Supply and Target Based Superstructure Synthesis of Heat and Mass Exchange Networks

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Abstract

This paper presents new methods for superstructure heat exchanger network synthesis (HENS) and mass exchanger network synthesis (MENS). The techniques developed in this study explore the use namely supply temperatures/compositions and target temperatures/ compositions in HENS and MENS to define the intervals of superstructures. Such superstructures are modelled as mixed integer non linear programmes (MINLP) with the objective of simultaneous minimisation of the total annual cost (TAC) of each network. The two superstructures presented in this paper are based on the supply based superstructure (SBS) developed previously [1]. The first uses the supply temperatures/compositions of hot/rich streams and the target temperatures/compositions of cold/lean streams, denoted supply and target based superstructure (S&TBS), while the second uses the target temperatures/compositions of hot/rich streams and the supply temperatures/compositions of cold/lean streams, denoted target and supply based superstructure (T&SBS). Three HEN examples and three MEN examples are presented, and the results obtained compare well with those in the literature.

1. Introduction

In this paper we will focus on the use of superstructure approaches for heat exchanger network synthesis (HENS) and mass exchanger network synthesis (MENS). As pointed out by Yee and Grossman [2] these approaches overcome a key shortcoming of the sequential techniques such as pinch technology which is that the different costs associated with the network design cannot be optimised simultaneously.

Yee and Grossman were the first to develop an insight based superstructure for optimization of the total annual cost (TAC) in HENS, which they called the stagewise superstructure (SWS). In the SWS the number of stages were determined by the maximum of the number of hot or cold streams present in the synthesis task. It is only recently that others have taken this kind of approach further. Isafiade and Fraser [3] developed the interval based MINLP superstructure (IBMS) for HENS using either the supply and target temperatures of hot streams in a hot based superstructure or the supply and target temperatures of cold streams in a cold based superstructure. Azeez, *et al.* [1] developed a supply-based superstructure (SBS) that is very similar to the IBMS, with the interval boundaries being set by the supply temperatures of the both the hot streams and the cold streams.

Comeaux was the first to apply such an approach for MENS [4]. Subsequently, Szitikai, *et al.* [5] used the key SWS idea of Yee and Grossman [2] to develop a similar superstructure for MENS. According to Szitkai, *et al.* the number of stages in the superstructure can be set arbitrarily but in a manner that is large enough to accommodate the optimal structure. They thus suggested adding the number of rich and lean streams in the synthesis task to set the maximum number of stages in the superstructure, for moderate numbers of streams. Isafiade and Fraser also developed the mass exchange analogue of the IBMS for MENS [6], as did Azeez, *et al.* for the SBS [1].

2. Motivation

In the SBS of Azeez, *et al.* [1] each of the streams originates from its supply temperature/composition. The hot/rich streams end at the lowest temperature interval boundary of the superstructure, while the cold/lean streams end at the highest interval boundary of the superstructure. The HEN grid diagram of the SBS with two hot streams and two cold streams is shown in Figure 1 below, with temperature decreasing from left to right. Note that the supply temperature T_{H1}^{s} of H1 is higher than the supply temperature T_{H2}^{s} of H2 while the supply temperature T_{C2}^{s} of C2 is higher than that of C1, T_{C1}^{s} but lower than that of H2. In the SBS, both process and utility streams are treated as process streams. An analogous structure exists for MENS [1].

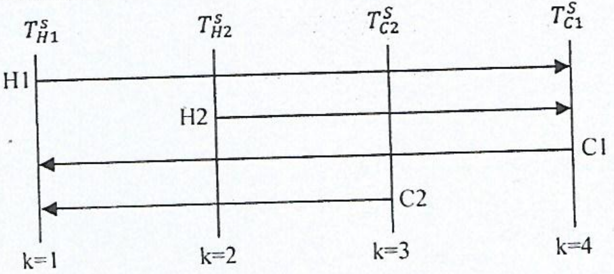

Figure 1. Grid representation for SBS with 2 hot streams and 2 cold streams

This study presents three new ways of defining the superstructure partitioning and compares the effect on the total annual cost in both HENS and MENS. As in the SBS, both process and utility streams are treated as process streams.

Conceptual consideration of the SBS led to the realisation that any combination of supply and target temperatures/compositions could conceivably be used to define the boundaries of the intervals This results in four possible combinations:

- A supply based superstructure (as in the SBS);
- A supply and target based superstructure (S&TBS);
- A target and supply based superstructure (T&SBS); and
- A target based superstructure (TBS).

Each of the three new options will be examined in turn. Note that in all three cases one or more additional boundaries are needed in order to create an interval or intervals at the extremes so as to cover all the possible stream conditions/matches in the superstructure.

3. New Superstructures

3.1 Supply and target based superstructure (S&TBS)

The first approach is the use of the supply temperatures of hot streams and the target temperatures of cold streams to define the interval boundaries of the superstructure. The grid diagram in Figure 2 below shows two hot streams and two cold streams with the hot streams running between the interval boundaries that correspond to their respective supply temperatures (T^S_{H1}, T^S_{H2}) and the last (additional) interval boundary in the superstructure T^s_{Cf}while the cold streams run between the last (additional) interval boundary T^s_{Cf} and the interval boundaries that correspond to their respective target temperatures (T^t_{C1}, T^t_{C2}).

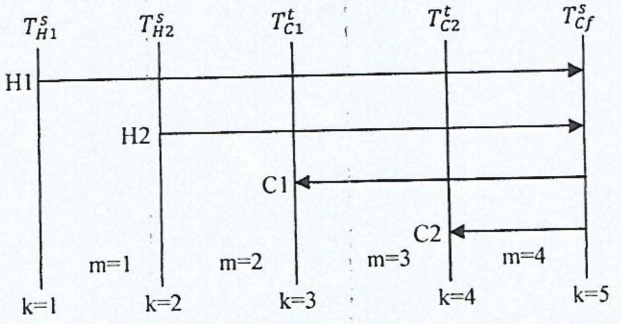

Figure 2. Grid representation for S&TBS

In the SBS, all the temperatures/ compositions fall within the superstructure. In S&TBS there is the need to use the lowest supply temperature/composition of the cold/lean streams to define the lowest interval boundary in the superstructure and ensure that all stream conditions fall within the superstructure. This is usually the supply temperature/ composition of the cold utility/external mass separating agent (MSA). Thus, the lowest temperature boundary in S&TBS is an additional interval boundary. Each hot/rich stream begins at the interval boundary that corresponds to its supply value and ends at the additional interval boundary, while each cold/lean stream begins at the additional interval boundary and ends at the interval boundary that corresponds to its target value. The exchange of heat between hot/rich streams and cold/lean streams in an interval within the superstructure is subject to the presence of such streams in that interval and to thermodynamic feasibility. An analogous structure to Figure 2 represents the MENS counterpart.

To ensure that a hot stream cannot exchange heat in any interval whose temperature is higher than its supply value while a cold stream cannot exchange heat in any interval where the temperature is higher than its target value, the superstructure works with two stream existence conditionals. The first conditional is that a hot stream is considered for matching in an interval m (between the boundaries k and $k+1$) if its supply temperature is greater than or equal to the temperature interval boundary that starts that interval (i.e. boundary k). The second conditional is that a cold stream is considered for matching in an interval m (between the boundaries k and $k+1$) if its supply temperature is less than or equal to the temperature interval boundary k that begins that interval. The superstructures with the above conditionals are labelled S&TBS Type 1 and the mathematical expression for them is as follows:

$$H_{i,m}\$(T^s_i \geq T_k) = 1 \tag{1}$$

$$C_{j,m}\$(T^s_j \leq T_k) = 1 \tag{2}$$

In S&TBS Type 2, the first conditional (for hot streams) is the same as in Type 1 but the second conditional is that a cold stream is considered for matching if its target temperature is greater than or equal to the temperature interval boundary that begins the interval, which is expressed as follows:

$$C_{j,m}\$(T^t_j \geq T_k) = 1 \tag{3}$$

The overall energy balances to ensure that streams get to their target temperatures and interval energy balances which refer to heat exchanged by hot stream i and cold stream j are similar to those of the SBS [1]. The differences lie only in the definition of the temperature interval boundaries. From Figure 2 above, with lower case variables being those that are optimised:

$$k = 1;\; T^s_{H1,1} \tag{4a}$$

$$k = 2;\; T^s_{H2,2} \quad t_{H1,2} \tag{4b}$$

$$k = 3;\; T^t_{C1,3} \quad t_{H1,3} \quad t_{H2,3} \tag{4c}$$

$$k = 4;\; T^t_{C2,4} \quad t_{H1,4} \quad t_{H2,4} \quad t_{C1,4} \tag{4d}$$

$$k = 5;\; T^S_{H1,5} \quad T^S_{H2,5} \quad T^S_{C1,5} \quad T^S_{C2,5} \tag{4e}$$

3.2 Target and supply based superstructure (T&SBS)

In the second approach, the target temperatures/compositions of hot streams and the supply temperatures/compositions of cold streams are used to define the interval boundaries of the superstructure. The grid diagram in Figure 3 shows two hot streams and two cold streams in the superstructure. In the superstructure, the hot streams run between the first (additional) temperature interval boundary T^s_{Hf} and the interval boundaries that correspond to their respective target temperatures (T^t_{H2} T^t_{H2}) while the cold streams run between the interval boundaries that correspond to their supply temperatures and the additional interval boundary.

As in the S&TBS, there is the need to introduce an extra interval boundary, using the highest supply temperature/composition of the hot/rich stream (usually the supply temperature of the hot utility in HENS) to ensure that all temperatures/compositions in the synthesis task fall within the superstructure. Thus, the highest temperature boundary $T_{Hf,1}^{s}$ in this superstructure is the additional interval where each of the hot streams begins and where the cold streams end.

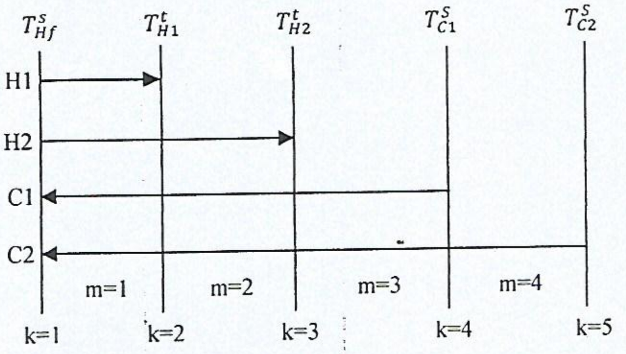

Figure 3. Grid representation for T&SBS

Heat exchange between hot and cold streams in any of the intervals depends on their presence in the interval and thermodynamic constraints. This superstructure works with the following stream existence conditionals: a hot stream should be considered for matching if its target temperature is less than or equal to the interval boundary that starts that interval, while a cold stream is to be considered for matching if its supply temperature is less than or equal to the interval boundary value that begins the interval.

$$H_{i,m}\$(T_i^t \le T_k) = 1 \qquad (5)$$

$$C_{j,m}\$(T_j^s \le T_k) = 1 \qquad (6)$$

The interval temperature boundaries in T&SBS are defined as follows (compare Equation 4):

$$k = 1;\ T_{Hf,1}^{s} \quad T_{H1,1}^{s} \quad T_{H2,1}^{s} \quad T_{C1,1}^{t} \qquad (7a)$$

$$k = 2;\ T_{H1,2}^{t} \quad t_{H2,2} \quad t_{C1,2} \qquad (7b)$$

$$k = 3;\ T_{H2,3}^{t} \quad t_{C1,3} \quad t_{C2,3} \qquad (7c)$$

$$k = 4;\ T_{C1,4}^{s} \quad t_{C2,4} \qquad (7d)$$

$$k = 5;\ T_{C2,5}^{s} \qquad (7e)$$

3.3 Target based superstructure (TBS)

The definition of a superstructure using the target temperatures/compositions of the hot/rich streams and the target temperatures/compositions of the cold/lean streams seems not to be feasible (see Figure 4). This is because even when two additional interval boundaries are created to ensure that all available hot and cold stream conditions in the synthesis task fall within the superstructure, it is not possible to match all the streams in the superstructure.

Examination of Figure 4 shows that the only interval where heat exchange is possible is Interval 3, where H2 and C1 may be matched. H1 and C2 cannot be matched with a stream of the opposite kind in any of the intervals.

Given that the TBS superstructure does not work, this paper will now consider the application of the S&TBS and T&SBS superstructures to the solution of HENS and MENS problems.

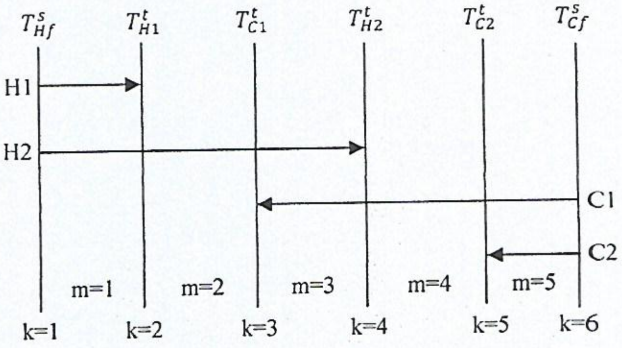

Figure 4. Grid representation for TBS

4. Solution and Initialisation

In the model equations of S&TBS and T&SBS, the temperature/composition feasibilities along the superstructure, the use of binary variables $Z_{i,j,m}$, in logical constraint equations to ensure the existence or otherwise of match *i,j* in interval *m*, the approach temperatures/compositions dt_{ijk}/dy_{rlk} to calculate the heat/mass exchanger driving force at the interval boundaries, and the objective functions in the two superstructures are as in the SBS of Azeez, *et al.* [1].

The S&TBS and T&SBS are modelled as MINLPs with the objective function being the minimum TAC. The models presented in this paper have been solved in the GAMS environment [7] with the solver DICOPT++, which uses CPLEX for the MILP and CONOPT for the NLP sub-problems, as done for the SBS. The solutions obtained gave results which are close to those in literature, as will be shown in the examples that follow.

The initialisation process is done through the exchanger minimum approach temperature (EMAT) in HENS and the exchanger minimum approach composition (EMAC) in MENS, while upper bounds are set for heat capacity flow rates of hot and cold utilities in HENS and external MSAs in MENS.

5. HENS Examples

5.1 Example 1 (4SP1)

This is the 4SP1 problem with two hot streams, two cold streams, one hot utility (steam) and one cold utility (water), taken from Lee, *et al.* [8]. The stream and cost data are shown in Table 1. Other workers that have solved this problem include Grossman and Sargent [9], Krishna and Murty [10] and Azeez, *et. al.* [1].

The S&TBS and the T&SBS were applied to this problem and the results compared well with those of previous workers as shown in Table 2. Note that Table 2 and all subsequent results tables are arranged in descending order of TAC for ease of comparison. The results for both types of S&TBS are very close (within 0.1%) to those of the SBS and Krishna and Murty [10], with S&TBS Type 1 being slightly lower than Type 2 and the SBS, whereas the T&SBS is about 4% higher than them.

Table 1. Stream and capital cost data for Example 1 [8]

Stream	T^s(°F)	T^t(°F)	Cp (Btu/(h °F))
H1	320	200	16,666.8
H2	480	280	20,000
C1	140	320	14,450.1
C2	240	500	11,530
S1	540	540	-
W1	100	180	-

Hot utility (S1) cost = \$12.76kBTU^{-1} yr^{-1}, Cold utility (W1) cost = \$5.24 kBTU^{-1} yr^{-1}, Heat exchangers annual cost = \$35×Area$^{0.6}$(Area in ft^2), U = 150 Btu/ft^2°F for all matches except those involving steam where U = 200 Btu/ft^2.

Table 2. Comparison of results for Example 1

Method	Stream Splits	No of units	TAC ($/year)
Branch and Bound Method of Lee, *et al.* [8]	0	5	13,481
T&SBS	2	5	11,204
S&TBS (Type 2)	1	5	10,795
SBS of Azeez, *et al.* [1]	1	5	10,794
S&TBS (Type 1)	1	5	10,786
DEM of Krishna and Murty [1]	0	5	10,782
Mathematical Optimisation Technique of Grossman and Sargent [9]	0	5	10,592

5.2 Example 2 (MAGNETS problem)

This example was taken from the MAGNETS User Manual and used for the analysis of the SWS method by Yee and Grossman [2] for cases that required stream splits. It involves five hot streams, one large cold stream, one hot utility (steam) and one cold utility (cooling water). The stream and cost data are shown in Table 3. The problem was expected to require many splits, which is reflected in the solutions obtained by them and other workers [3, 1]. The results of the present techniques compare well with those of previous workers, as shown in Table 4. In fact, apart from the one IBMS result, all the reported results are within less than 1% of the lowest one which was obtained by the SWS method. Of the methods being presented here, S&TBS Type 2 has the lowest cost. Yee and Grossman (SWS) set up a five stage superstructure and an NLP sub optimisation step to obtain a TAC which is 0.2% lower than the TAC obtained by S&TBS Type 2.

Table 3. Stream data for Example 2 [2].

Stream	T^s(°F)	T^t(°F)	Cp (kW/K)	Cost ($kW^{-1}yr^{-1})
H1	500	320	6	-
H2	480	380	4	-
H3	460	360	6	-
H4	380	360	20	-
H5	380	320	12	-
C1	290	660	18	-
S1	700	700	-	140
W1	300	320	-	10

U (kWm^{-2} K^{-1}) = 1 for all matches, annualized area cost = 1200(A)$^{0.6}$ for all exchangers where A is Area (m^2).

Table 4. Comparison of results for Example 2.

Method	Stream Splits	No of units	TAC ($/year)
Cold Stream Based IBMS of Isafiade and Fraser [3]	1	5	595,064
T&SBS	1	7	581,954
Hot Stream Based IBMS of Isafiade and Fraser [3]	1	7	581,942
S&TBS (Type 1)	1	7	581,942
SBS of Azeez, *et al.* [1]	1	8	580,023
S&TBS (Type 2)	1	10	577,602
SWS of Yee and Grossman [2]	1	7	576,640

5.3 Example 3 (Aromatic plant)

This is the Aromatic plant problem that involves the determination of a cost optimal network of heat exchangers for four hot streams and five cold streams having different heat transfer coefficients (Linnhoff and Ahmad [11]). The stream and cost data are shown in Table 5 and a comparison of costs with previous works in Table 6. The cost comparison shows that the new S&TBS and T&SBS methods are able to solve problems with different heat transfer coefficients.

Table 5. Stream data for Example 3 [11]

Streams	T^s(°C)	T^t(°C)	Cp (kWK^{-1})	H (kWm^{-2}K^{-1})
H1	327	40	100	0.50
H2	220	160	160	0.40
H3	220	60	60	0.14
H4	160	45	400	0.30
C1	100	300	100	0.35
C2	35	164	70	0.70
C3	85	138	350	0.50
C4	60	170	60	0.14
C5	140	300	200	0.60
Hot Oil	330	250	-	0.50
Water	15	30	-	0.50

Plant Lifetime = 5 yrs; Rate of interest = 0%; Exchanger cost (US\$) = 10,000 + 350 * S (S is Area in m^2); Hot oil Cost = 60 US\$.kW^{-1}yr^{-1}; Water Cost = 6 US\$.kW^{-1}yr^{-1}.

Table 6. Comparison of results for Example 3.

Method	Stream Splits	No of units	TAC (M$/year)
DEM of Krishna and Murty [10].	2	-	3.146
Block Decomposition Method of Zhu, *et al.* [12]	0	10	2.980
S&TBS (Type 1)	3	13	2.979
SBS of Azeez, *et al.* [1]	6	14	2.976
Linnhoff and Ahmad [11]	0	13	2.960
GA of Lewin [13]	0	11	2.946
DEM of Krishna and Murty [10].	0	15	2.942
S&TBS (Type 2)	1	11	2.940
GA of Lewin [13]	2	12	2.936
T&SBS	7	17	2.922
Match Reduction approach of Petersen [14]	7	17	2.905

6. MENS Examples

6.1 Example 4 (Ammonia removal)

This example is taken from Hallale [15] and been solved by a number of other workers [5, 16, 6, 1]. In the problem, ammonia is to be removed from five gaseous streams (mainly air). Two process MSAs and one external MSA, L1, L2 and L3 respectively, are available for ammonia removal. Packed column mass exchangers are to be used; stream and cost data for the problem are as shown in Table 7. The exchanger cost based on mass of Hallale (1998) is adopted in this study for comparison with previous workers.

Table 8 compares the results of this study with those of previous workers. The SBS method features the lowest TAC (1.2% lower than the next lowest one, which is T&SBS), while the methods of S&TBS and T&SBS give TACs that are within 0.7% of each other. They are all lower than the TACs of Szikai, *et al.* [5], Emhamed, *et al.* [16], and the IBMS technique of Isafiade and Fraser [6].

Table 7. Stream and cost data for Example 4 [15].

Rich Stream	R(kg/s)	Y(s)	Y(t)
R1	2	0.005	0.0010
R2	4	0.005	0.0025
R3	3.5	0.011	0.0025
R4	1.5	0.010	0.0050
R5	0.5	0.008	0.0025

Lean Stream	L (kg/s)	X(s)	X(t)	m	b	Cost ($/kg)
L1	1.8	0.0017	0.0071	1.2	0	0
L2	1	0.0025	0.0085	1	0	0
L3	α	0.017	0.0017	0.5	0	0.001

K_W = 0.02 kg NH_3/(s kg); Annualisation factor = 0.225; Annual operating time = 8150 hr.

Table 8. Comparison of results for Example 4.

Method	Splits: rich/lean	No of units	TAC ($/yr)
Hybrid method of Emhamed, *et al.* [16]	3/2	10	134,399
SWS of Szikai, *et al.* [5]	0/1	8	134,000
IBMS of Isafiade and Fraser [6]	1/1	7	133,323
S&TBS (Type 1)	2/1	9	132,372
S&TBS (Type 2)	2/1	9	132,331
T&SBS	2/1	9	131,524
SBS of Azeez, *et al.* [1]	1/2	9	129,901

6.2 Example 5 (Dephenolisation of aqueous wastes)

This example is taken from El-Halwagi [17]. In the problem, phenol is to be absorbed by solvent extraction from two aqueous streams, R1 and R2. Two process MSAs, namely gas oil (L1) and lube oil (L2), and one external MSA, light oil (L3) are available for the absorption. The problem specification is that the entire gas oil stream should be used. The mass exchangers are sieve tray columns. The capital cost data of Papalexandri, *et al.* [18] with the specification of $4552 per equilibrium stage per year was used. Stream data for the problem can be found in Table 9, while the cost comparison with previous workers can be found in Table 10.

Table 9. Stream and Cost data for Example 5 [17]

Rich Stream	R(kg/s)	Y(s)	Y(t)
R1	2	0.050	0.010
R2	1	0.030	0.006

Lean Stream	L^C (kg/s)	X(s)	X(t)	m	b	Cost ($/kg)
L1	5	0.005	0.015	2.00	0	0
L2	3	0.01	0.030	1.53	0	0
L3	∞	0.0013	0.015	0.71	0.001	0.01

Table 10. Comparison of results for Example 5.

Method	Splits: rich/lean	No of Units	TAC ($/yr)
S&TBS (Type 2)	0/1	5	421,147
Lean based IBMS of Isafiade and Fraser [6]	0/0	5	358,292
Pinch technique of Hallale and Fraser [19]	0/2	7	345,416
SBS	0/0	6	339,579
Rich based IBMS of Isafiade and Fraser [6]	0/0	6	338,168
1st option of Insight based technique of Comeaux [4]	0/2	7	333,300
2nd option of Insight based technique of Comeaux [4]	0/2	8	332,000

6.3 Example 6 (Coke oven gas problem)

This example was taken from El-Halwagi and Manousiouthakis [20]. It has been solved by Hallale and Fraser using pinch technology [19] and Isafiade [21] using the IBMS method. The problem involves the removal of hydrogen sulphide from two rich streams namely coke-oven gas, R1, and tail gas from a Claus unit, R2 One process MSA (aqueous ammonia), L1, and one external MSA (chilled methanol), L2, are available for this removal. The stream and cost data are shown in Table 11. The stream flowrates are assumed to be constant [20]. The columns used are stagewise columns and the cost per stage per year of Papalexandri, *et al.* [18] ($4552) is used in the column costing.

Table 11. Stream and cost data for Example 6 [20]

Rich Stream	R(kg/s)	Y(s)	Y(t)
R1	0.9	0.070	0.0003
R2	0.1	0.051	0.0001

Lean Stream	L^C (kg/s)	X(s)	X(t)	m	b	Cost ($/kg)
L1	2.3	0.0006	0.031	1.45	0	117,360
L2	∞	0.0002	0.0035	0.26	0	176,040

Table 12. Comparison of results for Example 6

Method	Splits: rich/lean	No of Units	TAC ($/yr)
Rich based IBMS of Isafiade [21]	0/0	4	530,471
T&SBS	0/2	4	526,471
S&TBS (Type 1)	0/2	4	524,244
S&TBS (Type 2)	0/2	4	524,244
SBS of Azeez, *et al.* [1]	0/0	5	469,968
Lean Based IBMS of Isafiade [21]	0/2	4	446,840
Pinch technique of Hallale and Fraser [19]	0/1	5	431,613

7. Conclusions

The present study demonstrates that in HENS and MENS interval boundaries of superstructures can be defined using combinations of key variables such as supply temperatures/compositions of hot/rich streams and target temperatures/compositions of cold/lean streams. The results obtained in this study show that neither the type of temperature/composition used to partition the superstructure interval boundary in HENS/MENS, nor the number of intervals (stages) in the superstructure appear have any significant effect on the network TAC.

This study demonstrates that, so far, the outcome of various techniques presented in the literature have been problem specific, since there is no particular technique that conclusively obtains the lowest cost for all HEN or MEN problems. This highlights the general problem with using mathematical programming techniques in process synthesis, namely the non-convexity of the problem specifications, which means that any gradient based tool may not locate the global optimum in the synthesis task (Lee and Grossman [22]).

As we apply these techniques to more problems we hope that a pattern may emerge which allows us to relate which technique is best for which kind of problem.

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