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Globally optimal synthesis of heat exchanger networks. Part I: Minimal networks

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Abstract

This article introduces the concept of minimal structure (MSTR) and presents an enumeration algorithm for the synthesis of heat exchanger networks based on MSTR. Minimal Structures refer to a class of heat exchanger networks featuring acyclic heat transfer networks without energy loops. The enumerations used are either exhaustive or smart with a stopping criterion. Without loss of generality we use the isothermal mixing Synheat model, that is, the method applies identically to other superstructures, with likely variations in the optimization models associated to each step. A conjecture is used to state that the algorithm renders solutions that are globally optimal. Literature examples are used to demonstrate the capabilities of the enumeration algorithm. Most of our solutions compare favorably with the best reported ones in literature, with exceptions where the reported solution is not minimal.

KEYWORDS

enumeration algorithm, global optimality, heat exchanger networks, minimal structures

1 | INTRODUCTION

Heat exchanger network (HEN) synthesis has been researched intensively over the last 40–50 years. Reviews were made by Furman and Sahinidis[1] followed by Morar and Agachi.[2] Of all this work, we especially review the combined use of mathematical programming and the use of superstructures.

Regarding superstructures, the most cited are the generalized superstructure by Floudas et al.[3] which considers nonisothermal mixing and the isothermal mixing stage-wise superstructure proposed by Yee and Grossmann.[4] The former was further generalized by Kim and Bagajewicz,[5] while the latter, more appealing to practitioners in industry and widely preferred in academia, was expanded to consider nonisothermal mixing by Björkand and Westerlund[6] and Huang et al.[7] In addition, Huang and Karimi[8,9] proposed extensions of the stage-wise superstructure that include recycles inside each stage as well as partial bypasses of the stages. Finally, regarding staged superstructures, another extension to consider substages and nonisothermal mixing was proposed by Jongsuwat et al.[10] and solved globally by Kim et al.[11] Bypasses and recycles, as well as several exchangers in series on each branch, were also considered by Barbaro and Bagajewicz[12] who proposed a superstructure that uses transshipment-type equations to obtain a rigorous linear model.

Regarding solution procedures, there are several approaches. In this brief overview, we omit most of the stochastic-based approaches like genetic algorithms (GA), particle swarm optimization (PSO), simulated annealing (SA), etc., because none of them guarantees global optimality. Some of these methods are worth mentioning, as they are capable of solving large-scale problems: GA by Ernst et al.[13] and Aguitoni et al.,[14] PSO by Silva et al.[15] and Huo et al.,[16] SA by Peng and Cui[17] and Pavão et al.[18]

There are several approaches proposed to solve the HEN synthesis mixed integer nonlinear model (MINLM)[19] using MINLP approaches; some use Lagrangian decomposition, very many use outer approximation (DICOPT) and a few use global optimization solvers. Some of the most relevant efforts made in the last 5 years that do not address global optimization are by Wu et al.,[20] who replace binaries by nonlinear approximations and solve an NLP using BARON because any other solver does not work without initial values. Hong et al.[21] developed a new transshipment model that considers splitting, by-passing and recycling of streams as well as non-isothermal mixing (counting exchangers in a similar way that Barbaro and Bagajewicz[12] proposed). Beck and Hofmann,[22] aiming at reducing solution time, presented a novel linearization approach for HEN synthesis based on stage-wise superstructure ending in a MILP problem whose solutions are used to initialize the MINLP model. Nemet et al.[23] developed a two-step approach, obtaining a structure in the first step by solving a MILP to find several solutions in acceptable time. In a second step, they run a "reduced" MINLP model where poor solutions obtained in the first step are forbidden. Nair and Karimi[24] studied HEN synthesis using a stage-less superstructure employing an effective outer-approximation algorithm.

Finally, several articles that guarantee globally optimal solutions were also developed recently. Bogataj and Kravanja[25] proposed an alternative global optimization strategy for HEN synthesis using an isothermal mixing stage-wise superstructure that has limitations for large-scale structures. Mistry and Misener[26] showed that the reverse logarithmic mean temperature difference (RLMTD) is convex and proposed an outer approximation that works well for small problems. Faria et al.[27] applied RYSIA, a bound contraction methodology, to solve HEN synthesis problems to global optimality based on the isothermal mixing stage-wise superstructure (they address medium size problems). Kim and Bagajewicz[5] developed a new generalized superstructure for HEN synthesis and solved it globally. Later, Kim et al.[11] presented a new substage superstructure for HEN synthesis that is also solved globally. Finally, Beck and Hofmann[28] proposed solving several MILP and NLP subproblems iteratively that allow to solve small-scale problems to global optimality, but the algorithms are not efficient for large-scale problems.

Our strategy departs completely from attempting to solve the full MINLM using local or global MINLP solvers. Instead, we resort to naïve or smart enumeration of structures guaranteeing global optimality.

This paper is organized as follows: We first present some HEN properties that aid understanding the procedure proposed. Next, we present the different optimization problems and algorithms that are used and then show the globally optimal smart search. We finish with showing results and the conclusions.

2 | HEN PROPERTIES

We start with a set of definitions, remarks, and lemmas that are put in the context of the Synheat stage-wise model and its nomenclature.

Match A match between streams *i* and *j* exists if there is a set of heat exchangers with finite area and non-negative heat transferred between the streams. In the nomenclature of our Synheat model (See Appendix A) a match is defined by $\sum_{k \in ST} z_{i,j,k} \geq 1$. For other superstructures, the equation is similar.

Unit A unit is a heat exchanger between two streams that has finite area and non-negative heat transferred. In the nomenclature of our Synheat model (see Appendix A) a unit is defined by $z_{i,j,k} = 1$.

Remark 1 The term *Match* is borrowed from heat exchanger network literature, and although it is commonly assumed that the heat transferred is strictly positive, in many studies where it is used, there is no clear distinction. The interpretation that a match can exist with $q_{i,j,k} = 0$ is used here.

Active unit A unit is active if $z_{i,j,k} = 1$, and has strictly positive heat exchanged, that is $q_{i,j,k} > 0$, strictly.

Inactive unit We define it as unit ($z_{i,j,k} = 1$) for which $q_{i,j,k} = 0$.

Structure A structure (*STR*) is a set of active units that makes all streams attain their target temperatures. Formally, we write:

$$STR = \left\{ \begin{array}{l} (i,j,k) \ni z_{i,j,k} = 1 \wedge zhu_j = 1 \wedge zcu_i = 1 \wedge q_{i,j,k} > 0 \wedge qhu_j > 0 \wedge qcu_i > 0; \\ i \in HP, j \in CP, k \in ST \end{array} \right\}$$

Minimal structure (MSTR): It is a structure that has a unique set of heat transferred $q_{i,j,k}$ for any utility usage $E = \sum_{j \in CP} qhu_j$ that makes the HEN feasible.

$$MSTR = \left\{ \begin{array}{l} Feasible\ STR \ni q_{i,j,k}, qhu_j, qcu_i\ are\ unique \\ for\ a\ fixed\ E = \sum_{j \in CP} qhu_j,\ \forall i \in HP, \forall j \in CP, \forall k \in ST \end{array} \right\}$$

Minimum number of units The concept of minimum number of units used in this article is derived from graph theory. For a bipartite graph, the minimum number of edges is given by:

$$N_{min} = NH + NC + NU - P \tag{1}$$

where *NH=Card(HP)*, *NC=Card(CP)*, *NU = 2*, where *NU* is the number of utility types and *Card*(*X*) is the cardinality of the set *X* (see Appendix A for explanation of the nomenclature). Additionally, *P* is the largest number of independent subsystems. A subsystem, in turn, is a subbipartite graph included in the complete bipartite graph with an empty intersection with other subbipartite graphs, that is, all subsystems are disjoint. Regarding *NU*, for example, if one uses one hot utility of type "Furnace" and a cold utility of type "cooling water," *NU* = 2. However, if one uses one hot utility of type "Furnace" and another hot utility of type "Condensing steam" and one cold utility of type "cooling water," *NU* = 3, but in this case of more than one utility per type, one should write $N_{min} < NH + NC + NU - P$, because one of the hot utilities may not be active. In this article, without loss of generality, we use only two types of utilities, one hot and one cold, each being able to fulfill the task using more than one unit.

Remark 2 The number of subsystems *P* is rarely larger than *P* = 1 for cost-optimal or sub-optimal heat exchanger networks.

Remark 3 The number of subsystems can be obtained easily by considering increasing number of hot streams and identifying how many cold streams' collective energy content add-up to the aggregated energy content of the hot streams considered. We use a different strategy to obtain this number, because the compatibility with the superstructure model needs to be taken into account. We offer an algorithm to determine *P* in Appendix B.

Remark 4 Other definitions of the minimum number of units have been presented. One well-known formula is that of the Pinch Design Method, which considers two systems, one above the pinch and one below the pinch (using $NU = 1$ for each system). Such definition almost always leads to a total number of units that is larger than N_{min} (as defined above), and consequently these structures are rarely MSTR structures. Similarly, structures with nonisothermal mixing and with bypasses that cannot be represented by the staged superstructure have been studied[29,30] and rendered values given by N_{min} that are virtually impossible using other limited superstructures.

Remark 5 There have been several studies in the literature regarding the a-priori calculation of the minimum number of units, sometimes referred to as minimum number of matches.[31,32] Letsios et al.[32] presented a proof that the minimum number is $N_{min} = NH + NC + NHU + NCU\text{-}L$, where *NHU* and *NCU* are the number of hot and cold utilities types respectively and $L \in [1, Min\{NH + NHU, NC + NCU\}]$. For these authors,[31] the big issue is to obtain the maximum value of *L*. They state the problem is *NP-hard*, and provide a series of theorems, lemmas, and approximation procedures that intend to obtain bounds of the solution. The issue is also complicated by the fact that the heat transfer is limited by the second law of thermodynamics, that is, temperature differences are limited to be higher than a certain minimum, an issue that complicates the proofs. Letsios et al.[32] make such a distinction when they introduce multiple temperature intervals. Even after this limitation is introduced, they cannot obtain a solution directly, and have to rely on "approximation" algorithms.

Remark 6 We believe that the aforementioned works[31,32] identify the problem as *NP-hard* correctly, but only because of their incomplete formulation when multiple intervals are introduced. Bagajewicz and Valtinson[30] showed that linear constraints can be added to solve the problem rigorously and globally using small computational time. The proposed procedure is a simplified version on an earlier MILP model[12] and avoids the aforementioned *NP-Hardness* by using a different modeling.

Remark 7 The above formula (Equation 1) is a formula that does not consider thermodynamic constraints. Bagajewicz and Valtinson[30] discussed the issue and showed that there are structures that can accomplish this number of units. Moreover, as stated above, there are always uninteresting structures featuring no heat recovery. Now, when one is confined to a certain superstructure, the solutions featuring the numbers predicted by the formula may not exist.

Lemma 1 Solutions of the Synheat model that feature minimum number using the correct number of subsystems (*P*) of units or fewer are MSTR.

Proof This is explained using graph theory invoking the absence of simple cycles. Such cycles consist of path of vertices connected by edges in such a way that the path ends in the first vertex. In Pinch Design Technology language, these simple cycles are called energy "loops."[30,33] *Q.E.D.*

Remark 8 For *E* fixed, the value of *EMAT* used has no impact in the answer when a solution sought is a MSTR network. This is true regardless of the superstructure model used. It is understood that $EMAT \le HRAT(E)$, where $HRAT(E)$ is the heat recovery approximation temperature corresponding to a specific value of *E*, a parameter that is not used in the Synheat Model. In Pinch technology, the procedure is inverted: *HRAT* is used to find the associated *E* and then the network is built.

Remark 9 Solutions that feature a number of units larger than the minimum (as defined above) are not MSTR because one more match in any subsystem creates a cycle (in graph theory nomenclature) or an energy loop (using pinch technology nomenclature). This is especially true for structures obtained using the pinch design method (PDM), which are very well known for proposing matches between the same pair of streams involving two units, one above and one below the pinch. Such structures are not minimal by definitions.

Lemma 2 The Total Annualized Cost (*TAC*) (see Appendix A for its definition) that corresponds to the same feasible MSTR is a continuous function of *E*.

Proof Any differential change $dE = dqhu_j$ causes differential changes $dq_{i,j,k}$ through a path from the heater to the cooler. As a result, only differential changes in temperatures $dT^H_{i,k}$ and $dT^C_{j,k}$ take place. Because the area is a smooth function of these temperatures, the *TAC* only changes differentially. *Q.E.D.*

Conjecture The Total Annualized Cost as a function of *E*, that is *TAC* (*E*) for a given MSTR, is a unimodal continuous function with one and only one global minimum between E_{Min} and E_{Max}.

This conjecture is based on the following observation: When the amount of utility decreases, the average temperature difference for the heat exchangers between process streams becomes smaller, and consequently the total area increases, which can be verified using Area Targeting algorithms. The trade-off is obvious and it rules out any local maximum of *TAC*. Finally, Pinch Technology Supertargeting always predicts either a minimum or a monotone increasing *TAC*. We discuss this issue briefly further in Appendix C. We now explain the concepts in more detail using the following illustration.

Illustration It consists of two hot and two cold streams from Faria et al.[27] The data is given in Table 1. The fixed annual cost of units is $5,500 and the annual area cost coefficient is 150 $/m^2. One feasible structure with five exchangers for this problem is shown in Figure 1.

For a certain range of E, the minimum number of units for this problem is N_{min} = 5. For this illustration, if one chooses E = 580 kW, this is the only possible MSTR. To show why this is an MSTR, that is, why the set of heat transferred $q_{i,j,k}$ is unique, we resort to graph theory[30,33] as shown in Figure 2.

Figure 2 shows that given the MSTR of Figure 1, there is no other set of heat values that can accomplish transferring heat from hot to cold streams than the one presented for the shown edges. This assertion stems from the fact that there is no "loop" (*Pinch Technology* terminology), to move around heat.

We now illustrate ***Lemma 1***. We verify that the MSTR of Figure 1 is only feasible for values of energy between E_{Min} = 575 kW and E_{Max} = 2,750 kW. They correspond to $HRAT_{min}$ = 18.3 K and $HRAT_{max}$ = 129.3 K. These values can be verified using the pinch method tableau. Figure 3 shows that the *TAC* is monotone increasing and therefore does not exhibit a minimum within the range of feasible E values, but rather in the left extreme of the feasible range (E = 575 kW).

Figure 4, in turn, shows the *TAC* calculated for the same range, but using a much lower cost of energy, that is $\hat{C}hu_j$ = 8.0 $/kWy $\forall j \in CP$, $\hat{C}cu_i$ = 1.5 $/kWy $\forall i \in HP$, for the purpose of illustrating the

TABLE 1 Data of Example 1

Stream	T_{IN} (K)	T_{OUT} (K)	h (kW/m^{2}K)	Fcp (kW/K)
H1	650.0	370.0	1.0	10.0
H2	590.0	370.0	1.0	20.0
C1	410.0	650.0	1.0	15.0
C2	350.0	500.0	1.0	13.0
CU	300.0	320.0	1.0	_
HU	680.0	680.0	5.0	_
$EMAT_{Min}$	10.0 K			
Utility cost coefficients		Chu_j = 80 $/kWy; Ccu_i = 15 $/kWy;		
Fixed cost coefficients		$\hat{C}f_{i,j} = \hat{C}cuf_i = \hat{C}huf_j$ = $5,500; $\hat{n}y$=1		
Area cost coefficients		$\hat{a}_{i,j} = \hat{a}cu_i = \hat{a}hu_j$=150 $/m^2 $\hat{b}_{i,j} = \hat{b}cu_i = \hat{b}hu_j$=1		

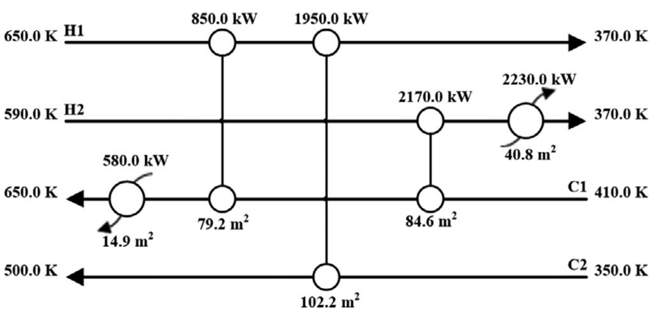

FIGURE 1 One heat transfer structure for Example 1 (N = 5)

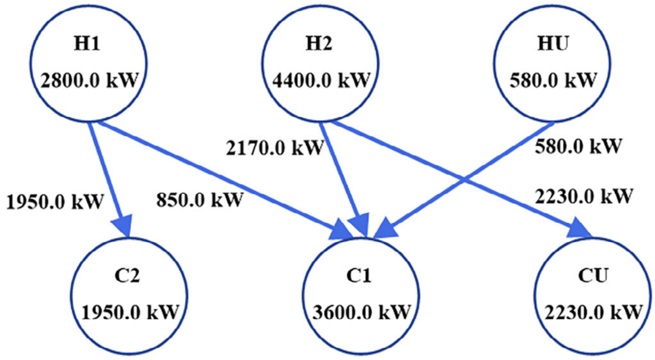

FIGURE 2 Graph representation of the MSTR for Example 1 (N = 5) [Color figure can be viewed at wileyonlinelibrary.com]

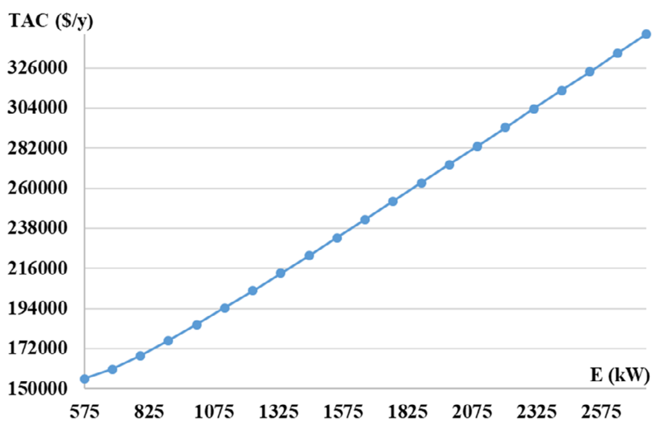

FIGURE 3 *TAC* vs. *E* for a fixed structure of Example 1 (Figure. 1) [Color figure can be viewed at wileyonlinelibrary.com]

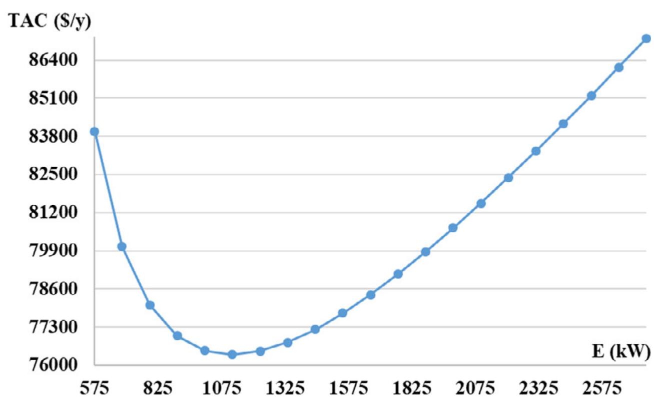

FIGURE 4 *TAC* vs. *E* for a fixed structure of Example 1 (Figure 1) and reduced energy cost [Color figure can be viewed at wileyonlinelibrary.com]

existence of a minimum inside the range. In this case, the minimum *TAC* takes place at E = 1,117.3 kW.

Based on the concepts and proofs offered above, we propose an exhaustive search algorithm that guarantees global optimality over the search space of MSTR. This search can be exhaustive or be smart, that is, have a stopping criterion. We start from a value of N_{min} that corresponds to the largest possible value of the number of subsystems (P), as obtained using the algorithm of Appendix B and then reduced until no MSTR exists.

- The enumeration of different solutions for heat transfer in a given MSTR, by calculating the heat transfer pattern for given values of E, starting from the smallest possible energy value until the largest in small steps is time consuming and the strict minimum may be missed, so some gap is expected on the *TAC* value and the associated energy consumption (E) and the minimum. This gap is dependent on the size of the step used. To improve this, one can take advantage that *TAC* is a univariate function of E. Several algorithms are available for this task, namely: Golden Search, Ternary Search, Polynomial Interpolation, etc. In this article, we use Golden Search.
- It is possible that the *TAC* vs. E has no local minimum with zero derivative, but rather has its extremum at the minimum or maximum value of energy. We identify this condition, which avoids the Golden Search by using a Monotonicity Test.
- Every single time an optimum value of E is identified for each MSTR, one can store an incumbent Upper Bound (UB) to be used by a stopping criteria (explained below).
- As an alternative to running Synheat without the area equations to obtain a MSTR, one can actually run a lower bound (LB) model, without fixing the structure and thus obtaining the MSTR from this run. To this effect, we extend the LB model proposed by Faria et al.[27] If such LB is larger than the incumbent UB, one can stop. The LB model is likely to identify very good MSTR candidates. As a result, subsequent MSTR obtained excluding previous ones may have a higher LB. When such LB has a cost higher than the incumbent UB, the process can stop.
- After identifying a MSTR by any method, one can run a LB model with fixed stucture and if the result of this LB is larger than the incumbent UB, the structure is abandoned without searching for its minimum value. The LB model with a structure fixed is considerably faster than the one without the structure fixed.

We now present formally the additional tools outlined in the above comments.

3 | NAÏVE METHOD TO OBTAIN MINIMAL STRUCTURES

Based on the discussion above, a naïve way to obtain a MSTR is proposed as follows:

$$PSTR = \underset{\forall (T,Q,Z) \in D_{Synheat}}{Min} \alpha \tag{2}$$

s.t.

$$\hat{E}MAT = \hat{E}MAT_{Min} \tag{3}$$

$$\sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} z_{i,j,k} + \sum_{i \in HP} zcu_i + \sum_{j \in CP} zhu_j = N \tag{4}$$

where α is a dummy variable, and N is the number of desired exchangers. This model renders any viable structure of matches, candidate to be a minimal structure, when N is sufficiently low.

Additional structures can be obtained using problem ***PSTRR***

$$PSTRR = \underset{\forall (T,Q,Z) \in D_{Synheat}}{Min} \alpha \tag{5}$$

s.t.

$$\hat{E}MAT = \hat{E}MAT_{Min} \tag{6}$$

$$\sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} z_{i,j,k} + \sum_{i \in HP} zcu_i + \sum_{j \in CP} zhu_j = N \tag{7}$$

$$\left(\sum_{i,j,k \in MSTR_{l'}} z_{i,j,k} + \sum_{i \in MSTR_{l'}} zcu_i + \sum_{j \in MSTR_{l'}} zhu_j \right) - \left(\sum_{i,j,k \notin MSTR_{l'}} z_{i,j,k} + \sum_{i \notin MSTR_{l'}} zcu_i + \sum_{j \notin MSTR_{l'}} zhu_j \right) \leq Card(MSTR_{l'}) - 1 \quad \forall l' = 1,\ldots,l-1 \tag{8}$$

Remark 10 Equation (8) is a classical set exclusion constraint. There is, however, a problem with this constraint, as applied to solving the Synheat model. Indeed, the same HEN structure of matches can be represented by locating the heat exchangers in different stages, especially if a larger number of stages than needed is used. Thus, when the constraint is used, the same structure can be obtained with matches in different stages, not acting as an exclusion constraint after all the possible equivalent structures with the same unit in different places are exhausted. To avoid the repeated equivalent structures, we developed a set of equations to generate a single number for a given structure, which excludes a network regardless of the stage location of the matches. This was done following the procedure proposed by Ji and Bagajewicz.[34] The corresponding equations are shown and explained at the end of the Supplemental Material. However, after implementing, we found that they add more computational time than the time they save by not repeating structures, so we propose to use the classical exclusion constraint to enumerate structures including the repeated equivalent ones. Later, in Section 9, we explore other alternatives to reduce computational time.

Remark 11 By using the lowest possible heat recovery approximation temperature $\hat{E}MAT_{Min}$, we guarantee that all possible structures and values of energy consumption E are part of the feasible region.

4 | ENERGY LIMITS FOR A FIXED MSTR

The minimum energy can be obtained using traditional pinch technology algorithms for $HRAT = EMAT_{Min}$. In practice, the minimum $EMAT_{Min}$ is larger than 5°C for shell and tube exchangers, depending of the case, sometimes lower for other type of exchangers. However, if what is sought is the minimum energy for a given MSTR, the minimum obtained using pinch technology, may be infeasible for the structure considered. Thus, we first obtain the minimum energy by running problem ***PEMin*** using the minimum value $EMAT_{Min}$.

$$PEMin = \underset{\forall(T,Q)\in D_{Synheat}}{Min} \; E \tag{9}$$

s.t.

$$E = \sum_{j\in CP} qhu_j \tag{10}$$

$$\hat{E}MAT = \hat{E}MAT_{Min} \tag{11}$$

$$E \geq \hat{E}^{User}_{Min} \tag{12}$$

$$\{z_{i,j,k} = 1, zhu_j = 1, zcu_i = 1\} \; \forall(i,j,k)\in STR_l \tag{13}$$

We use the constraint $E \geq \hat{E}^{User}_{Min}$, where $\hat{E}^{User}_{Min}$ is a user inserted minimum energy value to limit the energy consumption of the solutions to this minimum. We remark that $\hat{E}MAT$ is a limit, so no match is forced to have a temperature difference equal to it.

Any user might think of obtaining $\hat{E}^{User}_{Min}$ using a selected low value of HRAT (this is a term that was coined associated to pinch technology). Our algorithm calculates $\hat{E}^{User}_{Min}$ as the largest of the input value given by the user and the one obtained using a value of $HRAT = EMAT_{Min}$ using the classic LP problem equivalent to the Minimum Energy Tableau.[33]

In turn, an UB of the maximum energy consumption can be obtained as follows:

$$E_{\max} = \sum_{j\in CP} \hat{F}cp^C_j \left(\hat{T}^C_{OUT,j} - \hat{T}^C_{IN,j}\right) \tag{14}$$

However, this value is too large and is likely to be infeasible for a given structure because it implies that there is no heat recovery. To obtain a realistic UB for a given structure, one can use $\hat{H}RAT_{Max} = \hat{\Gamma}_{i,j}/1.01$, where $\hat{H}RAT_{Max}$ is provided by the user (or some default is used) and $\hat{\Gamma}_{i,j}$ is obtained using Equation (A-26) from Appendix A, and then run problem ***PEMin*** using $\hat{E}MAT = \hat{H}RAT_{Max}$. However, this might also be infeasible because $\hat{H}RAT_{Max} = \hat{\Gamma}_{i,j}/1.01$ may be too large for the structure selected. We therefore propose to obtain E_{Max} for the current MSTR, by running problem ***PEMax.***

$$PEMax = \underset{\forall(T,Q)\in D_{Synheat}}{Max} \; E \tag{15}$$

s.t.

$$E = \sum_{j\in CP} qhu_j \tag{16}$$

$$\hat{E}MAT = \hat{E}MAT_{Min} \tag{17}$$

$$\hat{E}^{User}_{Min} \leq E \leq \hat{E}^{User}_{Max} \tag{18}$$

$$q_{i,j,k} \geq \hat{\varepsilon}\; z_{i,j,k} \qquad i\in HP, j\in CP, k\in ST \tag{19}$$

$$qcu_i \geq \hat{\varepsilon}\; zcu_i \qquad i\in HP \tag{20}$$

$$qhu_j \geq \hat{\varepsilon}\; zhu_j \qquad j\in CP \tag{21}$$

$$\{z_{i,j,k} = 1, zhu_j = 1, zcu_i = 1\} \forall(i,j,k)\in STR_l \tag{22}$$

Equation (18) takes into account the energy limits set by the user. The value of maximum energy $\hat{E}^{User}_{Max}$ can also be obtained considering the use of pinch calculations associated to a maximum $HRAT$ that the user might consider using. Equations 19–21 are inserted so that the solution has the properties of a MSTR, that is, variables $z_{i,j,k}$, zcu_i and zhu_j are associated to matches where the heat transferred is strictly positive ($\hat{\varepsilon}$ is a small positive number), even though this might be true by construction. However, if users want to rule out exchangers with heat transferred smaller than a certain threshold, $\hat{\varepsilon}$ can be set to such a limit and individualized to each exchanger. We expect these constraints rarely be binding.

5 | HEAT TRANSFER PATTERN FOR A GIVEN MSTR

To obtain a heat distribution corresponding to each MSTR and each value of energy consumption E, we solve problem ***PESTR***

$$PESTR = \underset{\forall(T,Q)\in D_{Synheat}}{Min} \; \alpha \tag{23}$$

s.t.

$$\hat{E}MAT = \hat{E}MAT_{Min} \tag{24}$$

$$\hat{E} = \sum_{j\in CP} qhu_j \tag{25}$$

$$\{z_{i,j,k} = 1, zhu_j = 1, zcu_i = 1\} \; \forall(i,j,k)\in STR_l \tag{26}$$

where α is a dummy variable and $\hat{E}$ is fixed.

6 | TAC MONOTONY TEST

We now consider doing monotony test to detect whether the *TAC* solution of *E* is monotone or not, as shown in Figures 3 and 4 respectively. The test is the following:

1. Consider the extreme energy points E_{Min}, E_{Max} and a golden-section one $E_{Ratio} = E_{Min} + \frac{E_{Max} - E_{Min}}{GR}$ where *GR* is the golden ratio equal to $\left(1+\sqrt{5}\right)/2$. Obtain the total annualized costs TAC_{Min}, TAC_{Max}, and TAC_{Ratio} at these three points.
2. If TAC_{Ratio} = *Min* (TAC_{Min}, TAC_{Max}, TAC_{Ratio}), the solution is not monotone.
3. If TAC_{Min} = *Min* (TAC_{Min}, TAC_{Max}, TAC_{Ratio}), the solution may be monotone or not. Then, run ***PESTR*** for $E = E_{Min} + 0.01$ and obtain its total annualized cost namely TAC^{+}_{Min}.
   If $TAC^{+}_{Min} - TAC_{Min} > 0$, the solution is monotone and the optimum is TAC_{Min}.
   If $TAC^{+}_{Min} - TAC_{Min} < 0$, the solution is not monotone.
4. If TAC_{Max} = *Min* (TAC_{Min}, TAC_{Max}, TAC_{Ratio}), the solution may also be monotone or not. Then, run ***PESTR*** for $E = E_{Max} - 0.01$ and obtain its total annualized cost namely TAC^{-}_{Max}.
   If $TAC_{Max} - TAC^{-}_{Max} < 0$, the solution is monotone and the optimum is TAC_{Max}.
   If $TAC_{Max} - TAC^{-}_{Max} > 0$, the solution is not monotone.

7 | LOWER BOUND MODEL

A LB model proposed by Faria et al.[27] was adapted: A linear relaxation of the Chen's approximation[35] of the logarithmic mean temperature difference (*ΔT*), the area (*A*) and the cost of area (*ACEX*) was done. Thus, a LB featuring a given number of units *N* is obtained by solving problem ***PLB***.

$$PLB = \underset{\forall (T,Q,Z)\in D_{Synheat}}{Min} RTAC \tag{27}$$

s.t.

$$RTAC = \{FCEXL + ACEXL + HUCOST + CUCOST\} \tag{28}$$

$$FCEXL = \left(\sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST}\hat{C}fl_{i,j}z_{i,j,k} + \sum_{j\in CP}\hat{C}hufl_j zhu_j + \sum_{i\in HP}\hat{C}cufl_i zcu_i\right) \tag{29}$$

$$ACEXL = \left(\sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST}\hat{a}l_{i,j}A_{i,j,k} + \sum_{j\in CP}\hat{a}hul_j Ahu_j + \sum_{i\in HP}\hat{a}cul_i Acu_i\right) \tag{30}$$

$$\hat{E}_{Min} \le E \le \hat{E}_{Max} \tag{31}$$

$$q_{i,j,k} - \sum_{\forall l}\sum_{\forall m} H_{i,j,k,l,m}\hat{K}_{i,j,k,l,m} \le 0 \quad i\in HP, j\in CP, k\in ST \tag{32}$$

$$qcu_i - \sum_{\forall p} Hcu_{i,p}\hat{K}cu_{i,p} \le 0 \quad i\in HP \tag{33}$$

$$qhu_j - \sum_{\forall s} Hhu_{j,s}\hat{K}hu_{j,s} \le 0 \quad j\in CP \tag{34}$$

$$\sum_{\forall l} H_{i,j,k,l,m} - \hat{\psi}_{i,j}\, r_{i,j,k,m} \le 0 \quad i\in HP, j\in CP, k\in ST, \forall m \tag{35}$$

$$\sum_{\forall m} H_{i,j,k,l,m} - \hat{\psi}_{i,j}\, r_{i,j,k+1,l} \le 0 \quad i\in HP, j\in CP, k\in ST, \forall l \tag{36}$$

$$\sum_{\forall p} Hcu_{i,p} - \hat{\psi}cu_i\, rcu_i \le 0 \quad i\in HP \tag{37}$$

$$\sum_{\forall s} Hhu_{j,s} - \hat{\psi}hu_j\, rhu_j \le 0 \quad j\in CP \tag{38}$$

$$\sum_{\forall l}\sum_{\forall m} H_{i,j,k,l,m} - A_{i,j,k} = 0 \quad i\in HP, j\in CP, k\in ST \tag{39}$$

$$\sum_{\forall s} Hhu_{j,s} - Ahu_s = 0 \quad j\in CP \tag{40}$$

$$\sum_{\forall p} Hcu_{i,p} - Acu_i = 0 \quad i\in HP \tag{41}$$

$$\hat{E}MAT = \hat{E}MAT_{Min} \tag{42}$$

$$\sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST} z_{i,j,k} + \sum_{i\in HP} zcu_i + \sum_{j\in CP} zhu_j = N \tag{43}$$

$$r_{i,j,k,l}\in\{0,1\};\, rhu_{j,s}\in\{0,1\};\, rcu_{i,p}\in\{0,1\};\quad i\in HP, j\in CP, k\in ST, \forall l, \forall s, \forall p \tag{44}$$

where *HUCOST* and *CUCOST* are given by Equations A-33 and A-34 from Appendix A, and $\hat{\psi}$ is an UB of the area. Such a value can be obtained from considering the largest possible heat load among hot and cold streams, and using the smallest possible log-mean temperature difference, or *EMAT*, that is

$$\hat{\psi}_{i,j} = \frac{Min\left\{\hat{Q}h_i, \hat{Q}c_j\right\}}{\hat{U}_{i,j}\hat{E}MAT_{Min}} \quad i\in HP, j\in CP \tag{45}$$

Likewise, the values for the utilities are:

$$\hat{\psi}cu_i = \frac{\hat{Q}h_i}{\hat{U}_{CU,i}\hat{E}MAT_{Min}} \quad i\in HP \tag{46}$$

$$\hat{\psi}hu_j = \frac{\hat{Q}c_j}{\hat{U}_{HU,j}\hat{E}MAT_{Min}} \quad j\in CP \tag{47}$$

We also use the following parameters in the model:

$$\hat{K}_{i,j,k,l,m} = \hat{U}_{i,j}\sqrt[3]{\Delta\hat{T}^{D}_{i,j,k,l}\Delta\hat{T}^{D}_{i,j,k+1,m}\frac{\left(\Delta\hat{T}^{D}_{i,j,k,l} + \Delta\hat{T}^{D}_{i,j,k+1,m}\right)}{2}} \quad i\in HP, j\in CP, k\in ST, \forall l, \forall m \tag{48}$$

$$\hat{K}cu_{i,p} = \hat{U}_{CU,i}\sqrt[3]{\Delta\hat{T}^{D}_{CU,i,p}\left(\hat{T}^{H}_{OUT,i} - \hat{T}cu_{IN}\right)\frac{\left[\Delta\hat{T}^{D}_{CU,i,p} + \left(\hat{T}^{H}_{OUT,i} - \hat{T}cu_{IN}\right)\right]}{2}} \quad i\in HP, \forall p \tag{49}$$

$$\hat{K}hu_{j,s} = \hat{U}_{HU,j}\sqrt[3]{\Delta\hat{T}^{D}_{HU,j,s}\left(\hat{T}hu_{IN} - \hat{T}^{C}_{OUT,j}\right)\frac{\left[\Delta\hat{T}^{D}_{HU,j,s} + \left(\hat{T}hu_{IN} - \hat{T}^{C}_{OUT,j}\right)\right]}{2}} \quad j\in CP, \forall s \tag{50}$$

For notation purposes, we define the set of constraints of this LB as follows:

$$DR_{Synheat} = D_{Synheat} \cup \{(T,Q,Z,A) \ni equations\,(27-50)\ are\ satisfied\} \tag{51}$$

Also, *ACEXL* and *FCEXL* are linear versions of *ACEX* and *FCEX* (See Appendix A). The linear version *ACEXL* uses coefficients $\hat{a}l_{i,j}$, $\hat{a}hul_j$ and $\hat{a}cul_i$, and the linear version *FCEXL* uses coefficients $\hat{C}fl_{i,j}$, $\hat{C}hufl_j$ and $\hat{C}cufl_i$ to approximate $\hat{C}f_{i,j} + \hat{a}_{i,j}A_{i,j,k}^{\hat{b}_{i,j}}$ with $\hat{C}fl_{i,j} + \hat{a}l_{i,j}A_{i,j,k}$ over the range of area between a certain minimum and maximum. The cost of utility exchanger area is approximated in the same way. Finally, problem ***PLBR*** is composed of problem ***PLB*** plus the exclusion constraint in Equation (8) for excluding previous structures.

8 | SMART GLOBAL SEARCH ALGORITHM FOR MSTR NETWORKS

Our algorithm ***OPTMSTR*** is the following:

1. Set *UBTAC*, the best Upper Bound of the problem, to ∞.
2. Determine $\hat{E}^{User}_{Min}$ by choosing the maximum of the user given value or the one obtained using $HRAT=\hat{E}MAT_{Min}$ as a parameter of the LP problem equivalent to a minimum energy tableau proposed by Linhoff et al.[33]
3. Obtain the largest value of the number of units *N* that corresponds to a MSTR (largest *P* value in the minumn number of units expression). We call this number N_{start}. This can be obtained running the algorithm shown in Appendix B.
4. Set $N = N_{start}$
5. Obtain a viable minimal structure (MSTR). We use several different options for this.
   - ***Option 1***: To identify a viable structure, the lower bound model (***PLB***) is run with the energy and the matches free. The lower bound model excluding previous found structures (***PLBR***) is run to obtain subsequent structures.
   - ***Option 2***: The ***PSTR*** problem, which obtains one viable heat transfer pattern and gives a viable solution, thus providing the values of the binary variables to define the structure, is run and then the lower bound is run with the structure fixed. If the lower bound objective is larger than the incumbent upper bound *UBTAC*, then ***PSTRR*** (the ***PSTR*** problem excluding previous solutions) is run until a viable structure is found. Note that this cannot be used as a stopping criteria, because the structures are not generated using ***PLB.***
   - ***Option 3***: To identify a viable structure, we run the lower bound model ***PLB*** with *E* and *z* free, only the first time and use ***PSTRR*** **(**the ***PSTR*** problem excluding previous solutions) in all other subsequent runs.
   - ***Option 4*****:** use the model ***PSTR*** to find one viable solution at the first time and use ***PSTRR*** (model ***PSTR*** excluding previous solutions) afterwards.
6. For Option 1 if the problem is infeasible or *RTAC* > *UBTAC*, go to step 17. Otherwise if the solution is feasible, go to step 8.
7. For Options 2, 3, and 4, if the solution is feasible, go to step 8. If infeasible, go to step 17.
8. For the chosen structure, obtain the minimum energy consumption (E_{Min}) using ***PEMin***
9. For the chosen structure, obtain the maximum energy consumption (E_{Max}) using ***PEMax***
10. Consider extreme and golden-ratio values of *TAC* as follows:
    a. Run ***PESTR*** for $E = E_{Min}$. Evaluate the total annualized cost and call it TAC_{Min}.
    b. Run ***PESTR*** for $E = E_{ratio}$. Evaluate the total annualized cost and call it TAC_{ratio}.
    c. Run ***PESTR*** for $E = E_{Max}$. Evaluate the total annualized cost and call it TAC_{Max}.
11. If $TAC_{ratio} = Min\{TAC_{Min}, TAC_{ratio}, TAC_{Max}\}$, the solution is not monotone. Then go to step 14
12. If $TAC_{Min} = Min\{TAC_{Min}, TAC_{ratio}, TAC_{Max}\}$, the solution may be monotone or not. Then, run ***PESTR*** for $E = E_{Min} + 0.01$ and obtain its total annualized cost namely TAC^{+}_{Min}.
    - If $TAC^{+}_{Min} - TAC_{Min} > 0$, the solution is monotone and $TAC = TAC_{Min}$. Go to step 15.
    - If $TAC^{+}_{Min} - TAC_{Min} < 0$, the solution is not monotone and go to step 14.
13. If $TAC_{Max} = Min\{TAC_{Min}, TAC_{ratio}, TAC_{Max}\}$, the solution also may be monotone or not. Then, run ***PESTR*** for $E = E_{Max} - 0.01$ and obtain its total annualized cost namely TAC^{-}_{Max}.
    - If $TAC_{Max} - TAC^{-}_{Max} < 0$, the solution is monotone and $TAC = TAC_{Max}$. Go to step 15.
    - If $TAC_{Max} - TAC^{-}_{Max} > 0$, the solution is not monotone and go to step 14.
14. Apply the Golden Search to obtain the best *TAC* for the current structure.
    - Use ***PESTR*** to obtain the *TAC* for each point.
15. If *TAC* ≤ *UBTAC*, then update *UBTAC* as follows: *UBTAC* = *TAC*.
16. Set *N* = *N* – 1. Go to step 5.
17. *UBTAC* is the global optimum.

TABLE 2 Results of all examples (minimal networks)

Example	Item	Our optimal solution for minimal HENs using different options				Best result from literature	Literature source
		Option 1	Option 2	Option 3	Option 4		
1 (2H, 2C, 1HU, 1CU)	TAC ($/y)	155,413.1	155,413.1	155,413.1	155,413.1	154,995.0	Faria et al.[27]
	Ns	1	27	27	27	—	
	Time	3.0 s	45.6 s	32.6 s	55.7 s	250.0	
2 (2H, 2C, 1HU, 1CU)	TAC ($/y)	360,037.2	360,037.2	360,037.2	360,037.2	361,983.0	Escobar and Trierweiler[37]
	Ns	5	35	35	35	—	
	Time	6.2 s	82.5 s	62.3 s	96.6 s	80.1	
3 (2H, 2C, 1HU, 1CU)	TAC ($/y)	717,293.8	717,293.8	717,293.8	717,293.8	717,293.8	Gundersen et al.[38]
	Ns	1	5	5	5	—	
	Time	4.1 s	13.6 s	13.9 s	12.6 s	Not reported	
4 (3H, 2C, 1HU, 1CU)	TAC ($/y)	80,959.6	80,959.6	80,959.6	80,959.6	80,959.6	Bogataj and Kravanja[25]
	Ns	1	16	16	16	—	
	Time	3.3 s	199.6 s	185.5 s	206.6 s	726.0	
5 (3H, 2C, 1HU, 1CU)	TAC ($/y)	2,045,349.0	2,045,349.0	2,045,349.0	2,045,349.0	1,780,505.0	Kim et al.[11]
	Ns	3	57	57	57	—	
	Time	4.8 s	110.6 s	90.6 s	198.9 s	5,667.0	
6 (5H, 1C, 1HU, 1CU)	TAC ($/y)	724,506.4	724,506.4	724,506.4	724,506.4	634,849.1	Escobar and Grossmann[39]
	Ns	1	101	101	101	—	
	Time	1.8 s	112.6 s	102.5 s	163.6 s	3.6	
7 (3H, 4C, 1HU, 1CU)	TAC ($/y)	177,261.3	177,261.3	177,261.3	177,261.3	183,029.0	Wang et al.[40]
	Ns	76	325	325	325	—	
	Time	286.3 s	498.2 s	399.2 s	592.5 s	Not reported	
8 (5H, 5C, 1HU, 1CU)	TAC ($/y)	—	64,015.0	64,015.0	64,015.0	64,138.0	Mistry and Misener[26]
	Ns	—	2,158	2,158	2,158	—	
	Time	≧100 hr	12,793.9 s	12,362.5 s	10,025.6 s	9,600.0	
9 (5H, 5C, 1HU, 1CU)	TAC ($/y)	—	109,078.4	109,078.4	109,078.4	109,260.0	Daichendt and Grossmann[41]
	Ns	—	3,569	3,569	3,569	—	
	Time	≧100 hr	11,355.9 s	10,926.8 s	9,625.5 s	2,252.0	
10 (5H, 5C, 1HU, 1CU)	TAC ($/y)	—	43,329.2	43,329.2	43,329.2	43,359.0	Huang and Karimi[8]
	Ns	—	2,239	2,239	2,239	—	
	Time	≧100 h	19,563.9 s	17,436.5 s	10,329.5 s	Not reported	
11 (11H, 2C, 1HU, 1CU)	TAC ($/y)	—	3,865,163.0	3,865,163.0	3,865,163.0	3,456,649.0	Kim et al.[11]
	Ns	—	1,365	1,365	1,365	—	
	Time	≧100 hr	18,965.8 s	12,359.6 s	10,635.5 s	43,200.0	
12 (6H, 5C, 1HU, 1CU)	TAC ($/y)	—	139,398.1	139,398.1	139,398.1	139,438.0	Pavão et al.[18]
	Ns	—	3,826	3,826	3,826	—	
	Time	≧100 hr	40,929.3 s	39,959.5 s	29,955.7 s	1886.0	

(Continues)

TABLE 2 (Continued)

Example	Item	Our optimal solution for minimal HENs using different options				Best result from literature	Literature source
		Option 1	Option 2	Option 3	Option 4		
13 (6H, 10C, 1HU, 1CU)	TAC ($/y)	—	7,030,035.0	7,030,035.0	7,030,035.0	6,712,551.0	Pavão et al.[42]
	Ns	—	1,025	1,025	1,025	—	
	Time	≧100 hr	10,988.9 s	9,856.8 s	8,059.3 s	9,868.0	
14 (8H, 7C, 1HU, 1CU)	TAC ($/y)	—	1,501,004.0	1,501,004.0	1,501,004.0	1,507,290.0	Pavão et al.[18]
	Ns	—	4,956	4,956	4,956	—	
	Time	≧100 hr	49,936.5 s	45,725.3 s	39,985.6 s	4,231.0	
15 (13H, 7C, 1HU, 1CU)	TAC ($/y)	—	1,427,966.0	1,427,966.0	1,427,966.0	1,418,981.0	Zhang et al.[43]
	Ns	—	5,835	5,835	5,835	—	
	Time	≧100 hr	68,685.6 s	56,896.5 s	40,968.9 s	1,120.0	
16 (22H, 17C, 1HU, 1CU)	TAC ($/y)	—	1,958,836.0	1,958,836.0	1,958,836.0	1,900,614.0	Pavão et al.[18]
	Ns	—	6,235	6,235	6,235	—	
	Time	≧100 hr	72,809.6 s	69,898.8 s	59,967.6 s	24,492.0	

9 | RESULTS

Several examples of different sizes are presented in this section. The examples were implemented in GAMS (version 23.7)[36] and solved using CPLEX (version 12.1) as the MIP solver on a PC machine (i7 3.6GHz, 8 GB RAM). Results are shown in Table 2, where *Ns* is the number of structures visited for evaluation.

Sixteen examples taken from literatures were solved. They are described in detail in the Supplemental Material. We found the same or slightly better answers than those from literatures for examples 2, 3, 4, 7, 8, 9, 10, 12, 13 and 14, indicating that the methods used in the literature sources identify solutions close to the global ones many times with smaller time. Unfortunately, one cannot know how good these answers are because the methods are not guaranteeing global optimality. For examples 1, 5, 6, 11, 15, and 16, solutions from literature, which are nonminimal structures, are better. In part II, we explore nonminimal structures and find the same or better answers.

We note that when the size of the problem remains small, Option 1 renders the smallest time, and as the size increases, the time becomes too large and this option is not viable, even though we partitioned the variables in different number of intervals, depending on the problem. We tried different numbers of intervals, namely 2, 3, 5, 7, 8, 10, 20, 30, 40, 50, 60, 70, 80, etc. Then, we picked the ones that render the minimum time. For instance, for examples 1 through 7, we used 10, 3, 10, 10, 60, 10, and 8, respectively. We are leaving for future work to explore ways to reduce this time and perhaps making it competitive by trying smaller number of intervals in combination with other strategies.

We also note that Option 3 is slightly better than Option 2 in most cases and both better than Option 4 for small problems. Option 4 becomes better than Options 2 and 3 for larger problems. To illustrate the different times spent by the algorithm, Figure 5 presents the computing time of ***PLB***, ***PLBR***, ***PSTR***, ***PSTRR***, ***PEMin***, ***PEMax***, and ***PESTR*** for Example 7.

The large time consumption of the large size problems can be attributed to the fact that several structures keep repeating many times by allocating the matches in different stages. We mentioned above that the procedure inspired in the method proposed by Ji and Bagajewicz[34] (See supplemental Material) adds more time than it saves. The specific results are included at the end of the Supplemental Material. In addition, per the suggestion of an anonymous reviewer, we developed a few constraints that force isolated matches and certain families of exchangers to be in the earliest stage possible, and we leave other cases for future work.

The following constraint eliminates empty stages before stages with some exchangers.

$$\sum_{i \in HP}\sum_{j \in CP} z_{i,j,k} - 100 \sum_{i \in HP}\sum_{j \in CP} z_{i,j,k-1} \le 0 \quad k \in ST, k \ge 2 \tag{52}$$

Next, the following constraint considers only one exchanger between streams *i* and *j* in stage *k*, that is $z_{i,j,k}$ = 1 and both stream

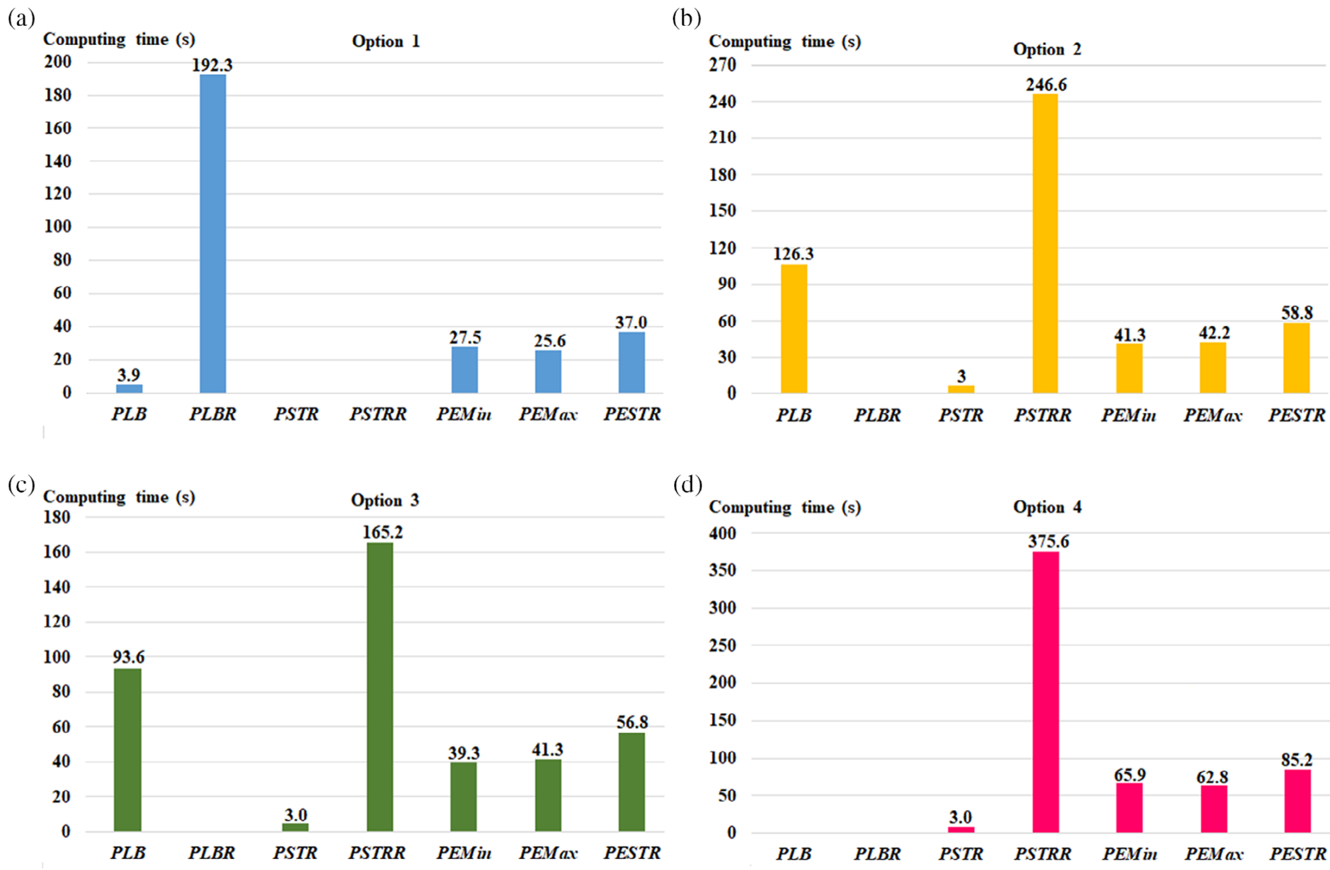

FIGURE 5 Computing times of example 7: (a) Option 1; (b) Option 2; (c) Option 3; (d) Option 4 [Color figure can be viewed at wileyonlinelibrary.com]

i and *j* are not split. It specifically forbids the single exchanger when it is actually feasible in stage *k*-1.

$$\left(\left(z_{i,j,k-1}+\sum_{j'\in CP, j'\neq j} z_{i,j',k-1}+\sum_{i'\in CP, i'\neq i} z_{i',j,k-1}\right) - z_{i,j,k}+\left(\sum_{j'\in CP, j'\neq j} z_{i,j',k}+\sum_{i'\in HP, i'\neq i} z_{i',j,k}\right)100\right)\geq 0 \quad i\in HP, j\in CP, k\in ST, k\geq 2 \tag{53}$$

In turn, the following Equation (54) forbids the split of hot stream *i* in stage *k* provided the cold streams involved in the split do not participate in turn in other splits when they are possible in stage *k*-1 (Figure 6). Similarly, Equation (55) is written for stream *j* in stage *k* when there is room for the match in stage *k*-1 (Figure 7).

$$\left(\begin{array}{l} z_{i,j,k-1}+z_{i,j',k-1} \\ +\sum_{j''\in CP, j''\neq j, j''\neq j'} z_{i,j'',k-1}+\sum_{i''\in HP, i''\neq i} z_{i'',j,k-1}+\sum_{i''\in HP, i''\neq i} z_{i'',j',k-1} \\ +\left(2-z_{i,j,k}-z_{i,j',k}\right)100+ \\ \left(\sum_{j''\in CP, j''\neq j, j''\neq j'} z_{i,j'',k}+\sum_{i''\in HP, i''\neq i} z_{i'',j,k}+\sum_{i''\in HP, i''\neq i} z_{i'',j',k}\right)100 \end{array}\right) \geq 1 \; i\in HP, j\in CP, j'\in CP, j\neq j', k\in ST, k\geq 2 \tag{54}$$

$$\left(\begin{array}{l} z_{i,j,k-1}+z_{i',j,k-1} \\ +\sum_{j''\in CP, j''\neq j} z_{i,j'',k-1}+\sum_{i''\in HP, i''\neq i, i''\neq i'} z_{i'',j,k-1}+\sum_{j''\in CP, j''\neq j} z_{i',j'',k-1} \\ +\left(2-z_{i,j,k}-z_{i',j,k}\right)100 \\ +\left(\sum_{j''\in CP, j''\neq j} z_{i,j'',k}+\sum_{i''\in HP, i''\neq i, i''\neq i'} z_{i'',j,k}+\sum_{j''\in CP, j''\neq j} z_{i',j'',k}\right)100 \end{array}\right) \geq 1 \; i\in HP, i'\in HP, j\in CP, i\neq i', k\in ST, k\geq 2 \tag{55}$$

Finally, the following constraint considers both streams split simultaneously (Figure 8).

$$\left(\begin{array}{l} z_{i,j,k-1}+z_{i,j',k-1}+z_{i',j,k-1} \\ +\sum_{j''\in CP, j''\neq j, j''\neq j'} z_{i,j'',k-1}+\sum_{i''\in HP, i''\neq i, i''\neq i'} z_{i'',j,k-1}+\sum_{j''\in CP, j''\neq j} z_{i',j'',k-1}+\sum_{i''\in HP, i''\neq i} z_{i'',j',k-1} \\ +\left(3-z_{i,j,k}-z_{i,j',k}-z_{i',j,k}\right)100+ \\ \left(\sum_{j''\in CP, j''\neq j, j''\neq j'} z_{i,j'',k}+\sum_{i''\in HP, i''\neq i, i''\neq i'} z_{i'',j,k}+\sum_{j''\in CP, j''\neq j} z_{i',j'',k}+\sum_{i''\in HP, i''\neq i} z_{i'',j',k}\right)100 \end{array}\right) \geq 1 \left\{\begin{array}{l} i\in HP, i'\in HP, \\ j\in CP, j'\in CP, \\ i\neq i', j\neq j', k\in ST, k\geq 2 \end{array}\right\} \tag{56}$$

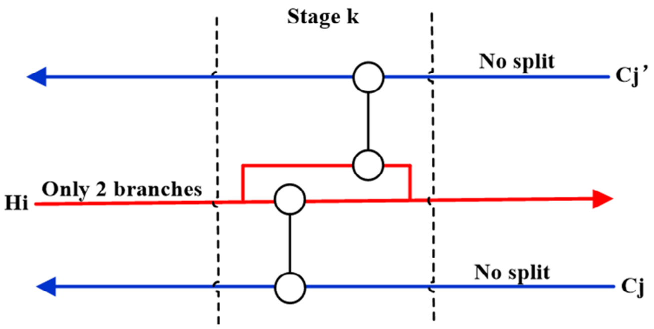

FIGURE 6 Stream *i* split in two branches at stage *k* and no other branching involved [Color figure can be viewed at wileyonlinelibrary.com]

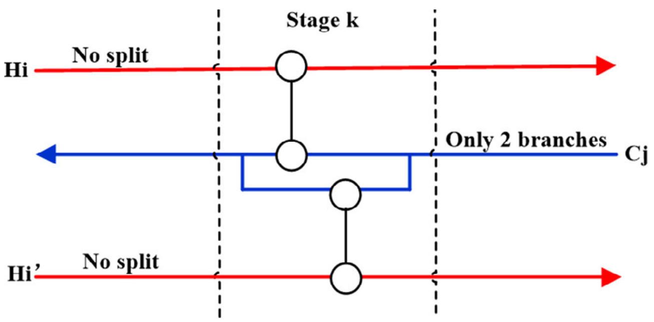

FIGURE 7 Stream *j* split in two branches at stage *k* and no other branching involved [Color figure can be viewed at wileyonlinelibrary.com]

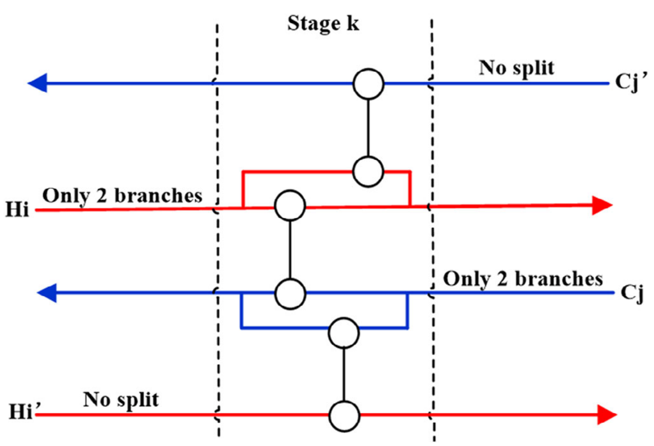

FIGURE 8 Stream *i* and *j* split in two branches at stage *k* and no other branching involved [Color figure can be viewed at wileyonlinelibrary.com]

The results of adding these constraints to selected examples 1–12 are shown in Table 3 using only Option 4. While the above constraints are a big advance, they do not solve the entire problem. For example, we did not develop constraints to prevent the repetition of families of heat exchangers in a stage containing, for example streams that are subject to a split of three or more streams. For instance, examples 1–5 exhibit no cases of repeated structures subject to a split of three or more streams, and example 6–10 exhibit 2, 7, 10, 19, and 12 such cases which are comparatively small amounts. However, examples 11 and 12 exhibit 912 (89%) and 625 (22%) repeated structures that are subject to a split of three or more streams. Note that example 11 has a cold stream with a large *Fcp*, which explains the outcome. Future work will take these opportunities to reduce computing time into account.

TABLE 3 Number of structures and time comparisons (minimal networks using Option 4)

Example	*Ns*	Time	*Ns* (*new*)	Time
1 (2H, 2C)	27	55.7 s	4	11.3 s
2 (2H, 2C)	35	96.6 s	5	16.9 s
3 (2H, 2C)	5	12.6 s	4	11.5 s
4 (3H, 2C)	16	206.6 s	2	19.2 s
5 (3H, 2C)	57	198.9 s	18	60.5 s
6 (5H, 1C)	101	163.6 s	30	51.2 s
7 (3H, 4C)	325	592.5 s	126	309.8 s
8 (5H, 5C)	2,158	10,025.0 s	986	5,136.9 s
9 (5H, 5C)	3,569	9,625.5 s	1,025	3,699.8 s
10 (5H, 5C)	2,239	10,329.5 s	1,325	6,109.3 s
11 (11H,2C)	1,365	10,635.5 s	1,028	9,068.7 s
12 (6H,5C)	3,826	29,955.7 s	2,962	26,365.8 s

10 | CONCLUSIONS

A new concept of Minimal HEN structures is presented and an algorithm to obtain globally optimal solutions for these types of networks is crafted. The algorithm is based on enumerating all possible structures, with or without a stopping criterion. The models are all linear. The strategy is based on the fact that for each structure, the total cost is a unimodal continuous function of *E* with one and only one global minimum. A Golden Search is employed to find the best solution with the lowest *TAC* for each minimal structure (MSTR). There are in total four alternative options for the proposed algorithm, each with advantages and disadvantages. Sixteen examples are tested for illustration purpose and most of our solutions compare favorably with literature results. The algorithm guarantees global optimality over the proposed search space.

We finally remark that the procedure above presented would render globally optimal solutions when using other superstructures, provided that the models are modified accordingly, even using isothermal mixing. For example, if the generalized superstructure by Floudas et al.[3] is used, then even assuming isothermal mixing can be used in models ***PSTR*** and ***PLB*** (a LB model proposed by Kim and Bagajewicz[5]), as well as ***PESTR***. Other extensions of the Synheat model, interesting for industry, like the stages/Substages model,[10,11] may require some changes in the ***PSTR*** and ***PESTR*** models, while a linear LB model was already developed.[5] Generating new constraints to avoid repeated structures is also ongoing work. Another issue is the consideration of nonisothermal mixing, which can be addressed at the level of the evaluation of the Golden Search. All these efforts are part of future work.

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NOTATION

Sets

HP	Set of hot process streams indexed by *i*
CP	Set of cold process streams indexed by *j*
HU	Hot utility
CU	Cold utility
K	Set of stages indexed by *k*
L, M, P, S	Set of discretization grids indexed by *l, m, p, s*

Parameters

N_{min}	Minimum number of units
NOK	Number of main stages
T_{IN}	Supply temperature of process stream
T_{OUT}	Target temperature of process stream
Fcp	Heat capacity flow rate of process stream
h	Film heat transfer coefficient of process stream
Chu	Hot utility price
Ccu	Cold utility price
$\hat{n}y$	The number of operation years for capital cost of heat exchanger
E	Total heating demand
EMAT	Exchanger minimum approach temperature
HRAT	Heat recovery approach temperature
N	Total number of the desired heat exchangers
α	A dummy variable
$\hat{\varepsilon}$	A small number
$\Delta\hat{T}^D$	Discrete point of temperature difference of heat recovery exchanger
$\Delta\hat{T}_{HU}^D$	Discrete point of temperature difference of heater
$\Delta\hat{T}_{CU}^D$	Discrete point of temperature difference of cooler
H	Discrete point of the partitioned heat recovery exchanger area
Hhu	Discrete point of the partitioned heater area
Hcu	Discrete point of the partitioned cooler area
$\hat{Q}h$	Heat content of hot process stream
$\hat{Q}c$	Heat content of cold process stream
$\hat{\psi}$	Maximum possible area of heat recovery exchanger
$\hat{\psi}hu$	Maximum possible area of heater
$\hat{\psi}cu$	Maximum possible area of cooler
Γ	Maximum temperature difference
Ω	Maximum heat load

Binary variables

z	Binary variable to denote heat recovery exchanger
zhu	Binary variable to denote heater
zcu	Binary variable to denote cooler
r	Binary variable related to the partitioned temperature difference of heat recovery exchanger
rhu	Binary variable related to the partitioned temperature difference of heater
rcu	Binary variable related to the partitioned temperature difference of cooler

Continuous variables

q	Heat exchanged between process streams
qhu	Hot utility demand for cold stream
qcu	Cold utility demand for hot stream
$T_{i,k}^H$	Temperature of hot stream *i* at stage *k*
$T_{j,k}^C$	Temperature of cold stream *j* at stage *k*
$\Delta T_{i,j,k}$	Heat transfer temperature difference between stream *i* and *j* at stage *k*
ΔThu	Hot utility temperature difference
ΔTcu	Cold utility temperature difference
A	Heat recovery exchanger area
Ahu	Heater area
Acu	Cooler area
ACEX	Total area cost of heat exchangers
FCEX	Total fixed cost of heat exchangers
HUCOST	Hot utility cost
CUCOST	Cold utility cost

MODEL ACRONYM LIST

PSTR	Problem rendering a viable structure of matches and candidates of Minimal Structures.
PSTRR	Problem to enumerate different structures for minimal networks
PEMin	Problem to obtain the minimum energy target for a fixed structure
PEMax	Problem to obtain the maximum energy target for a fixed structure
PESTR	Problem to obtain heat distribution for each MSTR with a fixed energy consumption
PLB	The lower bound model featuring a given number of units *N*
PLBR	problem containing problem ***PLB*** and the exclusion constraint Equation 8

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of this article.

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