Extending the Exergy–Pinch Methodology: A Multi-Layer HEN Optimization Framework

Sali EL SAYED[a], Hayato HAGI[b], Baptiste SAMAIN[b], Assaad ZOUGHAIB[a]

[a]*CEEP, Mines Paris, PSL University, Versailles, France*

[b]*TotalEnergies OneTech, TotalEnergies Research & Technology Gonfreville, P27 76700 Harfleur, France*

Abstract:

Traditional methodologies for heat exchanger network (HEN) synthesis are typically based on a sequential approach, where pinch analysis is first used to determine heat recovery targets and heat pump placement, followed by HEN synthesis using computational techniques. These approaches rely on fixed assumptions such as the minimum temperature difference ($\Delta \boldsymbol{T_{min}}$) and treat heat integration, heat pump design, and network synthesis independently, often leading to suboptimal configurations. This work proposes a multi-layer optimization framework for HEN synthesis, extending the Exergy-Pinch methodology by integrating pinch analysis, exergy analysis, and mixed-integer linear programming (MILP)-based network synthesis within a unified structure. The proposed approach enables the simultaneous and iterative optimization of heat exchanger matches, network structure, and thermodynamic conversion systems, while incorporating additional degrees of freedom such as refined temperature discretization and constrained stream matching. The methodology is demonstrated on an illustrative example and compared against a traditional approach based on the MILP transshipment formulation of Barbaro and Bagajewicz. The results show that the traditional method may lead to inconsistent designs, where the heat pump is no longer optimally integrated within the HEN, and in some cases is entirely replaced by conventional utilities. In contrast, the proposed framework ensures consistent and optimal integration, resulting in more structured, flexible, and practically implementable network configurations.

Keywords:

Heat exchanger network synthesis, Exergy-Pinch analysis, Heat pump integration, MILP.

1. Introduction

The industrial sector is responsible for 24% of the global greenhouse gas (GHG) emissions[1]. To address climate change and support the transition towards a more sustainable future, increasing attention has been directed toward the decarbonization of industrial heat. The electrification of industrial processes is becoming viable due to declining costs of low-carbon electricity and the rapid decarbonization of power systems. Heat pumps (HP) can be integrated into both new and existing industrial operations, enabling decarbonization through electrification while improving process energy efficiency. In particular, high-temperature heat pumps (HTHPs) are emerging as a key technology for industrial processes. These systems can provide process heat while recovering excess heat from various sources, including exhaust gases, condensate, and process streams. HTHPs are typically defined as heat pumps delivering heat above 100 °C and up to around 200 °C, although higher temperatures are also achievable. However, their level of technological maturity varies significantly across temperature ranges [2].

Numerous studies have investigated the performance of different high-temperature heat pump (HTHP) configurations, as well as their integration across various industrial sectors. Among these, Andersen et al. developed a comprehensive technology portfolio, evaluating 16 working fluids across 10 heat pump cycle configurations under 1124 high-temperature operating conditions, with source temperatures ranging from 0 °C to 100 °C and temperature lifts between 20 K and 150 K. The study also proposed an approximation of COP, enabling the identification of suitable working fluids and heat pump configurations across a wide range of operating conditions. The aforementioned studies, along with various others in the literature, provide valuable insight into HTHP cycles, refrigerant selection, and potentially promising results. However, the deployment of

HTHPs remains hindered due to the difficulty in industrial process integration. In many cases, industries struggle to identify the heat requirements of the industry, the optimal position of the HTHP, and their conditions. Consequently, the implementation of commercially available heat pumps is still limited, despite their availability and abundance in the market.

Traditionally, pinch analysis was used to identify the opportunities for placing the heat pump through the Grand Composite Curve (GCC). The GCC represents the minimum heating and cooling requirements and identifies the pinch temperature. Based on this, it can effectively identify the suitable temperatures in which the heat pump is placed within a heat exchanger network (HEN). One of the many studies in the literature, Schlosser et al. [3], provided a comprehensive review of heat pump integration using the GCC to identify appropriate source and sink locations. The study evaluated the conventional electrical closed vapor-compression cycle heat pumps (CCC_{el}), CO_2 heat pumps, 2-staged CCC_{el}, and mechanical vapor recompression heat pumps across various sectors, such as food processing, pulp and paper, and chemicals. However, relying solely on pinch analysis to guide heat pump integration is not sufficient. During HEN optimization, key design parameters such as the minimum temperature difference (ΔT_{min}) are often adjusted to balance energy costs and investment costs. These changes lead to shifts in the composite curves and, consequently, alter the optimal placement and operating conditions of the heat pump.

To better illustrate this gap, the following simple example is considered. A system composed of one hot stream, cooled from 65°C to 10°C with 200kW duty, and one cold stream, heated from 20°C to 70°C with 141.4kW duty. Pinch analysis is applied at three different ΔT_{min} (5,10,15), and the following grand composite curves (GCC) are obtained in Figure 1.

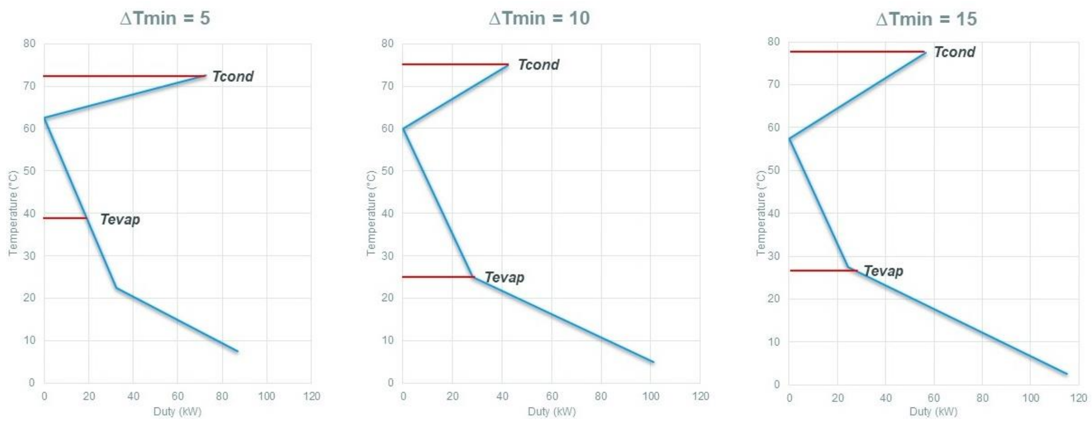

Figure 1: *GCCs at three different* ΔT_{min} .

The optimal placement of the heat pump is illustrated by the red lines on the GCCs in Figure 1. These were obtained using exergy-based optimization. It can be observed that the optimal position (evaporator and condenser temperature) varies with ΔT_{min} . As ΔT_{min} increases from 5 to 15 °C, internal heat recovery is reduced, leading to a greater reliance on the heat pump and consequently an increase in its required capacity. Each ΔT_{min} gives one unique solution, which defines a specific HEN with a fixed number of heat exchangers, a given heat transfer area, and an associated heat pump cost. However, this solution is not flexible from a design perspective. Once the HEN is synthesized, its structure and sizing are essentially fixed under the chosen ΔT_{min} .

In practice, during HEN design, ΔT_{min} is often adjusted to balance capital and operating costs. Increasing ΔT_{min} reduces the required heat exchanger area and investment cost, but at the expense of heat pump performance, leading to higher electricity consumption and lower COP with the increasing temperature lifts. This creates a fundamental trade-off between capital expenditure, operating costs, HEN complexity, and practical constraints. Conventional pinch-based approaches provide only a single solution for a fixed ΔT_{min} and therefore fail to capture this trade-off space. Consequently, a more flexible methodology is required. In particular, a multi-layer optimization framework is needed, in which HEN synthesis is performed iteratively with additional degrees of freedom, enabling key parameters to vary and allowing the exploration of multiple feasible solutions rather than a single fixed design.

In addition to the previously identified limitation, pinch analysis remains limited to thermal flows only. It can't ensure the practical and thermodynamic feasibility of the proposed heat integration. Pinch analysis overlooks other important aspects of process operation, including dynamic behavior, economic optimization, the integration of multiple heat pumps, and the presence of unreliable waste heat sources. In particular, pinch analysis does not account for the quality of energy or the conversion between different energy forms. This limitation becomes critical when integrating heat pumps or electrified heating systems, as these introduce electrical energy consumption into the heat recovery problem. To address this, researchers have developed a methodology combining exergy and pinch analysis. This methodology overcomes the main drawback of both techniques. Pinch analysis is unable to identify ways to utilize or valorize available excess energy within the process to further improve performance. Whereas the exergy analysis, which can indicate where improvements are possible but not whether they are practically feasible, should be complemented to become a design tool. Therefore, combining both methods enables their use as an effective design tool. Early work by Becker et al.[4] combined pinch and exergy analysis to identify optimal heat pump integration points using exergy-based composite curves. Building on this, Gourmelon et al. [5] developed the COOPERE methodology, which integrates optimization, pinch, and exergy analysis to improve industrial energy efficiency through process retrofitting and structural modifications. Similarly, Bou Malham et al.[6] proposed a systematic optimization framework combining process simulation with Exergy–Pinch analysis, enabling the identification of key operating variables and structural improvements, resulting in reduced utility demand and exergy destruction.

Beyond improvements in heat integration methodologies, several works have focused on HEN synthesis using a step-wise iterative approach with multilayer optimization. Early works by Papoulias and Grossmann [7] introduced a linear programming (LP) transshipment model to minimize utilities and a mixed-integer linear programming (MILP) transshipment model for HEN synthesis with a minimal number of heat exchangers. Based on this, Floudas et al. [8] developed a superstructure and a non-linear programming (NLP) model that minimizes the investment costs. Subsequent research has focused on improving accuracy, flexibility, and computational efficiency. Liu et al. [9] enabled intermediate utility placement using a genetic algorithm, and Nair & Karimi [10] designed a superstructure capable of modeling repeated matches, bypasses, and crossflows. In addition, Chen et al. [11] examined several strategies to solve large-scale complex transshipment MILP problems.

These advancements show a clear progression toward more intricate frameworks. However, important limitations remain. As previously demonstrated in the illustrative example, separating heat integration from process design, utility selection, and heat pump integration introduces inherent bias due to the assumptions embedded in pinch analysis. This is because economic targets, such as the minimum temperature difference, influence the pinch temperature and consequently the network structure. As a result, certain heat exchanger matches may be prematurely discarded, leading to designs that are not optimal when considering overall energy performance. Moreover, heat pumps optimized based on these initial assumptions may no longer be compatible with the final synthesized HEN. In addition, these approaches can be computationally heavy, particularly when large MILP problems are solved repeatedly. This can significantly increase computation time and limit their use for complex industrial systems.

This work extends the Exergy-Pinch methodology [12] to include a multi-layer HEN optimization framework. The proposed methodology integrates process integration, stream match selection, and detailed heat exchanger design within a unified framework. This ensures the simultaneous optimization of thermodynamic performance, process constraints, and equipment design. The integration of a heat pump model library allows for a more realistic representation of thermodynamic conversion systems, while industrial and design constraints are explicitly accounted for within the optimization framework, ensuring practical and economically feasible solutions.

2. Methodology

The following subsection describes the traditional approach based on pinch analysis combined with heat HEN synthesis, and illustrates the proposed methodology. The results of both approaches are compared in the subsequent sections.

2.1. Traditional Methodology

The traditional methodology utilizes the GCC to identify the optimal location for heat pump integration, followed by the synthesis of the corresponding heat exchanger network. Figure 2 illustrates the workflow of the traditional methodology.

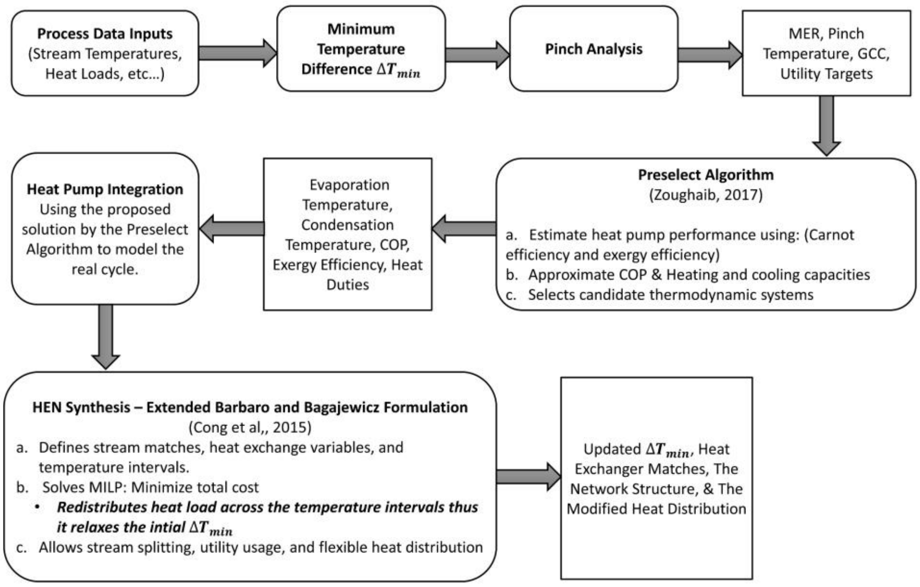

***Figure 2**: Traditional Methodology Workflow*

Pinch analysis is first applied using the Linnhoff and Flower problem table algorithm to determine the pinch temperature and the minimum energy requirements (MER) for a specified minimum temperature difference ΔT_{min} . Based on this, GCC is constructed from process stream data (temperatures and heat loads) to represent the cumulative heat source and sink profiles. From the GCC, the pinch temperature and the corresponding utility requirements at different temperature levels can be identified. The shape of the GCC and the location of the pinch directly determine both the placement and the operating conditions of the heat pump. Low-grade heat is recovered from below the pinch and upgraded by the heat pump to supply heat above the pinch. For many industrial processes, characteristic GCC profiles can therefore be used to identify suitable heat pump integration strategies, as illustrated in the introduction.

In the traditional methodology, the operating conditions of the heat pump are determined using a preselection algorithm based on the GCC, as described in [13]. This tool aims to identify suitable thermodynamic utilities by analyzing the GCC of the process and minimizing exergy destruction. A limited number of candidate thermodynamic systems are preselected, including heat pumps and other utilities. Each system is defined by fixed operating temperature levels and characterized by its performance, such as the COP or exergy efficiency.

The placement and operating conditions of the heat pump are therefore selected a priori using this preselection tool. The next step is the synthesis of the heat exchanger network (HEN). The HEN design must satisfy the fundamental pinch constraints: (1) no hot utilities are used below the pinch temperature, (2) no cold utilities are used above the pinch temperature, and (3) no heat is transferred from hot streams above the pinch to cold streams below the pinch. To facilitate the synthesis, particularly for large-scale problems, numerous computational methods have been developed, as discussed in the introduction.

Among these, the extended Barbaro and Bagajewicz formulation is selected as a representative approach and used as a benchmark for comparison with the proposed methodology. The formulation proposed by Barbaro [14] enables the cost-optimal design of heat exchanger networks in a single step, without relying on traditional sequential procedures such as nonlinear superstructure-based formulations [14]. In addition, it accounts for key design features such as stream splitting, non-isothermal mixing, and the explicit consideration of heat exchanger units. This formulation has been further extended in [15] to enhance its applicability to real industrial systems by accounting for the flexibility through determining the optimal outlet temperature of such streams simultaneously with the HEN design.

During the HEN synthesis, the ΔTmin is altered as the model redistributes heat loads to minimize cost. This directly impacts the utility requirements and resizes the heat pump within the network. As a result, the heat pump operating conditions selected a priori are no longer optimal and may become incompatible with the synthesized HEN. Consequently, multiple iterations are required, in which the ΔTmin and heat pump operating conditions are repeatedly updated based on the results of the HEN synthesis.

2.2. Proposed Methodology

2.2.1. General Workflow

The proposed methodology is implemented within a Python-based framework and is structured around three iterative feedback loops, as illustrated in Figure 3.

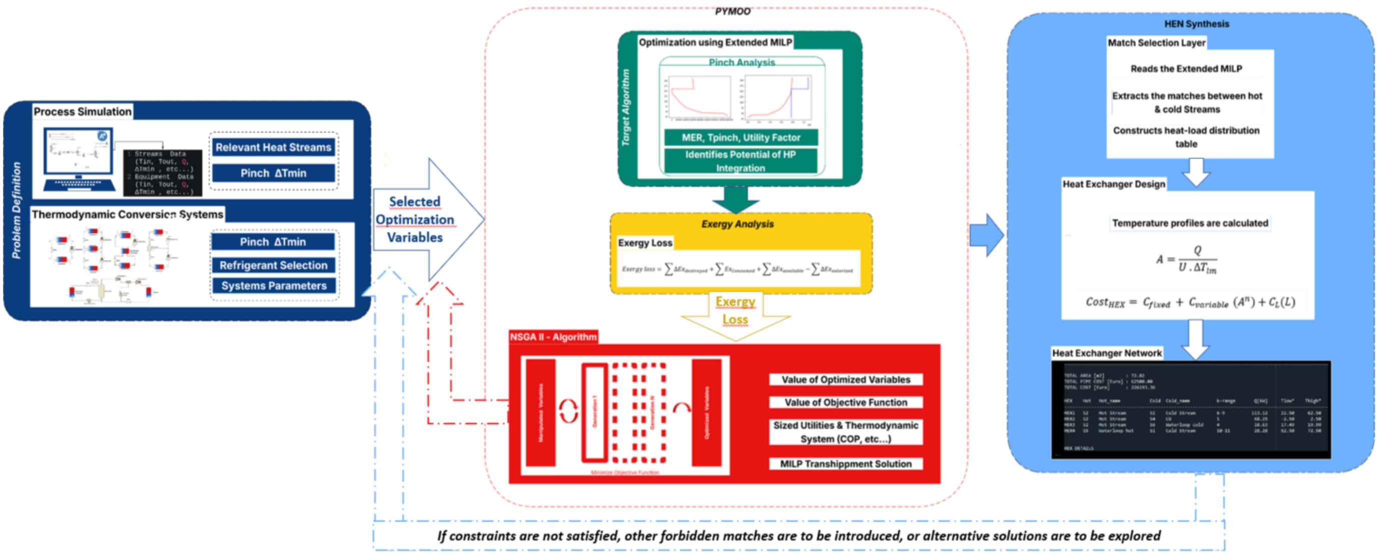

Figure 3: *Extended Exergy-Pinch Methodology Workflow*

The framework follows a multi-layer optimization approach and consists of four interconnected layers: Problem Definition, Process Integration, Match Selection, and Detailed Heat Exchanger Design.

a. Problem Definition

The methodology starts by collecting detailed process data, either directly from simulation software using a Python-based interface or via manual input. This includes all relevant equipment and stream information, particularly temperatures and heat duties. Suitable thermodynamic conversion systems are then selected from the Thermodynamic Systems Library (TSL), and key optimization variables, such as temperatures, pressures, and minimum temperature differences, are defined.

b. Process Integration Layer

This layer encompasses the Target, Exergy Analysis, and PYMOO blocks. Within this inner loop, pinch analysis is first performed to determine the minimum energy requirements (MER). Based on the composite curve analysis, hot and cold utilities are then allocated. The integration potential of thermodynamic conversion systems is subsequently evaluated at the defined operating conditions. Finally, exergy analysis is conducted to quantify the exergy content of process streams, components, and utilities, allowing the estimation of total exergy losses. The outer loop, implemented using a Genetic Algorithm (GA) solver, aims at minimizing the total exergy losses, which is the objective function. It iteratively updates the decision variables and evaluates the system performance at each iteration. These are detailed in [12].

c. Match Selection Layer

The match selection layer uses the results coming from the process integration layer to generate preliminary stream matches. A heat-load distribution table is constructed using the solution of the MILP transshipment model to organize heat exchange across feasible temperature intervals and to guide the selection of candidate matches.

d. Heat Exchanger Design

In this layer, heat exchangers are designed using the LMTD method to determine parameters such as heat transfer area, etc. Design constraints and economic considerations are evaluated, and if violations occur, the framework iterates by updating upstream conditions through the feedback loops. Otherwise, the HEN is synthesized and analyzed to aim for further enhancements.

2.2.2. Match Selection Layer

The MILP transhipment model used in this layer is based on the model developed by Papoulias and Grossmann [7]. In this approach, heat is treated as a commodity that is transferred from source nodes, corresponding to hot streams, to sink nodes, corresponding to cold streams, through intermediate nodes defined by temperature intervals. At each temperature interval, hot and cold streams are connected through variables representing the heat exchanged between stream pairs. In addition, a residual heat term is introduced for each hot stream, representing the amount of heat available for transfer to lower temperature intervals. Consequently, heat exchange is only allowed when both streams are present within compatible temperature intervals, ensuring thermodynamic feasibility. In this work, the original formulation is extended to incorporate additional features, including a refined temperature discretization, forbidden stream matches, and variable utility optimization through scaling factors that account for cost.

The resulting MILP transshipment formulation used is presented below. The model is defined in terms of sets, parameters, decision variables, constraints, and an objective function. It is formulated over a set of temperature intervals k, hot streams $i \in SHotStreams$, and cold streams $j \in SColdStreams$. Process and utility streams are placed in the sets $SProcStreams$ and $SUtStreams$, respectively. The variable $Qijk$ represents the heat exchanged between hot stream *i* and cold stream *j* in temperature interval *k*. $VRik$ denotes the residual heat of hot stream *i* across temperature intervals. The hot and cold utilities heat loads are represented in the variables $QHik$ and $QCjk$, respectively. Utility usage is modeled through the binary variable $UtEnabled$ and the continuous scaling factor $VFactUt$. The model is presented in the figure below.

$$\min \sum_{g \in SUtGroups} (costFix_g \cdot UtEnabled_g + costMult_g \cdot VFactUt_g) \quad \text{(Total utility cost)}$$

$$\begin{array}{lll}
\text{s.t.} \displaystyle\sum_{j \in SColdStreams} Q_{ijk} - VR_{i,k+1} + VR_{ik} - QH_{ik} = 0 & \forall i \in SHotStreams,\ k \in dk & \text{(Hot stream energy balance)} \\
\displaystyle\sum_{i \in SHotStreams} Q_{ijk} - QC_{jk} = 0 & \forall j \in SColdStreams,\ k \in dk & \text{(Cold stream energy balance)} \\
QH_{ik} = DQpk_{ik} & \forall i \in SProcStreams,\ k \in dk & \text{(Process hot streams)} \\
QC_{jk} = DQpk_{jk} & \forall j \in SProcStreams,\ k \in dk & \text{(Process cold streams)} \\
QH_{ik} = VFactUt_g \cdot DQuk_{ik} & \forall i \in SUtStreams,\ g,\ k & \text{(Hot utilities)} \\
QC_{jk} = VFactUt_g \cdot DQuk_{jk} & \forall j \in SUtStreams,\ g,\ k & \text{(Cold utilities)} \\
Q_{ijk} = 0 & \forall (i,j) \in SForbConn,\ k & \text{(Forbidden matches)} \\
VR_{ik} \geq 0 & \forall i, k & \text{(Heat cascade feasibility)} \\
VR_{i1} = 0,\ VR_{iK} = 0 & \forall i & \text{(No heat accumulation)} \\
f_{min,g} \cdot UtEnabled_g \leq VFactUt_g \leq f_{max,g} \cdot UtEnabled_g & \forall g & \text{(Utility bounds)} \\
Q_{ijk} \geq 0,\ VFactUt_g \geq 0 & \forall i, j, k, g & \text{(Non-negativity)} \\
UtEnabled_g \in \{0,1\} & \forall g & \text{(Binary variables)}
\end{array}$$

Figure 4: *Extended MILP Transshipment Model*

The refined temperature discretization increases the number of temperature intervals, allowing the model to explore a wider range of matching possibilities. This can lead to a reduced number of matches in some cases. Furthermore, industrial constraints are represented through the inclusion of forbidden matches. This feature allows the model to account for limitations such as the spatial separation between heat sources and sinks, while enabling the identification of alternative feasible matches where possible. In addition, the formulation introduces variable utility usage through scaling factors, allowing utility levels to be optimized rather than fixed.

In many MILP transshipment models, utilities are fixed, which limits the flexibility of the solution. In contrast, the proposed approach enables utility usage to be adjusted within the optimization, ensuring consistency with process integration and match selection decisions.

This formulation yields the scaling factors of the utilities and thermodynamic systems considered in the problem. It also determines the heat-load distribution, representing the amount of heat exchanged between all the hot and cold streams. These results are extracted and organized into a heat-load distribution table, Q_{load} table, which summarizes the identified stream matches, associated heat loads, and energy requirements.

2.2.3. Heat Exchanger Design

The heat exchanger network design layer aims to translate the results obtained from the match selection layer into physical heat exchangers. $Qijk$ representing the heat exchanged between streams *i* and *j* at temperature interval *k* is now interpreted as the heat duty of an individual heat exchanger.

The exchanger configuration is established by determining whether heat exchange between a given pair of streams occurs in series or in parallel. In cases where heat exchange spans multiple consecutive intervals, the corresponding duties are added and represented as a single heat exchanger. This is valid only for streams that are not involved in parallel heat exchange with other streams.

Subsequently, the temperature profiles are calculated through an interval-wise marching procedure, as illustrated in Figure 5.

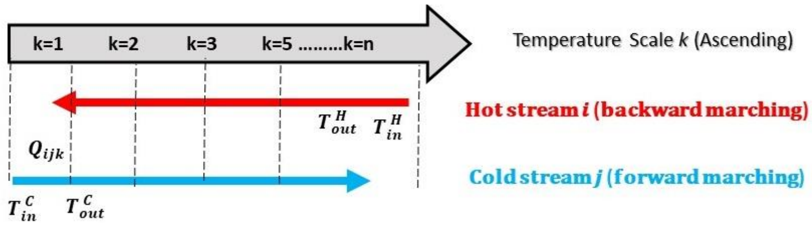

Figure 5: *Forward/backward marching logic*

For cold streams, the calculation proceeds in the direction of heat transfer, starting from the known inlet temperature at the first active temperature interval. For each interval, the outlet temperature is determined based on the exchanged heat load and the stream heat capacity. This outlet temperature then serves as the inlet temperature for the subsequent interval. For hot streams, the temperature calculation is performed in the opposite direction, starting from the known outlet temperature at the lowest temperature interval in which the stream is present. The inlet temperature at each interval is then determined by accounting for the heat released within that interval.

Once the inlet and outlet temperatures of the streams are determined, the heat exchanger area can be calculated using the Logarithmic Mean Temperature Difference (LMTD) method in equation 1. The LMTD represents an effective temperature driving force for heat transfer, accounting for the variation of temperature difference between the hot and cold streams along the exchanger.

$$\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\ln(\frac{\Delta T_1}{\Delta T_2})} \quad (1)$$

Whereby, ΔT_1 and ΔT_2 are the temperature differences between the hot and cold streams at each end of the heat exchanger.

The required heat transfer area is then obtained using the equation below.

$$A = \frac{Q}{U\,.\,\Delta T_{lm}} \quad (2)$$

Where U is the heat transfer coefficient.

An economic evaluation is performed for each heat exchanger to assess the investment cost. The total cost includes fixed, area-dependent, and piping contributions, and is expressed as:

$$Cost_{HEX} = C_{fixed} + C_{variable}\ (A^n) + C_L(L) \tag{3}$$

Whereby, the first term represents the fixed cost, the second term accounts for the nonlinear dependence of cost on heat transfer area, and the third term represents piping costs. For the subsequent case study, the piping cost term is neglected. The cost parameter C_{fixed} is taken as 5291.9 \$, $C_{variable}$ is equal to 77.79 \$/m^2, and the exponent n is taken as 1 [10].

The cost of the heat pump is evaluated using equation 4.This simplified cost approximation is based on the compressor work rather than the condenser duty, as is commonly done.

$$Cost_{HP} = W_{Compressor} \times 1000 \tag{4}$$

This is due to the fact that the compressor is typically the most capital-intensive component of the heat pump system[13].

Energy costs are evaluated using the following equation:

$$Cost_{Energy} = W_{Compressors} \times t_{op} \times C_{el} \tag{5}$$

Where, t_{op} is the operating time assumed to be 8000 h/year and C_{el} is the electricity price taken at 0.12 \$/kWh

2.2.4. Heat Exchanger Network Synthesis

The proposed methodology yields a complete HEN based on the MILP formulation. However, the resulting configurations may become complex, involving multiple exchangers arranged in both series and parallel. The multi-layer feedback structure enables iterative adjustment of the refined temperature discretization and forbidden matches, allowing the network structure to be improved. Furthermore, heat pump integration is optimized simultaneously within this framework, ensuring the adaptability of the heat pump to changing operating conditions. This is illustrated in the simple case study below.

3. Illustrative Example

To demonstrate the applicability of the proposed methodology, the same illustrative example introduced in the previous section is now revisited as a case study. The system consists of two process streams, one hot and one cold, along with a utility stream and a gas boiler, as summarized in Table 1

Table 1. *Steam table of the illustrative example.*

Stream	Tin (°C)	Tout (°C)	Q(kW)
Cold Stream	20	70	141,4
Hot Stream	65	10	200
Cold Utility	-5	0	1000
Gas Boiler	90,1	90	1000

For this case study, a simple heat pump model is selected from the thermodynamic systems' library, as described in our previous work [12]. Propane is set as the working fluid, and the compressor efficiency is fixed at 0.7. The heat pump relies on a water loop to recover the waste heat. The condensation and evaporation temperatures are selected as optimization variables. To evaluate the impact of key design parameters, several cases (A–D and B′–C′) are defined by varying the minimum temperature difference and the forbidden streams. In each case, the heat pump is reoptimized again. The corresponding operating conditions and optimization results for each case are summarized in Table 2.

__Table 2.__ Results summary of the simple case study.

Parameter		Cases					
		A	B	B'	C	C'	D
Minimum Temperature Difference ΔT_{min} (°C)		4	5	5	10	10	15
Forbidden Streams		None	None	Hot Stream & Heat Pump Evaporation Stream in k=5	None	Hot Stream & Heat Pump Evaporation Stream in k=5	None
Objective Function: Exergy Destroyed		11,5	13,12	18,5	29,5	33,9	45,7
Simple Heat Pump	Condensation Temperature (°C)	74,5	75	75	80,0	80,0	85,0
	Evaporation Temperature (°C)	35,7	33,1	15,0	20,7	12,5	21,4
	COP	4,6	4,31	2,93	2,88	2,56	2,47
	Duty (kW)	25,5	28,3	28,3	42,4	42,4	56,6
	Work of Comp (kW)	5,4	6,6	9,7	14,7	16,9	22,8
Cold Utility	Cold Utility (kW)	64,0	65,2	68,3	73,3	75,5	81,4
	Work of Comp (kW)	10,7	10,9	11,4	12,2	12,6	13,6
HEX	Number of HEX	6	6	4	6	4	4
	Total Area (m^2)	84,5	81,0	72,8	63,9	62,6	58,4
Economic Evaluation	Annualized Heat Pump Cost ($)	542,6	655,84	965,42	1472,77	1692,77	2279,37
	Annualized Energy Cost (k$)	15,5	16,7	20,2	25,9	28,3	34,9
	Annualized HEX Cost ($)	3832,5	3805,1	2683,2	3672,2	2603,6	2571,1
	TAC (k$)	19,8	21,2	23,8	31,0	32,6	39,8

i. Impact of changing ΔT_{min}

To evaluate the impact of the minimum temperature difference, Cases A, B, C, and D are analyzed, corresponding to ΔT_{min} values of 4°C, 5°C, 10°C, and 15°C, respectively. The optimal operating conditions of the heat pump are not fixed, but vary with the selected ΔT_{min}. As the ΔT_{min} is modified, the composite curves shift, altering the feasible temperature levels for heat integration. Consequently, the optimal evaporation and condensation temperatures of the heat pump change from case to case.

As the ΔT_{min} increases, a significant decrease in the COP is observed, dropping from 4.69 in Case A to 2.47 in Case D. This is accompanied by an increase in compressor work and utility consumption. The higher pinch temperature imposes larger temperature differences between streams, limiting the extent of direct heat exchange and increasing reliance on the heat pump and external utilities. From a design perspective, increasing the ΔT_{min} results in a reduction in the total heat transfer area due to higher temperature driving forces. However, this comes at the expense of overall system efficiency. These results highlight the trade-off between heat recovery and exchanger design, where lower ΔT_{min} values favor energy efficiency, while higher ΔT_{min} values simplify heat transfer requirements.

ii. Impact of incorporating forbidden streams.

The details of the HEN synthesized for Case B is presented in Table 3.

***Table 3**: HEN of Case B – Simple Case Study*

HEX	Hot Stream Name	Cold Stream Name	k-range	Q [kW]	A [m2]
HEX1	Hot Stream	Cold Stream	4	37,1	11,6
HEX2	Hot Stream	Cold Stream	5	7,1	1,9
HEX3	Hot Stream	Cold Stream	6-7	69	18,1
HEX4	Hot Stream	CU	1	65,2	34,5
HEX5	Hot Stream	Evaporation	5	21,7	5,2
HEX6	Condensation	Cold Stream	8-9	28,3	9

As observed, the heat pump is placed in interval 5, whereby the hot stream is split and forms two parallel heat exchangers. For this reason, the heat pump is forbidden in interval 5 in the following case B', in order to obtain a simpler and more practical network configuration. Figure 6 depicts the HENs of cases B and B'.

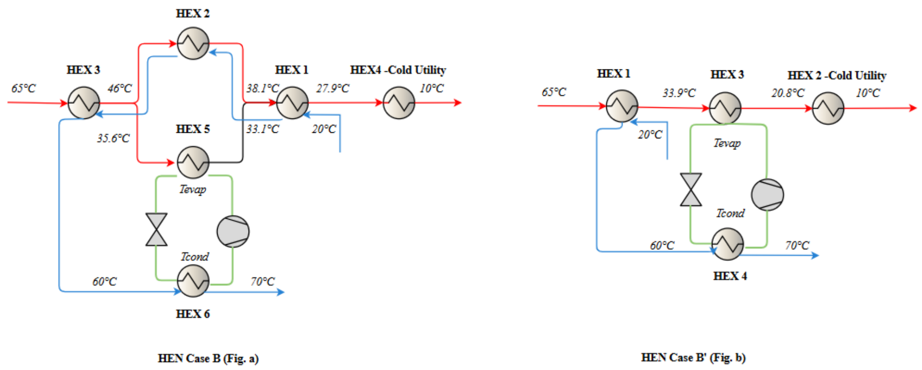

Figure 6: *HENs of Cases B & B' – Illustrative Case Study*

4. Comparison of Methodologies

To evaluate the performance of the proposed methodology, a comparison with the traditional methodology is carried out in this subsection. Multiple iterations are required to adjust the minimum temperature difference and the heat pump operating conditions in order to reach improved solutions. The results of these iterations are summarized in Table 4.

Table 4*: Iterations of the traditional methodology*

Iteration Num	**ΔT_{min} (Initial)**	**ΔT_{min} (Updated by HEN Algorithm)**	**HP Cond/Evap Temperatures (°C)**	**COP**	**Annualized Heat Pump Cost ($)**	**Energy Cost (k$)**	**TAC (k$)**	**Area (m²)**	**Key Observations**
1	10	5	80,1 / 20 (Preselect Algorithm)	2.88	2177,4	19,4	22,1	81,5	ΔT_{min} shift, non-optimal HEN
2	5	4	76,1 / 34,9 (Preselect Algorithm)	N/A	N/A	21,6	23,8	77,7	Heat pump removed, boiler used
3–6	4	4	78/25 (manual)	3,29	1804,7	18,1	20,82	92,77	Manual tuning required
7	4	4	76 / 27 (manual)	3,62	1721,3	16,7	19,6	99,34	Best Case Obtained

i. Iterations 1 & 2 (ΔT_{min} 10 & 5)

As shown in Table 4, the preselect algorithm identifies a heat pump with a condensation temperature of 80.1 °C and an evaporation temperature of 20°C for a ΔT_{min} of 10K. During HEN synthesis, the methodology shifts the ΔT_{min} toward approximately 5 °C in order to reduce costs. The resulting HEN is illustrated in Figure 7a. When compared with the results obtained from the proposed methodology, it can be observed that the solution lies between Cases B and B′. However, under these conditions, the selected heat pump is no longer optimal, as a more suitable configuration exists at ΔT_{min} of 5 °C. Consequently, the resulting heat exchanger network is suboptimal.

This motivates a second iteration, in which the heat pump is updated using the optimal operating conditions corresponding to ΔT_{min} of 5 °C determined by the preselect algorithm. The resulting heat exchanger network is shown in Figure 7b. However, the heat pump is no longer integrated within the network and is ultimately replaced by a gas boiler. This is due to the mismatch between the heat pump operating conditions and the modified ΔT_{min}. Although this leads to a reduction in overall cost, it represents an undesirable outcome, as the heat recovery potential is not utilized.

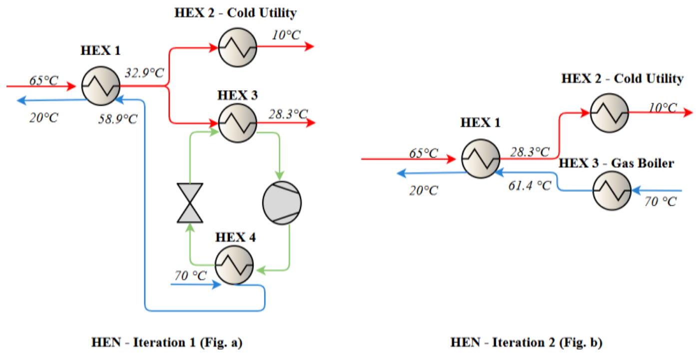

Figure 7: *HEN of the traditional methodology, Iterations 1 & 2*

ii. Iterations 3-7 ($\Delta \boldsymbol{T}_{min}$ of 4 °C)

Since the previously identified heat pump operating conditions are no longer suitable, further manual iterations are required to adjust the heat pump in order to better match the HEN. By modifying the evaporation temperature, a feasible network configuration can be obtained. The lowest TAC is obtained in iteration 7, as shown in Table 4.

iii. Comparison of solutions at ΔT_{min} of 4 °C (Case A and Iteration 7)

The traditional methodology (Iteration 7) yields a heat pump with a COP of 3.62 and a compressor work of 17.2 kW, delivering 62.4 kW. In comparison, the proposed methodology (Case A) identifies a more efficient heat pump with a COP of 4.69 and a significantly lower compressor work of 5.4 kW, delivering 25.5 kW. This results in a lower energy cost (15.5 k$ vs. 16.7 k$). While the traditional methodology achieves a slightly lower total cost (19.6 k$ vs. 19.8 k$) and fewer heat exchangers (4 vs. 6), this outcome is obtained through multiple manual iterations and does not ensure consistency between the heat pump and the HEN.

iv. Overall comparison between the two methodologies

Table 5 summarizes the main differences between the traditional and proposed methodologies.

Table 5: *Comparison between the traditional and the proposed methodologies*

Aspect	Traditional Methodology	Proposed Methodology
Approach	Sequential	
Heat pump selection	Preselected using GCC-based preselection tool (fixed a priori)	Simultaneously optimized with HEN from the Thermodynamic System's Library
$\Delta \boldsymbol{T}_{min}$ handling	Fixed initially, then implicitly shifted during HEN synthesis	Optimized dynamically within the framework
HEN synthesis	Independent step (full MILP formulation)	Independent step (match selection based on one MILP)
Computational effort	High (MILP solved at each iteration)	Reduced (MILP embedded within iterative framework, avoiding full re-solves)
Consistency (HP–HEN)	Not ensured (mismatch possible)	Ensured
Convergence	Not guaranteed	Converges to a consistent optimal solution
Design flexibility of HEN	High, due to flexible features (e.g., stream splitting, non-isothermal mixing, unit-level modeling), enabling compact networks	Structured through incorporating systematic constraints (e.g., forbidden matches, discretization)

The traditional approach is robust and capable of generating heat exchanger networks with fewer exchangers, primarily due to its flexibility in manipulating the network structure. However, this is associated with high computational effort as each iteration requires resolving the entire MILP problem. In addition, the use of the preselection algorithm fixes the heat pump operating conditions a priori based on the initial $\Delta \boldsymbol{T}_{min}$ which may become inconsistent once the HEN synthesis implicitly shifts this value. As a result, multiple manual adjustments of the heat pump operating conditions may be required. Furthermore, the preselection algorithm is limited to simple heat pump configurations and cannot be readily extended to more complex systems, such as mechanical vapor recompression cycles. In contrast, the proposed methodology integrates heat pump selection and HEN synthesis within a unified framework, allowing all key variables to be optimized simultaneously. This eliminates the need for manual tuning and avoids repeated full-scale optimizations, significantly reducing computational effort. Furthermore, it enables the systematic exploration of multiple scenarios under varying operating conditions. In addition, it incorporates a thermodynamic systems library based on industrial heat pump technologies, rather than being limited to simplified configurations.

5. Conclusion

This study highlights the limitations of traditional sequential methodologies for heat exchanger network synthesis, particularly the inconsistency between heat pump design and network configuration arising from fixed assumptions and decoupled optimization. The proposed methodology addresses these challenges by enabling simultaneous and iterative optimization of heat integration, heat pump optimization, and HEN synthesis. In addition, the incorporation of refined temperature discretization and forbidden streams introduces additional degrees of freedom, allowing for a more realistic HEN. Overall, the findings demonstrate that the proposed methodology provides a robust and efficient pathway for solving HEN design problems. Future work will explore the integration of artificial intelligence–based tools to enhance the framework, particularly manipulating the network structures through the introduction of constraints, such as manipulating forbidden matches.

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