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SYNTHESIS AND OPTIMIZATION OF WORK AND HEAT EXCHANGE NETWORKS USING AN MINLP MODEL WITH A REDUCED NUMBER OF DECISION VARIABLES

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Abstract –Integrating the energy available in industrial processes in the form of heat and work is fundamental to achieve higher energy efficiencies as well as to reduce process costs and environmental impacts. To perform this integration, a new framework for the optimal synthesis of work and heat exchange networks (WHEN) aiming to reduce capital and operating costs is presented. The main contribution of this paper is the elaboration of a new WHEN superstructure and mixed-integer nonlinear programming (MINLP) derived model. Strategies of changing variables are applied to reduce the number of decision variables from the model. The MINLP problem with a reduced number of decision variables is solved with a two-level meta-heuristic optimization approach, using Simulated Annealing in the combinatorial problem and Particle Swarm Optimization in the nonlinear programming problem. For the sake of validation, this methodology is applied to three case studies comprising two, five, and six process streams. Economic savings achieved outperform results reported in the literature from 1.0 to 7.2%. Also, the solutions obtained present non-intuitive WHENs that shows the importance of using super- structure-based mathematical programming for such a difficult decision-making task.

Keywords: Work and heat exchange networks. MINLP. Superstructure. Optimization. Change of variables. Third-level optimization.

1. Introduction

Industrial processes are responsible for the consumption of approximately 30 % of the total energy worldwide in tasks like heating, cooling, compressing, and expanding process streams for chemical reactions or separations, for example [1]. Simultaneous work and heat integration (SWHI) helps in reducing the use of external energy sources in industrial processes employing energy resources from within the process by the synthesis of work and heat exchange networks (WHEN) performing temperature-and-pressure-related process demands with minimum total annualized cost (TAC). The synthesis of optimum WHEN involves determining the existence of heat exchangers, heaters, coolers, and pressure manipulators, as well as their appropriated placement and sizes. Superstructure-based mathematical programming can be used in solving kind of problems providing mixed-integer nonlinear programming (MINLP) formulations related to equipment existence and sizes, cost calculations, mass and energy balances and thermodynamic and physical properties equations and constraints.

Considering only heat integration (HI) or heat exchanger networks (HEN) synthesis, superstructure-based mathematical programming was deeply explored with interesting results. The most used one is the stage-wise superstructure of HEN of Yee and Grossmann (1990) [2], in which streams are classified as hot and cold and divided into K stages. In a stage k, a hot stream could exchange heat in parallel with every cold one as long as isothermal mixing was hold. After K stages, hot and cold utilities were used to adjust final temperatures.

Much research attention was directed to adding pressure recovery in WHEN synthesis and optimization in recent years (Fu *et al*., 2018) [3] and thermodynamic-and-heuristic-based graphical methods and superstructure-based mathematical programming approaches have been used. Aspelund *et al*. (2007) [4] developed a graphical method for the synthesis of WHEN aiming to reduce the exergy consumption following heuristic rules for the appropriate placement of pressure manipulators and heat exchangers. Gundersen *et al*. (2009) [5] proposed the heuristic in which the optimum inlet temperature to the compression and expansion tasks should be the Pinch temperature in order to reduce the exergy consumption. Fu and Gundersen (2016a; 2016b) [6,7] augmented to the graphical method the rule that the inlet temperature to compression and expansion could be not only the Pinch one, but also the ambient, the hot utility, or the cold utility temperatures. Despite its non-linearity and non-convexity, which make the mathematical problem hard to solve, this kind of approach has presented interesting results in this research field.

Wechsung *et al*. (2011) [8]. published the first paper in WHEN synthesis and optimization using superstructure-based mathematical programming. They proposed a superstructure in which the process streams were classified as hot or cold, with fixed or variable pressure. Each process stream classification presented a pre-defined route of heating, cooling, compressing, and expanding in that superstructure. Also, those authors simplified their model using heuristics proposed by Gundersen *et al*. (2009) [5] for the appropriate placement of pressure manipulators, which stated that the inlet temperature to pressure manipulators should preferably be at the Pinch temperature. Therefore, the heating/cooling goal before pressure manipulation was known. The authors modeled the problem with an MINLP formulation that comprised Pinch analysis and irreversibilities calculation. The optimization problem to minimize the WHEN irreversibilities was implemented in GAMS and solved using BARON solver.

Razib *et al*. (2012) [9] proposed a multi-stage superstructure for work integration with temperature variation of process streams. In that superstructure, streams were classified as high pressure (HP) and low pressure (LP). For a HP stream, a stage would be composed by a heater with hot utility and an expansion work exchange network (WEN). In expansion WEN, a HP stream could be expanded in parallel in a valve, in a utility turbine to generate electricity, and/or in a turbine coupled to other turbines and compressors for work integration in several shafts, or bypass the WEN entirely. For a LP stream, a stage was a cooler with cold utility and a compression WEN, which was composed by a utility compressor in parallel with compressors in different shafts of work integration. The introduction of turbines and compressors coupled together in one shaft for work integration, called single-shaft-turbine-compressor (SSTC), was a major contribution. The authors proposed an MINLP formulation to treat the problem, aiming to minimize the total annualized cost (TAC). The problem was solved in GAMS using BARON solver.

Onishi *et al*. (2014a) [10] proposed a multi-stage superstructure inspired in the work of Razib *et al*. (2012) [9] and added the possibility of heat integration. Heaters and coolers were replaced by the well-known HEN superstructure from Yee and Grossmann (1990) [2], in which HP streams were considered cold streams and LP were considered hot streams. An MINLP formulation was proposed aiming the TAC minimization, and the problem was solved in GAMS using SBB solver. Using the same superstructure, Onishi *et al*. (2017) [11] presented a bi-objective optimization problem in order to minimize both TAC and environmental impacts. The authors solved the problem using DICOPT solver in GAMS.

Onishi *et al*. (2014b) proposed a WHEN superstructure based on Wechsung *et al*. (2011) [8]. The former Pinch analysis was substituted by the Yee and Grossmann (1990) [2] HEN superstructure, similar to Onishi *et al*. (2014a) [10]. Mathematical programming was used in the appropriate placement of pressure manipulators, avoiding heuristics use. SSTCs was allowed in the WHEN superstructure. Lastly, a final heater/cooler was added, depending on the stream identity to adjust the final streams temperature. An MINLP formulation was proposed to minimize the network TAC and the problem was solved using BARON solver in GAMS. Based on this work, Onishi et al. (2015) [13] developed a methodology for retrofitting HEN with streams with pressure change in subambient conditions [13].

Huang and Karimi (2016) [14] proposed some modifications to the work of Onishi *et al*. (2014b) [12]. One modification was to decide the type of final device to adjust stream temperature (heater/cooler) based on the stream need instead of its identity. These simple alterations showed to be important in some case studies. The authors proposed an MINLP formulation to the optimization problem, aiming to minimize the total annualized cost (TAC), and used BARON solver in GAMS to solve it.

Onishi *et al*. (2018) [15] presented a new superstructure to deal with unclassified streams. Compression and expansion WEN were unified, comprising the possibility of using a valve, a utility compressor, and a utility turbine, or bypassing the section. Generalized disjunctive programming was used to deal with pressure manipulator selection and streams classification. The optimization model included mathematical programming and Pinch location method to minimize the WHEN TAC. BARON solver in GAMS was used to solve the problem.

Nair *et al*. (2018) [16] added to the model equations to the model of Onishi *et al*. (2018) [15], considering streams phase change and variable heat capacity. Also, compression and expansion of streams with no net pressure change (*i.e.*, cycles) were allowed. An MINLP formulation to minimize the total annualized cost (TAC) was proposed and BARON solver in GAMS was used to solve the problem. The methodology was applied to two industrial cases: the natural gas liquefaction and C3 separation.

Pavão *et al*. (2019a) [17], inspired in the work of Onishi *et al*. (2014b) [12], proposed a new approach to treat the WHEN synthesis and optimization problem. The authors replaced the Yee and Grossmann (1990) [2] HEN superstructure by a new one (Pavão *et al*., 2018) [18], without considering isothermal mixing and allowing utilities in every HEN stage in parallel with the other heat transfer devices. The authors proposed a matrix formulation to the MINLP problem, which was implemented in C++ language. A two-level meta-heuristic optimization method, in which Simulated Annealing (SA) was used in combinatorial level and Rocket Fireworks Optimization in the continuous one, was proposed. This approach was applied to the industrial processes of natural gas liquefaction and carbon capture of exhausting gas using membrane separation. Employing the same framework, Pavão *et al*. (2019b) [19] considered in the model uncertainties in the energy price and different hot and cold utilities.

In the present paper a new approach for the WHEN synthesis and optimization is proposed. It includes the elaboration of a new four-section multi-stage WHEN superstructure and the derivation of an MINLP formulation model, which allows to reduce the optimization search space without losing the superstructure generality. Changes of variables and third-level optimization are used. The solution approach proposed to solve the the decision-variable-reduced MINLP is a two-level meta-heuristic optimization method. Finally, the methodology is validated by its application in three case studies.

2. Superstructure and derived MINLP model

The problem this paper tackles is to synthesize a WHEN of electric turbines and compressors, SSTCs, helper motors, electric generators, heat exchangers, heaters, and coolers that perform the required temperature and pressure changes of process streams with minimum operating and capital costs. To do so, the problem statement includes the set of S streams (s = 1,2,…,S), their initial and final states (T_{in} and P_{in}, T_{out} and P_{out}), heat capacity flow rates (CP) and individual heat exchange coefficients (h), hot and cold utilities with their inlet and outlet temperatures (TS_{in} and TW_{in}, TS_{out} and TW_{out}), individual heat exchange coefficients (h_s and h_w) and costs (C_{HU} and C_{CU}), prices of purchase and selling electricity (CE and PE), economic capital cost parameters (a, b, and c), polytropic exponent (κ), and compression and expansion efficiencies (η_c and η_e).

Model assumptions:

- Steady-state operation;
- All process streams are gaseous and considered ideal gases;
- Compression and expansion take place in electric compressors, electric turbines, or SSTCs with isentropic efficiencies;
- The SSTC operates at any speed and the number of units it can allocate it is not limited;
- Lacks of work in the SSTC is supplied by helper motor using electricity;
- Surplus of work is transformed into electricity in an electric generator;
- Heat capacities and heat transfer coefficients are constant;
- Pressure drop and heat losses in thermal devices and pipes are neglected;
- Mixers, splitters, and pipes cost is negligible.

In order to solve the problem stated, a multi-stage superstructure inspired by Onishi *et al*. (2018) [15] is proposed (Figure 1 presents the proposed superstructure for two process streams). Process streams are not pre-classified as HP, LP, hot or cold. Thus, an unclassified stream can be heated, cooled, compressed, and expanded without a fixed logic. One major difference in this superstructure is to divide the HEN superstructure into two sections: heat integration (heat exchangers between thermally classified process streams) and temperature adjustment of unclassified streams with hot or cold utilities. This novelty brings more generality to the network because, for instance, a stream that was treated as hot stream in heat integration section can be eventually heated up with hot utility to adjust its temperature for pressure manipulation.

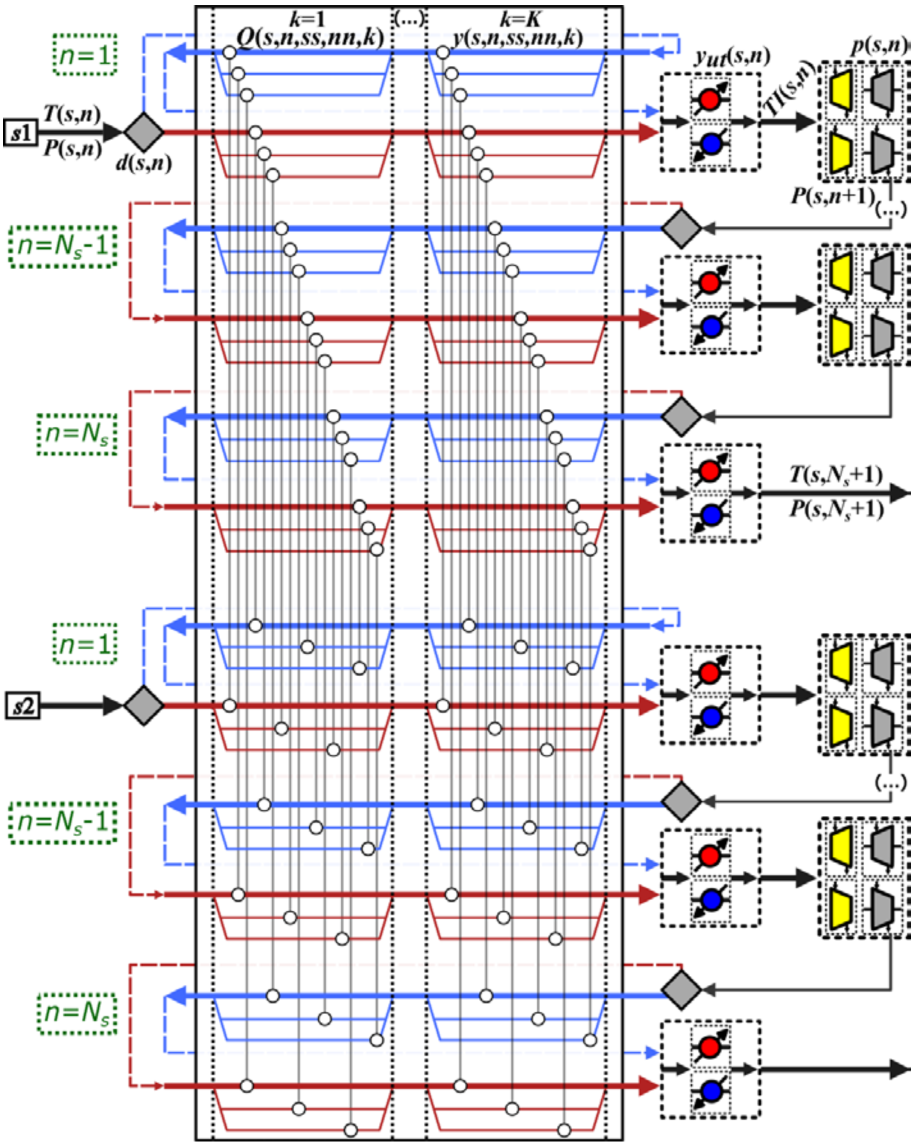

Figure 1. Proposed superstructure for two process streams.

This superstructure is composed by horizontal and vertical stages. Vertical stages refer to the heat integration and are described by index *k*, ranging from 1 to *K*. Horizontal stages correspond to WHEN and are described by index *n*, ranging from 1 to N_s. Figure 2 illustrates a horizontal stage with four sections: classification, HI, temperature adjustment and WEN.

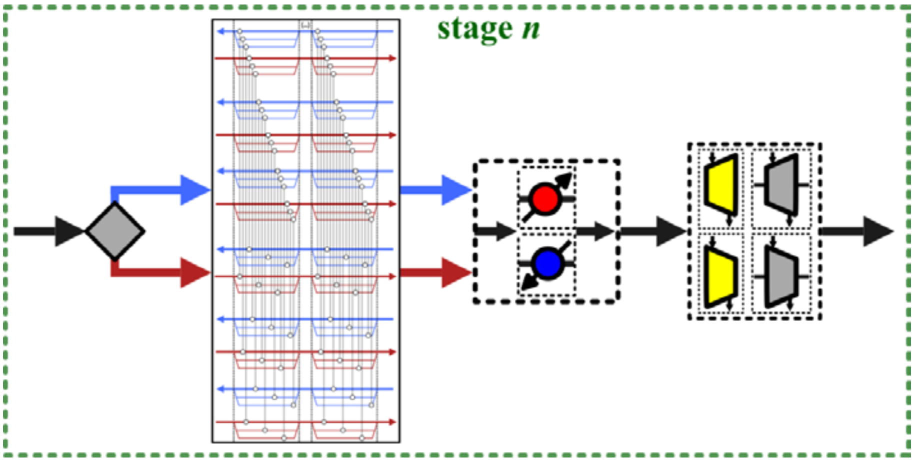

Figure 2. Four-section SWHI superstructure stage.

In the classification section, an unclassified stream can be hot or cold. Next, the thermally classified stream can exchange heat with other process streams in the HI section. In this section, each hot stream can exchange heat with every cold stream in parallel in each *k* stage considering isothermal mixing, like the HEN superstructure proposed by Yee and Grossmann (1990) [2]. Subsequently, in the temperature adjustment section, the stream temperatures are adjusted to their inlet temperature of pressure manipulations, using either hot or cold utilities, depending on their needs. Finally, after the temperature adjustment, streams can be compressed or expanded in electric compressors, electric turbines, or SSTCs in the WEN section. This four-section stage is repeated $N_s - 1$ times because in the last stage (N_s) the stream has to be in its final pressure and only temperature related operations take place.

From this superstructure, a model is derived with an MINLP formulation. The model comprises the four-section model equations, costs calculation, constraints, penalties and the objective function. The mathematical model with a degrees of freedom analysis for choosing the MINLP decision variables is presented in next topic. The degrees of freedom analysis allows to define the flexibility for the optimization problem, once each degree of freedom needs to be fulfilled with a decision variable, so that the mathematical problem is completely determined.

Before starting the classification section modeling, the initial and final values of state variables T (s, n) and P (s, n) must be established. These variables represent the temperature and pressure of the process stream $s \in [1, S]$ in stage $n \in [1, N_s+1]$. Therefore, the initial (n = 1) and final values (n = N_s for pressure and n = N_s+1 for temperature) are known accordingly with the problem statement (*Tin*, *Pin*, *Tout*, and *Pout*).

2.1. Classification section

In this section, mass and energy balances are performed in the streams classification prior to the HI. These balances result in a set of four equations for each $s \in [1, S]$, $n \in [1, N_s]$:

$$FH(s,n) = d(s,n).CP(s) \tag{1}$$

$$FC(s,n) = \left[1 - d(s,n)\right].CP(s) \tag{2}$$

$$TH(s,n,0) = T(s,n) \tag{3}$$

$$TC(s,n,K) = T(s,n) \tag{4}$$

This thermal classification is achieved using the binary variable $d(s,n)$, which states if the stream s in stage n will be considered a hot ($d = 1$) or a cold ($d = 0$) stream for HI. Therefore, either the hot stream thermal capacity (FH) or the cold one (FC) equals zero. It is worth noticing that FH, FC, and d are 2D matrixes. Their indexes $s \in [1, S]$ and $n \in [1, N_s]$ indicate that each element in these matrixes is a variable referring to stream s in horizontal stage n. Similarly, the temperatures of classified hot and cold streams (TH and TC) are 3D matrixes. Their indexes $s \in [1, S]$, $n \in [1, N_s]$ and $k \in [0, K]$ refer to stream s in horizontal stage n entering vertical stage k+1 for hot stream and k for cold stream in the HI section.

In this section, there are five variables (d, FH, FC, $TH_{k=0}$ e $TC_{k=K}$) for each $s \in [1, S]$ and $n \in [1, N_s]$, and there are four equations ((1), (2), (3), and (4)) for the same s and n. Therefore, there are $1.S.N_s$ degrees of freedom from this section. To fulfill this number, the binary variable $d(s, n)$ in each $s \in [1, S]$ and $n \in [1, N_s]$ is chosen as the decision variable.

2.2. Heat integration section

In this section, global energy balances are performed around every heat exchanger allocated in hot or cold stream s, stage n, and vertical stage k in the HI section. These energy balances result in a set of two equations for each $s \in [1, S]$, $n \in [1, N_s]$, and $k \in [1, K]$:

$$TH(s,n,k) = TH(s,n,k-1) - \frac{\sum_{ss=1}^{S}\sum_{nn=1}^{N_S} y(s,n,ss,nn,k-1).Q(s,n,ss,nn,k-1)}{FH(s,n)+eps} \tag{5}$$

$$TC(s,n,K-k) = TC(s,n,K+1-k) + \frac{\sum_{ss=1}^{S}\sum_{nn=1}^{N_s} y(ss,nn,s,n,K-k).Q(ss,nn,s,n,K-k)}{FC(s,n)+eps} \tag{6}$$

Each heat exchanger is indexed with five slots: s, n, ss, nn and k. The first two slots stand for the hot stream identification and its horizontal stage, respectively. The third and fourth slots stand for the cold stream identification and its horizontal stage, respectively. The fifth slot is the vertical stage in which this heat exchanger is placed. Therefore, y is a matrix of binary variables that state whether the heat exchanger (s, n, ss, nn, k) with a heat load of $Q(s, n, ss, nn, k)$ exists ($y = 1$) or not ($y = 0$). In order to avoid division by zero, a very small number (*eps*) is added to the denominator in both equations (5) and (6).

There are two variables (*TH* e *TC*) for each $s \in [1, S]$, $n \in [1, N_s]$ and $k \in [1, K]$, and two variables (y, Q) for each $s \in [1, S]$, $n \in [1, N_s]$, $ss \in [1, S]$, $nn \in [1, N_s]$ and $k \in [1, K]$. Also, there are two equations, (5) and (6), for each $s \in [1, S]$, $n \in [1, N_s]$ and $k \in [1, K]$. Therefore, it results in $2.S^2.N_s^2.K$ degrees of freedom in this section and it is necessary to choose two decision variables for each s, n, ss, nn and k belonging to these intervals, which are the binary variable $y(s, n, ss, nn, k)$ and the continuous variable $Q(s, n, ss, nn, k)$.

2.3. Temperature adjustment section

In this section, a global energy balance is performed around the possible heater or cooler in stream s, stage n resulting in a set of four equations for each $s \in [1, S]$ and $n \in [1, N_s]$:

$$T_{ut}(s,n) = d(s,n).TH(s,n,K) + (1 - d(s,n)).TC(s,n,0) \tag{7}$$

$$TI(s,n) = T_{ut}(s,n).(1 - y_{ut}(s,n)) + T_{adj}(s,n).y_{ut}(s,n) \tag{8}$$

$$Q_s(s,n) = \max(0, y_{ut}(s,n).CP(s).[TI(s,n) - T_{ut}(s,n)]) \tag{9}$$

$$Q_w(s,n) = \max(0, y_{ut}(s,n).CP(s).[T_{ut}(s,n) - TI(s,n)]) \tag{10}$$

In this equations, T_{ut} is the outlet temperature from the HI section, TI is the WEN inlet temperature and T_{adj} is the adjusted temperature in case there is a heater or cooler. The existence of heaters and coolers is controlled by the binary variable y_{ut} and their heat loads are Q_s and Q_w.

These four equations are interconnected. If $y_{ut} = 0$, then TI receives the value of T_{ut} due to equation (8). In addition, as TI and T_{ut} are the same, Q_s and Q_w are zero because of equations (9) and (10). On the other hand, if $y_{ut} = 1$, TI receives the value of T_{adj} and there will be either a heater, in case TI is greater than T_{ut}, or a cooler, otherwise. The heat load of this heater or cooler is calculated in equations (9) and (10).

In order to assure that $T(s, N_s+1) = Tout(s)$, T_{adj} in horizontal stage N_s must equal $Tout$. Therefore, a heater/cooler is always available to adjust the final temperature if needed. Mathematically, a set of two equations for each $s \in [1, S]$ is added:

$$T_{adj}(s, N_s) = Tout(s) \tag{11}$$

$$y_{ut}(s, N_s) = 1 \tag{12}$$

Finally, in this section there are six variables (y_{ut}, T_{adj}, T_{ut}, TI, Q_s and Q_w) for each $s \in [1, S]$ and $n \in [1, N_s]$, there are four equations ((7), (8), (9), and (10)) for each s and n belonging to the same interval and two equations ((11) and (12)) for each $s \in [1, S]$. Therefore, this section presents $2.S.(N_s - 1)$ degrees of freedom that are fulfilled by the binary $y_{ut}(s, n)$ and continuous $T_{adj}(s, n)$ in $s \in [1, S]$ and $n \in [1, N_s - 1]$ as decision variables. It is noted that the interval of n does not include the last stage N_s, because in this stage the adjusted temperature (T_{adj}) is known and equal to $Tout$.

2.4. Work exchange network

In the WEN section a global energy balance is performed around the possible electric compressor, electric turbine, single-shaft-compressor (SSC), or single-shaft-turbine (SST) in stream s, stage n. This energy balance result in a set of three equations for each $s \in [1, S]$ and $n \in [1, N_s]$:

$$c_{tmp}(s,n) = \frac{\max(0, p(s,n).[P(s,n+1) - P(s,n)])}{\max(eps, p(s,n).[P(s,n+1) - P(s,n)])} \tag{13}$$

$$e_{tmp}(s,n) = \frac{\max(0, p(s,n).[P(s,n) - P(s,n+1)])}{\max(eps, p(s,n).[P(s,n) - P(s,n+1)])} \tag{14}$$

$$T(s,n+1) = TI(s,n).\left\{1 + \left[\frac{c_{tmp}(s,n)}{\eta_c} + e_{tmp}(s,n).\eta_e\right].\left[\left(\frac{P(s,n+1)}{P(s,n)}\right)^{\frac{\kappa-1}{\kappa}} - 1\right]\right\} \tag{15}$$

Some binary variables are introduced in this section. Binary variable p indicates whether the stream s in stage n is considered for pressure change, so it activates ($p = 1$) or deactivates ($p = 0$) WEN section. Binary variables c_{tmp} and e_{tmp} control respectively the existence in stream s stage n of a compressor or a turbine, which can be electric of coupled in the shaft of work integration. The way it works is that if p equals 0 the WEN section is deactivated because c_{tmp} and e_{tmp} equal zero due to equations (13) and (14). In case p equals 1, the WEN section is activated because either c_{tmp} or e_{tmp} equals 1 depending on the value of the stream pressure in the next stage n+1 ($P(s,n+1)$). In case $P(s,n+1)$ is greater than $P(s,n)$, c_{tmp} equals 1 and compression is assured. Else, e_{tmp} equals 1 and expansion is assured.

The next horizontal stage inlet temperature ($T(s,n+1)$) changes due to pressure variation, and it is calculated in equation (15).

In order to guarantee that *P* reaches its final value *Pout*, it is necessary that *p* in $N_s - 1$ equals 1 so that a compressor or turbine can be installed depending on stream need for compression or expansion. Also, to ensure that in the last stage N_s there is no pressure change *p* must be equal zero. Mathematically, this set of four equations for each $s \in [1, S]$ is added:

$$p(s, N_s - 1) = 1 \tag{16}$$

$$p(s, N_s) = 0 \tag{17}$$

$$P(s, N_s) = Pout(s) \tag{18}$$

$$P(s, N_s + 1) = Pout(s) \tag{19}$$

In this section there are five variables (p, e_{tmp}, c_{tmp}, P_{n+1} e T_{n+1}) and three equations (13), (14) and (15) for each $s \in [1, S]$ and $n \in [1, N_s]$. There are also four equations (16), (17), (18), and (19) for each $s \in [1, S]$. Therefore, the resulting degrees of freedom number of this section is $2.S.(N_s - 2)$. So, are necessary two decision variables for each *s* and *n* of these intervals, the binary $p(s, n)$ and the continuous $P(s, n + 1)$ for $s \in [1, S]$ and $n \in [1, N_s - 2]$. Like in previous section, the interval of *n* is not complete. That is because in the last stage N_s there is no pressure manipulation and in the stage before last ($N_s - 1$) exit pressure is known and equal to *Pout*.

2.5. HEN cost calculation

The annualized HEN cost (*CostHEN*) is given by Equation (20), where *HOC* is the operating cost and *HCC* is the annualized HEN capital cost, which is a function of the area of heat exchangers, heaters and coolers, given by Equation (22) [20]. Global heat exchanger coefficients (*U*) and the logarithmic mean temperature differences (ΔT_{ml}) are calculated for each heat transfer device in equations (25), (28), and (31).

$$\mathrm{Cos}\,tHEN = HOC + f.HCC \tag{20}$$

$$HOC = \sum_{s=1}^{S} \sum_{n=1}^{N_s} \left(Q_s(s,n).C_{HU} + Q_w(s,n).C_{CU} \right) \tag{21}$$

$$HCC = \sum_{s=1}^{S} \sum_{n=1}^{N_s} \left\{ \begin{array}{l} \sum_{ss=1}^{S} \sum_{nn=1}^{N_s} \sum_{k=1}^{K} y(s,n,ss,nn,k).\left[a + b.A(s,n,ss,nn,k) + c.A(s,n,ss,nn,k)^2 \right] + \\ \dfrac{Q_s(s,n)}{Q_s(s,n) + eps}.\left[a + b.A_s(s,n) + c.A_s(s,n)^2 \right] + \dfrac{Q_w(s,n)}{Q_w(s,n) + eps}.\left[a + b.A_w(s,n) + c.A_w(s,n)^2 \right] \end{array} \right\} \tag{22}$$

$$A(s,n,ss,nn,k) = \frac{Q(s,n,ss,nn,k)}{U(s,ss).\Delta T_{ml}(s,n,ss,nn,k)} \tag{23}$$

$$U(s,ss)=\frac{h(s).h(ss)}{h(s)+h(ss)} \tag{24}$$

$$\Delta T_{ml}(s,n,ss,nn,k)=\begin{cases} if\left(\left[TH(s,n,k)-TC(ss,nn,k)\right]==\left[TH(s,n,k-1)-TC(ss,nn,k-1)\right]\right): \\ \qquad TH(s,n,k)-TC(ss,nn,k) \\ else: \\ \qquad \dfrac{\left[TH(s,n,k)-TC(ss,nn,k)\right]-\left[TH(s,n,k-1)-TC(ss,nn,k-1)\right]}{\ln\left(\dfrac{TH(s,n,k)-TC(ss,nn,k)}{TH(s,n,k-1)-TC(ss,nn,k-1)}\right)} \end{cases} \tag{25}$$

$$A_s(s,n)=\frac{Q_s(s,n)}{U_s(s).\Delta Ts_{ml}(s,n)} \tag{26}$$

$$U_s(s)=\frac{h(s).h_s}{h(s)+h_s} \tag{27}$$

$$\Delta Ts_{ml}(s,n)=\begin{cases} if\left(\left[TS_{out}-T_{ut}(s,n)\right]==\left[TS_{in}-TI(s,n)\right]\right): \\ \qquad TS_{out}-T_{ut}(s,n) \\ else: \\ \qquad \dfrac{\left[TS_{out}-T_{ut}(s,n)\right]-\left[TS_{in}-TI(s,n)\right]}{\ln\left(\dfrac{TS_{out}-T_{ut}(s,n)}{TS_{in}-TI(s,n)}\right)} \end{cases} \tag{28}$$

$$A_w(s,n)=\frac{Q_w(s,n)}{U_w(s).\Delta Tw_{ml}(s,n)} \tag{29}$$

$$U_w(s)=\frac{h(s).h_w}{h(s)+h_w} \tag{30}$$

$$\Delta Tw_{ml}(s,n)=\begin{cases} if\left(\left[T_{ut}(s,n)-TW_{out}\right]==\left[TI(s,n)-TW_{in}\right]\right): \\ \qquad T_{ut}(s,n)-TW_{out} \\ else: \\ \qquad \dfrac{\left[T_{ut}(s,n)-TW_{out}\right]-\left[TI(s,n)-TW_{in}\right]}{\ln\left(\dfrac{T_{ut}(s,n)-TW_{out}}{TI(s,n)-TW_{in}}\right)} \end{cases} \tag{31}$$

In these equations f is the annualization factor and a, b and c are the parameters of heat cost equation.

There are twelve variables: A and ΔT_{ml} for each $s \in [1, S]$, $n \in [1, N_s]$, $ss \in [1, S]$, $nn \in [1, N_s]$ and $k \in [1, K]$, A_s, ΔTs_{ml}, A_w, and ΔTw_{ml} for each $s \in [1, S]$ and $n \in [1, N_s]$, U for each $s \in [1, S]$ and $ss \in [1, S]$, U_s and U_w for each $s \in [1, S]$ and *CostHEN*, *HOC* and *HCC*.

There are also twelve equations: 2 (equations (23) and (25)) for each $s \in [1, S]$, $n \in [1, N_s]$, $ss \in [1, S]$, $nn \in [1, N_s]$ e $k \in [1, K]$; 4 (equations (26), (28), (29), and (31)) for each $s \in [1, S]$ and $n \in [1, N_s]$, 1 (Equation (24)) for each $s \in [1, S]$ and $ss \in [1, S]$; 2 (Equations (27) and (30)) for each $s \in [1, S]$ and equations (20), (21), and (22).

The resulting degrees of freedom from this section is null and there is no need for extra decision variables.

2.6. WEN cost calculation

Before calculating WEN cost, it is required to determine what pressure manipulator is used in stream s in the stage n whose $p(s,n)$ equals 1. The binary variables c_{tmp} and e_{tmp} already state respectively whether compression or expansion takes place. Therefore, it is needed to establish if this compressor or turbine is coupled to the work integration shaft or uses electric devices. In this regard, a set of four equations for each $s \in [1, S]$ and $n \in [1, N_s]$ is used:

$$c(s,n) = \max\left(0,\, p(s,n).m(s,n).c_{tmp}(s,n)\right) \tag{32}$$

$$e(s,n) = \max\left(0,\, p(s,n).m(s,n).e_{tmp}(s,n)\right) \tag{33}$$

$$uc(s,n) = \max\left(0,\, p(s,n).\left[1-m(s,n)\right].c_{tmp}(s,n)\right) \tag{34}$$

$$ue(s,n) = \max\left(0,\, p(s,n).\left[1-m(s,n)\right].e_{tmp}(s,n)\right) \tag{35}$$

The binary variables c, e, uc, and ue are introduced to determine respectively the existence of SSC, SST, electric compressors, and electric turbines. Binary variable m is responsible to determine whether the compressor or turbine is coupled to the work integration shaft (m = 1) or not (m = 0).

Equations (32), (33), (34), and (35) are formulated so that only one of the four binary variables c, e, uc, and ue is activated (equals 1) and the others equal 0. This formulation is based on a max function between 0 and a multiplication between three binary variables that are p, m (or $1 - m$), and c_{tmp} (or e_{tmp}). After determining what pressure manipulator exists, work duties are calculated based on the enthalpy change of gaseous streams (ideal gases) due to its temperature change in compression or expansion tasks. This calculation is performed in a set of four equations for each $s \in [1, S]$ and $n \in [1, N_s]$:

$$WC(s,n) = c(s,n).CP(s).\left(T(s,n+1) - TI(s,n)\right) \tag{36}$$

$$WE(s,n) = e(s,n).CP(s).\left(TI(s,n) - T(s,n+1)\right) \tag{37}$$

$$WUC(s,n) = uc(s,n).CP(s).\left(T(s,n+1) - TI(s,n)\right) \tag{38}$$

$$WUE(s,n) = ue(s,n).CP(s).\left(TI(s,n) - T(s,n+1)\right) \tag{39}$$

Variables WC, WE, WUC, and WUE correspond respectively to the work duty of SSC, SST, electric compressors, and electric turbines. Now, it is possible to check if the work integration shaft presents an energy surplus (*WG*) and an electric generator (*g*) is required, or if there is a lack of energy (*WM*) and an electric helper motor (*hm*) is required. These calculations are performed in equations (40), (41), (42), and (43).

$$hm = \frac{\max\left(0, \sum_{s=1}^{S}\sum_{n=1}^{N_s}\left[WC(s,n) - WE(s,n)\right]\right)}{\max\left(eps, \sum_{s=1}^{S}\sum_{n=1}^{N_s}\left[WC(s,n) - WE(s,n)\right]\right)} \tag{40}$$

$$g = \frac{\max\left(0, \sum_{s=1}^{S}\sum_{n=1}^{N_s}\left[WE(s,n) - WC(s,n)\right]\right)}{\max\left(eps, \sum_{s=1}^{S}\sum_{n=1}^{N_s}\left[WE(s,n) - WC(s,n)\right]\right)} \tag{41}$$

$$WM = hm.\sum_{s=1}^{S}\sum_{n=1}^{N_s}\left[WC(s,n) - WE(s,n)\right] \tag{42}$$

$$WG = g.\sum_{s=1}^{S}\sum_{n=1}^{N_s}\left[WE(s,n) - WC(s,n)\right] \tag{43}$$

Finally, the annualized WEN cost (*CostWEN*) is calculated by summing the operating cost (*WOC*) and annualized capital cost (*WCC*) in equations (44), (45), and (46). The capital cost of pressure manipulators is function of the work load (Couper *et al.*, 2012) [21].

$$CostWEN = WOC + f.WCC \tag{44}$$

$$WOC = \sum_{s=1}^{S}\sum_{n=1}^{N_s}\left[uc(s,n).WUC(s,n).CE - ue(s,n).WUE(s,n).PE\right] + hm.WM.CE - g.WG.PE \tag{45}$$

$$WCC = \sum_{s=1}^{S}\sum_{n=1}^{N_s}\begin{bmatrix} e(s,n).\left(a_e + b_e.WE(s,n)^{c_e}\right) + c(s,n).\left(a_c + b_c.WC(s,n)^{c_c}\right) \\ + ue(s,n).\left(a_{ue} + b_{ue}.WUE(s,n)^{c_{ue}} - a_g - b_g.WUE(s,n)^{c_g}\right) \\ + uc(s,n).\left(a_{uc} + b_{uc}.WUC(s,n)^{c_{uc}} - a_{hm} - b_{hm}.WUC(s,n)^{c_{hm}}\right) \end{bmatrix} + \begin{bmatrix} hm.\left(a_{hm} + b_{hm}.WM^{c_{hm}}\right) \\ + g.\left(a_g + b_g.WG^{c_g}\right) \end{bmatrix} \tag{46}$$

The parameters *CE* and *PE* stands for the purchase cost of electricity and the price of selling the electricity, whereas, a_i, b_i and c_i stand for the capital cost parameters of pressure manipulators.

In this section there are 16 variables: *m*, *e*, *c*, *ue*, *uc*, *WE*, *WC*, *WUE* and *WUC* for each $s \in [1, S]$ e $n \in [1,N_s]$ and *hm*, *g*, *WM*, *WG*, *CostWEN*, *WOC* and *WCC.*

Also, there are 15 equations: 8 (equations (32), (33), (34), (35), (36), (37), (38), and (39)) for each $s \in [1, S]$ e $n \in [1,N_s]$ and equations (40), (41), (42), (43), (44), (45), and (46).

Therefore, this section presents $1.S.N_s$ degrees of freedom that are fulfilled by binary variable *m* as decision variable for $s \in [1, S]$ and $n \in [1,N_s]$.

2.7. Constraints and penalty system

The WHEN synthesis and optimization problem is constrained to thermodynamic laws and industrial operating limitations. In order to ensure that a solution of the MINLP problem is in a feasible region, a penalty system is adopted to penalize the objective function of solutions outside this region. It is linearly proportional to the absolute value of how much a variable violated a constraint. Considering that there are more serious constraints than others, there must be different penalties. For instance, a violation in a thermodynamic law needs to be penalized more severely than violating a heuristically determined value of industrial operation, for example. Therefore, different values are considered for linear and angular coefficients of light (p_{lin}^{light} and p_{ang}^{light}) and severe (p_{lin}^{severe} and p_{ang}^{severe}) penalties.

One constraint is that the temperature (*TH* and *TC*), in each stage *k* of HI that presents at least one heat exchanger, must be between an upper (T_{up}) and lower (T_{low}) bounds (industrial limits). The violation of this constraints results in a light penalty. Beyond a lower bound, a hot stream must not reach below absolute zero temperatures. As this constraint is more serious than the former one, a severe penalty is resulted from this violation. These constraints are mathematically represented in inequations (47), (48), and (49). It is worth noticing that the summation of *y* over all *ss* and *nn* is used to activate the constraint only in stream *s* in the horizontal stage *n* and vertical stage *k* in which there is at least one heat exchanger. If this summation equals zero, then the inequation is true ($0 \leq 0, 0 \geq 0$) and no violation is considered. On the other hand, if the summation is greater than zero, it becomes a multiplication factor on both sides of the inequation, and it can be removed by dividing the whole inequation by this value and changing the constraint in its more intuitive format.

$$TH(s,n,k).\sum_{ss=1}^{S}\sum_{nn=1}^{N_s} y(s,n,ss,nn,k) \geq T_{low}.\sum_{ss=1}^{S}\sum_{nn=1}^{N_s} y(s,n,ss,nn,k) \tag{47}$$

$$TC(s,n,k).\sum_{ss=1}^{S}\sum_{nn=1}^{N_s} y(s,n,ss,nn,k) \leq T_{up}.\sum_{ss=1}^{S}\sum_{nn=1}^{N_s} y(s,n,ss,nn,k) \tag{48}$$

$$TH(s,n,k).\sum_{ss=1}^{S}\sum_{nn=1}^{N_s} y(s,n,ss,nn,k) \geq 0 \tag{49}$$

Similarly, in WEN section there is a constraint regarding upper and lower bounds of T_{n+1}, given by inequation (50). This temperature must also be positive as represented in inequation (51). It is also considered a constraint in the inlet temperature to pressure manipulators (*TI*) between and upper (TI_{up}) and lower (TI_{low}) bounds, as stated in inequation (52). This kind of constraint may appear due to compressor/turbine limitations. A positivity constraint in *TI* is not required because its value comes from *TH* and *TC* that would have already been penalized.

$$p(s,n).T_{up} \geq p(s,n).T(s,n+1) \geq p(s,n).T_{low} \tag{50}$$

$$p(s,n).T(s,n+1) \geq 0 \tag{51}$$

$$p(s,n).TI_{up} \geq p(s,n).TI(s,n) \geq p(s,n).TI_{low} \tag{52}$$

In the HEN cost calculation section, there are some constraints regarding the temperature difference between hot and cold streams, and hot or cold utilities and process stream in the terminal of a heat exchanger. These differences need to be greater than zero accordingly with the Second Law of Thermodynamics that is severely penalized in case of violation. Beyond positive, it also needs to be greater than a minimum approach temperature (ΔT_{min}) to secure industrial operation and its perturbations that is lightly penalized in the case of violation.

$$Q(s,n,ss,nn,k).\left(TH(s,n,k) - TC(ss,nn,k)\right) \geq Q(s,n,ss,nn,k).\Delta T_{\min} \tag{53}$$

$$Q(s,n,ss,nn,k).\left(TH(s,n,k) - TC(ss,nn,k)\right) \geq 0 \tag{54}$$

$$Q_s(s,n).\min\left(TS_{out} - T_{ut}(s,n), TS_{in} - TI(s,n)\right) \geq Q_s(s,n).\Delta T_{\min} \tag{55}$$

$$Q_s(s,n).\min\left(TS_{out} - T_{ut}(s,n), TS_{in} - TI(s,n)\right) \geq 0 \tag{56}$$

$$Q_w(s,n).\min\left(T_{ut}(s,n) - TW_{out}, TI(s,n) - TW_{in}\right) \geq Q_w(s,n).\Delta T_{\min} \tag{57}$$

$$Q_w(s,n).\min\left(T_{ut}(s,n) - TW_{out}, TI(s,n) - TW_{in}\right) \geq 0 \tag{58}$$

2.8. Objective function

The WHEN objective function is the TAC, which is given by:

$$TAC = CostHEN + CostWEN + pen \tag{59}$$

Finally, the optimization problem can be defined as the minimization of TAC (equation (59)) subjected to equations and inequalities (1) - (58).

$$\begin{aligned} \min_{d, y_{ut}, y, p, m, T_{adj}, Q, P} &: TAC = CostHEN + CostWEN + pen \\ & s.t. \left\{ \text{equations and inequations (1) - (58)} \right. \end{aligned} \tag{60}$$

2.9. Change of variables

One strategy proposed in the present approach, illustrated in Figure 3, is to reduce the search space of the optimization problem by a change of variables, (which was already included in the model) by replacing variables and adding extra equations based on logic relationship between the model variables in order to reduce the number of degrees of freedom and the number of decision variables.

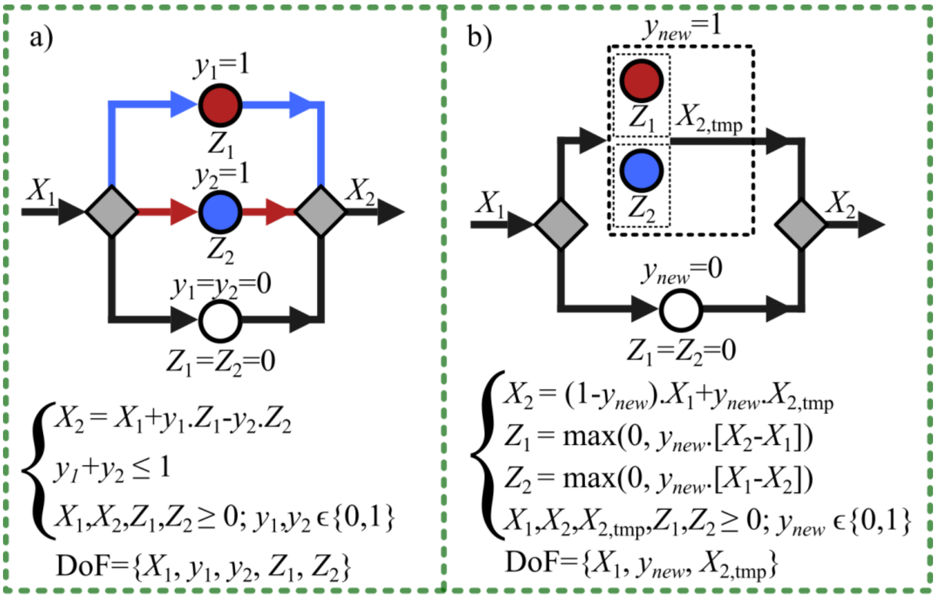

Figure 3. Generic exemple of modeling a) without and b) with change of variables.

The example illustrated in Figure 3 a) is a common situation in superstructure-based mathematical modeling. It is a problem in which there is a continuous variable X in two states: 1 and 2. Let X_2 be equal X_1 with an additional value of $y_1.Z_1$ minus $y_2.Z_2$, such that y_1 and y_2 are binary variables that state the existence of Z_1 and Z_2, respectively. Also, Z_1 and Z_2 cannot coexist accordingly with the constraint of $y_1+y_2 \leq 1$. In this context, the following logic is observed:

- The rate at which $X_2 - X_1$ change with respect to the change of Z_1 is always positive;
- The rate at which $X_2 - X_1$ change with respect to the change of Z_2 is always negative;
- Necessarily, either Z_1 or Z_2 is null.

From these logical relationships, it can be inferred that:

- In case X_2 is greater than X_1, Z_1 is greater than 0 (y_1 = 1), and Z_2 is null (y_2 = 0);
- In case X_1 is greater than X_2, Z_2 is greater than 0 (y_2 = 1), and Z_1 is null (y_1 = 0);
- In case X_2 equals X_1, both Z_1 and Z_2 are null (y_1 and y_2 are null);

Given this context, the change of variables proposed is substituting the binary variables y_1 and y_2 for the binary variable y_{new} and continuous variable $X_{2,\text{tmp}}$, as presented in Figure 3 b). The variable y_{new} determines either the exclusive existence of y_1 or y_2 in case y_{new} equals 1, or neither of them in case y_{new} equals 0. The variable $X_{2,\text{tmp}}$ represents the value of X_2 in case y_{new} equals 1. Regarding the inferences, it is mathematically equated using max-functions. In Z_1, the max-function assumes the value of 0 in case X_1 is greater than X_2, whereas, in Z_2, the max-function assumes value of 0 in case X_2 is greater than X_1. Lastly, in both Z_1 and Z_2, the max-function assumes value of 0 in case X_2 equals X_1. Thus, the max-functions guarantee the exclusive existence of Z_1 and Z_2.

Finally, in this generic example, before changing variables there were 6 variables and 1 equation or 5 degrees of freedom: X_1, y_1, y_2, Z_1 and Z_2. After changing variables, the number of variables stayed at 6, but the number of equations increased to 3 that results in 3 degrees of freedom: X_1, y_{new} and $X_{2,\mathrm{tmp}}$. Therefore, the strategy of changing variables reduced in 40 % the problem without losing the superstructure generality.

In the proposed model, two changes of variables were used. The first one is regarding temperature adjustment section, in which the changed variables y_{ut} and T_{adj} fully establish the section using max-functions in equations (8), (9), and (10), as illustrated in Figure 4. The similar to this section without change of variables would use 4 decision variables: the existence of heaters (y_s) and coolers (y_w), and the heat load of heaters (Q_s) and coolers (Q_w). Therefore, there is a reduction in 50 % in the number of decision variables.

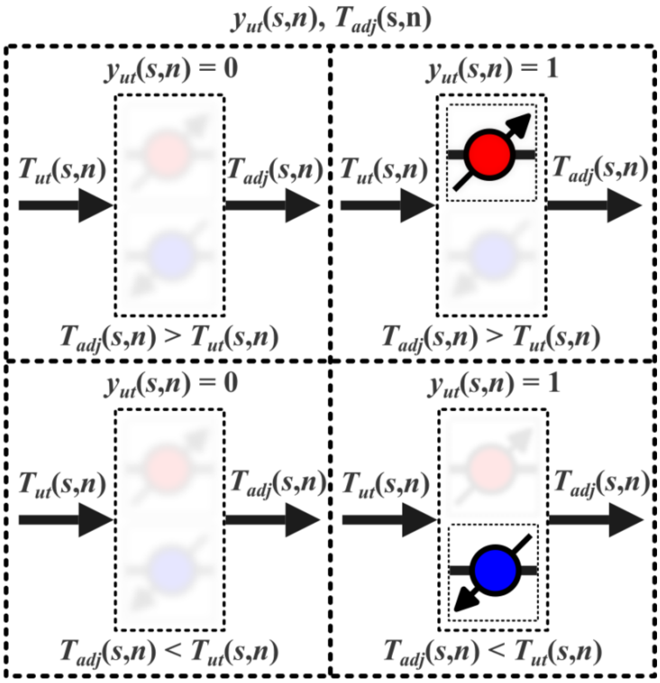

Figure 4. Changed variables y_{ut} and T_{adj} in the temperature adjustment section.

The same strategy is adopted in WEN and WEN cost sections, in which the changed variables p, m, and P_{n+1} fully establish the sections using max-functions in equations (13), (14), (32) , (33), (34), (35), (36), (37), (38), and (39), as illustrated in Figure 5. The similar of these sections without change of variables would use 5 decision variables: 4 to establish the existence of SS compressors (c), SS turbines (e), electric compressors (uc), and electric turbines (ue), and 1 to determine the energy duty of the pressure manipulator (W) or the pressure after this equipment (P_{n+1}). Therefore, there is a reduction in 40 % in the number of decision variables in these sections.

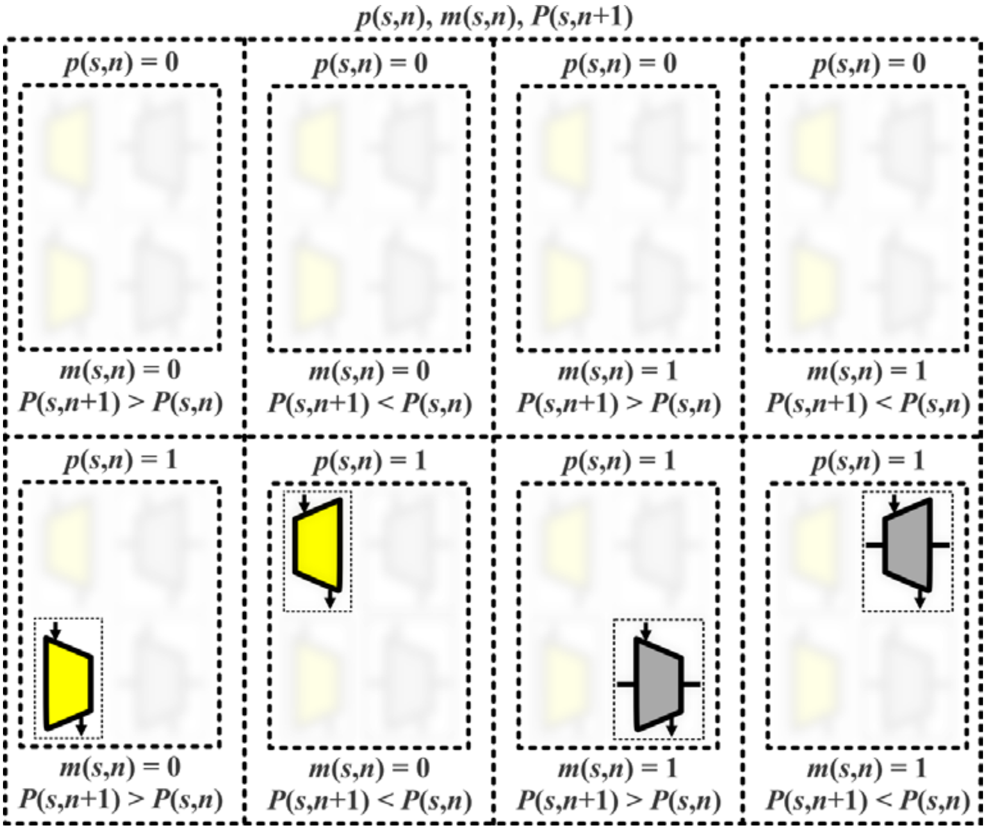

Figure 5. Changed variables p, m, and P_{n+1} in WEN and WEN cost sections.

3. Solution approach

Now it is presented the solution approach to the MINLP model, with the third-level optimization to reduce the number of decision variables from the original MINLP problem and the two-level meta-heuristic optimization approach, which includes SA for the combinatorial level and Particle Swarm Optimization (PSO) for the continuous level.

3.1. Model sequential implementation & third-level optimization

The mathematical model is implemented sequentially and is illustrated in Figure 6. It is given a set of decision variables configuration (d, y, y_{ut}, p, m, Q, T_{adj}, P), which determine one and only one WHEN. As can be noted in Figure 6, decision variable m is not included in the input configuration. The reason for that is because m is determined internally using third-level optimization. This strategy was applicable in the present approach since there is a subproblem in the MINLP such that its decision variables do not interact with equations other than the objective function. In other words, the value of WEN cost calculation section decision variable (m) only interacts with the objective function. Given that, third-level optimization can be defined as a strategy that reduces decision variables from an MINLP by determining them separately in an isolated optimization problem. Therefore, the $1.S.N_s$ degrees of freedom of the decision variable m are reduced from the original MINLP optimization problem, *i.e*. there is a reduction in the optimization search space.

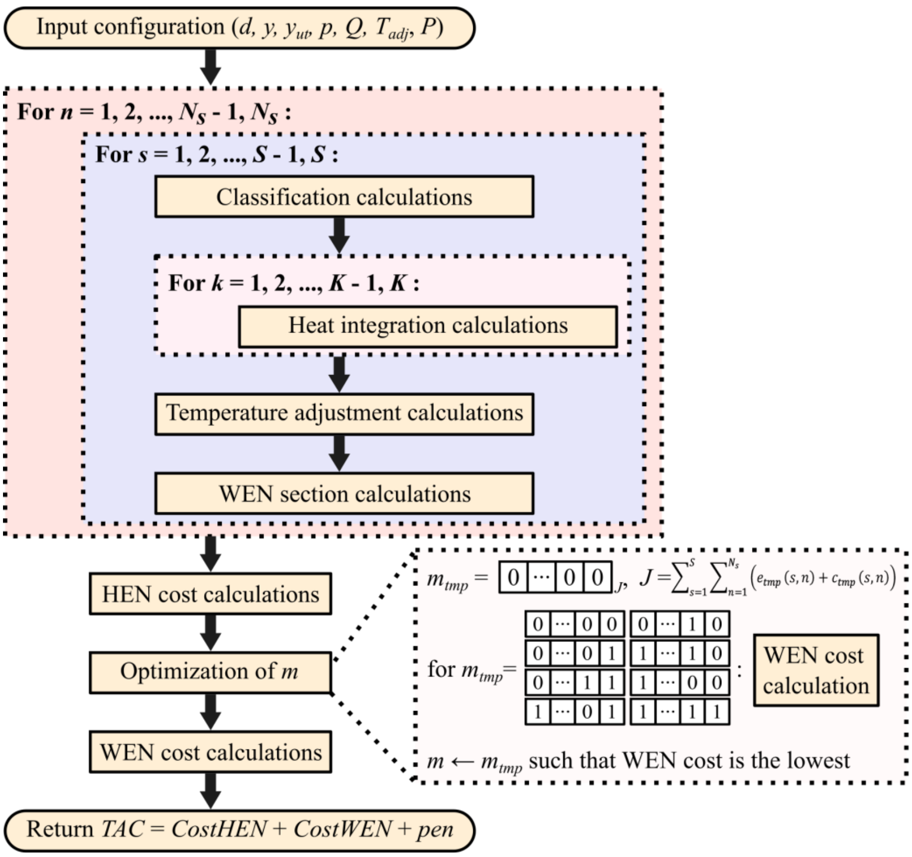

Figure 6. Mathematical model sequential implementation and third-level optimization.

Back to the algorithm, it starts receiving values of reduced input decision variables (d, y, y_{ut}, p, Q, T_{adj}, P). Then, the four-section calculations are performed inside their for-loops $n \in [1, N_s]$, $s \in [1, S]$, and $k \in [1, K]$. After ending the more external loop the calculations of HEN cost section are performed. Later, the values of variable m are determined using third-level optimization. As illustrated in Figure 6, the method applied for that is an exhaustive search, which is testing out every binary configuration of $m(s, n)$ for each (s, n) such that either $c_{tmp}(s, n)$ or $e_{tmp}(s, n)$ equals 1. In other words, this testing is performed for every (s, n) such that there exists a pressure manipulator. The first step of this exhaustive search is to declare an auxiliary binary vector $m_{tmp}(j)$ such that its size (J) equals the sum of $e_{tmp}(s,n)$ e $c_{tmp}(s,n)$ for $s \in [1, S]$ and $n \in [1, N_s]$. The meaning of this new variable m_{tmp} is the same as original m, which is determining whether the pressure manipulator is coupled (equals 1) or not (equals 0) to the work integration shaft. Next step is to open a loop of j so that the WEN cost is calculated for all 2^J binary permutations of m_{tmp}. Then, m receives the binary permutation of m_{tmp} for which the WEN cost was the lowest. Once this combinatorial problem is small (2^J possibilities), this exhaustive search optimization is not time prohibitive computationally and guarantees global optimality of pressure manipulation coupling configuration. Finally, with optimized m, the WEN cost is calculated as well as the objective function TAC.

3.2. Two-level optimization

In order to solve the remaining decision-variable-reduced MINLP, a two-level meta-heuristic optimization method is proposed. On an external level, binary decision variables (d, y, y_{ut}, and p) are dealt with a SA formulation to optimize the WHEN topology. On an internal level, continuous decision variables (Q, T_{adj}, and P) are manipulated accordingly with a Particle Swarm Optimization (PSO) to optimize the loads of WHEN units. Figure 7 presents a simplified algorithm for this optimization approach.

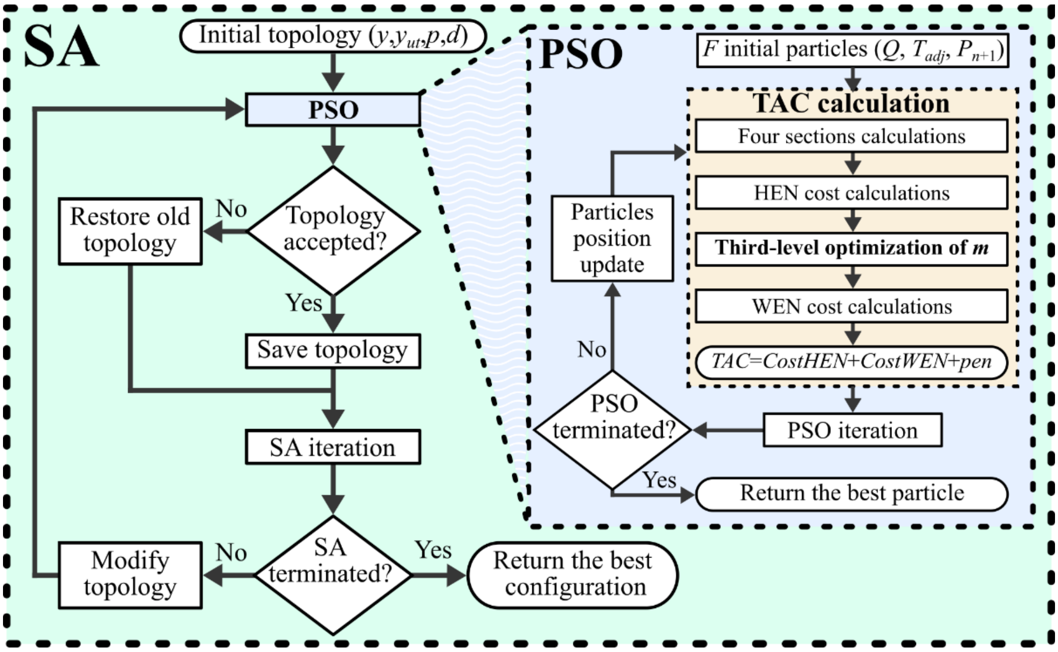

Figure 7. Two-level meta-heuristic optimization algorithm flowsheet.

In the first step of this algorithm, the initial WHEN topology is set to be the trivial one. Therefore, a topology in which compression and expansion (p) take place in the last stage of WEN ($N_s - 1$), heating and cooling are done with utilities ($y_{ut} = 0$ and $y_{ut} = 1$) in the last stage of temperature adjustment (N_s), and streams thermal identity (d) are hot for the ones that need to cool down or compress, and cold for the ones that need to heat up or expand.

Given a topology, F particles of PSO are initialized. Each particle stores a Q, a T_{adj}, and a P matrix that has its values randomly generated between a lower and an upper bound, accordingly with the topology. Mathematically:

$$y(s,n,ss,nn,k).Q_{up} \geq Q(s,n,ss,nn,k) \geq y(s,n,ss,nn,k).Q_{low} \quad (61)$$

$$y_{ut}(s,n).T_{up} \geq T_{adj}(s,n) \geq y_{ut}(s,n).T_{low} \quad (62)$$

$$p(s,n).\left(P_{up}-P(s,n)\right)+P(s,n)\geq P(s,n+1)\geq p(s,n).\left(P_{low}-P(s,n)\right)+P(s,n) \tag{63}$$

In the next step, TAC calculations are performed for each particle in the swarm accordingly Figure 6. After TAC calculations, the PSO is iterated, and the particles positions are updated if PSO termination criterion is not reached ($k_{PSO}<K_{PSO}$). The following calculations are performed to update Q, T_{adj}, and P values of each particle (i):

$$v_{Q,k_{PSO}+1}^{(i)}=y\left[\omega_{k_{PSO}}.v_{Q,k_{PSO}}^{(i)}+c_1.r_1.\left(Q_{pbest,k_{PSO}}^{(i)}-Q_{k_{PSO}}^{(i)}\right)+c_2.r_2.\left(Q_{gbest,k_{PSO}}-Q_{k_{PSO}}^{(i)}\right)\right] \tag{64}$$

$$v_{T_{adj},k_{PSO}+1}^{(i)}=y_{ut}\left[\omega_{k_{PSO}}.v_{T_{adj},k_{PSO}}^{(i)}+c_1.r_1.\left(T_{adj,pbest,k_{PSO}}^{(i)}-T_{adj,k_{PSO}}^{(i)}\right)+c_2.r_2.\left(T_{adj,gbest,k_{PSO}}-T_{adj,k_{PSO}}^{(i)}\right)\right] \tag{65}$$

$$v_{P,k_{PSO}+1}^{(i)}=p_{n-1}\left[\omega_{k_{PSO}}.v_{P,k_{PSO}}^{(i)}+c_1.r_1.\left(P_{pbest,k_{PSO}}^{(i)}-P_{k_{PSO}}^{(i)}\right)+c_2.r_2.\left(P_{gbest,k_{PSO}}-P_{k_{PSO}}^{(i)}\right)\right] \tag{66}$$

$$Q_{k_{PSO}+1}^{(i)}=Q_{k_{PSO}}^{(i)}+v_{Q,k_{PSO}+1}^{(i)} \tag{67}$$

$$T_{adj,k_{PSO}+1}^{(i)}=T_{adj,k_{PSO}}^{(i)}+v_{T_{adj},k_{PSO}+1}^{(i)} \tag{68}$$

$$P_{k_{PSO}+1}^{(i)}=P_{k_{PSO}}^{(i)}+v_{P,k_{PSO}+1}^{(i)} \tag{69}$$

The parameters $\omega_{k_{PSO}}$, c_1 e c_2 refer to the weight of inertia (proportional to previous step), of the individual i particle best position, and of the whole swarm best position. The variables $v_{Q,k_{PSO}+1}^{(i)}$, $v_{T_{adj},k_{PSO}+1}^{(i)}$, and $v_{P,k_{PSO}+1}^{(i)}$ are the steps that variables Q, T_{adj} and P of particle i take in iteration k_{PSO}. The subscript *pbest* stands for the best value of a particle i, whereas *gbest* refers to the best value of the whole swarm. The parameters r_1 and r_2 are randomly generated numbers between 0 and 1 that makes it more aleatory for the particle to go towards the individual best or swarm best directions.

Accordingly with Shi and Eberhart (1998) [22], a linear decay is considered as inertia damping, *i.e.* a velocity progressive reduction as the particles reach a final optimum. Being K_{PSO} the total number of PSO iterations, ω_{max} the initial inertia weight, and ω_{min} the final inertia weight, this inertia damping is calculated as follows:

$$\omega_{k_{PSO}+1}=\omega_{\max}-k_{PSO}.\frac{\omega_{\max}-\omega_{\min}}{K_{PSO}} \tag{70}$$

When the termination criterion of PSO is reached ($k_{PSO}=K_{PSO}$), then PSO is finished and the best particle (lowest TAC) is selected to continue the SA. This particle’s topology may or may not be accepted respecting SA criterion of acceptance that follows:

$$PoA = e^{\frac{-\Delta TAC}{T_{SA}}} \tag{71}$$

The variable PoA is the probability of acceptance of a new WHEN topology accordingly with SA, *i.e*. calculated like Boltzmann probability. ΔTAC is the difference between the TAC of the present configuration and the TAC of the old topology, and T_{SA} is the annealing temperature, which starts at $T_{SA,max}$. If the new topology is accepted, it is stored as the old topology. If it is not, the present topology receives back the values stored before as the old topology.

Afterwards, the algorithm takes a step of SA, which means incrementing one to the value of k_{SA}. When k_{SA} reaches K_{SA}, it returns to 0 and T_{SA} decays by a factor of α which is a parameter from 0 to 1. Then, if T_{SA} is higher than the parameter $T_{SA,min}$, the termination criterion of SA is not reached and the algorithm makes a modification in the topology to return to the PSO block. This modification is adding or removing randomly a heat exchanger (y), a heater/cooler (y_{ut}), a pressure manipulator (p), and/or changing a stream thermal identity (d). On the other hand, if T_{SA} is lower than $T_{SA,min}$, the SA termination criterion is reached, and the algorithm returns the best configuration stored.

4. Case studies

The presented WHEN synthesis and optimization approach was implemented in C++ language in Dev-C++ 5.11 in a 2.20 GHz Intel® Core™ i5-5200U computer with 8.00 GB of RAM and applied to three case studies of SWHI.

4.1. Case Study 1

This case is a 2-stream problem used by Pavão *et al*. (2019a) [17] and proposed by Onishi *et al*. (2014b) [12]. Table 1 presents streams and utilities data and Table 2 economic capital cost parameters.

Table 1. Process streams and utilities data for case study 1

Stream	T_{in} [K]	T_{out} [K]	CP [kW.K^{-1}]	h [kW.m^{-2}.K^{-1}]	P_{in} [MPa]	P_{out} [MPa]
$s1$	650	370	3	0.1	0.1	0.5
$s2$	410	650	2	0.1	0.5	0.1
HU	680	680	–	1.0	–	–
CU	300	300	–	1.0	–	–

Compression/expansion parameters: κ = 1.352; η_c = 1; η_e = 1.

Problem constraints: TI_{low} = 350 K; TI_{up} =750 K; ΔT_{min} = 1 K.

Operating cost parameters ($\$.kWy^{-1}$): C_{CU} = 100; C_{HU} = 337; CE = 455.04; PE = 364.03.

Table 2. Capital cost parameters for case study 1.

Equipment	*a*	*b*	*c*
Heat exchanger	106,017.23	618.68	0.1689
SS & electric compressors	0	47840.41	0.62
SS & electric turbines	0	2420.32	0.81
Motor/Generator	0	988.49	0.62

Optimization model parameters:

- Superstructure: K = 2; N_s = 3.
- SA: K_{SA} = 15; $T_{SA,max}$ = 10,000 $\$.y^{-1}$; $T_{SA,min}$ = 5 $\$.y^{-1}$; α = 0.8.
- PSO: F = 50; K_{PSO} = 200; c_1 = 1; c_2 = 1; ω_{max} = 0.75; ω_{min} = 0.5.
- Penalty system: p_{lin}^{light} = 100,000; p_{ang}^{light} = 10,000; p_{lin}^{severe} = 2,000,000; p_{ang}^{severe} = 20,000.

Figure 8 presents the WHEN achieved with the present approach. The TAC is $ 773,805.01/year, which is 7.2 % cheaper than the best result reported so far by Pavão *et al*. (2019a) [17], $ 834,204.00/year. Table 3 presents capital and operating costs of the WHEN devices. The computational time was around 5 minutes.

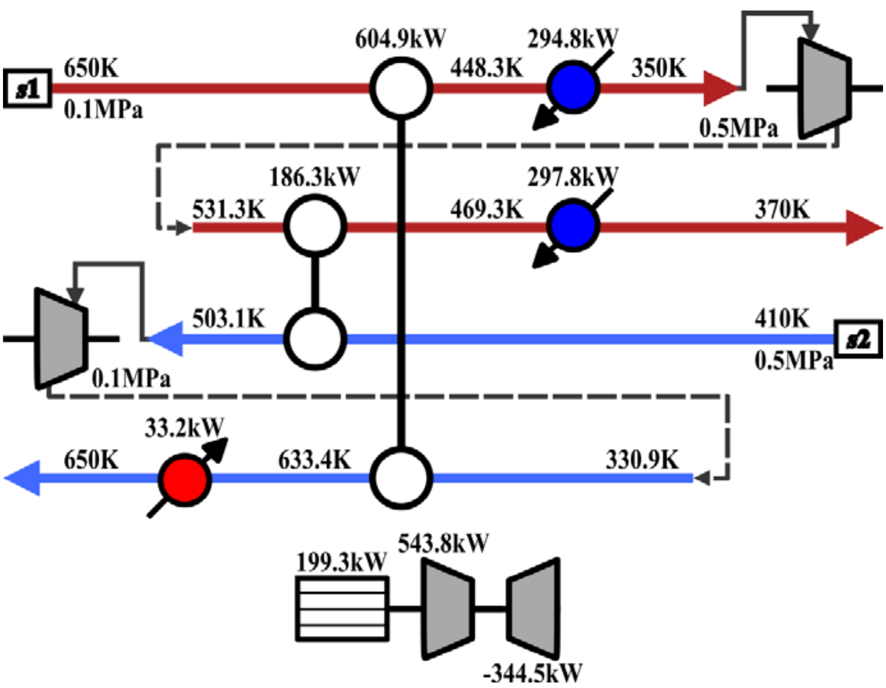

Figure 8. WHEN achieved for case study 1.

Table 3. Case study 1 capital and operating costs

Device	Capital cost ($/year)	Operating cost ($/year)
HE(s1,n1,s2,n2,k0)	49,629.78	-
HE(s1,n2,s2,n1,k0)	30,319.43	-
CU(s1,n1)	23,538.96	29,505.90
CU(s1,n2)	22,691.50	29,740.00
HU(s2,n2)	20,279.65	11,204.07
SSC(s1,n1)	418,705.65	-
SST(s2,n2)	42,800.01	-
HM	4,740.46	90,649.60
TOTAL	612,705.44	161,099.57

Figure 9 presents the WHEN obtained by Pavão *et al*. (2019a) [17].

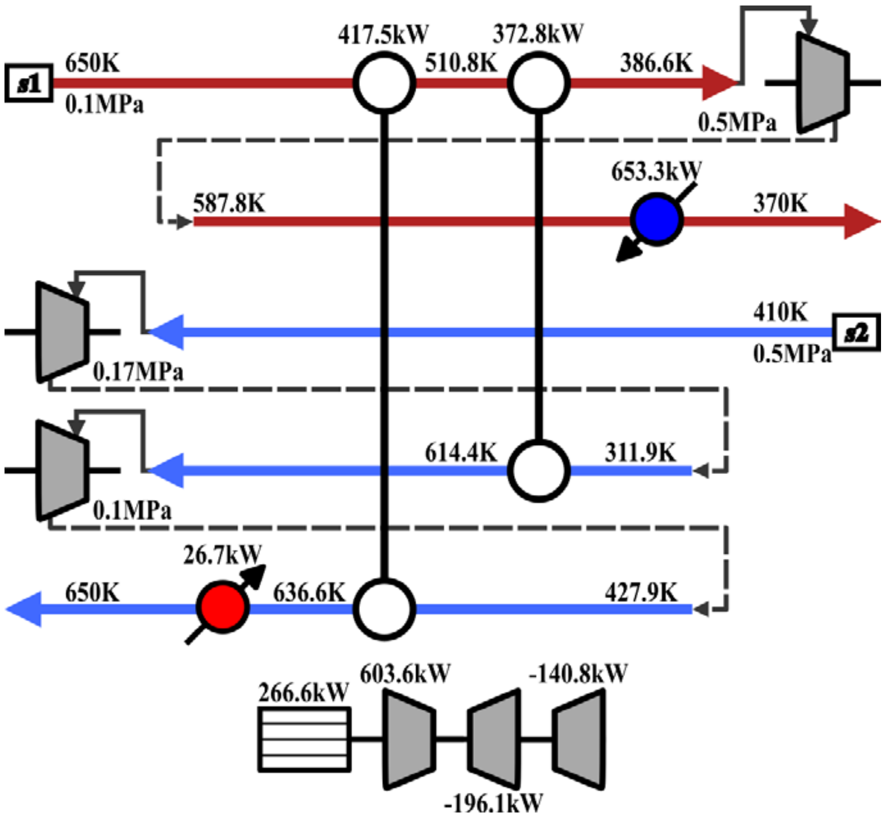

Figure 9. Pavão *et al*. (2019a) [17] WHEN for case study 1.

It can be noted that the compression inlet temperature of *s*1 using the present approach is 350 K, which is lower than 386.6 K, the value used by Pavão *et al*. (2019a) [17]. This difference implicates in energy savings in compression, from 603.6 to 543.8 kW. Also, as less energy is added to the stream in the compression, less cold utility is required to adjust its final temperature. In addition, the present

WHEN shows to be economically more interesting to heat up stream *s*2 before expansion rather than performing a two-stage expansion with heating in between. This becomes clear when comparing the difference in the work produced, from 336.9 to 344.5 kW and the capital costs decreased from $ 55,298.09/year to $ 42,800.10/year. Table 4 presents a simplified comparison.

Table 4: WHEN comparison overview of case study 1.

	Pavão *et al*. (2019a) [17]	Present paper
Total annualized cost ($.year^{-1})	834,3204.00	773,805.01
Heat recovered (kW)	790.3	791.2
Work recovered (kW)	336.9	344.5
Hot utility consumed (kW)	26.7	33.2
Cold utility consumed (kW)	653.3	592.6
Electricity consumed (kW)	266.6	199.3
Electricity produced (kW)	0	0
Number of heat transfer devices	4	5
Number of pressure manipulators	3	2

From this comparison overview, it can be concluded that both WHENs presented similar heat recovered, work recovered, hot utility consumed, number of heat transfer devices, and number of pressure manipulators. On the other hand, cold utility and electricity consumption was diminished considerably in the present WHEN.

4.2. Case Study 2

Case study 2 was used by Huang and Karimi (2016) [14] and first proposed by Onishi *et al*. (2014a) [10]. It is a 5-stream SWHI problem, whose process streams and utilities are presented in Table 5 and economic capital cost parameters are presented in Table 6.

Table 5. Process streams and utilities data for case study 2

Stream	T_{in} [K]	T_{out} [K]	CP [kW.K^{-1}]	h [kW.m^{-2}.K^{-1}]	P_{in} [MPa]	P_{out} [MPa]
*s*1	350	350	36.81	0.1	0.9	0.1
*s*2	350	350	14.73	0.1	0.85	0.15
s3	400	400	21.48	0.1	0.7	0.2
s4	390	390	25.78	0.1	0.1	0.7
s5	420	420	36.81	0.1	0.1	0.9

HU	680	680	–	1.0	–	–
CU	300	300	–	1.0	–	–

Compression/expansion parameters: κ = 1.4; η_c = 0.7; η_e = 0.7.

Problem constraints: T_{low} = TI_{low} = 288 K; T_{up} = TI_{up} =600 K; ΔT_{min} = 1 K.

Operating cost parameters ($.kWy^{-1}): C_{CU} = 8; C_{HU} = 280; CE = 960; PE = 800.

Table 6: Capital cost parameters for case study 2.

Equipment	*a*	*b*	*c*
Heat exchanger	3,000	30	0
SS & electric compressors	250,000	1000	1
SS & electric turbines	200,000	1000	1
Motor/Generator	50,000	1000	1

Optimization model parameters:

- Superstructure: K = 2; N_s = 3.
- SA: K_{SA} = 50; $T_{SA,max}$ = 100,000 $.y^{-1}; $T_{SA,min}$ = 20,000 $.y^{-1}; α = 0.8.
- PSO: F = 50; K_{PSO} = 300; c_1 = 1; c_2 = 1; ω_{max} = 0.75; ω_{min} = 0.5.
- Penalty system: p_{lin}^{light} = 10^7; p_{ang}^{light} = 3.10^6; p_{lin}^{severe} = 3.10^7; p_{ang}^{severe} = 6.10^6.

Huang and Karimi (2016) [14] used a different WEN cost function. Instead of using work load (*WC*, *WUC*, *WE* e *WUE*) in equation (46), they used heat capacity flow rates (*CP*). For coherence and comparison sake, in this case study *CP* is used in this equation.

Figure 10 presents the WHEN achieved with the present approach. TAC is $ 10,004,220.70/year, which is 1.8 % cheaper than $ 10,186,680.00/year, the result reported by Huang and Karimi (2016) [14]. Table 7 presents capital and operating costs. The elapsed time was around 85 minutes.

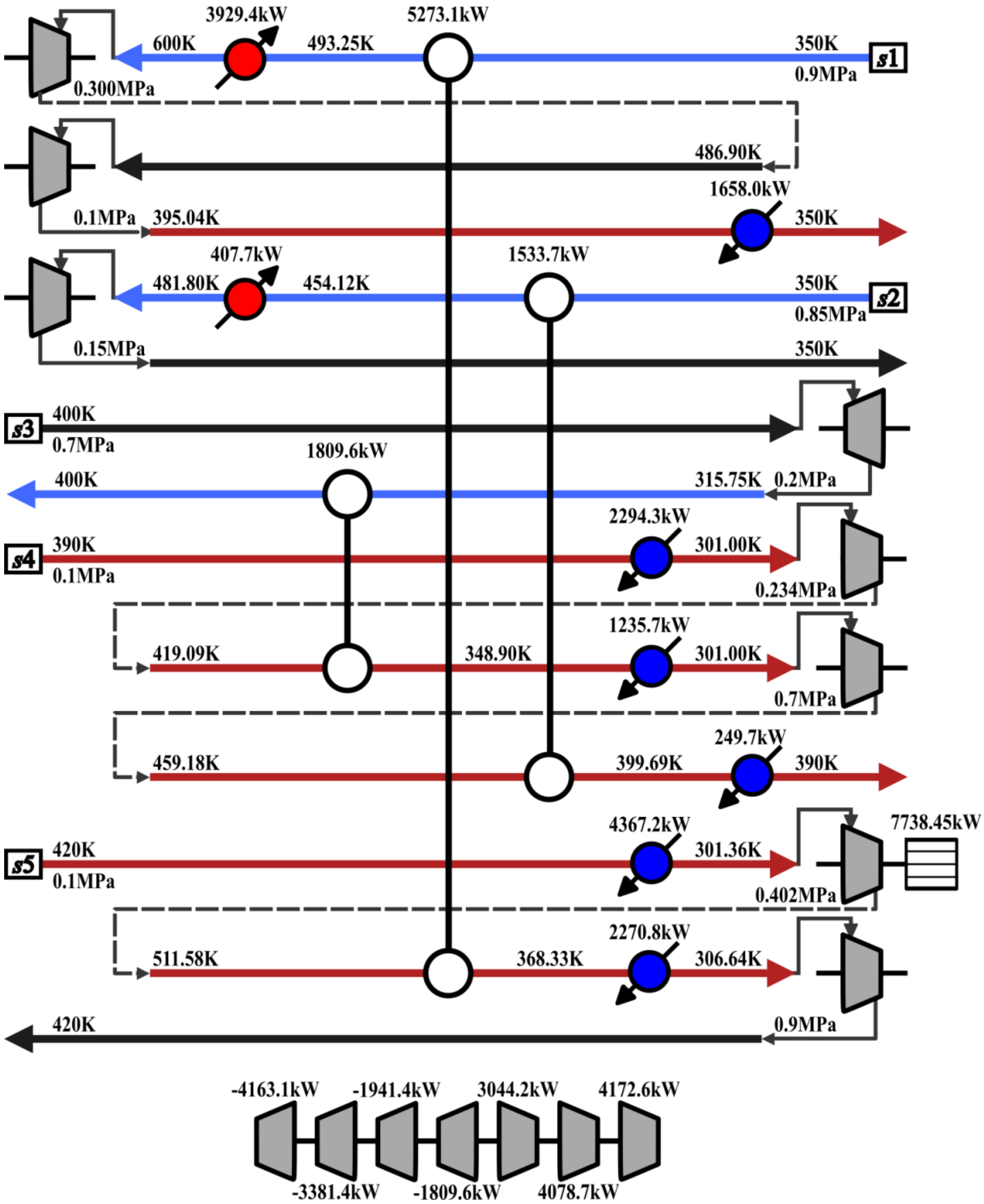

Figure 10. Final WHEN from present methodology for case study 2.

Table 7. Capital and operating cost of each unit in WHEN of case study 2.

Equipment	Capital cost ($/year)	Operating cost ($/year)
HE(s1,n1,s5,n2,k0)	176,070.00	-
HE(s2,n1,s4,n3,k0)	50,103.60	-
HE(s3,n2,s4,n2,k0)	45,626.50	-
CU(s1,n3)	10,802.10	13,263.76
CU(s4,n1)	41,236.40	18,358.40
CU(s4,n2)	36,387.30	9,887.72
CU(s4,n3)	3,869.81	1,998.17

CU(s5,n1)	57,710.90	34,946.56
CU(s5,n2)	31,301.00	18,150.64
HU(s1,n1)	13,297.6	1,100,220.80
HU(s2,n1)	3,635.44	114,161.60
SST(s1,n1)	76,810.00	-
SST(s1,n2)	76,810.00	-
SST(s2,n1)	54,730.00	-
SST(s3,n1)	61,480.00	-
SSC(s4,n1)	75,780.00	-
SSC(s4,n2)	75,780.00	-
C(s5,n1)	286,810.00	7,428,182.40
SSC(s5,n2)	86,810.00	-
TOTAL	1,265,050.65	8,739,170.05

Figure 11 presents a comparison with the results of Huang and Karimi (2016) [14].

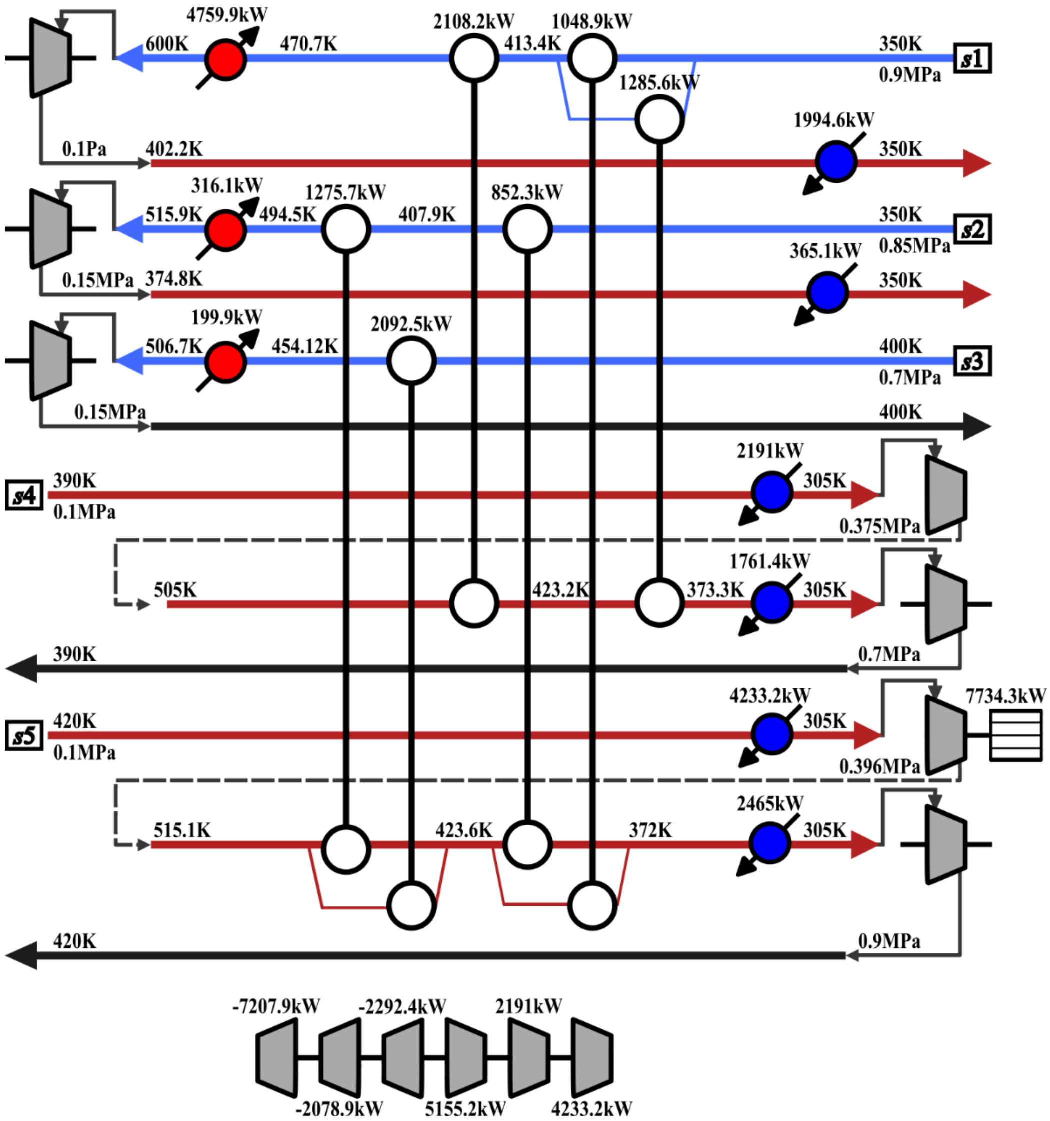

Figure 11. Final WHEN from Huang and Karimi (2016) [14] for case study 2.

The major difference between these networks is stream *s*1, which is expanded in two stages in the proposed network instead of in only one as Huang and Karimi (2016) [14] presented. The two-stage expansion even without heat exchanging in between showed to be a better path for increasing work production for this κ and η_e. The increased work production implicates in extracting more energy from this stream so that cold utility was saved afterwards. Another difference is regarding heat integration, which in the present network was performed in three heat exchangers in comparison with six from those authors to recover almost the same amount of energy.

It is interesting to notice that both WHENs presented thermal identity change of process streams. Beyond changing thermal identity, the use of hot and cold utilities in the same stream (*s*1) would be difficult to determine intuitively or based on heuristic process synthesis. Therefore, it expresses the potential of using superstructure-based mathematical programming for complex decision-making tasks like optimum WHEN synthesis. It is also interesting that final WHEN showed heat recovery between multi-stage compression (streams *s*4 and *s*5), *i.e.* recovering part of the energy added by compression. That justifies the importance of doing work and heat integration simultaneously. A simplified comparison overview is presented in Table 8.

Table 8. WHEN comparison overview of case study 2.

	Huang and Karimi (2016) [14]	Present paper
Total annualized cost ($\$.year^{-1}$)	10,186,680.00	10,004,220.70
Heat recovered (kW)	8,663.2	8,616.4
Work recovered (kW)	11,579.2	11,295.5
Hot utility consumed (kW)	5,275.9	4,337.1
Cold utility consumed (kW)	13,010.3	12,075.7
Electricity consumed (kW)	7,734.3	7,738.4
Electricity produced (kW)	0	0
Number of heat transfer devices	15	11
Number of pressure manipulators	7	8

From this comparison overview, it can be concluded that these WHENs have similar heat and work recovery, electricity consumption, and number of pressure manipulators. However, significant reductions in the amount of hot and cold utility consumed and in the number of heat transfer devices reinforce the improvement of the WHEN obtained with the proposed approach. In addition, energy savings of almost 1000 kW on both utilities, which represents about 20 % of the total hot utility consumed, may lead to extra benefits like the reduction of the industrial utility system size. Also, diminishing the number of heat transfer devices may be interesting for industries that have limited site area like offshore processes, for example.

4.3. Case Study 3

Case study 3 is based on a real industrial process of CO_2/N_2 membrane separation for carbon capture of exhausting gases. The problem was first presented by Fu and Gundersen (2016a) [7], and used by Pavão *et al*. (2019a) [17]. This is a six-stream problem and Table 9 and Table 10 presents streams and utilities data and economic capital cost parameters. In this case study, there is no hot utility available. To deal with that in the optimization model, a severe penalization is introduced proportional to the value of Q_s if hot utility is used.

Table 9. Process streams and utilities data for case study 3

Stream	T_{in} [K]	T_{out} [K]	CP [kW.K^{-1}]	h [kW.m^{-2}.K^{-1}]	P_{in} [MPa]	P_{out} [MPa]

*s*1	298.15	298.15	37.49	0.1	0.1	0.8
*s*2	298.15	298.15	10.09	0.1	0.1	0.8
s3	650.15	348.15	43.77	0.1	–	–
s4	298.15	298.15	27.40	0.1	0.8	0.1
s5	298.15	298.15	4.40	0.1	0.8	0.1
*s*6	298.15	600.15	34.7	0.1	–	–
CU	288.15	288.15	–	1.0	–	–

Compression/expansion parameters: κ = 1.4; η_c = 0.85; η_e = 0.9.

Problem constraints: ΔT_{min} = 1 K.

Operating cost parameters ($.kWy^{-1}): C_{CU} = 100; C_{HU} = -; CE = 455.04; PE = 364.03.

Table 10: Capital cost parameters for case study 3.

Equipment	*a*	*b*	*c*
Heat exchanger	93,500.12	602.96	0.149
SS & electric compressors	0	51,104.85	0.62
SS & electric turbines	0	2,585.47	0.81
Motor/Generator	0	985.47	0.62

Optimization model parameters:

- Superstructure: K = 2; N_s = 3.
- SA: K_{SA} = 75; $T_{SA,max}$ = 100,000 $.y^{-1}; $T_{SA,min}$ = 5,000 $.y^{-1}; α = 0.8.
- PSO: F = 50; K_{PSO} = 300; c_1 = 1.1; c_2 = 1.1; ω_{max} = 0.75; ω_{min} = 0.5.
- Penalty system: p_{lin}^{light} = 2.10^6; p_{ang}^{light} = 1.10^5; p_{lin}^{severe} = 2.10^7; p_{ang}^{severe} = 2.10^5.

Figure 12 shows the WHEN resulted from the present approach. TAC is $ 8,919,187.84/year, which is 1.0 % cheaper than the result reported by Pavão *et al*. (2019a) [17], $ 9,011,115.00/year. Table 11 presents capital and operating costs. The elapsed time to solve the problem was around 170 minutes.

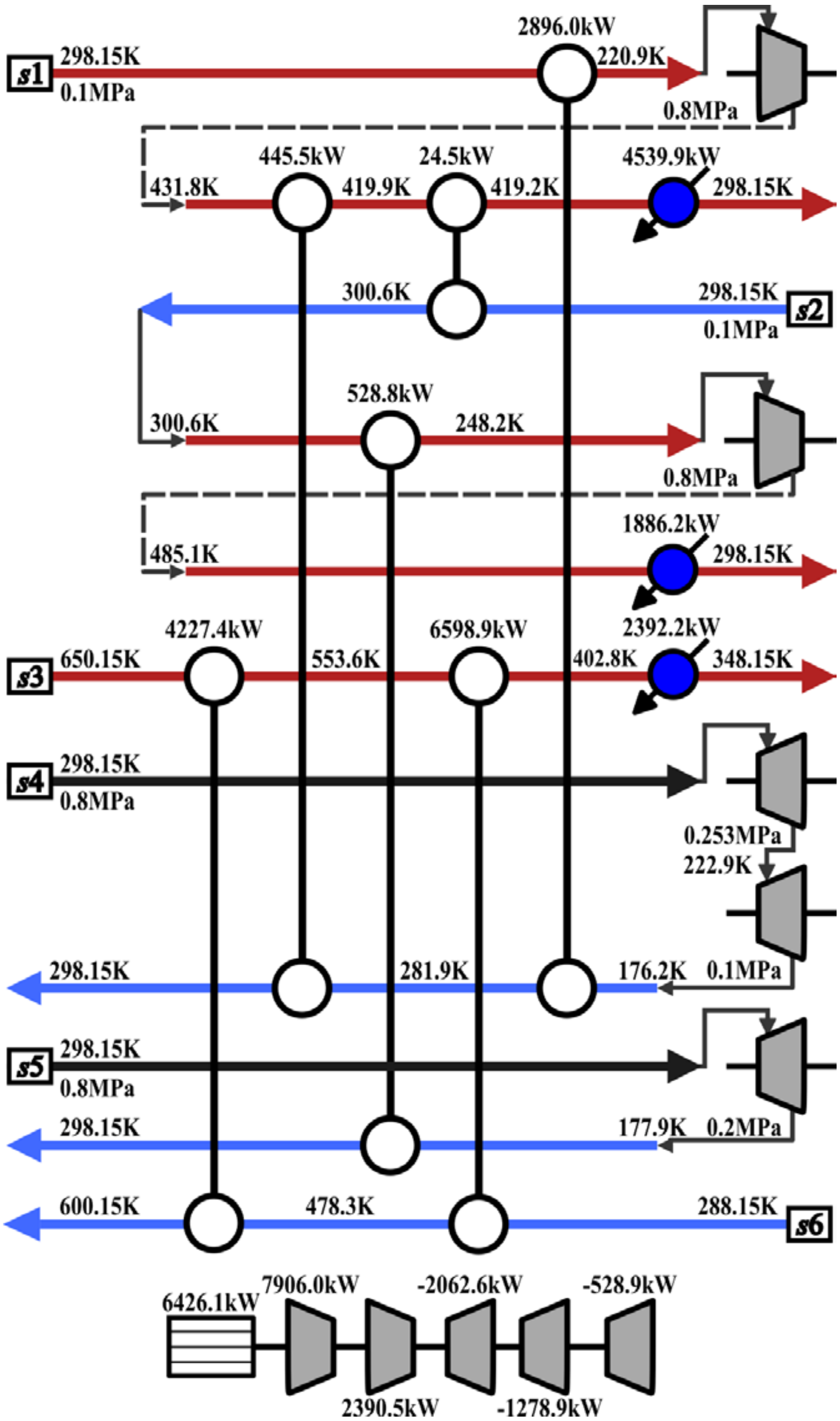

Figure 12. Final WHEN from present methodology for case study 3.

Table 11. Capital and operating costs of each unit in WHEN of case study 3.

Equipment	Capital cost ($/year)	Operating cost ($/year)
HE(s1,n1,s4,n2,k1)	354,095.00	-
HE(s1,n2,s4,n2,k0)	24,066.50	-
HE(s1,n2,s2,n1,k1)	17,273.40	-
HE(s2,n2,s5,n2,k0)	80,983.80	-

HE(s3,n1,s6,n1,k0)	223,263.00	-
HE(s3,n1,s6,n1,k1)	215,640.00	-
CU(s1,n2)	162,212.00	453,989.00
CU(s2,n3)	55,665.80	188,624.00
CU(s3,n1)	53,276.80	239,224.00
SSC(s1,n1)	2,355,110.00	-
SSC(s2,n2)	1,121,870.00	-
SST(s4,n1)	205,027.00	-
SST(s4,n2)	137,916.00	-
SST(s5,n1)	66,114.00	-
HM	40,723.20	2,924,114.34
TOTAL	5,113,236.50	3,805,951.34

Figure 13 presents the WHEN obtained by Pavão *et al*. (2019a) [17].

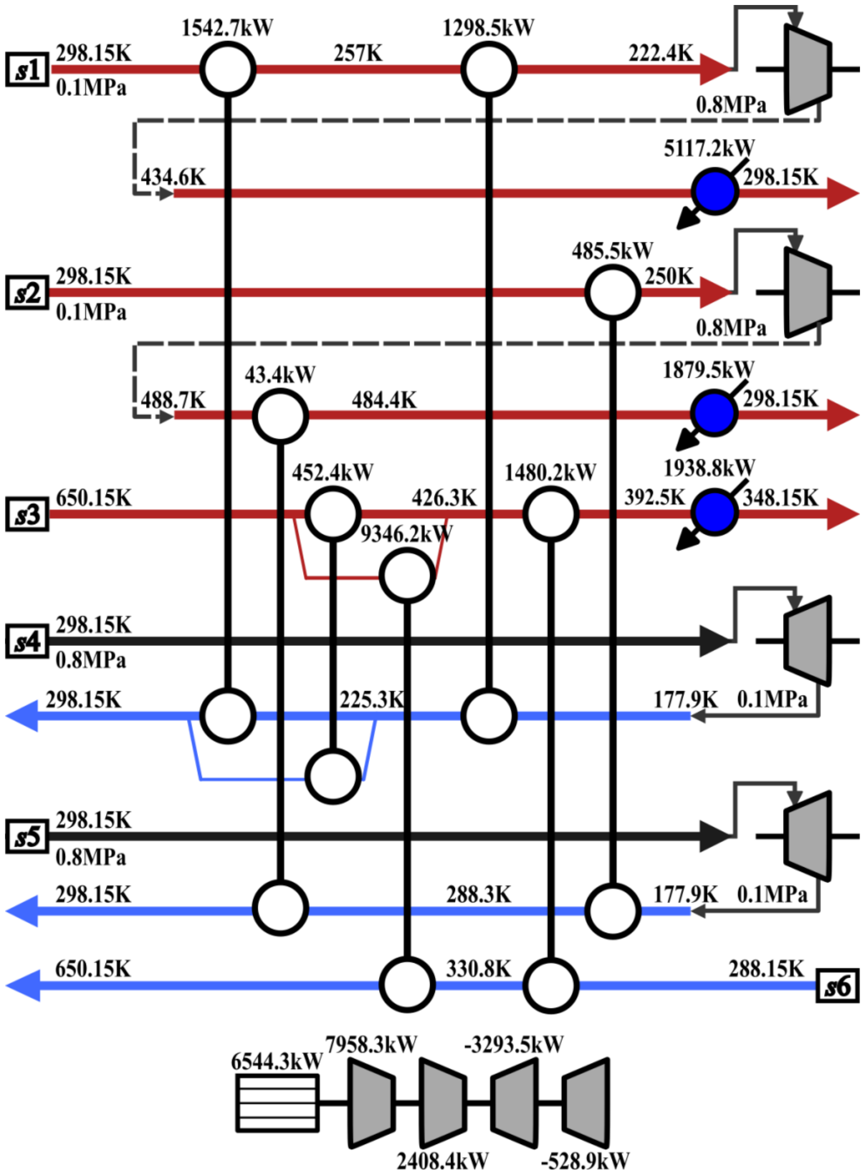

Figure 13. Final WHEN from Pavão *et al*. (2019a) [17] for case study 3.

One difference between these networks is the compressor inlet temperature of streams *s*1 and *s*2. In the present WHEN these temperatures are reduced, which lead to less work needed for compression. It is possible for stream *s*1 due to the two-stage expansion of stream *s*4. This expansion in two stages produces more work than the one-stage proposed by the other authors. Therefore, as more energy is removed from *s*4 during the expansion, more energy is received from *s*1 in the heat exchanger. Regarding stream *s*2, in the first stage this stream is thermally classified as cold and heats up just a little so it could break the minimum approach temperature and fully heat up stream *s*5. Thus, this identity change makes it possible to reduce the *s*2 compression inlet temperature and save electricity. A simplified comparison overview is presented in Table 12.

Table 12. WHEN comparison overview of case study 3.

	Pavão *et al*. (2019a) [17]	Present paper
Total annualized cost ($.year^{-1})	9,011,115.00	8,919,187.84
Heat recovered (kW)	14,648.9	14,721.1
Work recovered (kW)	3,822.4	3,870.4
Hot utility consumed (kW)	-	-
Cold utility consumed (kW)	8,935.5	8,818.3
Electricity consumed (kW)	6,544.3	6,426.1
Electricity produced (kW)	0	0
Number of heat transfer devices	10	9
Number of pressure manipulators	4	5

It can be observed that the present WHEN outperformed the one from Pavão *et al*. (2019a) [17] in every item, but the number of pressure manipulators. This better performance is possible because of non-intuitive aspects of the present WHEN such as the identity change of stream *s*2 and the two-stage expansion without heat exchanging units in between.

5. Conclusions

In the present paper, a new approach for the WHEN synthesis and optimization is proposed. It includes a new superstructure and an MINLP derived model. Also, two strategies of search space reduction are applied: change of variables and third-level optimization. The decision-variable-reduced MINLP model is implemented sequentially and solved with a two-level meta-heuristic optimization approach using SA and PSO. This approach was applied to three case studies and WHENs economic savings were between 1.0 and 7.2 % compared to the best results reported so far in the literature. Regarding the physical problem of SWHI, it is observed that superstructure-based mathematical programming approaches can determine networks that are far from intuitive, but very economically interesting. One example of that is in case study 3, in which stream *s*2 started as cold stream to exchange heat with stream *s*1 and increase its temperature a little, so it could fully heat up stream *s*5. Other examples are considering heat recovery between compression stages of streams *s*4 and *s*5 and the thermal identity change of stream *s*1 in case study 2. For the latter, this stream starts as cold stream to heat up for compression using hot utility, and after compression this stream is cooled with cold utility. Finally, it can be concluded that the proposed methodology is efficient in WHEN synthesis and optimization without severe computational efforts.

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Nomenclature

Superstructure

k	Vertical stage index in heat integration [-]
K	Number of vertical stages of heat integration [-]
n	Horizontal stage index in WHEN superstructure [-]
N_s	Number of horizontal stages [-]
s	Process stream identification index [-]
S	Number of process streams [-]

Simulated Annealing (SA)

k_{SA}	Current SA iteration [-]
K_{SA}	Number of iterations at each SA temperature [-]
PoA	Probability of accepting a new topology in SA [-]
T_{SA}	SA temperature [$.year^{-1}]
$T_{SA,max}$	Initial SA temperature [$.year^{-1}]
$T_{SA,min}$	Final SA temperature [$.year^{-1}]
α	SA temperature decay constant [-]

Particle Swarm Optimization (PSO)

c_1	Cognitive parameter of PSO [-]
c_2	Social parameter of PSO [-]
F	Number of particles in the swarm [-]
i	Index of particles in the swarm [-]
k_{PSO}	Index of the number of iterations of PSO [-]
K_{PSO}	Maximum number of iterations of PSO [-]
ω	Inertia factor [-]
ω_{max}	Initial inertia factor [-]
ω_{min}	Final inertia factor [-]

Problem parameters

a	Fixed capital cost of heat exchangers [$]

a_c	Fixed capital cost of SSCs [$]
a_e	Fixed capital cost of SSTs [$]
a_g	Fixed capital cost of electric generators [$]
a_{hm}	Fixed capital cost of helper motors [$]
a_{uc}	Fixed capital cost of electric compressors [$]
a_{ue}	Fixed capital cost of electric turbines [$]
b	Heat exchangers capital cost coefficient [$.m^{-2}]
b_c	SSCs capital cost coefficient [$.kW^{-cc}]
b_e	SSTs capital cost coefficient [$.kW^{-ce}]
b_g	Electric generators capital cost coefficient [$.kW^{-cg}]
b_{hm}	Helper motors capital cost coefficient [$.kW^{-chm}]
b_{uc}	Electric compressors capital cost coefficient [$.kW^{-cuc}]
b_{ue}	Electric turbines capital cost coefficient [$.kW^{-cue}]
c	Heat exchangers capital cost coefficient [$.m^{-4}]
c_c	Work exponent of SSCs capital cost [-]
C_{CU}	Cold utility cost [$.kWyear^{-1}]
CE	Electricity purchase cost [$.kWyear^{-1}]
c_e	Work exponent of SSTs capital cost [-]
c_g	Work exponent of electric generators capital cost [-]
c_{hm}	Work exponent of helper motors capital cost [-]
C_{HU}	Hot utility cost [$.kWyear^{-1}]
CP	Heat capacity flow rate of process streams [kW.K^{-1}]
c_{uc}	Work exponent of electric compressors capital cost [-]
c_{ue}	Work exponent of electric turbines capital cost [-]
eps	Relative precision of a float number in computation [-]
f	Annualization factor [year^{-1}]
h	Individual heat exchange coefficient of process streams [kW.m^{-2}.K^{-1}]
h_s	Individual heat exchange coefficient of hot utility [kW.m^{-2}.K^{-1}]
h_w	Individual heat exchange coefficient of cold utility [kW.m^{-2}.K^{-1}]
p_{lin}^{light}	Light penalties linear coefficient [-]
p_{ang}^{light}	Light penalties angular coefficient [-]
p_{lin}^{severe}	Severe penalties linear coefficient [-]
p_{ang}^{severe}	Severe penalties angular coefficient [-]
PE	Electricity selling price [$.kWyear^{-1}]

P_{in} Initial pressure of process streams [MPa]

P_{low} Lower limit of process streams pressure [MPa]

P_{out} Final pressure of process streams [MPa]

P_{up} Upper limit of process streams pressure [MPa]

Q_{low} Lower limit of heat exchangers heat load [kW]

Q_{up} Upper limit of heat exchangers heat load [kW]

TI_{low} Lower limit of inlet temperature to pressure manipulators [K]

T_{in} Initial temperature of process streams [K]

TI_{up} Upper limit of inlet temperature to pressure manipulators [K]

T_{low} Lower limit of temperature of process streams [K]

T_{out} Final temperature of process streams [K]

TS_{in} Hot utility inlet temperature [K]

TS_{out} Hot utility outlet temperature [K]

T_{up} Upper bound temperature for the process streams [K]

TW_{in} Cold utility inlet temperature [K]

TW_{out} Cold utility outlet temperature [K]

ΔT_{min} Heat exchanger minimal approach temperature [K]

η_c Isentropic efficiency for compressors [-]

η_e Isentropic efficiency for turbines [-]

κ Polytropic exponent [-]

Variables

A Area of heat exchanger [m^2]

A_s Area of heaters [m^2]

A_w Area of coolers [m^2]

c Binary variable that controls the existence of SSCs [-]

c_{tmp} Binary variable that controls the existence of compressors [-]

$CostHEN$ HEN annualized cost [\$.year^{-1}]

$CostWEN$ WEN annualized cost of WEN [\$.year^{-1}]

d Binary variable that for hot (equals 1) or cold (equals 0) streams

e Binary variable that controls the existence of SSTs [-]

e_{tmp} Binary variable that controls the existence of turbines [-]

FC Thermal capacity of cold streams [kW.K^{-1}]

FH Thermal capacity of hot streams [kW.K^{-1}]

g Binary variable that controls the existence of electric generator in the shaft [-]

HCC	Capital cost of HEN [$]
hm	Binary variable that controls the existence of helper motor in the shaft [-]
HOC	HEN operational cost [$.year^{-1}]
j	Pressure manipulator index in third-level optimization of *m*
J	Number of pressure manipulators
m	Binary variable that decides if the compressor or turbine is electric or couple to the work integration shaft [-]
m_{tmp}	Vector of *m* binary permutation [-]
p	Binary variable that controls the existence of pressure manipulators [-]
P	Pressure of process streams [MPa]
pen	Continuous variable that accounts for the network penalizations [$.year^{-1}]
Q	Heat exchanger heat load [kW]
Q_s	Heater heat load [kW]
Q_w	Cooler heat load [kW]
T	Temperature of unclassified process stream prior to classification [K]
TAC	Total annualized cost of a WHEN [$.year^{-1}]
T_{adj}	Temperature after adjustment with hot or cold utilities [K]
TC	Cold stream temperature [K]
TH	Hot stream temperature [K]
TI	Inlet temperature to pressure manipulators [K]
T_{ut}	Temperature after HI section [K]
U	Heat exchangers global heat exchange coefficient [kW.m^{-2}.K^{-1}]
uc	Binary variable that control the existence of electric compressors [-]
ue	Binary variable that control the existence of electric turbines [-]
U_s	Heaters global heat exchange coefficient of heaters [kW.m^{-2}.K^{-1}]
U_w	Coolers global heat exchange coefficient of coolers [kW.m^{-2}.K^{-1}]
WC	Work load of SSC [kW]
WCC	WEN capital cost [$]
WE	Work load of SST [kW]
WG	Work load of electric generator [kW]
WM	Work load of helper motor [kW]
WOC	WEN operating cost [$.year^{-1}]
WUC	Work load of electric compressors [kW]
WUE	Work load of electric turbines [kW]
y	Binary variable that controls the existence of heat exchangers [-]

y_{ut} Binary variable that activates the temperature adjustment section [-]

y_s Binary variable that controls the existence of heaters [-]

y_w Binary variable that controls the existence of coolers [-]

ΔT_{ml} Heat exchangers logarithmic mean temperature difference [K]

ΔTs_{ml} Heaters logarithmic mean temperature difference [K]

ΔTw_{ml} Coolers logarithmic mean temperature difference [K]

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