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Simultaneous Synthesis of Heat Exchanger Networks with Pressure Recovery: Optimal Integration between Heat and Work

Viviani C. Onishi

Dept. of Chemical Engineering, University of Alicante, Ap Correos 99, 03080, Alicante, Spain

Dept. of Chemical Engineering, State University of Maringá, Av. Colombo 5790, 87020-900, Maringá, PR, Brazil

CAPES Foundation, Ministry of Education of Brazil, 70040-20, Brasília, DF, Brazil

Mauro A. S. S. Ravagnani

Dept. of Chemical Engineering, State University of Maringá, Av. Colombo 5790, 87020-900, Maringá, PR, Brazil

José A. Caballero

Dept. of Chemical Engineering, University of Alicante, Ap Correos 99, 03080 Alicante, Spain

Correspondence concerning this article should be addressed to V. C. Onishi at pg51551@uem.br/ viviani.onishi@hotmail.com

The optimal integration between heat and work may significantly reduce the energy demand and consequently the process cost. This paper introduces a new mathematical model for the simultaneous synthesis of heat exchanger networks (HENs) in which the

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pressure levels of the process streams can be adjusted to enhance the heat integration. A superstructure is proposed for the HEN design with pressure recovery, developed via generalized disjunctive programming (GDP) and mixed-integer nonlinear programming (MINLP) formulation. The process conditions (stream temperature and pressure) must be optimized. Furthermore, the approach allows for coupling of the turbines and compressors and selection of the turbines and valves to minimize the total annualized cost, which consists of the operational and capital expenses. The model is tested for its applicability in three case studies, including a cryogenic application. The results indicate that the energy integration reduces the quantity of utilities required, thus decreasing the overall cost.

Keywords: Optimization, mathematical modeling, heat exchanger network (HEN), energy integration, pressure recovery

Introduction

Applying innovative strategies for energy conservation and efficiency is fundamental to reducing energy consumption in industrial processes. The increasing global energy demand, the current high cost of energy due to the rapid depletion of crude oil reserves, and the tightening environmental regulations on CO_2 emissions aimed at alleviating global warming are among the many driving forces behind the need for energy conservation and efficiency[1–4], and are often achieved by adopting more efficient processing technologies or by optimizing energy usage.

Heat and work are two forms of energy frequently available in industrial plants. Effective heat recovery is critical to solving the problem of energy efficiency and consequently decreasing the process cost[5,6]. Thus, analysis and optimization of thermal integration are imperative because a reduced energy consumption is directly associated with improved heat transfer[7,8]. Heat exchanger network (HEN) synthesis is responsible for the energy integration. Given the importance of the HEN in the total cost and its interdependence with other sectors of the process, HEN synthesis has been extensively studied in recent decades[6,9,10].

The synthesis of HENs began to attract attention during the oil crisis of the 1970s[6,11]. Hwa,[12] using separable programming methods, and Kesler and Parker,[13] using linear programming, were among the first to present solutions to the problem of HEN design. Since then, several studies have used different methods to solve the problem[14]. The recent trend in the development of more sustainable processes has renewed interest in the design of these systems[11].

Gundersen and Naess[10] and Furman and Sahinidis[6] published comprehensive reviews on HEN synthesis. Important lines of research were proposed, such as pinch analysis and mathematical programming. Pinch analysis is based on thermodynamic concepts and heuristics[15–18]. In mathematical programming, the HEN synthesis is treated as an optimization problem. According to Grossmann et al.[19], the use of the mathematical programming method has gradually evolved from sequential approaches in which one seeks a step-by-step solution to the problem[20–24] to work using simultaneous optimization in which all variables are optimized concurrently[25–27].

Yee and Grossmann[26] proposed a robust mathematical programming model for HEN synthesis. The Yee and Grossmann[26] model is among the most widely accepted superstructure-based simultaneous methods found in the literature. Although their objective function was highly nonlinear and non-convex, they were able to obtain good solutions. The simultaneous approach for HEN synthesis results in an NP-hard problem; however, even if the simultaneous strategy is more difficult to implement and solve, it can lead to larger economic benefits[28]. Conventional MINLP (mixed-integer nonlinear programming) methods are based entirely on optimization problems with discrete and continuous variables. In contrast, the approaches using generalized disjunctive programming (GDP)[29–31] combine logical and algebraic equations to represent discrete decisions.

Despite the numerous attempts to optimize heat recovery using HEN synthesis, literature sources regarding process optimization using pressure recovery to improve the heat integration are limited. Handling pressure is especially important in oil refineries and cryogenic processes, such as production of liquefied natural gas (LNG). In such plants, the compression and expansion of process streams that are subject to high pressures consume large quantities of energy. For example, in the LNG process depicted in Figure 1, high-pressure natural gas (NG) is pre-cooled with liquid carbon dioxide (LCO_2) through a heat exchanger and then expanded to a lower pressure to exchange heat with liquid inert nitrogen (LIN). Then, to achieve its storage pressure, the NG passes through a turbine that reduces the pressure further. The high-pressure liquid N_2 passes through two heat exchangers to cool the natural gas. Thus, the process utilizes one compressor and two turbines for cooling, which also produces work[3,4,32–35]. Clearly, an optimal integration between the heat and work could significantly reduce the energy demand, consequently reducing the process cost.

Wechsung et al.[3] presented an optimization model for synthesizing HENs using streams under sub-ambient conditions that are subject to compression and expansion. The formulation proposed by the authors combines pinch analysis, exergy analysis and mathematical programming (a non-convex MINLP model) to obtain an optimal HEN design by minimizing the total irreversibility of the system and varying the pressure levels in the process flows. The authors study an industrial application related to the production of LNG to demonstrate that the correct manipulation of the process stream pressure can significantly reduce the total irreversibility of the HENs. Nevertheless, this study lacked an analysis of the cost involved in the process and any consideration of other equipment arrangements, such as the possibility of coupling turbines to compressors and exchanging turbines for valves.

This paper introduces a new mathematical model for the simultaneous synthesis of HENs, in which the pressure levels of the process streams can be adjusted to enhance the heat integration. The proposed formulation involves generalized disjunctive programming (GDP) and mixed-integer nonlinear programming (MINLP) based on the superstructure presented by Yee and Grossmann[26] allowing for stream splits, while assuming constant heat capacity flow rates and isothermal mixing. The main difference between the proposed model and the Yee and Grossmann[26] superstructure is that the present study considers the stream temperature an unknown variable and includes a new optimization variable, the pressure of the process streams. Several possible HENs involving compressors, turbines and valves are studied to obtain an optimal HEN design to minimize the total annualized cost, including the capital and operational expenses. Three case studies are conducted to verify the applicability of the proposed model. In these examples, the optimal integration between the heat and work is found to decrease the quantity of utilities necessary in the HEN design. Consequently, the total annualized cost is reduced due to the reduction of the operational expenses related to heating and cooling the process flows.

Problem Statement

This model utilizes a set of hot and cold process streams with a known supply state (temperature, pressure and resulting phase), a target state in which some gaseous streams have pressures that differ from the inlet conditions, energy supplies for heating and cooling, and pressure manipulation equipment, with their respective costs. The primary objective of the model is to synthetize an optimal HEN with a pressure recovery of the streams that minimizes the total annualized cost, considering the operational expenses and the capital investment in the various units of the network.

A mathematical model for HEN synthesis based on the well-known superstructure of Yee and Grossmann[26] is proposed to solve the problem. The superstructure is composed of various stages wherein heat exchange may occur between hot and cold streams. Moreover, the HEN is designed allowing for stream splits, while assuming constant heat capacity flow rates (i.e., product of flow rate and heat capacity) and isothermal mixing. In addition, heaters and coolers are placed at the ends of the streams. As recommended by Yee and Grossmann[26], the number of stages is equal to the maximum number of possible exchanges between the hot and cold streams. Because some process streams are compressed and expanded, equipment for pressure manipulation—namely compressors, turbines and valves—is also required. Thus, the stream pressure and temperature become unknown variables at the inlet and outlet of the HEN superstructure.

In this approach, the hot and cold streams should follow a specific route for pressure manipulation, with a maximum number of possible expansions and compressions being n. Thus, if n = 3, a hot stream can potentially be cooled, compressed, cooled, expanded, heated, compressed, and cooled. Similarly, a cold stream can be heated, expanded, heated, compressed, cooled, expanded, and heated (see Figure 2). The selection of this route is based on the work of Wechsung et al.[3] in which the ''plus–minus'' principle[36] was used to identify the best direction for the pressure modifications to reduce the energy requirements. This definition is significantly more complex than the conventional problem of heat integration in HEN synthesis postulated by Yee and Grossmann[26] and extensively studied over the past decades primarily because both the stream pressure and temperature must be considered unknown variables that require optimization. The streams that are subject to pressure manipulation are connected to the HEN via compressors and expanders; thus, the stream state at the outlet of the pressure manipulation equipment should correspond to the inlet state in the HEN superstructure. If the aforementioned route is considered (n = 3), eight additional variables are involved: three intermediate inlet temperatures, three intermediate outlet temperatures, and two intermediate outlet pressures. Moreover, the need for an operator to manipulate the pressure of the streams increases the non-linearity and non-convexity of the model considerably. Wechsung et al.[3] also noted that this type of problem has no clear distinction between the hot and cold streams and between the process streams and utilities. In fact, the flows can change identity; thus, a cold stream can temporarily behave like a hot stream, and vice versa. Some process streams can also act as utilities, serving as energy sources or sinks at temperatures outside the range generated by the available utilities.

The flow properties, such as the phase, may also be modified by manipulating the pressure. In addition to the larger number of variables and constraints, the GDP formulation is needed to aid in the selection of expansion equipment (valves or turbines) and to consider the possibility of coupling a compressor with a turbine, often industrially referred to as a "compander". These factors, added to the high nonlinearity and non-convexity of the cost correlations, confer an even higher degree of complexity on the model.

Like the study presented by Wechsung et al.[3], this work models the expansion and compression of the streams as an isentropic process. For simplification, the ideal gas model is used for the thermodynamic behavior and the pressure variations in the streams. However, an isentropic efficiency factor is introduced to adjust for the inevitable loss of efficiency in real processes. As previously mentioned, when the cost-benefit ratio for the process is satisfied, the proposed formulation enables the exchange of turbines for valves. In these cases, the isenthalpic expansions are considered using the correct Joule-Thomson coefficient.

Mathematical Programming Model

The model formulation is based on the HEN superstructure and the mathematical model introduced by Yee and Grossmann[26]. Their MINLP model[26] allows the identification of the network within the superstructure with minimal cost by determining which heat exchangers are effectively required and the heat duty and temperatures of each stream. This is among the widely accepted models with similar methods based on superstructures.

The generation of the superstructure proposed in this work is based on three main ideas:

I- Representation in stages according to the temperatures. The superstructure consists of *Ns* stages. In each stage, each hot stream is believed capable of exchanging heat with all cold streams and vice versa (each cold stream could exchange heat with all hot streams). However, when a stream undergoes expansion or compression, its identity can temporarily change; hence, an expanded hot stream begins to behave as a cold stream, and a compressed cold stream behaves as a hot stream (see Figure 2). In this case, the heat exchange between these streams is forbidden (because they are, in fact, the same stream). The placement of thermal utilities (heaters and coolers) between the compression and expansion stages is also disallowed. However, these heat exchange constraints can be easily removed from the model.

II- Assumption of an isothermal mixing of streams. At each stage of the superstructure, the hot and cold streams are split into a number of sub-streams equal to the number of possible heat exchanges, and the outlet temperature after each of these exchanges should be the same. Thus, the energy balance at the point of mixing can be eliminated.

III- The hot and cold streams can follow a specific route of pressure manipulations. If this route of compression and expansion is chosen correctly (i.e., hot stream: compression, expansion and compression; cold stream: expansion, compression and expansion), pressure manipulation may be used to supply energy (heating or cooling) to the streams to reduce their need for hot or cold utilities, thus reducing the total cost of the process.

The following assumptions are considered for the formulation of the problem:

(i) A given stream is allowed to have a maximum of three (n = 3) pressure changes

(ii) All turbines and compressors are centrifugal

(iii) All compressions and expansions, except expansions through the valves, are isentropic

(iv) All expansions through the valves are isenthalpic (Joule-Thompson) with a constant Joule-Thompson coefficient

(v) The isentropic efficiencies of all compressors and turbines are known constants

(vi) All process streams have constant heat capacities and heat transfer coefficients

(vii) Pressure drop and heat losses in all thermal equipment are neglected

(viii) All equipment is built using carbon steel

The superstructure can easily be generated using the following procedure:

1. Selecting the number of stages, *Ns.* In the superstructure, the number of stages is set to be equal to the number of hot or cold streams, whichever is the largest:

$$N_S = \max\{N_H, N_C\}$$

In which N_H and N_C are the number of hot and cold streams, respectively. The number of possible matches is given by $N_H \times N_C \times N_S$, which means that potentially a hot stream and a cold stream could exchange heat in all the *Ns* stages. Nevertheless, the selection of *Ns* can be arbitrary and based on the observation that an optimal network does not generally contain a large quantity of heat-exchange equipment: a stream does not typically exchange heat with many other streams. The model allows this number to be easily changed. Obviously, an increase in the number of stages increases the size of the problem. A rigorous study of how to choose the number of stages to reduce the size of the superstructure was conducted by Daichendt and Grossmann[37].

2. In each stage, the streams are split into a number of sub-streams equal to the number of potential exchanges. The sub-streams outputs in a stage should be at the same temperature (assuming isothermal mixing) and should gather at the exit point, which is considered the entry point for the next stage. The outlet temperature of each stream at each stage is an unknown variable that requires optimization. According to the previous discussion, the hot and cold parts of the same stream resulting from the stages of compression and expansion, cannot exchange heat between them. In addition, no heaters and coolers can be placed on such streams. The following constraints, written as a function of binary variables are necessary for determining the existence or absence of the exchange (h, c) at each stage k and the exchanges between the process streams and the utilities.

$$\begin{aligned} Q_{h,c,k} &\leq y_{h,c,k} \cdot Q_{h,c,k}^{\max} \\ Q_{h,n} &\leq y_{h,n}^{cooler} \cdot Q_{h,n}^{\max} \\ Q_{m,c} &\leq y_{m,c}^{heater} \cdot Q_{m,c}^{\max} \end{aligned} \tag{1}$$

In which $Q_{h,c,k}$ is the quantity of heat exchanged between the hot and cold streams in stage k of the superstructure, $Q_{h,n}$ is the quantity of heat exchanged between the hot streams and the cold utilities, and $Q_{m,c}$ is the quantity of heat exchanged between the cold streams and the hot utilities. The term $y_{h,c,k}$ is a binary variable that defines the heat exchange between a hot stream h and a cold stream c in a stage k. Similarly, $y_{h,n}^{cooler}$ and $y_{m,c}^{heater}$ are the binary variables that define the existence of a cooler and a heater, respectively, for hot and cold streams; these binary variables define the heat exchange between the streams and the corresponding utilities.

Equation (1) was originally presented in the HEN design model proposed by Yee and Grossmann[26]. These equations ensure that the binary variable assumes the value $y = 1$ if there is heat exchange ($Q > 0$). To prohibit a given heat exchange, the corresponding binary variable is fixed at zero, and thus the heat exchanged is zero (which is equivalent to removing such a possibility from the superstructure).

3. In each stream that is subject to pressure manipulation, the possibility of using expanders or compressors is considered according to the previous discussion regarding the best route for manipulating the stream pressure to reduce the use of thermal utilities. In this case, the stream temperatures and pressures at the outlet of the HEN superstructure are connected to the inlet temperatures and pressures of the expanders and compressors. Therefore, the stream temperatures and pressures should be treated as optimization variables.

The operators for pressure manipulation—the coupling of turbines and compressors, the selection of turbines or valves, and the objective function—are presented as follows.

Operator for pressure manipulation

Consider a stream s with a supply state s_{in} and a target state defined by s_{out} in which (s_{in}, s_{out}) are the stream inlet and outlet states in the respective pressure manipulation equipment. Note that the stream inlet state in a compressor/expander should correspond to the stream outlet state in the HEN superstructure, and vice versa. Therefore, the reversible adiabatic process of manipulating the pressure of an ideal gas can be formulated as follows (this expansion and compression operator was originally presented in Wechsung et al.[3]):

$$
\begin{aligned}
&(\kappa-1)\cdot\left(\ln p_{s,in}-\ln p_{s,out}\right)=\kappa\left(\ln T_{s,in}-\ln \tilde{T}_{s,out}\right) \quad \forall\left(s_{in},s_{out}\right)\in CO\cup EX\\
&\eta_v=\left(\tilde{T}_{s,out}-T_{s,in}\right)/\left(T_{s,out}-T_{s,in}\right) \quad \forall\left(s_{in},s_{out}\right)\in CO\\
&\eta_t=\left(T_{s,in}-T_{s,out}\right)/\left(T_{s,in}-\tilde{T}_{s,out}\right) \quad \forall\left(s_{in},s_{out}\right)\in EX\\
&WC_v=F_sCp_s\left(T_{s,out}-T_{s,in}\right) \quad \forall\left(s_{in},s_{out}\right)\in CO\\
&WE_t=F_sCp_s\left(T_{s,in}-T_{s,out}\right) \quad \forall\left(s_{in},s_{out}\right)\in EX
\end{aligned} \tag{2}
$$

In which $\tilde{T}_{s,out}$ is the stream outlet temperature for a reversible process, κ is the polytrophic exponent, and η_v and η_t are the isentropic efficiencies of the compressors and turbines, respectively. Moreover, WC_v is the work consumed by the compressors and WE_t is the work generated by the turbines.

As suggested by Couper et al.[38], the compression work must be limited within a range of $18\ kW \le WC_v \le 950\ kW$. The expansion work produced by the turbines is held between $50\ kW \le WE_t \le 1500\ kW$.

The state described by Equation (2) is related only to positive physical quantities. Thus, all variables must be limited to prevent the logarithm from becoming undefined. The mathematical formulation can be easily modified for the case in which the thermodynamic properties explicitly describe the state equation in terms of volume. The work of both the compression and expansion are defined as non-negative quantities. Consequently, the net work produced is equal to the sum of the expansion work minus the sum of the compression work. This paper does not consider pressure drop in the heat exchangers, although a constant pressure drop can be easily considered within the model.

Operator for expander and compressor coupling

To save electricity, the coupling of turbines and compressors is typically considered. In this case, the work generated by the expander is used to rotate the shaft of the compressor, supplying the energy required by this equipment. In this case, the coupling of the compressor and turbine is considered without an extra motor, i.e., the turbine can satisfy the energy requirements of the compressor. Another advantage to using a compressor coupled to a turbine rotor in a single shaft is the reduction of the space required for construction.

Consider a binary variable y^{CoEx}, such that $y^{CoEx}=1$ determines the coupling of a compressor to a turbine. In this case, the compression work should be equal to the expansion work, and the compressor requires no electricity. If $y^{CoEx}=0$ the opposite occurs. The coupling of the expander and compressor can be obtained from the following mathematical formulation:

$$\begin{bmatrix} y_{v,t}^{CoEx} \\ WC_v = WE_t \\ C_{ele} = CE \cdot WC_v = 0 \end{bmatrix}$$

Using the big-M formulation, the disjunction may be expressed as follows:

$$
\begin{aligned}
& WC_v - WE_t \leq M_1\left(1 - y_{v,t}^{CoEx}\right) \\
& WC_v - WE_t \geq -M_1\left(1 - y_{v,t}^{CoEx}\right) \\
& C_{ele} \leq M_2\left(1 - y_{v,t}^{CoEx}\right) \\
& C_{ele} \geq CE \cdot WC_v - M_2 \cdot y_{v,t}^{CoEx}
\end{aligned}
\tag{3}
$$

In which M is a positive parameter that is large enough to validate the formulation (3). Clearly, this parameter must be as smaller as possible. In this case, the parameter M_1 is calculated as the difference between the upper bound of the expansion work (1500 kW) and the lower bound of the compression work (18 kW). Likewise, the parameter M_2 is calculated as the difference between the upper (10e2 kUS\$/year) and lower (10 kUS\$/year) bounds of the electricity cost.

Operator for selecting valves or turbines

In some cases, a valve can replace a turbine if it meets the pressure requirements (expansion) of the system. Whenever this occurs, the use of a valve must be considered because its capital cost is negligible compared with that of a turbine. Logically, no coupling occurs between a compressor and valve, and no electricity is generated. The following disjunction can be used to promote the selection between valves and turbines.

$$\begin{bmatrix} y_w^{val} \\ T_{s,in} = \left(T_{s,out} + \mu_s\left(p_{s,in} - p_{s,out}\right)\right) \\ WE_t = 0 \\ C_t = 0 \end{bmatrix} \veebar \begin{bmatrix} y_t^{ex} \\ T_{s,in} = \exp\left(\left(\kappa - 1/\kappa\right)\cdot\left(\ln p_{s,in} - \ln p_{s,out}\right) + \ln \tilde{T}_{s,out}\right) \\ T_{s,in} = \left(T_{s,in} - \tilde{T}_{s,out}\right)\eta_t + T_{s,out} \\ C_w = 0 \end{bmatrix}$$

Note that w and t indicate the position of the valves and turbines, respectively, in the process. If $y^{val} = 1$, a valve is chosen over a turbine. In this case, the expansion considered is isenthalpic (Joule-Thompson expansion with a constant coefficient μ_s), and the expansion work and capital cost for the turbines are considered zero. If $y^{ex} = 1$, a turbine is selected, the expansion considered is isentropic assuming a constant isentropic efficiency for this turbine, and the related cost of its construction is estimated. Obviously, turbines and valves cannot coexist; thus, $y^{val} = 1$ implies $y^{ex} = 0$, and vice versa. The following big-M formulation is used to ensure this decision:

$$\begin{aligned}
& y_w^{val} + y_t^{ex} = 1 \qquad \forall \;\; w = t \\
& T_{s,in} \le \left[T_{s,out} + \mu_s\left(p_{s,in} - p_{s,out}\right)\right] + M_3\left(1 - y_w^{val}\right) \\
& T_{s,in} \ge \left[T_{s,out} + \mu_s\left(p_{s,in} - p_{s,out}\right)\right] - M_3\left(1 - y_w^{val}\right) \\
& T_{s,in} \le \left[\exp\left(\left(\kappa - 1/\kappa\right)\cdot\left(\ln p_{s,in} - \ln p_{s,out}\right) + \ln \tilde{T}_{s,out}\right)\right] + M_3\left(1 - y_t^{ex}\right) \\
& T_{s,in} \ge \left[\exp\left(\left(\kappa - 1/\kappa\right)\cdot\left(\ln p_{s,in} - \ln p_{s,out}\right) + \ln \tilde{T}_{s,out}\right)\right] - M_3\left(1 - y_t^{ex}\right) \\
& T_{s,in} \le \left[\left(T_{s,in} - \tilde{T}_{s,out}\right)\eta_t + T_{s,out}\right] + M_3\left(1 - y_t^{ex}\right) \\
& T_{s,in} \ge \left[\left(T_{s,in} - \tilde{T}_{s,out}\right)\eta_t + T_{s,out}\right] - M_3\left(1 - y_t^{ex}\right)
\end{aligned} \qquad (4)$$

$$WE_t \le M_4\left(1-y_w^{val}\right)$$

$$WE_t \ge F_s Cp_s\left(T_{s,in}-T_{s,out}\right)-M_4\cdot y_w^{val}$$

$$C_t \le M_5\left(1-y_w^{val}\right)$$

$$C_t \ge \left[CPO_t\cdot FBM_t\right]-M_5\cdot y_w^{val}$$

$$C_w \le M_6\left(1-y_t^{ex}\right)$$

$$C_w \ge \left[CPO_w\cdot FBM_w\right]-M_6\cdot y_t^{ex}$$

Again, the parameter M must be positive and large enough to guarantee that Equation (4) is valid. Thus, the parameters M_3 to M_6 are calculated as the difference between the upper and lower bounds of the temperature (specified according to case studies), the expansion work (50–1500 KW), the cost of the turbines (10–10e2 kUS$/year) and the cost of valves (0,1–1 kUS$/year), respectively.

Objective function

The total annualized cost (C_{total}) is composed of the operational costs ($C_{operational}$) and the capital expenses ($C_{capital}$). The operational costs include the expenses inherent in the use of utilities and electricity services. In this paper, the expansion work produced by turbines is credited from the operational expenses related to electricity only in the case that occurs the coupling of turbines and compressors. The capital expenses involve the costs of construction, all equipment required for the HEN, and the pressure manipulation equipment, i.e., the compressors, turbines and valves. Thus, the objective function can be expressed by Equation (5).

$$C_{total} = C_{capital} + C_{operational}$$

$$C_{operational} = \sum_{h}\sum_{n} CC \cdot Q_{h,n} + \sum_{m}\sum_{c} CH \cdot Q_{m,c} + \sum_{v} CE \cdot WC_{v} \tag{5}$$

$$C_{capital} = f \cdot \left[\begin{array}{l} \sum_{Hex} CPO_{Hex} \cdot FBM_{Hex} + \sum_{Cooler} CPO_{Cooler} \cdot FBM_{Cooler} + \sum_{Heater} CPO_{Heater} \cdot FBM_{Heater} \\ + \sum_{v} CPO_{v} \cdot FBM_{v} + \sum_{t} CPO_{t} \cdot FBM_{t} + \sum_{w} CPO_{w} \cdot FBM_{w} \end{array} \right]$$

In which *CC*, *CH* and *CE* are the cost parameters for the cold and hot utilities, and the electricity, respectively. The term *FBM* is the correlation factor for the equipment cost, and *CPO* indicates the cost of an equipment unit (in US$), obtained from the correlation of Turton et al.[39] for heat exchangers and valves and from the correlations of Couper et al.[38] for turbines and compressors. These correlations were corrected according to the CEPCI index (Chemical Engineering Plant Cost Index) for 2012. The term f is the annualization factor for the capital cost defined by Smith[40].

Computational Aspects

Before presenting the case studies, some important computational aspects related to the solution of the previous model should be discussed. The proposed disjunctive model is formulated as an MINLP problem using big-M reformulation[41]. This type of relaxation is convenient when the problem size does not increase substantially when compared to the convex hull relaxation[42]. The big-M formulation is always competitive when good bounds can be provided for the variables[43]. However, generally the lower bound obtained by the big-M formulation is weaker, requiring more CPU time than the convex hull relaxation. The value of the parameter M must be chosen carefully: If M is smaller than the upper bound for the function; valid solutions may be cut off. If M is too large, the model may become numerically difficult to solve. Thus, the big-M parameter is determined according to upper and lower bounds of the variables in each equation.

The problem is written in GAMS (version 24.0.2) and can be solved using any standard MINLP solver. Nevertheless, this type of model produces a large number of local solutions due its non-convex and nonlinear features that often lead to suboptimal solutions. Although decomposition techniques, such as generalized Benders decomposition[44] (GBD) and outer-approximation (OA) are available for solving MINLP problems, if the master problem is sensitive to the non-convexities, important portions of the feasible region may be cut off. Thus, the results often get trapped in a local optimum[45]. Typically, the branch-and-bound (BB) algorithm is less sensitive to non-convexities. The initial values for each nonlinear programming (NLP) problem in the BB algorithm are provided by the parent node. Upper and lower bounds should be provided for the initial node (relaxed NLP problem) for each of the variables in the model. In addition, the large number of potentially infeasible solutions can aid in pruning the tree search, somehow mitigating the combinatorial nature of the problem[31]. Therefore, the use of a simple BB-based solver, such as an SBB solver under GAMS, should find a near-global optimal solution. Although deterministic global optimization solvers (i.e., BARON) can solve the problem with global optimality, the required CPU time is excessive. Therefore, in this work, the SBB solver was chosen to solve the model.

An attempt to solve the model with the DICOPT solver was undertaken, yet this solver did not outperform the SBB. The DICOPT solver is based on the OA method and typically requires fewer major iterations (i.e., between the NLP sub-problems and the MILP master problem). However, because the DICOPT solver is more sensitive to non-convexities, especially in the master (MILP) problem, it repeatedly failed to find a single feasible solution. The BARON solver was also utilized; however, this solver was unable to return solutions as the superstructure became more complex and can thus only be applied when the superstructure is evaluated without pressure manipulation.

All problems were solved using a personal computer with an Intel Core 2 Duo 2.40 GHz processor and 3.00 GB RAM running Windows 7 Ultimate. The tolerance on the GAMS termination, OptCR, was adjusted to 0.00 (only when using the SBB solver), while the absolute tolerance in GAMS, OptCA, used the default values. To solve the model, one must impose limits (i.e., upper and lower bounds) on all variables. Thus, the limits on the pressures and temperatures are specified individually in each studied example.

Case Studies

Three examples (Examples 2 and 3 were extracted from Wechsung et al.[3]) comprising different situations are studied to analyze the performance of the developed model for obtaining an optimum HEN design with process streams that are undergoing pressure manipulation.

Example 1. This example considers the heat integration between two process streams, one hot (H1) and one cold (C1). The hot stream H1 is compressed between 0.1 and 0.5 MPa and the cold stream C1 is expanded from 0.5 to 0.1 MPa. As previously mentioned, H1 can potentially be compressed, expanded and compressed again, while C1 can be expanded, compressed and expanded with the use of coolers and/or heaters at the end of these streams after all expansion and compression stages. When expanded, the hot stream temporarily behaves as a cold stream, while a compressed cold stream behaves as a hot stream. Thus, in the system, eight process streams are considered—four hot streams (H1, H2, H3 and H4) and four cold streams (C1, C2, C3 and C4). In this case, the heat capacity and flow rates of all streams are known constants. The problem data are presented in Table 1, and Figure 2 shows the possible arrangement of the streams for this example. For the HEN synthesis, a superstructure with four stages and possible stream splits is considered.

Moreover, $\Delta T_{\min}$ = 5 K, $T^{h}{}_{U}$ = 680 K, $T^{c}{}_{U}$ = 300 K, κ = 1.352, η_t = 1, η_v = 1, and μ_s = 1.961 K/MPa. Unknown inlet temperatures can vary between 350 and 750 K, the pressures of the H2 and C2 streams are restricted to 0.1–0.8 MPa, and the pressure of the C3 and H4 streams are limited to 0.1–0.7 MPa. The individual heat transfer coefficients for all streams are maintained at 0.1 kW/m^{2}K with a hot and cold utility coefficient of 1.0 kW/m^{2}K. The annualized capital cost factor is assumed to be f = 0.18 (10% interest rate over 8 years).

Different cases are studied. Initially, the pressure levels are adjusted to promote integration between the heat and work, and two additional cases are presented to consider different constraints and possible equipment arrangements. In all cases, the total annualized cost minimization, composed of the operational expenses and capital investment, is considered to be the objective function.

In Case 1, the pressure manipulation of the process streams is evaluated. In this case, the obtained HEN is composed of four heat exchangers and one cooler. The heat transfer areas (and the heat exchanged) are equal to 47.95 m^2 (170.92 kW); 227.31 m^2 (229.88 kW); 117.45 m^2 (162.51 kW); 196.91 m^2 (389.08 kW), and 47.57 m^2 (618.46 kW). Furthermore, the results indicate that the optimal network is obtained through the following steps: (*i*) compression (through the compressor CO1) of the H1 stream, followed by heat exchange in the HEN, compression (CO2), heat exchange and cooling (cooler C); and (*ii*) the crossing of C1 by the HEN, followed by expansion (EX3) and return to the network for exchanging heat requiring no additional hot utility. Thus, two compressors and one turbine are utilized to compress and expand and to heat and cool, respectively, the process streams immediately prior to the heat exchange in the HEN. Figure 3 presents the HEN obtained in this case. In the compressors, 730.85 kW (CO1 = 20.96 kW and CO2 = 709.89 kW) of power is consumed, and the cost of electricity is approximately 333 kUS$/year. The expander produces 472.391 kW, which is available to meet the energy requirements of the process. The total annualized cost of the network with this configuration is 1,207 kUS$/year, with a capital cost for equipment construction of 813 kUS$/year and operating costs of 394 kUS$/year considering cold services and electricity expenses.

In Case 2, the HEN is designed to enable a coupling of the turbines and compressors to save electricity. The optimum network is obtained with four different heat exchangers and one cooler. The heat exchange areas are 63.24, 171.69, 134.14, 80.88 and 48.26 m^2, and responsible for the following quantities of exchanged heat: 265.03, 237.30, 322.70, 127.36, and 635.69 kW, respectively. Again, two compressors (CO1 = 472.391 kW and CO2 = 275.689 kW) and one expander (EX2 = 472.391 kW) are required to manipulate the pressure of the process streams. However, the H1 stream is compressed in two stages after exchanging heat in the HEN, with an intermediate heat exchange, returned to the HEN and finally cooled with a cold utility (C). While the stream C1 is expanded after heat exchange to return to the HEN without requiring any hot utility in the end of the stream. Figure 4 provides the HEN configuration for this case. In addition, this result allow a compander to be obtained in which the first compressor (CO1) is coupled to the expander (EX2) so that all required work (472.391 kW) is generated by the turbine, reducing the electricity cost for this compressor (CO1) to zero. The work consumed by the compressor CO2 is equal to 275.689 kW, a value below that obtained for this compression in Case 1. These factors directly reflect in the total annualized cost, which, in this case, is 1,081 kUS$/year (composed by $C_{capital}$ = 892 kUS$/year and $C_{operational}$ = 189 kUS$/year, the last value derives from the cold services and electricity expenses), which represents a 10% savings in the total cost of the HEN over that obtained in the previous case.

In Case 3, the handling of the pressure is evaluated assuming the possibility of exchanging turbines for valves and coupling turbines with compressors. Figure 5 shows the configuration obtained for this case. The optimal network is achieved with two heat exchangers (A = 358.96 m^2 with Q = 470.203 kW and A = 7.736 m^2 with Q = 11.366 kW) and one 63.70 m^2 cooler (Q = 1128.63 kW). In this case, one compressor (CO2 = 770.203 kW) is utilized so that H1 is compressed in a single stage with an intermediate heat exchange in the HEN. After compression by CO2, the stream is cooled using the thermal utility C in the end of stream H3. Furthermore, one valve replaces the expander EX3. Thus, the cost associated with the construction of the equipment (heat exchangers, cooler, compressor and valve) is 690 kUS$/year, the cost of electricity is 350 kUS$/year, and approximately 113 kUS$/year is spent on cold services. These values together imply a total annualized cost of 1,153 kUS$/year, which corresponds to a 7% increase over that in the previous case in which coupling is considered. Despite the negligible capital cost of the valves compared with that of the turbines, the nature of the expansion causes slight variations in the temperature of the streams, requiring additional cold services to meet the thermal needs. The results of the decision variables and the HEN configurations for all three cases are provided in Table 2.

In Case 1, the mathematical model contains 466 continuous variables, 32 discrete variables and 500 constraints with 1,690 Jacobian elements (non-zeros), of which 304 are nonlinear. In Case 2, the mathematical model contains 475 continuous variables, 41 discrete variables and 530 constraints with 1,804 Jacobian elements (non-zeros), of which 328 are nonlinear. In Case 3, the mathematical model has 494 continuous variables, 47 discrete variables and 859 constraints with 2,771 Jacobian elements (non-zeros), of which 308 are nonlinear. In all cases, the CPU time did not exceed 20 seconds with the SBB solver under GAMS.

By considering additional passages to H1 and C1 one can increase the amount of pressure manipulation equipment; however, the investment cost may increase significantly, so that the economic infeasibility could outweigh any potential benefits. Moreover, increasing the number of stages increases the size of the model and, thus, the difficulty in solving it. In addition, one can model any losses in efficiency for real processes by adjusting the isentropic efficiencies of the compressors and expanders to below 1. Other factors affecting the capital cost annualization can be appreciated. The influence of these factors on the total cost of the HEN is analyzed in the next example.

Example 2. In this example, one hot stream H1 and one cold stream C1 are at constant pressure, whereas a second cold stream C2 is expanded from 0.4 to 0.1 MPa. The pressure manipulation route for C2 includes expansion, compression and expansion and requires a heat exchange in the HEN between stages. Thus, C2 behaves as C3 after the first expansion, as H2 after compression, and finally as C4 after the last expansion. The heat capacity and flow rates of all streams are known constants. The data are presented in Table 3. Figure 6 depicts a possible arrangement of the streams for this example. A superstructure with four stages and possible stream splits is considered for the HEN synthesis.

In this example, $\Delta T_{\min}$ = 4 K, $T^h{}_U$ = 383 K, $T^c{}_U$ = 93 K, κ = 1.352, η_t = 1, η_v = 1, and μ_s = 1.961 K/MPa. The unknown inlet temperatures can vary between 103 and 373 K, the pressure of the C3 stream is restricted to 0.1–0.4 MPa, and the pressure of the H2 stream is restricted to 0.1–0.6 MPa. The individual heat transfer coefficients for all streams are maintained at 0.1 kW/m^{2}K, and a hot and cold utility coefficient of 1.0 kW/m^{2}K is considered. An annualized capital cost factor of f = 0.18 (10% interest rate over 8 years) is assumed.

Different cases are studied. Initially, no expander and/or compressor are used. Then, the pressure levels are adjusted to promote integration between the heat and work, and three additional cases are presented with different constraints and possible equipment arrangements. In all cases, the total annualized cost minimization, consisting of the operating expenses and capital expenditures, is considered to be the objective function.

In Case 1, the HEN is designed without manipulating the pressure of stream C2, i.e., all streams are at constant pressure. The optimal HEN is obtained with three heat exchangers (A = 128.30 m^2, Q = 102.54 kW; A = 117.61 m^2, Q = 91.98 kW; and A = 126.47

m^2, Q = 168.76 kW), two heaters of the same area A = 7.74 m^2 located at the ends of streams C1 and C2 (Q = 47.46 and Q = 36.76 kW, respectively), and a cooler located in the end of H1 (A = 35.52 m^2, Q = 131.72 kW). In this case, no compression and/or expansion work is produced. The total annualized cost of the HEN with this configuration is 331 kUS$/year, in which 160 kUS$/year derives from the hot and cold services, and 171 kUS$/year is related to the capital investment in equipment.

Case 2 evaluates the manipulation of the pressure for C2. Thus, C2 is expanded between 0.4 and 0.1 MPa. Again, the optimal HEN consists of three heat exchangers, two heaters and one cooler. The respective areas of heat transfer (and heat exchange) equal 108.97 m^2 (122.39 kW); 100.85 m^2 (96.17 kW); 155.47 m^2 (204.63 kW); 7.74 m^2 (27.61 kW), 7.86 m^2 (84.04 kW), and 24.74 m^2 (71.82 kW). Furthermore, the process uses a turbine (EX1) with capacity of 87.34 kW. No compression work is consumed, so the electricity cost is zero. The optimal configuration of the HEN obtained for this case is depicted in Figure 7. The total annualized cost of the network with this configuration is 296 kUS$/year, with a capital expenditure for construction equipment of 187 kUS$/year and operational expenses of 109 kUS$/year. The total annualized cost is 11% below the total cost obtained for the previous case, which used no compression and/or expansion equipment, due to the reduced need for cooling services to cool the hot stream H1. In this case, the impact of the annualized cost factor f on the final HEN cost is evaluated by varying this factor. Therefore, values of f = 0.30 (25% interest rate over 8 years) and f = 0.43 (40% interest rate over 8 years) are considered. In both cases, the obtained network has the same configuration as that obtained previously for f = 0.18. However, the annualized total cost increases at a rate directly proportional to the increase in f. The respective values are 424 kUS$/year and 550 kUS$/year.

In Case 3, the HEN synthesis considers the possibility of coupling equipment with an efficiency of $\eta = 0.7$ and $\kappa = 1.51$ for both the turbine and the compressor. The results in this case indicate that the optimal HEN is obtained with three heat exchangers (A = 116.43 m^2, Q = 124.61 kW; A = 95.46 m^2, Q = 101.51 kW; and A = 154.1 m^2, Q = 188.44 kW), two heaters with areas of A = 7.74 and 7.89 m^2 located at the ends of streams C1 and C4 (Q = 25.39 and Q = 84.40 kW, respectively), and one cooler located in the end of H1 (A = 26.58 m^2, Q = 80.45 kW). In this case, only the second expander (EX2) is used, producing 76.84 kW. The total annualized cost of the HEN with this configuration is 303 kUS$/year, of which 117 kUS$/year derives from the hot and cold services, and 186 kUS$/year derives from the capital investment in equipment. Because no compressor is required, the cost of electricity equals zero. The value for the total annualized cost presents a saving of 8% over that of the HEN obtained without pressure manipulation (Case 1); even when the loss of efficiency is considered, the total cost of the process is reduced. Figure 8 depicts the configuration obtained for this case study.

In Case 4, the HEN synthesis allows for the selection between valves and turbines (i.e., the coupling operator is replaced by the selection operator for the expander equipment). In this case, the obtained HEN is formed by three heat exchangers, two heaters and one cooler with corresponding areas of thermal exchange (and heat exchange) of 128.27 m^2 (102.52 kW); 117.59 m^2 (92.03 kW); 126.71 m^2 (169.71 kW); 7.74 m^2 (47.48 kW), 7.74 m^2 (36.75 kW) and 35.38 m^2 (130.74 kW). Figure 9 depicts the configuration obtained for this case study. Furthermore, the expander (EX1) is replaced by a valve and no compressor is required. Thus, the electricity cost equals zero. However, because one valve is used to expand the streams, a larger quantity of cold services is required, increasing the operational expenses. The total annualized cost of the network with this configuration is 330 kUS$/year, with a capital expenditure for equipment construction of 171 kUS$/year and operational expenses of 159 kUS$/year. The total cost is 0.3 % below that obtained in Case 1, i.e., the expansion produced by the valve provides a small difference in the temperatures of the streams and thus in the quantity of heat available to reduce the required heat services. Because the expansion produced by the valve causes a temperature difference below that expected from a turbine, an increase of 9% is obtained relative to Case 3.

The results of the decision variables and HEN configurations for Cases 1 to 4 are presented in Table 4. In Case 1, the mathematical model has 65 continuous variables, 7 discrete variables and 67 constraints with 208 Jacobian elements (non-zeros), of which 32 are nonlinear. In Case 2, the mathematical model has 317 continuous variables, 23 discrete variables and 450 constraints with 1,382 Jacobian elements (non-zeros), of which 200 are nonlinear. In Case 3, the mathematical model has 322 continuous variables, 25 discrete variables and 460 constraints with 1,411 Jacobian elements (non-zeros), of which 200 are nonlinear. In Case 4, the mathematical model has 331 continuous variables, 29 discrete variables and 389 constraints with 1,264 Jacobian elements (non-zeros), of which 202 are nonlinear. The CPU time for Case 1 is 10 seconds (SBB solver) and 11 minutes (BARON solver) returning the same solution under both solvers; Cases 2 and Case 3 are solved in 42 seconds (SBB solver), and Case 4 is solved in 11 minutes (SBB solver). The BARON solver failed to return feasible solutions for Cases 2–4.

The accuracy of the model is evaluated under real conditions in the next example in which the proposed superstructure is used to optimize a process for producing LNG.

Example 3. In the offshore section of the energy chain for transporting and utilizing LNG, natural gas (NG) is liquefied to produce LNG, while liquid carbon dioxide (LCO_2) and liquid inert nitrogen (LIN) act as cold carriers (see Figure 1). The reheated nitrogen is emitted into the atmosphere under ambient conditions, while the high-pressure CO_2 is transferred to an offshore oil field. Because this is a real process, the heat capacity of the streams is not constant. Therefore, the flow rate of the NG is divided into three individual streams (H1–H3), which produce a reasonably good fit to the actual cooling curve. Likewise, the flow of liquid carbon dioxide is divided into two individual streams (C1 and C2), and the cold nitrogen stream is divided into three streams (C3–C5) to more precisely adjust the heat capacities. The inlet and outlet temperatures of the NG and LCO_2 streams and the inlet temperature of the LIN stream are fixed, as are the pressures of the NG and LCO_2 streams and the inlet and outlet pressures of the LIN stream. The intermediate temperatures and pressures and the outlet temperature of the LIN stream are the optimization variables in the problem. All stream flow rates are fixed, and the process design calculations are based on a production rate of 1.0 kg/s LNG. The stream data for this example are provided in Table 5. The nitrogen flow at high pressure (10 MPa) is expanded in accordance with Figure 10. Therefore, three possible cold streams and one hot stream result from two expansion cycles and one compression cycle, with heating and cooling during the intermediate cycle. The pressure manipulation route for C5 (LIN) is composed of expansion, compression and expansion and results in the streams C6, H4, and C7, respectively. In general, the process is modeled using four hot streams (H1–H4) and seven cold streams (C1–C7) with three possible pressure manipulations using EX1, CO1 and EX2 equipment. More details regarding the process can be obtained in references[3,32–35].

Given the high pressure and low temperature of the liquid nitrogen flow, the expansion and compression are far from ideal. Thus, a non-ideal polytrophic exponent of 1.51 and an efficiency factor of 0.7 are assumed. Moreover, $\Delta T_{\min}$ = 4 K and μ_s = 1.961 K/MPa. Additionally, water at 383.15 K is used as the hot utility and liquid inert nitrogen at a lower pressure is used as the cold utility ($T^c{}_U$ = 93.15 K). The unknown inlet temperatures can vary from 95 to 380 K, the pressure of the stream H4 is restricted between 1 and 3.5 MPa, and that of the stream C6 between 0.3 and 1 MPa. Thus, if the process can capture 90% of the generated carbon dioxide, the LCO_2 flow rate to the offshore process is 2.46 kg/s. The individual heat transfer coefficients for all streams are maintained at 0.1 kW/m^{2}K, and those for the hot and cold utilities at 1.0 kW/m^{2}K. The factor for the annualized capital cost f = 0.18 (10% interest rate over 8 years) is used. For the HEN synthesis, a superstructure with 7 stages and the possibility of stream splits are considered.

Three different cases are studied. Initially, the pressure levels are adjusted to promote integration between the heat and work, considering the possibility of coupling the equipment (turbines with compressors) and selecting between the valves and turbines. The total annualized cost, consisting of the operational expenses and capital investment is minimized. The LIN flow rate is fixed at 1.0 kg/s. In Case 1, the optimal HEN is obtained using five heat exchangers with areas equal to 50.26 m^2 (Q = 107.14 kW), 15.12 m^2 (Q = 77.27 kW), 7.74 m^2 (Q = 4.68 kW), 28.35 m^2 (Q = 85.86 kW), and 88.12 m^2 (Q = 162.97 kW); two coolers (A = 24.26 m^2 with Q = 262.63 kW and A = 80.61 m^2 with Q = 162.05 kW) and two heaters (A = 12.35 m^2 with Q = 163.14 kW and A = 15.37 m^2 with Q = 140.55 kW). Only two expansion cycles through the turbines EX1 and EX2 are required, and because no compressor is required, the electricity cost is zero. The expansion work produced by EX1 equals 97.67 kW, and the work produced by EX2 equals 90.59 kW, which becomes available for use in other aspects of the process. Figure 11 depicts the optimal HEN obtained for this case. The total annualized cost of the HEN with this configuration is 785 kUS$/year, of which 527 kUS$/year corresponds to expenses from the hot (102 kUS$/year) and cold services (425 kUS$/year), and 258 kUS$/year is related to the capital investment in equipment.

In Case 2, the HEN is designed by coupling the turbine and compressor. Thus, the possibility of equipment coupling is fixed (y^{CoEx} = 1). The optimal HEN is obtained with eight heat exchangers with areas of 9.86 m^2 (Q = 75.42 kW), 10.93 m^2 (Q = 49.48 kW), 21.29 m^2 (Q = 60.22 kW), 36.59 m^2 (Q = 28.27 kW), 46.11 m^2 (Q = 113.67 kW), 74.45 m^2 (Q = 25.64 kW), 16.04 m^2 (Q = 65.40 kW), and 39.58 m^2 (Q = 92.23 kW); two coolers (A = 21.23 m^2 with Q = 222.87 kW and A = 82.90 m^2 with Q = 178.89 kW) and one heater (A = 25.09 m^2 with Q = 247.69 kW). One must use two turbines and one compressor in which the expander EX2 is coupled to CO1 (WC = WE = 178.87 kW), thus the cost of electricity is zero. The expansion work produced by EX1 is equal to 101.67 kW, which becomes available for use in other sections of the process. Figure 12 presents the optimal HEN obtained for this case. The total annualized cost of the HEN with this configuration is 1,018 kUS$/year, of which 485 kUS$/year derives from the hot (83 kUS$/year) and cold (402 kUS$/year) services, and 533 kUS$/year is related to the capital investment in equipment. In this case, although the total cost of the network is 23% over that of the previous case, the costs related to the cold and hot services decrease by 5% and 18%, respectively, due to the use of the compressor. Thus, the addition of one more pressure manipulation stage can supply energy (heating and cooling) to the streams in such a way that the need for hot and cold utilities is significantly reduced.

The objectives of Case 3 are to devise a process without manipulating the pressure of the LIN stream (i.e., liquid nitrogen is available only as a cold utility) and to determine the point at which the pressure manipulation of LIN stream becomes economically viable. In this case, a superstructure with 3 stages and the possibility of stream splits is considered for the HEN synthesis. Hence, only the heat integration between the NG and LCO_2 streams is allowed. The optimal HEN is composed of three heat exchangers with areas of 44.45 m^2 (Q = 59.75 kW), 69.21 m^2 (Q = 129.33 kW) and 86.11 m^2 (Q = 103.39 kW); two coolers (A = 22.95 m^2 with Q = 245.10 kW and A = 99.22 m^2 with Q = 325.03 kW) and one heater (A = 13.16 m^2 with Q = 118.36 kW). Figure 13 depicts the optimal configuration obtained for this case. The total annualized cost of a HEN with this configuration is 766 kUS$/year, of which 610 kUS$/year derives from the hot (40 kUS$/year) and cold (570 kUS$/year) services, and 156 kUS$/year is related to the capital investment in equipment. In this case, total annualized network cost decreases by 2% over that in Case 1. However, the expenses related to the cold utilities increase by 34% (extremely expensive in this process) over that in Case 1.

In addition, the cost related to the cold utility versus the total cost of the network is studied. Thus, if the cost of the cold utility increases by 5% (i.e., 1,050 US$/year kW), the network obtained in Case 1 has a total cost of 807 kUS$/year, of which 446 kUS$/year derives from the cold services, and the network obtained in Case 3 (without pressure manipulation) has a total cost of 795 kUS$/year, of which the expenses related to the cold services are 599 kUS$/year. If the cost of cold utility increases 10% (i.e., 1,100 US$/year kW), the network obtained in Case 1 has a total cost of 828 kUS$/year, of which 467 kUS$/year derives from the cold services, and the network obtained in Case 3 (without pressure manipulation) has a total cost of 823 kUS$/year, of which 627 kUS$/year derives from the cold services. Given these results, the total cost of the network without pressure manipulation is below that of the network that utilizes expanders and compressors. However, if the cost of the cold utility is increased 15% (i.e., 1,150 US$/year kW), the network obtained in Case 1 has a total cost of 849 kUS$/year, of which 488 kUS$/year derives from the cold services, and the network obtained in Case 3 (without pressure manipulation) has a total cost of 852 kUS$/year, of which 656 kUS$/year derives from the cold services. Therefore, a 15% increase in the cost related to the cold utility is the point at which the HEN with pressure manipulation becomes economically beneficial.

The decision variables and the optimal HEN configurations obtained for the three case studies are presented in Table 6. In this example, the mathematical model contains 1,439 continuous variables, 173 discrete variables and 3686 constraints with 14163 Jacobian elements (non-zeros), of which 1,199 are nonlinear. The CPU times did not exceed 20 minutes with the SBB solver under GAMS.

Conclusions

A new mathematical model for HEN synthesis is proposed to optimize the integration between heat and work by manipulating the pressure of the process streams. The developed approach, implemented in GAMS, combines generalized disjunctive programming (GDP) and mixed-integer nonlinear programming (MINLP) formulation and is based on the HEN superstructure proposed by Yee and Grossmann[26]. The superstructure is comprised of various stages in which heat exchange may occur between hot and cold streams. Furthermore, in the HEN synthesis, stream splits are considered possible, constant heat capacity flow rate and isothermal mixing are assumed, and heaters and coolers are placed at the ends of the streams.

The conventional HEN synthesis problem is expanded to include process streams that may undergo changes in pressure via expanders and compressors. Thus, intermediate stream pressures and temperatures should be considered unknown variables requiring optimization. The streams that are subject to pressure manipulation must be connected to the HEN via compressors and expanders; therefore, the stream outlet state of the pressure manipulation equipment should correspond to the inlet state in the HEN superstructure. The hot and cold streams should follow a specific pressure manipulation route to reduce the energy requirements. If this route involving compression and expansion is chosen correctly (i.e., hot stream: compression, expansion and compression; cold stream: expansion, compression and expansion), it may supply energy to the streams, which should reduce the need for hot and cold utilities. Thus, the resulting design integrates the heat exchange and pressure manipulation equipment. Several possibilities for HENs involving compressors and expanders (turbines and valves) are studied to optimize the HEN design by minimizing the total annualized costs composed of the operational and capital expenses for the various network components.

The mathematical formulation is significantly more complex than that for a standard HEN synthesis problem because it involves a larger number of unknown variables and constraints, which, when combined with the variable process conditions (temperature and pressure), can make the problem difficult to solve in a reasonable time. Moreover, no clear distinction exists between the hot and cold streams or between the process streams and the utilities. The flows can change identity: a cold stream can temporarily behave like a hot stream, and vice versa. Some process streams can act as utilities, serving as energy sources or sinks at temperatures outside the range generated by the available utilities. In addition to the larger number of variables and constraints, a GDP formulation is required to select the equipment (valves or turbines) and to consider the possibility of coupling the compressor with a turbine.

Three examples are studied to verify the accuracy of the proposed model, including a cryogenic application. The first two examples demonstrate that optimizing the integration between the heat and work decreases the quantity of hot and cold utilities needed. Consequently, the total annualized costs are reduced due the reduction of operational expenses related to heating and cooling the process flows even when one considers the efficiency losses of the compressors and turbines inherent in real processes. The total annualized costs are also reduced when the turbines and compressors are coupled (companders) to allow the expansion work to satisfy the energy requirement of the compressors, which nullifies the electricity costs. In contrast, the use of valves generally increases the process cost despite its low initial capital investment because a larger quantity of cold utilities are required to promote stream cooling. In Example 3, the ability of the model to design a HEN with pressure recovery under real conditions is highlighted by the results of its application to an LNG processing plant. In this example, by appropriately expanding and compressing the process streams, the hot and cold utility requirements may be significantly reduced. Furthermore, the relationship between the expenses related to the cold utility and the total cost of the network reaches a point at which the implementation of the HEN with pressure manipulation provides economic benefits.

In all examples, a maximum of three pressure manipulations are allowed; however, additional compression and expansion stages can be easily considered in the model. Nevertheless, in the examples, most streams use only one or two stages of pressure manipulation, and the last stage is generally a simple bypass. Moreover, the marginal effect of additional pressure equipment does not justify the increase in capital cost.

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Notation

Roman letters

A = heat exchanger area

C = cost

CC = cost parameter for cooling

CE = cost parameter for electricity

CH = cost parameter for heating

Cp = heat capacity

CPO = cost of equipment unit

f = annualization factor for capital cost

F = streams flow rate

FBM = correlation factor for equipment cost

M = parameter for big-M formulation

N_C = number of cold streams

N_H = number of hot streams

N_S = number of stages in the superstructure

p = pressure

Q = heat duty

T = temperature

$\tilde{T}$ = temperature of reversible process

$\Delta T_{\min}$ = minimum temperature approach

WE = expansion work

WC = compression work

y = binary variable that define the heat exchange between hot and cold streams

y^{CoEx} = binary variable that define the coupling of expanders and compressors

y^{ex} = binary variable that define the choice of expanders

y^{heater} = binary variable that define the heat exchange between cold stream and hot utility

y^{val} = binary variable that define the choice of valves

y^{cooler} = binary variable that define the heat exchange between hot stream and cold utility

Acronyms

BB	branch-and-bound
CEPCI	chemical engineering plant cost index
GAMS	general algebraic modeling system
GBD	generalized benders decomposition
GDP	generalized disjunctive programming
HEN	heat exchanger network
LCO_2	liquid carbon dioxide
LIN	liquid inert nitrogen
LNG	liquefied natural gas
MILP	mixed-integer programming
MINLP	mixed-integer nonlinear programming
NG	natural gas
NLP	nonlinear programming
OA	outer-approximation

Greek letters

η = isentropic efficiency

μ = Joule-Thompson coefficient

κ = polytrophic exponent

Subscripts

c = cold fluid

ele = electricity

h = hot fluid

Hex = heat exchanger

k = stages of superstructure

m = number of heaters

n = number of coolers

s = process streams

t = expander

U = utilities

v = compressor

w = valves

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List of Figures Captions

Figure 11. Optimal HEN configuration obtained for Example 3 - Case 1.

Figure 12. Optimal HEN configuration obtained for Example 3 - Case 2.

Figure 13. Optimal HEN configuration obtained for Example 3 - Case 3.

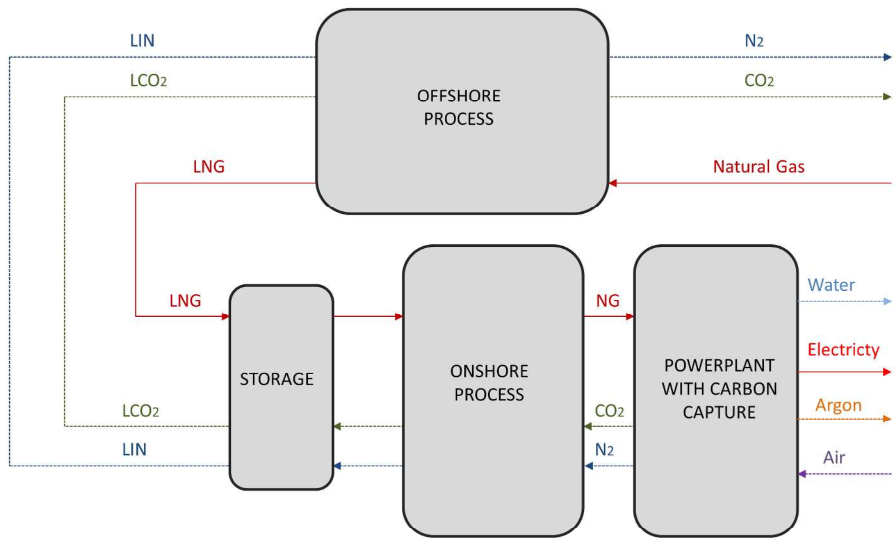

Figure 1. Energy chain for transport and utilization of liquefied natural gas (Adapted from Wechsung et al.3).
254x190mm (300 x 300 DPI)

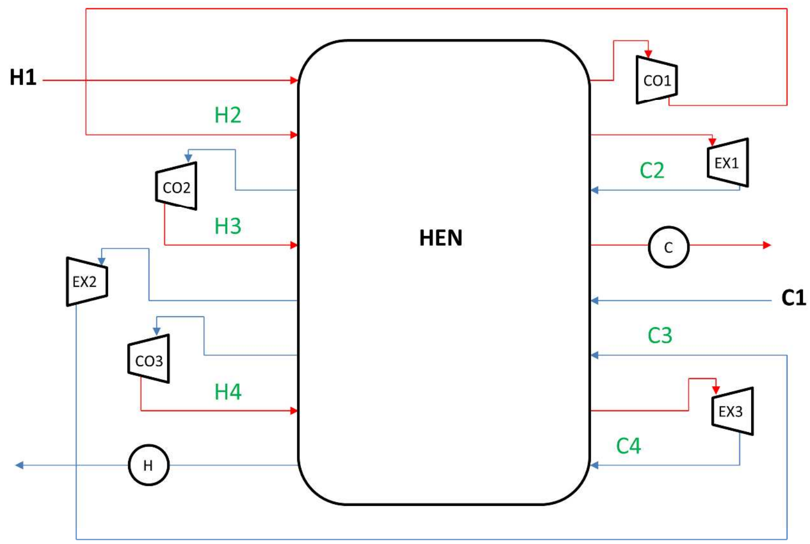

Figure 2. Possible streams arrangement for Example 1.
254x190mm (300 x 300 DPI)

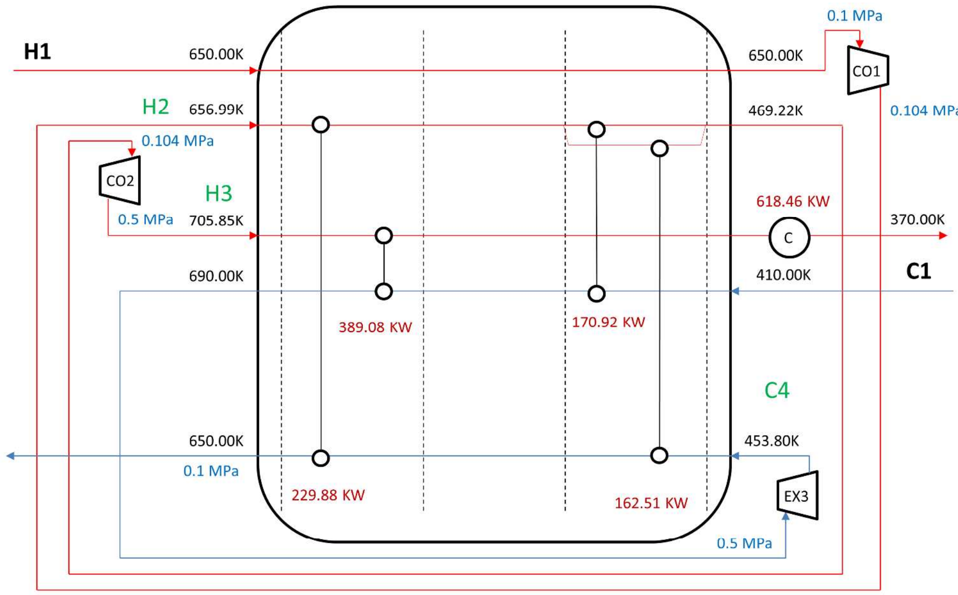

Figure 3. Optimal HEN configuration obtained for Example 1 - Case 1.
254x190mm (300 x 300 DPI)

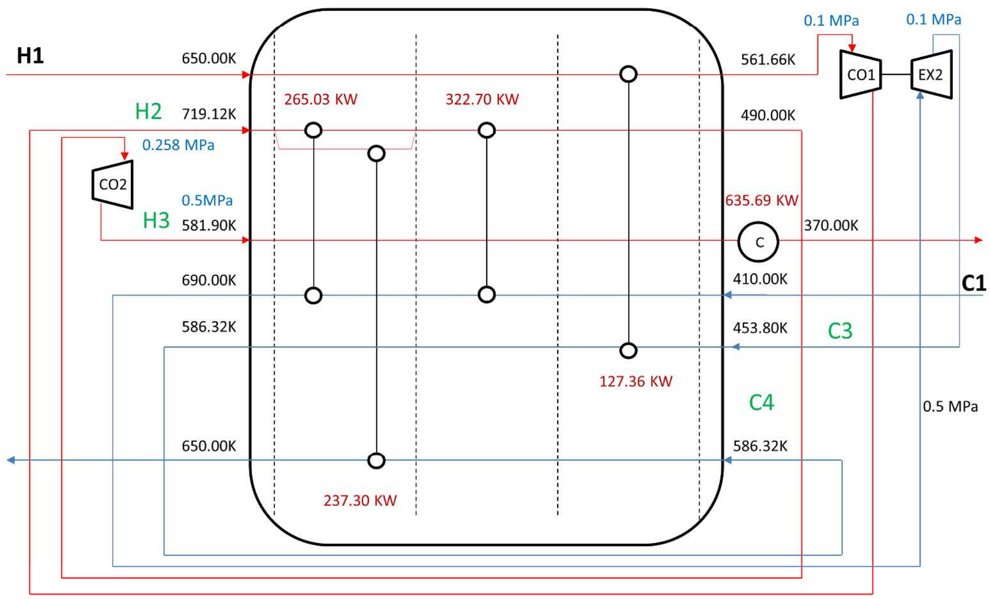

Figure 4. Optimal HEN configuration obtained for Example 1 - Case 2.
254x190mm (300 x 300 DPI)

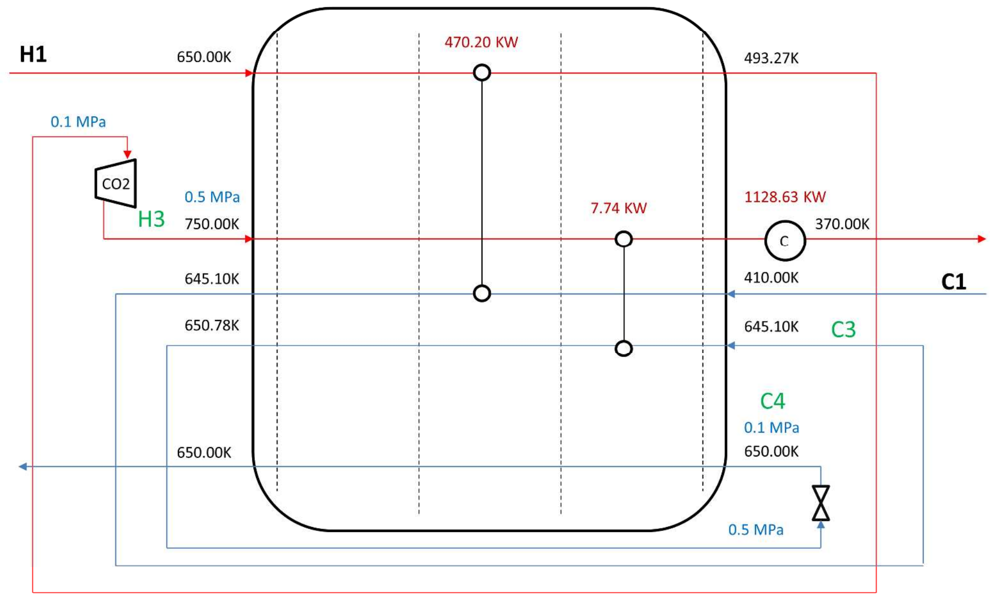

Figure 5. Optimal HEN configuration obtained for Example 1 - Case 3.
254x190mm (300 x 300 DPI)

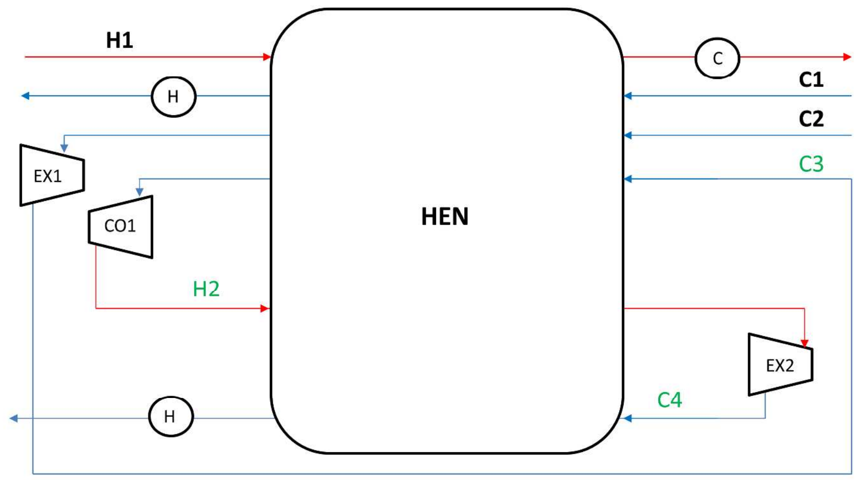

Figure 6. Possible streams arrangement for Example 2.
254x190mm (300 x 300 DPI)

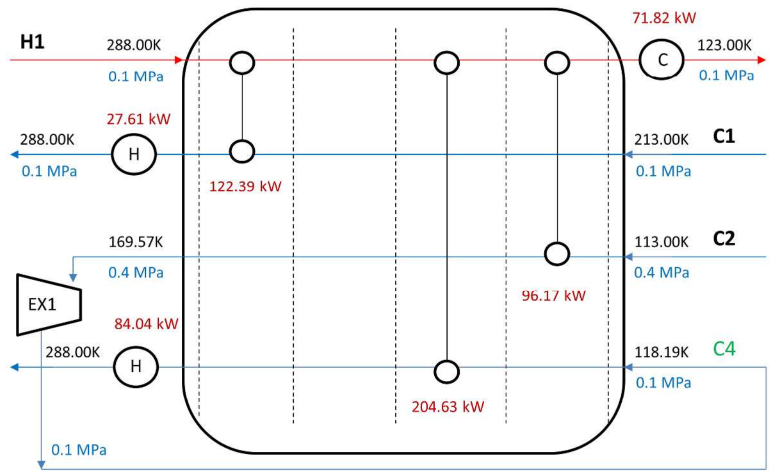

Figure 7. Optimal HEN configuration obtained for Example 2 - Case 2.
254x190mm (300 x 300 DPI)

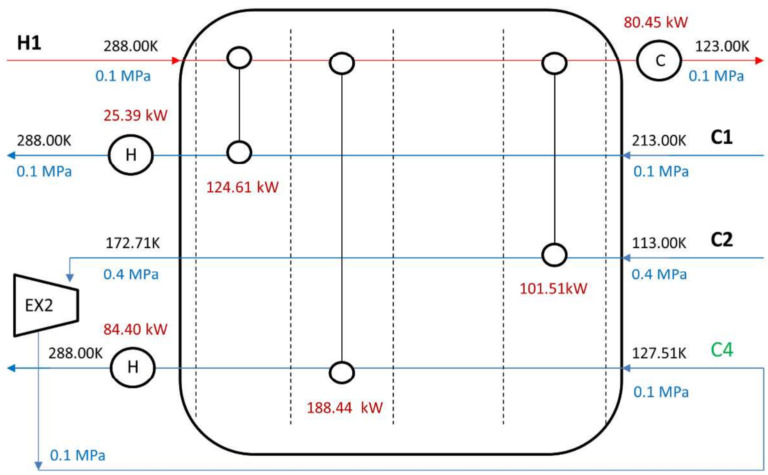

Figure 8. Optimal HEN configuration obtained for Example 2 - Case 3.
254x190mm (300 x 300 DPI)

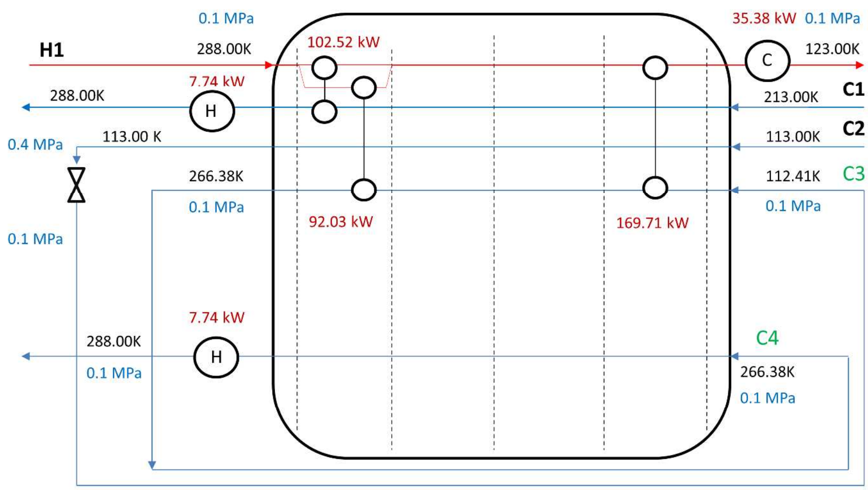

Figure 9. Optimal HEN configuration obtained for Example 2 - Case 4.
254x190mm (300 x 300 DPI)

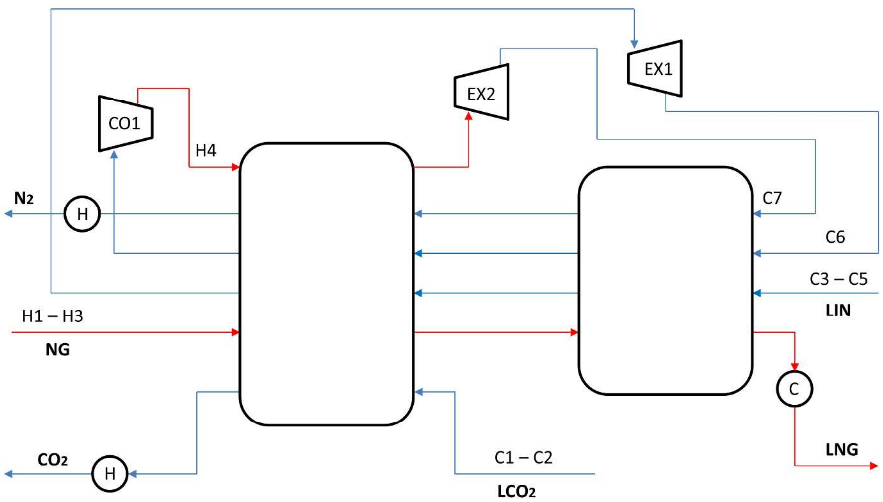

Figure 10. Process diagram for the production of LNG.
254x190mm (300 x 300 DPI)

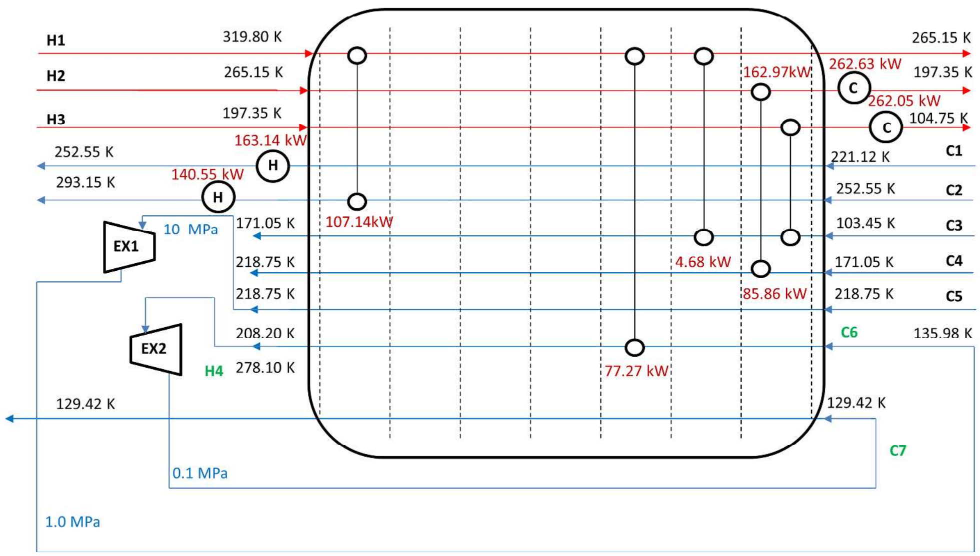

Figure 11. Optimal HEN configuration obtained for Example 3 - Case 1.
254x190mm (300 x 300 DPI)

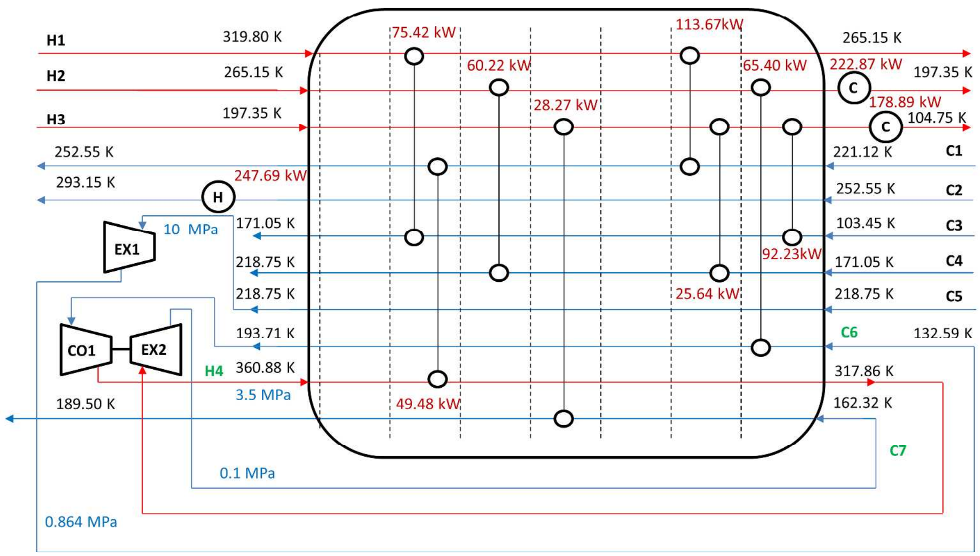

Figure 12. Optimal HEN configuration obtained for Example 3 - Case 2.
254x190mm (300 x 300 DPI)

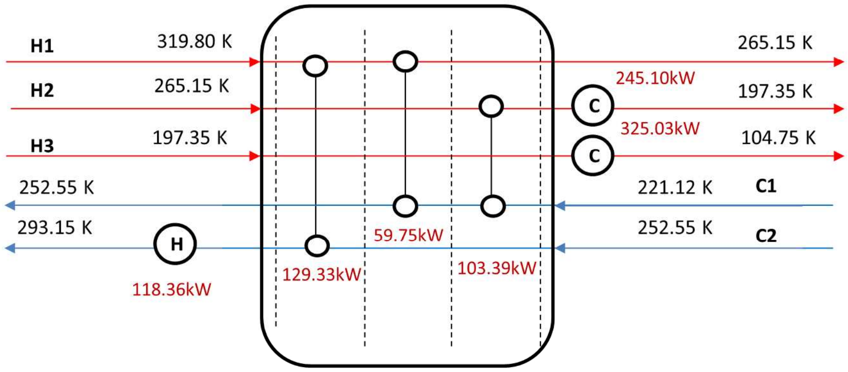

Figure 13. Optimal HEN configuration obtained for Example 3 - Case 3.
199x90mm (300 x 300 DPI)

Table 1. Stream Data for Example 1

Stream	h_s (kW/m^{2}K)	F_sCp_s (kW/K)	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)
H1	0.1	3.0	650	-	0.1
H2	0.1	3.0	-	-	-
C2	0.1	3.0	-	-	-
H3	0.1	3.0	-	370	0.5
C1	0.1	2.0	410	-	0.5
C3	0.1	2.0	-	-	-
H4	0.1	2.0	-	-	-
C4	0.1	2.0	-	650	0.1

Cost data: CC = 100 US$/year kW; CE = 455.04 US$/year kW; CH = 337 US$/year kW

Table 2. Results obtained for the Decision Variables in Example 1

Case 1				*Case 2*				*Case 3*			
Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)	Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)	Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)
H1	-	650.00	-	H1	-	561.66	-	H1	-	493.27	-
H2	656.99	469.22	0.104	H2	719.12	490.00	0.258	H2	493.27	493.27	0.100
C2	469.22	469.22	0.104	C2	490.00	490.00	0.258	C2	493.27	493.27	0.100
H3	705.85	-	-	H3	581.90		-	H3	750.00	-	-
C1	-	690.00	-	C1	-	690.00	-	C1	-	645.10	-
C3	690.00	690.00	0.500	C3	453.80	586.32	0.100	C3	645.10	650.78	0.500
H4	690.00	690.00	0.500	H4	586.32	586.32	0.100	H4	650.78	650.78	0.500
C4	453.80	-	-	C4	586.32	-	-	C4	650.00	-	-
HEN	Q (kW)	A (m^2)	W (kW)	HEN	Q (kW)	A (m^2)	W (kW)	HEN	Q (kW)	A (m^2)	W (kW)
H2.C4.k1	229.88	227.31	-	H2.C1.k1	237.30	171.69	-	H1.C1.k2	470.20	358.96	-
H3.C1.k1	389.08	196.91	-	H2.C4.k1	127.36	80.88	-	H3.C3.k3	11.37	7.74	-
H2.C1.k3	170.92	47.95	-	H2.C1.k2	322.70	134.14	-	H3	1128.63	63.70	-
H2.C4.k3	162.51	117.45	-	H1.C3.k3	265.03	63.24	-	CO2	-	-	770.20
H3	618.46	47.57	-	H3	635.69	48.26	-	valve	-	-	-
CO1	-	-	20.96	CO1	-	-	472.39				
CO2	-	-	709.89	CO2	-	-	275.69				
EX3	-	-	472.39	EX2	-	-	472.39				
C_{total} (kUS$/year)			1,207	C_{total} (kUS$/year)			1,081	C_{total} (kUS$/year)			1,153

Table 3. Stream Data for Example 2

Stream	h_s (kW/m^{2}K)	F_sCp_s (kW/K)	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)
H1	0.1	3.0	288	123	0.1
C1	0.1	2.0	213	288	0.1
C2	0.1	1.7	113	-	0.4
C3	0.1	1.7	-	-	-
H2	0.1	1.7	-	-	-
C4	0.1	1.7	-	288	0.1

Cost data: CC = 1,000 US$/year kW; CE = 455.04 US$/year kW; CH = 337 US$/year kW

Table 4. Results obtained for the Decision Variables in Example 2

Case 1

Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)
C2	-	-	-
C3	-	-	-
H2	-		-
C4	-	-	-

HEN	Q (kW)	A (m^2)	W (kW)
H1.C1.k1	102.54	128.30	-
H1.C2.k1	91.98	117.61	-
H1.C2.k2	168.76	126.47	-
C1	47.46	7.74	-
C2	36.76	7.74	-
H1	131.72	35.52	-
C_{total} (kUS$/year)			331

Case 2

Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)
C2	-	169.57	-
C3	118.19	118.19	0.1
H2	118.19	118.19	0.1
C4	118.19	-	-

HEN	Q (kW)	A (m^2)	W (kW)
H1.C1.k1	122.39	108.97	-
H1.C4.k3	204.63	155.47	-
H1.C2.k4	96.17	100.85	-
C1	27.61	7.74	-
C4	84.04	7.86	-
H1	71.82	24.74	-
EX1	-	-	87.34
C_{total} (kUS$/year)			296

Case 3

Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)
C2	-	172.71	-
C3	172.71	172.71	0.4
H2	172.71	172.71	0.4
C4	127.51	-	-

HEN	Q (kW)	A (m^2)	W (kW)
H1.C1.k1	124.61	116.43	-
H1.C4.k2	188.44	154.10	-
H1.C2.k4	101.51	95.46	-
C1	25.39	7.74	-
C4	84.40	7.89	-
H1	80.45	26.58	-
EX2	-	-	76.84
C_{total} (kUS$/year)			303

Case 4

Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)
C2	-	113.00	-
C3	112.41	266.38	0.1
H2	266.38	266.38	0.1
C4	266.38	-	-

HEN	Q (kW)	A (m^2)	W (kW)
H1.C1.k1	102.52	128.27	-
H1.C3.k1	92.03	117.59	-
H1.C3.k4	169.71	126.71	-
C1	47.48	7.74	-
C4	36.75	7.74	-
H1	130.74	35.38	-
valve	-	-	-
C_{total} (kUS$/year)			330

Table 5. Stream Data for Example 3

Stream	h (kW/m^{2}K)	F_s (kg/s)	Cp_s (kJ/kg K)	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)
H1	0.1	1.0	3.46	319.80	265.15	10.0
H2	0.1	1.0	5.14	265.15	197.35	10.0
H3	0.1	1.0	3.51	197.35	104.75	10.0
H4	0.1	-	1.15	-	-	-
C1	0.1	2.46	2.11	221.12	252.55	6.0
C2	0.1	2.46	2.48	252.55	293.15	6.0
C3	0.1	-	2.48	103.45	171.05	10.0
C4	0.1	-	1.80	171.05	218.75	10.0
C5	0.1	-	1.18	218.75	-	10.0
C6	0.1	-	1.07	-	-	-
C7	0.1	-	1.04	-	-	0.1

Cost data: CC = 1,000 US$/year kW; CE = 455.04 US$/year kW; CH = 337 US$/year kW

Table 6. Results obtained for the Decision Variables in Example 3

Case 1				***Case 2***				***Case 3***		
Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)	Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)	p_s (MPa)	Stream	$T_{s,in}$ (K)	$T_{s,out}$ (K)
C5	-	218.75	-	C5	-	218.75	-	C5	-	-
C6	135.98	208.20	1.0	C6	132.59	193.71	0.86	C6	-	-
H4	208.20	208.20	1.0	H4	360.88	317.86	3.50	H4	-	-
C7	129.42	129.42	-	C7	162.32	189.50	-	C7	-	-
HEN	Q (kW)	A (m^2)	W (kW)	HEN	Q (kW)	A (m^2)	W (kW)	HEN	Q (kW)	A (m^2)
H1.C2.k1	107.14	50.26	-	H1.C3.k2	75.42	9.86	-	H1.C2.k1	129.33	69.21
H1.C6.k5	77.27	15.12	-	H4.C1.k2	49.48	10.93	-	H1.C1.k2	59.75	44.45
H1.C3.k6	4.68	7.74	-	H2.C4.k3	60.22	21.29	-	H2.C2.k3	103.39	86.11
H2.C4.k7	85.86	28.35	-	H3.C7.k4	282.23	36.59	-	C2	118.36	13.16
H3.C3.k7	162.97	88.12	-	H1.C1.k6	113.67	46.11		H2	245.10	22.95
C1	163.14	12.35	-	H3.C4.k6	25.64	74.45		H3	325.03	99.22
C2	140.55	15.37	-	H2.C6.k7	65.40	16.04				
H2	262.63	24.26	-	H3.C3.k7	92.23	39.58				
H3	262.05	80.61	-	C2	247.69	25.09				
			-	H2	222.87	21.23	-			
EX1	-	-	97.67	H3	178.89	82.90				
EX2	-	-	90.59	CO1	-	-	178.87			
				EX1	-	-	101.67			
	-	-		EX2	-	-	178.87			
C_{total} (kUS$/year)			785	C_{total} (kUS$/year)			1,018	C_{total} (kUS$/year)		766