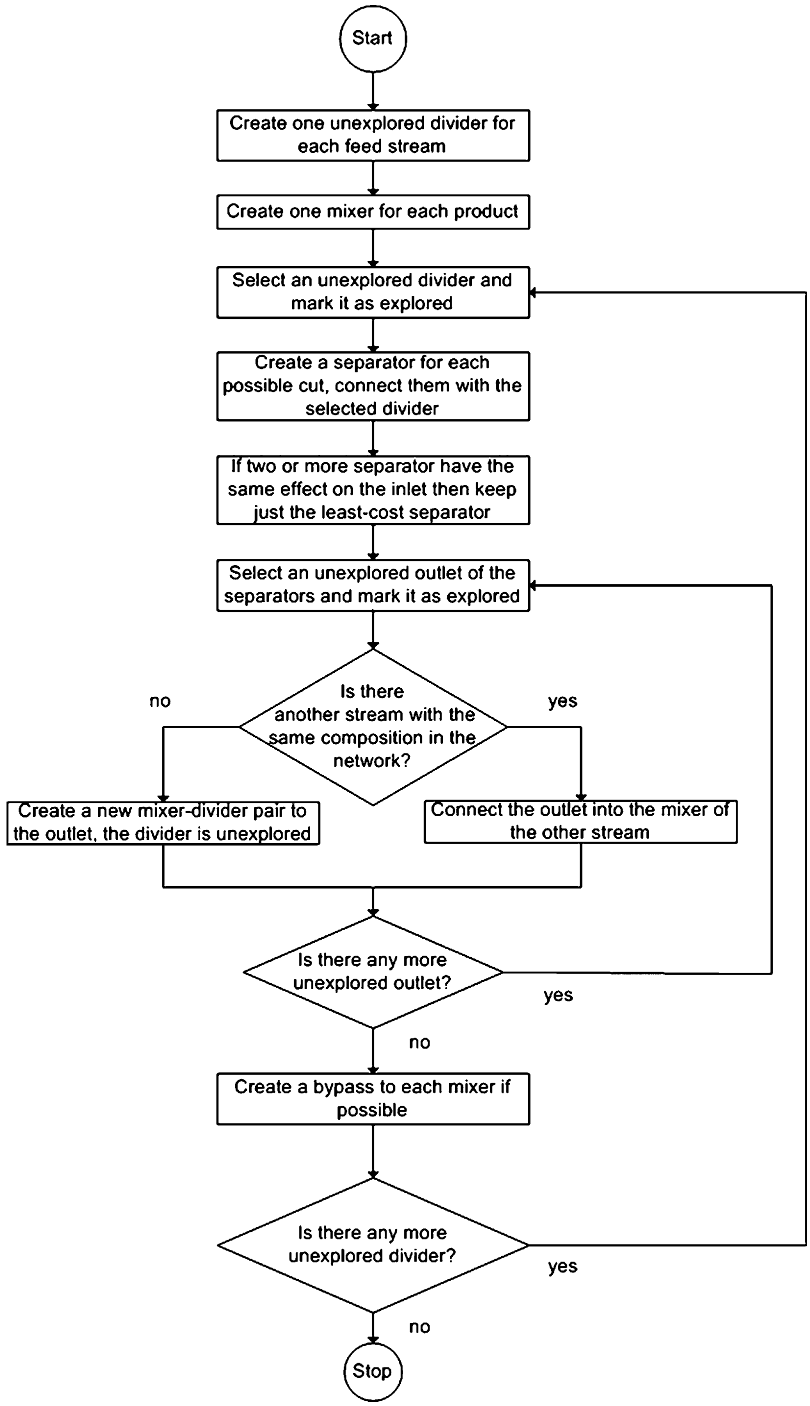

Fig. 8. Flowchart for generating the reduced super-structure.

precede the product streams; in contrast, in the reduced super-structure mixers can be found elsewhere. These new mixers are termed *inner mixers*; all their inlets have the same composition. The reduced super-structure is also a rigorous super-structure: the unreduced super-structure has been proved to be rigorous, and thus, the simplification only on the basis of the identical inlet composition does not exclude any potentially optimal structure; it only eliminates unnecessary duplications. Consequently, both the unreduced and reduced super-structures lead to optimal solutions. Moreover, these two solutions are identical if the problem under consideration has a unique optimum, and all possible simplifications are performed on the solution structures.

There are two possibilities to generate the reduced super-structure. The first generates the unreduced super-structure as described in an earlier work (Heckl et al., 2007) and then carries out all the possible mergers based on the identical inlet composition; the second generates the reduced super-structure directly from the input data. The streams originating from the same feed stream in the reduced super-structure are mixed if they have identical composition. In the reduced super-structure, therefore, an inner mixer precedes every divider, though the mixer might be equipped only with a single inlet; see Fig. 7. Introducing inner mixers does not magnify the size of the mathematical model: variables are assigned only to the outlets of each divider.

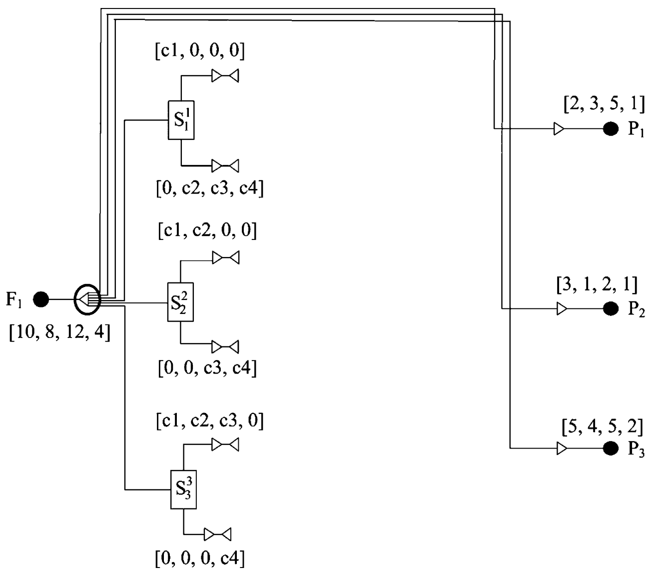

Fig. 9. Generation of the reduced super-structure: initialization and iteration 1.

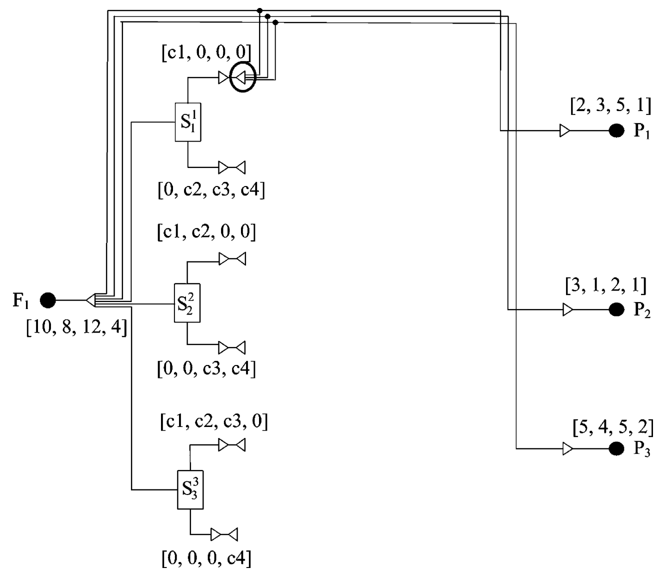

Fig. 10. Generation of the reduced super-structure: iteration 2.

What follows describes the stepwise generation of the reduced super-structure; see Fig. 8. In the initialization step, one divider is created for and linked to each feed stream, and one mixer is created for and linked to each product stream; see Fig. 9. Subsequently, an iteration is performed as long as some dividers remain unexplored. In the iteration, an unexplored divider is selected and a separator for each possible separation is created and connected to the selected divider. By taking into account several separator families, various separators linked to the selected divider, would yield identical outlet streams. Obviously, only the least-cost separator should be retained in the reduced super-structure in this case. Subsequently, the outlets from the separators created for each possible separation are examined. If the compositions of these outlets are the same as the composition of a stream, which is already in the network and connected to an inner mixer, the new outlet is also connected to the same mixer. Otherwise, a new mixer–divider pair is formed for and connected to this outlet. The new divider is marked unexplored. Afterward, a bypass is created from the selected divider to each product mixer created in the initialization step. The creation of a bypass between an outlet of any divider and the inlet of a product mixer is possible only when every component in the outlet of the divider appears in the product stream from the mixer. Finally, the selected divider is marked explored.

Figs. 9–12 illustrate the generation of the reduced super-structure of a five-component example. Fig. 9 shows the initialization and the first iteration. The encircled divider is selected at the iteration step. No inner mixer exists in the structure at this time; thus, a new mixer–divider pair is formed for every separator outlet. In Fig. 10 the inlet of the selected divider contains a single component, and thus, no further separation is possible; consequently, only bypasses are created in this iteration. The third iteration, exhibited in Fig. 11, indicates that a new mixer–divider pair is formed for the top outlet of separator S_4, but the bottom outlet is connected to an inner mixer already present in the network. The final reduced super-structure is displayed in Fig. 12.

5. Mathematical model

The mathematical model of the reduced super-structure is formulated in terms of the feed allocation ratios. Formulating the mathematical models on the basis of compositions or component flowrates gives rise to non-linear terms in the governing equations of either the separators or the dividers.

Let C, F, P, D, PM, IM, and S be the index sets for the components, feeds, products, dividers, product mixers, inner mixers, and separators, respectively. Consequently, $\mathrm{FE}_{k,c}$ is the flowrate of component c in feed k; $\mathrm{PR}_{k,c}$, the flowrate of component c in product k; and OC_s, the overall cost coefficient of separator s. prev(a) signifies the set of operating units preceding a, and prev3(a) is a shorthand for prev(prev(prev(a))). Similarly, next(a) signifies the set of operating units succeeding a. Thus, the objective function in terms of the

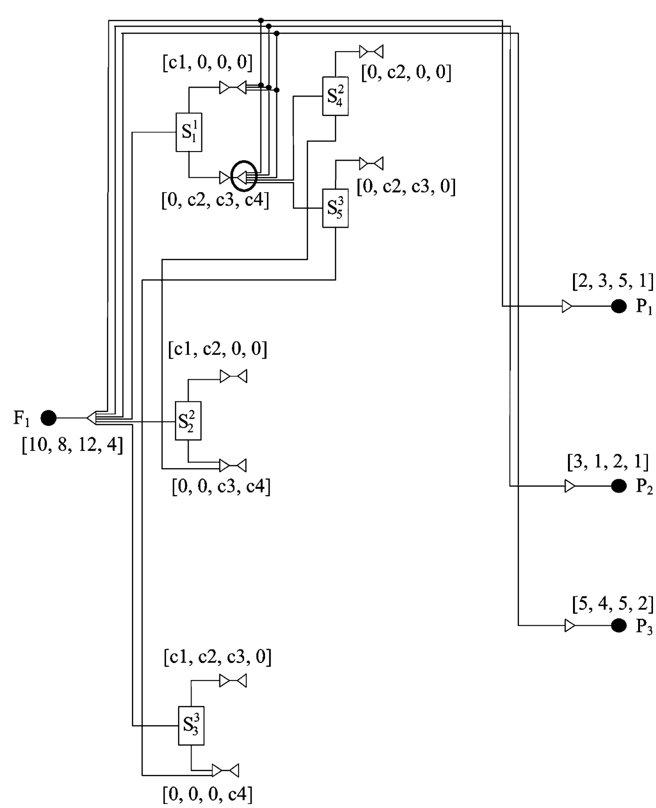

Fig. 11. Generation of the reduced super-structure: iteration 3.

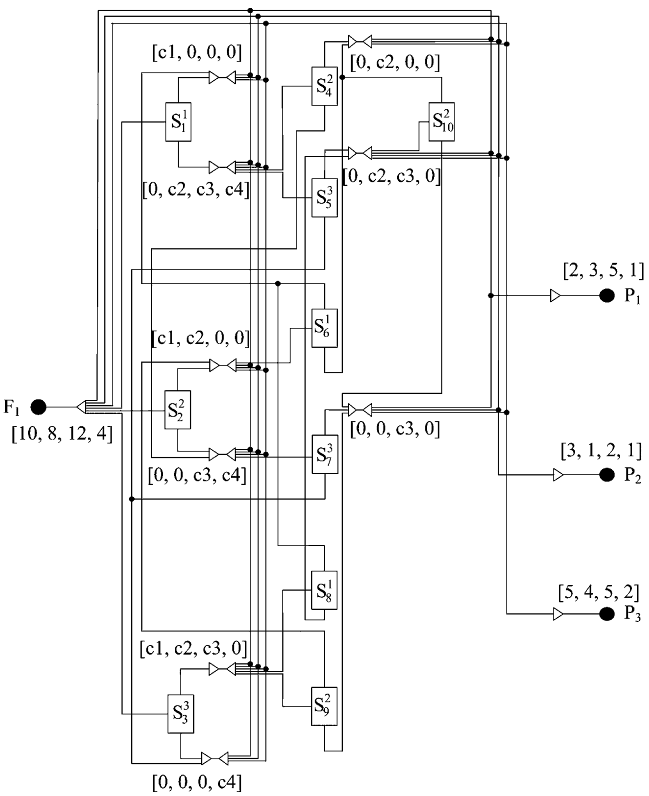

Fig. 12. Generation of the reduced super-structure: iteration 18 and final structure.

separation cost, comprising the cost of each separator, is

$$F=\sum_{\forall s\in S}\left(\mathrm{OC}_s x_{\mathrm{prev}(s),s}\sum_{\forall c\in \mathrm{CO}_{\mathrm{prev}(s),s}}\mathrm{FE}_{\mathrm{first}(s),c}\right), \tag{17}$$

which is to be minimized subject to the following constraints;

$$1=\sum_{\forall j\in \mathrm{next}(d)} x_{d,j},\quad \forall d\in \mathrm{next}(F) \tag{18}$$

$$\sum_{\forall i\in \mathrm{prev3}(d)} x_{i,\mathrm{next}(i)}=\sum_{\forall j\in \mathrm{next}(d)} x_{d,j},\quad \forall d\in D\setminus \mathrm{next}(F) \tag{19}$$

$$\sum_{\forall i\in \mathrm{prev}(m)}\sum_{\forall c\in \mathrm{CO}_i}(x_{i,m}\mathrm{FE}_{\mathrm{first}(i),c})=\mathrm{PR}_{\mathrm{next}(m),c},\quad \forall m\in \mathrm{PM},\forall c\in C \tag{20}$$

$$0\le x_{d,j}\le 1,\quad \forall (d,j)\in D\times\{S\cup \mathrm{PM}\} \tag{21}$$

The cost of each separator is calculated as the product of its overall cost coefficient, OC_s, and the flowrate of the separator's inlet stream. Moreover, $\mathrm{CO}_{\mathrm{prev}(s),s}$ is the set of components present in the stream at the inlet of separator s, and $x_{\mathrm{prev}(s),s}$ is the feed allocation ratio at this inlet. Note that several paths may lead backward from separator s in the reduced super-structure. An inner mixer represents a junction in a path while going backward from a separator; however, all these paths originate from the same feed, and thus, first(s) is unique. Eq. (18) signifies the dividers for the feed streams; at these dividers, the splitting ratio and the feed allocation ratio are identical. Eq. (19) represents the material balances around the inner mixer–divider pair. The sum of the feed allocation ratios at the inlets of the inner mixer is equal to the sum of the feed allocation ratios at the outlets of the succeeding divider. It is worth noting that the feed allocation ratios are not assigned to the inlets of inner mixers, and therefore, the feed allocation ratios at the inlets of the separators preceding the inner mixers are used. The separators do not alter the feed allocation ratios. Eq. (19) imposes a constraint on each component in every product. This equation states that the sum of the component flowrates at the inlets of a product mixer must be $\mathrm{PR}_{\mathrm{next}(m),c}$. It is possible to define a product without specifying the exact amounts of the components therein. For example, we can prescribe the ratios of the components, the upper and lower bounds of the flowrates of the components, or the minimum or maximum amount of the product. The model's capability is limited only by the requirement that all such constraints be linear as well. Eq. (21) is a natural assumption, indicating that $x_{i,j}$ cannot be negative or exceed one.

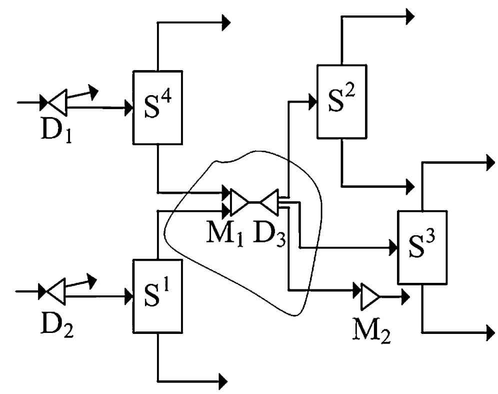

Fig. 13. Material balance around a mixer–divider pair.

The material balance around an inner mixer–divider pair is illustrated in the following with a specific example illustrated in Fig. 13; it gives

$$x_{D_1,S^4}+x_{D_2,S^1}=x_{D_3,S^2}+x_{D_3,S^3}+x_{D_3,M_2} \tag{22}$$

In this example, $\mathrm{prev3}(D_3)=\{D_1, D_2\}$, $\mathrm{next}(D_3)=\{S^2, S^3, M_2\}$.

Succeeding the generation, the sizes of the unreduced and reduced super-structures are compared quantitatively.

6. Mathematical complexity

As mentioned earlier, the optimal structures derived on the basis of the unreduced and reduced super-structures are identical if the optimum is unique. The profound advantage of the reduced super-structure is that it gives rise to the simplified mathematical model, thus facilitating the solution.

The size of the mathematical model derived from either the unreduced or reduced super-structures depends on the parameters of the specific example, such as the numbers of the components and available separators, as well as on the numbers and compositions of the feed and product streams. Let us suppose that the separation network has only one feed stream and the available separators belong to a single family. As such, the most important parameter affecting the size of the mathematical model is the number of components. The number of variables in the mathematical model equals the number of all the outlets of the dividers throughout the super-structure. These outlets are linked either to the separators or to the mixers. The number of divider outlets linked to the mixers for the products depends on the compositions in the products, thereby rendering it difficult to determine the exact number of variables. On the other hand, the number of separators in the unreduced and reduced super-structures can be given explicitly; thus, the super-structures will be characterized and compared on the basis of these numbers.

Let SN(n) be the number of separators in the unreduced super-structure, where n is the number of components. The following details the calculation and simplification of SN(n).

Suppose that the separation occurs between the ith and the $(i+1)$ st component, thus requires one separator. The number of separators continues to increase beyond one: additional separators are needed to process the outlets of the current separator. The top and bottom outlets contain i and $(n-i)$ components, respectively, and therefore $[\mathrm{SN}(i)+\mathrm{SN}(n-i)]$ additional separators are required. The initial separation can occur between the first and second components, the second and third components, and so on, thus yielding the following formula for SN(n) containing the sum;

$$\mathrm{SN}(n)=\sum_{i=1}^{n-1}[1+\mathrm{SN}(i)+\mathrm{SN}(n-i)]$$

$$=(n-1)+\sum_{i=1}^{n-1}[\mathrm{SN}(i)+\mathrm{SN}(n-i)] \tag{23}$$

where

$$\sum_{i=1}^{n-1}1\equiv n-1. \tag{24}$$

Obviously, no separation is needed for a pure component, i.e., $n=1$, and thus, $\mathrm{SN}(1)=0$.

$$\mathrm{SN}(n)=\begin{cases}1+\mathrm{SN}(1)+\mathrm{SN}(n-1)\\+1+\mathrm{SN}(2)+\mathrm{SN}(n-2)\\+1+\mathrm{SN}(3)+\mathrm{SN}(n-3)\\\dots\\\dots\\\dots\\+1+\mathrm{SN}(n-2)+\mathrm{SN}(2)\\+1+\mathrm{SN}(n-1)+\mathrm{SN}(1)\end{cases} \tag{25}$$

$$\mathrm{SN}(n)=\begin{cases}\left.\begin{matrix}1+\mathrm{SN}(1)+\mathrm{SN}(n-2)\\+1+\mathrm{SN}(2)+\mathrm{SN}(n-3)\\+1+\mathrm{SN}(3)+\mathrm{SN}(n-4)\\\dots\\\dots\\\dots\\+1+\mathrm{SN}(n-2)+\mathrm{SN}(1)\end{matrix}\right\}=\mathrm{SN}(n-1)\\+1+\mathrm{SN}(n-1)+\mathrm{SN}(n-1)\end{cases} \tag{26}$$

and thus,

$$\mathrm{SN}(n)=3\cdot\mathrm{SN}(n-1)+1 \tag{27}$$

To determine the growth of SN(n), the current recursive form must be reformulated. The first step is to unfold the sum; see Eq. (25). Subsequently, the terms must be reordered; see Eq. (26). It is worth noting that SN(n) contains SN($n-1$), and therefore, a different recursive form can be generated for SN(n); see Eq. (27). Adding 1/2 to both sides of Eq. (27) yields

$$\mathrm{SN}(n)+\frac{1}{2}=3\cdot\mathrm{SN}(n-1)+\frac{3}{2}=3\cdot\left[\mathrm{SN}(n-1)+\frac{1}{2}\right] \tag{28}$$

By defining

$$g(n)\equiv\mathrm{SN}(n)+\frac{1}{2}, \tag{29}$$

we obtain

$$g(n)=3\cdot g(n-1) \tag{30}$$

Continuing,

$$g(n)=3\cdot3\cdot g(n-2)=\cdots=3^{n-1}\cdot g(1) \tag{31}$$

Table 1
The number of separators in the unreduced, SN(n), and the reduced super-structure, CN(n), based on component number, n

n	2	3	4	5	6	7	8	9	10
SN(n)	1	4	13	40	121	364	1093	3280	9841
CN(n)	1	4	10	20	35	56	84	120	165

Table 2
Component flowrates of the feed and the product streams of the first example

	c1 (kg/s)	c2 (kg/s)	c3 (kg/s)	c4 (kg/s)
F_1	10	8	12	4
P_1	2	3	5	1
P_2	3	1	2	1
P_3	5	4	5	2

Since

$$g(1)=\mathrm{SN}(1)+\frac{1}{2}=0+\frac{1}{2}=\frac{1}{2}, \tag{32}$$

we have, from Eq. (31),

$$g(n)=\frac{3^{n-1}}{2} \tag{33}$$

Substituting the above expression into Eq. (29) yields

$$\mathrm{SN}(n)=\frac{3^{n-1}-1}{2} \tag{34}$$

This closed form indicates explicitly that SN(n) grows exponentially as n increases.

Let CN(n) be the number of separators in the reduced super-structure where n is the number of components. What follows details the evaluation and simplification of the formulae for CN(n). Suppose that all the available separators belong to a single family. Consequently, if a stream contains i adjacent components, $(i-1)$ separations can be carried out on this stream. Because of its configuration, the reduced super-structure contains $(n+1-i)$ streams with i components adjacent to each other where n is the number of components in the feed; i can be any integer number between 2 and n, thereby yielding

$$\mathrm{CN}(n)=\sum_{i=2}^{n}[(n+1-i)\cdot(i-1)] \tag{35}$$

or

$$\mathrm{CN}(n)=\sum_{i=2}^{n}(-i^2+n\cdot i+2\cdot i-n-1) \tag{36}$$

Table 3
The separators available in the first example

Separator designation	Top-product components	Bottom-product components	Overall cost coefficient, g_s
S^1	c1	c2, c3, c4	4
S^2	c1, c2	c3, c4	2
S^3	c1, c2, c3	c4	3

Table 4
Component flowrates of the feed and the product streams of the second example

	c1 (kg/s)	c2 (kg/s)	c3 (kg/s)	c4 (kg/s)	c5 (kg/s)	c6 (kg/s)	c7 (kg/s)
F_1	23	19	25	21	26	26	12
F_2	12	11	8	6	2	6	15
P_1	9	3	6	8	4	10	13
P_2	14	10	8	8	11	5	9
P_3	5	10	10	3	1	4	2
P_4	7	7	9	8	12	13	3

Table 5
The separators available in the second example

Separator designation	Top-product components	Bottom-product components	Overall cost coefficient, g_s
S^{R1}	c1	c2, c3, c4, c5, c6, c7	1.5
S^{R2}	c1, c2	c3, c4, c5, c6, c7	3
S^{R3}	c1, c2, c3	c4, c5, c6, c7	2
S^{R4}	c1, c2, c3, c4	c5, c6, c7	2.5
S^{R5}	c1, c2, c3, c4, c5	c6, c7	4
S^{R6}	c1, c2, c3, c4, c5, c6	c7	4
S^{E1}	c4	c6, c3, c1, c7, c2, c5	4.5
S^{E2}	c4, c6	c3, c1, c7, c2, c5	1
S^{E3}	c4, c6, c3	c1, c7, c2, c5	2.5
S^{E4}	c4, c6, c3, c1	c7, c2, c5	3.5
S^{E5}	c4, c6, c3, c1, c7	c2, c5	1.75
S^{E6}	c4, c6, c3, c1, c7, c2	c5	4.5
S^{K1}	c1, c5, c3, c4	c7, c2, c6	6.6

Partitioning the sum in the right-hand side of the above expression into 3 parts results in

$$\mathrm{CN}(n)=\sum_{i=2}^{n}(-i^2)+\sum_{i=2}^{n}[i\cdot(n+2)]+\sum_{i=2}^{n}(-n-1) \tag{37}$$

where

$$\sum_{i=2}^{n}(-i^2)=-\left[\sum_{i=1}^{n}(-i^2)-1\right]=-\left(\frac{2\cdot n^3+3\cdot n^2+n}{6}-1\right)$$
$$=\frac{-n^3}{3}-\frac{n^2}{2}-\frac{n}{6}+1 \tag{38}$$

$$\sum_{i=2}^{n}[i\cdot(n+2)]=(n+2)\cdot\sum_{i=2}^{n}i=(n+2)\cdot\left[\frac{n\cdot(n+1)}{2}-1\right]$$
$$=\frac{n^3}{2}+\frac{3\cdot n^2}{2}-2 \tag{39}$$

$$\sum_{i=2}^{n}(-n-1)=(n-2)\cdot(-n-1)=-n^2+1 \tag{40}$$

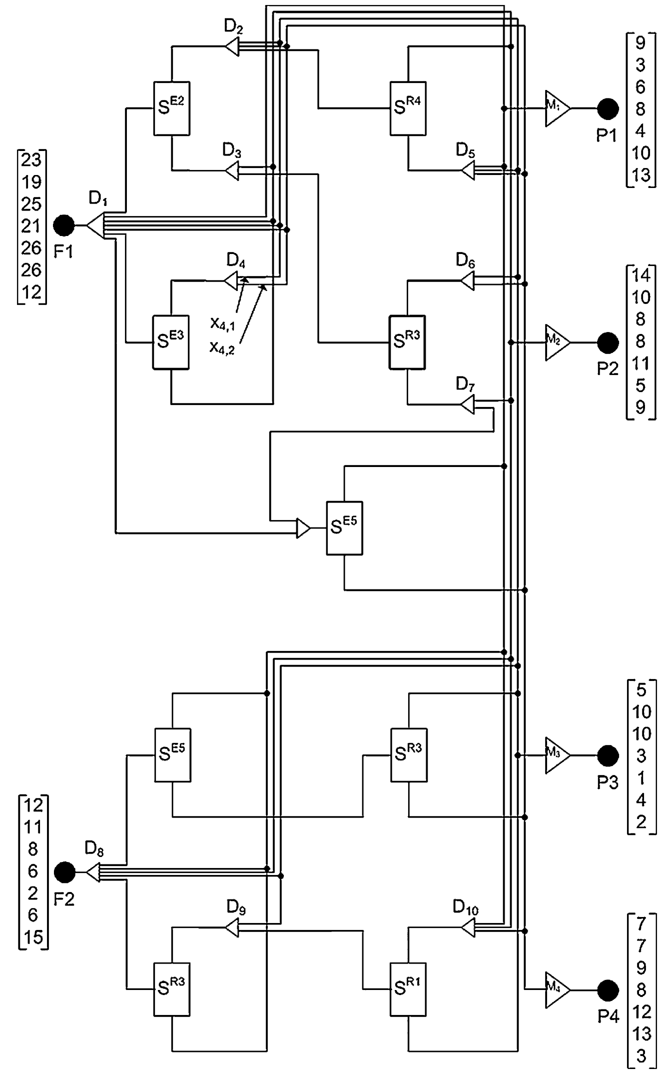

Fig. 15. Optimal structure of the second example.

Thus,

$$\mathrm{CN}(n)=\frac{n^3-n}{6} \tag{41}$$

Note that CN(n) grows polynomially with n.

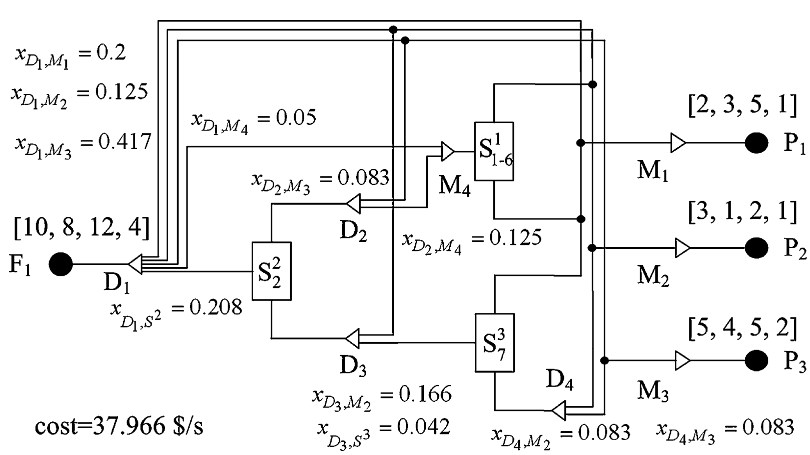

Fig. 14. Optimal structure of the first example.

Table 6
Component flowrates of the feed and the product streams of the third example

	c1	c2	c3	c4	c5	c6	c7	c8	c9	c10	c11	c12	c13	c14	c15
F_1	23	19	25	21	26	26	2	6	4	2	7	5	5	9	8
F_2	12	11	8	6	2	6	8	4	6	1	1	9	5	3	4
F_3	2	1	7	6	8	2	5	3	2	7	2	8	4	6	8
F_4	2	3	5	7	11	13	17	23	27	31	37	7	6	4	5
P_1	11	6	11	15	15	23	20	24	32	32	40	3	8	5	1
P_2	16	11	15	8	6	5	2	1	2	3	1	7	2	7	4
P_3	5	14	10	3	11	4	2	4	2	2	5	10	6	8	12
P_4	7	3	9	14	15	15	8	7	3	4	1	9	4	2	8

Table 7
The separators available in the third example

Separator designation	Top-product components	Bottom-product components	Overall cost coefficient, g_s
S^{R1}	c1	c2, c3, c4, c5, c6, c7, c8, c9, c10, c11, c12, c13, c14, c15	1.5
S^{R2}	c1, c2	c3, c4, c5, c6, c7, c8, c9, c10, c11, c12, c13, c14, c15	3
S^{R3}	c1, c2, c3	c4, c5, c6, c7, c8, c9, c10, c11, c12, c13, c14, c15	2
S^{R4}	c1, c2, c3, c4	c5, c6, c7, c8, c9, c10, c11, c12, c13, c14, c15	2.5
S^{R5}	c1, c2, c3, c4, c5	c6, c7, c8, c9, c10, c11, c12, c13, c14, c15	4
S^{R6}	c1, c2, c3, c4, c5, c6	c7, c8, c9, c10, c11, c12, c13, c14, c15	2
S^{R7}	c1, c2, c3, c4, c5, c6, c7	c8, c9, c10, c11, c12, c13, c14, c15	3
S^{R8}	c1, c2, c3, c4, c5, c6, c7, c8	c9, c10, c11, c12, c13, c14, c15	5
S^{R9}	c1, c2, c3, c4, c5, c6, c7, c8, c9	c10, c11, c12, c13, c14, c15	3
S^{R10}	c1, c2, c3, c4, c5, c6, c7, c8, c9, c10	c11, c12, c13, c14, c15	2
S^{R11}	c1, c2, c3, c4, c5, c6, c7, c8, c9, c10, c11	c12, c13, c14, c15	4
S^{R12}	c1, c2, c3, c4, c5, c6, c7, c8, c9, c10, c11, c12	c13, c14, c15	2.7
S^{R13}	c1, c2, c3, c4, c5, c6, c7, c8, c9, c10, c11, c12, c13	c14, c15	6
S^{R14}	c1, c2, c3, c4, c5, c6, c7, c8, c9, c10, c11, c12, c13, c14	c15	2.3
S^{E1}	c5	c15, c8, c9, c1, c6, c7, c3, c4, c10, c11, c14, c13, c12, c2	7
S^{E2}	c5, c15	c8, c9, c1, c6, c7, c3, c4, c10, c11, c14, c13, c12, c2	5
S^{E3}	c5, c15, c8	c9, c1, c6, c7, c3, c4, c10, c11, c14, c13, c12, c2	3
S^{E4}	c5, c15, c8, c9	c1, c6, c7, c3, c4, c10, c11, c14, c13, c12, c2	1
S^{E5}	c5, c15, c8, c9, c1	c6, c7, c3, c4, c10, c11, c14, c13, c12, c2	6
S^{E6}	c5, c15, c8, c9, c1, c6	c7, c3, c4, c10, c11, c14, c13, c12, c2	5.2
S^{E7}	c5, c15, c8, c9, c1, c6, c7	c3, c4, c10, c11, c14, c13, c12, c2	3.4
S^{E8}	c5, c15, c8, c9, c1, c6, c7, c3	c4, c10, c11, c14, c13, c12, c2	4.5
S^{E9}	c5, c15, c8, c9, c1, c6, c7, c3, c4	c10, c11, c14, c13, c12, c2	3.6
S^{E10}	c5, c15, c8, c9, c1, c6, c7, c3, c4, c10	c11, c14, c13, c12, c2	2
S^{E11}	c5, c15, c8, c9, c1, c6, c7, c3, c4, c10, c11	c14, c13, c12, c2	4
S^{E12}	c5, c15, c8, c9, c1, c6, c7, c3, c4, c10, c11, c14	c13, c12, c2	2.9
S^{E13}	c5, c15, c8, c9, c1, c6, c7, c3, c4, c10, c11, c14, c13	c12, c2	3
S^{E14}	c5, c15, c8, c9, c1, c6, c7, c3, c4, c10, c11, c14, c13, c12	c2	2.3
S^{K1}	c1, c2, c3, c4, c8, c9, c10, c11, c12, c13, c14	c15	0.2
S^{K2}	c1, c2, c9, c10, c11, c12, c13, c14	c15	0.1

It is worth noting that as discernable from their closed forms, the rates of growth of SN(n) and CN(n) are exponential and polynomial, respectively. Moreover, the latter is not noticeably steep. Table 1 illustrates the rates of growth of SN(n) and CN(n).

In the following, the method based on the reduced super-structure will be applied to three examples. Our theoretical exploration indicates that the computation and effort required will decrease substantially.

7. Examples

In the first example, 3 multi-component product streams are to be produced from a 4-component feed stream. All separators belong to a single separator family. Tables 2 and 3 contain the input data. The generation of the reduced super-structure is illustrated in Figs. 9–12. Subsequently, the mathematical programming model is generated from the reduced super-structure. This example features 10 separators and 10 dividers; each divider is connected to all 3 product mixers. Consequently, there are 40 divider outlets in the reduced super-structure, representing 40 variables in the mathematical programming model. If this model is based on the unreduced super-structure, the number of variables is 94. Fig. 14 exhibits the optimal structure of the example.

The second example comprises 7 components, 2 feed streams, 4 product streams, and 13 separators belonging to 3 separator families. Tables 4 and 5 list the input data. The optimal structure is exhibited in Fig. 15. The cost of the network is 261.1 $/s. The same optimal structure is obtained with either the reduced or unreduced super-structure; however, the computational time with the former is 0.453 s, and that with the latter 15 s on a PC (AMD-XP 3 GHz). As mentioned earlier, the difference in the solution time increases rapidly with the increase in the problem size.

The third example comprises 15 components, 4 feed streams, 4 product streams, and 30 separators from 3 different separator families. Tables 6 and 7 list the input data. The cost of the network is 1193.9 $/s. With the reduced super-structure, this problem has been solved within merely 86.1 s on the same PC mentioned above while with the unreduced super-structure the problem has failed to yield a solution.

The solver and the three examples together are available for downloading from web page http://www.dcs.vein.hu/capo/demo/sns/heckl2008.

8. Conclusions

The current work re-addresses a separation-network synthesis problem involving various separator families based on different separation methods. A systematic method is proposed for constructing the reduced super-structure of the problem. It has been proved that this reduced super-structure leads to the same optimal structure as that obtained with the unreduced super-structure. The closed form of the formulae has been derived to compute the sizes of the reduced as well as unreduced super-structures. With the increase in the problem size, the former magnifies only cubically, while the latter magnifies exponentially. Consequently, problems of the type considered in the current work can be solved substantially faster with the reduced super-structures than with the unreduced super-structures.

The main advantages of the proposed method are: it is algorithmic at each step; insures the generation of the optimal solution; and exceedingly effective so that it is applicable to problems of considerable sizes. Nonetheless, it has some limitations also: only single and sharp separators with proportional cost functions are taken into account. The future work would involve separators with various cost functions and/or non-sharp separators.

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Appendix A. Supplementary Data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2008.08.003.

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