Received: 22 October 2021 | Revised: 17 March 2022 | Accepted: 31 March 2022
DOI: 10.1002/aic.17878

AIChE JOURNAL

RESEARCH ARTICLE
Process Systems Engineering

Globally optimal design of Minimal WHEN systems using enumeration

Qucheng Lin[1] | Zuwei Liao[1] | Miguel J. Bagajewicz[2,3,4]

[1]State Key Laboratory of Chemical Engineering, College of Chemical and Biological Engineering, Zhejiang University, Hangzhou, Zhejiang, People's Republic of China

[2]Rio de Janeiro State University (UERJ), Rio de Janeiro, Brazil

[3]School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, Oklahoma, USA

[4]Federal University of Rio de Janeiro (UFRJ), Rio de Janeiro, Brazil

Correspondence
Zuwei Liao, State Key Laboratory of Chemical Engineering, College of Chemical and Biological Engineering, Zhejiang University, Hangzhou, Zhejiang 310027, People's Republic of China.
Email: liaozw@zju.edu.cn

Funding information
National Natural Science Foundation of China, Grant/Award Numbers: 21822809, 21978256

Abstract

The process synthesis problem referred to as work and heat exchange networks (WHENs) asks to determine the optimal heat exchanger network intertwined with compressors, expanders, and valves, all integrated into one single network, such that streams with certain initial temperature and pressure attain their temperature and pressure targets at minimum cost. This article presents a procedure that obtains the globally optimal solution of Minimal WHEN systems using an enumeration scheme, using only a few subproblems, each one solved using mathematical programming to global optimality. Minimal structures feature one compression/decompression task and one heat exchange task per stream. In addition, we depart from the ideal gas assumption and use a cubic equation of state for stream properties. Finally, the approach allows for the use of turboexpanders. Four examples are presented to show the effectiveness and accuracy of the proposed method.

KEYWORDS
global optimality, minimal structures, work and heat exchange networks

1 | INTRODUCTION

The optimal design and retrofit of work and heat exchange network (WHEN), which is an important part of energy recovery systems, plays an important role in reducing costs and CO_2 emissions. Compared with heat exchanger network (HEN) synthesis, WHEN synthesis simultaneously takes into consideration the pressure-change of the stream involved as well as the coupling between the pressure-change devices alongside heat recovery. This is especially important in ammonia synthesis,[1,2] oil refineries,[3] CO_2 capture processes,[4] and liquefied natural gas (LNG) production processes.[5–8] In these processes, for example, compression or decompression arrangements upgrade low-grade heat to reduce the consumption of hot and cold utilities, while heating or cooling of process streams can reduce the net consumption of shaft work. Thus, optimization results are often the result of the trade-off between work and heat.

Research on WHEN synthesis can be divided into heuristic and algorithmic methods based on pinch analysis or methods that use mathematical programming or metaheuristics/stochastic procedures.

In the case of heuristic and algorithmic methods, Aspelund et al.[9] first proposed an Extended Pinch Analysis and Design (ExPAnD) procedure, using exergy to represent the quality of energy. They used 10 heuristic rules for determining the appropriate pressure-change and temperature-change routes of process streams. Subsequently, Fu and Gundersen[10–14] discussed the appropriate placement of compressors and expanders in HENs based on thermodynamic analysis, using proposed heuristic rules. All these methods do not guarantee optimality, neither global nor local because of their nature.

In turn, the WHEN synthesis studies based on mathematical models, in particular mixed integer nonlinear models (MINLM), have the potential of identifying local and global optima and can be roughly divided into four categories according to the pressure-change routes design method.

In the first category of mathematical modeling, the pressure-change routes of process streams are fixed, predefined by the aforementioned ExPAnD method or other. Indeed, Wechsung et al.[15] first combined the pinch location method (PLM), proposed by Duran and Grossmann,[16] with exergy analysis and mathematical programming to minimize the exergy required. Later, Onishi et al.[17] expanded the method by introducing an expander and compressor coupling operator to consider the work recovery process and replaced the PLM with a stage-wise superstructure (SWS) proposed by Yee and Grossmann[18] to simultaneously consider the cost of equipment in WHENs. Recently, Pavão et al.[19] presented a novel alternative framework using a matrix-based implementation fit for the use of meta-heuristic solution approaches and used simulated annealing and rocket fireworks optimization (SA-RFO).

The second category uses a monotonic SWS to describe the pressure-change routes, that is, high pressure (HP) and low pressure (LP) process streams are monotonically depressurized or pressurized to target pressure, respectively. Based on this concept, Razib et al.[20] introduced operating curves to identify potential HP and LP process streams to be matched for work exchange via compressors and turbines running in the same single-shaft-turbine-compressor (SSTC), thereby establishing a WEN optimization model. Later, Onishi et al.[21] introduced the SWS model for heat integration into the framework but no longer considered operating curves for representing the relationship between discharge pressure and flow rate at the same shaft speed. The work was further extended by Huang and Karimi,[22] who developed a mixed-integer nonlinear model (MINLM) solved using mathematical programming (MINLP) that enables an optimizable selection of end-heaters and end-coolers. Recently, Zhuang et al.[23] proposed a step-by-step design strategy. The hot or cold identity of process streams are determined by exergy analysis, and then an MINLM model is used in synthesizing the WHEN to attain the minimal total annualized cost (TAC).

The third category uses a non-monotonic SWS, that is, the HP or LP identity of process streams in the pressure-change routes is no longer predefined. Onishi et al.[24] combined this kind of superstructure with the heat integration operator of PLM and considered unclassified streams in the WHEN synthesis problem. Using BARON, they found global optimal solutions quickly for small problems, mostly because of the PLM simplification. In the same year, Nair et al.[25] proposed a very rich superstructure model, introducing a phase identification operator that allows the model to consider both gas and liquid phases. However, even for small-scale problems, it takes a long time to find a good solution. Recently, Lin et al.[26] proposed a two-phase strategy, targeting, and design, which efficiently reduced the difficulty in solving the WHEN synthesis problem.

Finally, the fourth category assumes a single-stage pressure-change of process streams, whose purpose is to perform a rough target estimation before the detailed design of WHENs. Yu et al.[27] proposed a Mixed Integer Nonlinear model for determining the optimal thermodynamic paths of process streams in WHENs to minimize exergy consumption. Later, Vikse et al.[28] proposed a novel nonsmooth formulation for handling unclassified process streams, turning the original MINLP model into an NLP model, which somewhat reduced the computational difficulty.

Due to the highly nonlinear and nonconvex nature of MINLMs, only small-scale WHEN synthesis problems were solved, even under many simplifying assumptions, and aggravated when unclassified streams are considered. Among these assumptions, ideal gas and constant heat capacity are the two most common idealized assumptions used to reduce the computational difficulty but aggravated by the fact that in WHEN synthesis problems, the temperature, and pressure of process streams are both variables so that the range of physical property changes is usually large. The use of the above two assumptions inevitably affects the accuracy of the model and the credibility of the calculation results. In our opinion, if the accuracy of the model cannot be guaranteed, even if the calculation speed is fast, only results that severely deviate from reality or are even not feasible can be obtained.

In this article, we propose to use a decoupling method, which allows the accuracy that is absent in previous work, yet guarantees global optimality for a certain class of WHEN systems that we define.

The novelty of our work relies on departing significantly from previous work in various aspects:

- Instead of ideal gas assumptions, we use the Peng–Robinson equation of state (PR-EOS) to calculate the properties of gas process streams.
- We introduce the concept of Minimal WHEN structures, an extension of a concept of the same name introduced by Chang et al.[29] These structures typically feature a certain number of units or less (in HENs, it is the minimum number of exchangers guaranteed by the absence of energy loops). For each minimal structure, the temperatures and pressures are defined and therefore the units can be designed subsequently. In other words, each structure contains at most one heat exchange task and one pressure change task.
- We enumerate all possible Minimal WHEN structures or we use a smart enumeration method (introduced by Costa and Bagajewicz[30]) using lower bounds, a concept also used by Chang et al.[29] in a unique manner.
- While coupling compressors and expanders to save electricity is not a new feature, we introduce the splitting of streams for this coupling to take place.
- We use an assignment problem for the compressor-expanders coupling.
- The HEN is solved to global optimality using Minimal structures.
- Because our enumeration is exhaustive and because the WEN integration, as well as the HEN solutions, are global, our methodology guarantees global optimality.

We thought that it would be implicit in our claims, but a reviewer of this article has asked us to clarify that our claim of global optimality refers to the nature of the result of the optimization using the specific mathematical model corresponding to the class of WHEN structures we define (Minimal WHEN) and that we do not claim we are obtaining globally optimal structures among the universe of all possible WHEN structures.

The article is organized as follows: In Section 2, we provide our problem statement of the optimal WHEN synthesis. In Section 3, the concept of the Minimal WHEN structure and the corresponding superstructure are introduced. Section 4 discusses our calculations of work done by compressors and expanders as well as the temperature at the inlet or outlet of compressors, expanders, and valves. In Section 5, we present an enumeration algorithm to generate Minimal WHEN structures. In Sections 6 and 7, we give the design-optimization model for the HEN and WEN in Minimal WHEN structures, respectively. In Section 8, we present the optimization procedure for Minimal WHEN structures. In Section 9, three examples with different cases are presented to demonstrate the applicability of the proposed approach.

2 | PROBLEM STATEMENT

The general problem of WHENs is as follows: given a set of process streams, each with given supply and target temperatures and pressure, and considering a set of hot utilities (HU), a set of cold utilities (CU), and an electric utility (EU), determine a network of heat exchangers, compressors, expanders, valves, and work exchange units (compressors coupled with expanders), such that a minimum TAC is attained. The following assumptions are also used:

1. All compressions and expansions (except expansions via valves) are isentropic, corrected by efficiency, and calculated using a real gas equation of state. Previous work (Wechsung et al.[15] and others) assumed ideal gas behavior.
2. All expansion through valves is isenthalpic neglecting changes of kinetic energy, which is a common approximation.
3. Finally, we assume that the pressure drop and heat losses in piping are negligible.

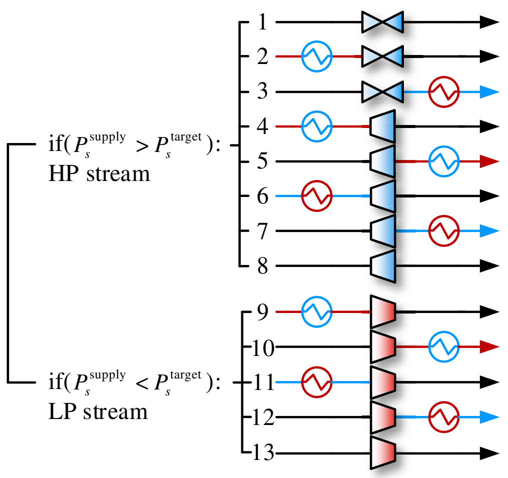

FIGURE 1 Stream path options in Minimal WHEN structures

3 | MINIMAL WHEN STRUCTURES

By definition, in Minimal structures, each stream undertakes one compression or decompression in only one unit (valve, compressor, expander, and/or a coupled compressor-expander) and one cooling/heating task in a Minimal HEN structure. Minimal HEN structures are structures without energy loops (see Chang et al.[29]). The temperature change and pressure change paths followed by each stream are depicted in Figure 1. We note that this definition excludes structures considered in prior work, where heat exchange can take place before and after a single compressor or expander even though the number of compression or expansion tasks is still only one.

One important feature of this definition is that the sub-networks, HEN, and WEN, of each Minimal WHEN structure are now independent. For each stream, the pressure change unit can only be placed at the beginning or end of its thermodynamic path (pressure change and temperature change path). Once the placement of the unit is known, the suction and discharge temperatures can be determined. Then the inlet and outlet temperatures of the stream in the HEN are fixed, and the total shaft work required or generated in the WEN is also fixed. Based on this feature, the optimal solution of each Minimal WHEN structure can be obtained by solving the HEN and WEN subproblems separately, the WEN problem being reduced to determine power integration, with known power demands. After enumerating/optimizing all Minimal WHEN structures, the best Minimal structure can be determined, that is, global optimality is guaranteed.

We use the following nomenclature: NPH and NPC for hot and cold streams without pressure change as well as HP and LP for streams whose target pressure is smaller and larger than the inlet pressure, respectively. The stream path options in Minimal WHEN structures (Figure 1) are as follows:

- Cases 1, 8, and 13 in Figure 1: These options, where heating/cooling corrections are not needed, are rare but not impossible. These cases should be tested first and only the work exchange of relevant compressors and expanders should be considered.
- Cases 3, 5, 7, 10, and 12 in Figure 1: These cases consist of allowing pressure change first followed by adjusting the temperature in the model. In these cases, the discharge temperature of the pressure-change unit (T_s^{dis}) for the known suction temperature ($T_s^{suc} = T_s^{supply}$) is calculated. The streams are then considered as hot or cold streams for the HEN synthesis. Figure 2A shows the situation for these cases

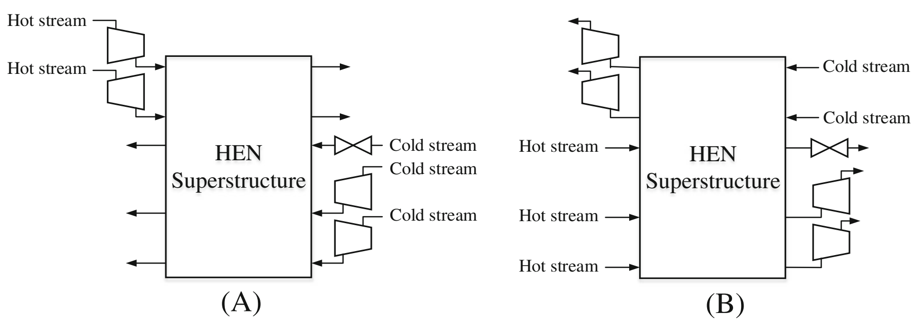

FIGURE 2 Path options: (A) Using pressure-change units first; (B) Using pressure-change units last

including HOT streams ($T_s^{dis} > T_s^{target}$) and COLD streams ($T_s^{dis} < T_s^{target}$). Valves are only placed before heat exchange for cold streams to generate larger heat transfer driving force.

- Cases 2, 4, 6, 9, and 11 in Figure 1: These cases consist of performing the pressure change last. In these cases, the suction temperature of the pressure-change unit (T_s^{suc}) needs to be calculated for a known discharge temperature ($T_s^{dis} = T_s^{target}$). The streams then are considered as hot or cold streams for the HEN synthesis. Figure 2B shows the situation for these cases including HOT streams ($T_s^{supply} > T_s^{suc}$) and COLD streams ($T_s^{supply} < T_s^{suc}$). Valves are only placed after heat exchange for hot streams to have larger driving force of heat transfer.

4 | PRESSURE EQUIPMENT CALCULATIONS

The most common assumptions in previous work[4,9–15,17,19,21–24,27,28] include constant heat capacities (C_p), ideal gas behavior, all compressions and expansions (except through valves) most of the time performed using the polytropic equation resulting from assuming $P/\rho^n = C$, where C is a constant, and all expansions through valves isenthalpic with a constant Joule–Thomson coefficient.

In this work, we depart from the ideal gas condition by using the Peng–Robinson equation of state (PR-EOS) (see Supporting Information). We also depart from the use of a polytropic equation to calculate the work of a compressor. Instead, we use a thermodynamics-based rigorous method to calculate the work as well as the suction/discharge temperature and enthalpy. Thus, the relation between the suction temperature and the isentropic discharge temperature is:

$$S\left(T_s^{suc}, \hat{P}_s^{supply}\right) = S\left(T_{s,pm}^{dis,isen}, \hat{P}_s^{target}\right), \quad \forall (s,pm) \in \{s \in HP\, pm = E\} \cup \{s \in LP\, pm = C\} \tag{1}$$

where $T_{s,pm}^{dis,isen}$ is the discharge temperature of compressors (pm = C) or expanders (pm = E) based on the isentropic path. T_s^{suc} is the suction temperature, which has a fixed value when the discharge temperature is calculated from the inlet condition, and it is a variable when the suction temperature is calculated from the discharge condition. The real discharge temperature T_s^{dis} can be obtained from $T_{s,pm}^{dis,isen}$:

$$H\left(T_s^{dis}, \hat{P}_s^{target}\right) - H\left(T_s^{suc}, \hat{P}_s^{supply}\right) = \left[H\left(T_{s,C}^{dis,isen}, \hat{P}_s^{target}\right) - H\left(T_s^{suc}, \hat{P}_s^{supply}\right)\right] / \hat{\eta}^C, \quad \forall s \in LP \tag{2}$$

$$H\left(T_s^{suc}, \hat{P}_s^{supply}\right) - H\left(T_s^{dis}, \hat{P}_s^{target}\right) = \left[H\left(T_s^{suc}, \hat{P}_s^{supply}\right) - H\left(T_{s,E}^{dis,isen}, \hat{P}_s^{target}\right)\right] \hat{\eta}^E, \quad \forall s \in HP \tag{3}$$

where $\hat{\eta}^C$ and $\hat{\eta}^E$ are the isentropic efficiency of compressors and expanders, respectively. In turn, the isenthalpic expansions can be expressed by:

$$H\left(T_s^{suc}, \hat{P}_s^{supply}\right) = H\left(T_s^{dis}, \hat{P}_s^{target}\right), \forall s \in HP \tag{4}$$

The above formulas as an equation-oriented model can be easily solved. The results include the discharge temperature ($T_{s,pm}^{dis}$) and enthalpy ($H_{s,pm}^{dis}$) of different pressure equipment under the condition of using pressure-change units first, as well as the suction temperature ($T_{s,pm}^{suc}$) and enthalpy ($H_{s,pm}^{suc}$) of different pressure equipment under the condition of using pressure-change units last.

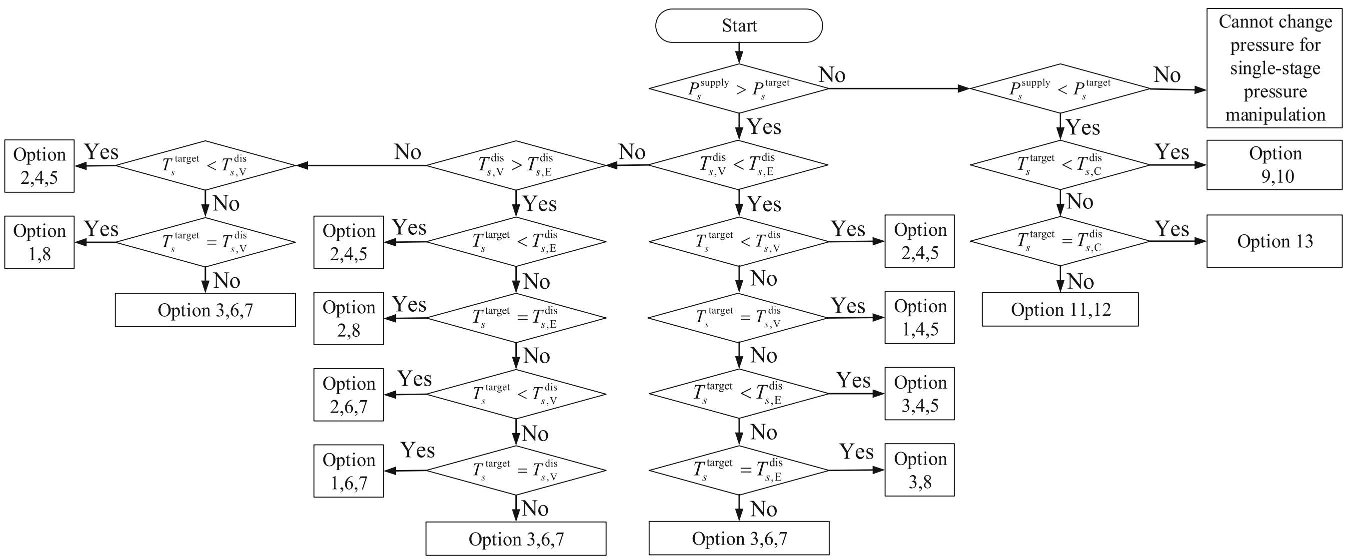

FIGURE 3 Screening all feasible path options of each process stream

5 | ENUMERATION PROCEDURE

The first step in the enumeration procedure is to screen all feasible path options of HP/LP streams in Minimal WHEN structures. This can be done by comparing the target temperature and discharge temperature of HP/LP streams in different pressure-change devices under the assumption of using pressure-change units first. For example, if $T_s^{\text{target}} < T_{s,\text{V}}^{\text{dis}} < T_{s,\text{E}}^{\text{dis}}$ for a HP stream, then it has feasible path options 2, 4, and 5, the number of feasible paths is 3. The complete screening process is shown in Figure 3.

Thus, once the possible pressure/heat exchange path for each stream has been determined, all possible Minimal WHEN structures (i.e., path combinations for all steams) are obtained. For example, if one has three HP streams with feasible options 3, 6, 7, and two LP streams with feasible options 9 and 10, then the number of Minimal WHEN structures are $3^3 \times 2^2 = 108$. However, because of the constraints of temperatures or duties of HU/CU streams in the HEN, not all structures are feasible. Therefore, a feasibility check needs to be performed before optimizing each Minimal WHEN structure.

6 | HEAT EXCHANGE NETWORK DESIGN

Process streams belong to sets I and J, composed of streams that need cooling (hot) and streams that need heating (cold), respectively. The heat capacities are determined by the inlet and outlet states of streams in the HEN for different path options. For the chosen Minimal WHEN structure, the average heat capacity flow rate ($\hat{F}cp$) of LP/HP streams in the HEN are calculated as follows:

$$\hat{F}cp_i = \begin{cases} \dfrac{\hat{H}_i^{\text{supply}} - \hat{H}_{i,pm}^{\text{suc}}}{\hat{T}_i^{\text{supply}} - \hat{T}_{i,pm}^{\text{suc}}} \text{ for option } 2,4,9 \\ \dfrac{\hat{H}_{i,pm}^{\text{dis}} - \hat{H}_i^{\text{target}}}{\hat{T}_{i,pm}^{\text{dis}} - \hat{T}_i^{\text{target}}} \text{ for option } 5,10 \end{cases} \quad \begin{matrix} \forall (i,pm) \in \{i \in \text{HP} \cap \text{I}, pm = \text{E},\text{V}\} \\ \cup \{i \in \text{LP} \cap \text{I}, pm = \text{C}\} \end{matrix} \tag{5}$$

$$\hat{F}cp_j = \begin{cases} \dfrac{\hat{H}_{j,pm}^{\text{suc}} - \hat{H}_j^{\text{supply}}}{\hat{T}_{j,pm}^{\text{suc}} - \hat{T}_j^{\text{supply}}} \text{ for option } 6,11 \\ \dfrac{\hat{H}_j^{\text{target}} - \hat{H}_{j,pm}^{\text{dis}}}{\hat{T}_j^{\text{target}} - \hat{T}_{j,pm}^{\text{dis}}} \text{ for option } 3,7,12 \end{cases} \quad \begin{matrix} \forall (j,pm) \in \{j \in \text{HP} \cap \text{J}, pm = \text{E},\text{V}\} \\ \cup \{j \in \text{LP} \cap \text{J}, pm = \text{C}\} \end{matrix} \tag{6}$$

In turn, inlet, and outlet temperatures of process streams in the HEN are the following:

$$T_i^{\text{IN}} = \begin{cases} \begin{cases} \hat{T}_i^{\text{supply}} \text{ for option } 2,4,9 \\ \hat{T}_{i,pm}^{\text{dis}} \text{ for option } 5,10 \end{cases}, \forall (i,pm) \in \{i \in \text{HP} \cap \text{I}, pm = \text{EV}\} \cup \{i \in \text{LP} \cap \text{I} pm = \text{C}\} \\ \hat{T}_i^{\text{supply}}, \forall i \in \text{NPH} \end{cases} \tag{7}$$

$$T_i^{\text{OUT}} = \begin{cases} \begin{cases} \hat{T}_{i,pm}^{\text{suc}} \text{ for option } 2,4,9 \\ \hat{T}_i^{\text{target}} \text{ for option } 5,10 \end{cases}, \forall (i,pm) \in \{i \in \text{HP} \cap \text{I}, pm = \text{EV}\} \cup \{i \in \text{LP} \cap \text{I} pm = \text{C}\} \\ \hat{T}_i^{\text{target}}, \forall i \in \text{NPH} \end{cases} \tag{8}$$

$$T_j^{\text{IN}} = \begin{cases} \begin{cases} \hat{T}_j^{\text{supply}} \text{ for option } 6,11 \\ \hat{T}_{j,pm}^{\text{dis}} \text{ for option } 3,7,12 \end{cases}, \forall (j,pm) \in \{j \in \text{HP} \cap \text{J}, pm = \text{EV}\} \cup \{j \in \text{LP} \cap \text{J} pm = \text{C}\} \\ \hat{T}_j^{\text{supply}}, \forall j \in \text{NPC} \end{cases} \tag{9}$$

$$T_j^{\text{OUT}} = \begin{cases} \begin{cases} \hat{T}_{j,pm}^{\text{suc}} \text{ for option } 6,11 \\ \hat{T}_j^{\text{target}} \text{ for option } 3,7,12 \end{cases}, \forall (j,pm) \in \{j \in \text{HP} \cap \text{J}, pm = \text{EV}\} \cup \{j \in \text{LP} \cap \text{J} pm = \text{C}\} \\ \hat{T}_j^{\text{target}}, \forall j \in \text{NPC} \end{cases} \tag{10}$$

For the HEN problem, now the heat capacities, inlet, and outlet temperatures of streams are obtained. With the values of heat transfer coefficients and flow rates given as parameters, the minimum TAC of the HEN (TAC^{HEN}) is given by:

$$Min\left\{TAC^{\text{HEN}} = IC^{\text{HEN}} + OPC^{\text{HEN}}\right\} \tag{11}$$

$$IC^{\text{HEN}} = \left(\begin{matrix} \sum_{k \in \text{ST}} \sum_{i \in \text{I}} \sum_{j \in \text{J}} \hat{a}^{\text{H}} z_{i,j,k} + \sum_{i \in \text{I}} \hat{a}^{\text{H}} zcu_i + \sum_{j \in \text{J}} \hat{a}^{\text{H}} zhu_j + \\ \sum_{k \in \text{ST}} \sum_{i \in \text{I}} \sum_{j \in \text{J}} \left(\hat{b}^{\text{H}} A_{i,j,k} + \hat{c}^{\text{H}} A_{i,j,k}^2 \right) + \sum_{i \in \text{I}} \left(\hat{b}^{\text{H}} Acu_i + \hat{c}^{\text{H}} Acu_i^2 \right) + \sum_{j \in \text{J}} \left(\hat{b}^{\text{H}} Ahu_j + \hat{c}^{\text{H}} Ahu_j^2 \right) \end{matrix} \right) \tag{12}$$

$$OPC^{\mathrm{HEN}} = \sum_{i \in I} \hat{C}cu \cdot qcu_i + \sum_{j \in J} \hat{C}hu \cdot qhu_j \tag{13}$$

where IC^{HEN} and OPC^{HEN} are the annualized capital cost and operational cost of the HEN, respectively.

The global optimal solution can be obtained using the Synheat superstructure proposed by Yee and Grossmann,[18] provided it is solved globally, or the enumeration procedure developed by Chang et al.,[29] which guarantees global optimality.

7 | WORK EXCHANGE NETWORK DESIGN

Three subsets are defined: VAL for streams that use valves for expansion, COM for streams that are compressed, and EXP, for streams that are decompressed in expanders. For the chosen Minimal WHEN structure, the compression, or expansion tasks are given by:

$$WLP_p^{\mathrm{real}} = \begin{cases} \hat{F}_p\left(\hat{H}_{p,C}^{\mathrm{dis}} - \hat{H}_p^{\mathrm{supply}}\right) \text{ for option } 10, 12, 13 \\ \hat{F}_p\left(\hat{H}_p^{\mathrm{target}} - \hat{H}_{p,C}^{\mathrm{suc}}\right) \text{ for option } 9, 11 \end{cases}, \forall p \in \mathrm{COM} \tag{14}$$

$$WHP_q^{\mathrm{real}} = \begin{cases} \hat{F}_q\left(\hat{H}_q^{\mathrm{supply}} - \hat{H}_{q,T}^{\mathrm{dis}}\right) \text{ for option } 5, 7, 8 \\ \hat{F}_q\left(\hat{H}_{q,T}^{\mathrm{suc}} - \hat{H}_q^{\mathrm{target}}\right) \text{ for option } 4, 6 \end{cases}, \forall q \in \mathrm{EXP} \tag{15}$$

We propose a new WEN model that considers turboexpanders for power integration by default, which means that the compression/expansion tasks can be split into more than one compressor/expander as shown in Figure 4A. Consider that $\hat{WLP}_p^{\mathrm{real}}$ and $\hat{WHP}_q^{\mathrm{real}}$ are the power of the compressors corresponding to COM and expanders corresponding to EXP (these are parameters at this stage). Consider also that $WTE_{p,q}$ are variables denoting the power exchanged between streams $p \in \mathrm{COM}$ and $q \in \mathrm{EXP}$ in turboexpanders. Finally, WLP_q^{res} and WHP_q^{res} are the residual power needed or produced.

We now write the model:

$$Min\left\{TAC^{\mathrm{WEN}} = IC^{\mathrm{WEN}} + OPC^{\mathrm{WEN}}\right\} \tag{16}$$

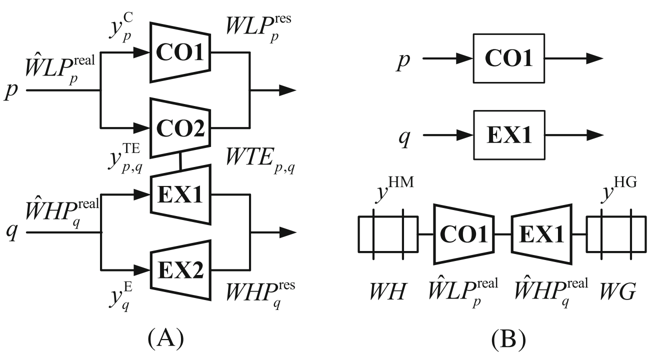

FIGURE 4 Work exchange networks considering. (A) Turboexpanders, (B) SSTCs

s.t

$$IC^{\mathrm{WEN}} = \hat{fac}\left[\sum_{p \in \mathrm{COM}} cpo_p^{\mathrm{C}} + \sum_{q \in \mathrm{EXP}} cpo_q^{\mathrm{E}} + \sum_{p \in \mathrm{COM}} \sum_{q \in \mathrm{EXP}} cpo_{p,q}^{\mathrm{TE}} + \hat{B}\left(cpo^{\mathrm{HM}} + cpo^{\mathrm{HG}}\right)\right] \tag{17}$$

$$OPC^{\mathrm{WEN}} = \left(1-\hat{B}\right)\left(\sum_{p \in \mathrm{COM}} \hat{COE}\, WLP_p^{\mathrm{res}} - \sum_{q \in \mathrm{EXP}} \hat{POE}\, WHP_q^{\mathrm{res}}\right) + \hat{B}\left(\hat{COE}\, WH - \hat{POE}\, WG\right) \tag{18}$$

$$\hat{WLP}_p^{\mathrm{real}} = \sum_{q \in \mathrm{EXP}} WTE_{p,q} + WLP_p^{\mathrm{res}}, \forall p \in \mathrm{COM} \tag{19}$$

$$\hat{WHP}_q^{\mathrm{real}} = \sum_{p \in \mathrm{COM}} WTE_{p,q} + WHP_q^{\mathrm{res}}, \forall q \in \mathrm{EXP} \tag{20}$$

$$WTE_{p,q} - \hat{BM}_{p,q}^{\mathrm{TE}} y_{p,q}^{\mathrm{TE}} \le 0, \forall p \in \mathrm{COM}, q \in \mathrm{EXP} \tag{21}$$

$$WLP_p^{\mathrm{res}} - \hat{BM}_p^{\mathrm{C}} y_p^{\mathrm{C}} \le 0, \forall p \in \mathrm{COM} \tag{22}$$

$$WHP_q^{\mathrm{res}} - \hat{BM}_q^{\mathrm{E}} y_q^{\mathrm{E}} \le 0, \forall q \in \mathrm{EXP} \tag{23}$$

$$cpo_p^{\mathrm{C}} = \hat{a}^{\mathrm{C}} y_p^{\mathrm{C}} + \hat{b}^{\mathrm{C}}\left(WLP_p^{\mathrm{res}}\right)^{\hat{c}^{\mathrm{C}}} - \hat{B}\left[\hat{a}^{\mathrm{M}} y_p^{\mathrm{C}} + \hat{b}^{\mathrm{M}}\left(WLP_p^{\mathrm{res}}\right)^{\hat{c}^{\mathrm{M}}}\right], \forall p \in \mathrm{COM} \tag{24}$$

$$cpo_q^{\mathrm{E}} = \hat{a}^{\mathrm{E}} y_q^{\mathrm{E}} + \hat{b}^{\mathrm{E}}\left(WHP_q^{\mathrm{res}}\right)^{\hat{c}^{\mathrm{E}}} - \hat{B}\left[\hat{a}^{\mathrm{G}} y_q^{\mathrm{E}} + \hat{b}^{\mathrm{G}}\left(WHP_q^{\mathrm{res}}\right)^{\hat{c}^{\mathrm{G}}}\right], \forall q \in \mathrm{EXP} \tag{25}$$

$$cpo_{p,q}^{\mathrm{TE}} = \begin{pmatrix} \left(\hat{a}^{\mathrm{C}} + \hat{a}^{\mathrm{E}}\right) y_{p,q}^{\mathrm{TE}} + \hat{b}^{\mathrm{C}}(WTE_{p,q})^{\hat{c}^{\mathrm{C}}} + \hat{b}^{\mathrm{E}}(WTE_{p,q})^{\hat{c}^{\mathrm{E}}} \\ -\left(\hat{a}^{\mathrm{M}} + \hat{a}^{\mathrm{H}}\right) y_{p,q}^{\mathrm{TE}} - \hat{b}^{\mathrm{M}}(WTE_{p,q})^{\hat{c}^{\mathrm{M}}} - \hat{b}^{\mathrm{G}}(WTE_{p,q})^{\hat{c}^{\mathrm{G}}} \end{pmatrix}, \forall p \in \mathrm{COM}, q \in \mathrm{EXP} \tag{26}$$

$$\sum_{p \in \mathrm{COM}} \hat{WLP}_p^{\mathrm{real}} + WG = \sum_{q \in \mathrm{EXP}} \hat{WHP}_q^{\mathrm{real}} + WH \tag{27}$$

$$WH - \hat{BM}^{\mathrm{HM}} y^{\mathrm{HM}} \le 0 \tag{28}$$

$$WG - \hat{BM}^{\mathrm{HG}} y^{\mathrm{HG}} \le 0 \tag{29}$$

$$cpo^{\mathrm{HM}} = \hat{a}^{\mathrm{M}} y^{\mathrm{HM}} + \hat{b}^{\mathrm{M}}(WH)^{\hat{c}^{\mathrm{M}}} \tag{30}$$

$$cpo^{\mathrm{HG}} = \hat{a}^{\mathrm{G}} y^{\mathrm{HG}} + \hat{b}^{\mathrm{G}}(WG)^{\hat{c}^{\mathrm{G}}} \tag{31}$$

The parameter $\hat{B}$ is used to control two design situations and is set to zero (0) by default. In this case, turboexpanders are used for work exchange as shown in Figure 4A. Equations (19) and (20) represent the work balance for the streams that belong to COM and EXP, respectively. Equations (21)–(23) are logical constraints to determine the existence of turboexpanders, compressors and expanders, respectively, where the symbol $\hat{BM}$ with different subscripts and superscripts represents the Big-M for relaxation of constraints. Equations (24)–(26) are capital cost relations for different equipment, where cpo_p^{C} is the capital cost of each compressor with a motor, cpo_q^{E} is the capital cost of each expander with a generator, $cpo_{p,q}^{TE}$ is the capital cost of each turboexpander. Equations (17) and (18) represent the composition of total capital cost (IC^{WEN}) and operational cost (OPC^{WEN}) of the WEN, respectively, where $\hat{fac}$ is the annualization factor for IC^{WEN}, $\hat{COE}$ is the purchase cost of electricity, $\hat{POE}$ is the price of selling the electricity.

If the parameter $\hat{B}$ is set to 1, the SSTC is used for work exchange. All compressors and expanders run on the same shaft. Besides, one helper motor or generator is required to make up the deficit work or use the surplus work to generate power as shown in Figure 4B. Equation (27) represents the work balance for the SSTC, where WH is the work provided by the help motor, WG is the work to generate power by the help generator. Equations (28) and (29) are logical constraints to determine the existence of the help motor and the help generator, respectively. Equations (30) and (31) are capital cost relations for the two units. Besides, cpo_p^{C} and cpo_q^{E} in Equations (24) and (25) need to subtract the capital cost of motors and generators, respectively. The total capital cost in Equation (17) need to add the cost of the help motor and help generator. The operational cost in Equation (18) is replaced by the purchase cost of WH subtracting the selling cost of WG.

In this work, we use Baron, a commercial solver to find the solution to the problem. Baron works well in solving this model, while it sometimes fails solving other models, needing initial values or taking too much time. If Baron is not accessible, there are alternatives that can guarantee global optimality in a robust manner. Indeed, the model can be reformulated by inserting Equations (24–26) and (30, 31) into (17) and (18), and then inserting (17) and (18) into the objective function (16) to obtain a problem with a nonlinear (nonconvex) objective function and linear constraints. In such a model, one can underestimate the nonconvex terms using piecewise linear functions based on several intervals. Solutions of such linear models can be used as initial points of an NLP local solver or the objective can be simply reevaluated, which will provide an upper bound. In such an approach, increasing the number of intervals reduces the gap between the solutions of the nonlinear solver and the linear solver. Alternatively, one can use partitioning, following a recently introduced robust bound contraction procedure named RYSIA.[31] Global optimality is guaranteed in these two approaches, thus avoiding the need for a global solver.

8 | OPTIMIZATION PROCEDURE FOR MINIMAL WHEN

The optimization procedure is the following:

1. Set $UBTAC^{WHEN}$, the best upper bound of the WHEN problem, to ∞.
2. Screen all feasible path options of process streams and generate a list of all Minimal WHEN structures.
3. Choose a structure if there is one left in the list and test its feasibility in the HEN problem. If the HEN problem is feasible, go to step 4. However, if the HEN problem is infeasible, which can happen only in cases where no utility can attend target temperatures, discard the structure, and choose a new one. If there is no structure left, go to step 7.
4. Solve the corresponding power integration problem (WEN) and obtain the TAC_{struc}^{WEN} as described above (the subscript *struc* denotes the chosen structure). If $TAC_{struc}^{WEN} \geq UBTAC^{WHEN}$, discard the structure, and go to step 3. Else, go to step 5.
5. Solve the HEN problem and obtain TAC_{struc}^{HEN}.
6. If $TAC_{struc}^{HEN} + TAC_{struc}^{WEN} < UBTAC^{WHEN}$, update the value of $UBTAC^{WHEN}$ to $TAC_{struc}^{HEN} + TAC_{struc}^{WEN}$ and go to step 3.
7. $UBTAC^{WHEN}$ is the global optimum.

9 | EXAMPLES

In this section, four examples with different conditions of synthesis are studied to illustrate the effectiveness of the proposed new method for the optimal WHEN synthesis. Example 1 emphasizes the difference between using a real gas model and an ideal gas model. Example 2 illustrates the risks of using a step-by-step approach of using the minimization of exergy followed by the HEN synthesis. Example 3 compares other solution procedures that do not guarantee global optimality with our globally optimal procedure. Santos et al.[32] proposed a mixed-integer nonlinear model (MINLM) and solved it using metaheuristics. Metaheuristics have proven to be powerful and time-wise effective to find solutions close to the global optimum without knowing if that is the case or not. However, the search parameters usually have a great influence on the convergence speed and solution quality, which sometimes only apply to the case study solved and are therefore not expert-independent. Finally, our Example 4 solves an LNG design problem that has been simplified in the literature to be proposed as a WHEN problem. All results were obtained using GAMS (30.2.0) in a computer with a 2.6 GHz Intel® Core™ i7-8850H processor with 16 GB of RAM.

Example 1. This is an illustrative example with only one HP stream and one NPH stream and it aims at quantifying the impact of the ideal assumptions used in previous works, that is, the polytropic work equations and the assumptions of ideal gas behavior as well as constant heat capacity, on the results. The stream data are listed in Table 1, and the capital cost parameters are listed in Table 2. Besides, we use $\hat{\eta}^{C} = 0.9$, $\hat{\eta}^{E} = 0.9$, $\hat{EMAT} = 5$ K, $\hat{fac} = 0.18$. Because there is only one pressure-change stream, the equipment for work exchange (turboexpanders and the SSTC) is not used in this example, and the parameter $\hat{B}$ is set to 0. To perform the analysis, we use two different approaches to

TABLE 1 Stream data for Example 1

Stream	T^{supply} (°C)	T^{target} (°C)	P^{supply} (MPa)	P^{target} (MPa)	F (mol)	Fcp (kW/K)	h (kW/m^{2}K)
HP1-N_2	−50	−10	10	1	100	—	0.1
NPH1-CH_4	0	−50	10	10	—	10	0.1
Hot utility	25	25	—	—	—	—	1.0
Cold utility	−180	−180	—	—	—	—	1.0
Cost data (US$/kW-year)							
$\hat{C}OE$	455.04	$\hat{P}OE$	364.03	$\hat{C}hu$	100	$\hat{C}cu$	1000

TABLE 2 Capital cost parameters

Equipment	$\hat{a}$	$\hat{b}$	$\hat{c}$
Heat exchanger	93500.12	602.96	0.149
Compressor with a motor	0	51104.85	0.62
Expander with a generator	0	2585.47	0.81
Motor/generator	0	985.47	0.62

obtain the optimal networks: The first uses the ideal gas law and the polytropic work equation. The second uses the method of this article, that is, the isentropic change with enthalpies corrected by efficiency. In the first approach, we use $cp/cv = 1.613$ and the constant $Fcp = 3.493\,\text{kW/K}$ which are the average heat capacity ratio and heat capacity flow rate of the supply and target state of stream HP1.

Figure 5 depicts the detailed WHEN configurations obtained using the two work calculation approaches. Due to the nonideality of the stream HP1, the results obtained under the ideal assumptions are far from the results obtained without these assumptions. Both networks contain two heat exchangers, where the heat transfer area is equal to 170.3 m^2 (E1, the number 1 of the process stream heat exchangers) and 12.9 m^2 (H1, the number 1 of the heaters) for Network a, 217.4 m^2 (E1), and 3.8 m^2 (C1, the number 1 of the coolers) for Network b. The main difference lies in the work generated in the expanders (230.2 vs. 409.1 kW), leading to two different structures of the HEN. The number of stream-path combinations explored is 2 (path options 6 and 7 in Figure 1 are feasible for the stream HP1) in both cases. The detailed comparison of the two networks is listed in Table 3. In terms of TAC, the value of Network a is −28,989 $/year, and the value of Network b is 58,860 $/year. The deviation is as high as 149.3%. This shows the importance of using the equation of state and isentropic paths corrected by efficiency instead of the polytropic equation for power. The global optimal solutions are both obtained in 2 s.

Example 2. This example uses some of the data in the example from Yu et al.[27] We have provided the composition and flow rate of each process stream to replace the fixed heat capacity flow rate (the heat capacity flow rate of each process stream in the supply state is the same as the value given in the literature). Also, we choose N_2 which has the heat capacity ratio that is close to the one used in the literature ($cp/cv \approx 1.4$) in the given range of temperature and pressure. The relevant data for this example are listed in Table 4. In addition, we use $\hat{\eta}^C = 1$, $\hat{\eta}^E = 1$, $\hat{f}ac = 0.18$. Yu et al.[27] first determined the thermodynamic paths of process streams by exergy minimization and then used the Synheat stages model to obtain the HEN. The capital cost parameters are the same as the ones in Table 2. We do not allow valves and we consider two cases: Case 1, where cost is minimized without turboexpander or SSTC, and Case 2, where cost is minimized allowing the use of turboexpanders.

Case 1. In this case, the turboexpanders and the SSTC are not considered, so that we fix the value of $y^{TE}_{p,q}$ and $\hat{B}$ to be zero. The results indicate that the minimum TAC is 1,544,845 $/year. Figure 6B depicts the WHEN configuration, in which the heat transfer area is equal to 40.3 m^2 (E1), 25.2 m^2 (H1), 36.4 m^2 (H2), 36.5 m^2 (C1), 56.3 m^2 (C2). Compared with the number of heat exchangers of the WHEN obtained by Yu et al.,[27] our network requires only 5 heat exchangers vs. 13. The reason lies in the different optimization objectives. Yu et al.[27] focus on the exergy target when determining the optimal thermodynamic path so that a large number of streams splits are required to minimize the exergy loss. The corresponding HEN obtained in the literature is therefore more complex. In contrast, this work focus on design optimization from a TAC point of view and finds that fewer heat exchangers are better.

Because Yu et al.[27] did not give the cost parameters, we use our cost correlations to calculate the TAC for their WHEN configuration obtaining a TAC of 1,992,493 $/year. Considering that, the literature results were obtained using ideal gas law and polytropic equations, we recalculated the solutions using our work evaluation method based on isentropic change corrected by efficiency; because the temperatures change the heat demand/supply of the streams is also readjusted. The recalculated TAC is 2,022,134 $/year. As shown in

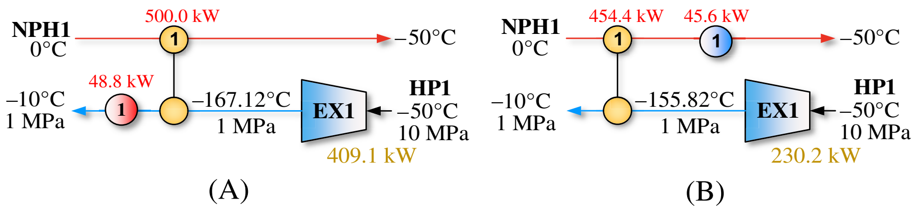

FIGURE 5 Optimal Minimal WHEN for Example 1: (A) Using the ideal gas law and the polytropic work equation. (B) Using the method of this article

TABLE 3 Comparison of results for Example 1

Items	Network a	Network b
Number of compressors and expanders	1	1
Work generated (kW)	409.1	230.2
WEN capital cost ($/year)	60,729	38,113
WEN operational cost ($/year)	−148,925	−83,789
Number of heat exchanger units	2	2
Total heat exchanger area (m^2)	183.2	221.2
Hot utility consumption (kW)	48.8	0
Cold utility consumption (kW)	0	45.6
HEN capital cost ($/year)	54,325	58,936
HEN operational cost ($/year)	4882	45,600
Total annualized cost ($/year)	−28,989	58,860

TABLE 4 Stream data for Example 2

Stream	T^{supply} (°C)	T^{target} (°C)	P^{supply} (MPa)	P^{target} (MPa)	F (mol)	h (kW/m^{2}K)	
HP1-N_2	350	350	0.2	0.1	66.08	0.1	
HP2-N_2	320	320	0.2	0.1	132.9	0.1	
HP3-N_2	110	110	0.2	0.1	102.5	0.1	
LP1-N_2	50	50	0.1	0.2	102.8	0.1	
LP2-N_2	190	190	0.1	0.2	339.5	0.1	
Hot utility	400	400	–	–	–	1.0	
Cold utility	15	15	–	–	–	1.0	
Cost data (US$/kW-year)							
$\hat{C}OE$	455.04	$\hat{P}OE$	364.03	$\hat{C}hu$	337	$\hat{C}cu$	100

Figure 6A, the WHEN structure of Yu et al.[27] is quite complex. To minimize the exergy losses of the WHEN, LP2 is separated into three sub-streams in their step 1, resulting in five heat exchangers to transfer heat between these sub-streams in step 2. Our WHEN structure, by contrast, is more concise and does not have energy loops. Although the hot/cold utility consumption and the corresponding operational cost of the HEN (295,157 $year) of our WHEN structure is larger than the result presented by Yu et al.[27] (43,062 $/year), the rest of the costs are all smaller, leading to a 23.6% lower TAC. Therefore, our approach achieves a good trade-off between energy consumption and capital cost. Results are listed in Table 5. Finally, from a computational point of view, Yu et al.[20] point out that it is impossible to find the global optimum with existing global MINLP solvers with their method. With our method, the global optimal solution of Case 1 is obtained in 18 s. The number of stream-path combinations explored is 32.

Case 2. In this case, the turboexpanders are used, so that we only fix the value of $\hat{B}$ to zero. The optimal Minimal WHEN structure is shown in Figure 7, where CO1 and EX2 form a turboexpander. The heat transfer area is the same as Case 1. As shown in Table 6, due to the use of the turboexpander, the WEN capital cost decreased by 8876 $/year, and the WEN operational cost decreased by 19,265 $/year, which reduces the TAC by 1.82% with respect to Case 1 and 25.0% with respect to the solution obtained by Yu et al.[27] The global optimal solution of Case 2 is obtained in 19 s.

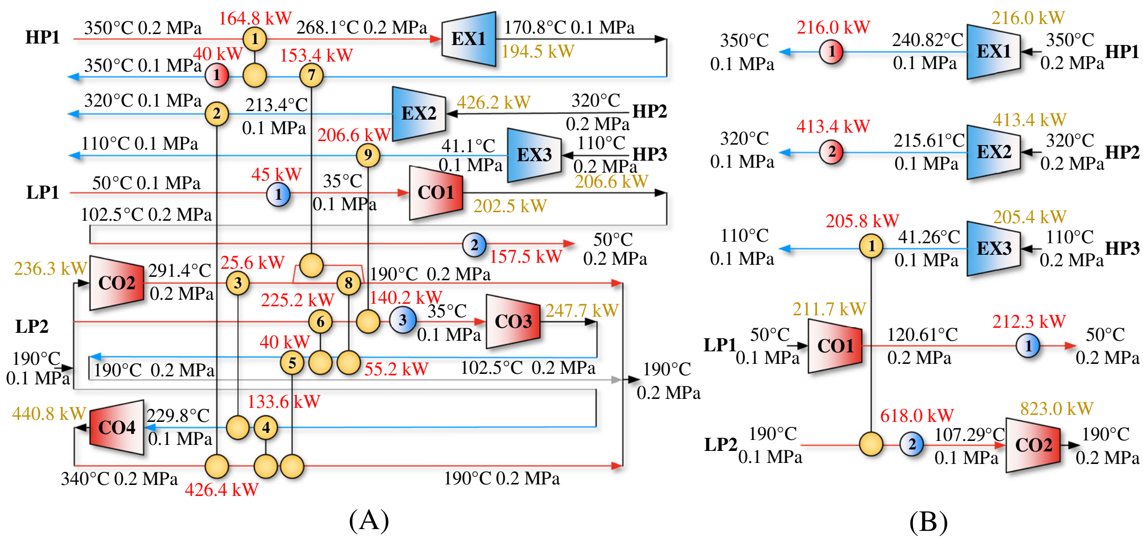

FIGURE 6 Optimal WHEN structure for Example 2-Case 1: (A) Yu et al.,[27] (B) Our Minimal WHEN

TABLE 5 Comparison of results for Example 2-Case 1

Items	Yu et al.[27]	Yu et al.[27] recalculated	Our procedure
Number of compressors and expanders	7	7	5
Work consumed (kW)	1127	1114	1035
Work generated (kW)	827.2	806.1	834.7
WEN capital cost ($/year)	1,332,645	1,321,442	977,249
WEN operational cost ($/year)	211,704	213,589	166,936
Number of heat exchanger units	13	13	5
Total heat exchanger area (m^2)	1748.4	1926.6	194.7
Hot utility consumption (kW)	40	27.8	629.2
Cold utility consumption (kW)	342.7	336.9	830.3
HEN capital cost ($/year)	400,394	444,041	105,503
HEN operational cost ($/year)	47,750	43,062	295,157
Total annualized cost ($/year)	1,992,493	2,022,134	1,544,845

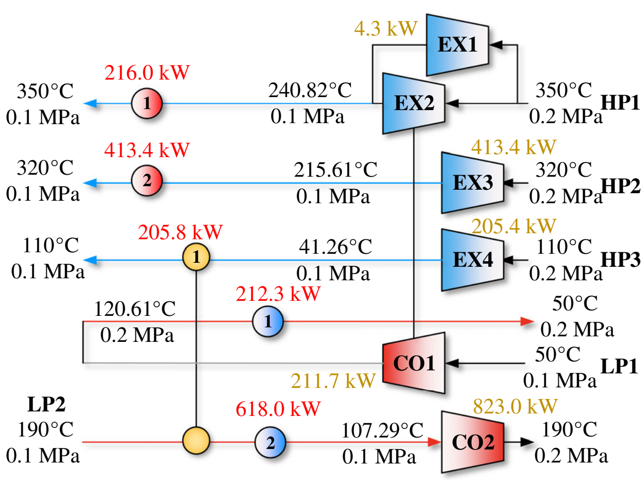

FIGURE 7 Optimal Minimal WHEN structure for Example 2-Case 2

TABLE 6 Comparison of results for Example 2-Case 2

Items	Case 1	Case 2
Number of compressors and expanders	5	6
Work consumed (kW)	1035	823.0
Work generated (kW)	834.7	623.1
WEN capital cost ($/year)	977,249	968,373
WEN operational cost ($/year)	166,936	147,671
Number of heat exchanger units	5	5
Total heat exchanger area (m^2)	194.7	194.7
Hot utility consumption (kW)	629.2	629.2
Cold utility consumption (kW)	830.3	830.3
HEN capital cost ($/year)	105,503	105,503
HEN operational cost ($/year)	295,157	295,157
Total annualized cost ($/year)	1,544,845	1,516,704

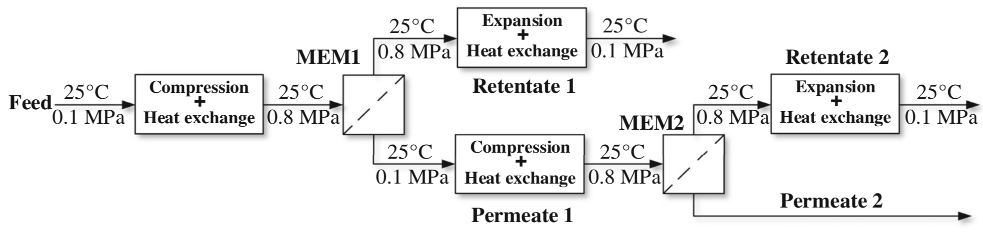

FIGURE 8 A two-stage membrane process for separating CO_2

TABLE 7 Stream data for Example 3

Stream	T^{supply} (°C)	T^{target} (°C)	P^{supply} (MPa)	P^{target} (MPa)	F (mol)	Composition (mole%)	Fcp (kW/K)	h (kW/m^{2}K)
LP1-Feed	25	25	0.1	0.8	1239.3	N_2: 86.0; CO_2: 14.0	–	0.1
LP2-Permeate 1	25	25	0.1	0.8	281	N_2: 51.3; CO_2: 48.7	–	0.1
HP1-Retentate 1	25	25	0.8	0.1	958.3	N_2: 96.2; CO_2: 3.8	–	0.1
HP2-Retentate 2	25	25	0.8	0.1	146.75	N_2: 89.1; CO_2: 10.9	–	0.1
NPH-FG	377	75	–	–	–	N_2: 75.7; CO_2: 12.3; H_2O: 12	43.77	0.1
NPC-Air	15	327	–	–	–	N2: 79.0; O2: 21	34.7	0.1
Cold utility	15	15	–	–	–	–	–	1.0
Cost data (US$/kW-year)								
$\hat{C}OE$	455.04		$\hat{P}OE$		364.03	$\hat{C}cu$	100	

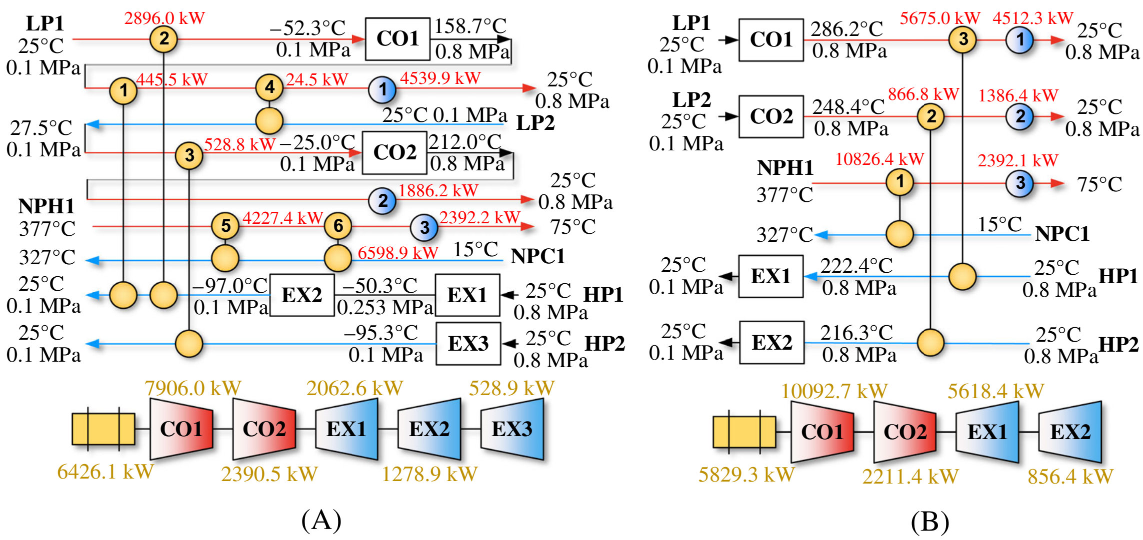

FIGURE 9 Optimal WHEN structure for Example 3-Case 1: (A) Santos et al.,[32] (B) Our Minimal WHEN

Example 3. The third example is an industrially inspired design of membrane separation of CO_2/N_2 in a post-combustion process, which was proposed by Zhao et al.[33] In this example, a two-stage membrane process is used for separating CO_2 from N_2 as shown in Figure 8, which is adapted from Fu and Gundersen.[4] In this figure only the compression tasks are shown. Later Pavão et al.[19] and Santos et al.[32] considered two more streams (Feed and Permeate 1). We also consider these six process streams. Because the flow rates and compositions of some pressure-change streams (Permeate 1, Retentate 1, and Retentate 2) are not listed in previous works, we calculated these parameters using a simulator (PRO II) using membrane parameters given by Zhao et al.[33] (see Table 7). In addition, we use $\hat{\eta}^C = 0.85$, $\hat{\eta}^E = 0.9$, $\hat{E}MAT = 5$ K, $\hat{f}ac = 0.18$ and we do not use valves. The capital cost parameters are the same as the ones in Table 2. We consider two cases: Case 1: where a single shaft turbine compressor (SSTC)[20] is used, and Case 2, where turboexpanders are used.

TABLE 8 Comparison of results for Example 3-Case 1

Items	Santos et al.[32]	Santos et al.[32] recalculated	Our procedure
Number of compressors and expanders	5	5	4
Work consumed (kW)	6426.1	5445.4	5829.3
WEN capital cost ($/year)	3,926,760	3,678,576	4,415,706
WEN operational cost ($/year)	2,924,114	2,477,876	2,652,573
Number of heat exchanger units	9	9	6
Total heat exchanger area (m^2)	7135.5	7081.5	6016.9
Cold utility consumption (kW)	8818.3	7907.4	8290.8
HEN capital cost ($/year)	1,186,477	1,176,800	1,044,823
HEN operational cost ($/year)	881,837	790,736	829,080
Total annualized cost ($/year)	8,919,188	8,123,989	8,942,178

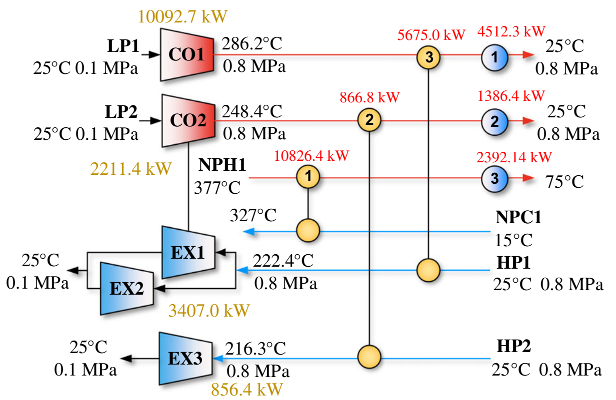

FIGURE 10 Optimal Minimal WHEN structure for Example 3-Case 2

TABLE 9 The results overview of Example 3-Case 2

Items	Case 2
Number of compressors and expanders	5
Work consumed (kW)	10092.7
Work generated (kW)	4263.4
WEN capital cost ($/year)	4,528,700
WEN operational cost ($/year)	3,040,583
Number of heat exchanger units	6
Total heat exchanger area (m^2)	6016.9
Hot utility consumption (kW)	–
Cold utility consumption (kW)	8290.8
HEN capital cost ($/year)	1,044,823
HEN operational cost ($/year)	829,080
Total annualized cost ($/year)	9,443,186

Case 1. In this case, the SSTC is used for work exchange. The results indicate that LP1 and LP2 are first compressed to 0.8 MPa (286.2 and 248.4°C, respectively) before they are both cooled to 25°C. HP1 and HP2 are first heated to 222.4 and 216.3°C, respectively before they are both expanded to 0.1 MPa (25°C). Figure 9B shows our optimal WHEN configuration (upper part where CO/EX in rectangles show the compression/expansion tasks) and the corresponding SSTC (lower part). In the WEN, a helping motor is required to make up for the deficient work (5829.3 kW). In the HEN, the heat transfer area is equal to 2779.4 m^2 (E1), 239.4 m^2 (E2), 1302.0 m^2 (E3), 1086.0 m^2 (C1), 298.5 m^2 (C2), and 311.8 m^2 (C3). The TAC for this case is 8,942,178 $/year, in which IC^{WEN} = 4,415,706 $/year, OPC^{WEN} = 2,652,573 $/year, IC^{HEN} = 1,044,823 $/year, OPC^{HEN} = 829,080 $/year.

Compared with Santos et al.,[32] our approach yields a WHEN structure with a similar TAC (0.26% higher than the minimum TAC in the literature[32]). However, as shown in Figure 9, our WHEN structure is simpler with a smaller number of heat exchanger units (6 vs. 9), the minimum number and consequently without energy loops. This is one reason why our cost is slightly higher than Santos et al.[32] In addition, the work consumed by CO1 in our WHEN structure is much higher because our Minimal WHEN structures only allow one heating/cooling task of each process stream. Therefore, the situation that LP1 had two cooling tasks in the literature is absent in our network, leading to higher TAC in our results. Another difference compared with the literature is that we do not use the polytropic work equations and the assumptions of ideal gas behavior as well as constant heat capacity. To estimate the influence of the different methods on pressure equipment calculations, one needs to recalculate the solutions using the method of isentropic compression/decompression adjusted by efficiency. Because the temperatures change the heat demand/supply of the streams is also readjusted. The results comparison is shown in Table 8. We remark that Santos et al.[32] used a metaheuristics that has a proven record of getting close to a global optimum, even though they cannot guarantee it.

First, the deviation between the reported values by Santos et al.[32] and the recalculated ones (~10%) illustrates the significant difference between the two calculation methods. However, the simpler solution obtained by our method also departs by approximately 10%

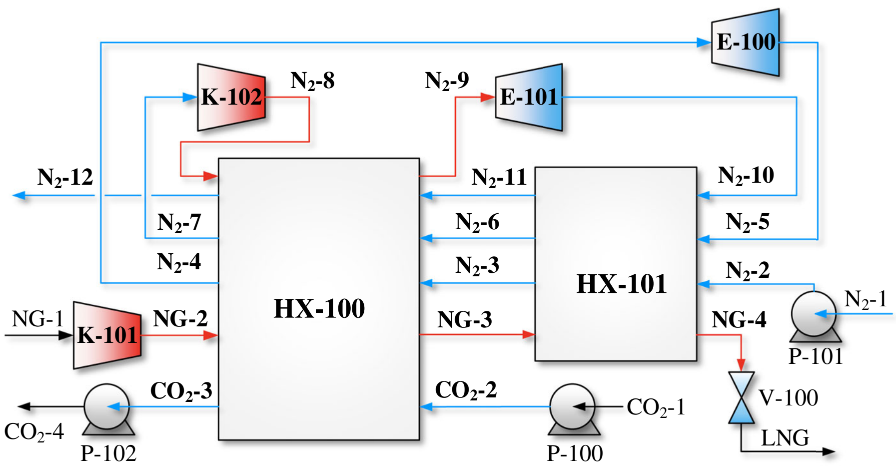

FIGURE 11 Process flow diagram for the offshore LNG process (Aspelund et al.[9])

TABLE 10 Stream data for Example 4

Stream	T^{supply} (°C)	T^{target} (°C)	P^{supply} (MPa)	P^{target} (MPa)	F (mol)	Fcp (kW/K)	h (kW/m^{2}K)
HP1 (N_2-4–N_2-7)	−54.4	−40	10	1	35.70	–	0.1
LP1 (N_2-7–N_2-9)	−40	−40	1	2	35.70	–	0.1
HP2 (N_2-9–N_2-12)	−40	20	2	0.1	35.70	–	0.1
NPH1 (NG-2–NG-4)	46.65	−8	10	10	–	3.46	0.1
NPH2 (NG-2–NG-4)	−8	−75.8	10	10	–	5.14	0.1
NPH3 (NG-2–NG-4)	−75.8	−168.4	10	10	–	3.51	0.1
NPC1 (CO_2-2–CO_2-3)	−52.03	−20.6	6	6	–	5.19	0.1
NPC2 (CO_2-2–CO_2-3)	−20.6	20	6	6	–	6.10	0.1
NPC3 (N_2-2–N_2-4)	−169.7	−102.1	10	10	–	2.48	0.1
NPC4 (N_2-2–N_2-4)	−102.1	−54.4	10	10	–	1.80	0.1
Hot utility	110	110	–	–	–	–	1.0
Cold utility	−180	−180	–	–	–	–	1.0
Cost data (US$/kW-year)							
$\widehat{COE}$	455.04	$\widehat{POE}$	0	$\widehat{Chu}$	337	$\widehat{Ccu}$	1000

TABLE 11 Capital cost parameters for Examples 4

Equipment	$\hat{a}$	$\hat{b}$	$\hat{c}$
Heat exchanger	111154.75	648.66	0.1771
Compressor with a motor	0	47840.41	0.62
Expander with a generator	0	2691.00	0.81
Motor/generator	0	0	0

from the recalculated solution of the literature. The difference can be explained by the fact that the structure of Santos et al.[32] is not a Minimal structure. Indeed, streams LP1 and LP2 have thermal tasks before and after the compressor. In addition, there are two expanders, which in principle could be considered as one because there is no heat exchange in between them. Incidentally, even though there are no fixed costs associated, a merging would be beneficial since the cost exponent is less than one. Nonminimal WHEN structures will be addressed in follow-up work.

As per computational aspects, the results in the literature are obtained in 20 min using meta-heuristic techniques. With our method, the global optimal solution of this case is obtained in 217 s. The number of stream-path combinations explored is 16.

Case 2. Although the use of the SSTC can be seen in many prior works on WHEN synthesis, it is a structure in which the work exchange of all compressors and expanders are achieved on the same shaft, possibly leading to control problems and not being flexible to parameter changes. In contrast, turboexpanders are structures in which only one compressor and one expander are located on the same shaft to achieve work exchange, and they are common in industry. In this case, turboexpanders are applied in the WEN. Figure 10 depicts the optimal WHEN configuration in this case, where the compressor CO_2 and the expander EX1 form

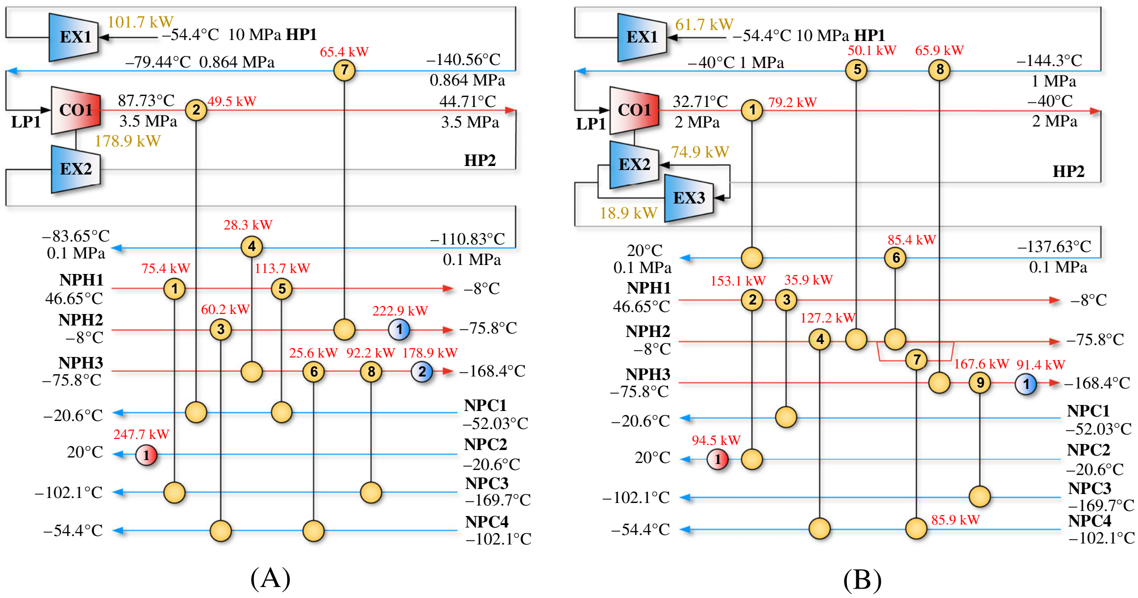

FIGURE 12 Optimal WHEN structure for Example 4: (A) Onishi et al.[17]; (B) Our Minimal WHEN

TABLE 12 Comparison of results for Example 4

Items	Onishi et al.[17]	Recalculated	Our procedure
Number of compressors and expanders	3	3	4
Work consumed (kW)	–	–	–
Work generated (kW)	101.7	64.4	80.61
WEN capital cost ($/year)	267,411	227,608	151,296
WEN operational cost ($/year)	0	0	0
Number of heat exchanger units	11	11	11
Total heat exchanger area (m^2)	384.1	351.8	901.4
Hot utility consumption (kW)	247.7	247.7	94.53
Cold utility consumption (kW)	401.8	369.0	91.44
HEN capital cost ($/year)	265,550	261,653	328,757
HEN operational cost ($/year)	485,232	452,491	123,293
Total annualized cost ($/year)	1,018,192	941,751	612,023

a turboexpander. The heat transfer area is the same as Case 1. The TAC is 9,443,186 $/year, in which IC^{WEN} = 4,528,700 $/year, OPC^{WEN} = 3,040,583 $/year, IC^{HEN} = 1,044,823 $/year, and OPC^{HEN} = 829,080 $/year. Although the TAC is larger than Case 1 (9,443,186 vs. 8,942,178 $/year), this WHEN configuration is more realistic. More information about the results are listed in Table 9. The global optimal solution is obtained in 202 s.

Example 4. This example is a design of an offshore LNG process, which was proposed by Aspelund et al.[9] In this example, natural gas is liquefied to produce LNG, whereas liquid carbon dioxide (LCO_2) and liquid inert nitrogen (LIN) act as cold carriers. Aspelund et al.[9] demonstrated, via extended pinch analysis and design (ExPAnD), that the use of a sequential expansion, compression and expansion route of the LIN stream can considerably reduce utility requirements. Figure 11 shows the process flow diagram of the offshore LNG process after applying the ExPAnD methodology. Wechsung et al.[15] provided the stream data for the optimization of the LNG process, where the streams (N_2, CO_2, and NG) are divided into several individual streams to fit the actual heating or cooling curves. A feature of the problem discussed in this example is that it is related to a specific choice of LNG system with specific stages and specific refrigeration cycles. We also remark that refrigeration cycles are not well described by the current WHEN problem framework. Indeed, the WHEN problem requires streams that are well defined having initial and final states. However, in cycles, there is no initial and final state, all the states in the cycle being variables. This issue has been sorted out by various authors by picking one state of the cycle and tearing the cycle, making the initial and final states coincide. The choice of this state is a simplification, which can only be avoided by generalizing the WHEN model, a task we do not undertake in this work. In addition, the heat capacity flow rate of the N_2 stream is constant with variable pressure (0.1–10 MPa), which may lead to infeasibility. For example, the specific heat capacity (*cp*) of N_2 varies from 29.21 to 40.77 kJ/(kmol K) with fixed temperature -54.4°C and the given range of pressure (0.1–10 MPa). In other words, there is a 40% fluctuation in the *cp* value, which corresponds to about 40% fluctuation in work consumed or generated in the WEN and about 40% fluctuation in the heat load of the N_2 stream in the HEN. To remedy these issues, we applied the process diagram shown in Figure 11 and fixed the outlet pressure of the expanders (E-100 and E-101) and the compressor (K-102) based on the design of Aspelund and Gundersen,[6] while the work consumed or generated in the WEN and the heat capacity of the N_2 stream are rigorously calculated based on PR-EOS as mentioned in Pressure Equipment Calculation. In addition, the outlet temperature of N_2 is fixed at 20°C. Same as Wechsung et al.,[15] the streams (N_2, CO_2, and NG) are divided into several individual streams to fit the actual heating or cooling curves. In general, there are 10 individual process streams considered in the WHEN synthesis problem, of which three streams are pressure-change streams. The stream data are listed in Table 10. In addition, we use $\hat{\eta}^{C}=0.7$, $\hat{\eta}^{E}=0.7$, $\hat{fac}=0.18$, $\hat{EMAT}=5$ K. The parameters for cost are listed in Table 11.

The results indicate that all pressure-change streams have a pressure-change first before they are heated or cooled to their target temperatures as shown in Figure 12. In the optimal WHEN the compressor CO1 and the expander EX2 form a turboexpander. In the HEN, the heat transfer area is equal to 111.4 m^2 (E1), 96.9 m^2 (E2), 33.9 m^2 (E3), 131.1 m^2 (E4), 50.2 m^2 (E5), 54.0 m^2 (E6), 94.5 m^2 (E7), 54.9 m^2 (E8), 218.4 m^2 (E9), 10.7 m^2 (H1), and 45.5 m^2 (C1). The TAC for this case is 613,023 \$/year, in which IC^{WEN} = 159,973 \$/year, IC^{HEN} = 328,757 \$/year, OPC^{HEN} = 123,293 \$/year.

Onishi et al.[17] first fixed a specific route of pressure changes and the position of heaters and coolers and then synthesized the WHEN. The TAC for the WHEN structure of Onishi et al.[17] using our cost correlations is 1,018,192 \$/year (Onishi et al.[17] did not provide the cost parameters), with capital and operational costs the same as the results in the reference. Considering that the literature results were obtained using ideal gas law and polytropic equations, we recalculated the solutions using our method of isentropic change adjusted by efficiency followed by recalculations of the thermal tasks. The recalculated TAC of the WHEN is 941,751 \$/year. Therefore, our approach yields a more economical WHEN structure with a 35.0% reduction of the TAC compared with the results presented by Onishi et al.[17] The main difference lies in the consumption of cold utility. Although more heat exchanger area is required by our WHEN (901.4 vs. 351.8 m^2), the hot and cold utility cost is greatly reduced (123,293 vs. 452,491 \$/year). More detailed information can be seen in Table 12. The global optimal solution of this case is obtained in 9 h, where the HEN calculations take the majority of the time, which is consistent with the time it takes for similar size problems. Unfortunately, few alternative approaches can guarantee global optimality for problems of this size. The number of stream-path combinations explored is 8.

10 | CONCLUSIONS

Work and heat consumption play an important role in the energy management of process industries. Because of the highly nonlinear and nonconvex nature of WHEN models, the synthesis problem is quite difficult to solve. To address this, we propose a new concept of Minimal WHEN structures and provide a framework to obtain globally optimal solutions for these types of WHENs. Based on enumerating possible combinations of feasible thermodynamic paths of streams, the framework decomposes the WHEN into a WEN and a HEN for each enumerated candidate structure, which are optimized separately. The PR-EOS is applied in pressure equipment calculation to guarantee the feasibility and accuracy of the obtained WHEN configuration. Turboexpanders and heat exchangers are applied for energy recovery. Also, our optimization procedure guarantees global optimality. Four examples from small-scale to large-scale problems are employed to illustrate the accuracy and effectiveness of the proposed approach. The results of each example compare favorably with literature results, except in one case, where the literature identifies a nonminimal network that is better than the minimal network we obtain. Addressing this case is part of subsequent work.

NOMENCLATURE

Subscripts

i	streams needing cooling in the HEN
j	streams needing heating in the HEN
k	HEN stages
p	streams that are compressed
pm	pressure manipulation units
q	streams that are decompressed in expanders
s	process streams
struc	WHEN structures

Sets

COM	streams using a compressor for compression
EXP	streams using a expander for expansion
HP	streams with target pressure smaller than inlet pressure
I	streams needing cooling in the HEN

J streams needing heating in the HEN
LP streams with target pressure larger than inlet pressure
NPC cold process streams with no pressure change
NPH hot process streams with no pressure change
PM pressure manipulation
VAL streams using a valve for expansion

Parameters

$\hat{a}$ cost correlation factor
$\hat{b}$ cost correlation factor
$\hat{B}$ parameter used to denote different design situations
$\hat{BM}$ big-M for relaxation of constraints
$\hat{c}$ cost correlation factor
$\hat{C}cu$ cold utility price
$\hat{C}hu$ hot utility price
$\hat{C}OE$ selling cost of electricity
$\hat{E}MAT$ exchanger minimum approach temperature
$\hat{F}$ flow rates of process streams
$\hat{f}ac$ annualization factor
$\hat{h}$ film heat transfer coefficient of process streams
$\hat{H}^{supply}$ supply specific enthalpy of process streams
$\hat{H}^{target}$ target specific enthalpy of process streams
$\hat{P}^{supply}$ supply pressure of process streams
$\hat{P}^{target}$ target pressure of process streams
$\hat{P}OE$ purchase cost of electricity
$\hat{T}^{supply}$ supply temperatures of process streams
$\hat{T}^{target}$ target temperatures of process streams
$\hat{W}LP^{real}$ power of the compressors required by LP streams
$\hat{W}HP^{real}$ Power of the expanders generated by HP streams
$\hat{\eta}^{C}$ isentropic efficiency of compressors
$\hat{\eta}^{E}$ isentropic efficiency of expanders

Binary variables

y^{C} binary variable to denote compressor
y^{E} binary variable to denote expander
y^{HG} binary variable to denote help generator
y^{HM} binary variable to denote help motor
y^{TE} binary variable to denote turboexpander
z Binary variable to denote heat recovery exchanger
zcu binary variable to denote cooler
zhu binary variable to denote heater

Continuous variables

cp specific heat capacities of process streams in the HEN
cpo capital cost of different equipment
H^{dis} discharge specific enthalpy of streams in pressure-change units
H^{suc} suction specific enthalpy of streams in pressure-change units
IC^{HEN} annualized capital cost of the HEN
IC^{WEN} annualized capital cost of the WEN
OPC^{HEN} annualized operational cost of the HEN
OPC^{WEN} annualized operational cost of the WEN
T^{dis} discharge temperature streams in pressure-change units
$T^{dis,isen}$ discharge temperature of streams following the isentropic process
T^{IN} inlet temperatures of process streams in the HEN
T^{OUT} outlet temperatures of process streams in the HEN
WG work provided by the help generator
WH work to generate power by the help motor
WHP^{res} residual power produced by HP streams
WLP^{res} residual power needed by LP streams
WTE power exchanged between process streams

AUTHOR CONTRIBUTIONS

Qucheng Lin: Conceptualization (equal); investigation (equal); methodology (equal); validation (lead); writing – original draft (equal); writing – review and editing (equal). **Zuwei Liao:** Funding acquisition (lead); methodology (supporting); project administration (equal); supervision (equal). **Miguel J. Bagajewicz:** Conceptualization (equal); investigation (equal); methodology (equal); writing – original draft (equal); writing – review and editing (equal).

ACKNOWLEDGMENTS

The financial support provided by the Project of National Natural Science Foundation of China (21822809 and 21978256). Miguel Bagajewicz performed part of this work with support of the Rio de Janeiro State University (Brazil) as a Visiting Researcher—PAPD Program and is now Visiting Professor at the Federal University of Rio de Janeiro (Brazil).

DATA AVAILABILITY STATEMENT

Data openly available in a public repository that issues datasets with DOIs.

ORCID

Qucheng Lin https://orcid.org/0000-0002-8946-4930
Zuwei Liao https://orcid.org/0000-0001-9063-1049
Miguel J. Bagajewicz https://orcid.org/0000-0003-2195-0833

REFERENCES

1. Amini-Rankouhi A, Huang Y. Prediction of maximum recoverable mechanical energy via work integration: a thermodynamic modeling and analysis approach. *AIChE J*. 2017;63(11):4814-4826.
2. Huang Y, Fan L. Analysis of a work exchanger network. *Ind Eng Chem Res*. 1996;35(10):3528-3538.
3. Yu H, Fu C, Gundersen T. Work exchange networks (WENs) and work and heat exchange networks (WHENs): a review of the current state of the art. *Ind Eng Chem Res*. 2020;59(2):507-525.
4. Fu C, Gundersen T. Heat and work integration: fundamental insights and applications to carbon dioxide capture processes. *Energ Conver Manage*. 2016;121:36-48.
5. Aspelund A, Tveit SP, Gundersen T. A liquefied energy chain for transport and utilization of natural gas for power production with CO_2 capture and storage—Part 3. The combined carrier and onshore storage. *Appl Energy*. 2009;86(6):805-814.
6. Aspelund A, Gundersen T. A liquefied energy chain for transport and utilization of natural gas for power production with CO_2 capture and

storage—Part 2. The offshore and the onshore processes. *Appl Energy*. 2009;86(6):793-804.
7. Aspelund A, Gundersen T. A liquefied energy chain for transport and utilization of natural gas for power production with CO_2 capture and storage—Part 1. *Appl Energy*. 2009;86(6):781-792.
8. Aspelund A, Gundersen T. A liquefied energy chain for transport and utilization of natural gas for power production with CO_2 capture and storage—Part 4. Sensitivity analysis of transport pressures and benchmarking with conventional technology for gas transport. *Appl Energy*. 2009;86(6):815-825.
9. Aspelund A, Berstad DO, Gundersen T. An extended pinch analysis and design procedure utilizing pressure based exergy for subambient cooling. *Appl Therm Eng*. 2007;27(16):2633-2649.
10. Fu C, Gundersen T. Correct integration of compressors and expanders in above ambient heat exchanger networks. *Energy*. 2016;116:1282-1293.
11. Fu C, Gundersen T. Appropriate placement of compressors and expanders in above ambient processes. *Chem Eng Trans*. 2015;45:643-648.
12. Fu C, Gundersen T. Sub-ambient heat exchanger network design including expanders. *Chem Eng Sci*. 2015;138:712-729.
13. Fu C, Gundersen T. Integrating compressors into heat exchanger networks above ambient temperature. *AIChE J*. 2015;61(11):3770-3785.
14. Fu C, Gundersen T. Integrating expanders into heat exchanger networks above ambient temperature. *AIChE J*. 2015;61(10):3404-3422.
15. Wechsung A, Aspelund A, Gundersen T, Barton PI. Synthesis of heat exchanger networks at subambient conditions with compression and expansion of process streams. *AIChE J*. 2011;57(8):2090-2108.
16. Duran MA, Grossmann IE. Simultaneous optimization and heat integration of chemical processes. *AIChE J*. 1986;32(1):123-138.
17. Onishi VC, Ravagnani MASS, Caballero JA. Simultaneous synthesis of heat exchanger networks with pressure recovery: optimal integration between heat and work. *AIChE J*. 2014;60(3):893-908.
18. Yee TF, Grossmann IE. Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis. *Comput Chem Eng*. 1990;14(10):1165-1184.
19. Pavão LV, Costa CBB, Ravagnani MASS. A new framework for work and heat exchange network synthesis and optimization. *Energy Convers Manage*. 2019;183:617-632.
20. Razib MS, Hasan MMF, Karimi IA. Preliminary synthesis of work exchange networks. *Comput Chem Eng*. 2012;37:262-277.
21. Onishi VC, Ravagnani MASS, Caballero JA. Simultaneous synthesis of work exchange networks with heat integration. *Chem Eng Sci*. 2014;112:87-107.
22. Huang K, Karimi IA. Work-heat exchanger network synthesis (WHENS). *Energy*. 2016;113:1006-1017.
23. Zhuang Y, Liu L, Liu Q, Du J. Step-wise synthesis of work exchange networks involving heat integration based on the transshipment model. *Chin J Chem Eng*. 2017;25(8):1052-1060.
24. Onishi VC, Quirante N, Ravagnani MASS, Caballero JA. Optimal synthesis of work and heat exchangers networks considering unclassified process streams at sub and above-ambient conditions. *Appl Energy*. 2018;224:567-581.
25. Nair SK, Rao HN, Karimi IA. Framework for work-heat exchange network synthesis (WHENS). *AIChE J*. 2018;64(7):2472-2485.
26. Lin Q, Liao Z, Sun J, Jiang B, Wang J, Yang Y. Targeting and design of work and heat exchange networks. *Ind Eng Chem Res*. 2020;59(27):12471-12486.
27. Yu H, Fu C, Vikse M, He C, Gundersen T. Identifying optimal thermodynamic paths in work and heat exchange network synthesis. *AIChE J*. 2019;65(2):549-561.
28. Vikse M, Watson HAJ, Barton PI, Gundersen T. Nonsmooth formulation for handling unclassified process streams in the optimization of work and heat exchange networks. *Ind Eng Chem Res*. 2019;58(22):9526-9539.
29. Chang C, Peccini A, Wang Y, Costa ALH, Bagajewicz MJ. Globally optimal synthesis of heat exchanger networks. Part I. Minimal networks. *AIChE J*. 2020;66(7):e162667.
30. Costa ALH, Bagajewicz MJ. 110th anniversary: on the departure from heuristics and simplified models toward globally optimal design of process equipment. *Ind Eng Chem Res*. 2019;58(40):18684-18702.
31. Faria DC, Bagajewicz MJ. A new approach for global optimization of a class of MINLP problems with applications to water management and pooling problems. *AIChE J*. 2012;58(8):2320-2335.
32. Santos LF, Costa CBB, Caballero JA, Ravagnani MASS. Synthesis and optimization of work and heat exchange networks using an MINLP model with a reduced number of decision variables. *Appl Energy*. 2020;262:114441.
33. Zhao L, Riensche E, Blum L, Stolten D. Multi-stage gas separation membrane processes used in post-combustion capture: energetic and economic analyses. *J Membr Sci*. 2010;359(1):160-172.

SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

How to cite this article: Lin Q, Liao Z, Bagajewicz MJ. Globally optimal design of Minimal WHEN systems using enumeration. *AIChE J*. 2023;69(1):e17878. doi:10.1002/aic.17878