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Solving a separation-network synthesis problem by interval global optimization technique

Adrian G. Szlama*[a], Karoly Kalauz[a], Botond Bertok[a], Istvan Heckl[a]

Department of Computer Science and Systems Technology, University of Pannonia, Veszprem, H-8200, Hungary
szlama@dcs.uni-pannon.hu

A new solution technique is proposed here for a specific kind of separation-network synthesis (SNS) problem, using Branch-and-Bound (B&B) framework and linear programming (LP). The suggested method determines effectively the structure and flowrates of the optimal separation network.
The method is illustrated by the solution of an SNS problem introduced in (Kovacs et al., 1995). The aim is to produce three pure product streams from two three-component feed streams with minimal cost. The rigorous super-structure of the problem is given by (Kovacs et al., 1995). The term itself was defined by Kovacs et al. (1999). The main idea is that it can be proved that the rigorous super-structure contains at least one optimal structure. The mathematical programming model generated from this rigorous super-structure is non-linear.
The goal of the present work is to determine the optimum of the aforementioned model effectively. The proposed method handles the splitting ratios of the dividers as intervals. A B&B method operates on these intervals. A branching step split one of the intervals. The bounding function approximates the concave cost functions of the separators. This function can be determined by solving LPs. The solution of the non-linear problem can be determined with arbitrary precision.

1. Introduction

Separation-network synthesis is an important area of process synthesis. It plays significant role in the chemical and allied industries, where almost every process needs some separation activity, for example, Huang et al. (2008), Marty et al. (1994), and Sutherland (2007). For a given problem, there are a plethora of separation networks yielding the desired product streams from the given feed streams. These networks differ in the separators they use and the connections between them, i.e., they have different structure. Our goal is to determine the solution structure with the lowest possible cost. In this work the mathematical model is formulated in terms of component flowrates and splitting ratios, where the non-convexities arise in the model of the dividers.
The examined problem contains simple and sharp separators, mixers, and dividers. A mixer merges two or more streams and the output stream is the sum of the corresponding component flowrates of the input streams. A divider splits its input stream into two output streams according to the corresponding splitting ratio as shown by Eq. 1.

$$f_{ST1,k} = \lambda_1 * f_{ST2,k} + (1-\lambda_1) * f_{ST3,k} \quad k \in \{C1, C2, C3\}; \; 0 \le \lambda_1 \le 1 \qquad (1)$$

$f_{st,k}$ is the flowrate of component k in stream st and λ_1 is the splitting ratio of the first output of the divider i. *ST1* is the inlet, *ST2* and *ST3* are the outlets of the divider.
A separator intends to separate its input stream into two output streams. In contrast to dividers, the compositions of the output streams of a separator differ from each other. In the ideal case, termed as

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sharp separation, each component of the input appears either in the top or in the bottom output. Simple separators have exactly one input and two output streams. In this paper simple and sharp separators are considered. The cost of the network is the sum of the costs of the separators and the cost of a separator is a concave function of its mass load.

2. Motivating example

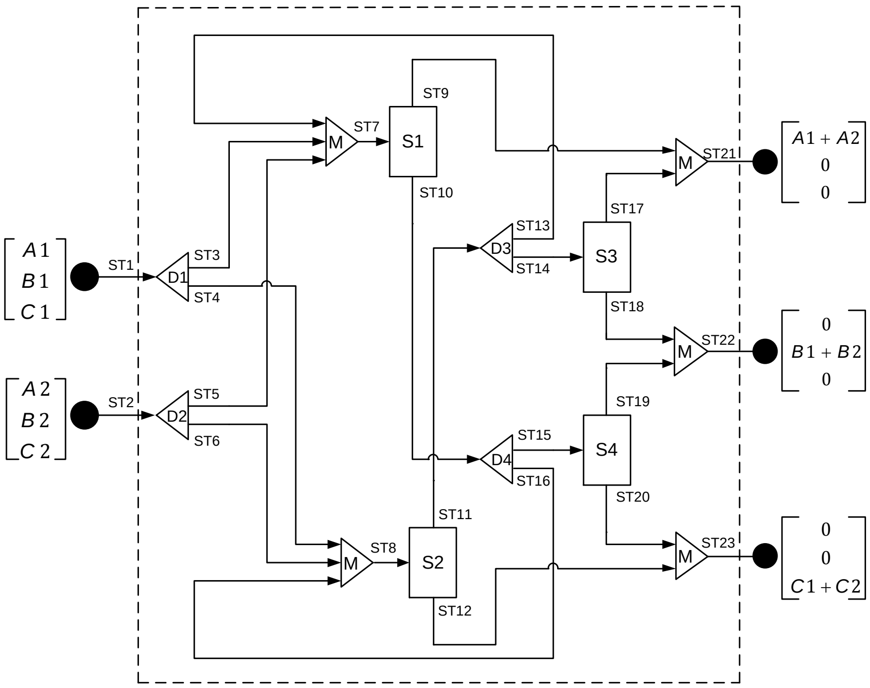

Figure 1: Rigorous super-structure for the example

An SNS problem, introduced in (Kovacs et al., 1995), is shown in Figure 1 to illustrate the operation and effectiveness of the proposed method. Two simple and sharp separator types are available here. S1 and S3 belong to the first type which separates between the first and the second components, S2 and S4 belong to the second type which separates between the second and the third components. The separators' cost function is $x^{0.6}$ in both cases, where x is the total flowrate at the inlet of the separator.

3. Optimization method

In the constructed component-based mathematical model the component flowrates and the splitting ratios are the variables. The splitting ratios clearly define the component flowrates, thus, the splitting ratios can be regarded as independent variables.

3.1 Causes of the non-linearity of the mathematical model

The non-linearity of the model can be traced back to two different causes. First, the equations of the dividers are non-linear in component flowrate based model. To resolve this problem, a splitting interval is introduced to replace the splitting ratio as shown in Figure 2. A B&B method is also introduced, which works on these intervals.

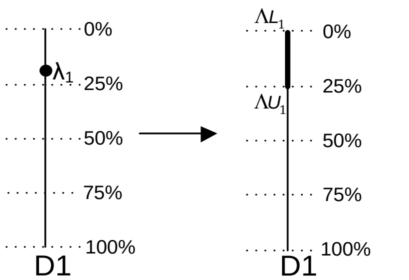

Figure 2: Replacing splitting ratio with splitting interval

Eq. 1 can be replaced by Eq. 3 and Eq. 3 where ΛL_1 and ΛU_1 represent the lower and upper bounds of the splitting interval corresponding to divider D1.

$$f_{ST1,k} * \Lambda L_1 \leq f_{ST3,k} \qquad k \in CI = \{C1, C2, C3\} \tag{2}$$

$$f_{ST1,k} * \Lambda U_1 \geq f_{ST3,k} \qquad k \in CI = \{C1, C2, C3\} \tag{3}$$

Second, the cost functions of the separators are concave. This problem is handled by constructing a linear lower estimating function of the original cost function in the specified interval. If a lower estimating function is determined for every separator then a lower bound can be also calculated for the total cost of the network.

3.2 Sub-problems and branching step

The rigorous super-structure in Figure1 contains four dividers; therefore, four splitting ratios should be managed together. Each splitting ratio is replaced by an interval, thus, a sub-problem can be described with 8 parameters (ΛL_1, ΛU_1, ΛL_2, ΛU_2, ...). Figure 3 shows a sub-problem where the four thin line represents the whole [0, 1] interval, i.e., the search space, corresponding to the four dividers. The bold lines mean the actual values of the splitting intervals in the current sub-problem.

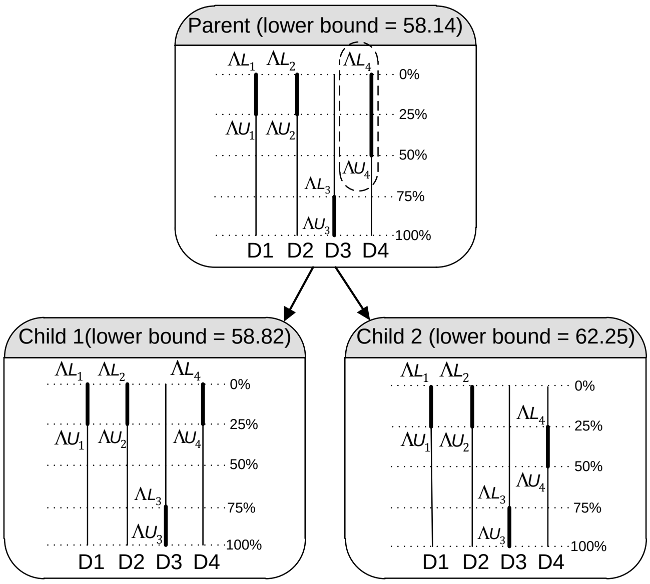

Figure 3: Branching step of the B&B method in the illustrative example

In a branching step, the widest interval is chosen and divided into two equal parts. If more than one interval has the same length then the first such interval is split. In the root of the B&B tree the [0, 1] interval is assigned to all dividers.

3.3 Sub-problem selection

The sub-problems generated during the branching step of the B&B method are stored in a list. The list is sorted according to the lower bounds of the sub-problem's costs. The first element of the list is chosen at sub-problem selection, which now has the lowest estimated cost, and the generated child problems are inserted to the proper positions according to given ordering. This method implements a directed depth-first search. Other sub-problem selection methods have been also examined, but they were inferior compared to the proposed one.

3.4 Minimum and maximum loads for the separators

The minimum, XL, and maximum, XU, loads of a separator has to be computed to determine the lower estimating function of a sub-problem. XL and XU are computed via LP's. The proposed LP's contain the material balances for dividers, the constraints for splitting intervals, the material balances for mixers, and the material balances for separators.

Figure 4 shows that eight LPs are generated and solved for the actual sub-problem. For clarity, only LP1 and LP2 are detailed. LP1 minimizes the total flowrate of stream ST7, the input of separator S1. LP2 maximizes the total flowrate of stream ST7. LP3 minimizes the total flowrate of stream ST8, the input of separator S2, and so on.

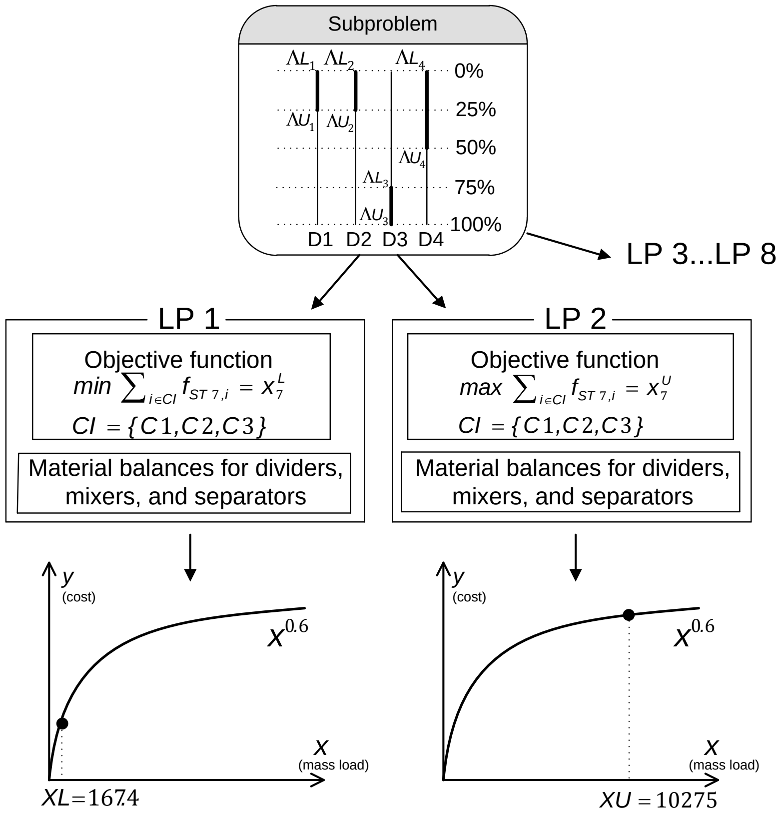

Figure 4: calculating the lower and upper bound for the separator's load

3.5 Calculation of the bounding functions

Now, our goal is to calculate a lower bound for a given sub-problem. The cost of the separation network is specified by the sum of the cost of separators, so we need lower estimation functions for the separators. The cost function of a separator is indicated by the solid line shown in Figure 5. The dashed line is the linear lower estimating function in the [XL, XU] interval. The XL and XU parameters, i.e., the lower and upper bounds of the specific separator's input in the corresponding sub-problem are calculated in the previous subsection. The corresponding cost of the minimum, YL, and maximum load, YU, are given by Eq. (4) and Eq. (5).

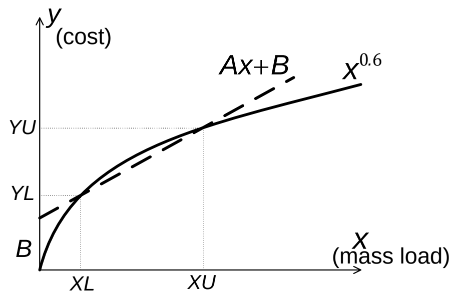

Figure 5: Linear lower estimation of the concave cost function

Eq. (6) and Eq. (7) define the A and B parameters of the lower estimating function, where A is the proportional part of the estimating function and B is the fixed part of the linear function.

$$YL = (XL)^{0.6} \tag{4}$$

$$YU = (XU)^{0.6} \tag{5}$$

$$A = (YU - YL)/(XU - XL) \tag{6}$$

$$B = YU - (A * XU) \tag{7}$$

At the beginning of the B&B method, the sub-problems contain wide intervals, so the difference of XL and XU is large as well. This results an inaccurate lower estimation. After a number of iterations, the length of the intervals decrease and the accuracy of the estimation increases.

3.6 Lower bound of a sub-problem

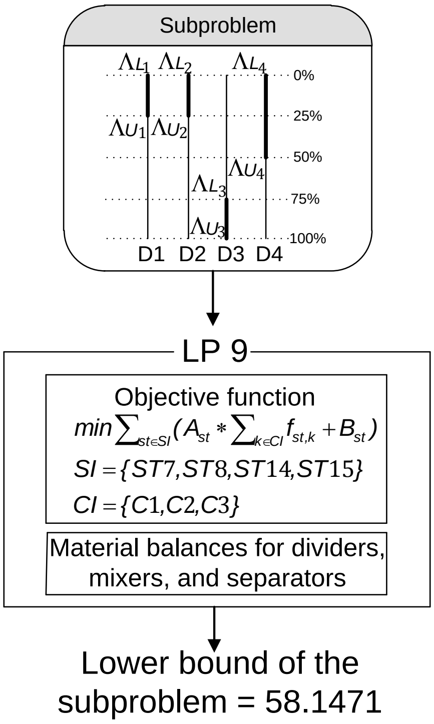

Figure 6: Calculating the lower bound of a sub-problem by solving the 9th LP

After the lower estimating functions for the separator's cost are determined, the lower bound for the sub-problem can be calculated by solving the 9th LP. This LP differs in the objective function from the previous LP's. Instead of minimizing or maximizing the load of a separator it aims to minimize the cost of the whole network. Figure 6 illustrates the computation of the lower bound of a sub-problem using LP 9. The objective function in Eq. 8 is the sum of the four lower estimating functions.

$$min \sum_{st \in SI}(B_{st} * \sum_{k \in CI} f_{st,k} + A_{st}) \qquad SI = \{ST7, ST8, ST14, ST15\}; \quad CI = \{C1, C2, C3\} \tag{8}$$

Two terminating criteria are considered for the B&B procedure. If the YL and YU values coincide then a leaf of the B&B tree is reached. In this case, the exact value, not only a lower bound, is obtained. In practice, the distance of YL and YU is calculated and if the distance is smaller than a predefined tolerance, e.g. 0.0001, then the two points is deemed coinciding. However, this method does not seem to be computationally effective. Consequently, another terminating criterion is proposed. If a splitting interval, $[\Lambda L, \Lambda U]$, is narrow enough then it is not divided any more. If all such intervals are narrow enough then the sub-problem is regarded as a leaf. It is worth noting that if the size of the interval [$\Lambda L, \Lambda U$] is small then the [XL, XU] and consequently the [YL, YU] intervals are also small. The tolerance value significantly affects the running time of the algorithm and the accuracy of the solution. Computational results with different parameters are presented in the following section.

4. Evaluation of results

Solving the motivating example with the proposed method results the optimal network with cost 62.5115, which is the same as in the literature. The intervals of the dividers are the following: $D1$: [0.999939, 1], $D2$: [0, 0.00006103], $D3$: [0.999939, 1], $D4$: [0.239197, 0.239258]. Practically, the whole input streams of dividers $D1$ and $D3$ proceeds to the first output stream and the whole input stream of divider $D2$ proceeds to the second output stream. These dividers do not perform splitting; therefore, the solution network does not contain them. 23.92% of the input stream of $D4$ proceeds to the first and 76.08% proceed to the second output stream.

Table 1: Results of the different solution algorithms

Algorithm	Cost	Time [s]	Iterations
OpenOpt NLP V1	66.6841	*11.35	614
OpenOpt NLP V2	70.9611	10.41	559
IGOS ε=0.01	62.4122	1.97	1787
IGOS ε=0.001	62.4998	3.25	3239
IGOS ε=0.0001	62.5115	**8.41	9337
Solution in literature	62.51		

Table 1 shows the results compared with the OpenOpt NLP solver (National Academy of Sciences of Ukraine, 2012) where V1 and V2 indicate the various stating points. OpenOpt is an open source, multi-platform optimization framework written in Python language. The built-in, R algorithm based ralg method is used with OpenOpt. IGOS (Interval Global Optimizer for SNS) denotes the presented algorithm and ε denotes the tolerance for the width of splitting intervals.

The proposed method** requires less computational time than the NLP solver*, even with tolerance ε=0.0001 and it guarantees the global optimum while the NLP did not.

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