OPTIMAL HEAT EXCHANGER NETWORK SYNTHESIS BY SEQUENTIAL SPLITTING OF PROCESS STREAMS

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Abstract

The paper introduces a new iterative sequential method for optimal heat exchanger network synthesis, that relies on an assignment problem. This method considers the splitting of hot and cold process streams, and uses a decomposition that fixes the split fractions for process streams at each subproblem. We apply this method to several heat integration problems to demonstrate its performance and efficiency. It is also compared with stage-wise superstructure optimization using mixed-integer nonlinear programming.

Keywords

Process synthesis; Mathematical programming**;** Heat exchanger networks; Heat integration; Assignment problem; Superstructure; Decomposition approach.

1. INTRODUCTION

The last few decades have witnessed a number of new methods for solving the problem of optimal heat exchanger network (HEN) synthesis aimed at reducing heat consumption by heat recovery in the process streams (Klemeš and Kravanja, 2013). These methods can be subdivided into three groups: the thermodynamic approach, mathematical programming, and stochastic optimization. In the thermodynamic approach, a pinch-based calculation method proposed by Linnhoff and Hindmarsh (1983) has found wide application, as well as a method based on estimating the minimum entropy production (Tsirlin et al., 2008).

The economic issues of the problem, however, are not accounted for in the pinch-based method. Mathematical programming (MP) methods convert the optimal heat exchanger network synthesis problem into a mixed-integer nonlinear programming (MINLP) problem (Biegler et al., 1997, Biegler, 2010, Zamora and Grossmann, 1998, Furman and Sahinidis, 2001, Yee and Grossmann, 1990), which is formulated from a superstructure containing many possible heat exchanger network designs. Due to the dimensionality of industrial HEN superstructures, this method becomes intractable for many realistic instances but can give better economic results than the thermodynamic approach. Additional disadvantages of MP include possibility of multiple local optima, a large number of optimization variables, and computational expense due to the combinatorial complexity of the HENS problem. These disadvantages are characteristic of simultaneous MP synthesis methods. It is possible to mitigate these disadvantages by using a sequential decomposition of the initial problem into subproblems, a technique adopted in this paper. Papoulias and Grossmann (1983) decompose this problem into three subproblems: minimizing external hot and cold utility consumption, minimizing the number of heat exchangers, and finding the minimum capital cost. These subproblems can be solved by using a transshipment model (Papoulias and Grossmann, 1983; Chen et al., 2015), or a transportation model (Cerda and Westerberg, 1983). The heuristic nature of this decomposition method, nevertheless, does not guarantee optimal heat exchanger networks (Biegler et al., 1997). Recently Bagajewicz and co-workers (Chang et al., 2020a, 2020b) have proposed global optimization approaches that rely on linear models for both minimal and non-minimal structures for heat exchanger networks.

Stochastic methods, such as simulated annealing (Athier et al., 1997), particle swarm optimization (Ghiasvand et al., 2014), and genetic algorithms (Ravagnani et al., 2005), are also used for solving HEN synthesis problems. However, taking into account high dimensionality of the optimization problem, these methods are very computationally expensive and do not guarantee optimal solutions.

Ziyatdinov et al. (2016) considered a single stage HEN synthesis problem where each of the hot and cold process streams can exchange heat only once. The solutions in this case on reference examples were compared to the results of pinch analysis. It was shown that the single stage optimal heat integration does not allow using potential energy recovery at its full capacity due to the limitation imposed by the single heat exchange between the hot and cold process streams. In the examples considered, a single-stage optimal heat integration provides energy recovery from 50% to 70% relative to the limiting values obtained as a result of pinch analysis. Ziyatdinov et al. (2018) showed that energy recovery can be improved using a multistage direct or counterflow heat exchange between the hot and cold process streams. This paper extends the multiple stage optimal HEN synthesis approach by splitting the hot and cold process streams, which expands the solution search area. The paper also reports results on a significant number of examples.

2. THEORETICAL BACKGROUND

2.1. Problem Formulation

Assume we are given a process system with M^{h} "hot" streams H_i, (i=1,…,M^{h}) and the M^{c} "cold" streams C_j, (j=1,…,M^{c}), with their flowrates F_i, F_j, initial temperatures T_i^{in}, (i=1,…,M^{h}), T_j^{in}, (j=1,…,M^{c}), and specific heat capacities at constant pressure c_i, c_j, correspondingly. The heat exchanger network synthesis problem (Seider et al., 2009) consists of finding the structure of a heat exchanger network involving heat exchangers for the hot and cold streams, and if needed, coolers for the hot streams and heaters for the cold streams. Furthermore, the heat exchange areas A^{he}, the areas for heaters A^{hr} and the areas of coolers A^{cr}, must be determined together with the consumption of cooling and heating utilities, F^{cu} and F^{hu} , respectively, to satisfy the outlet temperatures of the hot and cold streams,

$$T_i^{\text{out}}, (i=1,\dots,M^{\text{h}}), \quad T_j^{\text{out}}, (j=1,\dots,M^{\text{c}}),$$

that in turn define the heat content ΔH_i of the hot streams, and the heat content ΔH_j of the cold streams. The goal is to synthesize the network that minimizes the sum of annualized capital and operating costs.

The synthesis problem is a non-linear combinatorial optimization problem, which is hard to solve due to the presence of both continuous (heat loads in exchangers, consumption of utilities, areas, etc.) and discrete variables (presence or absence of potential heat exchangers as well as their interconnections).

We consider the problem of optimal heat exchanger network synthesis that takes into account the possibility of splitting the process streams. At the inlet of the hot (cold) streams, we place flow splitters D_i and D_j . They split the i^{th} hot stream H_i into L_i number of branches H_{l_i} (i=1,…,M^{h} , $l_i = 1,...,L_i$,) and the j^{th} cold stream C_j into L_j number of branches C_{l_j} (j=1,…,M^{c}, $l_j = 1,...,L_j$), correspondingly. Every hot and cold process stream of the system can be split into a different number of branches. For the j^{th} cold stream, the largest number of splits can be defined by the number of hot streams with temperatures higher than the j^{th} cold stream temperature by a value higher than the minimum permissible temperature difference. Similarly, for the i^{th} hot stream, the largest number of branches can be defined by the number of cold streams with initial temperatures lower than the set value of the minimum permissible temperature difference. The flowrates F_{l_i} , F_{l_j} of branches H_{l_i} and C_{l_j} will be equal to $\beta_{l_i} F_{l_i}$, $\beta_{l_j} F_{l_j}$, correspondingly, where β_{l_i} , β_{l_j} are the branch fractions satisfying the conditions:

$$\sum_{l_i=1}^{L_i} \beta_{l_i} = 1, \; i = 1,...,M^h, \sum_{l_j=1}^{L_j} \beta_{l_j} = 1, \; j = 1,...,M^{\text{c}}. \tag{1}$$

Clearly the branch temperatures H_{l_i} and C_{l_j} ($l_i = 1,...,L_i$, $l_j = 1,...,L_j$) are equal to the inlet streams temperatures T_i^{in} and T_j^{in}, correspondingly. After passing through the heat exchanger network, the streams obtained by splitting the i^{th} hot and the j^{th} cold streams are mixed in mixers G_i and G_j correspondingly. Using the equation for the mixer process stream balance, we obtain

$$\Delta H_i = \sum_{l_i=1}^{L_i} \Delta H_{l_i}, \quad F_i^{\text{out}} = \sum_{l_i=1}^{L_i} F_{l_i}, \quad i = 1,...,M^{\text{h}}, l_i = 1,...,L_i, \tag{2}$$

$$\Delta H_j = \sum_{l_j=1}^{L_j} \Delta H_{l_j}, \quad F_j^{\text{out}} = \sum_{l_j=1}^{L_j} F_{l_j}. \; j = 1,...,M^{\text{c}}, l_j = 1,...,L_j. \tag{3}$$

Next, we enumerate the hot and cold branches obtained after splitting the inlet streams. The numbers $M_{\text{S}}^{\text{h}}, M_{\text{S}}^{\text{c}}$ of the obtained hot and cold branches will be equal, correspondingly, to:

$$M_{\text{S}}^{\text{h}} = \sum_{i=1}^{M^{\text{h}}} L_i, \quad M_{\text{S}}^{\text{c}} = \sum_{j=1}^{M^{\text{c}}} L_j. \tag{4}$$

2.2. Splitting of Process Streams in a HEN Superstructure

We reduce the optimal heat exchanger network synthesis problem to the optimization problem of a certain flowsheet superstructure. All of the possible heat exchanger network configurations are particular cases of a global flowsheet. We postulate a superstructure characterized by the following parameters: 1) for every combination of the elementary l_i^{th} hot and l_j^{th} cold streams, a heat recovery exchanger can be installed; 2) for additional heating or cooling of the process streams, the HEN outlet allows for installing additional coolers and heaters (which may be eliminated in the course of the problem solution); 3) any hot and cold elementary streams can exchange heat (in a heat recovery exchanger) only once. The structure of the described global flowsheet is given in Fig.1.

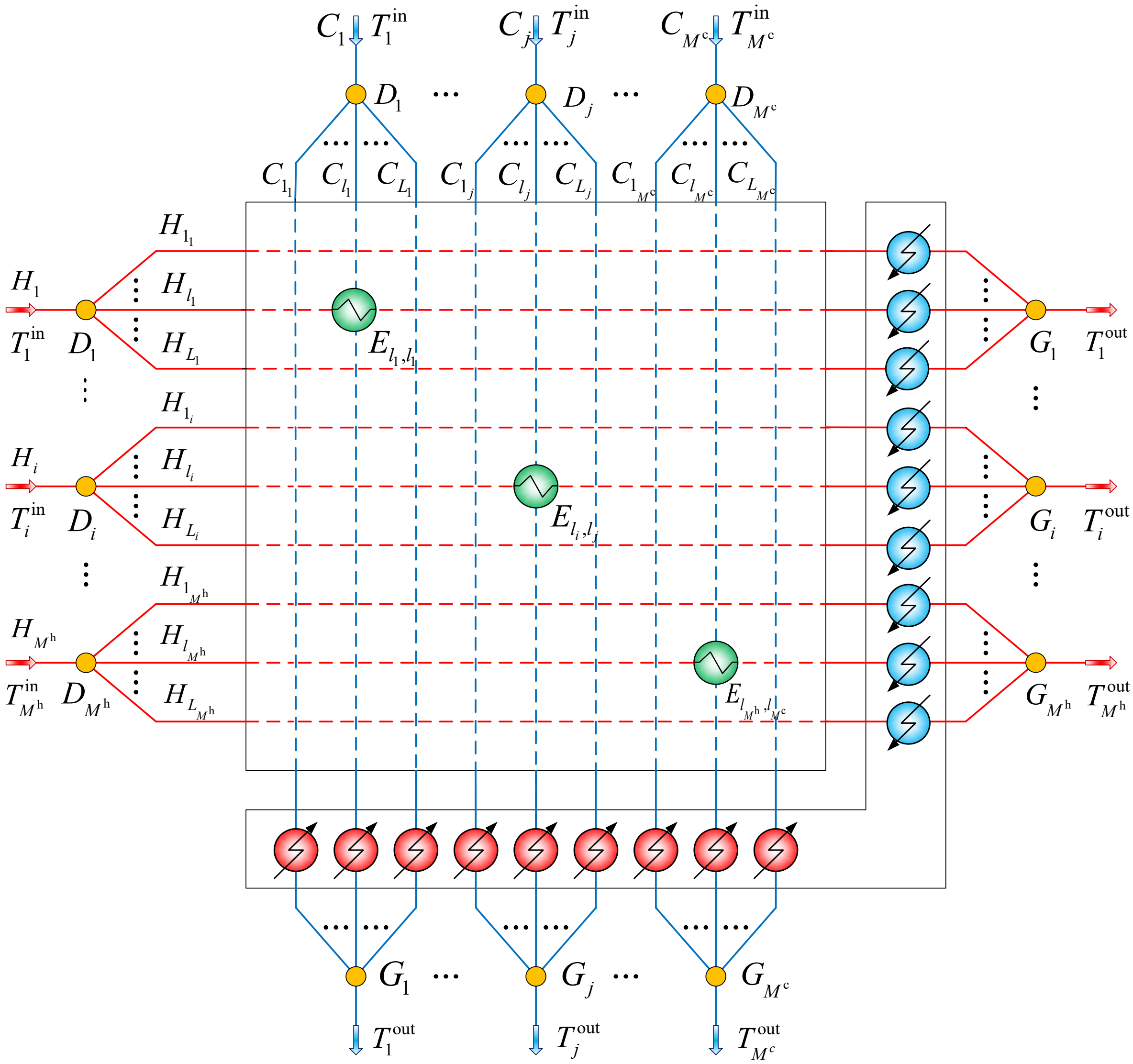

Figure 1 Splitting of Process Streams in a HEN Superstructure

A direct optimization of the global flowsheet may require significant computational effort and may lead to local minima. Therefore, we propose to solve the problem by decomposition. The method to solve the global flowsheet optimization problem is based on the principle of fixing the values of intermediate variables (Ostrovsky and Brusilovsky, 1977)). These variables are selected so as to eliminate the interactions between certain subsystems in a complex system when the variables are fixed. Thus, in case of known values for the fixed variables, the structures of certain subsystems in a complex system can be optimized independently.

Based on the principle of fixing the values of variables, the following iteration procedure can be developed. Two steps are taken at each iteration. In the first step, the optimal structures for certain subsystems are determined for the given values of the fixed variables. Using the new values of the fixed variables, the optimal structures for all subsystems are determined, and the iteration procedure starts again.

The proposed superstructure can be used in any HEN where process streams can be split. We define $T_{l_i}^{\text{in},(k)}, T_{l_i}^{\text{out},(k)}$ as the temperatures of the l_i^{th} hot elementary stream at the HEN inlet and outlet, $T_{l_j}^{\text{in},(k)}, T_{l_j}^{\text{out},(k)}$ are the temperatures of the l_j^{th} cold elementary stream at the HEN inlet and outlet at the k^{th} iteration. Clearly, $T_{l_i}^{\text{in},(k)} = T_i^{\text{in}}, T_{l_j}^{\text{in},(k)} = T_j^{\text{in}}$ for all values of k. We fix the process stream split fractions. At the k^{th} iteration, their values will be equal to $\beta_{l_i}^{(k)}, \beta_{l_j}^{(k)}, l_i = 1,...,(L_i - 1), l_j = 1,...,(L_j - 1)$, obtained from the $(k$-$1)^{\text{th}}$ iteration. At specified values of the fixed variables, we determine the optimal HEN structure with split process streams and multiple heat exchanger operating conditions. The optimal economic cost of heat exchange between the l_i^{th} hot and the l_j^{th} cold process streams is estimated using the HEN synthesis method without splitting the process streams as demonstrated by Ostrovsky et al. (2015). The method is based on structural decomposition of the system tested at the known values of $\Delta H_{l_j}, \Delta H_{l_i}$ .This method determines the optimal economic costs for the heat exchange in every pair of hot and cold process streams. The resulting matrix is used to find the optimal combination of coupled elementary process streams determining the structure and operation mode of the synthesized HEN.

For every combination of the l_i^{th} hot and the l_j^{th} cold process streams, we determine the optimal heat exchange unit structure and operating conditions of heat exchangers within this unit. We define a canonical form called the superstructure of HEN elementary units. An example of such a superstructure is shown in Figure 2. This superstructure is made up of the recovery heat exchanger E_{l_i,l_j}, where the l_i^{th} hot and the l_j^{th} cold process streams can exchange their heat, the cooler K_{l_i}, installed at the l_i^{th} hot process stream at the recovery heat exchanger outlet, and the heater B_{l_j}, installed at the l_j^{th} cold process stream at the heat exchanger outlet. Given the values of variables β_{l_i} and β_{l_j} we determine the optimal structure of the HEN elementary units, and operating conditions of the units within, so as to minimize the total costs $f_{l_i,l_j}(\beta_{l_i},\beta_{l_j})$. Using the defined superstructure, the problem is formalized as a nonlinear programming problem with equality constraints for the heat exchanger, cooler and heater mathematical models, and inequalities for the heat exchange feasibility. We chose the sum of capital and operating costs as the optimization criterion. The general problem definition for designing optimal HEN elementary units is given below in (5)-(13).

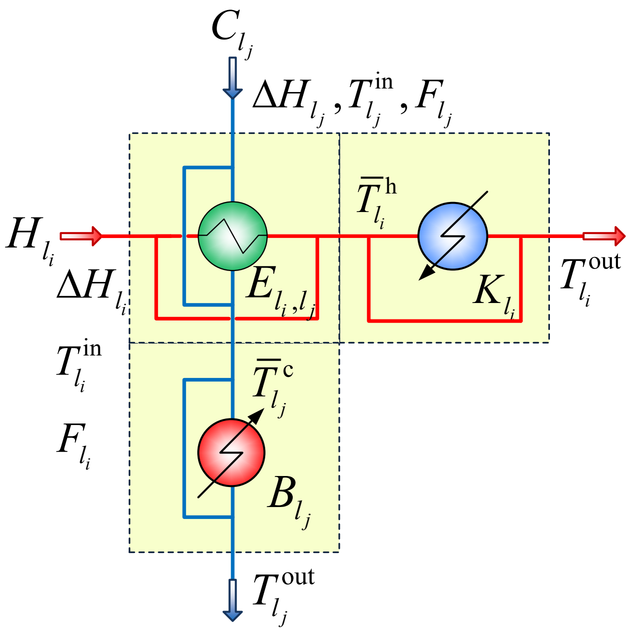

Figure 2 Superstructure of HEN Elementary Units

$$f^{\text{opt}}_{l_i,l_j} = \min_{A^{\text{he}}_{l_i,l_j}, A^{\text{cr}}_{l_i}, A^{\text{hr}}_{l_j}, F^{\text{cu}}_{l_i}, F^{\text{hu}}_{l_j}} f_{l_i,l_j}(A^{\text{he}}_{l_i,l_j}, A^{\text{cr}}_{l_i}, A^{\text{hr}}_{l_j}, F^{\text{cu}}_{l_i}, F^{\text{hu}}_{l_j}), \tag{5}$$

s.t. $\varphi^{\text{he}}(\bar{T}_{l_i}, \bar{T}_{l_j}, T^{\text{in}}_{l_i}, T^{\text{in}}_{l_j}, A^{\text{he}}_{l_i,l_j}, F_{l_i}, F_{l_j}, U^{\text{he}}_{l_i,l_j}) = 0,$ (6)

$$\varphi^{\text{cr}}(\bar{T}_{l_i}, T^{\text{out}}_{l_i}, T^{\text{cu,in}}_{l_i}, T^{\text{cu,out}}_{l_i}, A^{\text{cr}}_{l_i}, F_{l_i}, F^{\text{cu}}_{l_i}, U^{\text{cr}}_{l_i}) = 0, \tag{7}$$

$$\varphi^{\mathrm{hr}}(\overline{T}_{l_j}, T_{l_j}^{\mathrm{out}}, T_{l_j}^{\mathrm{hu,in}}, T_{l_j}^{\mathrm{hu,out}}, A_{l_j}^{\mathrm{hr}}, F_{l_j}, F_{l_j}^{\mathrm{hu}}, U_{l_j}^{\mathrm{hr}}) = 0, \tag{8}$$

$$T_{l_i}^{\mathrm{in}} = T_i^{\mathrm{in}},\ T_{l_j}^{\mathrm{in}} = T_j^{\mathrm{in}}, \tag{9}$$

$$i = 1, \ldots, M^{\mathrm{h}}, j = 1, \ldots, M^{\mathrm{c}},$$

$$l_i = 1, \ldots, L_i,\ l_j = 1, \ldots, L_j.$$

$$T_{l_i}^{\mathrm{in}} - \overline{T}_{l_j} \geq \Delta T_{\min},\ \overline{T}_{l_i} - T_{l_j}^{\mathrm{out}} \geq \Delta T_{\min}, \tag{10}$$

$$T_{l_j}^{\mathrm{hu,out}} - \overline{T}_{l_j} \geq \Delta T_{\min}, T_{l_j}^{\mathrm{hu,in}} - T_{l_j}^{\mathrm{out}} \geq \Delta T_{\min}, \tag{11}$$

$$T_{l_i}^{\mathrm{out}} - T_{l_i}^{\mathrm{cu,in}} \geq \Delta T_{\min},\ \overline{T}_{l_i} - T_{l_i}^{\mathrm{cu,out}} \geq \Delta T_{\min}. \tag{12}$$

$$Q_{l_i,l_j}^{\mathrm{he}} \geq 0, Q_{l_i}^{\mathrm{cr}} \geq 0, Q_{l_j}^{\mathrm{hr}} \geq 0. \tag{13}$$

where f_{l_i,l_j} is the objective function to be minimized for HEN elementary units; (6)-(8) are the mathematical models of the heat exchanger, cooler, and heater, correspondingly; (9) are the conditions imposed on the temperatures of the HEN inlet streams (the temperatures of the HEN inlet streams are to be kept to the set values); (10)-(13) are the limitations to the process driving force; $A_{l_i,l_j}^{\mathrm{he}}, A_{l_i}^{\mathrm{cr}}, A_{l_j}^{\mathrm{hr}}$ are heat exchange surface areas of the recuperative heat exchanger, cooler and heater, correspondingly; $Q_{l_i,l_j}^{\mathrm{he}}, Q_{l_i}^{\mathrm{cr}}, Q_{l_j}^{\mathrm{hr}}$ are duties of the heat exchanger, cooler and heater, correspondingly; $\overline{T}_{l_i}, \overline{T}_{l_j}$ are the heat exchanger outlet hot and cold temperatures; $\Delta T_{\min}$ is the minimum allowed temperature difference.

We next introduce a binary variable z_{l_i,l_j}, which is defined as follows:

$$z_{l_i,l_j} = \begin{cases} 1, \text{ elementary streams } H_{l_i} \text{ and } C_{l_j} \text{ exchange heat with each other,} \\ \quad \text{or with external utilities;} \\ 0, \text{ otherwise.} \end{cases}$$

Therefore, the arrangement problem of the optimal heat exchange structure can be reduced to a linear integer programming problem. In an ideal case, for $M_{\mathrm{S}}^{\mathrm{h}} = M_{\mathrm{S}}^{\mathrm{c}}$, the problem of determining the optimal structure is reduced to the following problem:

$$\min_{z_{l_i,l_j}} \sum_{i=1}^{M^{\mathrm{h}}} \sum_{l_i=1}^{L_i} \sum_{j=1}^{M^{\mathrm{c}}} \sum_{l_j=1}^{L_j} f_{l_i,l_j}^{\mathrm{opt}} z_{l_i,l_j}, \quad z_{l_i,l_j} \in \{0,1\}, \tag{14}$$

s.t.

$$\sum_{i=1}^{M^{\mathrm{h}}} \sum_{l_i=1}^{L_i} z_{l_i,l_j} = 1, \; \sum_{j=1}^{M^{\mathrm{c}}} \sum_{l_j=1}^{L_j} z_{l_i,l_j} = 1. \tag{15}$$

$$i = 1,\ldots,M^{\mathrm{h}}, \; j = 1,\ldots,M^{\mathrm{c}},$$

$$l_i = 1,\ldots,L_i, \; l_j = 1,\ldots,L_j.$$

This problem is the well-known assignment problem for which efficient solution methods are available (Kobayashi et al., 1971).

Based on the above, we propose the following iterative method for the optimal heat exchanger network synthesis. At the first step of each iteration, the assignment problem is solved using the given branch coefficients $\beta_{l_i}^{(k)}$ and $\beta_{l_j}^{(k)}$ for each of the hot and cold process streams obtained at the previous iteration. During the second step, the flowsheet optimization problem, shown in equations (16)–(23), is solved for the flowsheet structure obtained in the first step. Here, the values of the branch coefficients for the hot and cold process streams can be adjusted, taking into account the equations (1) – (3) for the process stream balance of the mixer and splitter, where:

Z is the total set of coupled branches with their HEN elementary units belonging to the HEN structure at the current iteration; and Φ is the total sum of the annualized capital costs in the heat recovery exchangers, together with the annualized capital and operating costs for the heaters and coolers.

$$\min_{F_{l_i}, F_{l_j}, A_{l_i,l_j}^{\mathbf{he}}, A_{l_i}^{\mathbf{cr}}, A_{l_j}^{\mathbf{hr}}, F_{l_i}^{\mathbf{cu}}, F_{l_j}^{\mathbf{hu}}} \Phi = \sum_{\forall (l_i,l_j) \in Z} (\varphi_{l_i,l_j}^{\mathbf{he}} + \varphi_{l_i,l_j}^{\mathbf{cr}} + \varphi_{l_i,l_j}^{\mathbf{hr}}) \tag{16}$$

$$\text{s.t.}\quad \varphi^{\text{he}}(\bar{T}_{l_i}, \bar{T}_{l_j}, T_{l_i}^{\text{in}}, T_{l_j}^{\text{in}}, A_{l_i,l_j}^{\text{he}}, F_{l_i}, F_{l_j}, U_{l_i,l_j}^{\text{he}}) = 0,\ \forall (l_i, l_j) \in Z\ , \tag{17}$$

$$\varphi^{\text{cr}}(\bar{T}_{l_i}, T_{l_i}^{\text{out}}, T_{l_i}^{\text{cu,in}}, T_{l_i}^{\text{cu,out}}, A_{l_i}^{\text{cr}}, F_{l_i}, F_{l_i}^{\text{cu}}, U_{l_i}^{\text{cr}}) = 0,\ \forall (l_i, l_j) \in Z, \tag{18}$$

$$\varphi^{\text{hr}}(\bar{T}_{l_j}, T_{l_j}^{\text{out}}, T_{l_j}^{\text{hu,in}}, T_{l_j}^{\text{hu,out}}, A_{l_j}^{\text{hr}}, F_{l_j}, F_{l_j}^{\text{hu}}, U_{l_j}^{\text{hr}}) = 0,\ \forall (l_i, l_j) \in Z, \tag{19}$$

$$T_{l_i}^{\text{in}} = T_i^{\text{in}},\ T_{l_j}^{\text{in}} = T_j^{\text{in}}, \tag{20}$$

$$T_{l_i}^{\text{in}} - \bar{T}_{l_j} \geq \Delta T_{\min},\ \bar{T}_{l_i} - T_{l_j}^{\text{out}} \geq \Delta T_{\min}, \tag{21}$$

$$T_{l_j}^{\text{hu,out}} - \bar{T}_{l_j} \geq \Delta T_{\min},\ T_{l_j}^{\text{hu,in}} - T_{l_j}^{\text{out}} \geq \Delta T_{\min}, \tag{22}$$

$$T_{l_i}^{\text{out}} - T_{l_i}^{\text{cu,in}} \geq \Delta T_{\min},\ \bar{T}_{l_i} - T_{l_i}^{\text{cu,out}} \geq \Delta T_{\min}. \tag{23}$$

$$Q_{l_i,l_j}^{\text{he}} \geq 0,\ Q_{l_i}^{\text{cr}} \geq 0,\ Q_{l_j}^{\text{hr}} \geq 0.$$

$$i = 1,\ldots,M^{\text{h}},\ j = 1,\ldots,M^{\text{c}},\ l_i = 1,\ldots,L_i,\ l_j = 1,\ldots,L_j.$$

The solution strategy can be accelerated with initial estimates for β_{l_i} and β_{l_j}, determined from the utility cost minimization problem using either the transshipment model by Papoulias and Grossmann (1983), or the transportation model by Cerda and Westerberg (1983).

We describe the components of the formulated problems (5) – (13) and (16) – (23). The objective function (5) is determined as a function of the total annualized capital and operating costs for the cooler and heater, and the annualized capital costs for the recuperative heat exchanger:

$$f_{l_i,l_j} = \left[\tilde{m}_1^{\text{he}} + \tilde{m}_2^{\text{he}}\left(A_{l_i,l_j}^{\text{he}}\right)^{\gamma^{\text{he}}}\right] + \left[\tilde{m}_1^{\text{hr}} + \tilde{m}_2^{\text{hr}}\left(A_{l_j}^{\text{hr}}\right)^{\gamma^{\text{hr}}} + \hat{m}^{\text{hr}} Q_{l_j}^{\text{hr}}\right] + \\ + \left[\tilde{m}_1^{\text{cr}} + \tilde{m}_2^{\text{cr}}\left(A_{l_i}^{\text{cr}}\right)^{\gamma^{\text{cr}}} + \hat{m}^{\text{cr}} Q_{l_i}^{\text{cr}}\right], \tag{24}$$

where $\tilde{m}_1^{\text{he}}, \tilde{m}_2^{\text{he}}, \tilde{m}_1^{\text{cr}}, \tilde{m}_2^{\text{cr}}, \tilde{m}_1^{\text{hr}}, \tilde{m}_2^{\text{hr}}$ are the price ratios for the corresponding heat exchanger, cooler, and heater, including the costs for the heat exchange equipment, its assembling and installation; $\gamma^{\mathrm{he}}, \gamma^{\mathrm{cr}}, \gamma^{\mathrm{hr}}$ are the cost exponent coefficients; and $\hat{m}^{\mathrm{cr}}, \hat{m}^{\mathrm{hr}}$ are the unit costs for the hot or cold heat carrier consumption.

The objective function (16) takes the form (25):

$$\Phi = \sum_{l_i}^{L_i} \sum_{l_j}^{L_j} \left[\left[\tilde{m}_1^{\mathrm{he}} + \tilde{m}_2^{\mathrm{he}} \left(A_{l_i, l_j}^{\mathrm{he}} \right)^{\gamma^{\mathrm{he}}} \right] + \left[\tilde{m}_1^{\mathrm{hr}} + \tilde{m}_2^{\mathrm{hr}} \left(A_{l_j}^{\mathrm{hr}} \right)^{\gamma^{\mathrm{hr}}} + \hat{m}^{\mathrm{hr}} Q_{l_j}^{\mathrm{hr}} \right] + \right.$$
$$\left. + \left[\tilde{m}_1^{\mathrm{cr}} + \tilde{m}_2^{\mathrm{cr}} \left(A_{l_i}^{\mathrm{cr}} \right)^{\gamma^{\mathrm{cr}}} + \hat{m}^{\mathrm{cr}} Q_{l_i}^{\mathrm{cr}} \right] \right], \tag{25}$$

The optimization problem given by (5) – (13) and (16) – (23) can be simplified with the following assumptions:

1) The outlet temperatures of all the utilities are specified. Therefore, the heat carrier consumption can be determined to maintain a fixed thermal capacity;

2) There are no phase transitions in the process streams.

The logarithmic mean temperature difference (LMTD) is used to calculate the areas of the heat exchangers, heaters and coolers. The following assumptions are introduced for the heat exchanger mathematical models:

1) the heat exchangers operate in counter flow mode;

2) the pressure drops across the exchangers are neglected;

3) the overall heat transfer coefficient of the heat exchanger is assumed to be given as a constant;

4) the average value of the specific heat capacity at constant pressure is used.

Therefore, the heat exchange areas can be determined from the heat transfer equation:

$$A_{l_i, l_j}^{\mathrm{he}} = \frac{Q_{l_i, l_j}^{\mathrm{he}}}{U_{l_i, l_j}^{\mathrm{he}} \Delta T_{LM}^{\mathrm{he}}}, \; A_{l_j}^{\mathrm{hr}} = \frac{Q_{l_j}^{\mathrm{hr}}}{U_{l_j}^{\mathrm{hr}} \Delta T_{LM}^{\mathrm{hr}}}, \; A_{l_i}^{\mathrm{cr}} = \frac{Q_{l_i}^{\mathrm{cr}}}{U_{l_i}^{\mathrm{cr}} \Delta T_{LM}^{\mathrm{cr}}}. \tag{26}$$

2.3. Algorithm for optimal HEN with splitting of process streams

The algorithm for the optimal HEN with splitting of process streams is as follows:

Step 1. Set the initial approximations for the branch coefficients $\beta_{l_i}^{(0)}, \beta_{l_j}^{(0)}, l_i = 1, \ldots, (L_i - 1),\ l_j = 1, \ldots, (L_j - 1)$.

$$\beta_{L_i}^{(0)} = 1 - \sum_{l_i=1}^{L_i-1} \beta_{l_i}^{(0)}, \quad i = 1,...,M^{\mathrm{h}},\ \beta_{L_j}^{(0)} = 1 - \sum_{l_j=1}^{L_j-1} \beta_{l_j}^{(0)}, \quad j = 1,...,M^{\mathrm{c}}.$$

We set the iteration counter k=1.

Step 2. Solve the $M_{\mathrm{S}}^{\mathrm{h}} \times M_{\mathrm{S}}^{\mathrm{c}}$ nonlinear mathematical programming problems (5)-(13) for every HEN elementary unit.

$$\min_{Q_{l_i,l_j}^{\mathrm{he},(k)}} f_{l_i,l_j}^{(k)},$$

where

$$f_{l_i,l_j}^{(k)} = \left[\tilde{m}_1^{\mathrm{he}} + \tilde{m}_2^{\mathrm{he}} \left(\frac{Q_{l_i,l_j}^{\mathrm{he},(k)}}{U_{l_i,l_j}^{\mathrm{he}} \Delta T_{LM}^{\mathrm{he},(k)}} \right)^{\gamma^{he}} \right] + \left[\tilde{m}_1^{\mathrm{hr}} + \tilde{m}_2^{\mathrm{hr}} \left(\frac{Q_{l_j}^{\mathrm{hr},(k)}}{U_{l_j}^{\mathrm{hr}} \Delta T_{LM}^{\mathrm{hr},(k)}} \right)^{\gamma^{\mathrm{hr}}} + \hat{m}^{\mathrm{hr}} Q_{l_j}^{\mathrm{hr},(k)} \right] + \left[\tilde{m}_1^{\mathrm{cr}} + \tilde{m}_2^{\mathrm{cr}} \left(\frac{Q_{l_i}^{\mathrm{cr},(k)}}{U_{l_i}^{\mathrm{cr}} \Delta T_{LM}^{\mathrm{cr},(k)}} \right)^{\gamma^{\mathrm{cr}}} + \hat{m}^{\mathrm{cr}} Q_{l_i}^{\mathrm{cr},(k)} \right] \tag{27}$$

$$U_{l_i,l_j}^{\mathrm{he}} = \frac{1}{\dfrac{1}{\alpha_{l_i}} + \dfrac{1}{\alpha_{l_j}}},\ U_{l_i}^{\mathrm{cr}} = \frac{1}{\dfrac{1}{\alpha_{l_i}} + \dfrac{1}{\alpha^{\mathrm{cu}}}},\ U_{l_j}^{\mathrm{hr}} = \frac{1}{\dfrac{1}{\alpha^{\mathrm{hu}}} + \dfrac{1}{\alpha_{l_j}}}, \tag{28}$$

$$\text{s.t.} \quad Q_{l_j}^{\mathrm{hr},(k)} = \Delta H_{l_j}^{(k)} - Q_{l_i,l_j}^{\mathrm{he},(k)},\ Q_{l_i}^{\mathrm{cr},(k)} = \Delta H_{l_i}^{(k)} - Q_{l_i,l_j}^{\mathrm{he},(k)}, \tag{29}$$

$$\Delta H_{l_j}^{(k)} = \beta_{l_j}^{(k-1)} \Delta H_j,\ \Delta H_{l_i}^{(k)} = \beta_{l_i}^{(k-1)} \Delta H_i, \tag{30}$$

$$F_{l_i}^{(k)} = \beta_{l_i}^{(k-1)} F_i, \quad F_{l_j}^{(k)} = \beta_{l_j}^{(k-1)} F_j, \tag{31}$$

$$\overline{T}_{l_j}^{(k)} = \frac{Q_{l_i,l_j}^{\mathrm{he},(k)}}{F_{l_j}^{(k)} c_j} + T_{l_j}^{\mathrm{in}},\ \overline{T}_{l_i}^{(k)} = T_{l_i}^{\mathrm{in}} - \frac{Q_{l_i,l_j}^{\mathrm{he},(k)}}{F_{l_i}^{(k)} c_i}, \tag{32}$$

$$T_{l_j}^{\mathrm{in}} = T_j^{\mathrm{in}},\ T_{l_i}^{\mathrm{in}} = T_i^{\mathrm{in}}, \tag{33}$$

$$T_{l_j}^{\mathrm{out}} = T_j^{\mathrm{out}},\ T_{l_i}^{\mathrm{out}} = T_i^{\mathrm{out}}, \tag{34}$$

$$\Delta T_{LM}^{p,(k)} = \frac{DT_1^{p,(k)} + DT_2^{p,(k)}}{\ln \dfrac{DT_1^{p,(k)}}{DT_2^{p,(k)}}},\ \forall p \in \Omega,\ \text{if } DT_1^{p,(k)} \neq DT_2^{p,(k)}; \tag{35}$$

$$DT_1^{\mathrm{he},(k)} = T_{l_i}^{\mathrm{in}} - \overline{T}_{l_j}^{(k)},\ DT_2^{\mathrm{he},(k)} = \overline{T}_{l_i}^{(k)} - T_{l_j}^{\mathrm{in}}, \tag{36}$$

$$DT_1^{\text{cr},(k)} = \overline{T}_{l_i}^{(k)} - T^{\text{cu,out}},\ DT_2^{\text{cr},(k)} = T_{l_i}^{\text{out}} - T^{\text{cu,in}}, \tag{37}$$

$$DT_1^{\text{hr},(k)} = T^{\text{hu,in}} - T_{l_j}^{\text{out}},\ \ DT_2^{\text{hr},(k)} = T^{\text{hu,out}} - \overline{T}_{l_j}^{(k)}, \tag{38}$$

$$DT_1^{p,(k)} - \Delta T_{\min} \ge 0,\ DT_2^{p,(k)} - \Delta T_{\min} \ge 0, \tag{39}$$

$$Q_{l_i,l_j}^{\text{he},(k)} \ge 0,\ Q_{l_i}^{\text{cr},(k)} \ge 0,\ Q_{l_j}^{\text{hr},(k)} \ge 0,$$

$$\Omega = \{\text{he, cr, hr}\}. \tag{40}$$

where $\alpha_{l_i}, \alpha_{l_j}$ are the film heat transfer coefficients of the hot and cold streams; $\alpha^{\text{hu}}, \alpha^{\text{cu}}$ are the film heat transfer coefficients of the hot and cold heat carriers; Ω is the set of heat exchangers in the HEN elementary unit structure.

Step 3. Solve the assignment problem in (14) and (15). As a result, the optimal HEN structure is determined for the fixed values of the stream branch fractions.

Step 4. Find the optimal operating conditions for the HEN with a fixed structure by solving the nonlinear programming problem in (16) – (23). The design and operating parameters of the heat exchangers, coolers and heaters are used as optimization variables.

$$\min_{\beta_{l_i}^{(k)},\beta_{l_j}^{(k)},Q_{l_i,l_j}^{\text{he},(k)}\ \forall(l_i,l_j)\in Z^k} \Phi^{(k)} \tag{41}$$

where

$$\Phi^{(k)} = \sum_{l_i}^{L_i}\sum_{l_j}^{L_j}\left[\left[\tilde{m}_1^{\text{he}} + \tilde{m}_2^{\text{he}}\left(\frac{Q_{l_i,l_j}^{\text{he},(k)}}{U_{l_i,l_j}^{\text{he}}\Delta T_{LM}^{\text{he},(k)}}\right)^{\gamma^{\text{he}}}\right] + \left[\tilde{m}_1^{\text{hr}} + \tilde{m}_2^{\text{hr}}\left(\frac{Q_{l_j}^{\text{hr},(k)}}{U_{l_j}^{\text{hr}}\Delta T_{LM}^{\text{hr},(k)}}\right)^{\gamma^{\text{hr}}} + \hat{m}^{\text{hr}}Q_{l_j}^{\text{hr},(k)}\right] + \right.$$
$$\left. + \left[\tilde{m}_1^{\text{cr}} + \tilde{m}_2^{\text{cr}}\left(\frac{Q_{l_i}^{\text{cr},(k)}}{U_{l_i}^{\text{cr}}\Delta T_{LM}^{\text{cr},(k)}}\right)^{\gamma^{\text{cr}}} + \hat{m}^{\text{cr}}Q_{l_i}^{\text{cr},(k)}\right]\right], \tag{42}$$

$$U_{l_i,l_j}^{\text{he}} = \frac{1}{\frac{1}{\alpha_{l_i}} + \frac{1}{\alpha_{l_j}}},\ U_{l_i,l_j}^{\text{cr}} = \frac{1}{\frac{1}{\alpha_{l_i}} + \frac{1}{\alpha^{\text{cu}}}},\ U_{l_i,l_j}^{\text{hr}} = \frac{1}{\frac{1}{\alpha^{\text{hu}}} + \frac{1}{\alpha_{l_j}}}, \tag{43}$$

$$\text{s.t.}\quad Q_{l_j}^{\text{hr},(k)} = \Delta\overline{H}_{l_j}^{(k)} - Q_{l_i,l_j}^{\text{he},(k)},\ Q_{l_i}^{\text{cr},(k)} = \Delta H_{l_i}^{(k)} - Q_{l_i,l_j}^{\text{he},(k)}, \tag{44}$$

$$\Delta H_{l_j}^{(k)} = \beta_{l_j}^{(k)} \Delta H_j, \Delta H_{l_i}^{(k)} = \beta_{l_i}^{(k)} \Delta H_i, \tag{45}$$

$$F_{l_i}^{(k)} = \beta_{l_i}^{(k)} F_i, \quad F_{l_j}^{(k)} = \beta_{l_j}^{(k)} F_j, \tag{46}$$

$$\overline{T}_{l_j}^{(k)} = \frac{Q_{l_i,l_j}^{\text{he},(k)}}{F_{l_j}^{(k)} c_j} + T_{l_j}^{\text{in}}, \overline{T}_{l_i}^{(k)} = T_{l_i}^{\text{in}} - \frac{Q_{l_i,l_j}^{\text{he},(k)}}{F_{l_i}^{(k)} c_i}, \tag{47}$$

$$\Delta T_{LM}^{p,(k)} = \frac{DT_1^{p,(k)} + DT_2^{p,(k)}}{\ln \dfrac{DT_1^{p,(k)}}{DT_2^{p,(k)}}}, \forall p \in \Omega, \text{ if } DT_1^{p,(k)} \neq DT_2^{p,(k)}; \tag{48}$$

$$DT_1^{\text{he},(k)} = T_{l_i}^{\text{in}} - \overline{T}_{l_j}^{(k)}, DT_2^{\text{he},(k)} = \overline{T}_{l_i}^{(k)} - T_{l_j}^{\text{in}}, \tag{49}$$

$$DT_1^{\text{cr},(k)} = \overline{T}_{l_i}^{(k)} - T^{\text{cu,out}}, DT_2^{\text{cr},(k)} = T_{l_i}^{\text{out}} - T^{\text{cu,in}}, \ \forall (l_i, l_j) \in Z^{(k)}, \tag{50}$$

$$DT_1^{\text{hr},(k)} = T^{\text{hu,in}} - T_{l_j}^{\text{out}}, DT_2^{\text{hr},(k)} = T^{\text{hu,out}} - \overline{T}_{l_j}^{(k)}, \tag{51}$$

$$DT_1^{p,(k)} - \Delta T_{\min} \geq 0, DT_2^{p,(k)} - \Delta T_{\min} \geq 0, \forall p \in \Omega, \tag{52}$$

$$Q_{l_i,l_j}^{\text{he},(k)} \geq 0, Q_{l_i}^{\text{cr},(k)} \geq 0, Q_{l_j}^{\text{hr},(k)} \geq 0,$$

$$\sum_{l_j=1}^{L_j} \beta_{l_j}^{(k)} - 1 = 0, \ \sum_{l_i=1}^{L_i} \beta_{l_i}^{(k)} - 1 = 0, \tag{53}$$

$$T_{l_i}^{\text{in}} = T_i^{\text{in}}, \ T_{l_j}^{\text{in}} = T_j^{\text{in}}, \tag{54}$$

$$T_{l_i}^{\text{out}} = T_i^{\text{out}}, \ T_{l_j}^{\text{out}} = T_j^{\text{out}}, \tag{55}$$

$$i = 1, \ldots, M^{\text{h}}, j = 1, \ldots, M^{\text{c}}, \ l_i = 1, \ldots, L_i \ l_j = 1, \ldots, L_j,$$

$$\Omega = \{\text{he, cr, hr}\}. \tag{56}$$

Step 5. If $\left|\Phi^{(k)} - \Phi^{(k-1)}\right| < \xi$, then the algorithm requirements are satisfied and the solution is obtained; otherwise set $k = k + 1$ and return to step 2.

2.4. Discussion

We denote the proposed synthesis method as SSHEN (Split Stream Heat Exchange Net). We can make the following remarks for the SSHEN method.

1) Equations in (34) and in (55) define the outlet temperatures of the branches and this assumption simplifies the problem. In some cases, however, they require additional heaters and coolers at the outlets of the branches, thus making it difficult to obtain the optimal value of the objective function. Therefore, the problem can be described more precisely by adding the optimization variables $T_{l_i}^{\text{out}} (i = 1,...,M^{\text{h}}, l_i = 1,...,L_i)$, $T_{l_j}^{\text{out}} \; (j = 1,...,M^{\text{c}}, l_j = 1,...,L_j)$ and limitations for the heat balance of the mixer (2) – (3). Thus, in non-isothermal mixing, Equations (57) and (58) are used.

$$T_i^{\text{out}} = \frac{\sum_{l_i=1}^{L_i} \beta_{l_i} F_i^{\text{in}} c_{l_i}^{\text{out}} T_{l_i}^{\text{out}},}{c_i^{\text{out}} F_i^{\text{out}}} \equiv \sum_{l_i=1}^{L_i} \beta_{l_i} T_{l_i}^{\text{out}}, \; T_j^{c,out} = \frac{\sum_{l_j=1}^{L_j} \beta_{l_j} F_j^{\text{in}} c_{l_j}^{\text{out}} T_{l_j}^{\text{out}}}{c_j^{\text{out}} F_j^{\text{out}}} \equiv \sum_{l_j=1}^{L_j} \beta_{l_j} T_{l_j}^{\text{out}}, \tag{57}$$

$$T_i^{\text{out}} - \sum_{l_i=1}^{L_i} \beta_{l_i} T_{l_i}^{\text{out}} = 0, \; T_j^{\text{out}} - \sum_{l_j=1}^{L_j} \beta_{l_j} T_{l_j}^{\text{out}} = 0, \tag{58}$$

$i = 1,...,M^{\text{h}}, j = 1,...,M^{\text{c}}, \; l_i = 1,...,L_i, \; l_j = 1,...,L_j.$

2) In the solution for the optimization problem in (27) – (40), some heat exchangers may be excluded from the optimal HEN elementary unit structure. We introduce the Boolean variables $\delta^{\text{he}}, \delta^{\text{hr}}, \delta^{\text{cr}}$, characterizing the presence or absence of units in the HEN structure:

$$\delta_{l_i,l_j}^{n,(k)} = \begin{cases} 1, \text{ if the } n^{\text{th}} \text{ unit for a combination of the } l_i^{\text{th}} \text{ hot and } l_j^{\text{th}} \text{ cold streams is present} \\ \text{in the HEN elementary unit structure at the } k^{\text{th}} \text{ iteration;} \\ 0, \text{ otherwise.} \end{cases}$$

Then, the optimization problem (41) – (56) can be simplified by adding the following conditions:

$$\left.\begin{cases} \text{if } (\delta^{\text{he}}_{l_i,l_j}=0)\wedge(\delta^{\text{hr}}_{l_i,l_j}=1)\wedge(\delta^{\text{cr}}_{l_i,l_j}=1), \\ \text{then } \Theta_{l_i,l_j}=\{\text{he}\}, Q^{\text{he}}_{l_i,l_j}=0, \overline{T}_{l_j}=T^{\text{in}}_{l_j}, \overline{T}_{l_i}=T^{\text{in}}_{l_i}; \\ \text{if } (\delta^{\text{he}}_{l_i,l_j}=1)\wedge(\delta^{\text{hr}}_{l_i,l_j}=0)\wedge(\delta^{\text{cr}}_{l_i,l_j}=1), \\ \text{then } \Theta_{l_i,l_j}=\{\text{hr}\}, Q^{\text{he}}_{l_i,l_j}=\Delta H_{l_i},\ \overline{T}_{l_j}=T^{\text{out}}_{l_j}; \\ \text{if } (\delta^{\text{he}}_{l_i,l_j}=1)\wedge(\delta^{\text{hr}}_{l_i,l_j}=1)\wedge(\delta^{\text{cr}}_{l_i,l_j}=0), \\ \text{then } \Theta_{l_i,l_j}=\{\text{cr}\}, Q^{\text{he}}_{l_i,l_j}=\Delta H_{l_j}, \overline{T}_{l_i}=T^{\text{out}}_{l_i}; \\ \text{if } (\delta^{\text{he}}_{l_i,l_j}=1)\wedge(\delta^{\text{hr}}_{l_i,l_j}=0)\wedge(\delta^{\text{cr}}_{l_i,l_j}=0), \\ \text{then } \Theta_{l_i,l_j}=\{\text{hr},\text{cr}\},\ Q^{\text{he}}_{l_i,l_j}=\Delta H_{l_j}=\Delta H_{l_i}, \\ \quad \overline{T}_{l_i}=T^{\text{out}}_{l_i}, \overline{T}_{l_j}=T^{\text{out}}_{l_j}. \end{cases}\right\} \begin{matrix} \forall(l_i,l_j)\in Z^{(k)}, \\ i=1,...,M^{\text{h}}, l_i=1,...,L_i, \\ j=1,...,M^{\text{c}}, l_j=1,...,L_j, \end{matrix} \quad (59)$$

where, and Θ_{l_i,l_j} is the set of heat exchangers excluded from the HEN elementary unit structure.

Based on the above conditions, the problem is solved for every sum of the l_ith hot and the l_jth cold branches for $\forall p \in \Omega / \Theta_{l_i l_j}$. Keep in mind that for the described cases, the heat exchanger load $Q^{\text{he}}_{l_i,l_j}$ is excluded from the list of optimization variables.

3) When solving the problem in (41)-(56) for cases where the heat exchanger, cooler and heater for the set of the l_ith hot and the l_jth cold branches ($(l_i,l_j)\in Z^{(k)}$) are present in HEN structure, the heat exchanger load $Q^{\text{he}}_{l_i,l_j}$ may also be excluded from the list of optimization variables considering that their operation costs significantly exceed capital costs. The thermal capacity is determined based on the following conditions:

$$\begin{cases} \nu<1:\ \overline{T}_{l_j}=T^{\text{in}}_{l_i}-\Delta T_{\min},\ Q^{\text{he}}_{l_i,l_j}=F_{l_j}c_j\left(\overline{T}_{l_j}-T^{\text{in}}_{l_j}\right); \\ \nu>1:\ \overline{T}_{l_i}=\Delta T_{\min}+T^{\text{in}}_{l_j},\ Q^{\text{he}}_{l_i,l_j}=F_{l_i}c_i\left(T^{\text{in}}_{l_i}-\overline{T}_{l_i}\right). \end{cases} \quad (60)$$

where $\nu=\dfrac{F_{l_j}c_j}{F_{l_i}c_i}$, $i=1,...,M^{\text{h}}, j=1,...,M^{\text{c}}, l_i=1,...,L_i, l_j=1,...,L_j$.

4) The assumption of no phase transitions can be easily eliminated by using detailed mathematical models. Thus, based on the heat balance equation for the heat exchanger model we derive the following:

$$\overline{T}_{l_j} = T_{l_j}^{\text{in}} + \frac{Q_{l_i,l_j}^{\text{he}} - rF_{l_j}}{F_{l_j} c_j}, \ \overline{T}_{l_i} = T_{l_i}^{\text{in}} - \frac{Q_{l_i,l_j}^{\text{he}} - rF_{l_i}}{F_{l_i} c_i}, \tag{61}$$

where r is the specific heat of evaporation.

5) In the general case, when $M_{\text{S}}^{\text{h}} \neq M_{\text{S}}^{\text{c}}$, for the optimal solution, it is suggested to reduce an asymmetric assignment problem to a symmetric problem by introducing additional rows $(M_{\text{S}}^{\text{c}} - M_{\text{S}}^{\text{h}})$ or additional $(M_{\text{S}}^{\text{h}} - M_{\text{S}}^{\text{c}})$ columns into the cost matrix. New rows contain optimal economic estimations for autonomous heating of the cold branches, while new columns contain economic estimations for autonomous cooling of the hot branches. As the assignment problem is to be solved for every sum of the hot and cold branches, the corresponding dummy cold and hot branches are introduced into the system. The economic value for heating and cooling these branches is zero.

The autonomous heating for the j^{th} cold branch together with the q^{th} imaginary hot branch f_{q,l_j}^{aut} is estimated based on the following equations:

$$f_{q,l_j}^{\text{aut}} = \tilde{m}_1^{\text{hr}} + \tilde{m}_2^{\text{hr}} \left(\frac{Q_{l_j}^{\text{hr}}}{U_{l_j}^{\text{hr}} \Delta T_{LM}^{\text{hr}}} \right)^{\gamma^{\text{hr}}} + \hat{m}^{\text{hr}} Q_{l_j}^{\text{hr}}, \tag{62}$$

$$\Delta Q_{l_j}^{\text{hr}} = \Delta H_{l_j}, \quad U_{l_j}^{\text{hr}} = \frac{1}{\dfrac{1}{\alpha^{\text{hu}}} + \dfrac{1}{\alpha_{l_j}}}, \tag{63}$$

$$\Delta T_{LM}^{\text{hr}} = \frac{DT_1^{\text{hr}} - DT_2^{\text{hr}}}{\ln \dfrac{DT_1^{\text{hr}}}{DT_2^{\text{hr}}}}, \text{ if } DT_1^{\text{hr}} \neq DT_2^{\text{hr}}; \tag{64}$$

$$DT_1^{\text{hr}} = T^{\text{hu,in}} - T_{l_j}^{\text{out}}, \ DT_2^{\text{hr}} = T^{\text{hu,out}} - T_{l_j}^{\text{in}}, \tag{65}$$

$$i = 1,\dots,M^{\text{h}}, \ j = 1,\dots,M^{\text{c}}, \ l_i = 1,\dots,L_i, \ l_j = 1,\dots,L_j.$$

In a similar way, the economic parameters $f_{l_i,w}^{\text{aut}}$ for autonomous cooling of the i^{th} hot branch together with the w^{th} imaginary cold branch are estimated based on the following equations:

$$f_{l_i,w}^{\text{aut}} = \tilde{m}_1^{\text{cr}} + \tilde{m}_2^{\text{cr}} \left(\frac{Q_{l_i}^{\text{cr}}}{U_{l_i}^{\text{cr}} \Delta T_{LM}^{\text{cr}}} \right)^{\gamma^{\text{cr}}} + \hat{m}^{\text{cr}} Q_{l_i}^{\text{cr}}, \tag{66}$$

$$Q_{l_i}^{\text{cr}} = \Delta H_{l_i},\ U_{l_i}^{\text{cr}} = \frac{1}{\dfrac{1}{\alpha_{l_i}^{\text{h}}} + \dfrac{1}{\alpha^{\text{cu}}}}, \tag{67}$$

$$\Delta T_{LM}^{\text{cr}} = \frac{DT_1^{\text{cr}} - DT_2^{\text{cr}}}{\ln \dfrac{DT_1^{\text{cr}}}{DT_2^{\text{cr}}}},\ \text{if } DT_1^{\text{cr}} \neq DT_2^{\text{cr}}; \tag{68}$$

$$DT_1^{\text{cr}} = T_{l_i}^{\text{in}} - T^{\text{cu,out}},\ DT_2^{\text{cr}} = T_{l_i}^{\text{out}} - T^{\text{cu,in}}, \tag{69}$$

$i = 1,...,M^{\text{h}},\ j = 1,...,M^{\text{c}},\ l_i = 1,...,L_i,\ l_j = 1,...,L_j.$

Therefore, the 0-1 linear optimization problem for determining the optimal HEN structure is as follows:

$$R = \max\{M_S^{\text{h}}, M_S^{\text{c}}\},\ f_{q,w} = \begin{cases} f_{l_j}^{\text{aut}},\ q = (M_{\text{S}}^{\text{h}}+1)...R,\ w \in \varnothing,\ M_S^{\text{h}} < M_S^{\text{c}}; \\ f_{l_i}^{\text{aut}},\ w = (M_{\text{S}}^{\text{c}}+1)...R,\ q \in \varnothing,\ M_S^{\text{h}} > M_S^{\text{c}}; \end{cases} \tag{70}$$

If $M_{\text{S}}^{\text{h}} < M_{\text{S}}^{\text{c}}$

$$\min_{z_{l_i,l_j}^{(k)}, z_{q,l_j}^{(k)}} \left(\sum_{i=1}^{M^{\text{h}}} \sum_{l_i=1}^{L_i} \sum_{j=1}^{M^{\text{c}}} \sum_{l_j=1}^{L_j} f_{l_i,l_j}^{\text{opt},(k)} z_{l_i,l_j}^{(k)} + \sum_{q=(M_S^{\text{c}}+1)}^{R} f_{q,l_j}^{\text{aut},(k)} z_{q,l_j}^{(k)} \right), \tag{71}$$

$$s.t.\ \sum_{i=1}^{M^{\text{h}}} \sum_{l_i=1}^{L_i} z_{l_i,l_j}^{(k)} + \sum_{q=(M_S^{\text{c}}+1)}^{R} z_{q,l_j}^{(k)} = 1,\ \sum_{j=1}^{M} \sum_{l_j=1}^{L_j} z_{l_i,l_j}^{(k)} = 1,\ \sum_{j=1}^{M} \sum_{l_j=1}^{L_j} z_{q,l_j}^{(k)} = 1, \tag{72}$$

$i = 1,...,M^{\text{h}},\ j = 1,...,M^{\text{c}},\ l_i = 1,...,L_i,\ l_j = 1,...,L_j,$

$z_{l_i,l_j} \in \{0,1\},\ z_{q,l_j} \in \{0,1\}.$

If $M_{\text{S}}^{\text{h}} > M_{\text{S}}^{\text{c}}$

$$\min_{z_{l_i,l_j}^{(k)}, z_{q,l_j}^{(k)}} \left(\sum_{i=1}^{M^{\text{h}}} \sum_{l_i=1}^{L_i} \sum_{j=1}^{M^{\text{c}}} \sum_{l_j=1}^{L_j} f_{l_i,l_j}^{\text{opt},(k)} z_{l_i,l_j}^{(k)} + \sum_{w=(M_S^{\text{h}}+1)}^{R} f_{l_i,w}^{\text{aut},(k)} z_{l_i,w}^{(k)} \right), \tag{73}$$

$$s.t. \sum_{i=1}^{M^{h}} \sum_{l_i=1}^{L_i} z_{l_i,l_j}^{(k)} = 1, \; \sum_{j=1}^{M^{c}} \sum_{l_j^{c}=1}^{L_j} z_{l_i,l_j}^{(k)} + \sum_{w=(M_S^{h}+1)}^{R} z_{l_i,w}^{(k)} = 1, \sum_{i=1}^{M^{h}} \sum_{l_i=1}^{L_i} z_{l_i,w}^{(k)} = 1, \quad (74)$$

$$i = 1,...,M^{h}, \; j = 1,...,M^{c}, \; l_i = 1,...,L_i, \; l_j = 1,...,L_j,$$

$$z_{l_i,l_j} \in \{0,1\}, \; z_{l_i,w}^{(k)} \in \{0,1\}. \quad (75)$$

3. COMPUTATIONAL RESULTS

3.1. Test problems

The operational performance and efficiency of the SSHEN method were first tested with four examples from the SYNHEAT software (Yee et al., 1990, Ponce-Ortega et al., 2008). SYNHEAT is based on a mixed-integer nonlinear programming model for optimizing a staged HEN superstructure. Two optimization algorithms were used when addressing the problem of heat exchange systems synthesis in the SYNHEAT program: DICOPT code and the global optimization code BARON. All examples were solved on a computer with an Intel Core i5-3570K processor, 3.4 GHz

3.2. Example 1

There are two hot and two cold streams which exchange heat. The data are given in Tables 1, 2. The total amount of heat to be recovered from the hot streams is $\Delta H_{\text{sum}}^{\text{h}} = 5000$ kW, the total amount of heat to be transferred to the cold streams is $\Delta H_{\text{sum}}^{\text{c}} = 4900$ kW.

Table 1 Stream data for Example 1

Hot stream	T_i^{in}, K	T_i^{out}, K	ΔH_i, kW	α, kW/m^{2}K	Cold stream	T_j^{in}, K	T_j^{out}, K	ΔH_j, kW	α, kW/m^{2}K
H_1	430	380	2,000	1.8	C_1	410	410	4,000	1.7
H_2	425	425	3,000	1.9	C_2	390	420	900	1.85
HU	627	627		2.5	CU	303	315		1.0

Table 2 Costs for Example 1

Cost of heating utility	($/kW-yr)	100.00

Cost of cooling utility	($/kW-yr)	10.00
Fixed charge for exchanger	($/yr)	0.00
Area cost coefficient for exchangers	($/m2)	380.00
Area cost coefficient for heaters	($/m2)	380.00
Area cost coefficient for coolers	($/m2)	380.00
Area cost exponent for exchangers		0.65

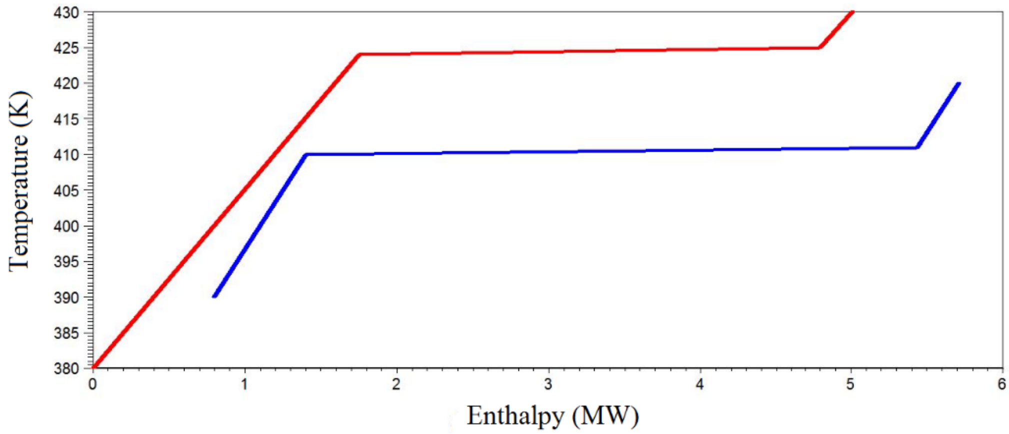

Figure 3 Composite Curves for Example 1 with $\Delta T_{\min} = 5°C$.

Pinch analysis for the lowest permissible temperature difference $\Delta T_{\min}$ of 5°C gives the following results:

a) In the area where the hot and cold composite curves coincide, the maximum possible amount of recovered heat is $Q_{\max}^{\text{he}} = 4,200$ kW;

b) The minimum amount of supply heat is $Q_{\min}^{\text{cr}} = 800$ kW;

c) The minimum amounts of removed heat is $Q_{\min}^{\text{hr}} = 700$kW .

Table 3 yields the results of solving the optimal synthesis problem by the SSHEN method

Table 3 Results the SSHEN method for Example 1

	Q, kW	T_i^{in}, K	T_i^{out}, K	T_j^{in}, K	T_j^{out}, K	A, m^2
Heat exchangers						
$E_{1_1 1_2}$	900	430	395	390	420	139
$E_{2_1 2_1}$	214.4	430	415	410	410	23.4
$E_{1_2 1_1}$	3,000	425	425	410	410	233.1
Coolers						

K_{1_1}	385.6	395	380	303	315	7.8
K_{2_1}	500	415	380	303	315	9
Heaters						
B_{1_1}	785.6	627	627	410	410	3.48

The HEN diagram obtained by using the proposed method (2.4 CPUs) is given in Figure 4.

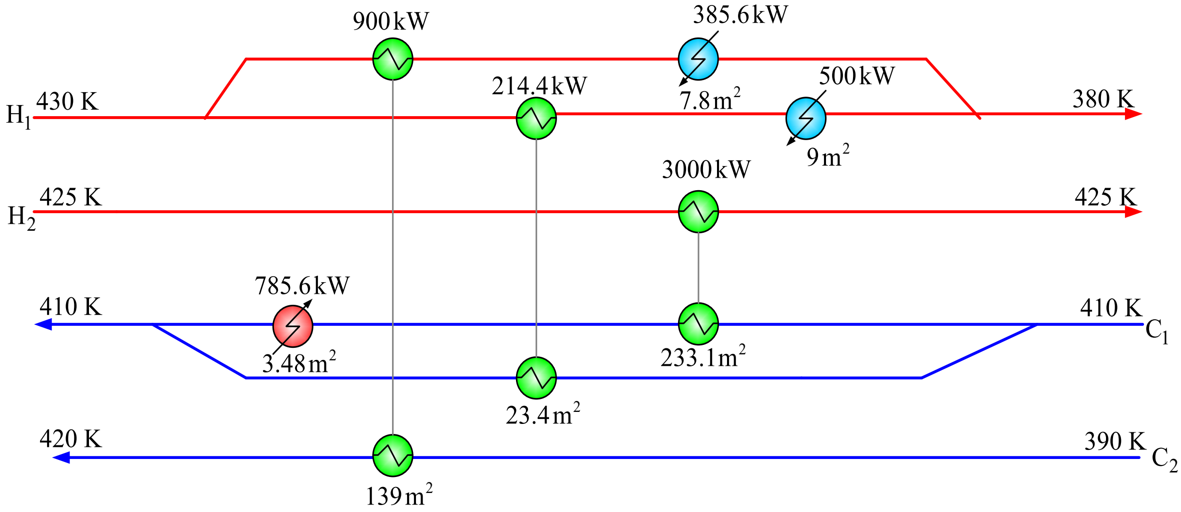

Figure 4 HEN diagram obtained by SSHEN method for Example 1.

The HEN Diagrams obtained by using SYNHEAT (DICOPT) (t=0.48 s) and SYNHEAT Software (BARON) (1,058 CPUs) are given in Figures 5 and 6.

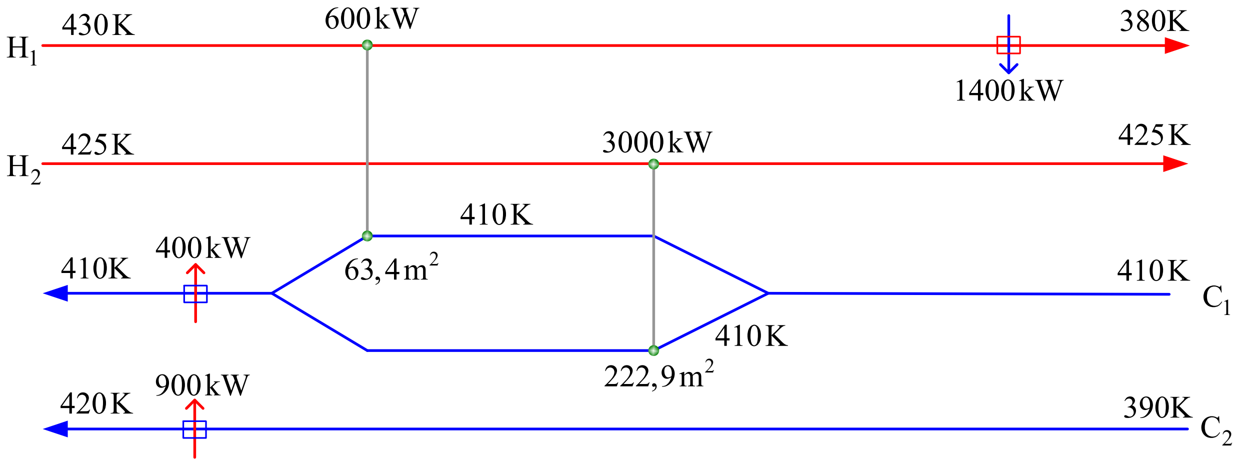

Figure 5 HEN diagram obtained by SYNHEAT (DICOPT) for Example 1.

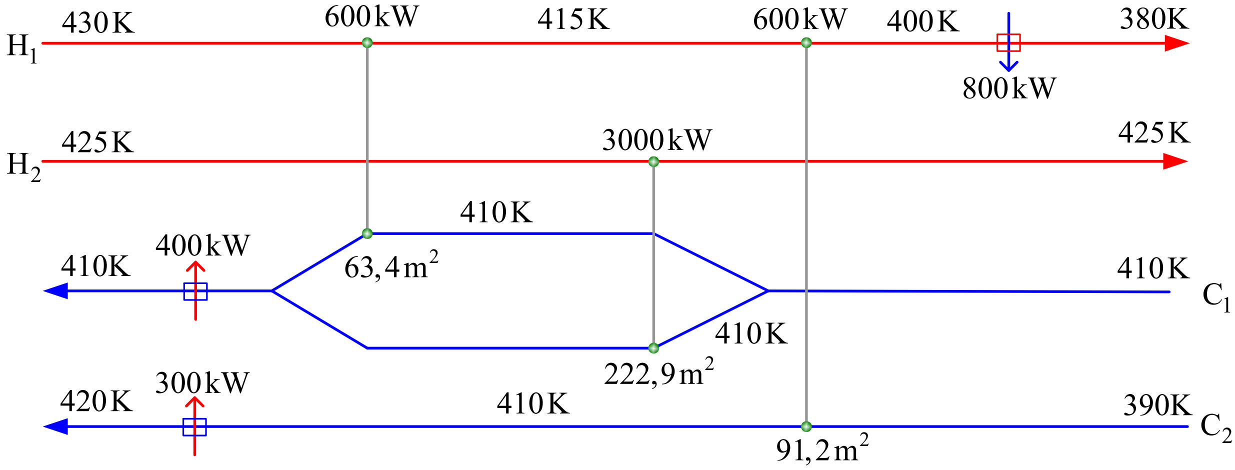

Figure 6 HEN diagram obtained by SYNHEAT (BARON) for Example 1.

Comparison of the obtained results is presented in Table 43.

Table 4 Results of the SSHEN and SYNHEAT Methods for Example 1

Name	SSHEN	DICOPT	BARON
Q^{he}, (kW)	4,114.1	3,600	4,200
Q^{hr}, (kW)	785.9	1300	700
Q^{cr}, (kW)	885.9	1400	800
n^{he}	3	2	3
n^{hr}	1	2	2
n^{cr}	2	1	1
E_{sum}, USD/year	87,420	144,000	78,000
K_{sum}, USD/year	29,454	22,951.3	28,828.4
A^{he}. m^2	395.5	286.4	377.5
A^{cr}, m^2	16.8	24.8	15.4
A^{hr}, m^2	3.48	5.7	3.15
Φ, USD/year TAC	116,874	166,951	106,828
CPU time, (s)	2.4	0.48	1,058

The results show that the HEN structure in Figure 4 is characterized by a lower total cost compared to the structure using the SYNHEAT (DICOPT) software (Figure 5). Also, its configuration is not significantly different from the HEN obtained in SYNHEAT (BARON) although it has a higher cost.

3.3. Example 2

There are three hot and four cold streams exchanging heat. The data are given in Tables 5, 6. The composite curves on temperature vs. enthalpy diagram for a ΔT_{min} of 5°C are shown in Figure 7.

Table 5 Stream data for Example 2

Hot stream	T_i^{in}, K	T_i^{out}, K	ΔH_i, kW	α, kW/m^{2}K	Cold stream	T_j^{in}, K	T_j^{out}, K	ΔH_j, kW	α, kW/m^{2}K
H_1	503	308	12,948	0.81	C_1	323	503	8,838	0.72
H_2	425	425	33,020	1.78	C_2	408	408	18,413.1	1.91
H_3	381	381	12,870	1.62	C_3	391	391	18,498.4	1.76
					C_4	353	353	16,347.7	1.84
HU	627	627		2.5	CU	303	315		1.0

Table 6 Costs for Example 2

Cost of heating utility	($/kw-yr)	100.00
Cost of cooling utility	($/kw-yr)	10.00
Area cost coefficient for exchangers	($/m2)	380.00
Area cost coefficient for heaters	($/m2)	380.00
Area cost coefficient for coolers	($/m2)	380.00
Area cost exponent for exchangers		0.65

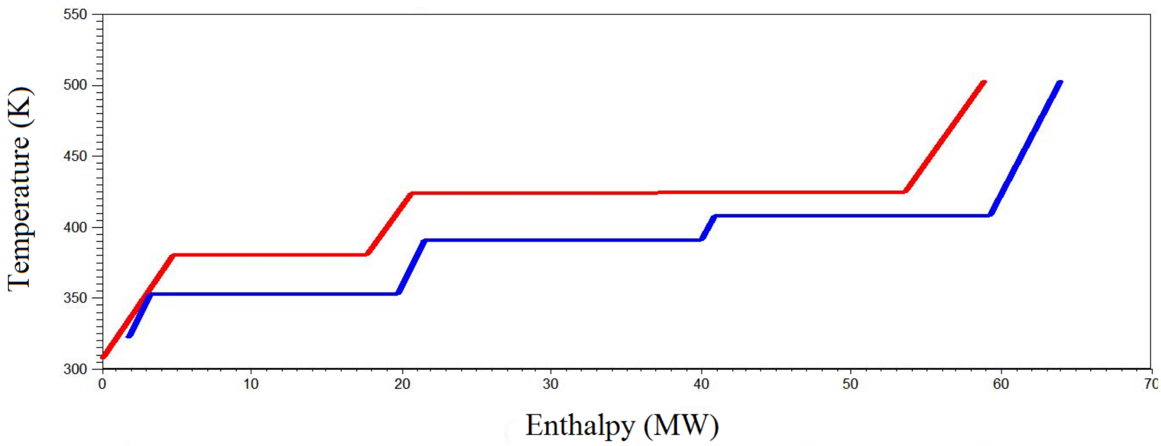

Figure 7 Composite Curves for Example 2 with ΔT_{min} = 5°C.

The results of pinch analysis are as follows:

$$\Delta H^{h}_{sum} = 58{,}838 \text{ kW}$$

$\Delta H^{c}_{sum} = 62{,}097$ kW

$Q^{he}_{max} = 56{,}991$ kW

$Q^{cr}_{min} = 1{,}847$ kW

$Q^{hr}_{min} = 5{,}106$kW

Table 7 gives the results of solving the optimal synthesis problem by the SSHEN method.

Table 7 Results the SSHEN method for Example 2

	Q, kW	T_i^{in}, K	T_i^{out}, K	T_j^{in}, K	T_j^{out}, K	A, m^2
Heat exchangers						
$E_{2_1 1_1}$	7,718.5	503	328	323	479.2	1,726.1
$E_{2_2 1_2}$	14,522	425	425	408	408	985
$E_{1_2 1_3}$	18,498	425	425	391	391	633.4
$E_{1_1 1_4}$	3,232.7	503	397.7	353	353	135.4
$E_{1_3 2_4}$	12,870	381	381	353	353	553.3
Coolers						
K_{2_1}	882.1	328	308	303	315	235.4
K_{1_1}	1,114.7	397.7	308	303	315	141
Heaters						
B_{1_1}	1,119.5	627	627	479.2	503	14.9
B_{1_4}	245.2	627	627	353	353	0.85
B_{2_2}	3,891.5	627	627	408	408	16.5

The HEN diagram obtained by using the SSHEN method (t=14.3 s) is given in Figure 8.

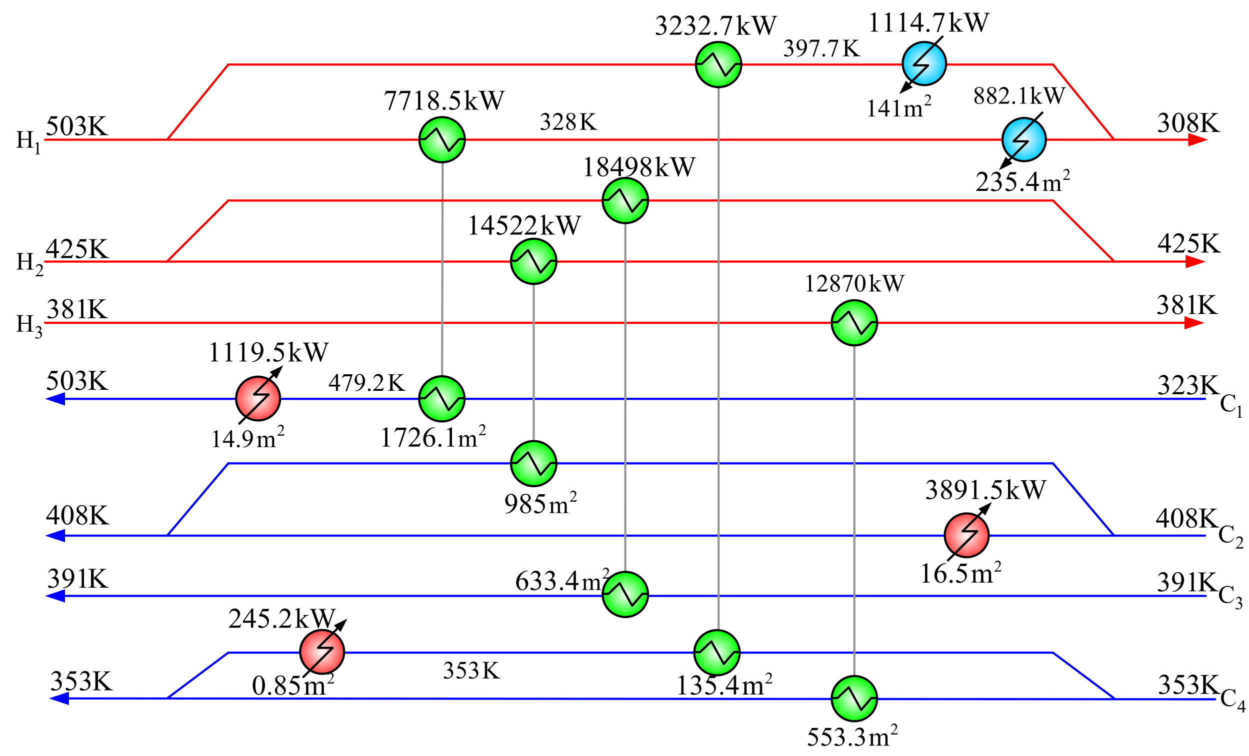

Figure 8 HEN diagram obtained by SSHEN method for Example 2.

The HEN diagrams obtained by using the SYNHEAT (DICOPT) (t=1.2 s) and SYNHEAT (BARON) (>24,126 CPU s) are given Figures 9 and 10.

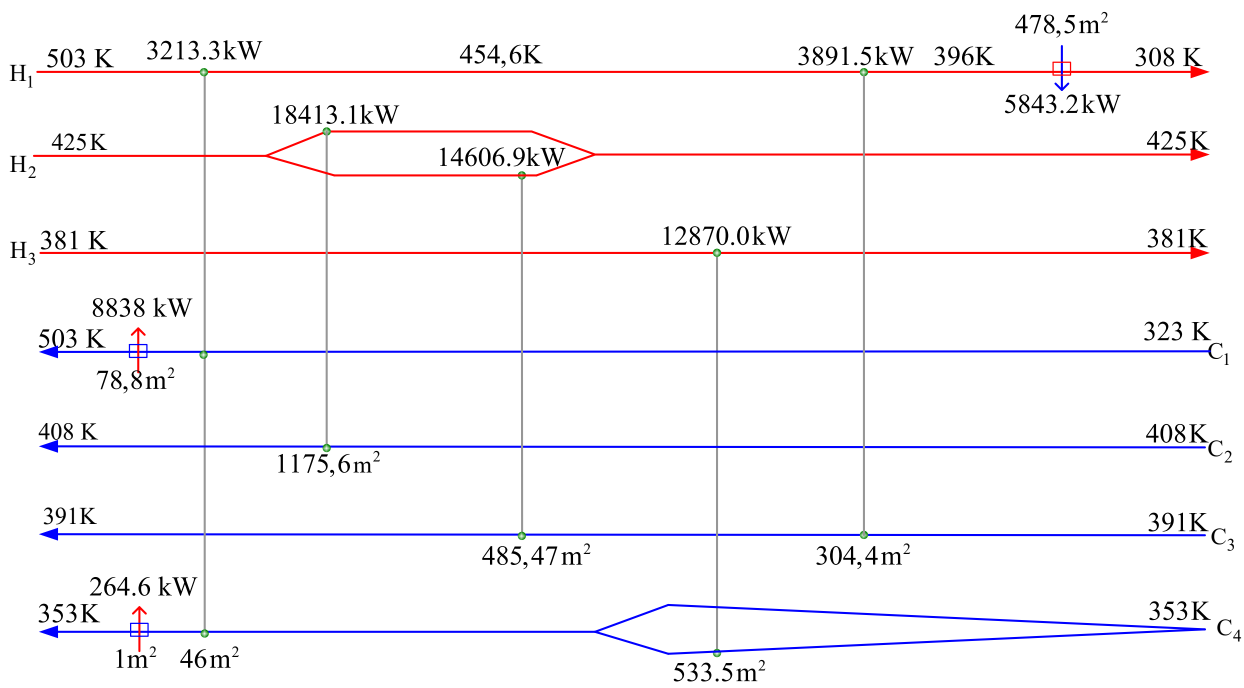

Figure 9 HEN diagram obtained by SYNHEAT (DICOPT) for Example 2.

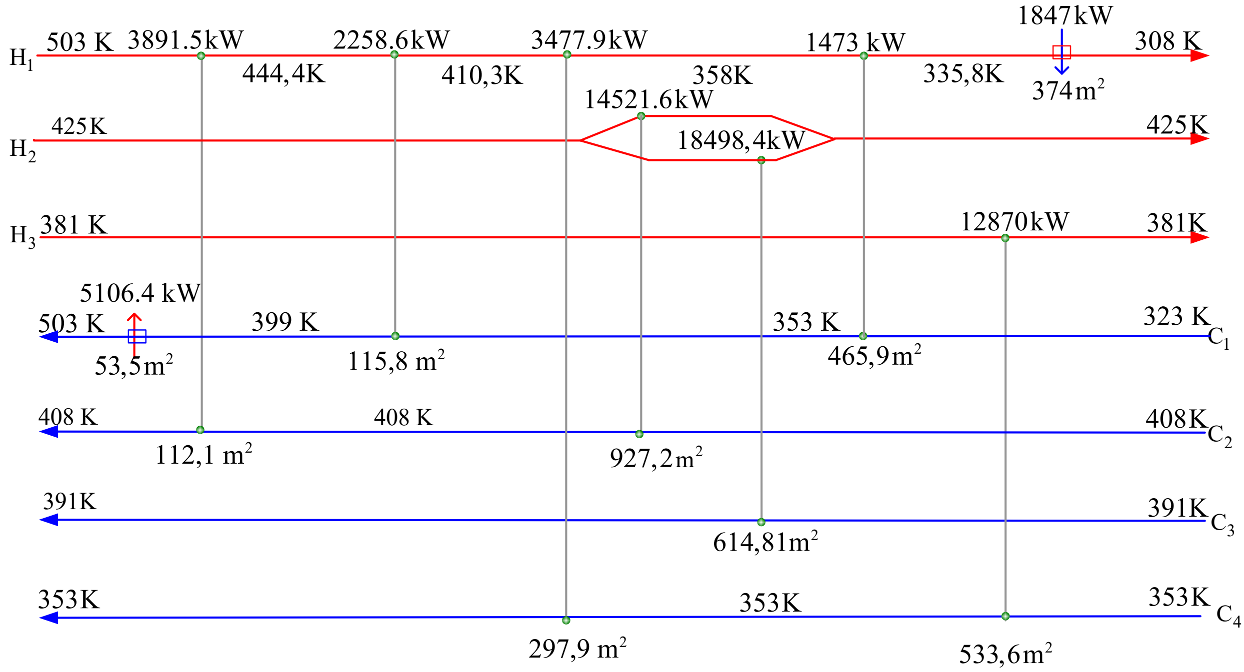

Figure 10 HEN diagram obtained by SYNHEAT (BARON) for Example 2.

Comparison of the obtained results is presented in Table 8.

Table 8 Results of the SSHEN and SYNHEAT methods for Example 2

Name	SSHEN	DICOPT	BARON
Q^{he}, (kW)	56,841.2	52,994.8	56,991
Q^{hr}, (kW)	5,256.2	9,102.6	5,106
Q^{cr}, (kW)	1,996.8	5,843.2	1,847
n^{he}	5	5	7
n^{hr}	3	2	1
n^{cr}	2	1	1
E_{sum}, USD/year	545,592	968,692	529,111
K_{sum}, USD/year	166,882	130,459	154,905
A^{he}. M^2	4,033.2	2,545	3,067.3
A^{cr}, m^2	376.5	504	374.1
A^{hr}, m^2	32.2	79.8	53.5
Φ, USD/year TAC	712,474	1,099,151	684,016
CPU time, (s)	14.3	1.2	24,126

The results in Table 8 show that the SSHEN method yields lower costs than SYNHEAT (DICOPT). However, SYNHEAT (BARON) showed slightly better results.

3.4. Example 3

There are four hot and four cold streams exchanging heat. The data are given in Tables 9, 10. The composite curves on temperature vs. enthalpy diagram for a ΔT_{min} of 10°C are shown in Figure 11.

Table 9 Stream data for Example 3

Hot stream	T_i^{in}, K	T_i^{out}, K	ΔH_i, kW	α, kW/m²K	Cold stream	T_j^{in}, K	T_j^{out}, K	ΔH_j, kW	α, kW/m²K
H_1	420	360	3,000	1.0	C_1	340	380	2,400	1.0
H_2	470	375	19,000	2.5	C_2	365	430	7,800	1.0
H_3	485	390	14,250	2.0	C_3	395	450	5,500	1.0
H_4	500	435	6,500	2.0	C_4	410	465	22,000	1.0
HU	620	620		5.0	CU	300	315		1.0

Table 10 Costs for Example 3

Cost of heating utility	($/kw-yr)	85.0
Cost of cooling utility	($/kw-yr)	15.0
Area cost coefficient for exchangers	($/m2)	380.00
Area cost coefficient for heaters	($/m2)	380.00
Area cost coefficient for coolers	($/m2)	380.00
Area cost exponent for exchangers		0.65

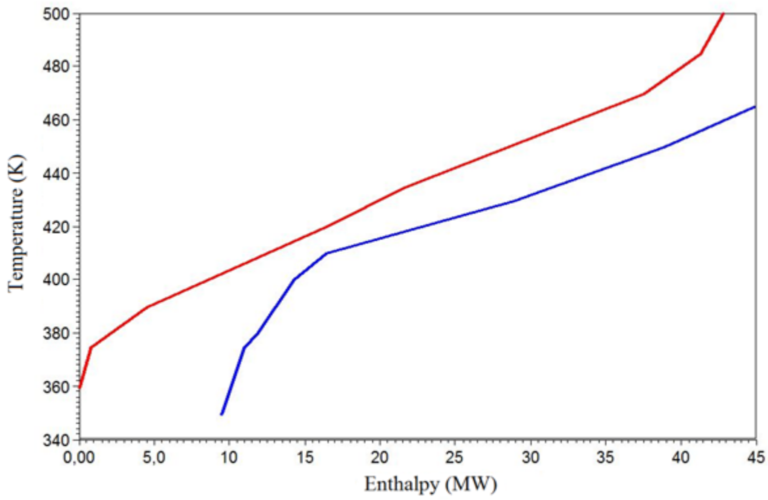

Figure 11 Composite Curves for Example 3 with ΔT_{min} = 5°C.

The results of pinch analysis are as follows:

$\Delta H^{h}_{sum} = 42.75$ MW, $\Delta H^{c}_{sum} = 37.7$ MW,

$Q^{he}_{max} = 35.55$ MW, $Q^{cr}_{min} = 9.5$ MW, $Q^{hr}_{min} = 2.15$MW.

HEN diagram obtained by using the SSHEN method (t=12.8 s) is given Figure 12.

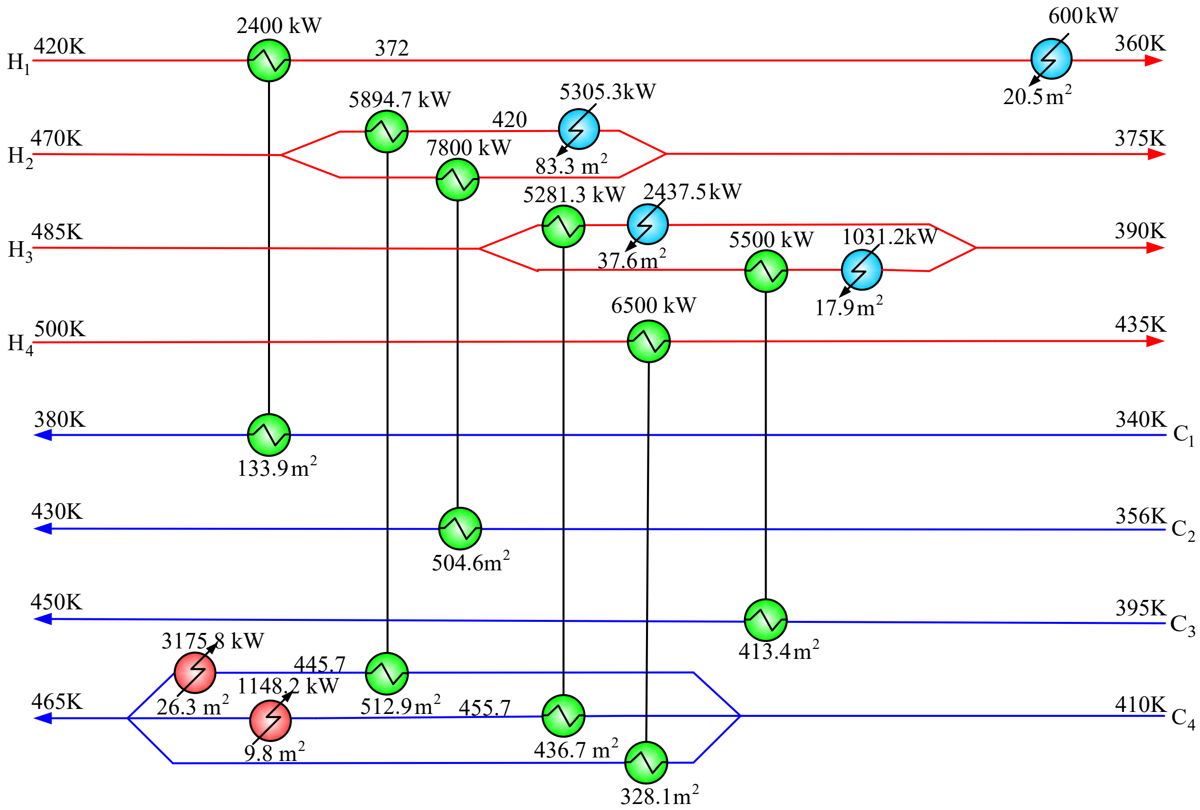

Figure 12 HEN diagram obtained by SSHEN method for Example 3.

The HEN Diagram obtained by using SYNHEAT (DICOPT) (t=0.85 s) and SYNHEAT (BARON) (34,752 CPUs) are given Figures 13 and 14.

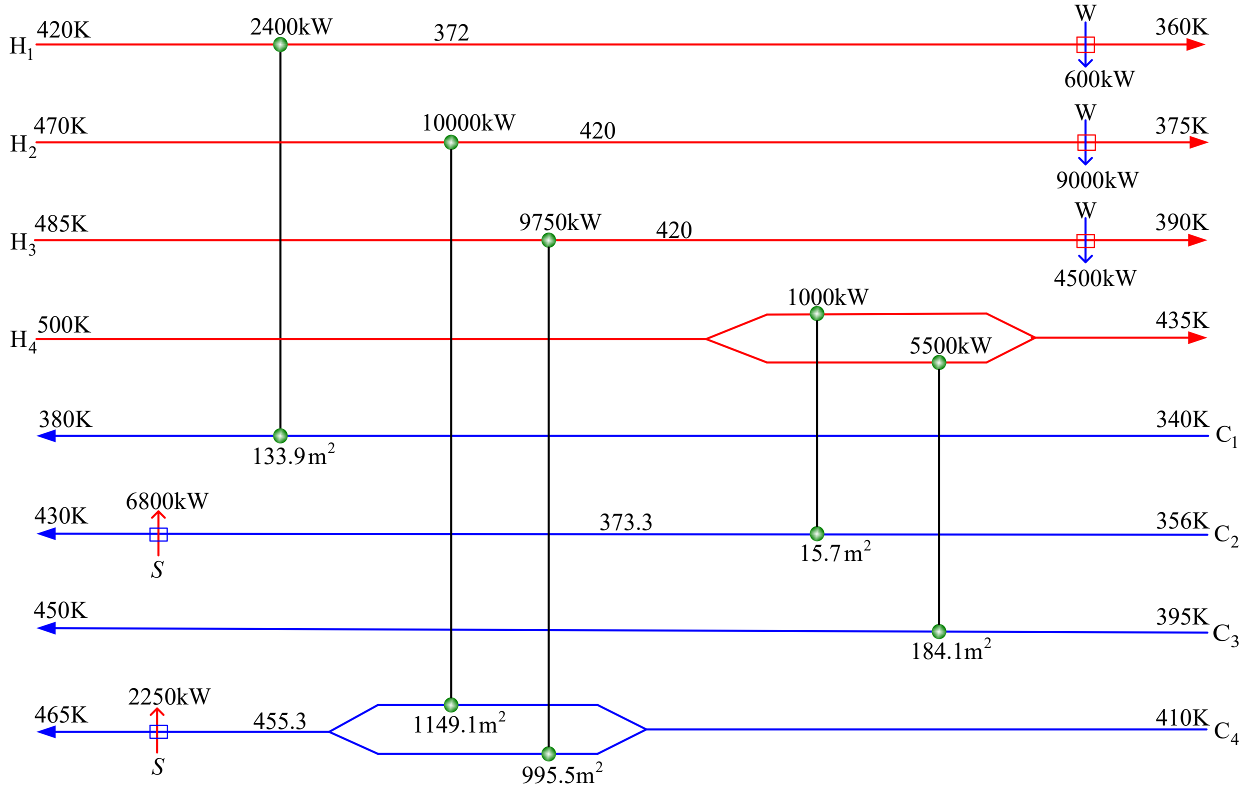

Figure 13 HEN diagram obtained by SYNHEAT (DICOPT) for Example 3.

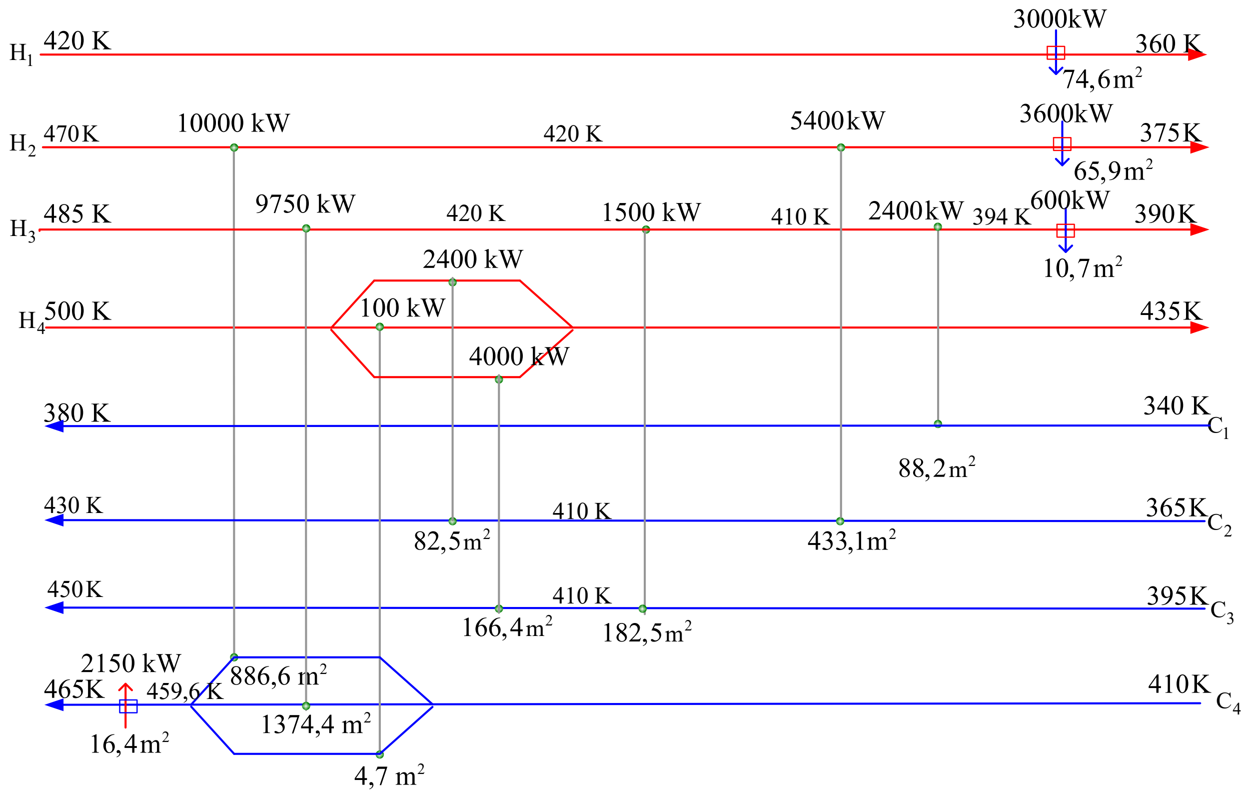

Figure 14 HEN diagram obtained by SYNHEAT (BARON) for Example 3.

Comparison of the obtained results is presented in Table 11.

Table 11 Results of the SSHEN and SYNHEAT Methods for Example 3

Name	SSHEN	DICOPT	BARON
Q^{he}, (kW)	33,376	28,650	35,550
Q^{hr}, (kW)	4,324	9,050	2,150
Q^{cr}, (kW)	9,374	14,100	7,200
n^{he}	6	5	8
n^{hr}	2	2	1
n^{cr}	4	3	3
E_{sum}, USD/year	508,150	980,750	290,750
K_{sum}, USD/year	128,798	118,164	145,283
A^{he}. M^2	36.1	54.7	3,218.4
A^{cr}, m^2	158.59	231.22	151.2
A^{hr}, m^2	2,329.6	2,478.3	16.4
Φ, USD/year TAC	636,948	1,098,914	436,012
CPU time, (s)	12.8	0.85	34,752

As in the previous examples, the proposed method gave a lower cost than SYNHEAT (DICOPT) but worse than the SYNHEAT (BARON) method, although at a much lower computational cost.

This example has been investigated of for the existence multiple local solutions. For this, we plotted the dependences of the optimal values of the objective function on two splitting coefficients of the streams, with fixed values of the others. The graphs in Figure 15 confirm the presence of many local minima.

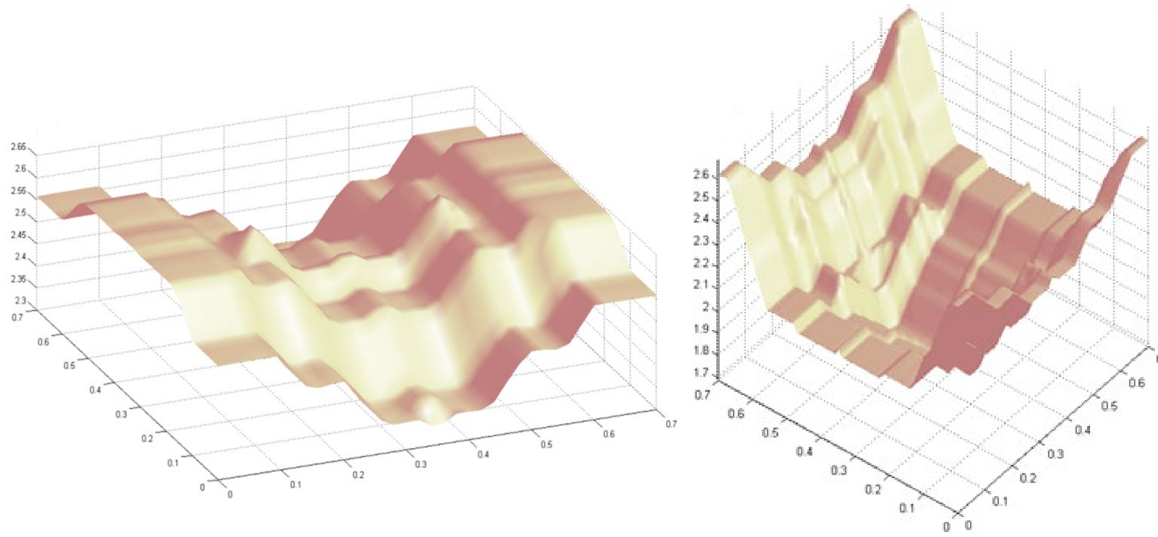

Figure 15 The dependence of the optimal values of the objective function (mln. USD) on two coefficients of splitting of streams.

3.5. Example 4

In this example there are four hot and three cold isothermal streams exchanging heat. The data are given in Tables 12, 13. The composite curves on temperature vs. enthalpy diagram for a $\Delta T_{\min}$ of 5°C are shown in Figure 16.

Table 12 Stream data for Example 4

Hot stream	T_i^{in}, K	T_i^{out}, K	ΔH_i, kW	α, kW/m^{2}K	Cold stream	T_j^{in}, K	T_j^{out}, K	ΔH_j, kW	α, kW/m^{2}K
H_1	340	340	1,900.0	1.52	C_1	350	350	992.5	1.81
H_2	390	390	1,493.1	1.63	C_2	375	375	1,801.2	1.72
H_3	420	420	2,594.4	1.75	C_3	400	400	4,361.6	1.64
H_4	475	475	1,999.1	1.58					
HU	627	627		2.5	CU	303	315		1.0

Table 13 Costs for Example 4

Cost of heating utility	($/kw-yr)	100.00
Cost of cooling utility	($/kw-yr)	10.00
Fixed charge for exchanger	($/yr)	0.00
Area cost coefficient for exchangers	($/m2)	380.00
Area cost coefficient for heaters	($/m2)	380.00
Area cost coefficient for coolers	($/m2)	380.00
Area cost exponent for exchangers		0.65

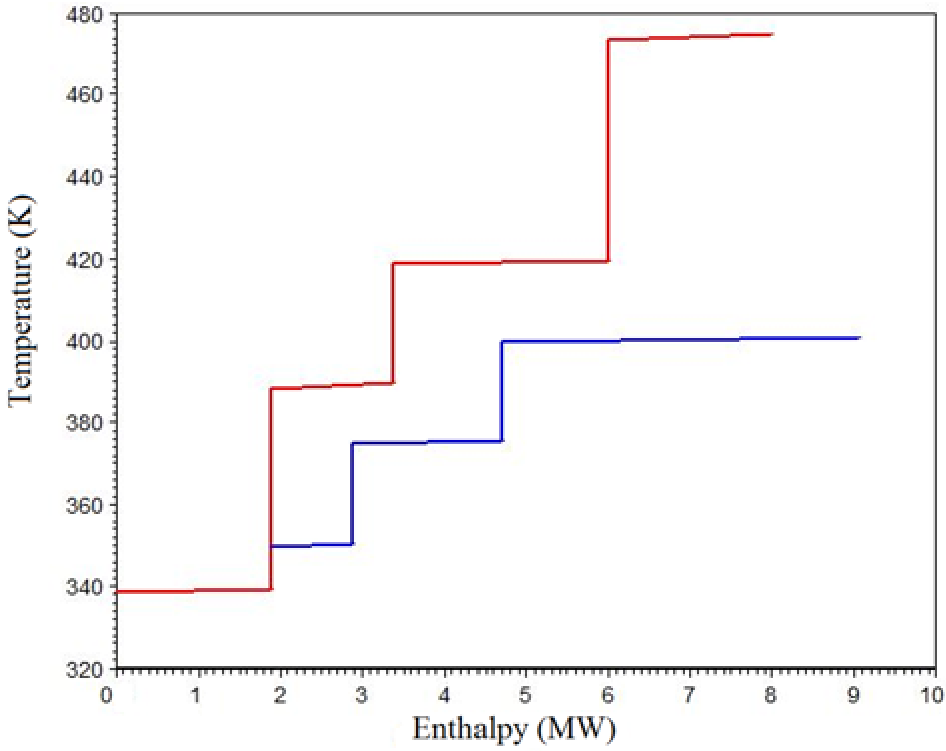

Figure 16 Composite Curves for Example 4 with $\Delta T_{\min}$ = 5°C.

The results of pinch analysis are as follows:

$\Delta H^{\mathrm{h}}_{\mathrm{sum}} = 7{,}986.6$ kW , $\Delta H^{\mathrm{c}}_{\mathrm{sum}} = 7{,}173.3$ kW ,

$Q^{\mathrm{he}}_{\max} = 6{,}086$ MW , $Q^{\mathrm{cr}}_{\min} = 1{,}900$ kW , $Q^{\mathrm{hr}}_{\min} = 1{,}068.7$kW.

The HEN diagram obtained by using the SSHEN method (t=6.5 s) is given in Figure 17.

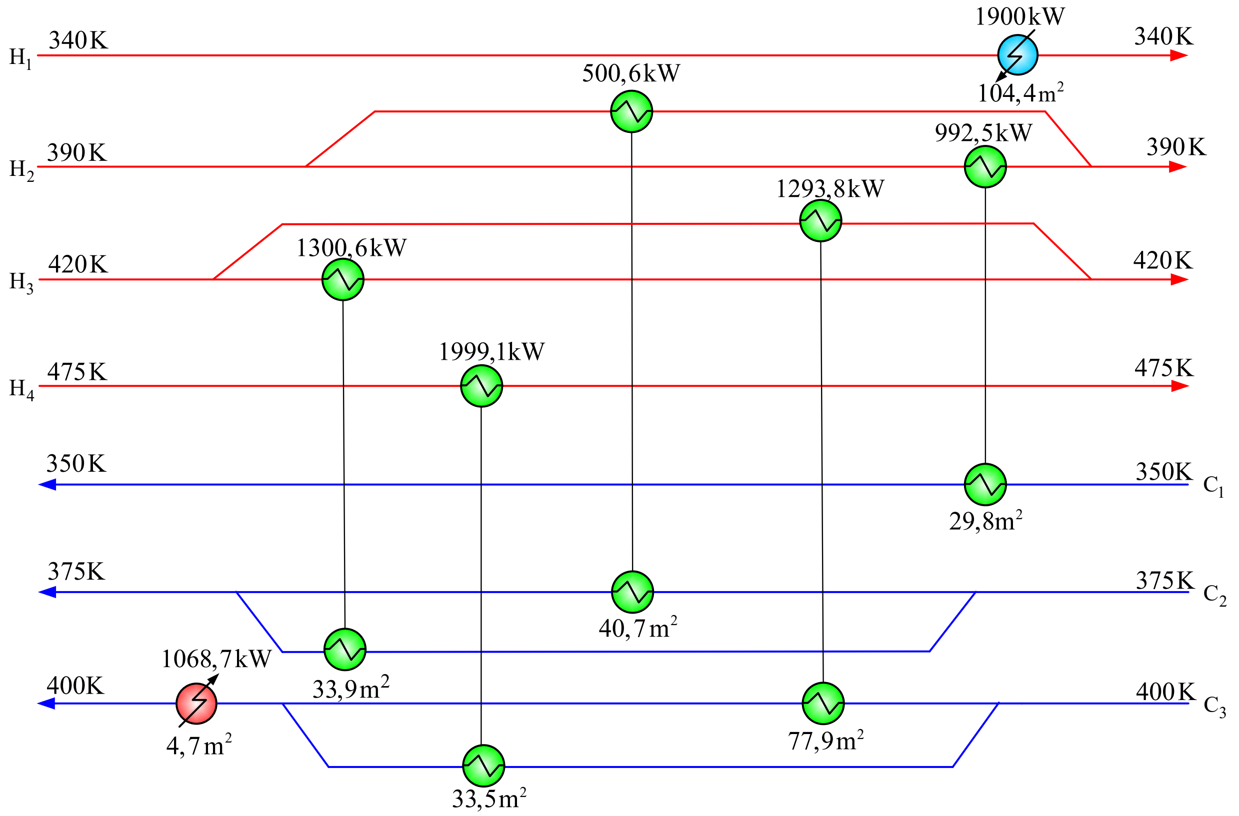

Figure 17 HEN diagram obtained by SSHEN method for Example 4.

The HEN diagram obtained by using SYNHEAT (DICOPT) (t=0.2 s) and SYNHEAT (BARON) (112,464 CPUs) is given in Figure 18.

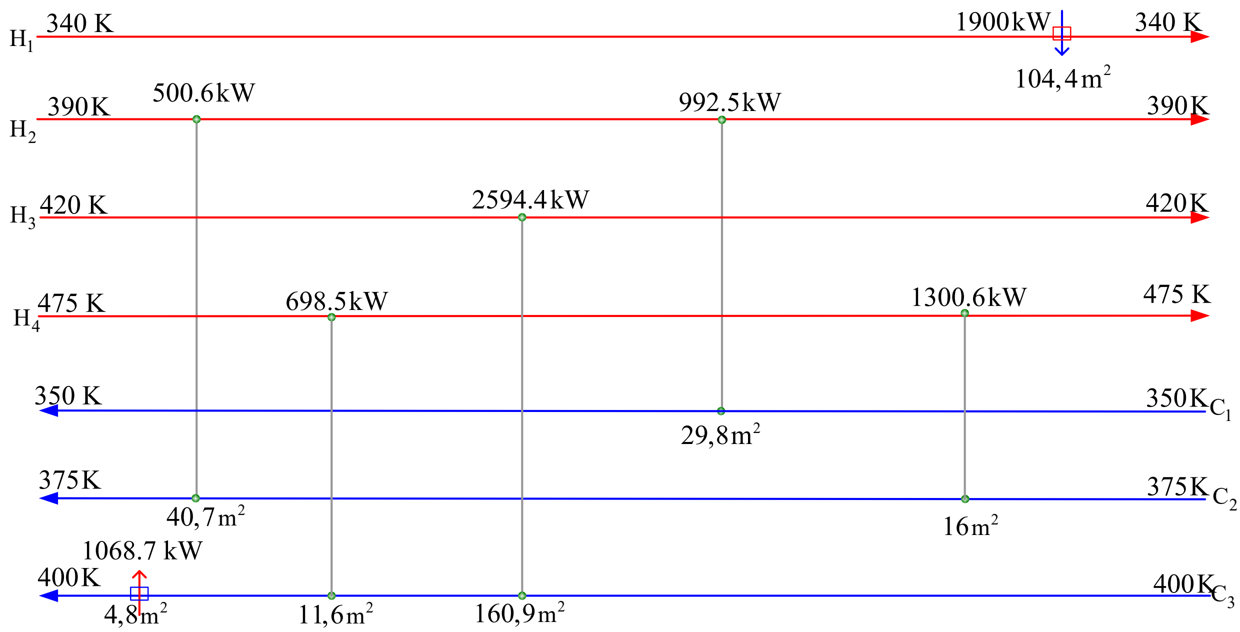

Figure 18 HEN diagram obtained by SYNHEAT (DICOPT/BARON) for Example 4

Comparison the obtained results are presented in Table 14.

Table 14 Results of the SSHEN and SYNHEAT Methods for Example 4

Name	SSHEN	DICOPT/BARON
Q^{he}, (kW)	6,086.6	6,086.6
Q^{hr}, (kW)	1,068.7	1,068.7
Q^{cr}, (kW)	1,900	1,900
n^{he}	5	5
n^{hr}	1	1
n^{cr}	1	1
E_{sum}, USD/year	125,870	125,870
K_{sum}, USD/year	30,467.2	30,438.4
A^{he}. M^2	216.2	215.8
A^{cr}, m^2	104.4	104.4
A^{hr}, m^2	4.7	4.7
Φ, USD/year	156,337.2	156,308.4
CPU time, (s)	6.5	0.2/112,464

As can be seen from Table 14, the results obtained are the same for two different synthesized structures. This phenomenon is most likely due to the isothermal conditions of the cold and hot streams.

3.6 Additional test problems

The proposed SSHEN method was tested on two problems studied by Ravagnani et al. (2005) and five problems studied by Escobar and Trierweiler (2013). The output generated by SSHEN was compared with the results published in these papers. The data are summarized in Appendix 1 and Appendix 2, respectively.

The number of hot streams ranges between 2 and 22 hot streams, and the cold streams between 2 and 17. As can be seen from tables A1-A3, the proposed method for five tasks yields cheaper and closer solutions, and higher cost for two other cases (CS03, CS05). The proposed SSHEN method solves these problems in a reasonable amount of time.

CONCLUSION

Synthesis methods for optimal heat exchanger networks based on superstructure optimization offer a general systematic approach. These problems result from the fact that the global flowsheet embeds all the possible alternatives for the heat exchanger configurations. The use of the BARON global optimization algorithm ensures the global optimum within the selected superstructure, although often at very high computational cost. The SSHEN method addresses the computational challenges of large scale HENS by reducing the problem to a sequence of assignment problems. In this case, the optimization problem can be solved for a number of fixed structure heat exchanger networks.

The SSHEN method has the advantage of extending the search area by splitting the streams and expanding the number of optimization variables. The basic procedure of HEN synthesis by the SSHEN method involves decomposing the problem into a sequence of assignment problems. To apply this procedure, it is necessary to estimate the optimal economic estimations of the possible heat exchanges between the hot and cold process streams. Therefore, the superstructure is decomposed into the elementary heat exchange units.

Computational results on four examples showed that the difference in the solutions found using the proposed method of schemes do not exceed an average of 10 percent of the optimal values obtained using SYNHEAT (BARON). At the same time, the time to solve the problems using the proposed method is several orders of magnitude smaller than the time spent by the BARON method. Additional results were presented in the Appendix to demonstrate the capabilities (good quality of solution, reduced CPU time) of the proposed SSHEN method.

ACKNOWLEDGEMENT

The research at Kazan National Research Technological University was supported by the Ministry of Science and Higher Education of the Russian

Federation grant “Energy and Resource-Saving Processes for Separation of Liquid Mixtures for the Separation of Industrial Solvents”.

SYMBOLS

A–heat exchange surface area, m^2;

B–outlet heater;

K–outlet cooler;

c–specific heat capacity at constant pressure, kW·h/kg·K;

E– heat exchanger;

E_{sum}–energy cost, USD/year

F–mass flow rate, kg/hour;

f–total reduced capital and operating costs, USD/year;

H–enthalpy, kW;

K_{sum}–annualized capital cost, USD/year

альфа

$\hat{m}_1$ –reduced price ratios of capital costs, USD/year;

$\hat{m}_2$ –reduced price ratios of capital costs, USD/year·m^2;

$\tilde{m}$ –unit cost for hot or cold heat carrier consumption, USD/kg;

T–stream temperature, K;

t – computational time of the case study, s

TAG–Total Annual Cost, USD/year

U– Total heat transfer coefficient, kW·h/m^2·K;

Q–heat quantity, kW;

ΔT_{min}–minimum allowed temperature difference, K;

r–specific heat of evaporation, kW·h/kg·K;

γ–correlation coefficient;

Φ–total sum of reduced capital and operating costs for heat exchanger network, USD/ year;

$Z^{(k)}$ –total sum of coupled branches with their HEN elementary units belonging to the HEN structure at current iteration.

INDICES

c–cold stream;

h–hot stream;

hu–heating steam;

cu–cooling water;

aut – autonomous heat exchange;

he–recuperative heat exchanger;

cr–cooler / condenser;

hr–heater/ boiler;

i–hot stream number;

j–cold stream number;

l –branch stream;

k–iteration number.

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Appendix 1. SSHEN comparison with other available methods

Table A1. Comparison of the SSHEN method with the methods by Frausto-Hernarndez et al. (2003), and Ravagnani et al. (2005). The case study dimension is 2H x 2C.

Name	**Frausto-Hernarndez et al. (2003)**	**Ravagnani et al. (2005)**	**SSHEN t(s)=2.4**
Hot utility (kW)	605.00	200.00	420
Cold utility (kW)	525.00	120.32	340
Total area (m^2)	423.26	706.45	577.4
Energy cost ($/year)	71800.00	23203.20	49600
Capital cost ($/year)	75553.75	93866.14	79204
Total cost ($/year)	**147353.75**	**117069.34**	**128804**

Table A2 Comparison of the SSHEN method with the methods by Ahmad (1985), and Ravagnani et al. (2005). The case study dimension is 6H x 4C

Name	**Ahmad (1985)**	**Ravagnani et al (2005)**	**SSHEN t(s)=7.2**
Hot utility (kW)	15400	20529.3	20759
Cold utility (kW)	9796	14923.8	15204
Total area (m^2)	–	56600.6	60712

Energy cost ($/y)	1686940	2276787	2303980
Capital cost ($/y)	5387060	3396034	3661944
Total cost ($/y)	**7074000**	**5672821**	**5965924**

Appendix 2. The results obtained by Escobar & Trierweiler (2013) for five case studies are complemented with the results obtained by SSHEN.

Table A3. Computational time and TAC for the MINLP solvers for each case study[b].

Problem	Case study	CS01	CS02	CS03	CS04	CS05
	Dimension	2Hx2C	5Hx5C	8Hx7C	13Hx7C	22Hx17C
	Solver	t(s)	t(s)	t(s)	t(s)	t(s)
P4	DICOPT	0.42	1.02	3.42	12.5	18.4
	SBB	2.70	6.98	17.5	18.2	25.1
	BARON	101.2	120.8	249.4	400.6	[a]
	OQNLP	7.22	182.3	221.8	[a]	[a]
P5	DICOPT	0.63	0.72	3.38	10.3	12.4
	SBB	0.17	2.35	2.46	50.0	71.8
	BARON	119.6	178.5	218.5	358.7	[a]
	OQNLP	80.1	15.2	47.6	327.2	[a]
AP	SSHEN	0.72	5.32	6.2	16.44	21.2
	Solver	TAC	TAC	TAC	TAC	TAC
		($ yr^{-1})	($$yr^{-1}$)	($$yr^{-1}$)	($$yr^{-1}$)	($$yr^{-1}$)
P4	DICOPT	368649.0	43705	1574948	1518187	2197653
	SBB	361982.8	43705	1769655	1758489	2197653
	BARON	362429.7	43242	1574948	1589810	[a]
	OQNLP	362459.9	43708	1594011	[a]	[a]
P5	DICOPT	399509.7	43570	1507654	1461006	2055421
	SBB	366006.7	43685	1506667	1467675	2055421
	BARON	377541.3	43689	1506667	1461276	[a]
	OQNLP	399509.8	43689	1518149	1467503	[a]
AP	SSHEN	290597.2[c]	43833	1891641	1519576	2223113

[a] Failed to converge; BARION within time limit (180000s)
[b] The table is borrowed from paper of Escobar and Trierweiler (2013) and supplemented by the results obtained using SSHEN.
[c] Problem was solved with data presented in the paper of Escobar and Trierweiler (2013). Discrepancy may be due to errors in the data presented in that paper.
P4: MINLP problem, Ciric & Floudas (1991).
P5: MINLP problem, Yee & Grossmann (1990).
AP: Assignment problem, Kobayashi S., Umeda T., & Ichikawa A. (1971).

Appendix 3. Step-by-step solution of Example 1

Step 1. Set the initial approximations for the branch coefficients:

$$L_i = 2, \quad L_j = 2, \quad i = 1,2, \quad j = 1,2;$$

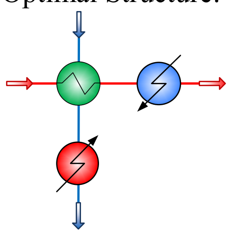
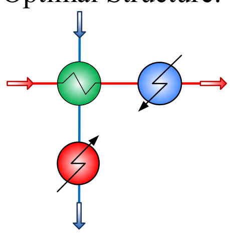
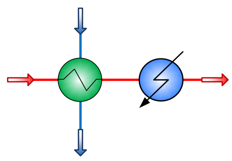
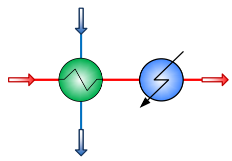
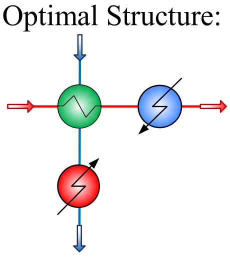
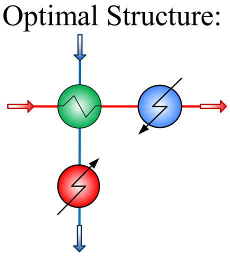
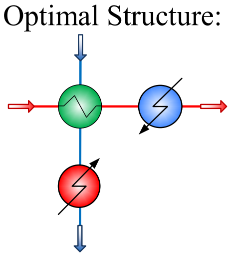
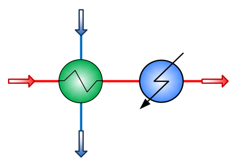
$$\beta_{1_1}^{\mathrm{h},(0)} = 0.55, \qquad \beta_{1_2}^{\mathrm{h},(0)} = 0.95;$$

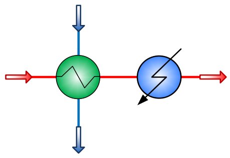
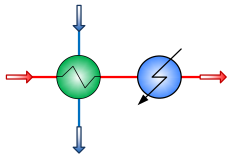
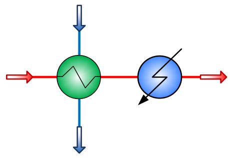
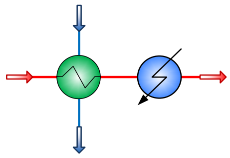
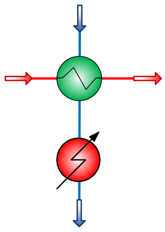
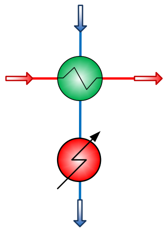
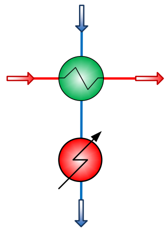
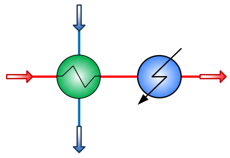
$$\beta_{1_1}^{\mathrm{c},(0)} = 0.55, \qquad \beta_{1_2}^{\mathrm{c},(0)} = 0.85;$$

$$\beta_{2_1}^{\mathrm{h},(0)} = 1 - \sum_{l_1=1}^{L_1^{\mathrm{h}}-1} \beta_{l_1}^{\mathrm{h},(0)} = 0.45, \qquad \beta_{2_2}^{\mathrm{h},(0)} = 1 - \sum_{l_2=1}^{L_2^{\mathrm{h}}-1} \beta_{l_2}^{\mathrm{h},(0)} = 0.05;$$

$$\beta_{2_1}^{\mathrm{c},(0)} = 1 - \sum_{l_1=1}^{L_1^{\mathrm{c}}-1} \beta_{l_1}^{\mathrm{c},(0)} = 0.45, \qquad \beta_{2_2}^{\mathrm{c},(0)} = 1 - \sum_{l_2=1}^{L_2^{\mathrm{c}}-1} \beta_{l_2}^{\mathrm{c},(0)} = 0.15;$$

Step 2. Solve the 4×4 nonlinear mathematical programming problems (5)-(13) for every HEN elementary unit. Optimization algorithm: SQP. Results:

Stream	C_1, 1st branch $\Delta H_{1_1}^{\mathrm{c},(1)} = 2200\,\mathrm{kW}$	C_1, 2nd branch $\Delta H_{2_1}^{\mathrm{c},(1)} = 2,200\,\mathrm{kW}$	C_2, 1st branch $\Delta H_{1_2}^{\mathrm{c},(1)} = 765\,\mathrm{kW}$	C_2, 2nd branch $\Delta H_{2_2}^{\mathrm{c},(1)} = 135\,\mathrm{kW}$
H_1, 1st branch $\Delta H_{1_1}^{\mathrm{h},(1)} = 1,100\,\mathrm{kW}$	Optimal Structure:  $f_{1_1,1_1}^{\mathrm{opt},(1)} = 202,143.3$ $Q_{1_1,1_1}^{\mathrm{he},(1)} = 330\,\mathrm{kW}$ $Q_{1_1}^{\mathrm{cr},(1)} = 770\mathrm{kW}$ $Q_{1_1}^{\mathrm{hr},(1)} = 1,870\mathrm{kW}$	Optimal Structure:  $f_{1_1,2_1}^{\mathrm{opt},(1)} = 161,923.8$ $Q_{1_1,2_1}^{\mathrm{he},(1)} = 330\,\mathrm{kW}$ $Q_{1_1}^{\mathrm{cr},(1)} = 770\mathrm{kW}$ $Q_{2_1}^{\mathrm{hr},(1)} = 1,470\mathrm{kW}$	Optimal Structure:  $f_{1_1,1_2}^{\mathrm{opt},(1)} = 12,903$ $Q_{1_1,1_2}^{\mathrm{he},(1)} = 765\,\mathrm{kW}$ $Q_{1_1}^{\mathrm{cr},(1)} = 335\mathrm{kW}$ $Q_{1_2}^{\mathrm{hr},(1)} = 0\mathrm{kW}$	Optimal Structure:  $f_{1_1,2_2}^{\mathrm{opt},(1)} = 13,398.8$ $Q_{1_1,2_2}^{\mathrm{he},(1)} = 135\,\mathrm{kW}$ $Q_{1_1}^{\mathrm{cr},(1)} = 965\mathrm{kW}$ $Q_{2_2}^{\mathrm{hr},(1)} = 0\mathrm{kW}$
H_1, 2nd branch $\Delta H_{2_1}^{\mathrm{h},(1)} = 900\,\mathrm{kW}$	Optimal Structure:  $f_{2_1,1_1}^{\mathrm{opt},(1)} = 206,050.6$ $Q_{2_1,1_1}^{\mathrm{he},(1)} = 270\,\mathrm{kW}$ $Q_{2_1}^{\mathrm{cr},(1)} = 630\mathrm{kW}$ $Q_{1_1}^{\mathrm{hr},(1)} = 1,930\mathrm{kW}$	Optimal Structure:  $f_{2_1,2_1}^{\mathrm{opt},(1)} = 165,833.1$ $Q_{2_1,2_1}^{\mathrm{he},(1)} = 270\,\mathrm{kW}$ $Q_{2_1}^{\mathrm{cr},(1)} = 630\mathrm{kW}$ $Q_{2_1}^{\mathrm{hr},(1)} = 1,530\mathrm{kW}$	Optimal Structure:  $f_{2_1,1_2}^{\mathrm{opt},(1)} = 23,894$ $Q_{2_1,1_2}^{\mathrm{he},(1)} = 630\,\mathrm{kW}$ $Q_{2_1}^{\mathrm{cr},(1)} = 270\mathrm{kW}$ $Q_{1_2}^{\mathrm{hr},(1)} = 135\mathrm{kW}$	Optimal Structure:  $f_{2_1,2_2}^{\mathrm{opt},(1)} = 11,103.4$ $Q_{2_1,2_2}^{\mathrm{he},(1)} = 135\,\mathrm{kW}$ $Q_{2_1}^{\mathrm{cr},(1)} = 765\mathrm{kW}$ $Q_{2_2}^{\mathrm{hr},(1)} = 0\mathrm{kW}$

Stream	C_1, 1st branch $\Delta H^{\mathrm{c},(1)}_{1_1} = 2200\,\mathrm{kW}$	C_1, 2nd branch $\Delta H^{\mathrm{c},(1)}_{2_1} = 2,200\,\mathrm{kW}$	C_2, 1st branch $\Delta H^{\mathrm{c},(1)}_{1_2} = 765\,\mathrm{kW}$	C_2, 2nd branch $\Delta H^{\mathrm{c},(1)}_{2_2} = 135\,\mathrm{kW}$
H_2, 1st branch $\Delta H^{\mathrm{h},(1)}_{1_2} = 2,850\,\mathrm{kW}$	Optimal Structure:  $f^{\mathrm{opt},(1)}_{1_2,1_1} = 18,898.8$ $Q^{\mathrm{he},(1)}_{1_2,1_1} = 2,200\,\mathrm{kW}$ $Q^{\mathrm{cr},(1)}_{1_2} = 650\,\mathrm{kW}$ $Q^{\mathrm{hr},(1)}_{1_1} = 0\mathrm{kW}$	Optimal Structure:  $f^{\mathrm{opt},(1)}_{1_2,2_1} = 22,103.8$ $Q^{\mathrm{he},(1)}_{1_2,2_1} = 1,800\,\mathrm{kW}$ $Q^{\mathrm{cr},(1)}_{1_2} = 650\mathrm{kW}$ $Q^{\mathrm{hr},(1)}_{2_1} = 0\mathrm{kW}$	Optimal Structure:  $f^{\mathrm{opt},(1)}_{1_2,1_2} = 29,165.3$ $Q^{\mathrm{he},(1)}_{1_2,1_2} = 765\,\mathrm{kW}$ $Q^{\mathrm{cr},(1)}_{1_2} = 2,085\mathrm{kW}$ $Q^{\mathrm{hr},(1)}_{1_2} = 0\,\mathrm{kW}$	Optimal Structure:  $f^{\mathrm{opt},(1)}_{1_2,2_2} = 32,671.6$ $Q^{\mathrm{he},(1)}_{1_2,2_2} = 135\,\mathrm{kW}$ $Q^{\mathrm{cr},(1)}_{1_2} = 2,715\mathrm{kW}$ $Q^{\mathrm{hr},(1)}_{2_2} = 0\,\mathrm{kW}$
H_2, 2nd branch $\Delta H^{\mathrm{h},(1)}_{2_2} = 150\,\mathrm{kW}$	Optimal Structure:  $f^{\mathrm{opt},(1)}_{2_2,1_1} = 208,493.5$ $Q^{\mathrm{he},(1)}_{2_2,1_1} = 150\,\mathrm{kW}$ $Q^{\mathrm{cr},(1)}_{2_2} = 0\mathrm{kW}$ $Q^{\mathrm{hr},(1)}_{1_1} = 2,050\mathrm{kW}$	Optimal Structure:  $f^{\mathrm{opt},(1)}_{2_2,2_1} = 168,279.9$ $Q^{\mathrm{he},(1)}_{2_2,2_1} = 150\,\mathrm{kW}$ $Q^{\mathrm{cr},(1)}_{2_2} = 0\,\mathrm{kW}$ $Q^{\mathrm{hr},(1)}_{2_1} = 1,650\mathrm{kW}$	Optimal Structure:  $f^{\mathrm{opt},(1)}_{2_2,1_2} = 63,308.9$ $Q^{\mathrm{he},(1)}_{2_2,1_2} = 150\,\mathrm{kW}$ $Q^{\mathrm{cr},(1)}_{2_2} = 0\mathrm{kW}$ $Q^{\mathrm{hr},(1)}_{1_2} = 615\mathrm{kW}$	Optimal Structure:  $f^{\mathrm{opt},(1)}_{2_2,2_2} = 1,925.1$ $Q^{\mathrm{he},(1)}_{2_2,2_2} = 135\,\mathrm{kW}$ $Q^{\mathrm{cr},(1)}_{2_2} = 15\mathrm{kW}$ $Q^{\mathrm{hr},(1)}_{2_2} = 0\mathrm{kW}$

Step 3. Solve the assignment problem in (14). As a result, the optimal HEN structure is determined for the fixed values of the stream branch fractions. Optimization algorithm: Hungarian algorithm.

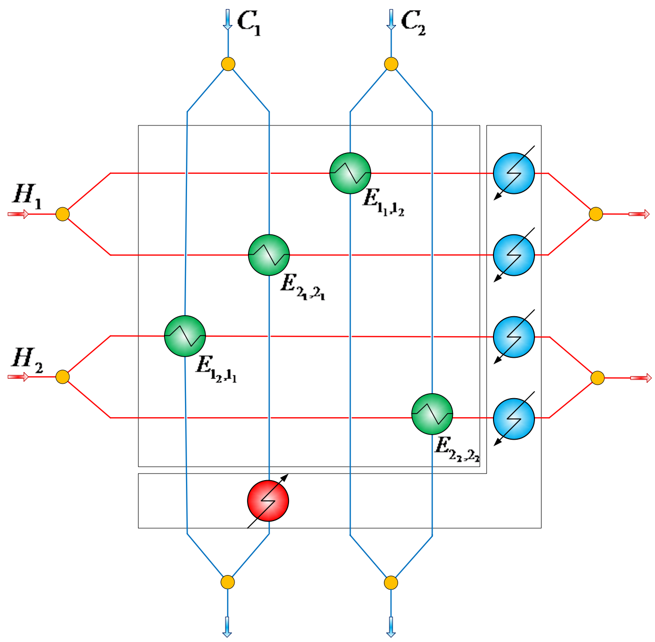
Result:

Stream	C_1, 1st branch	C_1, 2nd branch	C_2, 1st branch	C_2, 2nd branch
H_1, 1st branch	0	0	1	0
H_1, 2nd branch	0	1	0	0
H_2, 1st branch	1	0	0	0
H_2, 2nd branch	0	0	0	1

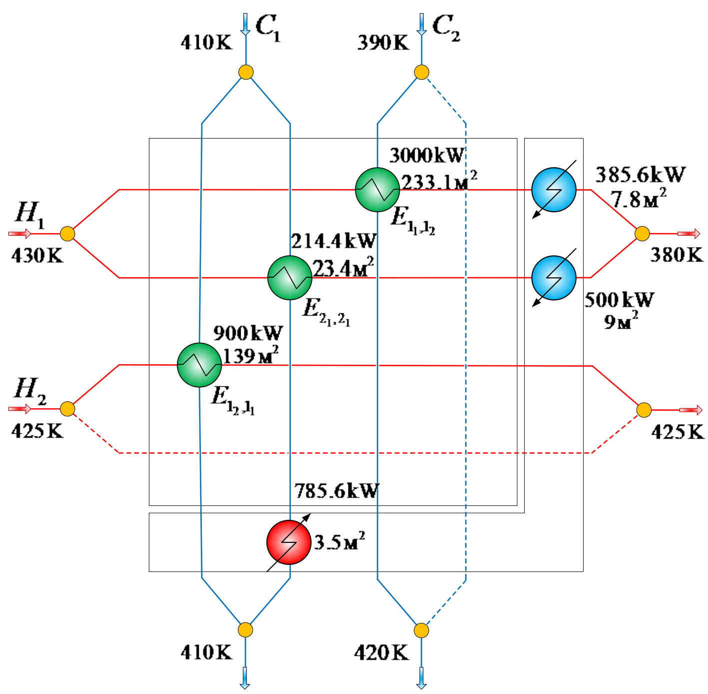
Criterion Value: 199,560.9

$\Phi^{(0)} = 199,560.9$

Optimal HEN structure:



Step 4. Find the optimal operating conditions for the HEN with a fixed structure by solving a nonlinear mathematical modeling problem in (16) – (23). Optimization algorithm: SQP. Results:



$\Phi^{(1)} = 116{,}874$

Optimal values of optimization variables:

$\beta_{1_1}^{h,(1)} = 0.643, \qquad \beta_{1_2}^{h,(1)} = 1.0;$

$\beta_{1_1}^{c,(1)} = 0.75, \qquad \beta_{1_2}^{c,(1)} = 1.0;$

$\beta_{2_1}^{h,(1)} = 0.357, \qquad \beta_{2_2}^{h,(1)} = 0;$

$\beta_{2_1}^{c,(1)} = 0.25, \qquad \beta_{2_2}^{c,(1)} = 0.$

Step 5. $\left|\Phi^{(1)} - \Phi^{(0)}\right| = \left|116{,}874 - 199{,}560.9\right| > 0.001$. Go to ***Step 2***. *k*=2.

At the second iteration, the value of the optimization criterion remains the same $\Phi^{(2)} = 116{,}874$. Calculation finished.

Appendix 4. Step-by-step results of Optimal HEN Synthesis using the SSHEN (Example 2)

Iteration Number	Q_{sum}^{he} kW	Q_{sum}^{hr} kW	Q_{sum}^{cr} kW	*Φ*, USD/year	n^{he}	n^{hr}	n^{col}
1	56,186	5,911.3	2,651.9	814,571.3	8	3	2
2	56,185	5,912.1	2,652.7	810,153.3	7	3	2
3	56,187	5,910.4	2,650.3	803,501.5	6	3	2
4	56,187	5,910	2,650.6	798,793.8	5	3	2
5	56,841.2	5,256.2	1,996.8	712,474.5	5	3	2
6	56,841.2	5,256.2	1,996.8	712,474.5	5	3	2

Appendix 5. Optimal heat exchanger network synthesis: A case study comparison (Escobar, M., & Trierweiler, J.O. (2013))

	Case study	CS01 ΔT_{min}=10 °C	CS01 ΔT_{min}=20 °C
	Solver	t(s)	t(s)
(P4)	DICOPT	**0.42**	**0.42**
	SBB	2.70	2.70
	BARON	101.2	101.2
	OQNLP	7.22	7.22
(P5)	DICOPT	0.63	0.63
	SBB	**0.17**	**0.17**
	BARON	119.6	119.6
	OQNLP	80.1	80.1

		t_i(s)	t_i(s)
(P4)		0.11	0.11
(P5)		0.78	0.78
AP	SSHEN	0.72	0.64
	Solver	TAC	TAC
		(\$ yr^{-1})	(\$ yr^{-1})
(P4)	DICOPT	368649.0	368649.0
	SBB	**361982.8**	**361982.8**
	BARON	362429.7	362429.7
	OQNLP	362459.9	362459.9
(P5)	DICOPT	399509.7	399509.7
	SBB	**366006.7**	**366006.7**
	BARON	377541.3	377541.3
	OQNLP	399509.8	399509.8
AP	SSHEN	290597.2	342000.4

We observe that in article Escobar and Trierweiler (2013), for the example of CS01, it is very likely that incorrect data for film heat transfer coefficients are reported.