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Globally optimal synthesis of heat exchanger networks. Part II: Non-minimal networks

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Abstract

In Part I of this work, the synthesis of minimal heat exchanger networks using the isothermal mixing stage-wise superstructure was presented. In this Part II, an extension of the algorithm presented in Part I is made to consider networks that allow multiple solutions regarding heat allocation, that is, they have energy loops where heat loads can be rearranged without changing the overall energy consumption. We extend the strategy of our Part I to use a set of nested loops to enumerate the number of units, the structure of matches, the energy consumption, different values of exchanger minimum approximation temperature (EMAT), and different locations where EMAT is active. All the models used are linear and are aided by capital cost evaluations. As in Part I, we claim global optimality based on our conjectures. Literature examples are solved to show the effectiveness of the algorithm.

KEYWORDS

global optimality, non-minimal heat exchanger networks

1 | INTRODUCTION

In Part I of this work, the latest advances in heat exchanger networks (HEN) synthesis were overviewed.[1] In addition, the fact that globally optimal solutions have been difficult to attain using mixed integer nonlinear programming (MINLP) approaches was also highlighted, a few articles notwithstanding. It was also pointed out that several stochastic-based algorithms do not guarantee global optimality, although they often achieve it in practice, as demonstrated in comparing our global solutions with some literature ones. It is also known that these types of algorithms require significant human interactions, that is, they are not automatic.

Our Part I defined the concept of minimal structure (MSTR) and connected it to the concept of minimum number of heat exchangers. However, the main feature that characterizes MSTR is that for a fixed energy consumption there is a unique set of temperatures throughout the network. After defining them, an enumeration algorithm was presented to obtain the globally optimal solution for HEN synthesis featuring this structure. This algorithm is based on generating structures of matches using linear models, evaluating the total annualized cost (TAC) of each, identifying the one with the lowest cost by using a Golden Search for the TAC versus energy consumption (E). One of the structures' enumeration algorithms uses a linear lower bound of the problem and therefore allows a stopping criterion for the enumeration. This enumeration algorithm proved to be more efficient in terms of computational time than the exhaustive enumeration of all other options for small- and medium-size problems.

This second part addresses the fact that non-minimal structure (non-MSTR) has additional features. First, non-MSTRs do not have a unique set of temperatures in the network for a fixed energy, that is, they are cyclic structures where heat can be moved around in what has been referred to as energy “loops” by Pinch technology (PT) in the 1980s. Indeed, for a given structure that has a number of exchangers larger than the minimum, heat can be shifted inside a cycle. Second, for every structure generated, the value of the exchanger minimum approximation temperature (EMAT) can vary, thus generating different solutions for the same structure (STR). Third, the place where the smallest temperature approximation takes place can vary in the cycle.

This article is organized as follows: we first present the additional HEN properties that we use to perform the global search. We follow with additional linear models needed for the global search algorithm that follows. We finish with examples.

2 | HEN PROPERTIES

The concepts of match, active and inactive matches, STR and MSTR were defined formally in our Part I. In addition, it was proven that

- Solutions of the HEN synthesis model that feature minimum number of units are MSTR (Lemma 1).
- The TAC values that correspond to the same feasible MSTR are a continuous function of E (Lemma 2).
- For a given MSTR, the TAC exhibits only one minimum (Conjecture 1 in our Part I).

We now extend Lemma 2 to any STR.

Lemma 3 The TAC that corresponds to a feasible STR is a continuous function of E.

Proof: Any differential change $dE = \sum_{j \in CP} dqhu_j$ causes differential changes $dq_{i,j,k}$ through the path to the cooler. As a result, only differential changes in temperature differences between $T^H_{i,k}$ and $T^C_{j,k}$ take place. Because the area is a smooth function of these temperature differences, the TAC only changes differentially. Q.E.D.

Remark 1 The proof of Lemma is exactly the same as the proof of Lemma 2, but it is repeated here because new features for structures are included.

Remark 2 The value of EMAT has an impact on the solution obtained for a given structure and a given energy consumption (E). In the case of minimal network structures, for E fixed, the heat transfer pattern is fixed and therefore the temperature differences in different matches are also fixed. Thus, the value of EMAT can only make a minimal network infeasible. In the case of non-MSTR networks, the value of EMAT has an impact in the answer. In other words, when changing EMAT the pattern of values of heat transferred in the exchangers may change.

We now define the following concepts:

- *Minimum network temperature difference*: This is defined as the minimum value of the temperature difference in all active units on both sides of the heat exchanger, that is,

$$\Delta T^*(\mathrm{STR}) = \underset{i,j,k \ni z_{i,j,k}=1 \vee z_{i,j,k-1}=1}{\mathrm{Min}} \left\{\Delta T_{i,j,k}\right\}. \quad (1)$$

- *EMAT-binding structures*: These are structures where $\Delta T^*(\mathrm{STR}) = \mathrm{EMAT}$. They are defined formally as follows:

$$\mathrm{STR}^*_s(E,\mathrm{EMAT}) = \left\{(i,j,k)_s \ni \sum_{j \in \mathrm{CP}} qhu_j = E \wedge \Delta T^*(\mathrm{STR}) = \mathrm{EMAT}\right\}, \quad (2)$$

where we introduce the index s to recognize that there could be more than one for each E and each EMAT.

To describe the locations of where the binding takes place formally, we introduce binary variables to indicate the position, where $\Delta T^*(\mathrm{STR}) = \mathrm{EMAT}$, namely, $y_{i,j,k}$, $y_{\mathrm{HU},j}$, $y_{\mathrm{CU},i}$. Note that the subindices (i,j,k) for these locations need not be the same as the corresponding heat exchanger because the exchanger has two sides. These binary variables satisfy the following equations:

$$\left(\Delta T_{i,j,k} - \mathrm{EMAT}\right) + \Gamma_{i,j}\left(1 - y_{i,j,k}\right) \geq 0 \; i \in \mathrm{HP}, j \in \mathrm{CP}, k \in \mathrm{ST} \wedge k\_\mathrm{NOK}+1;\; z_{i,j,k-1} = 1 \vee z_{i,j,k} = 1, \quad (3)$$

$$\left(\Delta T_{i,j,k} - \mathrm{EMAT}\right) - \Gamma_{i,j}\left(1 - y_{i,j,k}\right) \leq 0 \; i \in \mathrm{HP}, j \in \mathrm{CP}, k \in \mathrm{ST} \wedge k\_\mathrm{NOK}+1; z_{i,j,k-1} = 1 \vee z_{i,j,k} = 1, \quad (4)$$

$$\left(\Delta T_{\mathrm{HU},j} - \mathrm{EMAT}\right) + \Gamma_{\mathrm{HU},j}\left(1 - y_{\mathrm{HU},j}\right) \geq 0, \; j \in \mathrm{CP}, \; zhu_j = 1, \quad (5)$$

$$\left(\Delta T_{\mathrm{HU},j} - \mathrm{EMAT}\right) - \Gamma_{\mathrm{HU},j}\left(1 - y_{\mathrm{HU},j}\right) \leq 0, \; j \in \mathrm{CP}, zhu_j = 1, \quad (6)$$

$$\left(\Delta T_{\mathrm{CU},i} - \mathrm{EMAT}\right) + \Gamma_{\mathrm{CU},i}\left(1 - y_{\mathrm{CU},i}\right) \geq 0, \; i \in \mathrm{HP}, zcu_i = 1, \quad (7)$$

$$\left(\Delta T_{\mathrm{CU},i} - \mathrm{EMAT}\right) - \Gamma_{\mathrm{CU},i}\left(1 - y_{\mathrm{CU},i}\right) \leq 0, \; i \in \mathrm{HP}, zcu_i = 1. \quad (8)$$

Equations (3) and (4) state that when $y_{i,j,k} = 1$, the heat exchanger at stage location (k) has a temperature difference on its left side equal to EMAT, that is $\Delta T_{i,j,k}$ = EMAT and when $y_{i,j,k} = 0$, $\Delta T_{i,j,k} \geq$ EMAT. Note that the equations are also written for $z_{i,j,k-1} = 1$, which identifies the location of the equality on the right-hand side. We illustrate this in Figure 1. The same relations hold for the utility exchangers (Equations (5)–(8)).

When one structure is fixed and the total energy consumption is fixed, heat exchangers that do not participate in energy loops have their heat exchanged fixed (as in MSTRs), and only the exchangers participating in an energy loop (cycle in the graph) can have infinite number of heat transfer patterns subject only to a fixed value of total energy exchanged. Thus, attention is now shifted to the identification of the exchangers involved in the energy loop.

We illustrate the energy loop in Figure 2 (for Example 1 of our Part I) with $N = 6$ (not a MSTR). One location of ΔT^* is indicated by a star. Clearly, one can move heat around in infinitesimal values inside the loop resulting in different sets of areas for the exchangers that result in infinitesimal changes in TAC.

We now present the following conjecture:

Conjecture 2 The TAC that corresponds to the same STR and the same $\mathrm{STR}^*_s(E,\mathrm{EMAT})$, has only one extremum in EMAT and this extremum is a minimum.

One can attempt the same exercise as in Conjecture 1 (Part I), that is, to develop a first and second derivative of TAC and try to

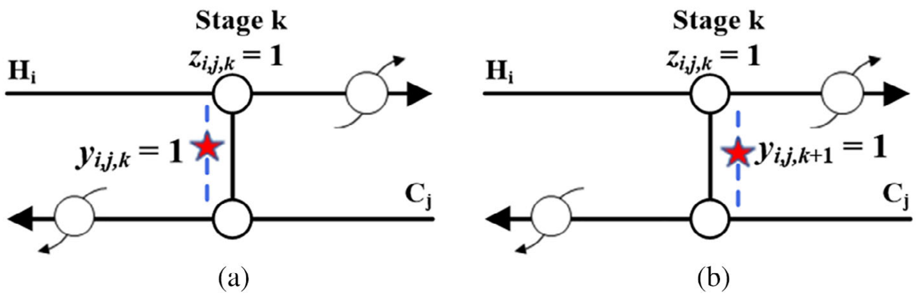

FIGURE 1 Illustration of binaries $y_{i,j,k}$ versus $z_{i,j,k}$: (a) left side; (b) right side [Color figure can be viewed at wileyonlinelibrary.com]

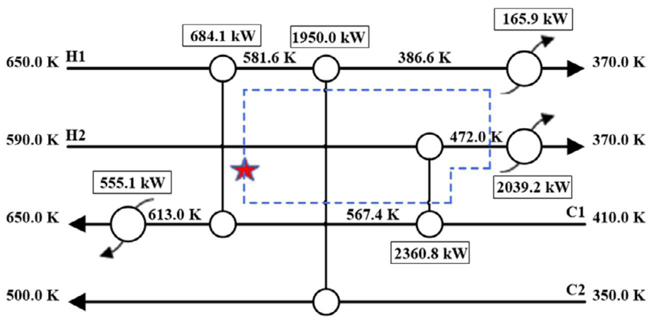

FIGURE 2 Loop in a feasible heat exchanger network of Example 1 [Color figure can be viewed at wileyonlinelibrary.com]

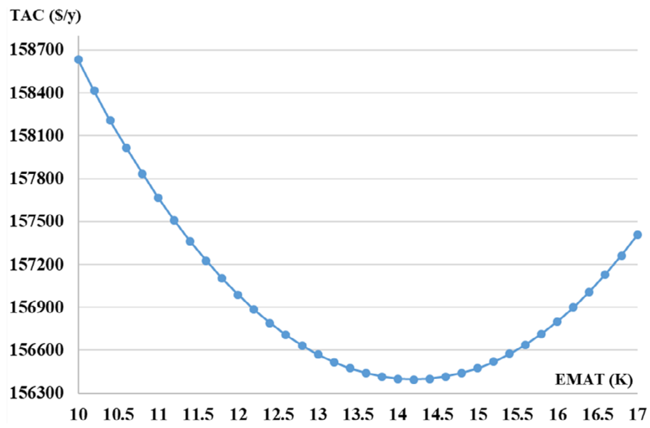

FIGURE 3 TAC versus EMAT, fixed structure (Figure 1), $N^* = 6$, $E^* = 555.1$ kW, $y_{\mathrm{H1,\,C1,\,K2}} = 1$ (Example 1) [Color figure can be viewed at wileyonlinelibrary.com]

prove that the latter is positive. Given the lack of success in the case of Conjecture 1, we did not attempt it here. We leave both statements as reasonable conjectures.

Remark 3 We point out that the minimum of TAC can be at the boundaries of the EMAT feasible interval ($\mathrm{EMAT_{Min}}$, $\mathrm{EMAT_{Max}}$) or inside the interval where the derivative of TAC w.r.t. EMAT is zero.

We have $z_{\mathrm{H1,C1,K1}} = z_{\mathrm{H1,C2,K2}} = z_{\mathrm{H2,C1,K2}} = zcu_{\mathrm{H1}} = zcu_{\mathrm{H2}} = zhu_{\mathrm{C1}} = 1$, which defines the STR with $N = 6$, and $E = 555.1$ kW, which corresponds to a value of heat recovery approach temperature (HRAT) = 17.0°C. Assuming the location SL = {(H1, C1, K2)}, Figure 3 shows the effect of varying EMAT in one location ($y_{\mathrm{H1,\,C1,\,K2}} = 1$) on the TAC.

The next goal is to identify automatically the energy loop and the potential locations of ΔT^*. The assumption is that all exchangers in STR are active, that is $q_{i,j,k} > 0$ for each $z_{i,j,k} = 1$, strictly. To do that we propose to identify all locations for ΔT^* of the energy loop. We remark that other locations outside the energy loop can be EMAT-binding. We propose the following problem to find the first location.

$$(\mathrm{PLOC1}) = \underset{\substack{\forall (T,Q)\in D_{\mathrm{Synheat}},\\ Y\in \mathrm{STR}}}{\mathrm{Min}} \; \beta, \tag{9}$$

$$\beta \geq \mathrm{EMAT_{Min}}, \tag{10}$$

$$\beta \leq \Delta T_{i,j,k}\; i\in \mathrm{HP}, j\in \mathrm{CP}, k\in \mathrm{ST} \wedge k\_\mathrm{NOK}+1;\; \forall \{z_{i,j,k-1} = 1 \vee z_{i,j,k} = 1\}, \tag{11}$$

$$\beta \leq \Delta T_{\mathrm{HU},j}\; j\in \mathrm{CP}, \forall zhu_j = 1, \tag{12}$$

$$\beta \leq \Delta T_{\mathrm{CU},i}\; i\in \mathrm{HP}, \forall zcu_i = 1, \tag{13}$$

$$(\Delta T_{i,j,k} - \beta) + \Gamma_{ij}(1 - y_{i,j,k}) \geq 0, i\in \mathrm{HP}, j\in \mathrm{CP}, k\in \mathrm{ST} \wedge k\_\mathrm{NOK}+1; \forall \{z_{i,j,k-1} = 1 \vee z_{i,j,k} = 1\}, \tag{14}$$

$$(\Delta T_{i,j,k} - \beta) - \Gamma_{ij}(1 - y_{i,j,k}) \leq 0,\; i\in \mathrm{HP}, j\in \mathrm{CP}, k\in \mathrm{ST} \wedge k\_\mathrm{NOK}+1;\; \forall \{z_{i,j,k-1} = 1 \vee z_{i,j,k} = 1\}, \tag{15}$$

$$(\Delta T_{\mathrm{HU},j} - \beta) + \Gamma_{\mathrm{HU},j}(1 - y_{\mathrm{HU},j}) \geq 0,\; j\in \mathrm{CP}, \forall zhu_j = 1, \tag{16}$$

$$(\Delta T_{\mathrm{HU},j} - \beta) - \Gamma_{\mathrm{HU},j}(1 - y_{\mathrm{HU},j}) \leq 0,\; j\in CP, \forall zhu_j = 1, \tag{17}$$

$$(\Delta T_{\mathrm{CU},i} - \beta) + \Gamma_{\mathrm{CU},i}(1 - y_{\mathrm{CU},i}) \geq 0, i\in \mathrm{HP}, \forall zcu_i = 1, \tag{18}$$

$$(\Delta T_{\mathrm{CU},i} - \beta) - \Gamma_{\mathrm{CU},i}(1 - y_{\mathrm{CU},i}) \leq 0,\; i\in \mathrm{HP}, \forall zcu_i = 1, \tag{19}$$

$$q_{i,j,k} > \varepsilon\; \forall z_{i,j,k} = 1 \in \mathrm{STR}, \tag{20}$$

$$qhu_j > \varepsilon\; \forall zhu_j = 1 \in \mathrm{STR}, \tag{21}$$

$$qcu_i > \varepsilon\; \forall zcu_i = 1 \in \mathrm{STR}. \tag{22}$$

In this problem, the network structure is fixed, that is, all $z_{i,j,k}$, zcu_i, and zhu_j are fixed to the corresponding one or zero values. Equations (14)–(19)

help identify the location where the minimum takes place (which needs not be equal to $EMAT_{Min}$). We also impose that all exchangers belonging to STR be active, that is, have a nonzero load (Equations (20)–(22)). We do that so the solution remains non-MSTR. Finally, we let E to vary between its minimum and maximum bounds, and we use EMAT = $EMAT_{Min}$. Note that the above model includes all the Synheat equations and minimizes the temperature difference in the network (for any energy consumption), that is, it accommodates all heat exchange loads so that there is a point where the temperature difference is the lowest. For example, in Figure 2, if $EMAT_{Min}$ = 5°C, then the candidate solutions for the location of the minimum are the ones in the loop and one more on the left side of the match (H1, C1), which does not vary with EMAT. This minimum value is likely to be equal to $EMAT_{Min}$, but nothing says it must be.

Once this problem is solved, one obtains optimal values E^*, q^*, $\Delta T^*_{i,j,k}$, y^*. In this solution, there is usually one y^* = 1. Let us call this $y^{**}_{i,j,k}$. Assuming that the location found is part of the energy loop, we now want to find all other locations of this loop. To do that, a perturbation of the heat transferred in the exchanger associated to $y^{**}_{i,j,k}$ (denoted by $z^{**}_{i,j,k}$), by a small amount ($\hat{\Delta} < \varepsilon$), will render the heat exchangers belonging to the loop change by the same amount, while the others stay unaltered. Examples of how heat increases and decreases in these cycles/loops abound in the Pinch Design literature. This is accomplished by solving the following problem:

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

s.t.

$$\sum_{j\in CP} qhu_j = E^*, \tag{24}$$

$$q^{**}_{i,j,k} = q^*_{i,j,k} - \hat{\Delta}. \tag{25}$$

Equation (25) states that the heat exchanged in exchanger $z^{**}_{i,j,k}$ is now fixed to a different value. The solution to this problem renders a set of $\Delta T_{i,\ j,\ k}$ values that are different from $\Delta T^*_{i,j,k}$ at the locations of the energy loop. However, if the problem is infeasible, then the location obtained by problem PLOC1 is not part of a loop. Thus, problem PLOC1 needs to be rerun excluding this solution until the loop is located by problem PLOC.

Remark 4 We point out that when $N = N_{\min} + 1$ ($N_{\min}$ was defined in our Part I), the number of loops is one, whereas when $N = N_{\min} + r$, the number of loops is smaller than or equal to r. However, in this article, we do not consider cases where $r > 1$, that is more than one loop.

To determine the minimum EMAT value ($EMAT_{Min}$), for each energy loop inside a fixed STR with fixed energy values we solve the following problem:

$$\text{PEMAT}_{\text{Min}} = \underset{(i,j,k)\in \text{STR}}{\text{Min}} \text{EMAT}, \tag{26}$$

s.t.

$$(\Delta T_{i,j,k} - \text{EMAT}) + \Gamma_{i,j}\left(1 - y^*_{i,j,k}\right) \geq 0, z_{i,j,k-1} = 1, \vee z_{i,j,k} = 1, \tag{27}$$

$$(\Delta T_{i,j,k} - \text{EMAT}) - \Gamma_{i,j}\left(y^*_{i,j,k} - 1\right) \leq 0, z_{i,j,k-1} = 1 \vee z_{i,j,k} = 1, \tag{28}$$

$$(\Delta T_{\text{HU},j} - \text{EMAT}) + \Gamma_{\text{HU},j}\left(1 - y^*_{\text{HU},j}\right) \geq 0,\ \ zhu_j = 1, \tag{29}$$

$$(\Delta T_{\text{HU},j} - \text{EMAT}) - \Gamma_{\text{HU},j}\left(1 - y^*_{\text{HU},j}\right) \leq 0, zhu_j = 1, \tag{30}$$

$$(\Delta T_{\text{CU},i} - \text{EMAT}) + \Gamma_{\text{CU},i}\left(1 - y^*_{\text{CU},i}\right) \geq 0, zcu_i = 1, \tag{31}$$

$$(\Delta T_{\text{CU},i} - \text{EMAT}) - \Gamma_{\text{CU},i}\left(1 - y^*_{\text{CU},i}\right) \leq 0, zcu_i = 1, \tag{32}$$

$$\sum_{j\in CP} qhu_j = E. \tag{33}$$

Next, the maximum value of EMAT ($EMAT_{Max}$) is found by solving:

$$\text{PEMAT}_{\text{Max}} = \underset{(i,j,k)\in \text{STR}}{\text{Max}} \text{EMAT}, \tag{34}$$

s.t.

$$(\Delta T_{i,j,k} - \text{EMAT}) + \Gamma_{i,j}\left(1 - y^*_{i,j,k}\right) \geq 0,\ \ z_{i,j,k-1} = 1 \vee z_{i,j,k} = 1, \tag{35}$$

$$(\Delta T_{i,j,k} - \text{EMAT}) - \Gamma_{i,j}\left(y^*_{i,j,k} - 1\right) \leq 0,\ \ z_{i,j,k-1} = 1 \vee z_{i,j,k} = 1, \tag{36}$$

$$(\Delta T_{\text{HU},j} - \text{EMAT}) + \Gamma_{\text{HU},j}\left(1 - y^*_{\text{HU},j}\right) \geq 0, zhu_j = 1, \tag{37}$$

$$(\Delta T_{\text{HU},j} - \text{EMAT}) - \Gamma_{\text{HU},j}\left(1 - y^*_{\text{HU},j}\right) \leq 0, zhu_j = 1, \tag{38}$$

$$(\Delta T_{\text{CU},i} - \text{EMAT}) + \Gamma_{\text{CU},i}\left(1 - y^*_{\text{CU},i}\right) \geq 0, zcu_i = 1, \tag{39}$$

$$(\Delta T_{\text{CU},i} - \text{EMAT}) - \Gamma_{\text{CU},i}\left(1 - y^*_{\text{CU},i}\right) \leq 0, zcu_i = 1, \tag{40}$$

$$\sum_{j\in CP} qhu_j = E. \tag{41}$$

3 | GLOBAL SEARCH ALGORITHM RATIONALE

The strategy to obtain the best HEN is based on fixing the number of exchangers to be the absolute minimum and then continue increasing the number of exchangers. Without loss of generality, we stop at a number of exchangers where the first non-MSTR structure is detected. This means that the number of exchangers is such that there is only one loop. Note that the non-MSTR solution may be of larger TAC than the best MSTR solution found.

For each number of heat exchangers, the same Options (1–4) as in our Part I are used. Then, for each structure, we determine all energy loops and all EMAT-binding locations. Then, for the structure identified, we establish a Golden Search for the energy *E*. In turn, for each *E*, we run the Golden Search for EMAT for each energy loop and each EMAT-binding location.

We now explain why we force at least one exchanger to have a temperature difference equal to EMAT. With both HRAT and EMAT fixed, when solving the minimum number of heat exchangers without forcing any temperature difference to be equal to EMAT one may obtain a structure that has temperature differences all strictly larger than EMAT, thus missing the solution with temperature difference equal to EMAT. Since we are interested in all the solutions, we force the temperature difference equal to EMAT in at least one exchanger, to capture all such alternatives. We note that solutions for the pair HRAT–EMAT that do not have this property will be captured when using a larger EMAT.

4 | GLOBAL SEARCH ALGORITHM

We now present the algorithm, which is based on a fixed value of energy *E*, a specific structure, and a specific set of EMAT locations $STR_s^*(E, EMAT)$ $s = 1, \ldots, s_{smax}$.

The Smart Enumeration Algorithm is the following:

1. The Synheat model is run by minimizing the number of heat exchangers, using the calculated bounds on energy. This number of heat exchangers is fixed and we call it *N*. Also, start by giving the incumbent cost a large value, that is, UBTAC = +∞.
2. For the current *N*, run one of the following options recursively, as explained in our Part I.
   - 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 model 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: It uses the model PSTR to find one viable solution at the first time and uses PSTRR (model PSTR excluding previous solutions) afterward.

   For each option, the first step is to identify if the structure is minimal or not. Thus, after the first problem, the sequence is to solve problems PLOC1 and PLOC. If PLOC is infeasible, there is no loop and the structure is minimal. Otherwise, it is non-minimal.

   If the structure is minimal, we run algorithm OPMSTR. Otherwise run the OPNMSTR algorithm. In each case, identify the best TAC. If TAC < UBTAC, then update UBTAC.
3. For Option 1, if the problem is infeasible or RTAC > UBTAC, stop. Otherwise, if the solution is feasible, go to 5.
4. For Options 2, 3, and 4, if the solution is infeasible, stop. Otherwise, if the solution is feasible, go to 5.
5. If the last structure was non-minimal, then stop. Otherwise, increase the number of exchangers by *N*=*N* + 1 and go to 2.

4.1 | OPMSTR algorithm

This algorithm is a portion of the algorithm presented in our Part I. We list it here for completeness.

1. For the chosen structure, obtain the minimum energy consumption (E_{Min}) using PE_{Min} (see Part I).
2. For the chosen structure, obtain the maximum energy consumption (E_{Max}) using PE_{Max} (see Part I).
3. Obtain the TAC for the extreme and golden-section energy (E_{Ratio}) as follows:
   - a Run PESTR which obtains one viable heat transfer pattern and gives a viable solution, thus providing the values of the binary variables to define the structure (see Part I). for $E = E_{Min}$. Evaluate the TAC and call it TAC_{Min}.
   - b Run PESTR (see Part I) for $E = E_{Max}$. Evaluate the TAC and call it TAC_{Max}.
   - c Run PESTR (see Part I) for $E = E_{Ratio}$. Evaluate the TAC and call it TAC_{Ratio}.
4. If $TAC_{ratio} = \mathrm{Min}\{TAC_{Min}, TAC_{ratio}, TAC_{Max}\}$, the solution is not monotone. Then, go to Step 7.
5. If $TAC_{Min} = \mathrm{Min}\{TAC_{Min}, TAC_{ratio}, TAC_{Max}\}$, the solution may be monotone or not. Then, run PESTR for $E = E_{Min} + 0.01$ and obtain its TAC, namely, TAC^+_{Min}.
   - If $TAC^+_{Min} - TAC_{Min} > 0$, the solution is monotone and $TAC = TAC_{Min}$. Go to Step 8.
   - If $TAC^+_{Min} - TAC_{Min} < 0$, the solution is not monotone and go to Step 7.
6. If $TAC_{Max} = \mathrm{Min}\{TAC_{Min}, TAC_{ratio}, TAC_{Max}\}$, the solution may be monotone or not. Then, run PESTR for $E = E_{Max} - 0.01$ and obtain its TAC, namely, TAC^-_{Max}.
   - If $TAC_{Max} - TAC^-_{Max} < 0$, the solution is monotone and $TAC = TAC_{Max}$. Go to 8.
   - If $TAC_{Max} - TAC^-_{Max} > 0$, the solution is not monotone and go to Step 7.
7. Apply the Golden Search for Energy. Use PESTR to obtain the TAC for each point.
8. If TAC ≤ UBTAC, then update UBTAC.

TABLE 1 Results of all examples (non-minimal networks)

Example	Item	Our optimal solution for non-minimal HENs using different options				Best literature result	Literature source
		Option 1	Option 2	Option 3	Option 4		
1 (2H, 2C, 1HU, 1CU)	TAC ($/year)	154,910.6	154,910.6	154,910.6	154,910.6	154,995.0	Faria et al.[3]
	Ns	3	42	42	42	–	
	Time	90.0 s	139.2 s	120.5 s	168.9 s	250.0	
2 (2H, 2C, 1HU, 1CU)	TAC ($/year)	360,037.2	360,037.2	360,037.2	360,037.2	361,983.0	Escobar and Trierweiler[4]
	Ns	7	38	38	38	–	
	Time	36.5 s	130.8 s	112.5 s	162.3 s	80.1	
3 (2H, 2C, 1HU, 1CU)	TAC ($/year)	715,962.9	715,962.9	715,962.9	715,962.9	717,293.8	Gundersen et al.[5]
	Ns	8	38	38	38	–	
	Time	69.1 s	159.3 s	135.0 s	196.2 s	Not reported	
4 (3H, 2C, 1HU, 1CU)	TAC ($/year)	80,959.6	80,959.6	80,959.6	80,959.6	80,959.6	Bogataj and Kravanja[6]
	Ns	3	56	56	56	–	
	Time	15.2 s	250.8 s	286.3 s	369.2 s	726.0	
5 (3H, 2C, 1HU, 1CU)	TAC ($/year)	1,758,381.0	1,758,381.0	1,758,381.0	1,758,381.0	1,780,505.0	Kim et al.[7]
	Ns	16	81	81	81	–	
	Time	125.6 s	392.5 s	365.1 s	598.2 s	5,667.0	
6 (5H, 1C, 1HU, 1CU)	TAC ($/year)	632,360.7	632,360.7	632,360.7	632,360.7	634,849.1	Escobar and Grossmann[8]
	Ns	8	146	146	146	–	
	Time	122.3 s	225.6 s	210.3 s	398.5 s	3.6	
7 (3H, 4C, 1HU, 1CU)	TAC ($/year)	177,261.3	177,261.3	177,261.3	177,261.3	183,029.0	Wang et al.[9]
	Ns	278	992	992	992	–	
	Time	652.3 s	1,656.3 s	1,388.2 s	1932.5 s	Not reported	
8 (5H, 5C, 1HU, 1CU)	TAC ($/year)	–	64,015.0	64,015.0	64,015.0	64,138.0	Mistry and Misener[10]
	Ns	–	5,236	5,236	5,236	–	
	Time	≧100 hr	51,668.9 s	46,892.6 s	31,502.8 s	9,600.0	
9 (5H, 5C, 1HU, 1CU)	TAC ($/year)	–	109,078.4	109,078.4	109,078.4	109,260.0	Daichendt and Grossmann[11]
	Ns	–	8,632	8,632	8,632	–	
	Time	≧100 hr	39,598.5 s	30,898.1 s	25,659.3 s	2,252.0	
10 (5H, 5C, 1HU, 1CU)	TAC ($/year)	–	43,329.2	43,329.2	43,329.2	43,359.0	Huang and Karimi[12]
	Ns	–	5,932	5,932	5,932	–	
	Time	≧100 hr	50,668.2 s	48,368.9 s	31,235.8 s	Not reported	
11 (11H, 2C, 1HU, 1CU)	TAC ($/year)	–	3,441,663.0	3,441,663.0	3,441,663.0	3,456,649.0	Kim et al.[7]
	Ns	–	3,962	3,962	3,962	–	
	Time	≧100 hr	75,892.6 s	69,925.3 s	55,689.3 s	43,200.0	
12 (6H, 5C, 1HU, 1CU)	TAC ($/year)	–	139,398.1	139,398.1	139,398.1	139,438.0	Pavão et al.[13]
	Ns	–	8,692	8,692	8,692	–	
	Time	≧100 hr	92,832.9 s	85,356.9 s	69,623.8 s	1886.0	
13 (6H, 10C, 1HU, 1CU)	TAC ($/year)	–	6,674,677.0	6,674,677.0	6,674,677.0	6,712,551.0	Pavão et al.[14]
	Ns	–	6,995	6,995	6,995	–	
	Time	≧100 hr	99,826.8 s	96,826.8 s	80,715.9 s	9,868.0	
14 (8H, 7C, 1HU, 1CU)	TAC ($/year)	–	1,501,004.0	1,501,004.0	1,501,004.0	1,507,290.0	Pavão et al.[13]
	Ns	–	9,823	9,823	9,823	–	

TABLE 1 (Continued)

Example	Item	Our optimal solution for non-minimal HENs using different options				Best literature result	Literature source
		Option 1	Option 2	Option 3	Option 4		
	Time	≧100 hr	102,368.2 s	97,629.3 s	89,625.9 s	4,231.0	
15 (13H, 7C, 1HU, 1CU)	TAC ($/year)	–	1,414,857.0	1,414,857.0	1,414,857.0	1,418,981.0	Zhang et al.[15]
	Ns	-	9,568	9,568	9,568	–	
	Time	≧100 hr	262,986.5 s	188,892.6 s	100,568.8 s	1,120.0	
16 (22H, 17C, 1HU, 1CU)	TAC ($/year)	–	1,912,763.0	1,912,763.0	1,912,763.0	1,900,614.0	Pavão et al.[13]
	Ns	–	15,369	15,369	15,369	–	

Abbreviations: HEN, heat exchanger network; TAC, total annualized cost.

4.2 | OPNMSTR algorithm

1 For the chosen structure, obtain the minimum energy consumption (E_{Min}) using PE_{Min}.

2 For the chosen structure, obtain the maximum energy consumption (E_{Max}) using PE_{Max}.

3 Obtain extreme values of TAC as follows:

a Run PESTR which obtains one viable heat transfer pattern and gives a viable solution, thus providing the values of the binary variables to define the structure, for $E = E_{Min}$. Then, run the problem PLOC1 that locates the first EMAT-binding location and then run the problem PLOC that finds the rest of the energy loop's locations to obtain the loop. Subsequently, run the Golden Search for EMAT, exploring all EMAT-binding locations in the loop. Evaluate the TAC and call it TAC_{Min}.

b Run PESTR for $E = E_{Max}$. Then, run PLOC1 and PLOC to obtain the loop running the Golden Search for EMAT, exploring all EMAT-binding locations in the loop. Evaluate the TAC and call it TAC_{Max}.

c Run PESTR for $E = E_{Ratio}$. Then, run PLOC1 and PLOC to obtain the loop running the Golden Search for EMAT, exploring all EMAT-binding locations in the loop. Evaluate the TAC and call it TAC_{Ratio}.

4 If $TAC_{ratio} = Min\{TAC_{Min}, TAC_{ratio}, TAC_{Max}\}$, the solution is not monotone. Then go to Step 7.

5 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 TAC, namely, TAC^{+}_{Min}.

- If $TAC^{+}_{Min} - TAC_{Min} > 0$, the solution is monotone and $TAC = TAC_{Min}$. Go to Step 8.
- If $TAC^{+}_{Min} - TAC_{Min} < 0$, the solution is not monotone and go to Step 7.

6 If $TAC_{Max} = Min\{TAC_{Min}, TAC_{ratio}, TAC_{Max}\}$, the solution may be monotone or not. Then, run PESTR for $E = E_{Max} - 0.01$ and obtain its TAC, namely, TAC^{-}_{Max}.

- If $TAC_{Max} - TAC^{-}_{Max} < 0$, the solution is monotone and $TAC = TAC_{Max}$. Go to Step 8.
- If $TAC_{Max} - TAC^{-}_{Max} > 0$, the solution is not monotone and go to Step 7.

TABLE 2 The extra computing time for non-minimal networks in examples

Example	Option 1 (s)	Option 2 (s)	Option 3 (s)	Option 4 (s)
1	87.0	93.6	87.9	113.2
2	30.3	48.3	50.2	65.7
3	65.0	145.7	121.1	183.6
4	11.9	51.2	100.8	162.6
5	120.8	281.9	274.5	399.3
6	120.5	113.0	107.8	234.9
7	366.0	1,158.1	989.0	1,340.0
8	–	38,875.0	34,530.1	21,477.2
9	–	28,242.6	19,971.3	16,033.8
10	–	31,104.3	30,932.4	20,906.3
11	–	56,926.8	57,565.7	45,053.8
12	–	51,903.6	45,397.4	39,668.1
13	–	88,837.9	86,970.0	72,656.6
14	–	52,431.7	51,904.0	49,640.3
15	–	194,300.9	131,996.1	59,599.9
16	–	236,182.4	189,027.2	96,917.4

7 Apply the Golden Search for Energy. For each point in this Golden Search, run PLOC1 and PLOC to obtain the loop running the Golden Search for EMAT, exploring all EMAT-Binding locations in the loop to obtain the best TAC for the current structure. Use PESTR to obtain the TAC for each point.

8 If TAC ≤ UBTAC, then update UBTAC.

5 | EXAMPLES

Sixteen examples from different literatures are solved using our proposed algorithm. These examples are all implemented in GAMS (Version 23.7)[2] and solved using CPLEX (Version 12.1) as the MIP solver on a PC machine (i7 3.6 GHz, 8 GB RAM). The example results are given in Table 1, where Ns is the number of structures

Example	Minimal network ($/year)	Non-minimal network ($/year)	TAC reduction (%)
1	155,413.1	154,910.6	0.3
3	717,293.8	715,962.9	0.2
5	2,045,349.0	1,758,381.0	14.0
6	724,506.4	632,360.7	12.7
11	3,865,163.0	3,441,663.0	11.0
13	7,030,035.0	6,674,677.0	5.1
15	1,427,966.0	1,414,857.0	0.9
16	1,958,836.0	1,912,763.0	2.4

TABLE 3 Comparisons between the total annualized costs (TACs) of minimal and non-minimal networks

enumerated. Note that in each example both minimal and non-minimal networks have been considered in the algorithm, but we pick the better one as our globally optimal solution. The extra computing time spent for non-minimal networks in examples is listed in Table 2. The solution results of Examples 1–16 are described in detail in Data S1 of this article. It can be seen clearly that for small scale Examples 1–7, Option 1 of our algorithm is the best approach, while for large scale Examples 8–16 Option 4 is the best approach.

Of all examples, we found the same or slightly better answers than those from the literature in Examples 1–15, indicating that our enumeration algorithm is effective in finding the global optima for minimal and non-minimal HEN with isothermal mixing. When the final structure is the same (see Data S1), these small differences can be attributed to the tolerances used in the original literature examples and/or the tolerances in our Golden Search. In Example 16, the literature solution is a network with non-isothermal mixing that is not considered in our study. Thus, the TAC of our solution is slightly higher than that of the reported one.

Finally, the optimal solutions of Examples 1, 3, 5, 6, 11, 13, 15, and 16 are non-minimal networks. For these examples, we compare their minimal and non-minimal networks' TACs in Table 3. The solutions of other examples (2, 4, 7–10, 12, 14) are all minimal networks that are the same as the results of our Part I.

6 | CONCLUSIONS

This article is a follow-up of the previous Part I article where MSTRs are defined. Here, we addressed non-MSTRs for HEN synthesis using stage-wise superstructure with isothermal mixing. All possible structures for HEN synthesis are firstly enumerated using linear Synheat model or its lower bound model. A smart enumeration algorithm is developed to solve HEN synthesis problem to global optimality, which is based on accepting the conjectures presented in Part I and this article. The proposed algorithm makes use of a Golden Search approach to enumerate solutions with different energy target and EMAT under each fixed structure. Since the TAC is a unimodal continuous function of E and EMAT, global optimality can be ensured by our algorithm. Sixteen literature examples are solved globally and all our solutions are better but the last one, because we have not considered nonisothermal mixing. All our solution results have illustrated the capabilities of the proposed enumeration algorithm for HEN synthesis.

Our comments of the conclusion section in the part I, regarding the use of other superstructures and nonisothermal mixing, are also valid here.

Finally, we believe that networks with more than one energy loop add fixed cost corresponding to the extra exchanger. We leave this for 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

Parameters

N_{min}	minimum number of units
NOK	number of stages
E	total heating demand
EMAT	exchanger minimum approach temperature
HRAT	heat recovery approach temperature
N	total number of the desired heat exchangers
ΔT^*	minimum network temperature difference

Binary variables

z	binary variable to denote heat recovery exchanger
zhu	binary variable to denote heater
zcu	binary variable to denote cooler
$y_{i,j,k}$	binary variable related to the location of the EMAT-binding for heat recovery exchanger
$y_{HU,j}$	binary variable related to the location of the EMAT-binding for heater
$y_{CU,i}$	binary variable related to the location of the EMAT-binding for cooler

Continuous variables

$q_{i,j,k}$	heat exchanged between process streams
qhu_j	hot utility demand for cold stream
qcu_i	cold utility demand for hot stream
$T^{H}_{i,k}$	temperature of hot stream *i* at stage *k*
$T^{C}_{j,k}$	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*
$\Delta T_{HU,j}$	hot utility temperature difference
$\Delta T_{CU,i}$	cold utility temperature difference
β	minimum value of the temperatures of all active heat exchangers

Model acronym list

PSTR	problem rendering any viable structure of matches and candidates of minimal structures.
PSTRR	problem to enumerate different structures for minimal networks
PE_{Min}	problem to obtain the minimum energy target for a fixed structure
PE_{Max}	problem to obtain the maximum energy target for a fixed structure
PESTR	problem to obtain heat distribution corresponding to each MSTR with a fixed energy target
PLB	the lower bound model featuring a given number of units *N*
PLBR	problem containing problem PLB and the exclusion constraint.
PLOC1	Problem to find the first location of ΔT^*
PLOC	Problem to detect if the location obtained is part of a loop.
$PEMAT_{Min}$	Problem to obtain the minimum EMAT under fixed structure, energy, and location
$PEMAT_{Max}$	Problem to obtain the maximum EMAT under fixed structure, energy, and location

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REFERENCES

1. Yee TF, Grossmann IE. Simultaneous optimization models for heat integration. II, Heat exchanger network synthesis. *Comput Chem Eng*. 1990;14(10):1165-1184.
2. Brooke A, Kendrick D, Meeraus A, Raman R. *GAMS: A Users Guide*. GAMS Development: Washington, DC; 2005.
3. Faria DC, Kim SY, Bagajewicz MJ. Global optimization of the stage-wise superstructure model for heat exchanger networks. *Ind Eng Chem Res*. 2015;54(5):1595-1604.
4. Escobar M, Trierweiler JO. Optimal heat exchanger network synthesis: a case study comparison. *Appl Therm Eng*. 2013;51(1):801-826.
5. Gundersen T, Traedal P, Hashemi-Ahmady A. Improved sequential strategy for the synthesis of near-optimal heat exchanger networks. *Comput Chem Eng*. 1997;21:S59-S64.
6. Bogataj M, Kravanja Z. An alternative strategy for global optimization of heat exchanger networks. *Appl Therm Eng*. 2012;43:75-90.
7. Kim SY, Jongsuwat P, Suriyapraphadilok U, Bagajewicz MJ. Global optimization of heat exchanger networks. Part 1: stages/substages superstructure. *Ind Eng Chem Res*. 2017;56(20):5944-5957.
8. Escobar, M, Grossmann, IE. *Mixed-Integer Nonlinear Programming Models for Optimal Simultaneous Synthesis of Heat Exchangers Network*. Available from Cyber Infrastructure for MINLP [www.minlp.org, a collaboration of Carnegie Mellon University and IBM Research] at: www.minlp.org/library/problem/index.php?i=93. 2010.
9. Wang J, Cui G, Xiao Y, Luo X, Kabelac S. Bi-level heat exchanger network synthesis with evolution method for structure optimization and memetic particle swarm optimization for parameter optimization. *Eng Optim*. 2017;49:401-416.
10. Mistry M, Misener R. Optimising heat exchanger network synthesis using convexity properties of the logarithmic mean temperature difference. *Comput Chem Eng*. 2016;94:1-17.
11. Daichendt MM, Grossmann IE. Preliminary screening procedure for the MINLP synthesis of process systems-II. Heat exchanger networks. *Comput Chem Eng*. 1994;18(8):679-709.
12. Huang KF, Karimi IA. Simultaneous synthesis approaches for cost-effective heat exchanger networks. *Chem Eng Sci*. 2013;98:231-245.
13. Pavão LV, Costa CBB, Ravagnani MASS, Jiménez L. Large-scale heat exchanger networks synthesis using simulated annealing and the novel rocket fireworks optimization. *AIChE J*. 2017;63(5):1582-1601.
14. Pavão LV, Costa CBB, Ravagnani MASS. A new stage-wise superstructure for heat exchanger network synthesis considering substages, sub-splits and cross flows. *Appl Therm Eng*. 2018;143:719-735.
15. Zhang H, Cui G. Optimal heat exchanger network synthesis based on improved cuckoo search via Lévy flights. *Chem Eng Res Design*. 2018;134:62-79.

SUPPORTING INFORMATION

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

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