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Generalized Simultaneous Optimization Model for Synthesis of Heat and Work Exchange Networks.

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Abstract

In this work, a new superstructure for simultaneous synthesis of work and heat exchange networks (WHEN) is presented. In the proposed model, an explicit modeling of the identity changes of the process streams is developed. The main idea behind this approach is to allow the pressure-change streams act as low-pressure hot streams as well as high-pressure cold streams in different stages of the WHEN without using any predefined manipulation routes. In this sense, using this novel approach, all possible thermodynamic paths of the process streams are considered into the synthesis problem. The novel formulation is done without incorporating new binary variables and nonlinear constraints in the problem. Therefore, the proposed superstructure allows to improve the obtained solution and to reduce the computational burden. These improvements are shown by using three case studies with different size and complexity. In most cases, savings of approximately 1-7% in total annualized cost were observed.

Keywords: WHEN, Simultaneous synthesis, Generalized modeling, MINLP, Optimization

1. Introduction

The growing consumption of energy is one of the major global concerns. World energy demand is expected to grow approximately 50% by 2050. This increase together with the

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expected higher consumption of fossil fuels encourages the development of strategies that improve the efficient use of energy and reduce the environmental impact. In the particular case of Argentina, the energy consumption doubled from 1990-2020, being the industrial sector responsible for consuming around 26% of the total energy demand in 2020 (Secretaría de Gobierno de Energía, 2020). In this sense, new strategies to increase the energy integration of the process will produce an improvement in the global process efficiency and the environmental impacts. It is well known that any industrial process presents available energy in the different streams that compose it. Usually, these streams could be: (i) cooled (called hot streams), (ii) heated (cold streams), (iii) compressed (low-pressure streams), and (iv) expanded (high-pressure streams) or (iv) they must have simultaneous changes in pressure and temperature. Without using an energy recovery system, most of these changes are produced by an additional external energy which increases the operating process costs. In this sense, in the last years, the work and heat integration has become a very important topic in the process systems engineering area. This problem aims to improve the use of available energy by installing of heat and work exchange equipments between the different process streams in order to minimize the energy consumption, i.e. by reducing the operating costs.

The heat integration through heat exchanger networks is one of the most studied topics of the last 60 years. Linnhoff and Flower (1978) were the first authors to introduce the energy integration and the pinch temperature concepts based on the previous work of Hohmann (1971). These concepts produced a large number of sequential (Cerdá et al., 1983; Floudas et al., 1986; Papoulias and Grossmann, 1983a,b) and simultaneous (Ciric and Floudas, 1991; Yee and Grossmann, 1990) methods to solve the HEN synthesis problem. This problem aims to obtain the best heat exchange combination between the process streams and utilities to achieve the network with the minimum total annualized cost, i.e. with the minimum investment and operating costs. Despite the fact that there have not been major conceptual contributions in the area of HEN synthesis, in the last few years, several publications addressed some modeling improvements. In this sense, some aspects incorporated into the synthesis problem are: (i) performance criteria for heat exchangers (Cotrim et al., 2021;

Frausto-Hernández et al., 2003; Li et al., 2022), (ii) non-isothermal mixtures of the streams (Faruque Hasan et al., 2010; Huang et al., 2012), and (iii) operation, control and flexibility criteria (Aaltola, 2002; Braccia et al., 2018; Zhang and Verheyen, 2006). A detailed review of these topics can be found in Furman and Sahinidis (2002) and Klemeš and Kravanja (2013).

Although the area of heat integration is a mature field, several strategies have emerged in the recent years to integrate compression/expansion work from turbines/compressors, using Work Exchange Networks (WENs). These networks were also integrated with Heat Exchanger Networks (HENs) generating a new energy recovery system called WHEN. The WHEN synthesis constitutes a more complex problem than the HEN and WEN synthesis problems (Fu and Gundersen, 2016a,b). Similarly to HEN synthesis, the aim of the WHEN problem is to obtain the best combination of heat (by heat exchangers) and work (by compressors/turbines) exchange trying to maximize the exergetic efficiency of the system or to minimize the total annualized cost. The formulations presented in the literature use different approaches to integrate the work of the compressors and turbines. While some methodologies propose integrating the work by using a single shaft for turbine and compressor, other formulations use indirect exchange through generators and motors. An excellent review of the problem and the different existing strategies in the area of heat and work integration is presented in Fu et al. (2018) and Yu et al. (2020). Moreover, Razib et al. (2012) present a list of processes where the use of HEN/WEN/WHEN are relevant.

Similarly to the HEN synthesis problem, the WHEN synthesis is solved by: (i) heuristic rules and graphical methods (Aspelund et al., 2007; Fu and Gundersen, 2016a,b) and (ii) optimization based on mathematical models (Huang and Karimi, 2016; Lin et al., 2021; Nair et al., 2018; Onishi et al., 2014a, 2017, 2014b; Pavão et al., 2019, 2021; Santos et al., 2020; Wechsung et al., 2011). Within the mathematical optimization works, Huang and Karimi (2016) present a WHEN synthesis model that improves the previous work of Onishi et al. (2014a). This new WHEN model incorporates: (i) constant-pressure streams, i.e. streams that do not exchange work and are only taken into account for heat integration and (ii) final heaters and coolers for pressure-changing streams in order to reach the desired temperature values. The authors show that with these modifications it is possible to reduce the total annualized cost by 3.1%, improving both the work exchanged by 10.6% and the heat exchanged by 81.0% according to the best solution obtained in the work. The authors also showed that the inclusion of the final heaters and coolers allows to obtain solutions that are infeasible for the model of Onishi et al. (2014a). It is important to highlight that the proposed WHEN superstructure was formulated as a set of interconnected networks, which were exclusively for: (i) the heat exchange (HEN) and (ii) the work exchange (WEN). In this superstructure, the different process streams alternately go through the HEN and WEN networks. In addition, the changes in the identity of the streams are not considered, instead, a pre-classification of the streams based on heuristic rules is used. While low-pressure (LP) streams are considered hot streams (HS) in the HEN, high-pressure (HP) streams are considered cold streams (CS). This heuristic pre-classification is based on the fact that the energy recoverable from the gas expansion increases with the temperature at which this gas enters at the turbine and, on the other hand, the energy required for compression decreases with the temperature at which this gas enters at the compressor. In this sense, considering the HP and LP streams as cold and hot streams, respectively, the HEN increases the energy recovery in the turbines by increasing the temperature of the HP streams and reduces the energy consumed in the compressors by decreasing the temperature of the LP streams. This treatment of the HP and LP streams within the WHEN constitutes a simplification since it does not contemplate that the HP or LP streams can be heated, cooled, compressed and expanded in different stages of the network.

A generalized treatment of the energy identities of the HP and LP streams was later incorporated in Lin et al. (2021), Nair et al. (2018), Onishi et al. (2018), Pavão et al. (2019), Santos et al. (2020), and Zhuang et al. (2020). Zhuang et al. (2020) propose a superstructure where only pressure-change streams are pre-classified, while hot and cold streams are considered unclassified streams. The authors demonstrate that considerable cost savings can be achieved with this superstructure compared to other solutions obtained from the literature. Later, Nair et al. (2018) provide a MINLP superstructure where unclassified high and low pressure streams and phase-changing streams are considered. Most recently, in Santos et al. (2020) the formulation presented by Onishi et al. (2018) is improved by incorporating hot and cold utilities after pressure manipulation and they are independent of the thermal identity of the process streams. In this case, the streams can potentially be heated or cooled using utilities based on their energy requirement. Thus, it is possible to adjust stream temperatures after the pressure manipulation. In this work, a two-level meta-heuristic method formed by SA (Simulated Anneling) to solve the combinatorial level and PSO (Particle Swarm Optimization) for the nonlinear level is used. It is important to note that the energy identity change modeling proposed in Onishi et al. (2018) and Santos et al. (2020) incorporates new nonlinearities to the original problem which increase its difficulty. Therefore, a better modeling approach would produce improvements on both the convergence time of the optimization algorithm as well as the quality of the obtained solution.

In this sense, this work proposes a novel MINLP formulation for WHEN synthesis with an explicit modeling of the identity changes of the process streams. The main idea behind the methodology is that the process streams can behave both as low-pressure hot streams as well as high-pressure cold streams at different stages of the WHEN. In this way, all possible thermodynamic paths for the streams are represented and alternative structures not considered by Huang and Karimi (2016) are included in this case. On the other hand, it is important to note that the explicit modeling of identity change is done in the following way: (i) the use of heuristic rules or predefined thermodynamic paths similar as used in Onishi et al. (2014a) and Onishi et al. (2014b) is avoided and (ii) new constraints to select the identity of the streams in each stage of the network are not used, thus new binary variables and nonlinearities are not included in the model. Therefore, with the proposed WHEN superstructure, it will be possible to obtain solutions not contemplated in previous works using a smaller number of binary variables and nonlinearities in the model.

This work is organized as follows: in section 1 the main contributions related to the WHENs synthesis are presented. In section 2 the definition of the synthesis problem of heat and work exchange networks is carried out and the proposed MINLP model is presented in the next section 3. Using this model, in sections 4.1, 4.2, and 4.3, three different case studies obtained from the bibliography are solved and their solutions are compared with previous works. Finally, section 5 summarizes the conclusions, discussions and future work.

2. Problem statement

Consider a set of process streams $S = \{1, 2, \ldots, \mathrm{S}\}$ where for each $s \in S$ it is known: (i) inlet temperature ($\mathrm{T}_s^{\mathrm{in}}$) and pressure ($\mathrm{P}_s^{\mathrm{in}}$), (ii) final target, i.e. outlet temperature ($\mathrm{T}_s^{\mathrm{out}}$) and pressure ($\mathrm{P}_s^{\mathrm{out}}$), (iii) mass flow ($\mathrm{F}_s$), (iv) heat capacity ($\mathrm{C}_{\mathrm{p}_s}$), (v) composition and phase, and (vi) heat transfer coefficient (h_s). Furthermore, heat exchange units and pressure manipulators are given with known efficiencies, design and operating costs, e.g. heat exchangers, cold and hot utilities, compressors and turbines (with the possibility of being coupled on a common shaft), valves, helper motors, and electric generators. The objective of the WHEN synthesis problem is to define the location and size of heat exchangers and cold/hot utilities, as well as pressure manipulation equipment, i.e. compressors, turbines, and valves, in order to minimize the total annualized cost. It is important to note that this cost is associated with a particular WHEN and includes the total capital cost, the operating cost and the revenue from electricity generation.

As in previous works, e.g. Huang and Karimi (2016); Onishi et al. (2014a); Santos et al. (2020), the following considerations are taken into account in order to simplify the problem:

- The heat capacities and the film heat transfer coefficient of each stream are known constants.
- In all heat exchangers, the pressure drops and the heat losses are negligible.
- For all compressors and turbines, the isentropic efficiency is known.
- The single-shaft-turbine-compressor can support an unlimited number of compressors and turbines operating at the appropriate speed.
- In the valves, the expansions are isenthalpic/adiabatic and irreversible (Joule-Thompson) with known constant Joule-Thompson coefficients.

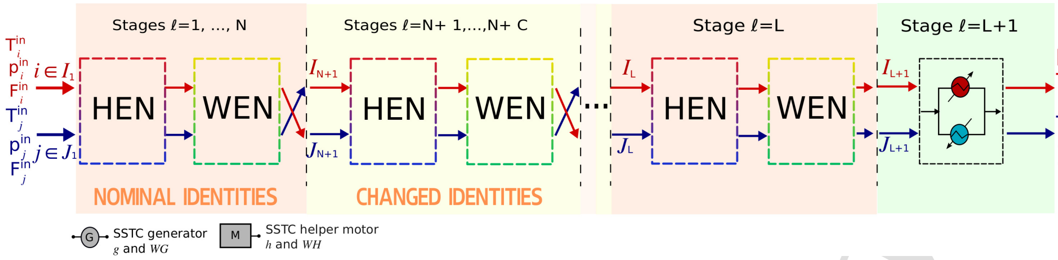


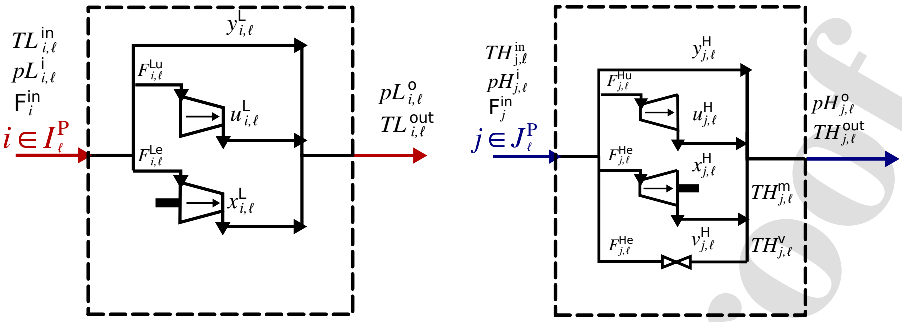
Figure 1: Proposed Superstructure for Heat and Work Exchange Networks Synthesis

- In the expansion, the gas streams are always below their inversion temperatures.

3. Simultaneous Work and Heat Exchange Network Synthesis Model

In this section, the superstructure for simultaneous synthesis of work and heat exchange networks (WHENs) is presented. This is based on the model proposed by Huang and Karimi (2016) to which an explicit modeling of the identity change in the streams is incorporated. This explicit modeling represents an improvement with respect to previous works (Onishi et al., 2018; Santos et al., 2020) since it avoids incorporating new binary variables and nonlinearities to the synthesis problem while maintaining the original model complexity (Huang and Karimi, 2016). The proposed WHEN superstructure, shown in Fig. 1, consists of L initial heat and work exchange stages formed by interconnected heat exchange networks (HENs) and work exchange networks (WENs). In the final additional stage (L + 1), the streams go through cold/hot utilities if necessary, in order to adjust their temperatures to target values.

The proposed superstructure contemplates the existence of streams with only relevant changes in: (i) pressure, (ii) temperature, or (iii) a combination of pressure and temperature. While the streams that change pressure go through all the stages of the WHEN, the streams that only change temperature go through only the HEN of the first stage, where they heat exchange and achieve the desired outlet temperatures. If the overall input and output states (pressures and temperatures) of the streams are taken into account and considering



(a) low-pressure stream i at stage ℓ. (b) high-pressure stream j at stage ℓ.

Figure 2: WEN superstructure

the criteria proposed by Huang and Karimi (2016), streams can be classified into: (i) hot streams, (ii) cold streams, (iii) high-pressure cold streams, and (iv) low-pressure hot streams. These overall identities constitute the nominal identities of the streams. The classification of streams will be further detailed in the section 3.1.

It is important to highlight that while HENs are modelled using the Synheat model proposed by Yee and Grossmann (1990), WENs are formed of single-stage and parallel equipment. Therefore, a low-pressure stream in the ℓ-th stage of the WHEN can: (i) bypass the stage, (ii) be compressed through a stand-alone compressor, and/or (iii) be compressed through an SSTC compressor, see Fig. 2(a). Similarly, a high-pressure stream in the ℓ-th stage of the WHEN can: (i) bypass the stage, (ii) be expanded through a stand-alone turbine, (iii) be expanded through an SSTC turbine, and/or (iv) go through the valve located in this stage, see Fig. 2(b).

As mentioned earlier, an explicit modeling of the identity change in the streams is incorporated into the superstructure to allow the pressure-changing streams to act as a low-pressure hot stream (i.e. they can be cooled and compressed) and as a high-pressure cold stream (i.e. they can be heated and expanded) at different stages of the network. In order to formulate these changes, the superstructure stages are separated into two sets N and C. These subsets indicate in which stages ℓ of the WHEN the streams take the nominal identities (equivalent to globally defined identity) or adopt the change identities (opposite identity of their global definition).

In each of these stages, when the streams act as low-pressure hot streams, they can be cooled (decreasing their temperature) in the HEN and compressed (increasing their pressure) in the WHEN and, when they act as high-pressure cold streams, they can be heated (increasing their temperature) and expanded (decreasing their pressure).

The superstructure (Fig. 1) is constructed in a such way that the streams present nominal identities during the first N stages ($\ell = \{1, \ldots, \mathrm{N}\} \in N$). Then, an identity crossover occurs which causes the streams pass through the next C stages with a changed identity, i.e. $\ell = \{\mathrm{N}+1, \ldots, \mathrm{N}+\mathrm{C}\} \in C$. After going through these C stages, the streams take their nominal identity again (new crossover). This change of energy identity every N stages of nominal identity and C stages of changed identity continues until the streams enter in the final utilities (at stage $\ell = \mathrm{L}+1$), where they adopt their nominal identities again. Using this model, all possible thermodynamic paths for the streams (Yu et al., 2020) can be represented. It is important to note that, in the Fig. 1, the streams going through the top of HENs/WENs act as low-pressure hot streams (low-pressure hot side of the WHEN), while the streams that enter below of WHEN act as high-pressure cold streams (high-pressure cold side of the WHEN).

This new modeling approach allows to improve the models proposed in previous works (Onishi et al., 2018; Santos et al., 2020), where the change in stream identity was formulated by: (i) splitting the streams into low-pressure hot sub-streams and high-pressure cold substreams before entering a stage, and (ii) using new constraints handled by binary variables to define the heat capacity flowrate of each substream. This modeling strategy: (i) generates a greater number of binary variables and (ii) transforms the heat capacity flowrate (a parameter in the original model) into a variable, which produces new nonlinear constraints. The above points show that these previous models are more complex and, therefore, the solvers could fail to obtain the optimal solution and they could use more computational burden. It is important to highlight that with the modeling proposed in this work, it is possible to maintain the difficulty of the original model since the heat capacity flowrate remains as a parameter in the model and additional binary variables are not incorporated.

Remark 1. *For all WHEN where $L \geq 4$, if $N = 2$ and $C = 2$, the obtained superstructure contemplates the heuristic rules used in Onishi et al. (2014a), in which: (i) a low-pressure stream can potentially be cooled, compressed, cooled, expanded, heated, compressed, and cooled and (ii) a high-pressure stream can be heated, expanded, heated, compressed, cooled, expanded, and heated. On the other hand, if $N = L$, the obtained superstructure is the same as that presented in Huang and Karimi (2016), where there is no identity change of the process streams. That is, the streams present nominal identity in all stages of the WHEN.*

3.1. Set Definitions

Before presenting the equations that describe the WHEN superstructure, it is necessary to define the sets involved in the modeling procedure. Given a set S of process streams whose compositions, phases, inlet and outlet temperatures ($\mathrm{T}_s^{\mathrm{in}}$ and $\mathrm{T}_s^{\mathrm{out}}$) and pressures ($\mathrm{P}_s^{\mathrm{in}}$ and $\mathrm{P}_s^{\mathrm{out}}$), flows and thermal and physicochemical properties are known, it can be classified in two subsets:

$$PC = \{\text{Pressure-Change streams}\} = \{s \mid s \text{ is gaseous and } \mathrm{P}_s^{\mathrm{in}} \neq \mathrm{P}_s^{\mathrm{out}}\}$$
$$NPC = \{\text{No-Pressure-Change streams}\} = \{s \mid s \text{ is gaseous or liquid and } \mathrm{P}_s^{\mathrm{in}} = \mathrm{P}_s^{\mathrm{out}}\}$$

The first set (PC) contains all gaseous process streams that change their pressure in the network (inlet and outlet pressure of the stream are different), i.e. PC has the streams that require a pressure manipulation by the turbines, compressors, valves, etc. In the second set (NPC), the gaseous or liquid streams whose pressures remain unchanged are considered. From a global point of view, taking into account the inlet ($\mathrm{P}_s^{\mathrm{in}}$) and outlet ($\mathrm{P}_s^{\mathrm{out}}$) pressures of each stream, the set PC can be partitioned as follows:

$$HPS = \{\text{High-Pressure streams}\} = \{s \mid s \in PC \wedge \mathrm{P}_s^{\mathrm{in}} > \mathrm{P}_s^{\mathrm{out}}\}$$
$$LPS = \{\text{Low-Pressure streams}\} = \{s \mid s \in PC \wedge \mathrm{P}_s^{\mathrm{in}} < \mathrm{P}_s^{\mathrm{out}}\}$$

That is, the set HPS includes all the streams that inlet pressure is higher than the outlet pressure (high-pressure streams) and the set LPS contains all low-pressure streams ($\mathrm{P}_s^{\mathrm{in}} <$

$\mathrm{P}_s^{\mathrm{out}}$). Similarly, the set NPC will be partitioned by considering the global input and output temperatures of the WHEN. Thus the following subsets can be specified:

$$HS = \{\text{No-Pressure-Change Hot streams}\} = \{s \mid s \in NPC \wedge \mathrm{T}_s^{\mathrm{in}} > \mathrm{T}_s^{\mathrm{out}}\}$$

$$CS = \{\text{No-Pressure-Change Cold streams}\} = \{s \mid s \in NPC \wedge \mathrm{T}_s^{\mathrm{in}} < \mathrm{T}_s^{\mathrm{out}}\}$$

where the set HS includes all streams without pressure changes for which their inlet temperature is higher than the outlet temperature (hot stream). On the other hand, CS contains the cold streams, i.e. streams that remain without pressure changes and their outlet temperature is higher than inlet temperature.

Although the proposed superstructure is flexible respect to the selection of the nominal identities of the streams, in this work the criteria proposed by Huang and Karimi (2016) is used, where the low-pressure and high-pressure streams are considered as hot and cold streams, respectively. Thus, the nominal identity of the pressure-changing streams is defined as low-pressure hot streams for streams in LPS and as high-pressure cold streams for streams in HPS.

As mentioned before, the new modeling approach presented in this work allows changes in the identity of the streams. In this way, regardless of how pressure-changing streams are globally classified, they can alternate their identity, acting in some stages of the WHEN with their nominal identity and with changed identity in the remaining stages. Thus, when the streams act as low-pressure hot streams, they will be cooled (i.e. their inlet temperature is higher than the outlet temperature in the HEN) and compressed (i.e. their inlet pressure is higher than the outlet pressure in the WEN). Similarly, when they act as high-pressure cold streams, they will be heated in the HEN and expanded in the WEN.

Due to these changes, it is necessary to classify the L stages of the WHEN in: (i) stages where the streams have a nominal identity and (ii) stages where the streams have a changed identity. Therefore, given the number of consecutive stages in which the streams have a nominal or changed identity, namely N and C, respectively, all stages of the WHEN can be classified by means of the function $f(\ell) = \left\lfloor \frac{\ell+\mathrm{C}-1}{\mathrm{C}+\mathrm{N}} \right\rfloor - \left\lfloor \frac{\ell-1}{\mathrm{C}+\mathrm{N}} \right\rfloor$, where $\lfloor . \rfloor$ is the floor function which returns the largest integer less than or equal to a given number. For each stage ℓ, this function returns zero if the streams have a nominal identity and one if they have a changed identity. Using this function the sets N and C result:

$$\begin{aligned} N &= \{\text{stages of WHEN where the streams have a nominal identity}\} \\ &= \left\{\ell \in L \mid \left\lfloor \frac{\ell + \mathrm{C} - 1}{\mathrm{C} + \mathrm{N}} \right\rfloor - \left\lfloor \frac{\ell - 1}{\mathrm{C} + \mathrm{N}} \right\rfloor = 0 \right\}, \\ C &= \{\text{stages of WHEN where the streams have a changed identity}\} \\ &= \left\{\ell \in L \mid \left\lfloor \frac{\ell + \mathrm{C} - 1}{\mathrm{C} + \mathrm{N}} \right\rfloor - \left\lfloor \frac{\ell - 1}{\mathrm{C} + \mathrm{N}} \right\rfloor = 1 \right\}. \end{aligned}$$

As an example, the values returned by this function for each stage ($\ell = 1, 2, \ldots, 4$) using different values of N and C are given in Table 3.1. It is important to note that regardless of how parameters N and C are set, in the first stage of the WHEN the streams have their nominal identities.

Table 1: Classification function, $f(\ell)$

N	C	Stage ℓ			
		1	2	3	4
1	1	0	1	0	1
2	1	0	0	1	0
1	2	0	1	1	0
2	2	0	0	1	1

Total number of stages, L = 4

Once N and C are defined, the streams that act as low-pressure or high-pressure streams at each stage are represented by the following sets:

$$\begin{aligned} I_\ell^{\mathrm{P}} &= \{\text{Low-Pressure streams at stage } \ell\} \\ &= \{s \mid s \in LPS \text{ if } \ell \in N, s \in HPS \text{ if } \ell \in C\} \quad \forall \ell = 1, \ldots, \mathrm{L} \\ J_\ell^{\mathrm{P}} &= \{\text{High-Pressure streams at stage } \ell\} \\ &= \{s \mid s \in HPS \text{ if } \ell \in N, s \in LPS \text{ if } \ell \in C\} \quad \forall \ell = 1, \ldots, \mathrm{L} \end{aligned}$$

These sets determine the energy identity of the streams according to the stage of the WHEN considered. Therefore, low-pressure streams in stage ℓ of the WHEN are included in the set I_ℓ^{P}, i.e. (i) streams in the set LPS at stages in N, and (ii) streams in the set HPS at stages in C. The streams in this set could increase their pressure in the WENs, i.e. $pL_{s,\ell}^{\mathrm{i}} \leq pL_{s,\ell}^{\mathrm{o}}$. Similarly, the set J_ℓ^{P} contains the streams that act as high-pressure streams in different stages of the WHEN, i.e. the streams that can be expanded, $pH_{s,\ell}^{\mathrm{i}} \geq pH_{s,\ell}^{\mathrm{o}}$.

Finally, if the hot and cold streams are added in sets I_ℓ^{P} and J_ℓ^{P}, respectively, two additional sets are defined as follows:

$$\begin{aligned} I_\ell &= \{\text{Low-Pressure Hot streams at stage } \ell\} \\ &= \{s \mid s \in I_\ell^{\mathrm{P}} \cup HS \text{ if } \ell = 1, s \in I_\ell^{\mathrm{P}} \text{ if } \ell \neq 1\} \quad \forall \ell = 1, \ldots, \mathrm{L} \\ J_\ell &= \{\text{High-Pressure Cold streams at stage } \ell\} \\ &= \{s \mid s \in J_\ell^{\mathrm{P}} \cup CS \text{ if } \ell = 1, s \in J_\ell^{\mathrm{P}} \text{ if } \ell \neq 1\} \quad \forall \ell = 1, \ldots, \mathrm{L} \end{aligned}$$

Thus, the sets I_ℓ and J_ℓ contain the low-pressure hot and high-pressure cold streams at each stage, respectively.

Remark 2. *It is important to highlight that the nominal thermal identity of low-pressure and high-pressure streams are defined according to the criteria used in Huang and Karimi (2016). However, the superstructure proposed in this work can be used even if these identities are defined using other criteria, e.g. by considering the inlet and outlet temperatures of the streams, by heuristic approaches, etc. This is possible given that the sets I_ℓ, J_ℓ, I_ℓ^P, and J_ℓ^P are defined in order to change the identities of the streams at different stages of the network and this modeling is sufficiently general to contemplate all possible behavior of the streams.*

3.2. Mathematical Programming Model

This section presents the equations of HEN, WEN, and final utilities that constitute each stage of WHEN. The objective function to be minimized is defined by:

$$TAC = f\,CAPEX + t\,(OPEX - REV) \qquad (1)$$

In this equation, TAC corresponds to the total annualized cost ($/year) and it is composed by the total capital cost $CAPEX$ ($/year), the total operating cost $OPEX$ ($/h) and revenue from electricity generation REV ($/h). On the other hand, f is the annualization factor for the capital cost and t is the operating hours per annum (h/year).

If the fixed (CF) and variable (C) costs associated with installing a stand-alone compressor/turbine, SSTC compressor/turbine, valve, heat exchanger, hot/cold utilities, an electric generator, and an auxiliary motor are known, then the total capital cost ($CAPEX$) will be defined as follows:

$$
\begin{aligned}
CAPEX = \sum_{\ell=1}^{\mathrm{L}} \Bigg[& \sum_{i\in I_\ell^{\mathrm{P}}} \left(\mathrm{CF}_i^{\mathrm{UC}}\, u_{i,\ell}^{\mathrm{L}} + \mathrm{C}_i^{\mathrm{UC}}\, F_{i,\ell}^{\mathrm{Lu}} + \mathrm{CF}_i^{\mathrm{SC}}\, x_{i,\ell}^{\mathrm{L}} + \mathrm{C}_i^{\mathrm{SC}}\, F_{i,\ell}^{\mathrm{Le}}\right) + \\
& \sum_{j\in J_\ell^{\mathrm{P}}} \left(\mathrm{CF}_j^{\mathrm{UT}}\, u_{j,\ell}^{\mathrm{H}} + \mathrm{C}_j^{\mathrm{UT}}\, F_{j,\ell}^{\mathrm{Hu}} + \mathrm{CF}_j^{\mathrm{ST}}\, x_{j,\ell}^{\mathrm{H}} + \mathrm{C}_j^{\mathrm{ST}}\, F_{j,\ell}^{\mathrm{He}} + \right. \\
& \left. \mathrm{CF}_j^{\mathrm{v}}\, v_{j,\ell}^{\mathrm{H}} + \mathrm{C}_j^{\mathrm{v}}\, F_{j,\ell}^{\mathrm{Hv}}\right) + \sum_{i\in I_\ell} \sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall j\neq i\\ j\in J_{\ell'}}} \sum_{k=1}^{\mathrm{K}-1} \left(\mathrm{CF}_{i,j}\, z_{i,\ell,j,\ell',k} + \mathrm{C}_{i,j}\, a_{i,\ell,j,\ell',k}\right) + \\
& \sum_{i\in I_\ell} \left(\mathrm{CF}_i^{\mathrm{cu}}\, zcu_{i,\ell} + \mathrm{C}_i^{\mathrm{cu}}\, acu_{i,\ell}\right) + \sum_{j\in J_\ell} \left(\mathrm{CF}_j^{\mathrm{hu}}\, zhu_{j,\ell} + \mathrm{C}_j^{\mathrm{hu}}\, ahu_{j,\ell}\right) \Bigg] + \\
& \sum_{i\in LPS} \left(\mathrm{CF}_i^{\mathrm{cu}}\, zcu_i^{\mathrm{L}} + \mathrm{C}_i^{\mathrm{cu}}\, acu_i^{\mathrm{L}} + \mathrm{CF}_i^{\mathrm{hu}}\, zhu_i^{\mathrm{L}} + \mathrm{C}_i^{\mathrm{hu}}\, ahu_i^{\mathrm{L}}\right) + \\
& \sum_{j\in HPS} \left(\mathrm{CF}_j^{\mathrm{cu}}\, zcu_j^{\mathrm{H}} + \mathrm{C}_j^{\mathrm{cu}}\, acu_j^{\mathrm{H}} + \mathrm{CF}_j^{\mathrm{hu}}\, zhu_j^{\mathrm{H}} + \mathrm{C}_j^{\mathrm{hu}}\, ahu_j^{\mathrm{H}}\right) + \\
& \mathrm{CF}^{\mathrm{G}}\, g + \mathrm{C}^{\mathrm{G}}\, W^{\mathrm{G}} + \mathrm{CF}^{\mathrm{H}}\, h + \mathrm{C}^{\mathrm{H}}\, W^{\mathrm{H}}
\end{aligned} \tag{2}
$$

where the binary variables $u_{i,\ell}^{\mathrm{L}}$, $x_{i,\ell}^{\mathrm{L}}$, $u_{j,\ell}^{\mathrm{H}}$, $x_{j,\ell}^{\mathrm{H}}$, y $v_{j,\ell}^{\mathrm{H}}$ define the existence of utility compressors, SSTC compressor, utility turbine, SSTC turbine, and valves, respectively, for the i-th low-pressure streams and j-th high-pressure streams at each stage ℓ of the WHEN. On the one hand, the flow rates through (utility or SSTC) compressors, (utility or SSTC) turbines, and valves are defined by the variables F^{Lu}, F^{Le}, F^{Hu}, F^{He}, and F^{Hv}, respectively. In addition, while the binary variables z, zcu, and zhu define the existence of a heat exchanger, a cold utility, and a hot utility, the variables a, acu, and ahu define their areas. Also, the binary variable $z_{i,\ell,j,\ell',k}$ indicates if the i-th hot stream in the ℓ-th stage of the network exchanges heat with the j-th cold stream defined in the ℓ'-th stage by the heat exchanger located at the k-th stage of the HEN. It is important to note that in this model the heat exchange between the same stream located in different stage of the WHEN is not allowed ($j \neq i$ is set to calculate the fixed cost of the exchangers). On the other hand, the binary variables zcu^{L}, zhu^{L}, zcu^{H}, and zhu^{H} represent the existence of the final cold and hot utilities for the low and high-pressure streams, and their areas are defined by the variables acu^{L}, ahu^{L}, acu^{H}, and ahu^{H}. Finally, while the binary variables g and h define the existence of electric generators and helper motors, the continuous variables W^{G} and W^{H} represent their capacity. Taking into account the operating cost for each unit (CO), the total operating cost ($OPEX$) is given by:

$$OPEX = \sum_{\ell=1}^{\mathrm{L}} \left(\sum_{i \in I_\ell} \mathrm{CO}^{\mathrm{cu}}\, qcu_{i,\ell} + \sum_{j \in J_\ell} \mathrm{CO}^{\mathrm{hu}}\, qhu_{j,\ell} + \sum_{i \in I_\ell^{\mathrm{P}}} \mathrm{CO}^{\mathrm{UC}}\, W_{i,\ell}^{\mathrm{Cu}} \right) + \sum_{i \in LPS} \left(\mathrm{CO}^{\mathrm{cu}}\, qcu_i^{\mathrm{L}} + \mathrm{CO}^{\mathrm{hu}}\, qhu_i^{\mathrm{L}} \right) + \sum_{j \in HPS} \left(\mathrm{CO}^{\mathrm{cu}}\, qcu_j^{\mathrm{H}} + \mathrm{CO}^{\mathrm{hu}}\, qhu_j^{\mathrm{H}} \right) + \mathrm{CO}^{\mathrm{H}}\, W^{\mathrm{H}} \quad (3)$$

In this equation, the continuous variable $qcu_{i,\ell}$ ($qhu_{j,\ell}$) represents the heat associated with the coolers (the heaters) for the i-th hot stream (j-th cold stream) in the ℓ-th stage of the WHEN. On the other hand, for the final heater and cooler, while the variables qcu_i^{L} and qhu_i^{L} are the heat exchanged for the i-th low-pressure stream, the variables qcu_j^{H} and qhu_j^{H} represent the heat exchanged for j-th high-pressure stream. Finally, the continuous variable $W_{i,\ell}^{\mathrm{Cu}}$ defines the capacity of the utility compressor associated to i-th low-pressure stream located at the ℓ-th stage of the HEN. As mentioned above, in this model the revenue from electricity generation (REV) is considered. In this way, if the price of energy is given by CE, the REV is defined by the following expression:

$$REV = \sum_{\ell=1}^{\mathrm{L}} \sum_{j \in J_\ell^{\mathrm{P}}} \mathrm{CE}\, W_{j,\ell}^{\mathrm{Tu}} + \mathrm{CE}\, W^{\mathrm{G}} \quad (4)$$

where $W_{j,\ell}^{\mathrm{Tu}}$ is the power generated by the j-th high-pressure stream in the utility turbine located at the ℓ-th stage of the WHEN and W^{G} is the auxiliary generator capacity.

3.2.1. Heat Exchanger Network (HEN) model

In this section the model of each HEN located at the ℓ-th stage of the WHEN is detailed. As it is suggested in the Yee and Grossmann (1990) model, the design equation for heat exchangers, heaters, and coolers is defined by:

$$\frac{q_{i,\ell,j,\ell',k}}{(a_{i,\ell,j,\ell',k})^{1/\beta}} - \frac{2}{3}\mathrm{U}_{i,j}\left(\sqrt{\Delta th_{i,\ell,j,\ell',k}\,\Delta tc_{i,\ell,j,\ell',k}} - \frac{1}{6}\Delta th_{i,\ell,j,\ell',k} - \frac{1}{6}\Delta tc_{i,\ell,j,\ell',k}\right) \leq 0, \quad \forall i \in I_\ell,\ \forall j \neq i \wedge j \in J_{\ell'},\ \forall \ell = 1,\ldots \mathrm{L},\ \forall \ell' = 1,\ldots,\mathrm{L},\ \forall k = 1,\ldots,\mathrm{K}-1 \tag{5}$$

$$\frac{qcu_{i,\ell}}{(acu_{i,\ell})^{1/\beta}} - \frac{2}{3}\mathrm{Ucu}_i\left(\sqrt{\Delta th^{\mathrm{cu}}_{i,\ell}\,\Delta tc^{\mathrm{cu}}_{i,\ell}} - \frac{1}{6}\Delta th^{\mathrm{cu}}_{i,\ell} - \frac{1}{6}\Delta tc^{\mathrm{cu}}_{i,\ell}\right) \leq 0, \quad \forall i \in I_\ell,\ \forall \ell = 1,\ldots \mathrm{L} \tag{6}$$

$$\frac{qhu_{j,\ell}}{(ahu_{j,\ell})^{1/\beta}} - \frac{2}{3}\mathrm{Uhu}_j\left(\sqrt{\Delta th^{\mathrm{hu}}_{j,\ell}\,\Delta tc^{\mathrm{hu}}_{j,\ell}} - \frac{1}{6}\Delta th^{\mathrm{hu}}_{j,\ell} - \frac{1}{6}\Delta tc^{\mathrm{hu}}_{j,\ell}\right) \leq 0, \quad \forall j \in J_\ell,\ \forall \ell = 1,\ldots \mathrm{L} \tag{7}$$

In these equations the variables Δth and Δtc are used to calculate the temperature difference between cold an hot stream at the ends of each exchanger. In this work the approximation proposed by Paterson (1984) is used to obtain the logarithmic mean temperature difference, however the Chen (1987) approximation could be used instead. It is important to recall that while the Paterson (1984) approximation slightly underestimates the areas of the heat exchangers, the Chen (1987) approximation overestimates them. In addition, the Paterson (1984) approximation has better accuracy than the Chen (1987) approximation and, for this reason, it is adopted in this work.

The global energy balance for each stream in the ℓ-th stage of the WHEN is given by:

$$\mathrm{F}^{\mathrm{in}}_i(Th^{\mathrm{in}}_{i,\ell} - Th^{\mathrm{out}}_{i,\ell}) = \sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall j \neq i \\ j \in J_{\ell'}}} \sum_{k=1}^{\mathrm{K}-1} q_{i,\ell,j,\ell',k} + qcu_{i,\ell}, \quad \forall i \in I_\ell,\ \forall \ell = 1,\ldots \mathrm{L} \tag{8}$$

$$\mathrm{F}_j^{\mathrm{in}}(Tc_{j,\ell}^{\mathrm{in}} - Tc_{j,\ell}^{\mathrm{out}}) = \sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall i \neq j \\ i \in I_{\ell'}}} \sum_{k=1}^{\mathrm{K}-1} q_{i,\ell',j,\ell,k} + qhu_{j,\ell}, \quad \forall j \in J_\ell,\ \forall \ell = 1, \ldots \mathrm{L} \tag{9}$$

where the continuous variables $Th_{i,\ell}^{\mathrm{in}}$ ($Tc_{j,\ell}^{\mathrm{in}}$) and $Th_{i,\ell}^{\mathrm{out}}$ ($Tc_{j,\ell}^{\mathrm{out}}$) represent the inlet and outlet temperature of the low-pressure hot streams (high-pressure cold stream) associated to the HEN located at the ℓ-th stage of the WHEN. In a similar way, the energy balances for the k-th stage of the HEN located in the ℓ-th stage of the WHEN can be computed by:

$$\mathrm{F}_i^{\mathrm{in}}(Th_{i,\ell,k} - Th_{i,\ell,k+1}) = \sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall j \neq i \\ j \in J_{\ell'}}} q_{i,\ell,j,\ell',k}, \quad \forall i \in I_\ell, \forall \ell = 1, \ldots \mathrm{L},\ \forall k = 1, \ldots \mathrm{K}-1 \tag{10}$$

$$\mathrm{F}_j^{\mathrm{in}}(Tc_{j,\ell,k} - Tc_{j,\ell,k+1}) = \sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall i \neq j \\ i \in I_{\ell'}}} q_{i,\ell',j,\ell,k}, \quad \forall j \in J_\ell, \forall \ell = 1, \ldots \mathrm{L},\ \forall k = 1, \ldots \mathrm{K}-1 \tag{11}$$

where the variables $Th_{i,\ell,k}$ and $Tc_{j,\ell,k}$ define the hot and cold temperatures of the streams at each stage of the HEN located at the ℓ-th stage of the WHEN. On the other hand, the energy balance of the coolers and heaters in the HENs is given by:

$$\mathrm{F}_i^{\mathrm{in}}(Th_{i,\ell,\mathrm{K}} - Th_{i,\ell}^{\mathrm{out}}) = qcu_{i,\ell}, \quad \forall i \in I_\ell, \forall \ell = 1, \ldots \mathrm{L} \tag{12}$$

$$\mathrm{F}_j^{\mathrm{in}}(Tc_{j,\ell}^{\mathrm{out}} - Tc_{j,\ell,1}) = qhu_{j,\ell}, \quad \forall j \in J_\ell, \forall \ell = 1, \ldots \mathrm{L} \tag{13}$$

Also, the following equations are defined to assign the HEN inlet temperatures:

$$Th_{i,\ell,1} = Th_{i,\ell}^{\mathrm{in}}, \quad \forall i \in I_\ell, \forall \ell = 1, \ldots \mathrm{L} \tag{14}$$

$$Tc_{j,\ell,\mathrm{K}} = Tc_{j,\ell}^{\mathrm{in}}, \quad \forall j \in J_\ell, \forall \ell = 1, \ldots \mathrm{L} \tag{15}$$

and the feasibility of temperature is given by:

$$Th_{i,\ell,k} \geq Th_{i,\ell,k+1}, \quad \forall i \in I_\ell, \forall \ell = 1, \ldots \mathrm{L},\ \forall k = 1, \ldots \mathrm{K}-1 \tag{16}$$

$$Tc_{j,\ell,k} \geq Tc_{j,\ell,k+1}, \quad \forall j \in J_\ell, \forall \ell = 1, \ldots \mathrm{L},\ \forall k = 1, \ldots \mathrm{K}-1 \tag{17}$$

$$Th_{i,\ell,\mathrm{K}} \geq Th^{\mathrm{out}}_{i,\ell}, \quad \forall i \in I_\ell, \forall \ell = 1, \ldots \mathrm{L} \tag{18}$$

$$Tc^{\mathrm{out}}_{j,\ell} \geq Tc_{j,\ell,1}, \quad \forall j \in J_\ell, \forall \ell = 1, \ldots \mathrm{L} \tag{19}$$

These equations allow to guarantee for the ℓ-th stage of the network that, on the one hand, the temperatures of the streams in the set I_ℓ decrease as they cross the HEN (i.e. they can be cooled) and, on the other hand, the streams in the set J_ℓ increase their temperature (i.e. they can be heated). As it is presented in Yee and Grossmann (1990), the logical constraints on heat exchanged are given by:

$$q_{i,\ell,j,\ell',k} \leq \Omega_{i,j} z_{i,\ell,j,\ell',k}, \quad \forall i \in I_\ell,\ \forall j \neq i\ \wedge j \in J_{\ell'}, \\ \forall \ell = 1, \ldots \mathrm{L},\ \forall \ell' = 1, \ldots \mathrm{L}, \\ \forall k = 1, \ldots \mathrm{K} - 1 \tag{20}$$

$$qcu_{i,\ell} \leq \Omega^{\mathrm{cu}}_i zcu_{i,\ell}, \quad \forall i \in I_\ell,\ \forall \ell = 1, \ldots \mathrm{L} \tag{21}$$

$$qhu_{j,\ell} \leq \Omega^{\mathrm{hu}}_j zhu_{j,\ell}, \quad \forall j \in J_\ell,\ \forall \ell = 1, \ldots \mathrm{L} \tag{22}$$

where $\Omega_{i,j}$, Ω^{cu}_i, and Ω^{hu}_j are the upper bound for heat exchanged taking into account the identity changes. On the other hand, the following constraints to approach temperatures are used:

$$\Delta th_{i,\ell,j,\ell',k} \leq Th_{i,\ell,k} - Tc_{j,\ell',k} + \Gamma_{i,j}(1 - z_{i,\ell,j,\ell',k}), \quad \forall i \in I_\ell,\ \forall j \neq i\ \wedge j \in J_{\ell'}, \\ \forall \ell = 1, \ldots \mathrm{L},\ \forall \ell' = 1, \ldots \mathrm{L}, \\ \forall k = 1, \ldots \mathrm{K} - 1 \tag{23}$$

$$\Delta tc_{i,\ell,j,\ell',k} \leq Th_{i,\ell,k+1} - Tc_{j,\ell',k+1} + \Gamma_{i,j}(1 - z_{i,\ell,j,\ell',k}), \quad \forall i \in I_\ell,\ \forall j \neq i\ \wedge j \in J_{\ell'}, \\ \forall \ell = 1, \ldots \mathrm{L},\ \forall \ell' = 1, \ldots \mathrm{L}, \\ \forall k = 1, \ldots \mathrm{K} - 1 \tag{24}$$

$$\Delta th^{\text{cu}}_{i,\ell} \leq Th_{i,\ell,\text{K}} - \text{Tcu}^{\text{out}} + \Gamma^{\text{cu}}_i (1 - zcu_{i,\ell}), \quad \forall i \in I_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{25}$$

$$\Delta tc^{\text{cu}}_{i,\ell} \leq Th^{\text{out}}_{i,\ell} - \text{Tcu}^{\text{in}} + \Gamma^{\text{cu}}_i (1 - zcu_{i,\ell}), \quad \forall i \in I_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{26}$$

$$\Delta th^{\text{hu}}_{j,\ell} \leq \text{Thu}^{\text{out}} - Tc_{j,\ell,1} + \Gamma^{\text{hu}}_j (1 - zhu_{j,\ell}), \quad \forall j \in J_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{27}$$

$$\Delta tc^{\text{hu}}_{j,\ell} \leq \text{Thu}^{\text{in}} - Tc^{\text{out}}_{j,\ell} + \Gamma^{\text{hu}}_j (1 - zhu_{j,\ell}), \quad \forall j \in J_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{28}$$

The parameters $\Gamma_{i,j}$, Γ^{cu}_i, and Γ^{hu}_j are calculated according to the work presented by Yee and Grossmann (1990) and taking into account the changes in the identity of the streams.

3.2.2. Work Exchanger Network (WEN) Model

The constraints related to the pressure change for each WEN located at the ℓ-th stage of the WHEN are presented in eqs 29 and 30. In this sense, the mass balance for each splitter of the streams that act as low and high pressure streams, is given by the following set of equations:

$$\text{F}^{\text{in}}_i - (1 - y^{\text{L}}_{i,\ell})\text{F}^{\text{in}}_i + F^{\text{Lu}}_{i,\ell} + F^{\text{Le}}_{i,\ell} = 0 \quad \forall i \in I^{\text{P}}_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{29}$$

$$\text{F}^{\text{in}}_j - (1 - y^{\text{H}}_{j,\ell})\text{F}^{\text{in}}_j + F^{\text{Hu}}_{j,\ell} + F^{\text{He}}_{j,\ell} + F^{\text{Hv}}_{j,\ell} = 0 \quad \forall j \in J^{\text{P}}_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{30}$$

These equations allow to calculate the flow passing through the pressure manipulator units and take into account if the streams enter ($y^{\text{L/H}}_{s,\ell} = 1$) or bypass ($y^{\text{L/H}}_{s,\ell} = 0$) the WEN. Also, the following constraints define the flow in the pressure manipulator units according to their existence:

$$u^{\text{L}}_{i,\ell}\text{F}^{\text{min}} \leq F^{\text{Lu}}_{i,\ell} \leq u^{\text{L}}_{i,\ell}\text{F}^{\text{in}}_i \quad \forall i \in I^{\text{P}}_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{31}$$

$$x^{\text{L}}_{i,\ell}\text{F}^{\text{min}} \leq F^{\text{Le}}_{i,\ell} \leq x^{\text{L}}_{i,\ell}\text{F}^{\text{in}}_i \quad \forall i \in I^{\text{P}}_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{32}$$

$$u^{\text{H}}_{j,\ell}\text{F}^{\text{min}} \leq F^{\text{Hu}}_{j,\ell} \leq u^{\text{H}}_{j,\ell}\text{F}^{\text{in}}_j \quad \forall j \in J^{\text{P}}_\ell,\ \forall \ell = 1, \ldots \text{L} \tag{33}$$

$$x^{\mathrm{H}}_{j,\ell}\mathrm{F}^{\min} \le F^{\mathrm{He}}_{j,\ell} \le x^{\mathrm{H}}_{j,\ell}\mathrm{F}^{\mathrm{in}}_{j} \quad \forall j \in J^{\mathrm{P}}_{\ell},\ \forall \ell = 1,\dots \mathrm{L} \tag{34}$$

$$v^{\mathrm{H}}_{j,\ell}\mathrm{F}^{\min} \le F^{\mathrm{Hv}}_{j,\ell} \le v^{\mathrm{H}}_{j,\ell}\mathrm{F}^{\mathrm{in}}_{j} \quad \forall j \in J^{\mathrm{P}}_{\ell},\ \forall \ell = 1,\dots \mathrm{L} \tag{35}$$

In these equations, the parameter $\mathrm{F}^{\min}$ defines the minimum stream flow through the units. That is, if there is a pressure manipulator unit, the flow in this unit must be greater than a minimum flow and less than the maximum flow of the stream ($\mathrm{F}^{\mathrm{in}}_{s}$). Then logical constraints on pressures are used:

$$pL^{\mathrm{o}}_{i,\ell} \ge pL^{\mathrm{i}}_{i,\ell} + \Delta\mathrm{P}^{\min} y^{\mathrm{L}}_{i,\ell} \quad \forall i \in I^{\mathrm{P}}_{\ell},\ \forall \ell = 1,\dots \mathrm{L} \tag{36}$$

$$pL^{\mathrm{o}}_{i,\ell} \le pL^{\mathrm{i}}_{i,\ell} + \Delta\mathrm{P}^{\max}_{i} y^{\mathrm{L}}_{i,\ell} \quad \forall i \in I^{\mathrm{P}}_{\ell},\ \forall \ell = 1,\dots \mathrm{L} \tag{37}$$

$$pH^{\mathrm{o}}_{j,\ell} \le pH^{\mathrm{i}}_{j,\ell} - \Delta\mathrm{P}^{\min} y^{\mathrm{H}}_{j,\ell} \quad \forall j \in J^{\mathrm{P}}_{\ell},\ \forall \ell = 1,\dots \mathrm{L} \tag{38}$$

$$pH^{\mathrm{o}}_{j,\ell} \ge pH^{\mathrm{i}}_{j,\ell} - \Delta\mathrm{P}^{\max}_{j} y^{\mathrm{H}}_{j,\ell} \quad \forall j \in J^{\mathrm{P}}_{\ell},\ \forall \ell = 1,\dots \mathrm{L} \tag{39}$$

These equations state that if the i-th (j-th) streams in set I^{P}_{ℓ} (J^{P}_{ℓ}) enter the WEN located at the ℓ-th stage of the network, their pressure are limited between a minimum ($\Delta\mathrm{P}^{\min}$) and a maximum value ($\Delta\mathrm{P}^{\max}$). Additionally, the temperature of the i-th low-pressure hot stream changes significantly when this stream goes through a compressor located at the ℓ-th stage of the WHEN. Therefore, given the inlet temperature $TL^{\mathrm{in}}_{i,\ell}$, the inlet pressure $pL^{\mathrm{i}}_{i,\ell}$, and the outlet pressure $pL^{\mathrm{o}}_{i,\ell}$, the exit temperature from the adiabatic mover $TL^{\mathrm{out}}_{i,\ell}$ can be calculated using the following expression:

$$TL^{\mathrm{out}}_{i,\ell} = TL^{\mathrm{in}}_{i,\ell}\left\{1 + \frac{1}{\eta_i}\left[\left(\frac{pL^{\mathrm{o}}_{i,\ell}}{pL^{\mathrm{i}}_{i,\ell}}\right)^{\frac{r_i-1}{r_i}} - 1\right]\right\} \quad \forall i \in I^{\mathrm{P}}_{\ell},\ \forall \ell = 1,\dots \mathrm{L} \tag{40}$$

Similarly, if the j-th high-pressure cold stream goes through a turbine located at the ℓ-th stage of the WHEN and its inlet temperature $TH^{\mathrm{in}}_{j,\ell}$, inlet pressure $pH^{\mathrm{i}}_{j,\ell}$, and outlet pressure $pH^{\mathrm{o}}_{j,\ell}$ are known, then the exit temperature from the adiabatic mover $TH^{\mathrm{m}}_{j,\ell}$ is obtained by:

$$TH^{\mathrm{m}}_{j,\ell} = TH^{\mathrm{in}}_{j,\ell}\left\{1 + \eta_j\left[\left(\frac{pH^{\mathrm{o}}_{j,\ell}}{pH^{\mathrm{i}}_{j,\ell}}\right)^{\frac{r_j-1}{r_j}} - 1\right]\right\} \quad \forall j \in J^{\mathrm{P}}_{\ell},\ \forall \ell = 1,\dots \mathrm{L} \tag{41}$$

In 40 and 41, η_s is the efficiency of the mover for the stream s and r_s is its heat capacity ratio ($\mathrm{Cp}_s/\mathrm{Cv}_s$). As well as compressors and turbines, when a high-pressure cold stream is expanded through a valve, its temperature changes according to:

$$TH^{\mathrm{v}}_{j,\ell} = TH^{\mathrm{in}}_{j,\ell} + \mu_j \left(pH^{\mathrm{o}}_{j,\ell} - pH^{\mathrm{i}}_{j,\ell} \right) \quad \forall j \in J^{\mathrm{P}}_{\ell},\ \forall \ell = 1, \ldots \mathrm{L} \tag{42}$$

where μ_j is the average Joule-Thomson coefficient of the j-th stream. At the end of the WENs, the substreams are mixed to reform the j-th stream, thus, the outlet temperature $TH^{\mathrm{out}}_{j,\ell}$ can be calculated according to the following energy balance:

$$\begin{aligned} \mathrm{F}^{\mathrm{in}}_j\, TH^{\mathrm{out}}_{j,\ell} = (1 - y^{\mathrm{H}}_{j,\ell})\, \mathrm{F}^{\mathrm{in}}_j\, TH^{\mathrm{in}}_{j,\ell} + \\ (F^{\mathrm{Hu}}_{j,\ell} + F^{\mathrm{He}}_{j,\ell})\, TH^{\mathrm{m}}_{j,\ell} + F^{\mathrm{Hv}}_{j,\ell}\, TH^{\mathrm{v}}_{j,\ell}, \qquad \forall j \in J^{\mathrm{P}}_{\ell}, \forall \ell = 1, \ldots \mathrm{L} \end{aligned} \tag{43}$$

After the inlet and outlet temperatures and flowrates are known, the power obtained by the turbines ($W^{\mathrm{T}}_{j,\ell}$) and consumed by the compressors ($W^{\mathrm{C}}_{i,\ell}$) connected by a common shaft (SSTC) are defined by:

$$W^{\mathrm{C}}_{i,\ell} = F^{\mathrm{Le}}_{i,\ell}(TL^{\mathrm{out}}_{i,\ell} - TL^{\mathrm{in}}_{i,\ell}) \quad \forall i \in I^{\mathrm{P}}_{\ell}, \forall \ell = 1, \ldots \mathrm{L} \tag{44}$$

$$W^{\mathrm{T}}_{j,\ell} = F^{\mathrm{He}}_{j,\ell}(TH^{\mathrm{in}}_{j,\ell} - TH^{\mathrm{m}}_{j,\ell}) \quad \forall j \in J^{\mathrm{P}}_{\ell}, \forall \ell = 1, \ldots \mathrm{L} \tag{45}$$

On the other hand, the power consumed by stand-alone compressors ($W^{\mathrm{Cu}}_{i,\ell}$) and generated by stand-alone turbines ($W^{\mathrm{Tu}}_{j,\ell}$) are calculated by:

$$W^{\mathrm{Cu}}_{i,\ell} = F^{\mathrm{Lu}}_{i,\ell}(TL^{\mathrm{out}}_{i,\ell} - TL^{\mathrm{in}}_{i,\ell}) \quad \forall i \in I^{\mathrm{P}}_{\ell}, \forall \ell = 1, \ldots \mathrm{L} \tag{46}$$

$$W^{\mathrm{Tu}}_{j,\ell} = F^{\mathrm{Hu}}_{j,\ell}(TH^{\mathrm{in}}_{j,\ell} - TH^{\mathrm{m}}_{j,\ell}) \quad \forall j \in J^{\mathrm{P}}_{\ell}, \forall \ell = 1, \ldots \mathrm{L} \tag{47}$$

For turbines and compressors connected by a common shaft, the following power balance must be satisfied:

$$\sum_{\ell=1}^{\mathrm{L}} \sum_{j \in J^{\mathrm{P}}_{\ell}} W^{\mathrm{T}}_{j,\ell} + W^{\mathrm{H}} = \sum_{\ell}^{\mathrm{L}} \sum_{i \in I^{\mathrm{P}}_{\ell}} W^{\mathrm{C}}_{i,\ell} + W^{\mathrm{G}} \tag{48}$$

where W^{H} and W^{G} are the capacity of helper motor and electric generator, respectively. Finally, the following constraints are established on the capacity of these units:

$$W^{\mathrm{H}} \leq h\ \mathrm{WH}^{\mathrm{UB}} \tag{49}$$

$$W^{\mathrm{G}} \leq g\ \mathrm{WG}^{\mathrm{UB}} \tag{50}$$

The eq. 49 determines that if a helper motor is used ($h = 1$), then its capacity will be less than an upper bound ($\mathrm{WH}^{\mathrm{UB}}$), otherwise ($h = 0$), the power must be zero. A similar analysis can be done with the constraint related to the electric generator (eq. 50).

3.2.3. Final Cold/Hot Utilities

After the pressure-change streams leave the last WEN, they enter with their nominal identities (equal to stage 1 of the network) at the final hot or cold utilities where they reach their final target temperature. This approach was incorporated in the model proposed by Huang and Karimi (2016) and is adopted here by the proposed superstructure. The constraints presented in eqs. 51 to 54 allow to define the final utilities existence (heaters or coolers) for each stream $s \in PC$. Similarly to the design equations used for heat exchangers and utilities for the HENs case, it can be defined for this final stage:

$$\frac{qcu_i^{\mathrm{L}}}{(acu_i^{\mathrm{L}})^{1/\beta}} - \frac{2}{3}\mathrm{Ucu}_i\left(\sqrt{\Delta th_i^{\text{cu-L}}\,\Delta tc_i^{\text{cu-L}}} - \frac{1}{6}\Delta th_i^{\text{cu-L}} - \frac{1}{6}\Delta tc_i^{\text{cu-L}}\right) \leq 0, \quad \forall i \in I_1^{\mathrm{P}} \tag{51}$$

$$\frac{qhu_i^{\mathrm{L}}}{(ahu_i^{\mathrm{L}})^{1/\beta}} - \frac{2}{3}\mathrm{Uhu}_i\left(\sqrt{\Delta th_i^{\text{hu-L}}\,\Delta tc_i^{\text{hu-L}}} - \frac{1}{6}\Delta th_i^{\text{hu-L}} - \frac{1}{6}\Delta tc_i^{\text{hu-L}}\right) \leq 0, \quad \forall i \in I_1^{\mathrm{P}} \tag{52}$$

$$\frac{qcu_j^{\mathrm{H}}}{(acu_j^{\mathrm{H}})^{1/\beta}} - \frac{2}{3}\mathrm{Ucu}_j\left(\sqrt{\Delta th_j^{\text{cu-H}}\,\Delta tc_j^{\text{cu-H}}} - \frac{1}{6}\Delta th_j^{\text{cu-H}} - \frac{1}{6}\Delta tc_j^{\text{cu-H}}\right) \leq 0, \quad \forall j \in J_1^{\mathrm{P}} \tag{53}$$

$$\frac{qhu_j^{\mathrm{H}}}{(ahu_j^{\mathrm{H}})^{1/\beta}} - \frac{2}{3}\mathrm{Uhu}_j\left(\sqrt{\Delta th_j^{\text{hu-H}}\,\Delta tc_j^{\text{hu-H}}} - \frac{1}{6}\Delta th_j^{\text{hu-H}} - \frac{1}{6}\Delta tc_j^{\text{hu-H}}\right) \leq 0, \forall j \in J_1^{\mathrm{P}} \tag{54}$$

The energy balance for the final utilities is given by:

$$\mathrm{F}_i^{\mathrm{in}}(TL_i^{\text{in-ut}} - TL_i^{\text{out-ut}}) = qcu_i^{\mathrm{L}} - qhu_i^{\mathrm{L}}, \quad \forall i \in I_1^{\mathrm{P}} \tag{55}$$

$$\mathrm{F}_j^{\mathrm{in}}(TH_j^{\text{out-ut}} - TH_j^{\text{in-ut}}) = qhu_j^{\mathrm{H}} - qcu_j^{\mathrm{H}}, \quad \forall j \in J_1^{\mathrm{P}} \tag{56}$$

Also, the logical constraints on the heat exchanged in the final utilities are given by:

$$qcu_i^{\mathrm{L}} \leq \Omega_i^{\mathrm{cu}} zcu_i^{\mathrm{L}}, \quad \forall i \in I_1^{\mathrm{P}} \tag{57}$$

$$qhu_i^{\mathrm{L}} \leq \Omega_i^{\mathrm{hu}} zhu_i^{\mathrm{L}}, \quad \forall i \in I_1^{\mathrm{P}} \tag{58}$$

$$qcu_j^{\mathrm{H}} \leq \Omega_i^{\mathrm{cu}} zcu_j^{\mathrm{H}}, \quad \forall j \in J_1^{\mathrm{P}} \tag{59}$$

$$qhu_j^{\mathrm{H}} \leq \Omega_j^{\mathrm{hu}} zhu_j^{\mathrm{H}}, \quad \forall j \in J_1^{\mathrm{P}} \tag{60}$$

On the other hand, the temperature approaches for the final cooler associated with the stream LPS are given by:

$$\Delta th_i^{\text{cu-L}} \leq TL_i^{\text{in-ut}} - \mathrm{Tcu}^{\mathrm{out}} + \Gamma_i^{\mathrm{cu}}(1 - zcu_i^{\mathrm{L}}), \quad \forall i \in I_1^{\mathrm{P}} \tag{61}$$

$$\Delta tc_i^{\text{cu-L}} \leq TL_i^{\text{out-ut}} - \mathrm{Tcu}^{\mathrm{in}} + \Gamma_i^{\mathrm{cu}}(1 - zcu_i^{\mathrm{L}}), \quad \forall i \in I_1^{\mathrm{P}} \tag{62}$$

and for the final heaters:

$$\Delta th_i^{\text{hu-L}} \leq \mathrm{Thu}^{\mathrm{out}} - TL_i^{\text{in-ut}} + \Gamma_i^{\mathrm{hu}}(1 - zhu_i^{\mathrm{L}}), \quad \forall i \in I_1^{\mathrm{P}} \tag{63}$$

$$\Delta tc_i^{\text{hu-L}} \leq \mathrm{Thu}^{\mathrm{in}} - TL_i^{\text{out-ut}} + \Gamma_i^{\mathrm{hu}}(1 - zhu_i^{\mathrm{L}}), \quad \forall i \in I_1^{\mathrm{P}} \tag{64}$$

Similarly, the temperature approaches for the cooler associated with the streams HPS are defined as follow:

$$\Delta th_j^{\text{cu-H}} \leq TH_j^{\text{in-ut}} - \mathrm{Tcu}^{\mathrm{out}} + \Gamma_j^{\mathrm{cu}}(1 - zcu_j^{\mathrm{H}}), \quad \forall j \in J_1^{\mathrm{P}} \tag{65}$$

$$\Delta tc_j^{\text{cu-H}} \leq TH_j^{\text{out-ut}} - \mathrm{Tcu}^{\mathrm{in}} + \Gamma_i^{\mathrm{cu}}(1 - zcu_j^{\mathrm{H}}), \quad \forall j \in J_1^{\mathrm{P}} \tag{66}$$

and for the final heaters as below:

$$\Delta th_j^{\text{hu-H}} \leq \mathrm{Thu}^{\mathrm{out}} - TH_j^{\text{in-ut}} + \Gamma_j^{\mathrm{hu}}(1 - zhu_j^{\mathrm{H}}), \quad \forall j \in J_1^{\mathrm{P}} \tag{67}$$

$$\Delta tc_j^{\text{hu-H}} \leq \mathrm{Thu}^{\mathrm{in}} - TH_j^{\text{out-ut}} + \Gamma_i^{\mathrm{hu}}(1 - zhu_j^{\mathrm{H}}), \quad \forall j \in J_1^{\mathrm{P}} \tag{68}$$

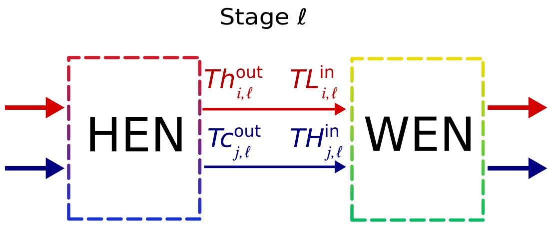


Figure 3: Connections between the HEN and the WEN located at the ℓ-th stage of the WHEN.

3.2.4. WHEN Connections

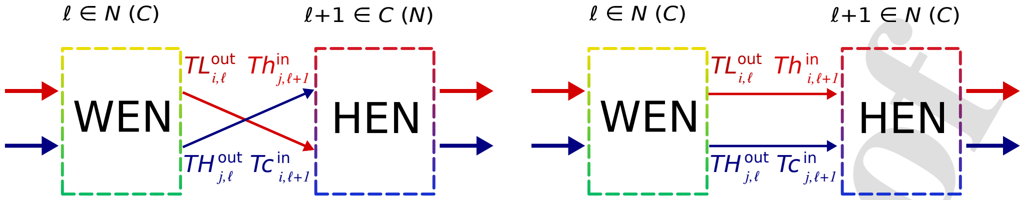
In this section, a set of constraints that allow modeling the connections between WHEN stages and the identity changes of the streams are presented. In this sense, the eqs. 69 and 70 define the relationship between the outlet temperature of the HEN and the inlet temperature of the WEN. It is important to note that, in the ℓ-th stage of the WHEN, streams maintain their identity, i.e. they take the same identity (low-pressure hot or high-pressure cold identity) in the HEN and WEN of this stage (see Fig. 3):

$$Th^{\text{out}}_{i,\ell} = TL^{\text{in}}_{i,\ell},\ \forall i \in I_\ell,\ \forall \ell = 1, \dots, \text{L} \tag{69}$$

$$Tc^{\text{out}}_{j,\ell} = TH^{\text{in}}_{j,\ell},\ \forall j \in J_\ell,\ \forall \ell = 1, \dots, \text{L} \tag{70}$$

Once the connection between the HEN and WEN of the same stage has been defined, it is necessary to determine the relationships between the outlet temperatures of the WEN located at the ℓ-th stage and the inlet temperatures of the HEN at the next stage $(\ell + 1)$. With this purpose, it is defined 3 cases: (i) the stream is located at a stage with nominal identity $(\ell \in N)$ and, in the next stage, this stream presents a changed identity $(\ell + 1 \in C)$, (ii) the stream has a changed identity $(\ell \in C)$ and, in the next stage, this stream presents a nominal identity $(\ell + 1 \in N)$, and (iii) the stream keeps its identity (nominal or changed) in the next stage $(\ell + 1)$. In this sense, for the first two cases, it can be stated that if $(\ell \in N \wedge \ell + 1 \in C) \vee (\ell \in C \wedge \ell + 1 \in N)$, then a change of stream identity must be done (see Fig. 4(a)):

$$TL^{\text{out}}_{i,\ell} = Tc^{\text{in}}_{i,\ell+1},\ \forall i \in I_\ell \tag{71}$$



(a) with an identity crossover.

(b) without an identity crossover.

Figure 4: Connections between the WEN and the HEN located at different stages of the WHEN.

$$TH^{\text{out}}_{j,\ell} = Th^{\text{in}}_{j,\ell+1},\ \forall j \in J_\ell \tag{72}$$

otherwise, if $(\ell \in N \wedge \ell + 1 \in N) \vee (\ell \in C \wedge \ell + 1 \in C)$, then the stream keep their identity (see Fig. 4(b)):

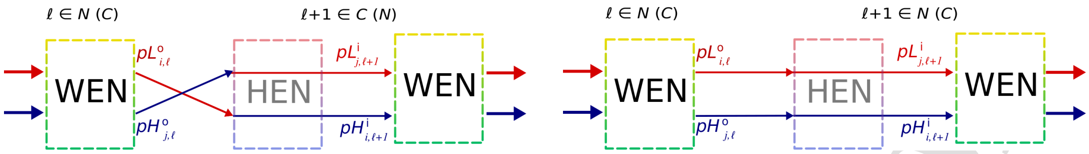
$$TL^{\text{out}}_{i,\ell} = Th^{\text{in}}_{i,\ell+1},\ \forall i \in I_\ell \tag{73}$$

$$TH^{\text{out}}_{j,\ell} = Tc^{\text{in}}_{j,\ell+1},\ \forall j \in J_\ell \tag{74}$$

Therefore, in the case where an identity change is done (eqs. 71 and 72), the outlet temperature of the stream acting as a low-pressure hot stream (high-pressure cold stream) is equal to its inlet temperature at the HEN of the next stage $(\ell + 1)$, where it will act with a changed identity, i.e. the stream will act as high-pressure cold stream (low-pressure hot stream). On the other hand, in the case where there is no identity change, the outlet temperature of the low-pressure (high-pressure) stream is equal to the inlet temperature of the next stage (eqs. 73 and 74), where the stream continues acting as a low-pressure hot stream (high-pressure cold stream). In a similar way, the outlet pressures of the streams that go through the WEN located at the stage ℓ and the inlet pressures to the WEN of the next stage $(\ell + 1)$ can be analyzed. Therefore, if $(\ell \in N \wedge \ell + 1 \in C) \vee (\ell \in C \wedge \ell + 1 \in N)$, an identity change will be produced:

$$pL^{\text{o}}_{i,\ell} = pH^{\text{i}}_{i,\ell+1} \quad \forall i \in I^{\text{P}}_\ell, \tag{75}$$

$$pH^{\text{o}}_{j,\ell} = pL^{\text{i}}_{j,\ell+1} \quad \forall j \in J^{\text{P}}_\ell, \tag{76}$$



(a) with an identity crossover. (b) without an identity crossover.

Figure 5: Connections between the WENs located in the ℓ-th and $\ell+1$-th stage of the WHEN.

otherwise, if $(\ell \in N \wedge \ell+1 \in N) \vee (\ell \in C \wedge \ell+1 \in C)$, then the streams keep acting with their identities (see Fig. 4(b)):

$$pL^{\mathrm{o}}_{i,\ell} = pL^{\mathrm{i}}_{i,\ell+1} \quad \forall i \in I^{\mathrm{P}}_{\ell}, \tag{77}$$

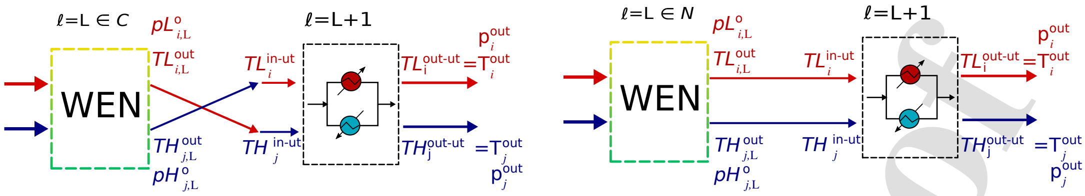
$$pH^{\mathrm{o}}_{j,\ell} = pH^{\mathrm{i}}_{j,\ell+1} \quad \forall j \in J^{\mathrm{P}}_{\ell}, \tag{78}$$

From equations 75 to 78, it can be concluded that the outlet pressure of a stream acting as a LP (HP) stream is equal to its inlet pressure at the next WEN where it acts as HP (LP) stream. On the other hand, for all cases where an identity change is not done, the outlet pressure of the LP (HP) stream is equal to its inlet pressure in the next stage, where it keeps acting as a LP (HP) stream (eqs. 77 and 78). Subsequently, it is necessary to define the relationships between the outlet temperature of the WEN at the stage L and the inlet temperature of the final utilities, see Fig. 6. Recalling that the superstructure states that the streams have nominal identities at the stage L + 1, these relationships are defined by:

$$TL^{\mathrm{out}}_{i,\mathrm{L}} = TL^{\text{in-ut}}_{i} \text{ if } \mathrm{L} \in N \text{ else } TH^{\text{in-ut}}_{i},\ \forall i \in I_{\ell} \tag{79}$$

$$TH^{\mathrm{out}}_{j,\mathrm{L}} = TH^{\text{in-ut}}_{j} \text{ if } \mathrm{L} \in N \text{ else } TL^{\text{in-ut}}_{j},\ \forall j \in J_{\ell} \tag{80}$$

These equations state that, if in the last stage the streams have a nominal identity ($\mathrm{L} \in N$), then the inlet temperatures of the final utilities are equal to the outlet temperatures of the WEN without identity crossover, since the streams in the L-th stage have their nominal identities. Otherwise, a new identity crossover is needed since the streams defined globally as LPS (HPS) streams are located in the high-pressure (low-pressure) side of the WHEN.



(a) with an identity crossover.

(b) without an identity crossover.

Figure 6: Connections between the WEN located in the stage L and the final utilities.

For this, the outlet temperature of the i-th low-pressure stream ($TL_{i,\mathrm{L}}^{\mathrm{out}}$) must be equal to the inlet temperature of the final utility located in the high-pressure side ($TH_i^{\text{in-ut}}$), and the outlet temperature of the j-th high-pressure stream ($TH_{j,\mathrm{L}}^{\mathrm{out}}$) must be equal to the inlet temperature of the final utility located in the low-pressure side ($TL_j^{\text{in-ut}}$). Furthermore, it is necessary to define the global inlet and outlet temperatures and pressures of the WHEN. In this sense, the inlet temperatures of the WHEN are given by:

$$Th_{i,1}^{\mathrm{in}} = \mathrm{T}_i^{\mathrm{in}},\ \forall i \in I_1 \tag{81}$$

$$Tc_{j,1}^{\mathrm{in}} = \mathrm{T}_j^{\mathrm{in}},\ \forall j \in J_1 \tag{82}$$

In these equations, $\mathrm{T}_i^{\mathrm{in}}$ ($\mathrm{T}_j^{\mathrm{in}}$) are the global inlet temperatures of the hot streams (cold strems) and low-pressure hot streams (high-pressure cold streams). On the one hand, the global outlet temperatures of the WHEN for streams that do not change pressure are defined by:

$$Th_{i,1}^{\mathrm{out}} = \mathrm{T}_i^{\mathrm{out}},\ \forall i \in HS \tag{83}$$

$$Tc_{j,1}^{\mathrm{out}} = \mathrm{T}_j^{\mathrm{out}},\ \forall j \in CS \tag{84}$$

On the other hand, for the streams that change pressure, their global outlet temperature can be defined according to the following cases: (i) for streams that present a fixed outlet target temperature:

$$TL_i^{\text{out-ut}} = \mathrm{T}_i^{\mathrm{out}},\ \forall i \in LPS \tag{85}$$

$$TH_i^{\text{out-ut}} = \mathrm{T}_j^{\text{out}},\ \forall j \in HPS \tag{86}$$

and (ii) for streams that have an outlet temperature between a lower and upper limit:

$$\mathrm{TLB}_j^{\text{out}} \le TL_i^{\text{out-ut}} \le \mathrm{TUB}_i^{\text{out}},\ \forall i \in LPS \tag{87}$$

$$\mathrm{TLB}_j^{\text{out}} \le TH_j^{\text{out-ut}} \le \mathrm{TUB}_i^{\text{out}},\ \forall j \in HPS \tag{88}$$

Finally the global inlet and outlet pressure of the WHEN is given by (see Fig. 6):

$$pL_{i,1}^{\mathrm{i}} = \mathrm{P}_i^{\text{in}} \quad \forall i \in LPS \tag{89}$$

$$pH_{j,1}^{\mathrm{i}} = \mathrm{P}_j^{\text{in}} \quad \forall j \in HPS \tag{90}$$

$$pL_{i,\mathrm{L}}^{\mathrm{o}} = \mathrm{P}_i^{\text{out}} \quad \forall i \in LPS \tag{91}$$

$$pH_{j,\mathrm{L}}^{\mathrm{o}} = \mathrm{P}_j^{\text{out}} \quad \forall j \in HPS \tag{92}$$

3.2.5. Structural Constraints

The set of constraints presented in equations 93 to 109 defines the existence of the WHEN units. In these sense, the constraints 93 to 95 state both if the $i \in I_\ell^{\mathrm{P}}$ stream enters or not the WEN of the ℓ-th stage, and the existence of a compressor in this stage:

$$(1 - y_{i,\ell}^{\mathrm{L}}) + u_{i,\ell}^{\mathrm{L}} + x_{i,\ell}^{\mathrm{L}} \ge 1, \quad \forall i \in I_\ell^{\mathrm{P}},\ \ell = 1, \ldots, \mathrm{L} \tag{93}$$

$$(1 - y_{i,\ell}^{\mathrm{L}}) + u_{i,\ell}^{\mathrm{L}} \le 1, \quad \forall i \in I_\ell^{\mathrm{P}},\ \ell = 1, \ldots, \mathrm{L} \tag{94}$$

$$(1 - y_{i,\ell}^{\mathrm{L}}) + x_{i,\ell}^{\mathrm{L}} \le 1, \quad \forall i \in I_\ell^{\mathrm{P}},\ \ell = 1, \ldots, \mathrm{L} \tag{95}$$

On the other hand, the income of the streams $j \in J_\ell^{\mathrm{P}}$ to the WEN of the ℓ-th stage and the existence of the turbines and valves is given by the following constraints:

$$(1 - y_{j,\ell}^{\mathrm{H}}) + u_{j,\ell}^{\mathrm{H}} + x_{j,\ell}^{\mathrm{H}} + v_{j,\ell}^{\mathrm{H}} \ge 1, \quad \forall j \in J_\ell^{\mathrm{P}},\ \ell = 1, \ldots, \mathrm{L} \tag{96}$$

$$(1 - y^{\mathrm{H}}_{j,\ell}) + u^{\mathrm{H}}_{j,\ell} + v^{\mathrm{H}}_{j,\ell} \leq 1, \quad \forall j \in J^{\mathrm{P}}_{\ell},\ \ell = 1, \ldots, \mathrm{L} \tag{97}$$

$$(1 - y^{\mathrm{H}}_{j,\ell}) + x^{\mathrm{H}}_{j,\ell} \leq 1, \quad \forall j \in J^{\mathrm{P}}_{\ell},\ \ell = 1, \ldots, \mathrm{L} \tag{98}$$

The streams in LPS (HPS) have to enter at least one WEN acting with this identity to reach the target outlet pressure. For this reason, the following (optional) constraints are used:

$$\sum_{\ell \in N} y^{\mathrm{L}}_{i,\ell} \geq 1, \quad \forall i \in LPS \tag{99}$$

$$\sum_{\ell \in N} y^{\mathrm{H}}_{j,\ell} \geq 1, \quad \forall j \in HPS \tag{100}$$

Furthermore, the constraints 101 to 103 are used to define the existence of electric generators and helper motor.

$$g + h \leq 1 \tag{101}$$

$$g + h \leq \sum_{\ell=1}^{\mathrm{L}} \sum_{i \in I^{\mathrm{P}}_{\ell}} x^{\mathrm{L}}_{i,\ell} \tag{102}$$

$$g + h \leq \sum_{\ell=1}^{\mathrm{L}} \sum_{j \in J^{\mathrm{P}}_{\ell}} x^{\mathrm{H}}_{j,\ell} \tag{103}$$

The eq. 101 states that an electric generator and a helper motor cannot exist simultaneously. On the one hand, if the electric generator or helper motor exist, then there must be at least one compressor (eq. 102) and one turbine (eq. 103) connected by a common shaft. Also, logical constraints on the existence of the final utilities are used:

$$zcu^{\mathrm{L}}_{i} + zhu^{\mathrm{L}}_{i} \leq 1, \quad \forall i \in LPS \tag{104}$$

$$zcu^{\mathrm{H}}_{j} + zhu^{\mathrm{H}}_{j} \leq 1, \quad \forall j \in HPS \tag{105}$$

these constraints state that a hot and cold utility cannot exist simultaneously. Finally, the constraints presented below determine whether or not a stream enters (bypasses) the HEN located in the stage ℓ of the WHEN. In this sense, for the low-pressure hot streams:

$$\sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall j \neq i \\ j \in J_{\ell'}}} \sum_{k}^{\mathrm{K}-1} z_{i,\ell,j,\ell',k} + zcu_{i,\ell} \leq \mathrm{M_{LP}}(1 - zL_{i,\ell}^{\mathrm{Hen}}), \quad \forall i \in I_\ell,\ \forall \ell = 1, \ldots, \mathrm{L} \tag{106}$$

$$\sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall j \neq i \\ j \in J_{\ell'}}} \sum_{k}^{\mathrm{K}-1} z_{i,\ell,j,\ell',k} + zcu_{i,\ell} \geq (1 - zL_{i,\ell}^{\mathrm{Hen}}), \quad \forall i \in I_\ell,\ \forall \ell = 1, \ldots, \mathrm{L} \tag{107}$$

where the parameter $\mathrm{M_{LP}} = \mathrm{J}(\mathrm{K}-1) + (|LPS|-1)\left\lceil \frac{\mathrm{L}-1}{2} \right\rceil (\mathrm{K}-1) + |HPS| \left\lfloor \frac{\mathrm{L}-1}{2} \right\rfloor (\mathrm{K}-1) + 1$ defines all possible heat exchanger for the i-th stream, $|\ |$ indicates the number of elements in a set, and $\lceil . \rceil$ is the roof function. These constraints state that if the i-th low-pressure hot stream bypasses the HEN located at the ℓ-th stage ($zL_{i,\ell}^{\mathrm{Hen}} = 1$), then there should be no heat exchanger or utility in that stage. Otherwise, the stream enters to the HEN ($zL_{i,\ell}^{\mathrm{Hen}} = 0$) and there should be at least one heat exchanger or utility. Similarly, for the streams in the set J_ℓ:

$$\sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall i \neq j \\ i \in I_{\ell'}}} \sum_{k}^{\mathrm{K}-1} z_{i,\ell',j,\ell,k} + zhu_{j,\ell} \leq \mathrm{M_{HP}}(1 - zH_{j,\ell}^{\mathrm{Hen}}), \quad \forall j \in J_\ell,\ \forall \ell = 1, \ldots, \mathrm{L} \tag{108}$$

$$\sum_{\ell'=1}^{\mathrm{L}} \sum_{\substack{\forall i \neq j \\ i \in I_{\ell\mathrm{H}}}} \sum_{k}^{\mathrm{K}-1} z_{i,\ell',j,\ell,k} + zhu_{j,\ell} \geq (1 - zH_{j,\ell}^{\mathrm{Hen}}), \quad \forall j \in J_\ell,\ \forall \ell = 1, \ldots, \mathrm{L} \tag{109}$$

where the parameter $\mathrm{M_{HP}} = \mathrm{J}(\mathrm{K}-1) + (|LPS|-1)\left\lceil \frac{\mathrm{L}-1}{2} \right\rceil (\mathrm{K}-1) + |HPS| \left\lfloor \frac{\mathrm{L}-1}{2} \right\rfloor (\mathrm{K}-1) + 1$ defines all possible heat exchangers for the j-th stream. As defined for the low-pressure hot streams, if the j-th high-pressure cold stream bypasses the HEN located at the ℓ-th stage ($zH_{j,\ell}^{\mathrm{Hen}} = 1$), then there should be no heat exchanger or utility in that stage. Otherwise, there should be at least one heat exchanger or utility.

Table 2: Cost parameters for Examples 1, 2, and 3

Process unit	Fixed cost [k$/year]		Cost coefficient [k$/year]		Energy cost [k$/kWh]	
Utility turbine	CF_s^{UT}	200	C_s^{UT}	1	CE	0.10
Utility compressor	CF_s^{UC}	250	C_s^{UC}	1	CO_{UC}	0.12
SSTC turbine	CF_s^{ST}	40	C_s^{ST}	1	-	-
SSTC compressor	CF_s^{SC}	50	C_s^{SC}	1	-	-
Generator	CF_G	2	C_G	1	CE	0.10
Helper motor	CF_H	2	C_H	1	CO_G	0.12
Valve	CF_s^V	2	C_s^V	1	-	-
Heat Exchanger	$CF_{i,j}$	3	$C_{i,j}$	0.03	-	-
Heater	CF_j^{HU}	3	C_j^{HU}	0.03	CO_{HU}	0.035
Cooler	CF_i^{CU}	3	C_i^{CU}	0.03	CO_{CU}	0.001
Operating time $t = 8000$ h/year						

4. Case studies

In this section, three cases are presented to show the improvements of the novel formulation developed in this work. The overall problem is implemented in Pyomo/Python environment and the Bonmin 1.8 code is used as MINLP solver. All problems are solved on an Intel(R) Core(TM) i7-8700 CPU @ 3.20GHz with 16 gb ram. In table 2, the fixed and variable costs associated with each unit and the utilities used in the problems are presented.

4.1. Case 1

This case was previously presented by Huang and Karimi (2016) and Onishi et al. (2014b). The problem consists of two streams whose pressures remain unchanged and two streams whose pressures are changed. On the one hand, within the set of streams without pressure changes, there are a hot stream that needs to be cooled and a cold stream that needs to be heated. On the other hand, within the streams with pressure changes, there

Table 3: Problem Data for Case 1 (Huang and Karimi, 2016; Onishi et al., 2014b).

Stream	T^{in} [K]	T^{out} [K]	h [$kW\,K^{-1}$ m^{-2}]	F^{in} [kW K^{-1}]	P^{in} [MPa]	P^{out} [MPa]
HS1 (s_1)	550	450	0.1	1	–	–
CS1 (s_2)	320	350	0.1	2	–	–
LP1 (s_3)	410	660	0.1	2	0.1	0.5
HP1 (s_4)	400	310	0.1	3	0.5	0.1
Hu	680	680	1			
Cu	300	300	1			

$\Delta T^{min} = 5\,K, \eta_s = 1, r_s = 1.4, \mu_s = 1.961\,K/MPa$

L = 3, N = 1, C = 1

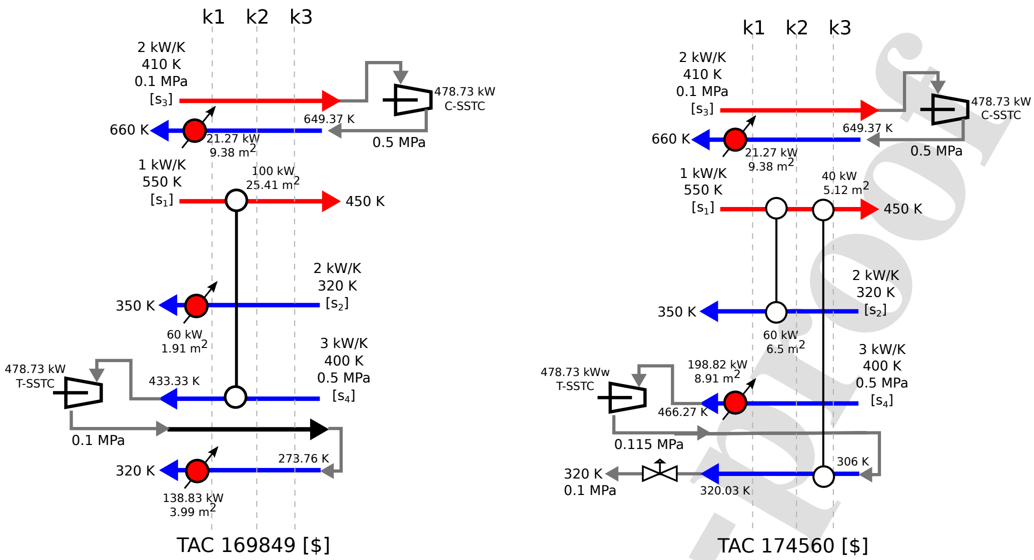
are a globally defined low-pressure stream (i.e. its outlet pressure is higher than its inlet pressure) and a globally defined high-pressure stream (i.e. its inlet pressure is higher than its outlet pressure). While the data of each stream used in this problem are presented in the table 3, the Fig. 7(a) shows the final WHEN configuration obtained by using the modeling approach proposed in section 3. The obtained WHEN has a total annualized cost equal to 169849 \$/year with a total capital cost of 108.22 \$/year, a total operating cost of 7.7 \$/year and zero revenue from electricity generation. The WHEN has (i) a heat exchanger with an area of $25.41\,m^2$ and a heat exchanged of 100 kW between the hot stream HS1 (s_1) and the stream s_4 acting as high-pressure cold stream at the first stage ($\ell = 1$) of the WHEN, (ii) three final hot utilities for the streams CS1 (s_2), LP1 (s_3), and HP1 (s_4) whose areas and heat exchanged are $9.38\,m^2$ - 21.27 kW, $1.91\,m^2$ - 60 kW, and $3.99\,m^2$ - 138.83 kW, respectively. In table 4 the final solution for this example and the solutions obtained in previous works are compared. It can be observed that, while the WHEN obtained in the work presented by Huang and Karimi (2016) (see Fig. 7(b)) has a total annualized cost of 174560 \$/year, in Onishi et al. (2014b) it is impossible to obtain a feasible solution. It is

Table 4: Solutions Obtained for Case 1.

Solution	Huang and Karimi (2016)	Onishi et al. (2014b)	Proposed Model
TAC [$/year]	174560	**	169846
CAPEX [$/year]	112.935	**	108.220
OPEX [$/year]	61.625	**	61.625
REV [$/year]	0	**	0
Number of heat transfer devices	4	**	4
Number of pressure manipulators	3	**	2
Constraints	478	604	377
Continuous Variables	357	407	320
Binary Variables	86	106	67
Nonlinear Terms	277	282	187
time [seg]	153	**	577

** no feasible solution.

important to note that the solution obtained here, by the new modeling approach, has a 2.7 % less TAC than the network proposed by Huang and Karimi (2016). The main difference relies on the heat exchange and the pressure management relationships with the stream HP1 (s_4). While the network proposed by Huang and Karimi (2016) uses two heat exchangers between the stream s_1 and the streams s_2 and s_4, the final WHEN obtained in this work: (i) has only one heat exchanger between the streams s_1 - s_4 and (ii) incorporates a hot utility for the stream s_2. On the other hand, the stream s_4 achieves its target pressure at the end of the SSTC turbine without using the additional valve proposed by Huang and Karimi (2016). A comparison between the thermodynamic paths made by the stream s_4 in each studied WHEN can be observed in the figure 8. If the two designs are compared, the final proposed structure presents a 4.17 % lower total capital cost than Huang and Karimi (2016). Finally, it is important to highlight that in both WHENs the work exchanged between SSTC compressor and turbine is 478.73 kW.



(a) Proposed Model. (b) Huang and Karimi (2016).

Figure 7: Final WHEN Configuration for Case 1.

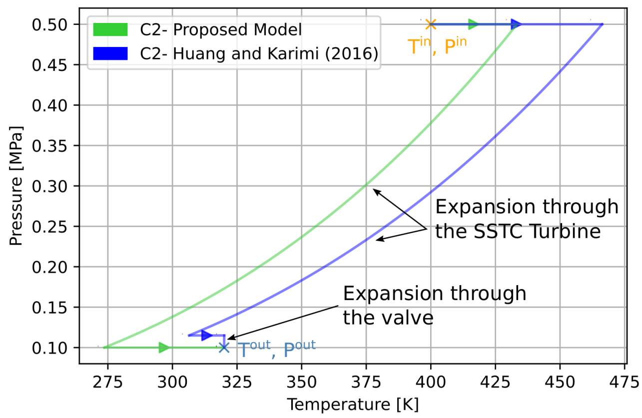


Figure 8: Thermodynamic Paths of the stream C2.

4.2. Case 2

This case study was presented and solved by Santos et al. (2020) and Pavão et al. (2019). The overall problem is defined as: (i) a globally defined low-pressure stream ($LP1$) whose inlet conditions ($\mathrm{T^{in}}$,$\mathrm{P^{in}}$) are 605 K and 0.1 MPa and outlet targets ($\mathrm{T^{out}}$,$\mathrm{P^{out}}$) are 370 K y 0.5 MPa; (ii) a globally defined high-pressure stream ($HP1$) whose inlet and outlet conditions are 410 K, 0.5 MPa and 650 K, 0.1 MPa, respectively. The data of this example are presented in the table 5.

In order to compare the results obtained here, with the new modeling approach, and the proposed solutions in previous works (Pavão et al., 2019; Santos et al., 2020), the eq. 2 is replaced by the $CAPEX$ proposed by these authors. Also, a term associated with the cost of the valves is incorporated in this objective function since it is not considered in these previous works. Concretely, the $CAPEX$ is defined as:

$$CAPEX = \sum_{\ell=1}^{\mathrm{L}} \Bigg\{ \sum_{j\in J_\ell^{\mathrm{P}}} F_{j,\ell}^{\mathrm{Hv}} + \sum_{i\in I_\ell}\sum_{\ell'=1}^{\mathrm{L}}\sum_{\substack{\forall j\neq i\\ j\in J_{\ell'}}}\sum_{k=1}^{\mathrm{K}-1} (106017.23\, z_{i,\ell,j,\ell',k} + 618.68\, a_{i,\ell,j,\ell',k} +$$

$$0.1689 a_{i,\ell,j,\ell',k}^2) + \sum_{i\in I_\ell} \left(106017.23\, zcu_{i,\ell} + 618.68\, acu_{i,\ell} + 0.1689\, acu_{i,\ell}^2\right) +$$

$$\sum_{j\in J_\ell} \left(106017.23\, zhu_{j,\ell} + 618.68\, ahu_{j,\ell} + 0.1689\, ahu_{j,\ell}^2\right) +$$

$$47840.41 \sum_{i\in I_\ell} \left[(W_{i,\ell}^{\mathrm{C}})^{0.62} + (W_{i,\ell}^{\mathrm{Cu}})^{0.62}\right] + 2420.32 \sum_{j\in J_\ell} \left[(W_{j,\ell}^{\mathrm{T}})^{0.81} + (W_{j,\ell}^{\mathrm{Tu}})^{0.81}\right] \Bigg\}$$

$$\sum_{i\in LPS} \Big[106017.23\, zcu_i^{\mathrm{L}} + 618.68\, acu_i^{\mathrm{L}} + 0.1689\, (acu_i^{\mathrm{L}})^2 +$$

$$106017.23\, zhu_i^{\mathrm{L}} + 618.68\, ahu_i^{\mathrm{L}} + 0.1689\, (ahu_i^{\mathrm{L}})^2\Big] + \sum_{j\in HPS} \Big[106017.23\, zcu_j^{\mathrm{H}} +$$

$$618.68\, acu_j^{\mathrm{H}} + 0.1689\, (acu_j^{\mathrm{H}})^2 + 106017.23\, zhu_j^{\mathrm{H}} + 618.68\, ahu_j^{\mathrm{H}} + 0.1689\, (ahu_j^{\mathrm{H}})^2\Big] +$$

$$988.49 \left[(W^{\mathrm{G}})^{0.62} + (W^{\mathrm{H}})^{0.62}\right]$$

The main difference between this new $CAPEX$ and the given by equation 2 is the way to obtaining the capital cost of heat exchangers, hot/cold utilities, turbines, compressors, electric generators and helper motors. While the capital cost of the heat exchangers, hot/cold utilities are obtained with a function $a + b\,(\mathrm{Area}) + c\,(\mathrm{Area})^2$ that depends on their areas, the capital cost associated to turbines, compressors, electric generator and helper motor is obtained through a function that depends on their capacity: $a(\mathrm{Work})^b$. It is important to

Table 5: Problem Data for Case 2 (Pavão et al., 2019; Santos et al., 2020).

Stream	T^{in} [K]	T^{out} [K]	h [kW K^{-1} m^{-2}]	F^{in} [kW K^{-1}]	P^{in} [MPa]	P^{out} [MPa]
LP1 (s_1)	650	370	0.1	3	0.1	0.5
HP1 (s_2)	410	650	0.1	2	0.5	0.1
Hu	680	680	1			
Cu	300	300	1			

$\Delta T^{min} = 1\,K, \eta_s^{HP} = 1, \eta_s^{LP} = 1, r_s^{HP} = 1.51, r_s^{LP} = 1.352, \mu_s = 1.961\,K/MPa,$
$N = 1,\ C = 1$

note that the calculation of the $CAPEX$ presented in Pavão et al. (2019); Santos et al. (2020) incorporates new nonlinearities into the model, increasing its difficulty.

This case is solved considering different number of stages for the WHEN (L = 3 and 4). The solution obtained here is presented in the figure 9(c), which has a total annualized cost (TAC) of 721241.67 \$/year with a total capital cost ($CAPEX$) of 564097 \$/year, a total operating cost ($OPEX$) of 157145 \$/year, and without revenue from electricity generation ($REV = 0$). A comparison with the solutions obtained by Pavão et al. (2019) (Fig. 9(a)) and Santos et al. (2020) (Fig. 9(b)) is made in Table 6. While the WHENs obtained by these works use two heat exchangers, the methodology proposed here suggests a network with a single heat exchanger (area = $267.5\,m^2$ and exchanged heat = 731.9 kW). This heat exchanger is associate to the stream s_1 at the stage 1 of the WHEN (acting as a low-pressure hot stream) and the stream s_2 at the stage 3 (acting as a high-pressure cold stream). Considering the total area of heat exchangers and hot and cold utilities, it can be observed that while the network proposed here has a total heat exchangers area of $267.9\,m^2$ and a total area for hot and cold utilities of $155.37\,m^2$, in the network obtained by Pavão et al. (2019) and Santos et al. (2020), they are: $433.4\,m^2/73.3\,m^2$ and $323.9\,m^2/98.2\,m^2$, respectively. Similarly, the total exchanged heat by heat exchangers and utilities is: (i) 731.9 Kw and 613.21 Kw, respectively, for our network, (ii) 790.3 Kw and 680 Kw for the WHEN proposed by Pavão et al. (2019), and (iii) 791.2 Kw and 625.8 Kw for the WHEN obtained by Santos et al. (2020). It is important to note that the smaller area in heat exchangers (one equipment eliminated in the structured proposed here) produces a larger area in the hot/cold utilities. In addition, the structure proposed here has the lowest exchanged heat in the utilities, which implies lower operating costs when compared against the previous publications. Let us consider the network pressure management differences between the proposed solution and previous works. It can be observed that while Pavão et al. (2019) suggests 3 pressure management equipment, the solution found here uses only 2 pressure management units with a smaller capacity generator (195.5 kW). Furthermore, compared with Pavão et al. (2019), the proposed network in Fig. 9(c) presents a reduction of 2.5% in total operating costs (due to the lower consumption of heaters, coolers and the elimination of an utility compressor) and a saving of 7.9% in the total capital cost (due to the lower area of the heat exchangers). Therefore, the mentioned costs reduction produces a saving of 6.8% in the total annualized cost.

Observing the computational burden, it can be concluded that the proposed new energy identity change modeling reduces the complexity of the synthesis problem and, therefore, reduces the computation times. In this context, comparing with the computational time presented in Santos et al. [27], it can be observed an improvement of 65.2% and 23% when the new modeling approach suggested here is solved by considering 3 or 4 stages, respectively. The increase in the number of stages implies a higher computational burden. This is related to the increase in the number of constraints and variables.

4.3. Case 3

This example was previously solved and analyzed in Onishi et al. (2014b), Huang and Karimi (2016), and Santos et al. (2020). The process consists of 2 low-pressure streams and 3 high-pressure streams. In table 7, it can be seen the inlet and outlet conditions of each stream. While the stream s_1 has inlet conditions of (390 K, 0.1 MPa) and outlet conditions of (390 K, 0.7 MPa), the inlet and outlet conditions of the stream s_2 are: (420 K, 0.1 MPa) and (420 K, 0.9 MPa), respectively. On the other hand, the streams defined globally as high-

Table 6: Solutions Obtained for Case 2.

Solution	Pavão et al. (2019)	Santos et al. (2020)	Proposed Model L = 3 [L = 4]
TAC [$/year]	834204	773805	721242
CAPEX [$/year]	638558	612705	564097
OPEX [$/year]	195646	161099	157145
REV [$/year]	0	0	0
Number of heat transfer devices	4	5	4
Number of pressure manipulators	3	2	2
time [seg]	**	3600	1251.09 [2770.84]

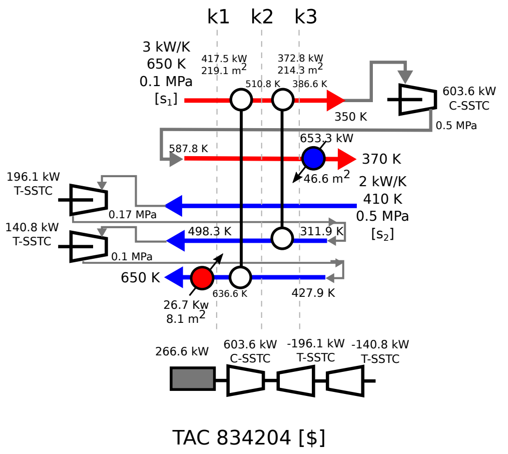
** Not Reported.

Table 7: Problem Data for Case 3 (Huang and Karimi, 2016; Onishi et al., 2014b; Santos et al., 2020).

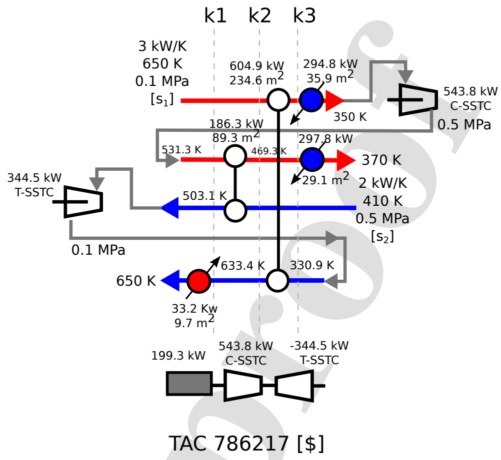
Stream	T^{in} [K]	T^{out} [K]	h [$kW\,K^{-1}\,m^{-2}$]	F^{in} [$kW\ K^{-1}$]	P^{in} [MPa]	P^{out} [MPa]
LP1 (s_1)	390	390	0.1	25.78	0.1	0.7
LP2 (s_2)	420	420	0.1	36.81	0.1	0.9
HP1 (s_3)	350	350	0.1	36.81	0.9	0.1
HP2 (s_4)	350	350	0.1	14.73	0.85	0.15
HP3 (s_5)	400	400	0.1	21.48	0.7	0.2
Hu	680	680	1			
Cu	300	300	1			

$\Delta T^{min} = 5\,K, \eta_s = 0.7, r_s = 1.4, \mu_s = 1.961\,K/MPa,$

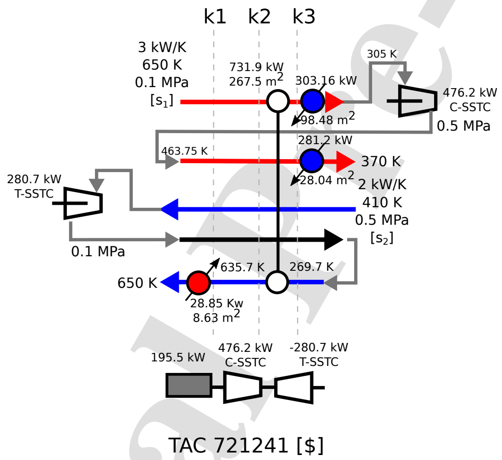
pressure streams (streams s_3, s_4, and s_5) need to be transitioned from the following input conditions: (350 K, 0.9 MPa), (350 K, 0.85 MPa), and (400 K, 0.7 MPa) to the following outlet conditions: (350 K, 0.1 MPa), (350 K, 0.15 MPa), and (400 K, 0.2 MPa). As can



(a) Pavão et al. (2019).



(b) Santos et al. (2020).



(c) Proposed Model - L = 3 and 4.

Figure 9: Final WHEN Configuration for Case 2.

be seen, all the process streams require a change in their pressures while their temperatures remain unchanged, i.e. they present equal inlet and outlet temperature. In table 8, the solution obtained here is compared with the suggested ones in previous works. It is worth mentioning that the minimum temperature approach (ΔT^{min}) used by Onishi et al. (2014b) and Huang and Karimi (2016) is 5K, while the same parameter used in Santos et al. (2020) is 1K. Regardless of this difference, the new modeling approach proposed here adequately reproduced the results in both cases. Using a $\Delta T^{min} = 5$ K, the solution proposed in this work is compared against the solution reported by Huang and Karimi (2016). The network obtained in this work presents a TAC of 10130 \$/year with a total capital cost ($CAPEX$) of 1338 \$/year, a total operating cost ($OPEX$) of 8793 \$/year and without revenue from electricity generation. This total annualized cost represents a saving of 0.6 % compared to the network given by Huang and Karimi (2016) ($TAC = 10187$). If the structures of both solutions (Fig. 10 and 11) are compared, it can be observed that the network proposed here has two less hot utilities but uses two more heat exchangers. On the other hand, taking into account the pressure management, the final WHEN obtained in this work adds one more SSCT compressor and turbine respect to Huang and Karimi (2016). It is important to note that the additional SSTC compressor is incorporated in parallel with the utility compressor, causing its capacity to be reduced. These changes produce that the network recovers 20.8 % more heat and 4.6 % more work compared to the WHEN of Huang and Karimi (2016). While in this network the work and heat recovered is 9647.5 kW and 12112.3 kW, respectively, in the WHEN of Huang and Karimi (2016) are 7989.0 kW and 11580.4 kW. This greater integration of heat and work generates an operating cost reduction of 2.4%. Finally, this decrease in operating costs implies an increase of 13.3 % in the total capital cost.

5. Conclusion and Future Works

In this work a novel model for the synthesis of work and heat exchange networks with changes in the identity of the process streams is presented. The proposed new modeling approach allows considering different thermodynamic paths for the streams without incorporating new nonlinear constraints and binary variables into the model, i.e without increasing the synthesis problem complexity. It can be concluded, by solving different problems with increasing complexities, that the new modeling approach allows to obtain better solutions with lower computational burden when comparing against other previous works. Analyzing the results, it was observed that the obtained network structures improve the integration of heat and work of the processes. This better integration of the energy impacts directly on the

Table 8: Solutions Obtained for Case 3.

Solution	Onishi et al. (2014b)	Huang and Karimi (2016)	Santos et al. (2020)	Proposed Model
TAC [$/year]	10502	10187	10004	10130
CAPEX [$/year]	1461	1180	1183	1338
OPEX [$/year]	9042	9006	8858	8793
REV [$/year]	0	0	0	0
Number of heat transfer devices	13	15	15	15
Number of pressure manipulators	9	7	7	9
Heat recovered [kW]	8794	7989	8663	9647
Hot utility consumed [kW]	1680	5951	5275.0	6323
Cold utility consumed [kW]	10521	13415	13010	13525
Work recovered [kW]	10474	11580	11579	12112
Electricity consumed [kW]	8840	7734	7734	7202
Electricity produced [kW]	0	0	0	0

total annualized cost, generating an important reduction of this index when compared with previous works. In most cases, savings of approximately 2% in the operating costs and 4 to 7% in the total capital cost were observed, which represent a saving of 1% to 7% in total annualized cost. Finally, as future works, it is necessary to extend the proposed modeling approach with several existing methodologies for HENs, WENs, and WHENs. For example, it is necessary to consider: (i) pressure drop in the heat exchanger and heat losses in the pressure manipulating equipment, (ii) phase change of the streams, (iii) several shafts for turbines and compressors, (iv) multiple utilities and multistage pressure manipulations, and (iv) pressure management equipment with different efficiencies.

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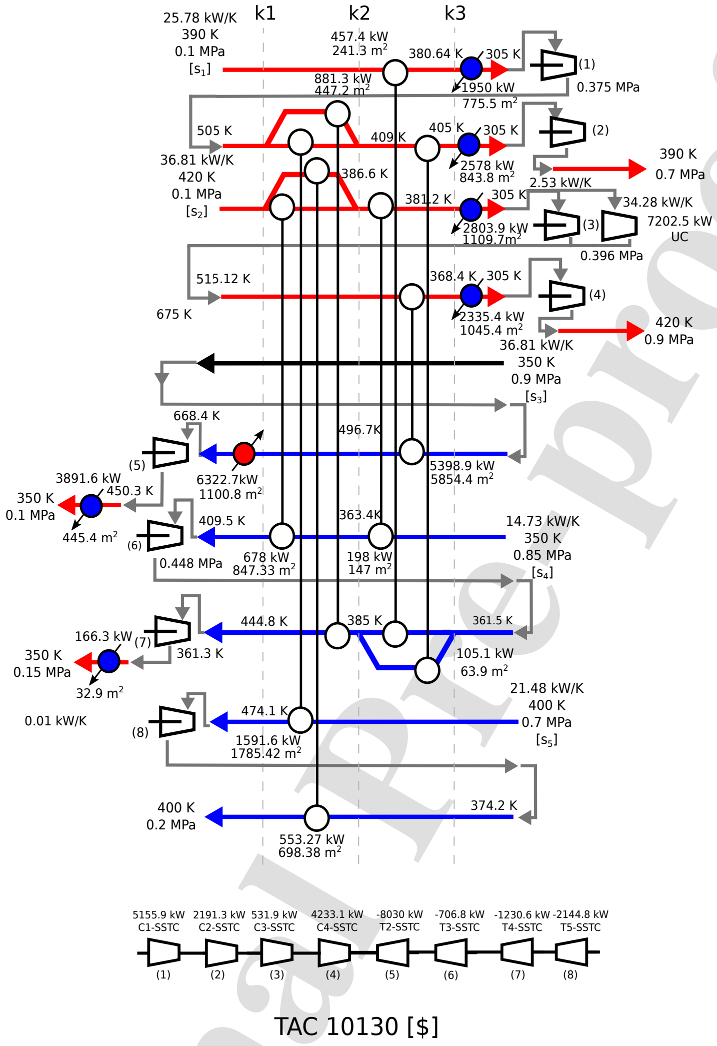

Figure 10: Final WHEN Configuration for Case 3 - Proposed Model

de la Información y Sistemas), and ANPCYT (Agencia Nacional de Promoción Científica y Tecnológica, PICT 2018-2313 and PICT 2019-0605)

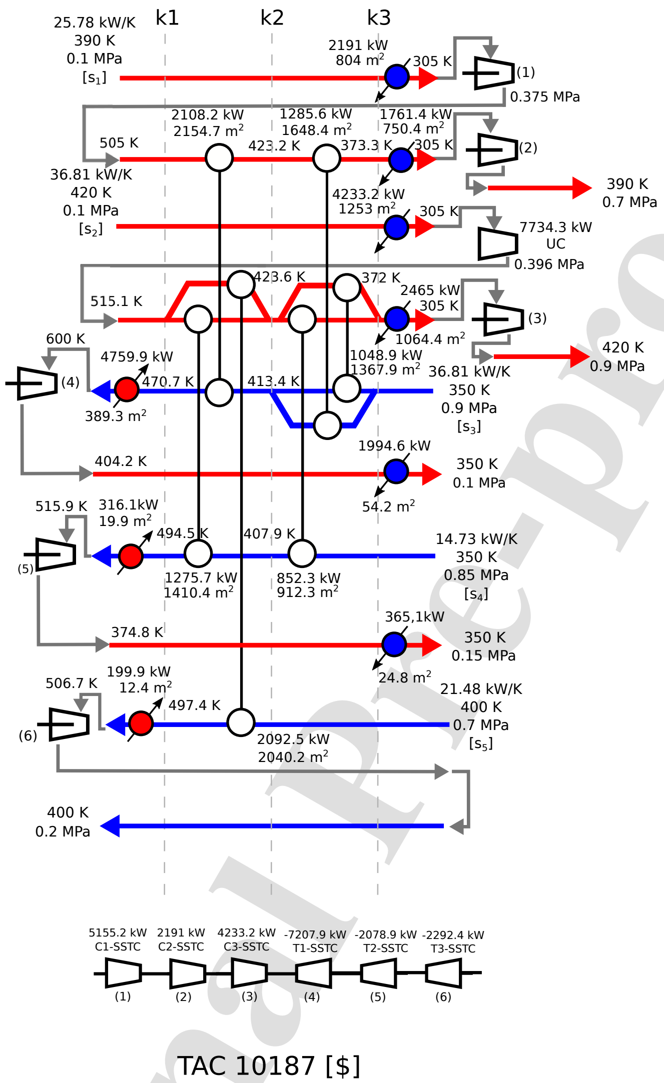

Figure 11: Final WHEN Configuration for Case 3 - Huang and Karimi (2016).

Nomenclature

Acronyms

CS: Cold Streams.

HEN: heat exchanger network.

HP: High-Pressure.

LP: Low-Pressure.

HS: Hot Streams.

MINLP: mixed-integer nonlinear programming.

WEN: work exchanger network.

WHEN: work and Heat exchanger network.

SSTC: single-Shaft-Tubine-Compressor.

TAC: total annualized cost.

Sets and Indices

C: set of stages where the streams have changed identities.

CS: set of cold streams.

HPS: set of high-pressure streams.

HS: set of hot streams.

$i \in I_\ell$: low-pressure hot streams at ℓ-th stage of the WHEN.

I_ℓ^{P}: set of low-pressure streams at ℓ-th stage of the WHEN.

$j \in J_\ell$: high-pressure cold streams at ℓ-th stage of the WHEN.

J_ℓ^{P}: set of high-pressure streams at ℓ-th stage of the WHEN.

$k \in K$: stage of the HEN.

$\ell \in L$: stage of the WHEN.

LPS: set of low-pressure streams.

N: set of stages where the streams have nominal identities.

NPC: set of no-pressure-change streams.

PC: set of pressure-change streams.

Continuous variables

a, acu, and ahu: area of heat exchangers and utilities, raised to the power of β

acu^{L} and ahu^{L}: area of the final cold/hot utilities for the low-pressure streams, raised to the power of β.

acu^{H} and ahu^{H}: area of the final cold/hot utilities for the high-pressure streams, raised to the power of β.

F^{Lu} and F^{Le} : flow rate through the compressors.

F^{Hu}, F^{He}, and F^{Hv}: flow rate through the turbines and valve.

pL^{i} and pL^{o}: inlet and outlet pressure for the low-pressure streams.

pH^{i} and pH^{o}: inlet and outlet pressure for the high-pressure streams.

q, qcu, and qhu: heat associated with the heat exchangers and the cold/hot utilities.

qcu^{L} and qhu^{L}: heat associated with the cold/hot utilities for low-pressure streams.

qcu^{H} and qhu^{H}: heat associated with the cold/hot utilities for high-pressure streams.

Th^{in} and Th^{out}: stage inlet and outlet temperatures of the hot streams.

Tc^{in} and Tc^{out}: stage inlet and outlet temperatures of the cold streams

Th and Tc: local temperatures of the hot and cold streams in the HENs.

TL^{in} and TL^{out}: inlet and outlet temperatures of the WENs for the low-pressure streams.

TH^{in} and TH^{out}: inlet and outlet temperatures of the WENs for the low-pressure streams.

TH^{m} and TH^{v}: outlet temperatures of the high pressure stream from the adiabatic mover and the valves.

$TL^{\text{in-ut}}$ and $TL^{\text{out-ut}}$: inlet and outlet temperatures of the low-pressure streams from the final utilities.

$TH^{\text{in-ut}}$ and $TH^{\text{out-ut}}$: inlet and outlet temperatures of the high-pressure streams from the final utilities.

W^{Cu} and W^{C}: compressor capacities.

W^{Tu} and W^{T}: turbine capacities.

W^{G} and W^{H}: capacity of the generator ant the helper motor

Δth, Δth^{cu}, and Δth^{hu} : temperature differences on the hot end of the heat exchanger and cold/hot utilities.

Δtc, Δtc^{cu}, and Δtc^{hu} : temperature differences on the cold end of the heat exchanger and cold/hot utilities.

$\Delta th^{\text{cu-H}}$ and $\Delta th^{\text{hu-H}}$: temperature differences on the hot end of the final hot and cold utilities for high-pressure streams.

$\Delta th^{\text{cu-L}}$ and $\Delta th^{\text{hu-L}}$: temperature differences on the hot end of the final hot and cold utilities for low-pressure streams.

$\Delta tc^{\text{cu-H}}$ and $\Delta tc^{\text{hu-H}}$: temperature differences on the cold end of the final hot and cold utilities for high-pressure streams.

$\Delta tc^{\text{cu-L}}$ and $\Delta tc^{\text{hu-L}}$: temperature differences on the cold end of the final hot and cold utilities for low-pressure streams.

Binary Variables

u^{L} and x^{L}: existence of compressors.
u^{H}, x^{H}, and v^{H}: existence of turbines and valves.
z, zcu, and zhu: existence of exchangers and cold/hot utilities.
zcu^{L}, zcu^{H}, zhu^{L}, and zhu^{H}: existence of final cold/hot utilities.
y^{L} and y^{H}: existence of the bypass over the WENs.
zL^{Hen} and zH^{Hen}: existence of the bypass over the HENs.

Parameters

C: variable cost.
CE: selling price of electricity.
CF: fixed cost.
CO: operation cost.
F^{in}: inlet flowrate.
F^{min}: minimum flowrate.
P^{in} and P^{out}: global inlet and outlet pressure.
TUB^{out} and TLB^{out}: upper and lower bounds for outlet temperatures.
T^{in} and T^{out}: global inlet and outlet temperatures for low-pressure hot streams.
U, Ucu, and Uhu: the overall heat transfer coefficient.
WG^{UB} and WH^{UB}: maximum capacity for electric generator and helper motor.
$\Delta\text{P}^{\text{min}}$ and $\Delta\text{P}^{\text{max}}$: minimum and maximum pressure drop.

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Highlights

- New MINLP model for heat and work exchange network synthesis based on total annualized cost.
- Mathematical formulation based on the SYNHEAT and WEN models for heat and work exchange network stages.
- Stage-wise superstructure for WHEN synthesis considering identity changes of the process streams.
- New identity changes modelling approach without adding alternative nonlinear constraints and binary variables.
- The generalized modelling approach includes all possible thermodynamic paths of process streams avoiding the manipulation heuristic routes definition.

CRediT author statement

Braccia L.: Conceptualization, Methodology, Software, Investigation, Writing - Original Draft.

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Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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