

Author's Accepted Manuscript

Simultaneous synthesis of work exchange networks with heat integration

Viviani C. Onishi, Mauro A.S.S. Ravagnani, José A. Caballero



www.elsevier.com/locate/ces

PII: S0009-2509(14)00129-8
DOI: <http://dx.doi.org/10.1016/j.ces.2014.03.018>
Reference: CES11569

To appear in: *Chemical Engineering Science*

Received date: 31 October 2013
Revised date: 23 January 2014
Accepted date: 17 March 2014

Cite this article as: Viviani C. Onishi, Mauro A.S.S. Ravagnani, José A. Caballero, Simultaneous synthesis of work exchange networks with heat integration, *Chemical Engineering Science*, <http://dx.doi.org/10.1016/j.ces.2014.03.018>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Simultaneous synthesis of work exchange networks with heat integration

Viviani C. Onishi ^{a,b,c,*}, Mauro A. S. S. Ravagnani ^a, José A. Caballero ^b

^a Department of Chemical Engineering, State University of Maringá, Av. Colombo 5790, 87020-900, Maringá, PR, Brazil. E-mail addresses: pg51551@uem.br, ravag@deq.uem.br

^b Department of Chemical Engineering, University of Alicante, Ap Correos 99, 03080 Alicante, Spain. E-mail address: caballer@ua.es

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

* Corresponding author. Tel: +34 965903400. E-mail address: pg51551@uem.br, viviani.onishi@hotmail.com (Viviani C. Onishi).

Abstract

The optimal integration of work and its interaction with heat can represent large energy savings in industrial plants. This paper introduces a new optimization model for the simultaneous synthesis of work exchange networks (WENs), with heat integration for the optimal pressure recovery of process gaseous streams. The proposed approach for the WEN synthesis is analogous to the well-known problem of synthesis of heat exchanger networks (HENs). Thus, there is work exchange between high-pressure (HP) and low-pressure (LP) streams, achieved by pressure manipulation equipment running on common axes. The model allows the use of several units of single-shaft-turbine-compressor (SSTC), as well as stand-alone compressors, turbines and valves. Helper motors and generators are used to respond to any demand and excess of energy. Moreover, between the WEN stages the streams are sent to the HEN to promote thermal recovery, aiming to enhance the work integration. A multi-stage superstructure is proposed to represent the process. The WEN superstructure is optimized in a mixed-integer nonlinear programming (MINLP) formulation and solved with the GAMS software, with the goal of minimizing the total annualized cost. Three examples are conducted to verify the accuracy of the proposed method. In all case studies, the heat integration between WEN stages is essential to improve the pressure recovery, and to reduce the total costs involved in the process.

Keywords: Optimization; Mixed-integer nonlinear programming (MINLP); Work exchange network (WEN); Heat exchanger network (HEN); Heat integration; Pressure recovery

1. Introduction

The energy efficiency is crucial in transformation processes, since it is responsible for a large portion of expenditures and acts decisively on environmental aspects. One of the main reasons to develop techniques for efficient and sustainable energy use is the increasing global demand, allied to the high cost of energy due to the rapid decrease in the availability of fossil fuels. Other significant reasons include the technological barriers and forbidding prices of renewable energy, the strict standards that regulate carbon dioxide emissions, as an attempt to palliate the greenhouse effect and its consequences (Gharaie et al., 2013; Hasan et al., 2010; Huang and Karimi, 2013; Razib et al., 2012; Wechsung et al., 2011). The minimization of environmental impacts can be achieved by increasing energy efficiency in industrial plants, particularly through the reduction of energy consumption, adoption of innovative strategies and development of more efficient processing techniques (Lara et al., 2013; Morar and Agachi, 2010).

The optimization of heat recovery is critical to solve the problem of the efficient use of energy and, consequently, to promote the reduction of gaseous emissions and consumption of oil and natural gas, since the reduction of energy consumption is closely linked to improvement of heat transfer (Cheng and Liang, 2012a; Kaluri and Basak, 2011; Onishi et al., 2013a; Wang et al., 2011). Thereby, harnessing energy from process streams through thermal integration between heat exchangers and cooling and/or heating systems is one of the most effective ways to reduce costs. The optimal synthesis of heat exchanger networks (HENs) consists in promoting the thermal integration of the system via an efficient network design, in economic and thermodynamic terms, in which the number of heat exchangers units and utilities consumption are minimal. This result can be obtained by minimizing the heat exchange area (Gorji-Bandpy et al., 2011; Serna and Jiménez, 2004),

and/or the total cost of the HEN—relative to the cost of capital investment in the units of the network and operational expenses—(Al-mutairi, 2010; Björk and Nordman, 2005; Escobar and Trierweiler, 2013; Frausto-Hernández et al., 2003; Huang and Karimi, 2013; Ravagnani and Caballero, 2007; Serna-González and Ponce-Ortega, 2011; Sors and Kravanja, 2002; Vaskan et al., 2012), and/or by minimizing other parameters such as exergy or entropy of the system (Cheng and Liang, 2012b, 2012c; Wechsung et al., 2011).

The HEN is essential in many industrial processes, including food and pharmaceutical industries, chemical plants, distillation of crude oil and cooling water systems. These industries are responsible for the consumption of large amounts of energy, being the process of heat transfer one of the most expensive (Allen et al., 2009; Vaklieva-Bancheva et al. 1996). For this reason, over the past few decades, the research in the area of HEN synthesis has received large attention from the scientific community, and significant progress has been made with considerable impact on the industry (Al-mutairi, 2010; Escobar and Trierweiler, 2013; Furman and Sahinidis, 2002; Huang and Karimi, 2013). Among the first works published with proposals to solve the problem of HEN synthesis are the papers of Hwa (1965), using separable programming methods, and Kesler and Parker (1969), using linear programming. Important literature reviews were also published by Jezowski (1994a, 1994b), Gundersen and Naess (1988), and Furman and Sahinidis (2002).

Despite the considerable effort to optimize heat integration and the outstanding results already achieved in HEN synthesis, other forms of energy are often available in processing plants such as, for example, work. Handling pressure is responsible for considerable energy consumption, and it is especially important in oil refineries, synthetic processes like ammonia and methanol synthesis, and cryogenic processes such as the production of liquefied natural gas (LNG). This source of energy—work—has been poorly

explored in synthesis of process, in spite of its higher cost in comparison with heat. In fact, compressors and turbines correspond to some of the most expensive equipment in industries, surpassing the value of heat exchange equipment. Given the urgency of achieving this important industrial goal focused on improving energy efficiency, the integration of work, and a closer interaction between work and heat should be considered as viable alternatives. Therefore, it is possible to integrate both work and heat in the same network for the purpose of energy conservation (Razib et al., 2012).

Aspelund et al. (2007) presented a heuristic graphical method based on Extended Pinch Analysis and Design (ExPANd) to minimize energy requirements under sub-ambient conditions. In their work, compressors and turbines are used separately, and no mention is made to the use of combinations between these pressure manipulation equipment operating on a same axis. Furthermore, the economic aspects have not been examined, only the aspects related to the exergy analysis of the system were evaluated. This type of analysis can lead to processes that on one hand are highly effective, but on the other hand are economically impracticable. Moreover, it is necessary to consider that the very nature of heuristic methods can take to sub-optimal solutions.

Wechsung et al. (2011) proposed a model for the HENs synthesis, wherein the streams are subjected to pressure manipulation. The authors combine pinch analysis, exergy analysis and mathematical programming to obtain an optimal network with minimal irreversibility. In this study, an industrial application, relating to the LNG production, demonstrates that a particular route of compression and expansion of gas flows can significantly reduce the total irreversibility in HENs. In Onishi et al. (2013b), a superstructure for simultaneous synthesis of HENs is presented, considering the adjustment of pressure levels of process streams to improve heat integration. The model is formulated

using generalized disjunctive programming (GDP) and reformulated in mixed-integer nonlinear programming (MINLP). Several configuration possibilities involving compressors, turbines and valves are studied, with the goal of minimizing the total annualized cost of the network. The authors demonstrate that the optimal integration between heat and work can reduce the amount of necessary utilities, decreasing the costs involved in the process. However, in these works the pressure manipulation equipment were considered independently, i.e., as stand-alone equipment, or just allowing the coupling between one compressor and one turbine on a single common shaft, as in Onishi et al. (2013b).

Huang and Fan (1996) define the WEN as a work exchange network between two or more transfer units, and propose the operational principles for work exchange among two streams. Razib et al. (2012) introduces the WEN terminology to denote the synthesis problem of work exchange networks, analogously to the well-studied HEN synthesis problem. An optimization model for the preliminary WEN synthesis is proposed, by formulating a superstructure in mathematical programming. The aim is the minimization of the total annual cost for a single-shaft-turbine-compressor (SSTC) running at constant speed. Operational curves of turbines and compressors are used to identify high and low-pressure flows for the work exchange through expansion and compression stages in equipment located in a single axis unit. Though, the authors did not consider the possibility of thermal integration of the process streams, such that the heat exchange between process streams was disallowed. Thus, heaters and coolers are just arranged at the end of each stage. Moreover, the possibility of using several shafts has not been evaluated, the model is restricted to a fixed rotational speed of the shaft, and all costs are considered as linear functions, not being able to realistically translate the process costs.

The present paper introduces a new model for the synthesis of work exchange networks (WENs), with heat integration of process gaseous streams obtained by the simultaneous design of the HEN. The WEN synthesis consists in optimal work integration between streams at high-pressure (HP) and low-pressure (LP), using pressure manipulation equipment acting on a common SSTC axis and stand-alone equipment to minimize the total annualized cost. The objective function is composed by capital costs associated to the various units of the network and operational expenses. The handling pressure of streams is performed in a multi-stage superstructure, allowing the use of several shafts units. Generators and helper motors are used, respectively, to convert work excess into electricity and to fill for power shortage on the SSTC units. Between the compression and expansion stages of the WEN, the streams are sent to the HEN to promote heat integration. The HEN formulation is based on the model of Yee and Grossmann (1990), in which isothermal mixing and constant heat transfer coefficients are assumed, and the possibility of stream splits is considered. The main difference of the proposed model to the Razib et al. (2012) model relies in the thermal integration of the streams occurring simultaneously to the work integration. As a consequence, the inlet and outlet temperatures in the HEN are dependent to the WEN synthesis; thus, they should be considered as optimization variables of the process. The WEN superstructure with heat integration is optimized as a mixed-integer nonlinear programming (MINLP) formulation, and solved with the GAMS software. Three case studies are conducted to verify the accuracy of the proposed model. In all cases, it is shown that the heat integration between WEN stages is essential to enhance the pressure recovery. It is also responsible for the reduction of the total annualized cost, as result of using a smaller amount of hot and cold utilities.

2. Problem statement

Consider a set of gaseous streams at high-pressure (HP) and low-pressure (LP) with known mass flows, heat capacities, supply state (inlet pressure and temperature), and target state (outlet pressure and temperature). In addition, thermal utilities for heating and cooling, electricity, equipment for handling pressure and heat transfer, and their respective costs, are also provided. The main objective is to synthesize an optimal WEN through pressure recovery between the HP and LP streams, using compressors and turbines running on a common shaft. The heat recovery is realized concurrently in the HEN, so that the total annualized cost of the network is minimized. The contributions of operational expenses and capital costs of the various units that constitute the network are considered in the objective function, including the revenue from electricity generation.

The WEN synthesis with heat integration is a complex process, which seeks to obtain the optimal configuration of the network, using the least amount of equipment for the pressure manipulation and heat exchange, and with a minimum consumption of electricity and thermal utilities.

For the WEN synthesis, the use of the following equipment is considered:

- (i) turbines and compressors running on a common shaft (SSTC)
- (ii) stand-alone turbines for electricity generation (utility turbines)
- (iii) stand-alone compressors that consume electricity (utility compressors)
- (iv) valves for expansion of streams via Joule-Thompson isenthalpic expansion
- (v) turbines generators to produce electricity from excess power
- (vi) helper motors to fill for power shortage
- (vii) mixers and splitters

For the heat integration, the use of the following equipment is considered:

- (viii) heat exchangers (two-stream or multi-stream)
- (ix) heaters using heating steam
- (x) coolers using cooling water
- (xi) mixers and splitters

3. WEN-HEN Superstructure

In this paper, the proposed model for the WEN synthesis with heat integration is formulated in mixed-integer nonlinear programming (MINLP). The development of the superstructure is based on the following ideas:

- I. A WEN superstructure must contain s stages of compression and expansion, in which the work exchange occurs between HP and LP streams. The pressure recovery is performed by means of single-stage and parallel equipment—namely compressors and turbines—associated to a common shaft (SSTC). Several units of SSTC axes can be used. However, the global energy balance in each SSTC unit should be respected, i.e., the expansion work should be equal to the compression work. For this, helper motors and generators (turbines) allocated on the axes, or even stand-alone compressors, turbines and/or valves, denominated utilities, can be allowed.
- II. At each compression and expansion stage, the overall mass flow is splitted between various flows, through the pressure manipulation equipment that compose each of these stages. In the end of each stage, the sub-streams pass

through a mixer, reforming the parent streams. Although the outlet pressure is the same in all equipment of each expansion stage, the temperature in the outlet of each device is different. For this reason, energy and mass balances should be performed at the mixing points.

- III. Between stages of handling pressure, the streams must be sent to the HEN for heat recovery. The thermal integration is carried out to improve pressure recovery, since the temperature of the streams is crucial in the processes of compression and expansion. It should be highlighted that high temperatures favor the expansion process, while lower temperatures favor the compression process of streams.

In order to simplify the mathematical formulation, the following assumptions are considered:

- (i) All the SSTC axes units operate at any speed
- (ii) Effect of surging and choking are disregarded. In other words, it is assumed that each compressor/turbine is designed to properly work at a given rotation speed with the optimized flow rate provided by the model
- (iii) All the compressions and expansions (except through valves) are adiabatic
- (iv) All expansions through valves are isenthalpic, with constant Joule-Thompson coefficient
- (v) All streams behave as ideal gases
- (vi) All turbines and compressors are centrifugal and are built with carbon steel
- (vii) Starter energy required for any compressor or turbine is neglected

- (viii) Streams temperatures through valves are always below the inversion temperature
- (ix) All the SSTC compressors and turbines are single-stage. Though, multi-stage compressors (turbines) with intermediate cooling (heating) naturally appear as a sequence of single-stage compressors (turbines) and heat exchangers
- (x) All heat capacities of streams are constant
- (xi) All heat transfer coefficients are constant
- (xii) Pressure drop and heat losses in all thermal equipment are neglected
- (xiii) Costs of mixers and splitters are negligible

The proposed WEN superstructure is composed by several stages of compression or expansion for each stream. Consequently, each HP stream goes through s expansion stages and, analogously, each LP stream undergoes s compression stages. Before each of these stages, as well as after leaving the last stage of the WEN, the streams are conducted to the HEN to promote heat integration. As result, heat exchangers, and heaters or coolers are placed at the beginning of each stage and at the end of the last pressure manipulation stage. Splitters are used after each heat exchanger, while a mixer is placed at the end of each stage. The splitter at the entrance of each stage gives rise to k sub-streams that enter in k parallel SSTC turbines/compressors, a sub-stream that passes through a turbine/compressor utility, a sub-stream for the bypass and, in the case of an HP stream, gives rise to a sub-stream that goes into a valve. Fig. 1 shows the stage s of compression of LP streams and Fig. 2 presents the stage s of expansion of HP streams. Fig. 3 shows the multi-stage superstructure for each stream, in which the HEN has been highlighted.

The leading idea of the WEN synthesis is to promote the work exchange between HP and LP streams, using equipment for pressure manipulation—namely turbines and compressors—running on a common axis denominated single-shaft-turbine-compressor, or simply SSTC. The SSTC is a direct extension of the coupling between turbines and compressors on a common shaft, with the difference that in the SSTC the HP streams replace the steam/gas that drive turbines (Razib et al., 2012). Furthermore, the SSTC allows the exchange of work among different process streams in various stages of expansion and compression through single-stage units, and the use of helper motors and generators to respond to any lack or excess of energy, respectively. To compose the WEN, stand-alone compressors and turbines, and/or valves are also used. As WEN utilities, steam or electricity can be used to move the stand-alone compressors and helper motors. When the possibility of thermal integration is considered, the HEN is synthesized simultaneously to the WEN, by recovering heat from process streams. Thus, while the HEN only involves the heat integration of process streams—via heat exchangers, heaters and coolers—the WEN involves the pressure integration or pressure and heat integration, using for it SSTC equipment, stand-alone turbines and compressors, valves, helper motors and generators, and, when necessary, heat exchangers, heaters and coolers.

In this paper, the thermal integration is achieved through the synthesis of HEN, based on the superstructure of Yee and Grossmann (1990), which considers heat exchange between hot and cold streams in several stages, and the possibility of streams splits, and assumes constant heat transfer coefficients and isothermal mixing. Moreover, heaters and coolers are placed at the ends of the streams. Nevertheless, in the proposed model the hot and cold streams are connected to WEN, such that heat exchange occurs between the stages of compression and expansion. Therefore, the inlet and outlet temperatures of the HEN are

unknown variables that must be optimized, which confer a higher degree of complexity to the model.

The heat integration process is entirely governed by the temperature difference of streams that compose the HEN, whereas no driving force acts on the WEN. Additionally, in the WEN synthesis with heat recovery, the temperatures much as the pressures play a critical role during the design of the network. As the compression work and, hence, the efficiency are favored by low inlet temperatures, the cooling of streams occurs between compression stages. In other words, the LP streams are considered as hot streams in terms of heat integration in the HEN. Similarly, the expansion work and, consequently, the efficiency are favored by higher inlet temperatures, so the heating of streams occurs among two successive expansion stages. Thus, the HP streams are treated as cold streams in the HEN synthesis.

The simultaneous synthesis of WEN with heat integration, results in a highly complex model due to the requirement to optimize all parameters related to the two networks—WEN and HEN—synchronously. With regard to the WEN design, the difficulties are to guarantee the equality of the outlet pressure of all sub-streams in compression and expansion stages, for the reason that streams at different pressures cannot be mixed unlike what happens in the HEN, in which the isothermal mixing can be assumed. Furthermore, single-stage and parallel compressors and turbines share the same SSTC axis in the WEN, and hence must operate properly to ensure equal flow rates.

This is an extremely difficult process, since the operations with pressure manipulation equipment are highly nonlinear functions of temperature, pressure, heat capacity and process efficiency. It is important to emphasize that the mechanical work is a highly nonlinear function of the stream pressure, though it is a linear function of the

temperature difference. In addition, the new unknown variables for the HEN synthesis (wherein the outlet temperatures of the heat network must meet inlet temperatures in the WEN stages of expansion and compression, and vice versa), the nonlinearity inherent in the calculation of temperature approximation, and the functions for cost estimation are factors that increase further the complexity of the model.

For simplicity, the ideal gas model is used to describe the thermodynamic behavior of real gases. However, an isentropic efficiency factor is considered to adjust inevitable losses of efficiency of real processes.

4. Mathematical programming model

The mathematical model is presented in the following sections, in which the WEN superstructure is generated according to the steps below.

4.1 Sets/Indices definitions

The definition of the following sets is required for the development of the model:

$$HP = \{j / j = 1, 2, \dots, HP \text{ are high pressure streams}\}$$

$$LP = \{i / i = 1, 2, \dots, LP \text{ are low pressure streams}\}$$

$$E = \{e / e = 1, 2, \dots, E \text{ are the number of SSTC axes units}\}$$

$$S = \{s / s = 1, 2, \dots, S \text{ are the number of WEN stages}\}$$

$$K = \{k / k = 1, 2, \dots, K \text{ are the number of stream splits}\}$$

The selection of the number e of SSTC axes units, and of the number s of stages of compression and expansion in the WEN is arbitrary. However, the number of stages must be chosen so that the maximum compression ratio allows reaching the desired target temperature. It should be emphasized that the higher the number of shafts, and the number of stages, the larger the problem to be solved will be. It is recommended to use a maximum of three equipment in parallel at each stage (i.e., $k = 3$), to avoid very small equipment.

4.2 Logical constraints

The following definition of binary variables is necessary to promote the selection between the equipment that will compose the WEN:

$$y_{i,s,e,k} = \begin{cases} 1 & \text{if stream } i \text{ uses a compressor on SSTC unit } e \text{ in stage } s \text{ and split } k \\ 0 & \text{otherwise} \end{cases} \quad i \in LP, s \in S, e \in E, k \in K$$

$$y_{j,s,e,k} = \begin{cases} 1 & \text{if stream } j \text{ uses a turbine on SSTC unit } e \text{ in stage } s \text{ and split } k \\ 0 & \text{otherwise} \end{cases} \quad j \in HP, s \in S, e \in E, k \in K$$

$$y_{i,s}^U = \begin{cases} 1 & \text{if stream } i \text{ uses a compressor utility in stage } s \\ 0 & \text{otherwise} \end{cases} \quad i \in LP, s \in S$$

$$y_{j,s}^U = \begin{cases} 1 & \text{if stream } j \text{ uses a turbine utility in stage } s \\ 0 & \text{otherwise} \end{cases} \quad j \in HP, s \in S$$

$$y_{j,s}^V = \begin{cases} 1 & \text{if stream } j \text{ uses a valve in stage } s \\ 0 & \text{otherwise} \end{cases} \quad j \in HP, s \in S$$

To simplify the model, the auxiliary binary variables $y_{i,s,e}^a$ and $y_{j,s,e}^a$ are defined to promote the selection of compressors and turbines, respectively, in the SSTC axis independent of split k :

$$y_{i,s,e}^a = \begin{cases} 1 & \text{if stream } i \text{ uses a compressor on SSTC unit } e \text{ in stage } s \\ 0 & \text{otherwise} \end{cases} \quad i \in LP, s \in S, e \in E$$

$$y_{j,s,e}^a = \begin{cases} 1 & \text{if stream } j \text{ uses a turbine on SSTC unit } e \text{ in stage } s \\ 0 & \text{otherwise} \end{cases} \quad j \in HP, s \in S, e \in E$$

It is convenient to introduce some logical relationships that ensure only feasible alternatives and, at the same time, constraint the search space by avoiding sub-optimal solutions or solutions without physical meaning:

The binary variables $y_{i,s,e,k}$ ($y_{j,s,e,k}$) and $y_{i,s,e}^a$ ($y_{j,s,e}^a$) are related so that if a variable exists, the other variable should also exist (Eq. (1)-(4)). In other words, if there is at least one compressor (turbine) on the shaft e in a split k , and in a stage s , then there is one compressor (turbine) on the same shaft e and stage s . Or still, if $y_{i,s,e,k} = 1$ (and/or $y_{j,s,e,k} = 1$) then $y_{i,s,e}^a = 1$ (and/or $y_{j,s,e}^a = 1$).

$$1 - y_{i,s,e,k} + y_{i,s,e}^a \geq 1 \quad i \in LP, s \in S, e \in E, k \in K \quad (1)$$

$$1 - y_{i,s,e}^a + \sum_{k=1}^K y_{i,s,e,k} \geq 1 \quad i \in LP, s \in S, e \in E, 1 \leq k \leq K \quad (2)$$

$$1 - y_{j,s,e,k} + y_{j,s,e}^a \geq 1 \quad j \in HP, s \in S, e \in E, k \in K \quad (3)$$

$$1 - y_{j,s,e}^a + \sum_{k=1}^K y_{j,s,e,k} \geq 1 \quad j \in HP, s \in S, e \in E, 1 \leq k \leq K \quad (4)$$

At each stage of expansion and compression, stand-alone compressors and turbines can be used. This type of pressure manipulation equipment can operate in multi-stage or not. However, in the stages of expansion, valves may be also used to replace turbines. It is

important to note that due to the ability of the expansion by turbines to recover more energy in comparison with the expansion through valves; these expanders cannot coexist in the same stage. Thus, in an expansion stage may exist a single-stage turbine (maximum three in parallel) associated to the SSTC axis, and/or a stand-alone turbine, or a valve, or bypass.

Similarly, a stage of compression may exist a single-stage SSTC compressor (maximum three in parallel), and/or a stand-alone compressor, or bypass. To allow the selection of bypass the following binary variables are defined:

$$y_{i,s}^B = \begin{cases} 1 & \text{if stream } i \text{ bypasses stage } s \\ 0 & \text{otherwise} \end{cases} \quad i \in LP, s \in S$$

$$y_{j,s}^B = \begin{cases} 1 & \text{if stream } j \text{ bypasses stage } s \\ 0 & \text{otherwise} \end{cases} \quad j \in HP, s \in S$$

Obviously, if the HP or LP stream bypasses the stage s then no device is allocated at this stage. As all sub-streams should have the same pressure at the end of a stage, a partial bypass cannot exist.

For each LP stream, the next logical relationships are used to promote the selection between the bypass and the utility compressor (Eq. (5)), and to define the existence of at least one SSTC compressor and/or stand-alone compressor (Eq. (6)). Thus, the Eq. (5) indicates that for each LP stream i in each stage s , the bypass or the utility compressor or none of them, may be selected.

$$y_{i,s}^B + y_{i,s}^U \leq 1 \quad i \in LP, s \in S \quad (5)$$

$$1 - y_{i,s}^B + 1 - y_{i,s,e}^a \geq 1 \quad i \in LP, s \in S, e \in E \quad (6)$$

In the same way, for each HP stream the following logical relationships are used to ensure the selection of the bypass, or utility turbine, or valve. Eq. (8) defines the existence of at least one stand-alone turbine and/or SSTC turbine.

$$y_{j,s}^B + y_{j,s}^U + y_{j,s}^V \leq 1 \quad j \in HP, s \in S \quad (7)$$

$$1 - y_{j,s}^B + 1 - y_{j,s,e}^a \geq 1 \quad j \in HP, s \in S, e \in E \quad (8)$$

It is clear that if the bypass occurs in a stage, it also will occur in all subsequent stages. This fact ensures that the bypass occurs only in the case that the target stream pressure has already been reached:

$$1 - y_{i,s}^B + y_{i,s+1}^B \geq 1 \quad i \in LP, s \in S \quad (9)$$

$$1 - y_{j,s}^B + y_{j,s+1}^B \geq 1 \quad j \in HP, s \in S \quad (10)$$

The model allows the allocation of up to k SSTC compressors and turbines units in parallel in a stage. In this case, if the split k is selected then the split $k-1$ must also be selected:

$$1 - y_{i,s,e,k} + y_{i,s,e,k-1} \geq 1 \quad i \in LP, s \in S, e \in E, k \in K \quad (11)$$

$$1 - y_{j,s,e,k} + y_{j,s,e,k-1} \geq 1 \quad j \in HP, s \in S, e \in E, k \in K \quad (12)$$

Moreover, the WEN superstructure enables the use of e SSTC units. Then, the possibility of multiple equal solutions (i.e., select only shaft 1, or only shaft 2 with the same assignment of compressors and turbines) should be avoided. Therefore, considering the ordered E set, the shaft e should only be selected if the previous shaft $e-1$ has already been chosen:

$$1 - y_{i,s,e}^a + \sum_{i=1}^{LP} \sum_{s=1}^S y_{i,s,e-1}^a + \sum_{j=1}^{HP} \sum_{s=1}^S y_{j,s,e-1}^a \geq 1 \quad 1 \leq i \leq LP, 1 \leq j \leq HP, s \in S, e \in E \quad (13)$$

$$1 - y_{j,s,e}^a + \sum_{i=1}^{LP} \sum_{s=1}^S y_{i,s,e-1}^a + \sum_{j=1}^{HP} \sum_{s=1}^S y_{j,s,e-1}^a \geq 1 \quad 1 \leq i \leq LP, 1 \leq j \leq HP, s \in S, e \in E \quad (14)$$

Finally, each stage of compression and expansion should be selected only once:

$$y_{i,s}^B + y_{i,s}^U + \sum_{e=1}^E y_{i,s,e}^a = 1 \quad i \in LP, s \in S, 1 \leq e \leq E \quad (15)$$

$$y_{j,s}^B + y_{j,s}^V + y_{j,s}^U + \sum_{e=1}^E y_{j,s,e}^a = 1 \quad j \in HP, s \in S, 1 \leq e \leq E \quad (16)$$

4.3 Compression and expansion stages

Between stages of compression and expansion, the streams pressure is kept unchanged, due to the assumption that there are no pressure losses in heat exchangers. In each of these WEN stages, the inlet and outlet pressure of all streams are limited between the minimum and the maximum value of the inlet and outlet pressures in the WEN. Additionally, the inlet pressure at the first stage is always equal to the pressure of the inlet

stream in the WEN. In the same manner, the outlet pressure at the last stage is always the same as the outlet pressure in the WEN.

Consider P_{IN} ($\forall i \in LP, j \in HP$) and P_{OUT} ($\forall i \in LP, j \in HP$), respectively, as the inlet and outlet pressures of HP and LP streams in the WEN, and Pin ($\forall i \in LP, j \in HP$) and $Pout$ ($\forall i \in LP, j \in HP$), respectively, as the inlet and outlet pressures of streams in each stage of pressure manipulation. Thus, the assignment of the streams pressure at the inlet and at the outlet of the WEN is ensured by the equations Eq. (17)-(20).

$$P_{INi} = Pin_{i,1} \quad i \in LP, s = 1 \quad (17)$$

$$Pout_{i,S} = P_{OUTi} \quad i \in LP, s = S \quad (18)$$

$$P_{INj} = Pin_{j,1} \quad j \in HP, s = 1 \quad (19)$$

$$Pout_{j,S} = P_{OUTj} \quad j \in HP, s = S \quad (20)$$

In which,

$$MIN [P_{IN}, P_{OUT}] \leq Pin \leq MAX [P_{IN}, P_{OUT}] \quad \forall i \in LP, j \in HP, s \in S$$

$$MIN [P_{IN}, P_{OUT}] \leq Pout \leq MAX [P_{IN}, P_{OUT}] \quad \forall i \in LP, j \in HP, s \in S$$

The streams pressures in the WEN are connected so that for each HP (LP) stream, the outlet pressure of each stage of expansion (compression) is equal to the inlet pressure in the subsequent stage:

$$Pout_{i,s} = Pin_{i,s+1} \quad i \in LP, 1 \leq s < S \quad (21)$$

$$Pout_{j,s} = Pin_{j,s+1} \quad j \in HP, 1 \leq s < S \quad (22)$$

At the entrance of each stage of the WEN, the streams are splitted into sub-streams that will pass through the different equipment of the stage. The streams are reformed to their parent state at the end of each stage by mixers. Thus, F_i and F_j are the inlet total flows at the WEN of the LP and HP streams, respectively. Mass balances at the mixing point of the entrance and/or exit of a stage are such that:

$$F_i = Fu_{i,s} + Fb_{i,s} + \sum_{e=1}^E \sum_{k=1}^K Fe_{i,s,e,k} \quad i \in LP, s \in S, 1 \leq e \leq E, 1 \leq k \leq K \quad (23)$$

$$F_j = Fv_{j,s} + Fu_{j,s} + Fb_{j,s} + \sum_{e=1}^E \sum_{k=1}^K Fe_{j,s,e,k} \quad j \in HP, s \in S, 1 \leq e \leq E, 1 \leq k \leq K \quad (24)$$

In which, Fu and Fb correspond to the sub-streams flow of HP and LP streams through utilities (stand-alone compressors for compression stages, and stand-alone turbines for expansion stages), and the flow through the bypass, respectively. Fv is the flow rate through valves for expansion stages, and Fe is the flow rate through compressors and turbines units associated with the SSTC. All these flows are limited to a maximum value equal to the inflow of HP and LP stream in the WEN, i.e., $Fv_{j,s} \leq F_j$, $Fu_{j,s} \leq F_j$, $Fe_{j,s,e,k} \leq F_j$, $Fb_{j,s} \leq F_j$, $Fu_{i,s} \leq F_i$, $Fe_{i,s,e,k} \leq F_i$, and $Fb_{i,s} \leq F_i$.

The streams temperature is an especially critical factor in processes of compression and expansion. In addition to physical factors that limit the temperature in compressors and turbines (as the selection of the material of construction to avoid damage), energy recovery is strongly dependent of the streams temperature. Hence, the turbine efficiency increases

while the compressor efficiency decreases with increasing operational temperature. With these considerations, the operation of turbines and compressors within a limited range of temperature is considered in this model.

Besides the mass balance, the energy balance across the mixers is needed due to the streams splits in each stage. However, this energy balance is unnecessary in compression stages if the same efficiency is considered for all equipment in a given stage. In contrast, in stages of expansion even if the outlet pressure is the same for all the equipment, the outlet temperatures are distinct, which should be taken into account (i.e., expansion through a valve and a turbine with the same outlet pressure yields different temperatures).

Consider $Tval_{j,s}$ as the outlet temperature of the valve, $Tturb_{j,s}$ as the outlet temperature of the utility or SSTC turbine, and $Tin_{j,s}$ as the temperature in case of bypass. Tin ($\forall i \in LP, j \in HP, s \in S$) and $Tout$ ($\forall i \in LP, j \in HP, s \in S$) are defined as the inlet and outlet temperatures of the streams, respectively, at each stage of the WEN. As the value of the heat capacity Cp is the same for all streams, it can be eliminated of the equation.

$$F_j \cdot Tout_{j,s} = Fb_{j,s} \cdot Tin_{j,s} + Fv_{j,s} \cdot Tval_{j,s} + \left(Fu_{j,s} + \sum_{e=1}^E \sum_{k=1}^K Fe_{j,s,e,k} \right) \cdot Tturb_{j,s} \quad j \in HP, s \in S, 1 \leq e \leq E, 1 \leq k \leq K \quad (25)$$

In which,

$$T_{\min} \leq Tin_{j,s} \leq T_{\max}, T_{\min} \leq Tout_{j,s} \leq T_{\max}, T_{\min} \leq Tval_{j,s} \leq T_{\max}, T_{\min} \leq Tturb_{j,s} \leq T_{\max}.$$

In compression stages, the increase of the streams pressures and temperatures are expected:

$$Pout_{i,s} \geq Pin_{i,s} \quad i \in LP, s \in S \quad (26)$$

$$Tout_{i,s} \geq Tin_{i,s} \quad i \in LP, s \in S \quad (27)$$

In expansion stages, pressures and temperatures of the streams should decrease:

$$Pout_{j,s} \leq Pin_{j,s} \quad j \in HP, s \in S \quad (28)$$

$$Tout_{j,s} \leq Tin_{j,s} \quad j \in HP, s \in S \quad (29)$$

In each stage of the WEN superstructure, the stream outlet pressure is limited to a maximum compression ratio:

$$Pout_{i,s} \leq CR_{\max} Pin_{i,s} \quad i \in LP, s \in S \quad (30)$$

The equipment for compression and expansion are responsible for the pressure and temperature variations of the streams, even if only a small change in temperature is generated, such as in the case of isenthalpic valves. In a compression stage, the outlet temperature is equal for all compressors. In this case, a bypass can be considered as a compressor in which the work is equal to zero. Considering an adiabatic operation of compression of an ideal gas, in which η_i is the isentropic efficiency and γ is the heat capacity ratio:

$$Tout_{i,s} = Tin_{i,s} \left[1 + \eta_i \left(Pout_{i,s} / Pin_{i,s} \right)^{(\gamma-1/\gamma)-1} \right] \quad i \in LP, s \in S \quad (31)$$

Similarly, the outlet temperature is the same for all turbines in a stage of expansion in an adiabatic process.

$$T_{turb_{j,s}} = T_{in_{j,s}} \left[1 + \eta_j \left(P_{out_{j,s}} / P_{in_{j,s}} \right)^{(\gamma-1/\gamma)-1} \right] \quad j \in HP, s \in S \quad (32)$$

To model the expansion of HP streams through valves, it is considered the isenthalpic process in which μ_j is the expansion coefficient of Joule-Thompson.

$$T_{val_{j,s}} = T_{in_{j,s}} + \mu_j \left(P_{out_{j,s}} - P_{in_{j,s}} \right) \quad j \in HP, s \in S \quad (33)$$

Consider $Wu_{i,s}$ as the compression work of the LP stream consumed by the stand-alone compressors in stage s , and $We_{i,s,e,k}$ as the compression work of the LP stream consumed on a SSTC in a stage s , and split k . For an adiabatic process, the energy required by the utility compressors and the energy required by the SSTC compressors are linear functions of inlet and outlet temperature in each compression stage:

$$Wu_{i,s} = Fu_{i,s} Cp_i \left(T_{out_{i,s}} - T_{in_{i,s}} \right) \quad i \in LP, s \in S \quad (34)$$

$$We_{i,s,e,k} = Fe_{i,s,e,k} Cp_i \left(T_{out_{i,s}} - T_{in_{i,s}} \right) \quad i \in LP, s \in S, e \in E, k \in K \quad (35)$$

Analogously, $Wu_{j,s}$ and $We_{j,s,e,k}$ can be defined as the energy generated by utility turbines and energy generated by turbines associated to SSTC, respectively, to HP streams in stages s of the WEN:

$$Wu_{j,s} = Fu_{j,s} Cp_j (Tin_{j,s} - Tturb_{j,s}) \quad j \in HP, s \in S \quad (36)$$

$$We_{j,s,e,k} = Fe_{j,s,e,k} Cp_j (Tin_{j,s} - Tturb_{j,s}) \quad j \in HP, s \in S \quad (37)$$

As suggested by Couper et al. (2010), the compression work and the expansion work must be limited between a lower and an upper bound:

$$100 W \leq Wu_{j,s} \leq 1500 W, \quad 100 W \leq We_{j,s} \leq 1500 W, \quad 18 W \leq Wu_{i,s} \leq 950 W \quad \text{and} \\ 18 W \leq We_{i,s} \leq 950 W.$$

If the bypass exists in a stage, then the inlet and outlet pressures and temperatures of the streams should be equal. To ensure this, the formulation in generalized disjunctive programming (GDP) followed by big-M reformulation are considered. Therefore, for each stage of compression the following disjunction is used:

$$\left[\begin{array}{l} y_{i,s}^B \\ Tout_{i,s} = Tin_{i,s} \\ Pout_{i,s} = Pin_{i,s} \end{array} \right]$$

$$Tin_{i,s} - Tout_{i,s} \leq M_{1i,s} (1 - y_{i,s}^B) \quad (38)$$

$$Tin_{i,s} - Tout_{i,s} \geq -M_{1i,s} (1 - y_{i,s}^B) \quad (39)$$

$$Pin_{i,s} - Pout_{i,s} \leq M_{2i,s} (1 - y_{i,s}^B) \quad (40)$$

$$Pin_{i,s} - Pout_{i,s} \geq -M_{2i,s} (1 - y_{i,s}^B) \quad (41)$$

In which, $M_{1i,s} = Tin_{i,s}^{UP} - Tout_{i,s}^{LO}$ and $M_{2i,s} = Pin_{i,s}^{UP} - Pout_{i,s}^{LO}$.

Note that M is a positive parameter large enough to validate the formulation (Eq. (38)-(41)), that must, however, be as small as possible. In this case, the parameter M_1 is calculated as a difference between the upper bound for the inlet temperature in the stage and the lower bound for the outlet temperature in the stage. In the same way, the parameter M_2 is calculated as a difference between the upper bound for the inlet pressure in the stage and the lower bound for the outlet pressure in the stage. The disjunctions for expansion stages and consequent big-M reformulation are very similar and, for this reason, they will be omitted in this article.

If the bypass does not exist in a stage of compression and/or expansion, the streams flowing through the bypass should be zero:

$$Fb_{i,s} \leq Fb_{i,s}^{UP} \cdot y_{i,s}^B \quad i \in LP, s \in S \quad (42)$$

$$Fb_{j,s} \leq Fb_{j,s}^{UP} \cdot y_{j,s}^B \quad j \in HP, s \in S \quad (43)$$

Likewise, if there is no valve in a stage of expansion, the flow rate through this valve should be zero:

$$Fv_{j,s} \leq Fv_{j,s}^{UP} \cdot y_{j,s}^V \quad j \in HP, s \in S \quad (44)$$

Otherwise, there must be a minimum pressure drop, and a minimum flow rate through this valve to avoid equipment with very small capacity.

$$Pin_{j,s} - Pout_{j,s} \geq P_{\min} - (Pin_{j,s}^{UP} - Pout_{j,s}^{LO}) \cdot (1 - y_{j,s}^V) \quad j \in HP, s \in S \quad (45)$$

$$Fv_{j,s} \geq F_{\min j} - F_j (1 - y_{j,s}^V) \quad j \in HP, s \in S \quad (46)$$

For the same reason, stand-alone compressors and turbines are forced to undertake a minimum work if they exist in a stage.

$$Wu_{i,s} \geq W_{\min} - Wu_{i,s}^{UP} (1 - y_{i,s}^U) \quad i \in LP, s \in S \quad (47)$$

$$Wu_{j,s} \geq W_{\min} - Wu_{j,s}^{UP} (1 - y_{j,s}^U) \quad j \in HP, s \in S \quad (48)$$

If these stand-alone turbines and compressors do not exist in their respective stages of compression and expansion, the flow through such equipment as well as their work must be zero:

$$Fu_{i,s} \leq Fu_{i,s}^{UP} \cdot y_{i,s}^U \quad i \in LP, s \in S \quad (49)$$

$$Wu_{i,s} \leq Wu_{i,s}^{UP} \cdot y_{i,s}^U \quad i \in LP, s \in S \quad (50)$$

$$Fu_{j,s} \leq Fu_{j,s}^{UP} \cdot y_{j,s}^U \quad j \in HP, s \in S \quad (51)$$

$$Wu_{j,s} \leq Wu_{j,s}^{UP} \cdot y_{j,s}^U \quad j \in HP, s \in S \quad (52)$$

The same occurs with the SSTC compressors and turbines. If the pressure manipulation equipment exists in a stage, they must carry out a minimum work of compression and expansion:

$$We_{i,s,e,k} \geq W_{\min} - We_{i,s,e,k}^{UP} (1 - y_{i,s,e,k}) \quad i \in LP, s \in S, e \in E, k \in K \quad (53)$$

$$We_{j,s,e,k} \geq W_{\min} - We_{j,s,e,k}^{UP} (1 - y_{j,s,e,k}) \quad j \in HP, s \in S, e \in E, k \in K \quad (54)$$

Otherwise, if there are no compressors and expanders in a stage, flow rates across these SSTC equipment and the work performed by them must be null:

$$Fe_{i,s,e,k} \leq Fe_{i,s,e,k}^{UP} \cdot y_{i,s,e,k} \quad i \in LP, s \in S, e \in E, k \in K \quad (55)$$

$$Fe_{j,s,e,k} \leq Fe_{j,s,e,k}^{UP} \cdot y_{j,s,e,k} \quad j \in HP, s \in S, e \in E, k \in K \quad (56)$$

$$We_{i,s,e,k} \leq We_{i,s,e,k}^{UP} \cdot y_{i,s,e,k} \quad i \in LP, s \in S, e \in E, k \in K \quad (57)$$

$$We_{j,s,e,k} \leq We_{j,s,e,k}^{UP} \cdot y_{j,s,e,k} \quad j \in HP, s \in S, e \in E, k \in K \quad (58)$$

4.4 Global energy balance for each SSTC

The turbines associated to the SSTC produce energy, while the SSTC compressors consume energy. The helper motor is allocated on the shaft to fill for any energy (electricity) shortage, and the generator is placed to convert any energy excess into electricity that can be used in other parts of the industrial plant, providing energy savings to the process.

The total expansion work produced in a SSTC unit must be equal to the total work of compression consumed in each single axis. In this context, the global energy balance on each SSTC unit is expressed by Eq. (59).

$$Wg_e + \sum_{i=1}^{LP} \sum_{s=1}^S \sum_{k=1}^K We_{i,s,e,k} = Wm_e + \sum_{j=1}^{HP} \sum_{s=1}^S \sum_{k=1}^K We_{j,s,e,k} \quad i \in LP, j \in HP, s \in S, k \in K, e \in E \quad (59)$$

4.5 Thermal integration (HEN synthesis)

To promote the heat integration of streams between each stage of compression and expansion, the synthesis of heat exchange network (HEN) is performed simultaneously with the WEN design. The formulation is based on the superstructure for HENs synthesis developed by Yee and Grossmann (1990), and the MINLP model proposed by the same authors (please see the Appendix).

The mathematical formulation for the HEN synthesis is centered the following key ideas:

- I. The HEN superstructure presents t stages of heat exchange divided according to the temperature at the mixing point. In each of these stages, it is postulated the possibility of heat exchange between all hot streams and all cold streams. For this purpose, the streams at high-pressure (HP) are considered as cold streams, and the streams at low-pressure (LP) as hot streams, since the expansion process is improved with increasing temperature and the compression process is enhanced with lowering temperature.
- II. The energy balance at the mixing point at the end of each HEN stage can be eliminated, as a result of considering the isothermal mixing of the streams. In each of the stages, the streams are splitted according to the maximum number of possible heat exchanges, but the outlet temperature is the same for each sub-stream.

- III. The heat exchange occurs between the stages of expansion and compression. Consequently, the inlet and outlet temperatures of the HEN must be connected with the temperatures of each WEN stage. Thus, the inlet temperatures of streams in the HEN correspond to the outlet temperatures of the stages of the WEN; and the HEN outlet temperatures correspond to the inlet temperatures of the stages of the WEN (please see Fig. 3). Due to this fact, all intermediate temperatures of a stream at the entrance and exit of the HEN are unknown variables that must be optimized.
- IV. Heaters are placed at the end of cold streams, and coolers are allocated at the end of hot streams to guarantee that the target temperatures of the process can be achieved.
- V. Due to the connection among the HEN and WEN temperatures, each stream from a compression and expansion stage is considered as a new stream in the HEN. Consequently, the number of cold streams in the HEN is always equal to the number of HP streams multiplied by the number of expansion stages, plus two streams that correspond to the inlet stream—it is also considered the heat exchange before the first stage of the WEN—and the outlet stream of the last stage of the WEN, which will enter the heater. Thus, two HP streams in four stages of expansion in the WEN, for example, will give rise to ten streams in the HEN. The number of hot streams in the HEN is calculated in a similar way.

For simplification, the number of stages in the HEN is considered equal to the number of stages in the WEN. Clearly, the selection of the number of stages is arbitrary and must be based on the fact that, in general, an optimal network does not need a lot of

equipment. It is noted that a very large number of stages increases the complexity of the model. The design equations of the HEN are presented in the Appendix.

4.6 Objective function

The total cost of the WEN with thermal integration consists of the total cost of the WEN plus the total cost of the HEN. The total annualized cost of both WEN and HEN is composed by the capital cost of investment in all units of the respective networks, and the operational expenses. Therefore, the calculus of the total cost of capital includes the cost of valves, SSTC compressors, stand-alone compressors, SSTC turbines, stand-alone turbines, helper motors, and generators for the WEN, as well as heat exchangers, heaters and coolers for the HEN. The calculation of operating expenses contains the expenditure with the thermal utilities (heating and cooling) and electrical services. It is also considered the sale of electricity to other sectors of the process. The objective function is expressed by the equation Eq. (60).

$$C_{total} = C_{total}^{WEN} + C_{total}^{HEN} = C_{capital}^{WEN} + C_{operational}^{WEN} + C_{capital}^{HEN} + C_{operational}^{HEN} \quad (60)$$

In which,

$$C_{capital}^{WEN} = f \cdot \left[\begin{aligned} & F_{BM}^V \cdot \sum_{j=1}^{HP} \sum_{s=1}^S C_{po}^V \cdot y_{j,s}^V + F_{BM}^{TU} \cdot \sum_{j=1}^{HP} \sum_{s=1}^S C_{po}^{TU} + F_{BM}^{CU} \cdot \sum_{i=1}^{LP} \sum_{s=1}^S C_{po}^{CU} + \\ & 1.2 F_{BM}^{TA} \cdot \sum_{j=1}^{HP} \sum_{s=1}^S \sum_{e=1}^E \sum_{k=1}^K C_{po}^{TA} + 1.2 F_{BM}^{CA} \cdot \sum_{i=1}^{LP} \sum_{s=1}^S \sum_{e=1}^E \sum_{k=1}^K C_{po}^{CA} + \\ & F_{BM}^{HM} \cdot \sum_{e=1}^E C_{po}^{HM} + F_{BM}^{GE} \cdot \sum_{e=1}^E C_{po}^{GE} \end{aligned} \right] \quad (60a)$$

$$C_{operational}^{WEN} = CE \cdot \left[\sum_{i=1}^{LP} \sum_{s=1}^S Wu_{i,s} + \sum_{e=1}^E Wm_e \right] - CV \cdot \left[\sum_{j=1}^{HP} \sum_{s=1}^S Wu_{j,s} + \sum_{e=1}^E Wg_e \right] \quad (60b)$$

$$C_{capital}^{HEN} = f \cdot \left[F_{BM}^{HE} \cdot \sum_{h=1}^H \sum_{c=1}^C \sum_{t=1}^T C_{po\ h,c,t}^{HE} + F_{BM}^{Cooler} \cdot \sum_{h=1}^H \sum_{n=1}^N C_{po\ h,n}^{HE} + F_{BM}^{Heater} \cdot \sum_{m=1}^M \sum_{c=1}^C C_{po\ m,c}^{HE} \right] \quad (60c)$$

$$C_{operational}^{HEN} = CW \cdot \sum_{h=1}^H \sum_{n=1}^N Q_{h,n} + CS \cdot \sum_{m=1}^M \sum_{j=1}^J Q_{m,j} \quad (60d)$$

In which, CE , CV , CW and CS are the cost parameters for electricity, sale of electricity, cooling and heating, respectively. f is the annualization factor for the capital cost defined by Smith (2005). Given r as the fractional interest rate per year and ny as the number of years:

$$f = \frac{(1+r)^{ny} - 1}{r} \quad (61)$$

In the equations Eq. (60a) and Eq. (60c), F_{BM} is the correction factor for the basic unit cost, in which the materials of construction and the operational pressure of the equipment are considered. C_{po} is the basic cost of an equipment unit (in US\$) operating with the pressure next to the ambient conditions. C_{po} is calculated according to the correlations of Turton et al. (2003) for heat exchangers, heaters, coolers and valves. For the cost estimation of compressors, turbines, generators and helper motors the correlations of Couper et al. (2010) are used. The costs of SSTC compressors and turbines are considered 20% higher than the same equipment outside the shaft. All the cost correlations used must

be corrected for the relevant year with the CEPCI index (Chemical Engineering Plant Cost Index).

5. Computational aspects

Some important computational aspects are related to the solution of the model presented above. As previously mentioned, the proposed superstructure for the WEN synthesis is optimized with a MINLP formulation. Because of its highly nonlinear and non-convex character, this type of problem generates a large number of local solutions that, as result, can lead to obtaining sub-optimal solutions. Among the main methods developed to solve MINLP problems are the branch-and-bound (BB) algorithm, in which NLP sub-problems are solved at each node, and decomposition techniques such as the iterative algorithms of generalized Benders decomposition (GBD) and outer approximation (OA), through which alternative NLP sub-problems with fixed binary variables, and MILP master problems are solved sequentially (Grossmann et al., 2000). According to Caballero and Grossmann (2013), all these methods are based on solving a number of sub-problems of easier solution obtained from the general formulation of the problem. Moreover, the convexity of the functions is considered to ensure convergence to the global optimum, or at least, to solutions very close to this value.

According to Grossmann (2002), the BB method is generally attractive when NLP sub-problems are relatively small, or only when some of them need to be solved. Thus, the difficulty of obtaining solutions by this method is enlarged with the increase in the complexity of the problem. Hence, the WEN superstructure proposed in this paper is written in GAMS (version 24.02) and is solved with the DICOPT solver. This solver is

based on extensions of the OA method to solve MINLP problems, through relaxation strategies of the master problem. Therefore, the MINLP algorithm is solved by decomposition into NLP and MIP sub-problems. Any solver available in GAMS can be used—as sub-solvers—to solve these NLP and MIP problems; however the CONOPT and CPLEX solvers are chosen, respectively, for each of these problems. It is important to remark that while the DICOPT solver algorithm contains provisions to deal with non-convexities, the high nonlinearity of the model does not always guarantee the global optimum solution. Nevertheless, some numerical experiments with this model showed that increasing the number of major iterations (i.e., 15), and solving feasibility problems that may arise from NLP, allow obtaining good solutions.

All cases studied are solved using a personal computer with an Intel Core 2 Duo 2.40 GHz processor and 3.00 GB RAM under Windows 7 Ultimate. For the solution of the model is essential that the limits of all variables are well established. It should be highlighted that the lower and upper bounds for the pressure, temperature, mass flow, and work variables are especially critical for the WEN design, as well as the limits applied on the temperature variables and the heat exchange quotas between streams are crucial for the HEN synthesis.

6. Case studies

Three examples considering different situations were conducted, to verify the accuracy of the proposed approach for the simultaneous synthesis of WEN with heat integration.

Example 1. In this example, the WEN is designed to allow the work integration between two streams at high-pressure (HP1 and HP2), and two streams at low-pressure (LP1 and LP2). The streams HP1 and HP2 are expanded from 850 kPa to 100 kPa and from 980 kPa to 180 kPa, respectively. While the streams LP1 and LP2 are subjected to compression from an initial state of 100 kPa to a final state of 520 kPa and 850 kPa, respectively. For the WEN synthesis, a maximum number of four stages of compression and four stages of expansion of the streams are considered. The thermal integration among the streams at high-pressure and at low-pressure is allowed. Thus, the process streams are sent to the HEN to promote heat recovery. As the heat exchange occurs at the entrance and exit of the WEN, like as between all stages of pressure manipulation, the outlet streams from each stage of the WEN are connected to the inlet streams in the HEN. Furthermore, all intermediate temperatures of the HEN are unknown variables that must be optimized. The high-pressure streams HP1 and HP2 are considered as cold streams, and the low-pressure streams LP1 and LP2 are regarded as hot streams for the HEN synthesis. The stream HP1 originates five new cold streams (C1–C5), and similarly, the stream HP2 gives rise to five new cold streams (C6–C10) in the HEN. The stream LP1 originates hot streams H1 to H5 and the stream LP2 gives rise to hot streams H6 to H10. As a consequence, the heat integration between ten cold streams and ten hot streams needs to be performed. For the HEN synthesis, four heat exchange stages and the possibility of streams splits are considered.

The flow rates and heat capacities of all the streams are known constants. The problem data are presented in Table 1. The hot and cold utilities are available on 500 K and 288 K, respectively. The individual coefficients of heat transfer (h) to all the streams are equal to 0.1 kW/m²K and for the hot and cold utilities this coefficient is equal to 1.0 kW/m²K. In addition, all unknown intermediate temperatures of streams are restricted

between 288 K and 600 K. To calculate the cost of all the equipment an annualized cost factor $f = 0.18$ is considered, which corresponds to an interest rate of 10% per year over a period of eight years.

In this first example, two case studies are carried out with the aim of identifying the optimal configuration for the WEN with heat integration. In all cases, the minimization of the objective function composed by the total annualized cost is evaluated.

In Case 1, the WEN is designed with only one SSTC axis unit. In this case, the optimal WEN obtained is composed by two valves, two stand-alone turbines, four stand-alone compressors, four SSTC turbines, and three SSTC compressors associated with the single shaft. Thus, the stream HP1 undergoes three stages of expansion through two parallel SSTC turbines (1,480.1 kW and 100 kW), one valve, and one utility turbine (848.4 kW). The stream HP2 is subjected to four expansion stages through one valve, two subsequent single-stage SSTC turbines (950 kW and 100 kW), and one stand-alone turbine (698.3 kW). Both streams LP1 and LP2 undergo three stages of compression. Initially, the stream LP1 passes through two stand-alone compressors (282 kW and 950 kW), and then is compressed by one single-stage SSTC compressor (950 kW). The stream LP2 passes through one stand-alone compressor (950 kW), two parallel SSTC compressors (950 kW and 730.1 kW), and one stand-alone compressor (950 kW). The total work of expansion (compression) performed (consumed) by the SSTC turbines (SSTC compressors) is equal to 2,630.1 kW.

In the HEN design, four heat exchangers with heat exchanger areas (A) of 390.5 m² (H1.C2.t3- $Q = 603.6$ kW), 432.7 m² (H1.C5.t1- $Q = 742.1$ kW), 581.3 m² (H7.C5.t2- $Q = 1,083.7$ kW) and 918.2 m² (H7.C10.t1- $Q = 1,748.6$ kW) are needed. In addition, two coolers ($A = 424.1$ m² with $Q = 836.2$ kW, and $A = 462.7$ m² with $Q = 747.9$ kW) allocated,

respectively, on the streams H1 and H7 are used for the heat recovery. Fig. 4 shows the optimal WEN configuration with heat integration obtained for this case.

In Case 2, the WEN the use of two axes is forced. In this case, the optimal WEN obtained is composed by the same equipment used in the previous case; however, distributed in two different axes. Thus, the network is also composed by two valves, two stand-alone turbines, four stand-alone compressors, four SSTC turbines, and three SSTC compressors. The stream HP1 is subjected to three stages of expansion through two parallel SSTC turbines (1,480.1 kW and 100 kW) associated to the shaft 2, one valve, and one stand-alone turbine (848.4 kW). The stream HP2 undergoes four expansion stages through one valve, two single-stage SSTC turbines (950 kW and 100 kW) located on shaft 1 and shaft 2, respectively, and one utility turbine (698.3 kW). Both streams LP1 and LP2 undergo three stages of compression. Initially, the stream LP1 passes through two stand-alone compressors (282 kW and 950 kW), and then is compressed by one single-stage SSTC compressor (950 kW) located on the shaft 1. The stream LP2 passes through one utility compressor (950 kW), two parallel SSTC compressors (950 kW and 730.1 kW) associated to the shaft 2, and one stand-alone compressor (950 kW). The total work of expansion (compression) performed (consumed) by the SSTC turbines (SSTC compressors) is equal to 950 kW for the shaft 1, and 1,680.1 kW for the shaft 2.

In the HEN design, the same thermal equipment obtained for Case 1 are needed. Thus, four heat exchangers (H1.C2.t3 with $A = 390.5 \text{ m}^2$ and $Q = 603.6 \text{ kW}$, H1.C5.t1 with $A = 432.7 \text{ m}^2$ and $Q = 742.1 \text{ kW}$, H7.C5.t2 with $A = 581.3 \text{ m}^2$ and $Q = 1,083.7 \text{ kW}$, and H7.C10.t1 with $A = 918.2 \text{ m}^2$ and $Q = 1,748.6 \text{ kW}$) are also used. Moreover, two coolers ($A = 424.1 \text{ m}^2$ with $Q = 836.2 \text{ kW}$, and $A = 462.7 \text{ m}^2$ with $Q = 747.9 \text{ kW}$) allocated,

respectively, on the streams H1 and H7 are used for heat recovery. Fig. 5 shows the optimal WEN configuration with heat integration obtained for this case.

In Case 1 and Case 2, as there are no remains or lacks of energy in the shafts, no helper motor or generator is needed to satisfy the energy balance. However, two stand-alone turbines are used in both the network configurations. Consequently, 1,546.7 kW of energy are produced in the WEN, and can be used in other stages of the process and/or for sale of electricity. The results obtained for both cases are shown in Table 2. Clearly, the networks obtained in both cases differ only in the number of SSTC axes used; as result, both have the same cost. Thus, the total annualized cost estimated is 6,279k US\$/year, in which 5,314k US\$/year are the capital costs of investment in equipment, 158k US\$/year corresponds to the total expenses of heating and cooling streams, and 807k US\$/year is the annual cost of electricity already discounted the revenue generated by utility turbines (619k US\$/year). Moreover, if the use of three SSTC axes units is forced, the objective function increases which represents a sub-optimal solution.

In Case 1, the mathematical model contains 3,476 continuous variables, 104 binary variables and 4,363 constraints with 15,010 Jacobian elements (non-zeros), in which 2,046 are nonlinear. In Case 2, the mathematical model contains 3,900 continuous variables, 232 binary variables and 5,105 constraints with 17,710 Jacobian elements (non-zeros), in which 2,482 are nonlinear. The CPU times are 1.11 min for Case 1 and 6.46 min for Case 2, the optimal solutions are found in the fifth and sixth major iterations, respectively.

In this example, the same WEN with heat integration can be designed with the use of one or two SSTC axes units. Thus, besides the economic factor, the space available in the processing plant for the arrangement of the shafts (SSTC units) and equipment should be considered to choose the best WEN design. The larger number of equipment running on

the same SSTC unit, the larger the difficulty to keep them under the same operating conditions will be, since all must be kept under the same rotational speed. In contrast, the use of a larger number of shafts may request a bigger space in the plant for allocating network equipment. In processes, such as the offshore section of the LNG production, where space is a very critical factor, it may represent a large problem.

Example 2. In this example, the WEN synthesis is performed with the objective of work integration among three streams at high-pressure (HP1, HP2 and HP3) and two low-pressure streams (LP1 and LP2). The stream HP1 is expanded from an initial pressure of 900 kPa to a final pressure of 100 kPa, the stream HP2 is expanded from 850 kPa to 150 kPa, and the stream HP3 is expanded from 700 kPa to 200 kPa. In contrast, the streams LP1 and LP2 are both compressed from inlet pressure of 100 kPa to 700 kPa and 900 kPa, respectively. The pressure recovery in the WEN takes place in, at most, four expansion stages and four stages of compression. The temperatures of all streams are equal in the entrance and exit of the WEN. The network is designed to get the maximum use of the available energy in the system, through the optimal integration between work and heat. Thus, the thermal integration of streams occurs in the HEN between all stages of compression and expansion. Since the HEN design is carried out simultaneously with the WEN synthesis, all inlet temperatures of the streams in the HEN are dependent of the WEN, consequently, they are unknown variables that must be optimized. For the HEN design, the streams HP1–HP3 are considered as cold streams, while the streams LP1 and LP2 are considered as hot streams in the HEN. The outlet streams of each stage of pressure manipulation are connected to the inlet streams in the HEN. For this reason, the stream HP1 originates the cold streams C1–C5, the stream HP2 gives rise to streams C6–C10, the

stream HP3 originates the cold streams C11–C15, and similarly, LP1 originates H1–H5 and LP2 gives rise to hot streams H6–H10. As consequence, the HEN is designed to exchange heat between 15 cold streams and 10 hot streams. The possibility of streams splits is considered, and heaters and coolers can be used to meet any thermal needs of streams. The data streams are shown in Table 1. For simplification, four stages of heat exchange in the HEN are considered. Furthermore, the flow rates and heat capacities of all streams are known constants.

In this example, two cases studies are performed to obtain the optimal WEN design with heat integration. In all cases, the minimization of the total annualized cost is considered. The intermediate inlet temperatures of the streams in the HEN are restricted from 288 K to 600 K. Hot and cold utilities are available on 500 K and 288 K, respectively.

In Case 1, the WEN is designed with a single SSTC axis unit. The optimal WEN obtained is composed by four expansion stages for the stream HP1, three stages for the stream HP2 and two expansion stages for the stream HP3, as well as three stages of compression for both streams LP1 and LP2. In this case, the stream HP1 is expanded through one stand-alone turbine (1,170.8 kW), followed by one single-stage SSTC turbine (200 kW) allocated on the shaft, two parallel SSTC turbines (1,500 kW and 200 kW), and one single-stage SSTC turbine (1473 kW). The stream HP2 is expanded through one valve, followed by expansion through one single-stage SSTC turbine (837.7 kW), one more valve and, finally, by one single-stage SSTC turbine (454.4 kW). The stream HP3 passes across two stages of expansion through one valve, and one single-stage SSTC turbine (1,500 kW). The stream LP1 is compressed through two subsequent stand-alone compressors (950 kW and 421.6 kW), followed by two parallel SSTC compressors (950 kW and 750 kW). The stream LP2 is compressed in three stages through two parallel SSTC compressors (950 kW

and 733.9 kW), followed by one stand-alone compressor (950 kW), and three parallel SSTC compressors (950 kW, 950 kW and 881.16 kW) associated with the shaft. Fig. 6 shows the optimal configuration for the WEN obtained for this case. The total work produced (consumed) by the turbines (compressors) on the shaft is equal to 6,165.1 kW. As there are no remains or lacks of energy on the shaft, no helper motor or generator is needed to satisfy the energy balance. However, one stand-alone turbine is used in the network. Consequently, 1,170.3 kW of energy are produced in the WEN, and can be used in other stages of the process and/or for sale of electricity.

The thermal integration of process streams is carried out after the first and the last expansion stages for the stream HP1 ($H1.C5.t1-Q = 631.4$ kW, $H6.C5.t3-Q = 378.4$ kW, $H7.C2.t3-Q = 2,261.6$ kW and $H7.C5.t4-Q = 1,272.4$ kW), after the second and the last expansion stages for the stream HP2 ($H1.C8.t2-Q = 379.4$ kW and $H1.C10.t2-Q = 913.3$ kW), and before the last expansion stage for the stream HP3 ($H6.C15.t4-Q = 1,502.7$ kW). The heat recovery of the streams LP1 and LP2 occurs before and after the first compression stage. Therefore, seven heat exchangers ($Q = 631.4$ kW with $A = 348.81$ m²; $Q = 378.4$ kW with $A = 163.3$ m²; $Q = 2,261.6$ kW with $A = 1,291.9$ m²; $Q = 1,272.4$ kW with $A = 830.6$ m²; $Q = 379.4$ kW with $A = 230.4$ m²; $Q = 913.3$ kW with $A = 875.3$ m²; and, $Q = 1,502.7$ kW with $A = 927.9$ m²) are used. In addition, one cooler allocated in the stream H2 ($Q = 1,147.5$ kW with $A = 352.3$ m²) is needed to meet the thermal demand of streams. The total annualized cost of the network is 9,099k US\$/year, composed by the capital cost of investment in equipment (8,396k US\$/year), and by the operational expenses with electricity (588k US\$/year) and thermal utilities (115k US\$/year).

In Case 2, the WEN is designed with two SSTC axes units. In this case, the optimal WEN obtained is composed by the same equipment used in Case 1. As result, the optimal

WEN obtained is also composed by four expansion stages for the stream HP1, three stages for the stream HP2 and two expansion stages for the stream HP3, as well as three stages of compression for both streams LP1 and LP2. The stream HP1 is expanded through one stand-alone turbine (1,170.8 kW), followed by one single-stage SSTC turbine (200 kW) allocated on the shaft 2, two parallel SSTC turbines (1,500 kW and 200 kW) on the shaft 1, and one single-stage SSTC turbine (1473 kW) on the shaft 1. The stream HP2 is expanded through one valve, followed by expansion through one single-stage SSTC turbine (837.7 kW) located on the shaft 1, one more valve and, finally, by one single-stage SSTC turbine (454.4 kW) on the shaft 1. The stream HP3 passes across two stages of expansion through one valve, and one single-stage SSTC turbine (1,500 kW) associated with the shaft 2. While LP1 is compressed through two subsequent stand-alone compressors (950 kW and 421.6 kW), followed by two parallel SSTC compressors (950 kW and 750 kW) located on the shaft 2. The stream LP2 is compressed in three stages through two parallel SSTC compressors (950 kW and 733.9 kW) located on shaft 1, followed by one stand-alone compressor (950 kW), and three parallel SSTC compressors (950 kW, 950 kW and 881.16 kW) associated with shaft 1. Fig. 7 shows the optimal configuration for the WEN obtained for this example. The total work produced (consumed) by the turbines (compressors) on each shaft is equal to 4,465.1 kW for shaft 1, and 1,700 kW for the shaft 2. Again, as there are no remains or lacks of energy in the shafts, no helper motor or generator is needed to satisfy the energy balance. However, one stand-alone turbine is used in the network. Thus, 1,170.3 kW of energy are produced in the WEN, and can be used in other stages of the process and/or for sale of electricity.

In the HEN design, the same heat exchange equipment obtained in the previous case is needed. Thus, seven heat exchangers ($Q = 631.4$ kW with $A = 348.81$ m²; $Q = 378.4$ kW

with $A = 163.3 \text{ m}^2$; $Q = 2,261.6 \text{ kW}$ with $A = 1,291.9 \text{ m}^2$; $Q = 1,272.4 \text{ kW}$ with $A = 830.6 \text{ m}^2$; $Q = 379.4 \text{ kW}$ with $A = 230.4 \text{ m}^2$; $Q = 913.3 \text{ kW}$ with $A = 875.3 \text{ m}^2$; and, $Q = 1,502.7 \text{ kW}$ with $A = 927.9 \text{ m}^2$) are used. Moreover, one cooler allocated in the stream H2 ($Q = 1,147.5 \text{ kW}$ with $A = 352.3 \text{ m}^2$) is needed to meet the thermal demand of streams. The results obtained for Case 1 and for Case 2 are shown in Table 3. The networks obtained in both cases differ only in the number of SSTC axes used; as result, both have the same total cost. Thus, in this case, the total annualized cost of the WEN is also 9,099k US\$/year, composed by the capital cost of investment in equipment (8,396k US\$/year), and by the operational expenses with electricity (588k US\$/year) and thermal utilities (115k US\$/year). As in Example 1, if the use of three axes is forced, the objective function leads to sub-optimal solutions.

In Case 1, the mathematical model contains 5,053 continuous variables, 132 binary variables and 6,287 constraints with 21,837 Jacobian elements (non-zeros) in which 2,975 are nonlinear. In Case 2, the mathematical model contains 5,581 continuous variables, 292 binary variables and 7,213 constraints with 25,377 Jacobian elements (non-zeros) in which 3,531 are nonlinear. The CPU times of solution with the DICOPT solver are 3.45 min for Case 1 and 8.15 for Case 2, the optimal solutions are found in the sixth and ninth major iterations, respectively.

In this example, it is again shown that the same WEN with heat integration can be designed with the use of one or two SSTC axes units. Thus, besides the economic factor, the space available in the processing plant for the arrangement of the shafts (SSTC) and equipment should be considered to choose the best WEN design.

The proposed model proved suitable for the synthesis of WEN in which the integration of work between five process streams is evaluated [three streams at high-

pressure (HP1 to HP3) and two streams at low-pressure (LP1 and LP2)]. However, the model can be used for pressure recovery of a larger number of process streams. Moreover, a larger number of compression and expansion stages in the WEN, as well as a larger number of heat exchange stages in HEN, and restrictions prohibiting exchange between streams can be easily implemented in the model. Though, a large number of stages in the WEN superstructure should be avoided so as not to increase the complexity of the problem to the point that it is only possible to obtain unfeasible solutions.

Example 3. In this example, the WEN synthesis with heat integration is performed to promote the work integration between streams, which need to achieve a target state distinct from the initial state. Thus, the pressure recovery is carried out between two streams at high-pressure (HP1 and HP2) and two streams at low-pressure (LP1 and LP2). The stream HP1 has an initial state of 410 K and 900 kPa, and needs to reach the final state of 600 K and 100 kPa. The stream HP2 enters in the process at 355 K and 850 kPa, and must attain a target state of 500 K and 150 kPa. In the same way, the streams LP1 and LP2 must change from the initial state of 100 kPa and 600 K to a final state of 700 kPa and 350 K, and 900 kPa and 360 K, respectively. The data streams for this case study are shown in Table 1. Again, the WEN is designed to allow up to four stages of compression and expansion, in which occurs the thermal integration of streams in the HEN. The stream HP1 gives rise to five cold streams C1–C5, and HP2 originates the inlet streams C6–C10 in the HEN. Similarly, LP1 gives rise to H1–H5 and LP2 originates H6–H10. Thus, the heat recovery is performed between 10 cold streams and 10 hot streams, given that all cold streams can exchange heat with all hot streams.

In this example, the intermediate inlet temperatures of the streams in the HEN are restricted from 288 K to 700 K. The hot utilities are available at 700 K and the cold utilities at 288 K. The possibility of streams splits is allowed, and heaters and coolers can be used to meet the needs of heat for streams. For simplification, four stages of heat exchange in the HEN are considered. Moreover, the flow rates and heat capacities of all the streams are known constants. The WEN design allows the use of up to three SSTC units to obtain an optimal network by minimizing the total annualized cost, which consists of the operational expenses and capital cost of investment in equipment.

In Case 1, the WEN is designed with only one SSTC axis unit. In this case, the optimal WEN design obtained is composed by four stages of expansion and three compression stages. Thus, the stream HP1 is subjected to four expansion stages through one single-stage SSTC turbine (1,276.1 kW) associated with the shaft, followed by one stand-alone turbine (1,026.3 kW), two parallel SSTC turbines (1,500 kW and 130.6 kW), and one valve. The stream HP2 undergoes four stages of expansion through one single-stage SSTC turbine (243.3 kW) associated with the shaft, one valve, and two subsequent single-stage SSTC turbines (1,500 kW and 100 kW). The stream LP1 undergoes compression through three subsequent stand-alone compressors (489.6 kW, 950 kW and 950 kW). The stream LP1 bypasses the last stage of compression. Likewise, the stream LP2 passes across three stages of compression through one stand-alone compressor (950 kW) in the first stage, three parallel SSTC compressors (950 kW each one), followed by two parallel SSTC compressors (950 kW each one) associated with the shaft. The last stage of compression for stream LP2 is a bypass. Fig. 8 shows the optimal configuration obtained for the WEN with heat integration. The total work produced (consumed) by the turbines (compressors) is equal to 4,750 kW on the shaft. As there are no remains or lacks of energy

in the shaft, no helper motor or generator is needed to satisfy the energy balance. However, one stand-alone turbine is used in the network. Thus, 1,026.3 kW of energy are produced in the WEN, and can be used in other stages of the process and/or for sale of electricity.

The thermal integration of the high-pressure streams occurs after the first and the last expansion stages for the stream HP1, and before the first and after the last stages for the stream HP2. The heat recovery for the low-pressure streams occurs before all compression stages for the streams LP1 and LP2. In this case, five heat exchangers to recover heat between the streams H6.C2.t2 ($Q = 1,518.1$ kW with $A = 469.6$ m²), H1.C5.t1 ($Q = 4,835.5$ kW with $A = 1,778.2$ m²), H6.C5.t1 ($Q = 2,293.5$ kW with $A = 1,000$ m²), H6.C6.t4 ($Q = 1,163.8$ kW with $A = 654.6$ m²) and H6.C10.t1 ($Q = 3,242.9$ kW with $A = 511.3$ m²) are required. One heater ($Q = 881.6$ kW with $A = 84.8$ m²) and six coolers ($Q = 1,572.8$ kW with $A = 459.3$ m², $Q = 575.8$ kW with $A = 344.1$ m², $Q = 775.5$ kW with $A = 277.8$ m², $Q = 4,791.1$ kW with $A = 1,000$ m², $Q = 1,427.6$ kW with $A = 943.5$ m², and $Q = 1,864.3$ kW with $A = 455.4$ m²) located in the streams C5, H1–H3, and H6–H8, respectively, are also needed. The total annualized cost of the WEN is 10,695k US\$/year, which 1,398k US\$/year corresponds to the operational costs associated with the thermal services, and 1,109k US\$/year are expenses related to electricity. The capital cost of investment in equipment is equal to 8,188k US\$/year.

In Case 2, the WEN is designed to allow the use of up to three SSTC axes units. In this case, the optimal WEN design obtained is composed by four stages of expansion and three compression stages. Thus, three SSTC axes units are required in the WEN configuration. The stream HP1 is subjected to four stages of expansion through two parallel SSTC turbines (1,500 kW and 1,364.8), followed by three subsequent single-stage SSTC turbines (100 kW, 588.3 kW and 705.3 kW) associated to shafts 1, 3 and 2, respectively.

The stream HP2 passes through four stages of expansion through four single-stage SSTC turbines (1,211.8 kW, 100 kW, 100 kW and 649.6 kW) associated to shafts 2, 1 and 2, respectively. The stream LP1 undergoes compression through one stand-alone compressor (844.4 kW), followed by one single-stage SSTC compressor (588.3 kW) on the shaft 3, and one stand-alone compressor (950 kW). The stream LP1 bypasses the last stage of compression. Likewise, the stream LP2 passes across three stages of compression through one stand-alone compressor (465.5 kW) in the first stage, three parallel SSTC compressors (950 kW each one) associated with shaft 2, followed by three parallel SSTC compressors (950 kW, 950 kW and 781.5 kW) allocated on shaft 2. The last stage of compression for stream LP2 is a bypass. Fig. 9 shows the optimal configuration obtained for the WEN with heat integration. The total work produced (consumed) by the turbines (compressors) is equal to 200 kW for the shaft 1, 5,531.5 kW for the shaft 2, and 588.3 kW for the shaft 3. Any utility turbine is used in the network; however, one energy generator (200 kW) is needed to satisfy the energy balance on the shaft 1.

The thermal integration of the high-pressure streams occurs after the first and the last expansion stages for the stream HP1, and before the first and after the last stages for the stream HP2. The heat recovery for the low-pressure streams occurs before all compression stages for the stream LP1, as well as before the stages 2 and 3 for the stream LP2. In this case, five heat exchangers to recover heat between the streams H1.C2.t3 ($Q = 2,245.6$ kW with $A = 748.2$ m²), H1.C6.t4 ($Q = 1,851.1$ kW with $A = 692.2$ m²), H7.C2.t3 ($Q = 4,558.4$ kW with $A = 1,446.1$ m²), H7.C5.t2 ($Q = 2,336.4$ kW with $A = 1,000$ m²) and H7.C10.t3 ($Q = 2,773.4$ kW with $A = 993.7$ m²) are required. One heater ($Q = 713.1$ kW with $A = 70.2$ m²) and five coolers ($Q = 2,363.4$ kW with $A = 594.9$ m², $Q = 851.3$ kW with $A = 387.9$ m², $Q = 441.3$ kW with $A = 196.2$ m², $Q = 3,936.6$ kW with $A = 1,000$ m² and $Q = 2,993.4$ kW

with $A = 1,000 \text{ m}^2$) located in the streams C5, H1–H3, H7 and H8, respectively, are also needed. The total annualized cost of the WEN is 11,322k US\$/year, which 1,299k US\$/year corresponds to the operational costs associated with the thermal services and 948k US\$/year are expenses related to electricity. The capital cost of investment in equipment is equal to 9,075k US\$/year. The results obtained for both cases are shown in Table 4.

In Case 1, the mathematical model contains 3,688 continuous variables, 168 discrete variables and 4,734 constraints with 16,360 Jacobian elements (non-zeros) in which 2,264 are nonlinear. In Case 2, the mathematical model contains 3,900 continuous variables, 232 discrete variables and 5,105 constraints with 17,710 Jacobian elements (non-zeros) in which 2,482 are nonlinear. The model is solved with the DICOPT solver, the CPU times are 6.30 min for Case 1 and 11.20 min for Case 2, the optimal solutions are obtained in the sixth and ninth major iterations, respectively.

In this example, the proposed superstructure is used for optimal WEN synthesis with heat integration of streams that need to achieve a target temperature state. The results show that the model can be successfully used to solve this kind of problem. However, it is noted that to satisfy the thermal demand of streams is required the use of a large number of equipment for heat exchange, i.e., heat exchangers, heaters and coolers. Consequently, a larger amount of thermal utilities (steam and cooling water) are also required, increasing the total annualized cost of the network in comparison to the previous examples, in which intermediate heat exchange between stages of expansion and compression is only used to improve the process of pressure recovery. Moreover, the use of three SSTC axes units proved to be less economically attractive, because although a smaller amount of thermal

services are needed, a larger number of equipment is required in this configuration, increasing the total annualized cost of the network.

In all cases studied, the heat recovery between stages of the WEN is essential to improve the processes of compression and expansion. In this way, the heat integration among process streams is economically interesting since the use of heating and cooling utilities (heaters and coolers) is reduced, which results in decrease of costs. It must be remembered that the reduction of the use of hot and cold external services, such as cooling water and steam is also responsible for the reduction of environmental impacts.

7. Conclusions

A new model for the simultaneous synthesis of WEN with thermal integration is proposed. The superstructure developed is formulated in mathematical programming, with the aim of obtaining the optimal integration of work, between streams at high-pressure and low-pressure. For this purpose, pressure manipulation equipment running on the same SSTC unit are used in various stages of expansion and compression. The model allows the use of several SSTC axes units, and between the WEN stages the streams are sent to the HEN to promote heat integration, as well as to improve the pressure recovery process. In addition to SSTC turbines and compressors, stand-alone (utility) equipment—namely compressors, turbines and valves—can be used to satisfy the energy demand of the streams. The WEN superstructure is optimized using a mixed-integer nonlinear programming (MINLP) formulation. The objective is to synthesize a network that presents a minimum total annualized cost, composed by the capital cost of investment in the various units of the

network, and the operational expenses related to electricity, heating, and cooling of process flows.

The WEN synthesis with heat integration is a highly complex process. It seeks to find the optimal configuration of the network using the least amount of equipment for the handling pressure and heat exchange, as well as the minimum consumption of electricity, and thermal utilities. The complexity of the resulting model is due to the requirement to simultaneously optimize all parameters relating to both networks (i.e., WEN and HEN). With regard to the optimal WEN design, it is necessary to ensure that all outlet pressures of the sub-streams in stages of compression and expansion should be equal, since streams at different pressures cannot be mixed. Moreover, the SSTC compressors and turbines share a common single shaft, and so should operate properly to guarantee the same flow rate. For the HEN synthesis, the standard problem is increased to include the unknown intermediate temperatures of the streams connected to the WEN.

The proposed WEN superstructure is written in GAMS, and solved with the DICOPT solver. The CONOPT and CPLEX solvers are used—as sub-solvers—to solve the NLP and MIP problems, respectively. While the DICOPT solver algorithm contains provisions for dealing with non-convexities, the high nonlinearity and non-convexity of the model does not always guarantee the global optimum. However, some numerical experiments with this model showed that increasing the number of major iterations, and solving feasibility problems that may arise from NLP, allow obtaining good solutions. For the solution of the model is crucial to adequately establish all limits of the variables. The lower and upper bounds for the variables pressure, temperature, mass flow, and work are especially critical for the network design.

Three examples covering different situations were studied to verify the accuracy of the proposed methodology. In all cases, it was showed that the heat integration between stages of the WEN is essential to enhance the processes of compression and expansion. Therefore, the heat recovery of the streams proved to be economically attractive, due to reduced capital cost and operating expenses related to heating and cooling fluids, because of using a smaller amount of hot and cold utilities. It was also observed that the total annualized cost of the network can be reduced with the use of power generators, and stand-alone turbines. In this case, the cost is reduced by the revenue obtained of the electricity generated from the excess of expansion work in the shafts and stand-alone turbines, which can be used in other stages of the process and/or for sale of electricity.

For the selection of the best WEN design, besides the economic factor, the available space in the process plant must also be considered. It is important to note that the larger the number of equipment operating on the same SSTC unit, the larger the difficulty in keeping them under the same operating conditions will be. In contrast, the use of a large number of SSTC units may request larger space for allocation of the equipment. In addition to allowing the use of several SSTC units, the present model can be used to promote the integration of work in a larger number of process streams. A higher number of stages of compression and expansion in WEN, as well as a larger number of heat exchange stages in HEN, and constraints prohibiting heat exchange between streams can be easily implemented in the WEN superstructure. However, a large number of stages in the WEN superstructure and constraints should be avoided, due to the complexity of the problem that can lead to infeasible solutions, or at least far from the global optimum. Likewise, the proposed model for the WEN design can be used to enable the integration between heat and work of streams needing to attain a target temperature state. In this case, the use of a larger

number of utilities is required to meet the streams thermal demand and reach the required output state in the process. Nevertheless, the model was also able to synthesize a network in a reduced CPU time providing good solutions.

Nomenclature

Roman letters

A	heat exchanger area
C	cost
CE	cost parameter for electricity
C_p	heat capacity
C_{po}	cost of equipment unit
CR_{max}	maximum compression ratio
CS	cost parameter for the heating
CV	cost parameter for the electric power revenue
CW	cost parameter for the cooling
E	number of SSTC units
f	annualization factor for the capital cost
F	flow rate streams
F_b	flow rate through the bypass
F_{BM}	correction factor for cost
F_e	flow rate through the SSTC equipment
F_v	flow rate through the valve
F_u	flow rate through the stand-alone equipment
h	individual coefficient of heat transfer

HP	high-pressure streams
K	number of stream splits
LP	low-pressure streams
M	big-M formulation parameter
ny	number of years
P_{IN}	inlet pressure
P_{in}	stage inlet pressure
P_{OUT}	outlet pressure
P_{out}	stage outlet pressure
Q	heat duty
r	fractional interest rate per year
S	number of stages in the work exchange network
T	temperature
T_{IN}	inlet temperature
T_{in}	stage inlet temperature
T_{OUT}	outlet temperature
T_{out}	stage outlet temperature
T_{turb}	turbine outlet temperature
T_{val}	valve outlet temperature
ΔT_{\min}	temperature minimal approximation
W_e	SSTC compressor/turbine work
W_g	generator work
W_m	helper motor work

W_u	compressor/turbine utility work
y	binary variable that defines the use of SSTC compressor/turbine
y^a	variable auxiliary for y
y^B	binary variable that defines the bypass
y^U	binary variable that defines the use of compressor/turbine utility
y^V	binary variable that defines the use of valve

Acronyms

BB	branch-and-bound
CEPCI	chemical engineering plant cost index
ExPAnD	extended pinch analysis and design
GAMS	general algebraic modeling system
GBD	generalized benders decomposition
GDP	generalized disjunctive programming
HEN	heat exchanger network
HP	high-pressure
LNG	liquefied natural gas
LP	low-pressure
MIP	mixed-integer programming
MILP	mixed-integer linear programming
MINLP	mixed-integer nonlinear programming
NLP	nonlinear programming
OA	outer approximation
SSTC	single-shaft-turbine-compressor

WEN work exchange network

Greek letters

γ heat capacity ratio

η isentropic efficiency

μ Joule-Thompson coefficient

Subscripts

c cold streams

e SSTC axes

h hot streams

i LP streams

j HP streams

k streams splits

m heating utility

n cooling utility

s stages in the WEN

t stages in the HEN

Acknowledgments

The authors gratefully acknowledge the financial support by the Brazilian agency “Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – CAPES”, under process

number 10758/12-7; and the Spanish Ministry of Science and Innovation and Ministry of Economy and Competitiveness, under project CTQ2012-37039-C02-02.

References

- Allen, B., Savard-Goguen, M., Gosselin, L., 2009. Optimizing heat exchanger networks with genetic algorithms for designing each heat exchanger including condensers. *Appl. Therm. Eng.* 29, 3437–3444.
- Al-mutairi, E.M., 2010. Optimal design of heat exchanger network in oil refineries. *Chem. Eng. Trans.* 21, 955–960.
- Aspelund, A., Berstad D.O., Gundersen, T., 2007. An extended pinch analysis and design procedure utilizing pressure based exergy for subambient cooling. *Appl. Therm. Eng.* 27, 2633–2649.
- Björk, K.-M., Nordman, R., 2005. Solving large-scale retrofit heat exchanger network synthesis problems with mathematical optimization methods. *Chem. Eng. Process. Process Intensif.* 44, 869–876.
- Caballero, J.A., Grossmann, I.E., 2013. A review of the state of the art in optimization. *J. Rev. Iberoam. Autom. In.* 4, 5–23.
- Chen, J.J., 1987. Letter to editor: Comments on improvement on a replacement for the logarithmic mean. *Chem. Eng. Sci.* 42, 2488.
- Cheng, X., Liang, X., 2012a. Optimization principles for two-stream heat exchangers and two-stream heat exchanger networks. *Energy* 46, 421–429.
- Cheng, X., Liang, X., 2012b. Computation of effectiveness of two-stream heat exchanger networks based on concepts of entropy generation, entransy dissipation and entransy-dissipation-based thermal resistance. *Energy Convers. Manag.* 58, 163–170.

- Cheng, X., Liang, X., 2012c. Heat-work conversion optimization of one-stream heat exchanger networks. *Energy* 47, 421–429.
- Couper, J.R., Penney, W.R., Fair, J.R., Walas, S.M., 2010. *Chemical Process Equipment, Selection and Design*, second ed., Elsevier, USA.
- Escobar, M., Trierweiler, J.O., 2013. Optimal heat exchanger network synthesis: A case study comparison. *Appl. Therm. Eng.* 51, 801–826.
- Frausto-Hernández, S., Rico-Ramírez, V., Jiménez-Gutiérrez, A., Hernández-Castro, S., 2003. MINLP synthesis of heat exchanger networks considering pressure drop effects. *Comput. Chem. Eng.* 27, 1143–1152.
- Furman, K.C., Sahinidis, N.V., 2002. A critical review and annotated bibliography for heat exchanger network synthesis in the 20th century. *Ind. Eng. Chem. Res.* 41, 2335–2370.
- Gharaie, M., Zhang, N., Jobson, M., Smith, R., Panjeshahi, M.H., 2013. Simultaneous optimization of CO₂ emissions reduction strategies for effective carbon control in the process industries. *Chem. Eng. Res. Des.* 91, 1483–1498.
- Gorji-Bandpy, M., Yahyazadeh-Jelodar, H., Khalili, M., 2011. Optimization of heat exchanger network. *Appl. Therm. Eng.* 31, 779–784.
- Grossmann, I.E., Caballero, J.A., Yeomans, H., 2000. Advances in mathematical programming for the synthesis of process systems. *Latin Am. Appl. Res.* 284, 263–284.
- Gundersen, T., Naess, L., 1988. The synthesis of cost optimal heat exchanger networks: An industrial review of the state of the art. *Comput. Chem. Eng.* 12, 503–530.
- Hasan, M.M.F., Jayaraman, G., Karimi, I.A., 2010. Synthesis of heat exchanger networks with nonisothermal phase changes. *AIChE J.* 56, 930–945.

- Huang, K.F., Karimi, I.A., 2013. Simultaneous synthesis approaches for cost-effective heat exchanger networks. *Chem. Eng. Sci.* 98, 231–245.
- Hwa, C.S., 1965. Mathematical formulation and optimization of heat exchanger networks using separable programming, in: *AIChE-I Chem. Symp.* 101–106.
- Grossmann, I.E., 2002. Review of nonlinear mixed-integer and disjunctive programming techniques. *Optim. Eng.* 3, 227–252.
- Jezowski, J., 1994a. Heat exchanger network grassroot and retrofit design. The review of the state-of-the-art: Part I. Heat exchanger network targeting and insight based methods of synthesis. *Hungar J. Ind. Chem.* 22, 279–294.
- Jezowski, J., 1994b. Heat exchanger network grassroot and retrofit design. The review of the state-of-the-art: Part II. Heat exchanger network synthesis by mathematical methods and approaches for retrofit design. *Hungar J. Ind. Chem.* 22, 295–308.
- Kaluri, R.S., Basak, T., 2011. Entropy generation due to natural convection in discretely heated porous square cavities. *Energy* 36, 5065–5080.
- Kesler, M.S., Parker, R.O., 1969. Optimal networks of heat exchanger. *Chem. Eng. Prog. Symp. Ser.* 65, 111–120.
- Lara, Y., Lisbona, P., Martínez, A., Romeo, L.M., 2013. Design and analysis of heat exchanger networks for integrated Ca-looping systems. *Appl. Energy* 111, 690–700.
- Morar, M., Agachi, P.S., 2010. Review : Important contributions in development and improvement of the heat integration techniques. *Comput. Chem. Eng.* 34, 1171–1179.
- Vaklieva-Bancheva, N., Ivanov, B.B., Shah, N., Pantelides, C.C., 1996. Heat exchanger network design for multipurpose batch plants. *Comput. Chem. Eng.* 20, 989–1001.

- Onishi, V.C., Ravagnani, M.A.S.S., Caballero, J.A., 2013a. Mathematical programming model for heat exchanger design through optimization of partial objectives. *Energy Convers. Manag.* 74, 60–69.
- Onishi, V.C., Ravagnani, M.A.S.S., Caballero, J.A., 2013b. Simultaneous synthesis of heat exchanger networks with pressure recovery: Optimal integration between heat and work. *AIChE J.* doi:10.1002/aic.14314.
- Ravagnani, M.A.S.S., Caballero, J.A., 2007. Optimal heat exchanger network synthesis with the detailed heat transfer equipment design. *Comput. Chem. Eng.* 31, 1432–1448.
- Razib, M.S., Hasan, M.M.F., Karimi, I.A., 2012. Preliminary synthesis of work exchange networks. *Comput. Chem. Eng.* 37, 262–277.
- Serna, M., Jiménez, A., 2004. An area targeting algorithm for the synthesis of heat exchanger networks. *Chem. Eng. Sci.* 59, 2517–2520.
- Serna-González, M., Ponce-Ortega, J.M., 2011. Total cost target for heat exchanger networks considering simultaneously pumping power and area effects. *Appl. Therm. Eng.* 31, 1964–1975.
- Smith, R., 2005. *Chemical Process Design and Integration*, second ed., John Wiley and Sons Ltda., England.
- Sors, A., Kravanja, Z., 2002. Simultaneous MINLP synthesis of heat exchanger networks comprising different exchanger types. *Comput. Chem. Eng.* 26, 599–615.
- Turton, R., Bailei, R.C., Whiting, W.B., Shaeiwitz, J.A., 2003. *Analysis, Synthesis and Design of Chemical Process*, second ed., McGraw-Hill, New York.
- Vaskan, P., Guillén-Gosálbez, G., Jiménez, L., 2012. Multi-objective design of heat-exchanger networks considering several life cycle impacts using a rigorous MILP-based dimensionality reduction technique. *Appl. Energy* 98, 149–161.

- Wang, R.Z., Xia, Z.Z., Wang, L.W., Lu, Z.S., Li, S.L., Li, T.X., Wu, J.Y., He, S., 2011. Heat transfer design in adsorption refrigeration systems for efficient use of low-grade thermal energy. *Energy* 36, 5425–5439.
- Wechsung, A., Aspelund, A., Gundersen, T., Barton, P.I., 2011. Synthesis of heat exchanger networks at subambient conditions with compression and expansion of process streams. *AIChE J.* 57, 2090–2108.
- Huang, Y.L., Fan, L.T., 1996. Analysis of a work exchanger network. *Ind. Eng. Chem. Res.* 35, 3528–3538.
- Yee, T.F., Grossmann, I.E., 1990. Simultaneous optimization models for heat integration - II. Heat exchanger network synthesis. *Comput. Chem. Eng.* 14, 1165–1184.

APPENDIX: MINLP model of Yee and Grossmann

Yee and Grossmann (1990) proposed a model based on mathematical programming for the HENs synthesis. This is one of the most studied models among the simultaneous methods based on superstructures that can be found in the literature. The solution of this MINLP model allows identifying which heat exchangers are required, as well as the heat duty and temperatures of each stream through the minimization of the total cost of the network. In addition, one of the important advantages provided by this model is the easy implementation of heat exchange constraints. The algorithm is presented as follows.

1. The definition of the following indices is necessary in the model:

$$\begin{aligned}
 HS &= \{i / i \text{ is a hot stream}\} \\
 CS &= \{j / j \text{ is a cold stream}\} \\
 ES &= \{t / t \text{ is a stage in the network}\}
 \end{aligned}$$

2. The following input data are required:

C	area cost coefficient
CCU	unit cost for cold utility
CF	fixed cost of heat exchangers
CHU	unit cost for hot utility
F	mass flow of each stream
NT	total number of stages
T_{in}	inlet temperature of process streams

T_{out}	outlet temperature of process streams
U	overall coefficient of heat transmission
β	exponent in the cost area
Ω	upper limit to the heat exchanged in a heat exchanger
Γ	upper limit for the temperature difference

3. The variables of the problem are defined as follows:

$dt_{i,j,t}$	temperature difference for the exchange (i,j) at stage t
$dctu_i$	temperature difference for the exchange between the hot stream i and cold utility
$dthu_j$	temperature difference for the exchange between the cold stream j and hot utility
$q_{i,j,t}$	heat exchanged between hot stream i and cold stream j in stage t
qcu_i	heat exchanged between hot stream i and cold utility
qhu_j	heat exchanged between cold stream j and hot utility
$T_{i,t}$	temperature of hot stream i at hot extreme of stage t
$T_{j,t}$	temperature of the cold stream j at hot extreme of stage t
$z_{i,j,t}$	binary variable that indicates the existence of exchange (i,j) in stage t
zcu_i	binary variable that indicates the heat exchanged between cold utility and stream i
zhu_j	binary variable that indicates the heat exchanged between hot utility and stream j

4. The model comprises the following equations:

Global energy balance for each stream. This balance is essential to guarantee enough heating or cooling for each process stream. Therefore, the sum of the amount of heat that each stream exchanges with all other process streams in all stages, plus the heat exchanged with the utility stream must equal the total heat transferred for each stream.

$$\begin{aligned} (Tin_i - Tout_i)F_i &= \sum_{t \in ES} \sum_{j \in CS} q_{i,j,t} + qcu_i & i \in HS \\ (Tout_j - Tin_j)F_j &= \sum_{t \in ES} \sum_{i \in HS} q_{i,j,t} + qhu_j & j \in CS \end{aligned} \quad (A.1)$$

Energy balance in each stage. The energy balance is required in each stage of the HEN superstructure to determine the temperatures. Due the assumption of isothermal mixing, flow rate variables are not required.

$$\begin{aligned} (T_{i,t} - T_{i,t+1})F_i &= \sum_{j \in CS} q_{i,j,t} & i \in HS, t \in ES \\ (T_{j,t} - T_{j,t+1})F_j &= \sum_{i \in HS} q_{i,j,t} & j \in CS, t \in ES \end{aligned} \quad (A.2)$$

Assignment of inlet temperatures in the superstructure. Fixed input temperatures (Tin) of all process streams are attributed to the inlet temperatures of the superstructure.

$$\begin{aligned} Tin_i &= T_{i,1} & i \in HS \\ Tin_j &= T_{j,NT+1} & j \in CS \end{aligned} \quad (A.3)$$

Feasibility of temperatures. The temperature through the subsequent stages should decrease. Thus, it is crucial to specify that the stage outlet temperature must be lower than the final outlet temperature for each stream.

$$\begin{aligned}
 T_{i,t} &\geq T_{i,t+1} & i \in HS, t \in ES \\
 T_{j,t} &\geq T_{j,t+1} & j \in CS, t \in ES \\
 Tout_i &\leq T_{i,NT+1} & i \in HS \\
 Tout_j &\geq T_{j,1} & j \in CS
 \end{aligned} \tag{A.4}$$

Calculation of the utility heat duty. The necessary hot and cold utilities are estimated for each process stream with an energy balance at the exit points of each stream.

$$\begin{aligned}
 (T_{i,NT+1} - Tout_i)F_i &= qcu_i & i \in HS \\
 (Tout_j - T_{j,1})F_j &= qhu_j & j \in CS
 \end{aligned} \tag{A.5}$$

Logical constraints. The logical constraints are required to verify the existence of the heat exchanged between hot and cold streams (i, j) at each stage t , as well as the exchanges between utilities and process streams.

$$\begin{aligned}
 q_{i,j,t} - \Omega z_{i,j,t} &\leq 0 & i \in HS, j \in CS, t \in ES \\
 qcu_i - \Omega zcu_i &\leq 0 & i \in HS \\
 qhu_j - \Omega zhu_j &\leq 0 & j \in CS
 \end{aligned} \tag{A.6}$$

Calculation of approximation temperatures among streams. The required area for a particular exchange is considered in the objective function. The determination of the approximation temperature at each extreme of the heat exchanger is needed for the calculation of these areas. However, these temperature differences are only active if heat exchange occurs. Hence, binary variables are used to enable or disable the calculation of these differences.

$$\begin{aligned}
 dt_{i,j,t} &\leq T_{i,t} - T_{j,t} + \Gamma(1 - z_{i,j,t}) & i \in HS, j \in CS, t \in ES \\
 dt_{i,j,t+1} &\leq T_{i,t+1} - T_{j,t+1} + \Gamma(1 - z_{i,j,t}) & i \in HS, j \in CS, t \in ES \\
 dtcu_i &\leq T_{i,NT+1} - Tout_{CU} + \Gamma(1 - zcu_i) & i \in HS \\
 dthu_j &\leq Tout_{HU} - T_{j,1} + \Gamma(1 - zhu_j) & j \in CS
 \end{aligned} \tag{A.7}$$

It is adequate to stipulate a minimum approach temperature in the network, such that the difference of temperature among the hot and cold streams at any point in the HEN is at least equal to this value.

$$dt_{i,j,t} \geq EMAT \quad i \in HS, j \in CS, t \in ES \tag{A.8}$$

Objective function. The objective function can be defined as the total cost of the network. The total cost includes the cost of utilities, the costs of the heat exchangers and the cost linked to each heat exchanger area. The logarithmic mean temperature difference is required for the calculation of the exchange area of the heat exchanger. Yee and Grossmann (1990) proposed the use of Chen's (1987) approximation:

$$\Delta T m_{i,j} = (\theta^1_{i,j} - \theta^2_{i,j}) / \ln(\theta^1_{i,j} / \theta^2_{i,j}) \approx [\theta^1_{i,j} \cdot \theta^2_{i,j} (\theta^1_{i,j} + \theta^2_{i,j}) / 2]^{1/3} \quad i \in HS, j \in CS \quad (A.9)$$

This method avoids numerical difficulties related with the logarithmic mean when temperature differences ($\theta^1_{i,j}$; $\theta^2_{i,j}$) on both sides of the heat exchanger are equal. Moreover, if the temperature difference on both sides tends to zero, the approximation of Chen (1987) also tends to zero. Therefore, the objective function is defined as follows:

$$\begin{aligned} \min : & \sum_{i \in HS} CCU \cdot qcu_i + \sum_{j \in CS} CHU \cdot qhu_j + \sum_{i \in HS} \sum_{j \in CS} \sum_{t \in ES} CF_{i,j} \cdot z_{i,j,t} + \sum_{i \in HS} CF_{i,CU} \cdot zcu_i + \\ & \sum_{j \in CS} CF_{j,HU} \cdot zhu_j + \sum_{i \in HS} \sum_{j \in CS} \sum_{t \in ES} C_{i,j} \left\{ q_{i,j,t} / U_{i,j} \left[dt_{i,j,t} \cdot dt_{i,j,t+1} (dt_{i,j,t} + dt_{i,j,t+1}) / 2 \right]^{1/3} \right\}^{\beta_{i,j}} + \\ & \sum_{i \in HS} C_{i,CU} \left\{ qcu_i / U_{i,CU} \left[dtcu_i (T_{out_i} - T_{in_{CU}}) (dtcu_i + (T_{out_i} - T_{in_i})) / 2 \right]^{1/3} \right\}^{\beta_{i,CU}} + \\ & \sum_{j \in CS} C_{HU,j} \left\{ qhu_j / U_{HU,j} \left[dthu_j (T_{in_{HU}} - T_{out_j}) (dthu_j + (T_{in_{HU}} - T_{out_j})) / 2 \right]^{1/3} \right\}^{\beta_{HU,j}} \end{aligned} \quad (A.10)$$

In which,

$$1/U_{i,j} = 1/h_i + 1/h_j; \quad 1/U_{i,CU} = 1/h_{CU} + 1/h_i; \quad 1/U_{HU,j} = 1/h_j + 1/h_{HU} \quad (A.11)$$

The resulting MINLP model contains the objective function and all constraints mentioned before. It is crucial to highlight that all constraints presented on this approach are linear. Nonlinearities exist only in the objective function. In spite of this, due to the non-convex character of the solution of this problem, a local minimum can be found. A significant characteristic of the model is that it allows, in general, avoiding configurations

in which streams splits are generated. This is achieved through the condition that sets a maximum of one exchange at each stage per stream. In mathematical language, this is expressed as follows:

$$\sum_{i \in HS} z_{i,j,t} \leq 1 \quad j \in CS, t \in ES, \quad \sum_{j \in CS} z_{i,j,t} \leq 1 \quad i \in HS, t \in ES \quad (\text{A.12})$$

List of Figures Captions

Fig 1. WEN superstructure for the compression stage s .

Fig 2. WEN superstructure for the expansion stage s .

Fig 3. Multi-stage superstructure for two streams in WEN synthesis with the HEN highlighted.

Fig 4. Optimal WEN configuration with heat integration obtained for Example 1 - Case study 1.

Fig 5. Optimal WEN configuration with heat integration obtained for Example 1 - Case study 2.

Fig 6. Optimal WEN configuration with heat integration obtained for Example 2 - Case study 1.

Fig 7. Optimal WEN configuration with heat integration obtained for Example 2 - Case study 2.

Fig 8. Optimal WEN configuration with heat integration obtained for Example 3 - Case study 1.

Fig 9. Optimal WEN configuration with heat integration obtained for Example 3 - Case study **Table 1**

Stream data for the different examples.

Stream	F (kg/s)	C_p (kJ/kg K)	h (kW/m ² K)	T_{IN} (K)	T_{OUT} (K)	P_{IN} (kPa)	P_{OUT} (kPa)
<i>Example 1</i>							
HP1	15	1.432	0.1	380	380	850	100
HP2	18	0.982	0.1	400	400	980	180
LP1	15	1.432	0.1	400	400	100	520
LP2	18	1.432	0.1	400	400	100	850
<i>Example 2</i>							
HP1	15	2.454	0.1	350	350	900	100
HP2	15	0.982	0.1	350	350	850	150
HP3	15	1.432	0.1	400	400	700	200
LP1	18	1.432	0.1	390	390	100	700
LP2	15	2.454	0.1	420	420	100	900
<i>Example 3</i>							
HP1	12	2.454	0.1	410	600	900	100
HP2	18	0.982	0.1	355	500	850	150
LP1	15	1.432	0.1	600	350	100	700
LP2	18	2.454	0.1	600	360	100	900
<i>Additional data</i>							
$\Delta T_{\min} = 5$ K	$\eta = 0.7$	$\mu = 1.961e^{-3}$ K/kPa	$RC_{\max} = 3$	$f = 0.18$			
<i>Cost data (US\$/year kW)</i>							
$CE = 455.04$	$CV = 400.00$	$CS = 337.00$	$CW = 100.00$				

Table 2

Optimal WEN design obtained for Example 1.

<i>Case 1</i>			<i>Case 2</i>		
WEN	Stream.Stage	W (kW)	WEN	Stream.Stage	W (kW)
Stand-alone turbines	HP1.s4	848.4	Stand-alone turbines	HP1.s4	848.4
	HP2.s4	698.3		HP2.s4	698.3
SSTC turbines	HP1.s1	100.0	SSTC turbines	HP1.s1	100.0
	HP1.s1	1,480.1		HP1.s1	1,480.1
	HP2.s2	950.0		HP2.s2	950.0
Stand-alone compressors	HP2.s3	100.0	Stand-alone compressors	HP2.s3	100.0
	LP1.s1	282.0		LP1.s1	282.0
	LP1.s2	950.0		LP1.s2	950.0
SSTC compressors	LP2.s1	950.0	SSTC compressors	LP2.s1	950.0
	LP2.s3	950.0		LP2.s3	950.0
	LP1.s3	950.0		LP1.s3	950.0
Valves	LP2.s2	950.0	Valves	LP2.s2	950.0
	LP2.s2	730.1		LP2.s2	730.1
Shaft 1	HP1.s2	-	Shaft 1	HP1.s2	-
	HP2.s1	-		HP2.s1	-
Shaft 2	-	2,630.1	Shaft 2	-	950.0
HEN	Q (kW)	A (m ²)	HEN	Q (kW)	A (m ²)
H1.C2.t3	603.6	390.5	H1.C2.t3	603.6	390.5
H1.C5.t1	742.1	432.7	H1.C5.t1	742.1	432.7
H7.C5.t2	1,083.7	581.3	H7.C5.t2	1,083.7	581.3
H7.C10.t1	1,748.6	918.2	H7.C10.t1	1,748.6	918.2
H1	836.2	424.1	H1	836.2	424.1
H7	747.9	462.7	H7	747.9	462.7
C_{total} (kUS\$/year)		6,279	C_{total} (kUS\$/year)		6,279

Table 3

Optimal WEN design obtained for Example 2.

<i>Case 1</i>			<i>Case 2</i>		
WEN	Stream.Stage	W (kW)	WEN	Stream.Stage	W (kW)
Stand-alone turbines	HP1.s1	1,170.8	Stand-alone turbines	HP1.s1	1,170.8
	HP1.s2	200.0		HP1.s2	200.0
	HP1.s3	1,500.0		HP1.s3	1,500.0
SSTC turbines	HP1.s3	200.0	SSTC turbines	HP1.s3	200.0
	HP1.s4	1,473.0		HP1.s4	1,473.0
	HP2.s1	837.7		HP2.s1	837.7
	HP2.s4	454.4		HP2.s4	454.4
	HP3.s4	1,500.0		HP3.s4	1,500.0
Stand-alone compressors	LP1.s1	950.0	Stand-alone compressors	LP1.s1	950.0
	LP1.s2	421.6		LP1.s2	421.6
	LP2.s2	950.0		LP2.s2	950.0
SSTC compressors	LP1.s3	950.0	SSTC compressors	LP1.s3	950.0
	LP1.s3	750.0		LP1.s3	750.0
	LP2.s1	950.0		LP2.s1	950.0
	LP2.s1	733.9		LP2.s1	733.9
	LP2.s3	950.0		LP2.s3	950.0
	LP2.s3	950.0		LP2.s3	950.0
	LP2.s3	881.2		LP2.s3	881.2
Valves	HP2.s1	-	Valves	HP2.s1	-
	HP2.s3	-		HP2.s3	-
	HP3.s1	-		HP3.s1	-
Shaft 1	-	6,165.1	Shaft 1	-	4,465.1
Shaft 2	-	-	Shaft 2	-	1,700.0
HEN	Q (kW)	A (m ²)	HEN	Q (kW)	A (m ²)
H1.C5.t1	631.4	348.8	H1.C5.t1	631.4	348.8
H6.C5.t3	378.4	163.3	H6.C5.t3	378.4	163.3
H7.C7.t3	2,261.6	1,291.9	H7.C7.t3	2,261.6	1,291.9
H7.C5.t4	1,272.4	830.6	H7.C5.t4	1,272.4	830.6
H1.C8.t2	379.4	230.4	H1.C8.t2	379.4	230.4
H1.C10.t2	913.3	875.3	H1.C10.t2	913.3	875.3
H6.C15.t4	1,502.7	927.9	H6.C15.t4	1,502.7	927.9
H2	1,147.5	352.3	H2	1,147.5	352.3
C_{total} (kUS\$/year)		9,099	C_{total} (kUS\$/year)		9,099

Table 4 Optimal WEN design obtained for Example 3.

<i>Case 1</i>			<i>Case 2</i>		
WEN	Stream.Stage	W (kW)	WEN	Stream.Stage	W (kW)
Stand-alone turbines	HP1.s2	1,026.3		HP1.s1	1,364.8
	HP1.s1	1,276.1		HP1.s1	1,500.0
SSTC turbines	HP1.s3	130.6	SSTC turbines	HP1.s2	100.0
	HP1.s3	1,500.0		HP1.s3	588.3
	HP2.s1	243.3		HP1.s4	705.3
	HP2.s3	1,500.0		HP2.s1	1,211.8
	HP2.s4	100.0		HP2.s2	100.0
Stand-alone compressors	LP1.s1	489.6	Stand-alone compressors	HP2.s3	100.0
	LP1.s2	950.0		HP2.s4	649.64
	LP1.s3	950.0		LP1.s1	844.4
SSTC compressors	LP2.s1	950.0	SSTC compressors	LP1.s3	950.0
	LP2.s2	950.0		LP2.s1	465.5
	LP2.s2	950.0		LP1.s2	588.3
	LP2.s2	950.0		LP2.s2	950.0
	LP2.s3	950.0		LP2.s2	950.0
Valves	LP2.s3	950.0	SSTC compressors	LP2.s2	950.0
	HP1.s4	-		LP2.s3	781.5
	HP2.s2	-		LP2.s3	950.0
			LP2.s3	950.0	
			Generator	-	200.0
Shaft 1	-	4,750.0	Shaft 1	-	200.0
Shaft 2	-	-	Shaft 2	-	5,531.5
Shaft 3	-	-	Shaft 3	-	588.3
HEN	Q (kW)	A (m ²)	HEN	Q (kW)	A (m ²)
H6.C2.t2	1,518.1	469.6	H1.C2.t3	2,245.6	748.2
H1.C5.t1	4,835.5	1,778.2	H1.C6.t4	1,851.1	692.2
H6.C5.t1	2,293.5	1,000	H7.C2.t3	4,558.4	1,446.1
H6.C6.t4	1,163.8	654.6	H7.C5.t2	2,336.4	1,000.0
H6.C10.t1	3,242.9	511.3	H7.C10.t3	2,773.4	993.7
C5	881.6	84.8	C5	713.1	70.2
H1	1,572.8	459.3	H1	2,363.4	594.9
H2	575.8	344.1	H2	851.3	387.9
H3	775.5	277.8	H3	441.3	196.2
H6	4,791.1	1,000	H7	3,936.6	1,000.0
H7	1,427.6	943.5	H8	2,993.4	1,000.0
H8	1,864.3	455.4			

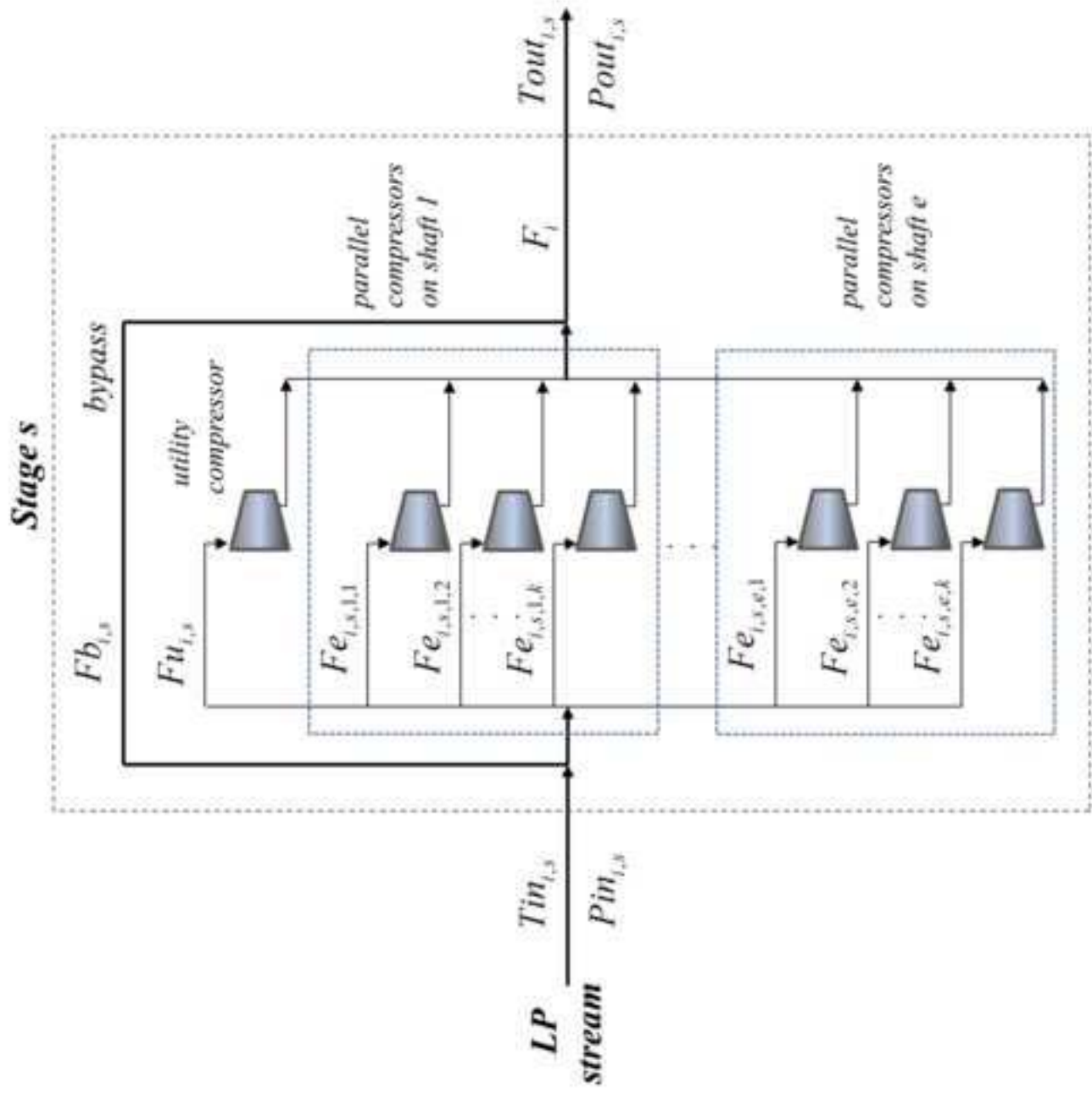
C_{total} (kUS\$/year)

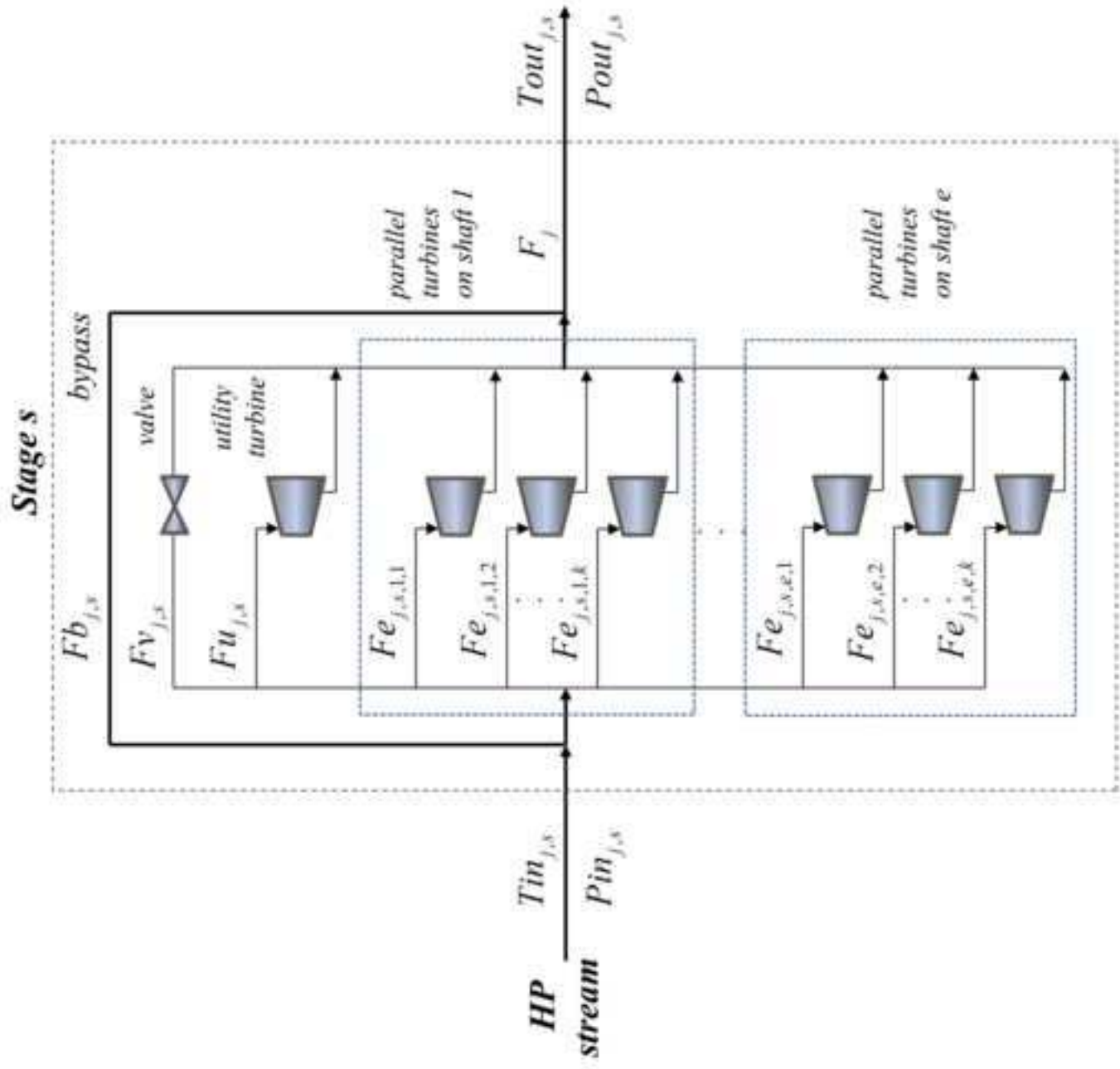
10,695

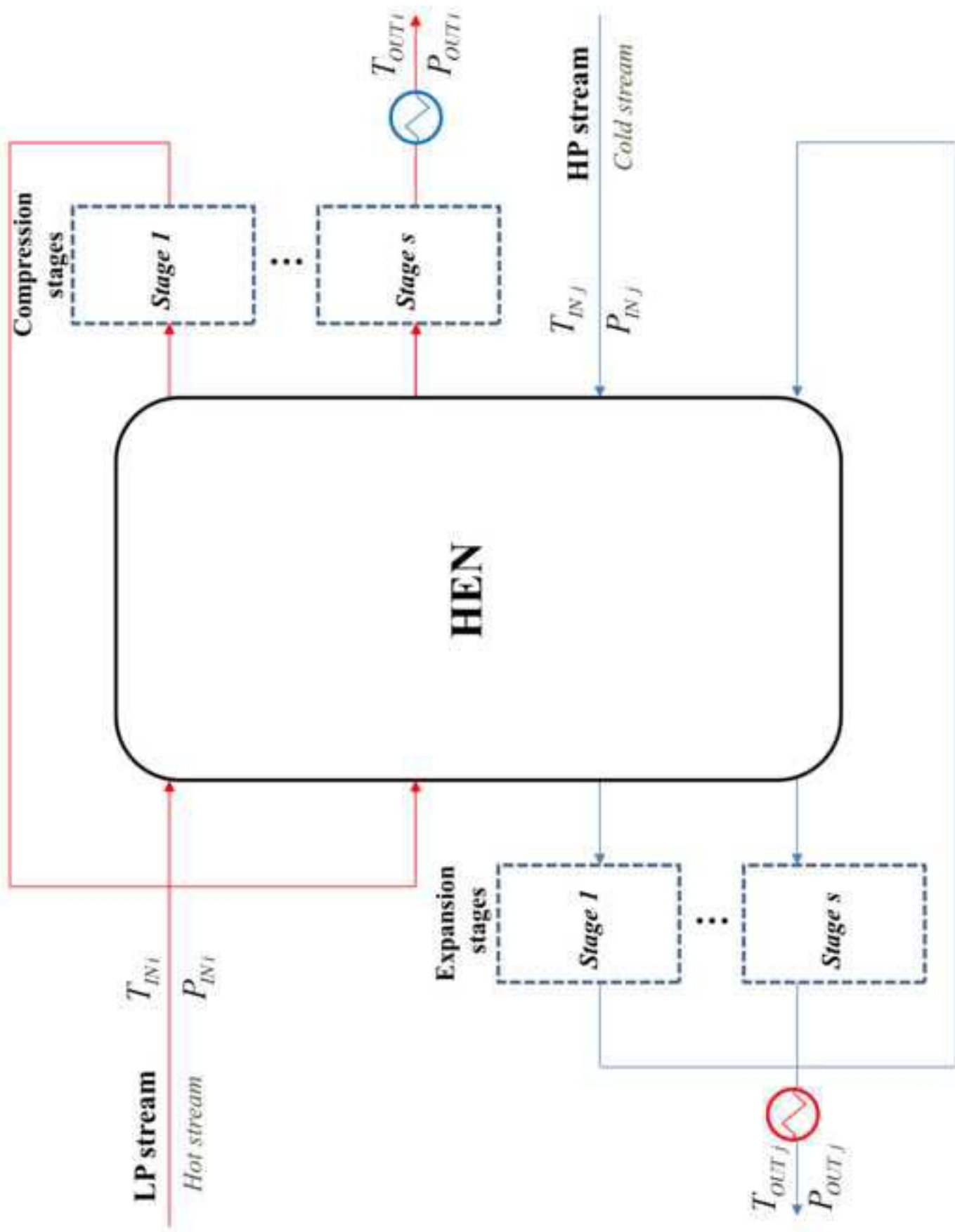
 C_{total} (kUS\$/year)11,322

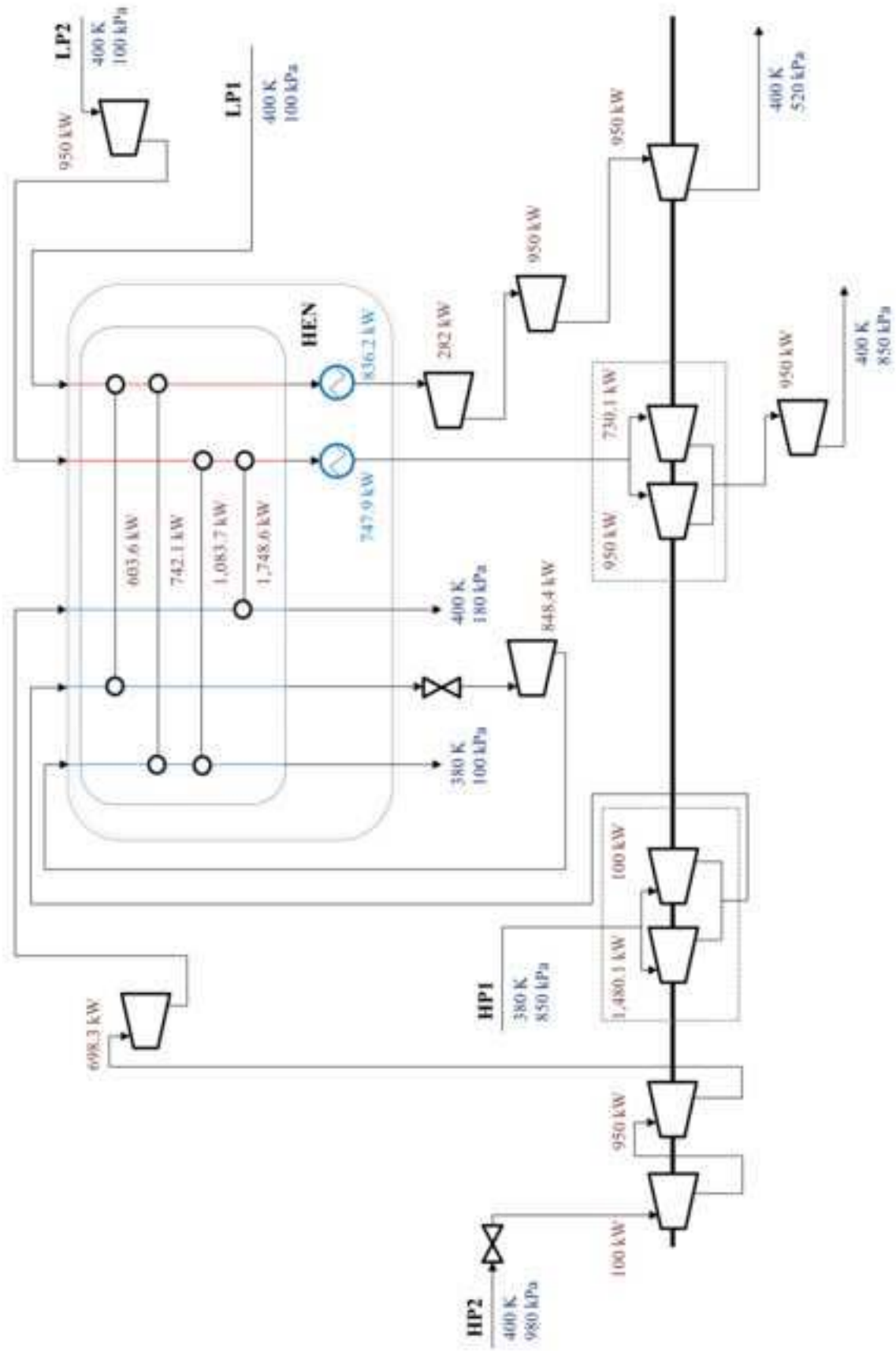
Highlights

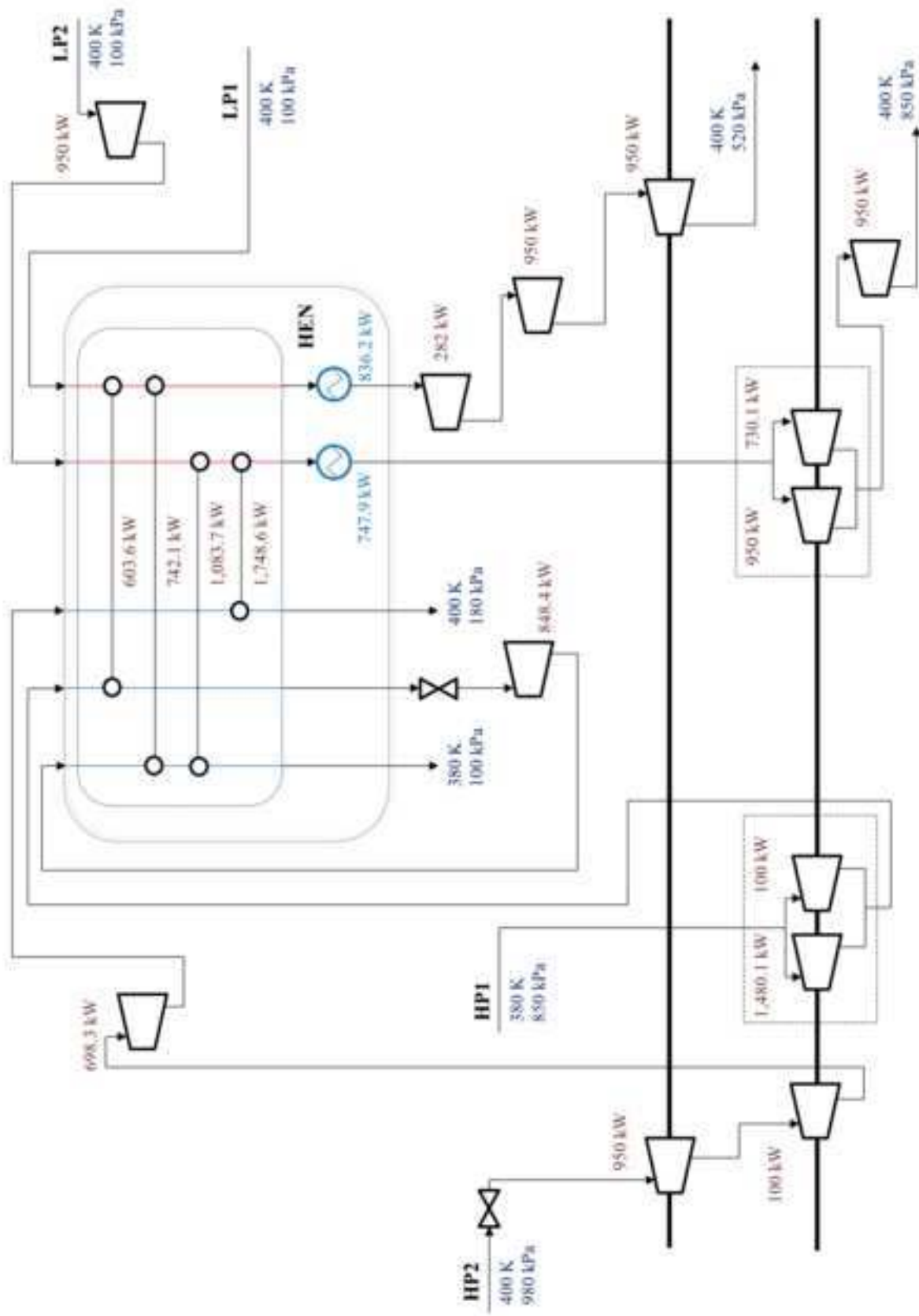
1. New MINLP model for the synthesis of work exchange networks with heat integration
2. Work integration of streams at high and low-pressure in a multi-stage superstructure
3. Pressure manipulation equipment acting on several shafts and stand-alone equipment
4. Heat integration between pressure manipulation stages in the work exchange network
5. Use of a smaller amount of utilities reducing capital cost and operational expenses

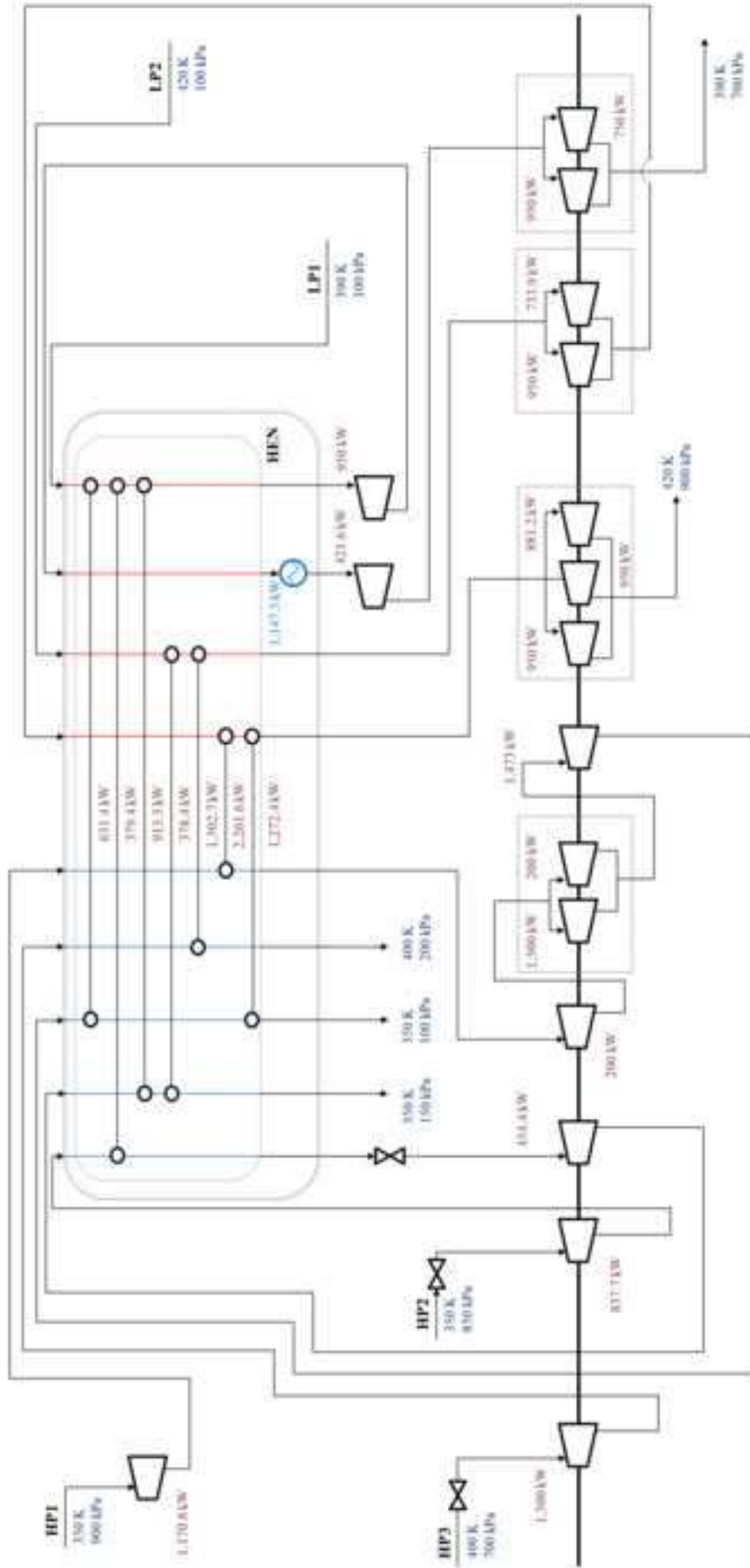


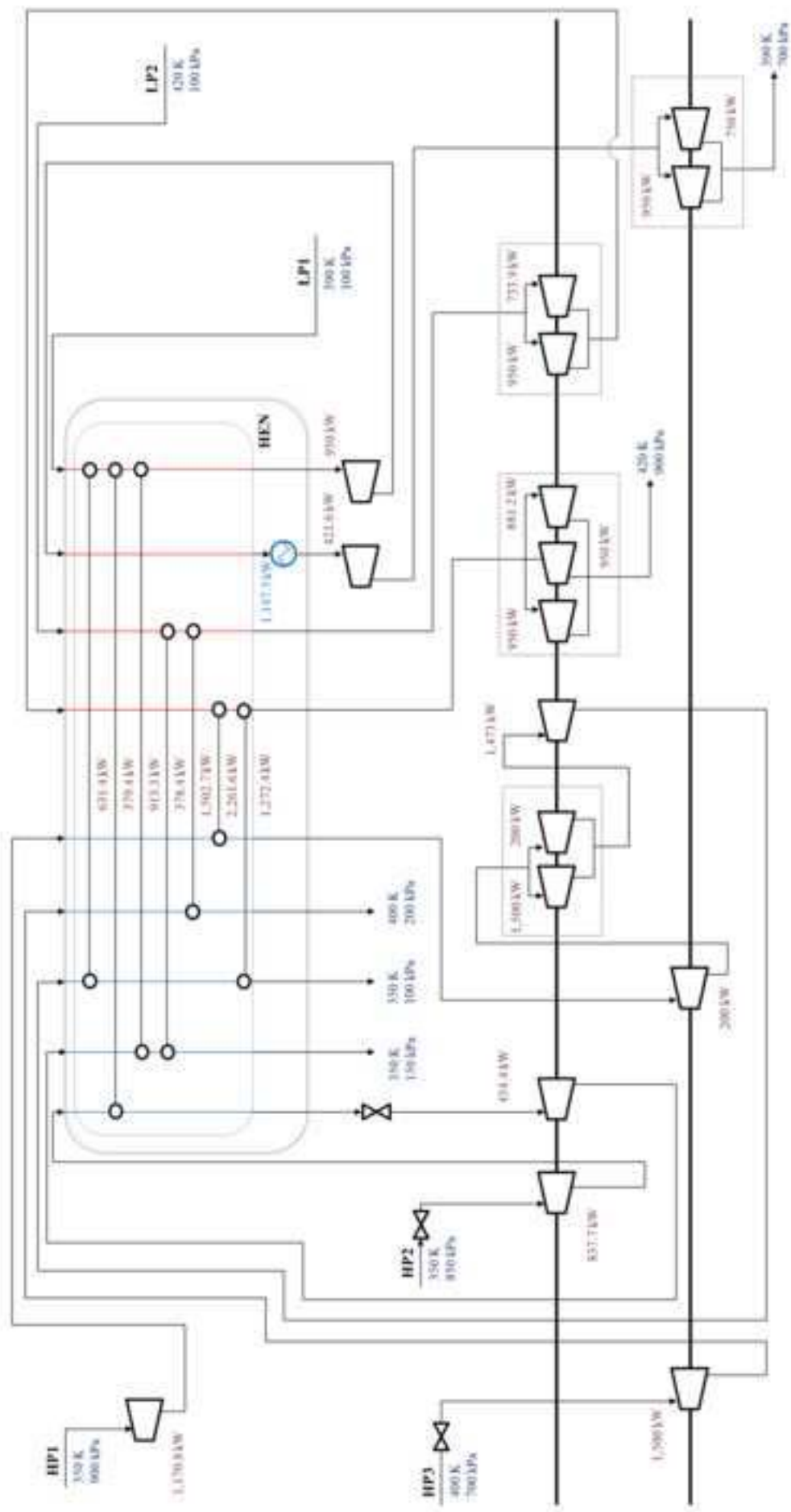


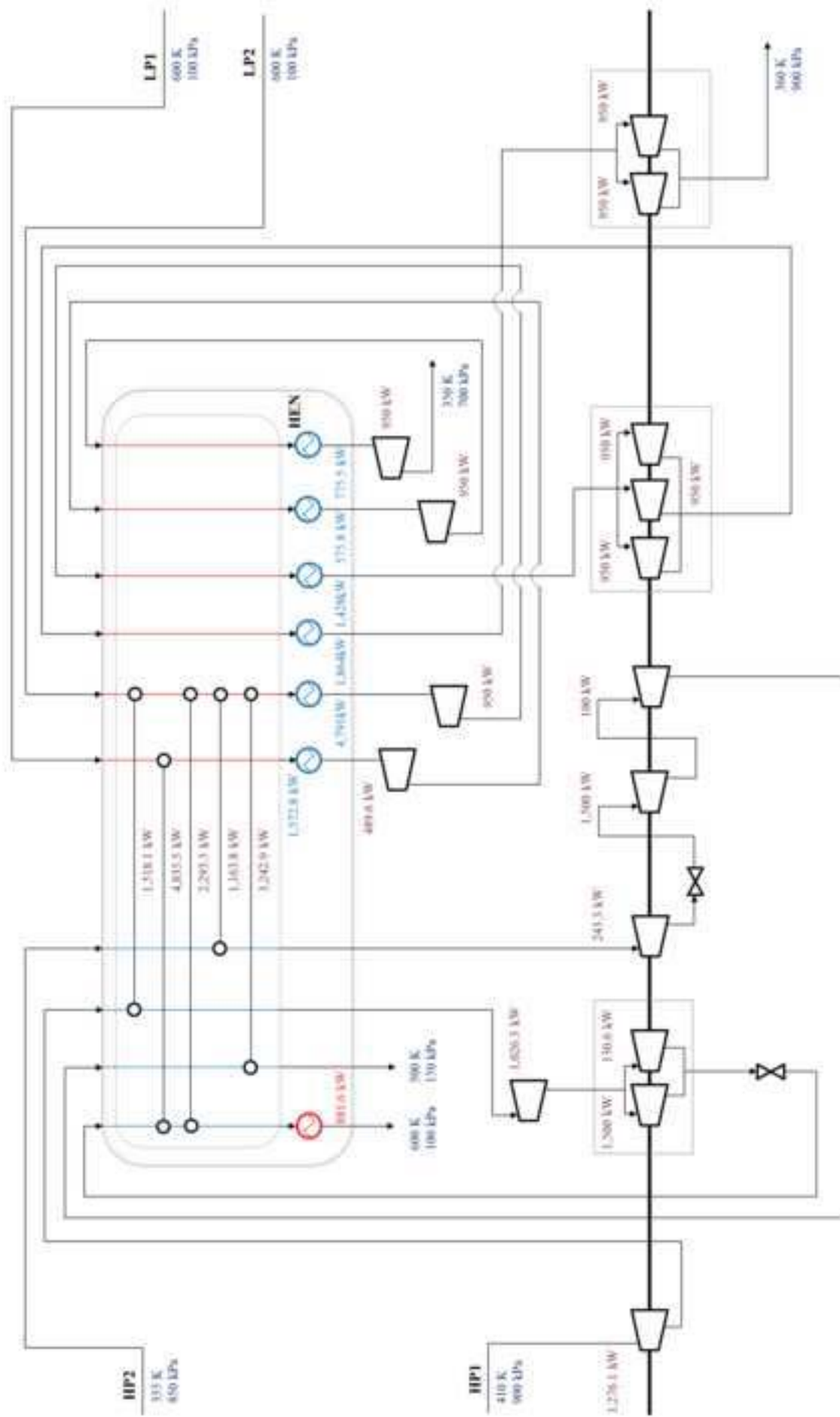












Figure

