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Multiperiod work and heat integration

Leandro V. Pavão [a1], *Camila B. Miranda*[a], *Jose A. Caballero*[b], *Mauro A. S. S. Ravagnani* [a], *Caliane B. B. Costa* [a]

[a]Department of Chemical Engineering, State University of Maringá, Av. Colombo, 5790, Bloco D90, CEP 87020900, Maringá, PR, Brazil

[b]Institute of Chemical Process Engineering, University of Alicante, Ap. Correos 99, 03080 Alicante, Spain

Abstract

The synthesis of multiperiod heat exchanger networks (HEN) is a well-studied topic in heat integration. Several methods for identifying heat exchanger network designs that are able to feasibly operate under multiple conditions have been presented. Multiperiod models are certainly a notable form of achieving such resilient designs. In work and heat integration, however, solutions presented so far are for nominal conditions only. This work presents a step-wise optimization-based multiperiod work and heat exchange network synthesis framework. Hybrid meta-heuristic methods are used in the optimization steps. The methodology is able to obtain work and heat exchanger networks (WHENs) that are able to operate under multiple known scenarios. A set of critical conditions for stream properties in work integration is proposed. When these scenarios are modeled as finite operating periods (which are here referred to as non-nominal periods), a WHEN which can feasibly operate under nominal and critical conditions can be obtained. An example is tackled in two cases: the first, with one nominal and six critical, non-nominal periods; the second with two nominal and twelve non-nominal periods. Note that with that number of periods, the problem is considerably more complex than in multiperiod HEN synthesis (which usually comprises three or four periods). Solutions obtained with the present method are compared to those obtaining by simply merging single-period solutions obtained for each period individually. Capital investments are 30.2 % and 58.2 % lower in Cases 1 and 2 than in straightforwardly merged solutions. The capacity utilization parameters also demonstrate that the overdesign issue is notably reduced in these solutions.

Keywords: Optimization; Work and Heat Integration; Multiperiod Work and Heat Exchange Networks; Meta-heuristics; Process Synthesis

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[1] Corresponding author. Tel: +55 (44) 3011-4774, Fax: +55 (44) 3011-4793

E-mail address: leandropavao@gmail.com

1 Introduction

Work and heat integration (WHI) has become, in recent years, a noteworthy research field in process synthesis. The design and optimization of work and heat exchange networks (WHEN) is central in these discussions. WHEN synthesis shares much common ground with heat integration (HI) via heat exchanger networks (HEN). Briefly, the synthesis of WHEN consists in, given a set of process streams having high/low/constant pressure classifications, which may as well be classified as hot/cold/constant regarding operating temperature ranges, a set of pressure manipulation equipment (compressors, expanders, valves, work exchange machinery) must be allocated so that pressures reach their target values, as well as a set of temperature manipulation units (heaters, coolers, heat exchangers) for target temperatures. Heat and work may be exchanged among the process streams by heat exchangers and via direct/indirect work exchangers. Hence, energy may be recovered, leading to important monetary savings, as well as possible reduction in emissions caused by utility and power production.

Please, note that when we refer to work integration (WI), heat integration (HI) or work and heat integration (WHI), we are describing the procedures involved in designing energy-effective solutions for cases that require, respectively, pressure manipulation units only, temperature manipulation units only and both pressure and temperature manipulation units. These definitions, in general, comprise the synthesis of work exchange networks (WEN), heat exchanger networks (HEN) or work and heat exchange networks (WHEN). Note also that there are particular industrial cases of each of these matters. In this work, we approach the third one (WHEN synthesis), but the main WHI problem may be divided into sub-problems that may comprise WI only or HI only.

In preliminary design stages, HEN and WHEN are synthesized for nominal conditions. It must be noted, however, that material streams in industrial plants may undergo important disturbances in their supply conditions (temperatures, pressures, flowrates). Note that streams may originate not only from the process feed, but from unit operation outlets as well. Hence, these stream property disturbances may be due to raw material quality variations, possible malfunctions in separation unit operations, efficiency reduction in reactors (e.g., catalyst activity loss), fouling in heat exchangers, improper isolation, etc. These changes may also occur in well-defined cycles (for instance, according to seasons), giving rise to multiperiod synthesis problems. From authors' experience and flexibility-related works from the literature, some examples are: oilseed extraction plants which may use different raw materials biorefinery production quantities which may be altered among sugar, ethanol (first/second generation) and electricity [1,2], stream supply temperature in general industrial plants which may vary due to cyclical changes on weather conditions [3], etc.

In heat integration, flexibility and multiperiod optimization are mature topics. Several studies have approached the issues by proposing methodologies for synthesizing flexible or multiperiod HEN. Pioneer studies on the field were published in the 1980's. Floudas and Grossmann's methodology was based on sequential optimization models for the HEN structure and final configuration [4], which was later extended for heat exchanger sizing/by-pass optimization [5]. A flexibility analysis was performed for checking the feasibility of the network under uncertain conditions. In another study, Floudas and Grossmann [6] proposed a sequential multiperiod model for synthesizing HEN able to operate under a finite set of conditions. Several recent methods for considering flexibility in heat integration are based on the multiperiod concept for developing optimization models. The network must be able to feasibly operate under those conditions. In these models, in general, weights are assigned to each period (based on their estimated yearly duration or probability of occurrence). In the objective functions (total annual costs), operating costs are considered according to these durations. Aiming for automaticity, prominent studies have led to the development of simultaneous optimization models for multiperiod HEN synthesis. The works of Aaltola [7] and Verheyen and Zhang [8] used Yee and Grossmann's stagewise superstructure (SWS) concept [9] for developing multiperiod HEN synthesis models. In Aaltola's work [7], heat exchanger areas were calculated as a weighted average among all period areas, which would slightly underestimate costs. On the other hand, Verheyen and Zhang [8] were later able to formulate the problem considering, for capital cost calculations, the maximum area needed among those required for each period. Furthermore, some recent works are worth highlighting. For instance, the simultaneous model of Isafiade and Fraser [10] for multiperiod heat exchanger network synthesis, which used a superstructure based on temperature intervals (Interval Based MINLP Superstructure, IBMS); the improved version of Floudas and Grossmann's framework [6] presented by Miranda et al. [11]; the method of Kang et al. [12], which was based on the most representative duration of periods, the meta-heuristic-based method of Pavão et al. [13], and Jiang and Chang's [14] timesharing mechanism (TSM), which considered that a single set of heat exchangers could match different streams depending on the operating conditions. The TSM scheme was improved by Miranda et al. [15], who achieved solutions with lower TAC with a mathematical model solved via deterministic methods, and by Pavão et al. [16], who included a post-optimization step for the final structure. Jiang and Chang's TSM concept was also applied to the process integration project of a biorefinery by Oliveira et al. [17]. The interested reader is also referred to a state-of-the-art review on the flexibility topic for heat integration by Kang et al. [18].

Different from heat integration, simultaneous work and heat integration (WHI) via work and heat exchange networks (WHEN) is a more recent research field. The problem can be seen as an extension of heat integration in the sense that streams require not only temperature manipulations, but pressure changes as well. Hence, these processes may involve not only heaters, coolers and heat exchangers, but also pressure manipulation units such as compressors, turbines and valves. Work may be "exchanged" directly or indirectly. Direct work exchange is performed with machinery such as flow work exchangers [19]. Indirect work exchange is obtained via single-shaft coupling of turbines and compressors (i.e., conversion of pressure energy to mechanical energy and back to pressure energy) or by electricity generation from turbines that may be reused within the process in compressors (i.e., pressure energy to electricity and back to pressure energy). Note that work exchange equipment is not a recent technology. For instance, the aforementioned flow work exchanger was presented in 1967 [19], and an example of single-shaft-turbine-compressor (SSTC) coupling has been used in power recovery trains of fluid catalytic cracking plants since the 1960s [20]. However, first discussions on synthesizing work exchange networks (WEN) have arisen only in the 1990s [21]. The WEN synthesis problem is defined as, given a set of high- and low-pressure streams, defining a set of pressure manipulation units, including work exchangers for energy recovery. In the referred work [21], direct work exchangers are considered. This sort of apparatus consists in chambers divided by a floating piston head that transfers pressure energy from high pressure (HP) to low pressure (LP) fluids. More recent contributions considering this type of machinery include, for instance, the graphical method of Zhuang et al. [22]. An important contribution considering indirect work exchange via SSTC units in WEN was published by Razib et al. [23]. An optimization model based on total annual costs (TAC) was employed.

Discussion regarding synthesis of work and heat exchange networks are even more recent, and come forward as a promising field. The problem may be described as a merged WEN/HEN synthesis problem, i.e., given a set of process streams that can be classified either as hot, cold or of constant temperature and as high-, low- or constant-pressure, a set of temperature and pressure manipulation units must be allocated so that all streams reach their target conditions. These units may include recovery units such as heat exchangers and work exchange machinery. The work of Aspelund et al. [24] established fundamental heuristic rules for the placement of pressure manipulation units aiming for the optimal energy use in sub-ambient processes. Wechsung et al. [25] extended those concepts and included a mathematical programming exergy-based approach for minimizing irreversibility in the process. In the framework, streams could pass through a heat recovery region, which was modeled as a HEN. That concept was improved by Onishi et al. [26], who included the possibility of using SSTC units and used an annual capital/operating costs function to be minimized. Later, Onishi et al. [27] included aspects to their framework such as stream splits in work exchange stages and the possibility of SSTC coupling of several units in multiple shafts. Huang and Karimi [28] took as basis the WHEN synthesis model of Razib et al. [23] and replaced stages of heating/cooling via thermal utilities by heat exchange stages using Yee and Grossmann’s SWS [9]. Nair et al. [29] presented a detailed framework that comprises aspects such as phase-changing streams. Pavão et al. [30] presented the block-based superstructure, where calculation blocks for each unit type were placed in the pressure manipulation region, and also included the concept of each stream passing multiple times through a heat exchange region, previously used by Wechsung et al. [25] and Onishi et al. [26]. The method was later extended to evaluate multiple electricity-related scenarios [31] and practical operating constraints such as maximum number of coupled units and more realistic temperature limits for compressors and turbines [32]. A pinch-based approach was developed by Pavão et al. [33] for efficient determination of pressure manipulation routes in WHEN. The reader is also referred to state-of-the-art reviews on the WHEN matter including key concepts and promising research opportunities [34,35].

As it can be noted, WHI is an emergent area. Several topics that were approached and are even mature branches of HI have been scarcely or not yet studied for WHI. Multiperiod synthesis remains a literature gap for WHI. Not only the existence of such a gap must be highlighted, but also rationale for the development of such a multiperiod model. It is notable that temperature variations are often observed in process streams of industrial plants, which led to the development of several heat integration multiperiod models. In early design stages, this leads to a more efficiently integrated project than the application of oversizing a posteriori, after a nominal design. This is given to the fact that some interactions between heat exchange matches are not trivial to observe when multiple periods are being handled. Process stream pressure fluctuations occur in the industry as well, and also lead to oversizing of pressure manipulation equipment for proper control conditions [36]. This issue is, in general, dealt with locally by evaluation and sizing of each unit during late design stages, taking into account more specific factors such as controllability and placement in the factory layout. However, it is important that, as in HEN synthesis, we handle these issues in early design stages, when the general work and heat integration project is being developed. This is even more necessary since, as seen in previous works [37], pressure/temperature interactions are frequently non-intuitive in a single-period design, and may even be more difficult to predict when uncertainties in inlet conditions are accounted for.

This work aims to present a framework for multiperiod WHEN synthesis. Critical conditions (e.g., occasional temperature and flowrate changes) are analyzed, as well as operating conditions that vary cyclically on the plant. Note that multiperiod analysis gives rise to a considerably more complex problem than that for nominal conditions only. One must find a single set of units that is able to perform under all operating conditions scenarios, which implies additional areas in heat exchangers and power requirements for compressors and turbines. Hence, overdesign must be limited to a certain extent so that the additional investment is acceptable. Given the simultaneous alterations in temperature and pressure by pressure manipulation units (compressors/turbines/valves) and the nonlinearity of these functions, WHEN synthesis is a non-intuitive task. Furthermore, one needs to simultaneously consider all known period conditions which, in short, multiplies the number of problem decision variables by the number of periods. These aspects imply important additional intricacies to the problem in comparison to solving for nominal conditions only, and enables optimization-based approaches as efficient options for the task.

1.1 Multiperiod WHEN synthesis - problem statement

A set of process streams is given. These streams may be individually classified according to their supply/target temperatures (hot/cold/constant temperature) and pressures (high-/low-/constant-pressure). Temperature manipulations are performed by heaters (using a hot utility, HU), coolers (using a cold utility, CU) or heat exchangers matching two process streams for heat recovery. Pressure manipulations may be performed by compressors, turbines or valves. Compressors and turbines may be coupled by a single shaft. Coupled units are here called single-shaft-turbine-compressor (SSTC) units. Streams are assumed as ideal gases, with known heat capacities and polytropic exponents. Isentropic efficiencies for pressure manipulation units are known.

Nominal stream conditions may vary, giving rise to a finite set of known conditions. Each set is named as a “period”. Total annual costs are calculated from known functions for capital costs (CC) and operating costs (OC). Maximum heat exchanger area, compressor/turbine capacity or motor/generator power values among all periods are assumed for sizing units. Total annual costs must be minimized.

In this work, we assume a “nominal” period as one with plant design conditions. Note that under this definition a plant may operate under more than one “nominal” period, each with known yearly duration. Periods defined as “non-nominal” are those considered with critical conditions, which are due to, for instance, variations in raw material quality, flowrate fluctuations, etc., and whose durations may be estimated, but are not pre-established as in nominal periods. For instance, for the sake of resiliency, one may take into account the prediction that a plant operates with 5 % higher flowrate for a given stream than in its nominal conditions for around 2 % of its operating time. This is, to some extent, in line with the HEN resiliency concept described by Marseille et al. [38] by using a table of critical conditions. We discuss those conditions further in Section 2, and present a set of critical conditions to be used in WHEN synthesis.

2 Multiperiod work and heat integration framework

The multiperiod WHEN synthesis framework developed in this work involves the sequential utilization of WI, HI and WHI models. Consider the process streams set mentioned in the problem statement.

2.1 WI, HI and WHI mathematical models

This first model is named SP_PINCH (where SP stands for single-period, given that it is applied to each period separately):

$$\begin{array}{lll} (SP\_PINCH) & min & \{TAC = AreaCC + WorkCC + UtilOC + WorkOC\} \\ & s.t. & \text{Pinch-based equations [30]} \end{array} \quad (1)$$

where *AreaCC* regards the capital costs due to the total heat exchange area prediction provided by the Pinch-based model, *WorkCC* is the total capital costs for compressors and turbines, *UtilOC* are the total thermal utility costs obtained from the Pinch-based model and *WorkOC* are the total sales/costs from electricity production/requirements (note that *WorkOC* assumes a negative value if the plant yields electricity surplus to be sold).

The SP_PINCH model is a single-period model for defining pressure manipulation routes by considering predictions for operating and capital costs via Pinch-based concepts. Presence/absence of pressure manipulation units and their inlet/discharge temperatures are decision variables related to work integration. For instance, consider a hot, low-pressure stream at 300 K and 0.1 MPa with target conditions of 0.5 MPa and 250 K. A pressure manipulation route for that stream with a single compressor with inlet temperature of 270 K and discharge temperature of 350 K is identified. That means the original stream becomes two streams for heat integration: the first with supply/target temperatures of 300-270 K, and the second, which begins at the compressor discharge, with 350-250 K as supply/target temperatures. All these streams can be considered as comprising a heat integration problem. Pinch technology has heuristic methods for predicting minimum energy requirements for such a problem [39], as well as its minimal area [40,41] for a given heat recovery approach temperature (*HRAT*) value. Hence, *HRAT* is a decision variable in SP_PINCH as well. With minimum area and thermal utility predictions, as well as work-related decision variable values, it is possible to obtain an estimation for total annual costs. SP_PINCH thus attempts to minimize such a TAC value. The SP_PINCH model allows the coupling of unlimited pressure manipulation units to a single shaft with the possibility of including a helper motor/generator in case of power shortage/surplus. This is a simplifying assumption that may be difficult to implement in industry due to rotation speed and space limitations for the coupled units. However, it is satisfactory for cost estimation purposes.

SP_HEN (Eq. 2) is a HEN synthesis simultaneous model derived from Yee and Grossmann's SWS [9], with non-isothermal mixing assumption [42]. This sort of superstructure is well-studied in the literature. It is relatively simple in comparison to other simultaneous HEN synthesis models and with a proper solution approach it is able to find low-cost solutions efficiently. The MP_HEN model (Eq. 3) is a multiperiod HEN synthesis model that was developed in our previous study [13] as an extension of the single-period one (SP_HEN) presented in Ref. [42]. In-depth description of the models can be found in the referred works. Some important aspects of multiperiod HENs are worth stressing out. For instance, consider that $Area_{i,j,k,t}$ is a variable that stores required area for the heat exchanger matching streams i and j, in stage k of the SWS during period t. Assume that $Area_{1,1,1,1}$ = 100 m^2 and that $Area_{1,1,1,2}$ = 120 m^2. The MP_HEN model considers the maximum value between those two (120 m^2) for proceeding with capital costs related calculation.

The SP_WHEN model (Eq. 4) is a simultaneous model for single-period WHEN synthesis. This model gathers concepts from Wechsung et al. [25] and Onishi et al. [26] (multiple passes of streams through a heat recovery region with pressure manipulation units between these passes). The model is presented in detail in our previous study [32]. Decision variables are presence/absence of heat exchangers, their heat loads and stream split fractions, presence/absence of pressure manipulation units and their inlet/discharge temperatures. In the SP_WHEN model multiple shafts can be considered for units coupling. The number of coupled units in each shaft may be limited, which is a more realistic scenario. Moreover, this model allows the use of auxiliary valves for streams depressurizing, whose costs are much lower than those of turbines.

$$\begin{aligned} (SP\_HEN) \quad min \quad & \{TAC = AreaCC + UtilOC\} \\ s.t. \quad & \text{SWS-related equations [37]} \end{aligned} \tag{2}$$

In Eq. (2), *AreaCC* are the total capital costs for the heat exchanger set in the HEN and *UtilOC* are the operating costs for the required thermal utilities.

$$\begin{aligned} (MP\_HEN) \quad min \quad & \{TAC = AreaCC + \sum_t UtilOC_t \cdot D_t\} \\ s.t. \quad & \text{MP-SWS-related equations [10]} \end{aligned} \tag{3}$$

In Eq. (3), *AreaCC* are the sum of the capital costs of the largest heat exchanger for each match considered among the operating periods, $UtilOC_t$ are the total thermal utility costs for each period and D_t is the duration of each period (a real number between 0.0 and 1.0).

$$\begin{aligned} (SP\_WHEN) \quad min \quad & \{TAC = AreaCC + WorkCC + UtilOC + WorkOC\} \\ s.t. \quad & \text{WHEN equations [29]} \end{aligned} \tag{4}$$

In Eq. (4), the variables are similar to those in Eq. (1), but *AreaCC* and *UtilOC* are obtained from a HEN synthesis model rather than from Pinch-based predictions, and *WorkCC* and *WorkOC* are obtained considering practical operating constraints such as maximum number of couplings.

Finally, Table 1 shows a summary of specific features present in each presented model, with proper citations of works these features are based on. The last column of the referred table presents the MP_WHEN model, which is developed in the present work and presented in detail in Section 2.2.

Table 1. Summary of the models used in this work

Model	SP_PINCH	SP_HEN	MP_HEN	SP_WHEN	MP_WHEN
Periods	Single	Single	Multiple	Single	Multiple
Heat integration	Simplified (Pinch-based) [40,41]	SWS-based [9] w/ non-isothermal mixing	SWS-based [9] w/ non-isothermal mixing	Enhanced SWS with multiple passes [30]	Enhanced SWS with multiple passes [30]

Work integration	Simplified (All coupled) [30]	Absent	Absent	Block-based w/ practical constraints [32]	Block-based w/ practical constraints [32]
Developed in:	Ref. [33]	Ref. [42]	Ref. [13]	Ref. [32]	Present work

2.2 *Multiperiod WHEN (MP_WHEN) synthesis model*

The model developed in this work consists in a complete revamp of the simultaneous WHEN synthesis model presented in our previous study [32]. That WHEN model is based on the idea of streams passing multiple times through a heat exchange area. Between passes, pressure manipulation units are placed. These units are conceived as calculation blocks to be placed in free “slots” between the passes. The derivation of the model is similar regarding energy balances, pressure/temperature-related, shaft-work rate and heat exchange area calculations. The detailed derivation of these equations is presented in the referred work [32]. Figure 1 illustrates the master superstructure concept and the blocks used in the model. In the figure, two streams (one hot, low-pressure and one cold, high-pressure) are shown. As presented in the figure, the possible blocks that can be chosen in the structure may contain single compressors, turbines and valves, cooler/compressor and heater/turbine/valve sets. Final heaters/coolers are always placed at stream ends for final temperature corrections. Note that, for simplicity, some blocks such as individual compressors/turbines that were present in Ref. [32] were removed, since equivalent structures can be obtained with the hybrid blocks presented in Figure 1.

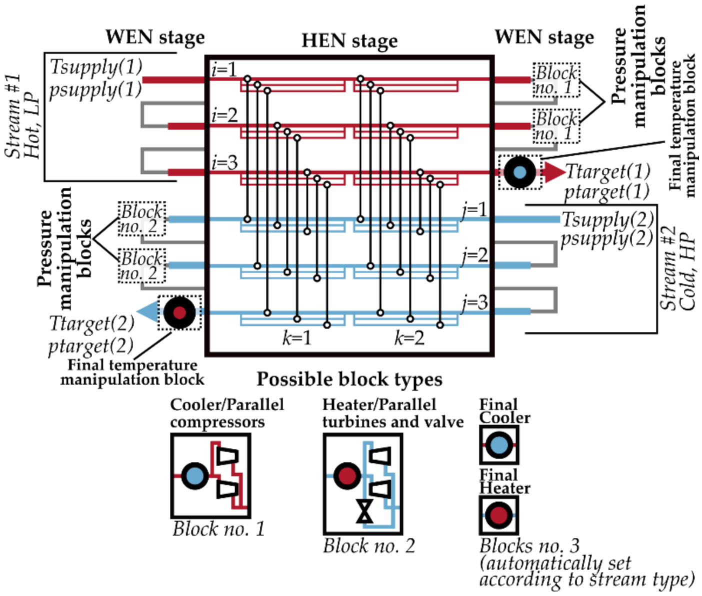

Figure 1. Simplified master WHEN synthesis superstructure [32] and its block types

In the new multiperiod model several variables are period-dependent, which means data for each period must be stored. This is performed by including a period-related set (*NP*) to the model, and adding its related index *t* to these variables. Note that these period-dependent variables are specifically design related ones, such as heat loads and compressors/turbines shaft-work rates. The superstructure here relates only to binary variables denoting presence/absence of units and is the same for all periods. If, for instance, a heat exchanger is "activated" in the superstructure, it is theoretically present in all periods, even if in some periods its heat load is null. The statement is also true for compressors/turbines existence and shaft-work rates.

This section presents equations for calculating operating and capital costs in order to provide some grasp regarding the multiperiod concept in WHI, as well as the objective function in the MP_WHEN model. The complete model with multiperiod-adapted energy balances and equations related to calculations of temperature, pressure and shaft-work rate are presented in Appendix A. Equations related to the multiperiod HEN stage are analogous to those derived in our previous meta-heuristic-based framework for multiperiod HEN synthesis [13].

Area-related capital costs are calculated according to the following equation:

$$\begin{aligned} AreaCC = & \sum_{i\in NH}\sum_{j\in NC}\sum_{k\in NS} AreaCost\left[\max_t\left(A_{i,j,k,t}\right)\right] \\ & + \sum_{w\in NG} AreaCost\left[\max_t\left(Acu_{w,t}\right)\right] + \sum_{w\in NG} AreaCost\left[\max_t\left(Ahu_{w,t}\right)\right] \\ & + \sum_{w\in NG} AreaCost\left[\max_t\left(Apre_{w,t}\right)\right] \end{aligned} \quad (5)$$

where *AreaCost* is a heat exchanger capital cost calculation function that requires area as input. These functions, in general, have the form $B+C\ [Area\ (m^2)]^{\beta}$. The *max* function returns the maximum value among those in all *t* periods for the respective area variable. $A_{i,j,k,t}$ are areas for heat exchangers matching process streams. $Acu_{w,t}$ and $Ahu_{w,t}$ are areas for final coolers and heaters in a given stream pass. The *w* index is a generic one and refers to stream passes through heat exchange region regardless of its identity. The matrix-based method used for linking stream pass index *w* to the *i* and *j* notation of the SWS as well as the *oi* and *oj* indexes (that refers to original identity of streams without considering passes) is described in Ref. [32]. $Apre_{w,t}$ are areas for pre-heaters/coolers that are present in compressor/turbine blocks.

Capital cost calculations related to pressure manipulation units are calculated as follows:

$$
\begin{aligned}
WorkCC = \sum_{w \in NG} \sum_{f \in NF} Comp_w \cdot ComCost\left[\max_t\left(ParWork_{w,f,t}\right)\right] \\
+ \sum_{w \in NG} Exp_w \\
\cdot \left\{ \sum_{f \in NF | f < Par(w)} TurCost\left[\max_t\left(ParWork_{w,f,t}\right)\right] + ValCost\left[\max_t\left(ParWork_{w,F,t}\right)\right] \right\} \\
+ \sum_{s \in NSh} MotCost\left\{\max_t\left[\max\left(0, \left(ComWork_{s,t} - TurWork_{s,t}\right)\right)\right]\right\} \\
+ \sum_{s \in NSh} GenCost\left\{\max_t\left[\max\left(0, \left(TurWork_{s,t} - ComWork_{s,t}\right)\right)\right]\right\}
\end{aligned}
\tag{6}
$$

where $Comp_w$ and Exp_w denote existence/absence of the compression/expansion block in the structure, *ComCost*, *TurCost* and *ValCost* are capital cost functions for compressors/turbines/valves, and *MotCost*/*GenCost* are capital cost functions for auxiliary motors/generators. $ParWork_{w,f,t}$ is the shaft-work in compressors/turbines (or relieved energy in valves) in the fraction f of given stream pass w, at period t. Note that, in the expansion case, the last stream split fraction ($f = F = Par_w$, where Par_w is the number of parallel units in a block) in the expansion block is always a valve. *ComWork* and *TurWork* are total shaft-work rate values for coupled compressors/turbines. Note that the inner *max* function guarantees motors/generators shaft-work as zero or with a positive value, which means only a motor or a generator is applied in a coupling at a given period.

The thermal utility-related operating costs in a given period t is given as follows:

$$
\begin{aligned}
UtilOC_t = & \sum_{oj \in NOC} Chu \cdot Qhu_{oj,t} + \\
& \sum_{oi \in NOH} Ccu \cdot Qcu_{oi,t} + \\
& \sum_{w \in NG} Comp_w \cdot Chu \cdot Qpre_{w,t} + \\
& \sum_{w \in NG} Exp_w \cdot Ccu \cdot Qpre_{w,t}
\end{aligned}
\tag{7}
$$

where *Chu*/*Ccu* are costs per *kWy* for hot and cold utilities, *Qhu*/*Qcu* are total heat loads required of hot and cold utilities in a given *oi* or *oj* stream. This is a sum of heat loads in pre-heaters/coolers in compression/expansion blocks and final temperature corrector blocks.

Operating costs for pressure manipulation units are calculated as follows:

$$WorkOC_t = Cel \cdot \left(SACompWork_t + \sum_{s \in NSh} \max\left[0, \left(ComWork_{s,t} - TurWork_{s,t}\right)\right] \right) - Rel \cdot \left(SATurbWork_t + \sum_{s \in NSh} \max\left[0, \left(TurWork_{s,t} - ComWork_{s,t}\right)\right] \right) \tag{8}$$

where *Cel* and *Rel* are electricity costs and revenue prices. *SACompWork* and *SATurbWork* are total shaft-work rates for standalone compressor and turbines (i.e., units that are not coupled to others).

The MP_WHEN optimization model is finally written as follows:

$$\begin{array}{lll} (MP\_WHEN) & min & \left\{ TAC = AreaCC + WorkCC + \sum_{t \in NP} \left(UtilOC_t + WorkOC_t\right) \cdot D_t \right\} \\ & s.t. & \text{Eqs. (5)-(8), (A-1)-(A-27) and HEN equations [10]} \end{array} \tag{9}$$

where D_t is the duration of a given period *t*.

Apart from total annual costs, another simple parameter that can be used in order to evaluate a multiperiod WHEN efficiency is the unit total required to total available capacity ratio (or, for simplicity, capacity ratio, *CR*). This parameter can be used for each unit individually, or in a more general manner, in a weighted average for each type of unit. That is, for a unit type, taking the weighted average of the total required capacity per period over the total available capacity. The weighting factors are period durations. The parameter is calculated after the model application. A generic definition is presented as follows:

$$CR = \sum_{t \in NP} D_t \cdot \left[\frac{\sum_{x \in NX} Cap_{x,t}}{\sum_{x \in NX} \left(\max_{tt \in NP} \left(Cap_{x,tt}\right) \right)} \right] \tag{10}$$

where *x* is a generic index for unit number, *tt* is an auxiliary period index, *Cap* is the unit capacity and may regard, in the WHEN case, to compressor/turbine shaft-work, motor/generator power or heat exchanger areas.

2.3 Model application scheme

For elucidation, Figure 2 can be followed along with the explanations in the present section. In the flow diagram, the number of nominal periods is represented as *N*. Every nominal scenario has *CS* associated critical scenarios, which are non-nominal periods. Period numbering (*t*) is standardized with nominal scenarios coming first (i.e., $t \leq$ N). For instance, a problem with two nominal periods has *N*=2. Non-nominal periods associated to a nominal period *t* are numbered from $N+(t\text{-}1)\ CS+1$ to $N+t\ CS$ ($t \leq N$). For instance, consider the aforementioned two-nominal-periods case (N = 2) with six critical scenarios each (CS = 6). The non-nominal periods for the nominal period 1 are from 3 to 8, and for period 2 are from 9 to 14.

A system was proposed to properly label solutions. These labels contain information regarding:

(i) if a period solution is a nominal or non-nominal one (N and/or NN);

(ii) the number of the period(s), which is placed between parentheses;

(iii) if the solution regards work (W), heat (H) or work and heat (WH) integration;

(iv) a solution number, used to differentiate solutions of the same type.

Following are some examples of solution nomenclature: N(1)-WH-1 regards a single-period work and heat integration solution for the nominal period 1. If, for instance, that solution is reused in another model as initial solution, the final solution for that optimization procedure will be named N(1)-WH-2. A multiperiod work and heat integration solution containing all nominal periods, without non-nominal ones may be N(All)-WH-1. An example containing nominal and non-nominal periods is N(All)-NN(All)-WH-1.

The multiperiod WHEN synthesis methodology consists, briefly, in: (i) work integration of each period individually considering simplified (Pinch-based) heat recovery; (ii) extraction of streams from (i) and heat integration model application to these streams; (iii) merging of work and heat integration solutions; (iv) application of multiperiod WHEN model to merged solutions. The detailed steps are as follows.

Step 1: for a nominal period t, the procedure begins with applying the SP_PINCH model to problem data for that period. The obtained solution is N(t)-W-1, and comprises pressure manipulation routes for the problem data and a prediction for the total heat exchange area. That topology is recorded and passed to non-nominal periods associated to it. As seen in Figure 2, in Step 1 for non-nominal periods, SP_PINCH is applied with the aforementioned fixed pressure manipulation topology, yielding solution NN(t)-W-1. Note that a fixed topology means that binary variable values are fixed. The set of pressure manipulation units may not change, only their sizes.

Step 2: for each nominal period t, in step 2.1 stream data is extracted from N(t)-W-1. That is, inlet/discharge temperatures from the pressure manipulation units present in the routes are considered as temperature data for a HEN synthesis problem. SP_HEN is then applied to these extracted streams. Pressure manipulation is omitted during the application of SP_HEN (i.e., pressure information is not even an input to the model). An illustration of streams extraction can be observed in Figure 3a. SP_HEN yields the solution N(t)-H-1. Here, in case that only one nominal period exists, Step 2 ends. Otherwise, we proceed to Step 2.2 and solutions N(1)-H-1 to N(N)-H-1 are then merged, rendering solution N(All)-H-1, which is a multiperiod solution. That means it is feasible in all periods considered (in this case, all nominal ones). The merging of a HEN solution is analogous to the WHEN merging presented in Figure 3b without the work-related variables. N(All)-H-1 is used as initial solution for the application of the MP_HEN model, which “refines” it, yielding solution N(All)-H-2. In case that $N = 1$, neither the merging nor the MP_HEN model is applied, and N(All)-H-2 is the same solution as N(1)-H-1. The HI topology of solution N(All)-H-2 (or N(1)-H-1 for $N = 1$) is then passed to all non-nominal periods. That HI structure is fixed, and SP_HEN is applied in all periods with it (i.e., binary variable values related to HI are fixed). Thus, for all non-nominal periods, a NN(*t*)-H-1 solution with the same topology as N(All)-H-2 is obtained.

Step 3: for nominal periods, the multiperiod heat integration solution N(All)-H-2 (N(1)-H-1 if only one nominal period is present) is merged to single-period work integration solutions for all nominal periods (N(1)-W-1 to N(*N*)-W-1), yielding a multiperiod work and heat integration solution for nominal periods (N(All)-WH-1). The MP_WHEN model is then applied to such a solution, refining it and yielding N(All)-WH-2. Regarding non-nominal periods, for a given $t > N$, a work integration solution NN(*t*)-W-1 obtained in Step 1 is merged to its respective heat integration solution NN(*t*)-H-1, obtained in Step 2. Such a merged solution is a work and heat integration single period solution NN(*t*)-WH-1. Given that, in general, non-nominal periods are critical conditions whose durations are expected to be much shorter that nominal ones, refinement via MP_WHEN is not applied to NN(*t*)-WH-1 for lowering total processing time.

Step 4: this stage begins with merging the nominal WHEN solution N(All)-WH-2 to all non-nominal single-period ones (NN(*N*+1)-WH-1 to NN(*T*)-WH-1, where *T* is the total number of periods), which yields N(All)-NN(All)-WH-1, i.e., a multiperiod solution comprising all nominal and non-nominal periods. MP_WHEN is then applied to that solution, yielding the final multiperiod WHEN solution of the methodology, N(All)-NN(All)-WH-2.

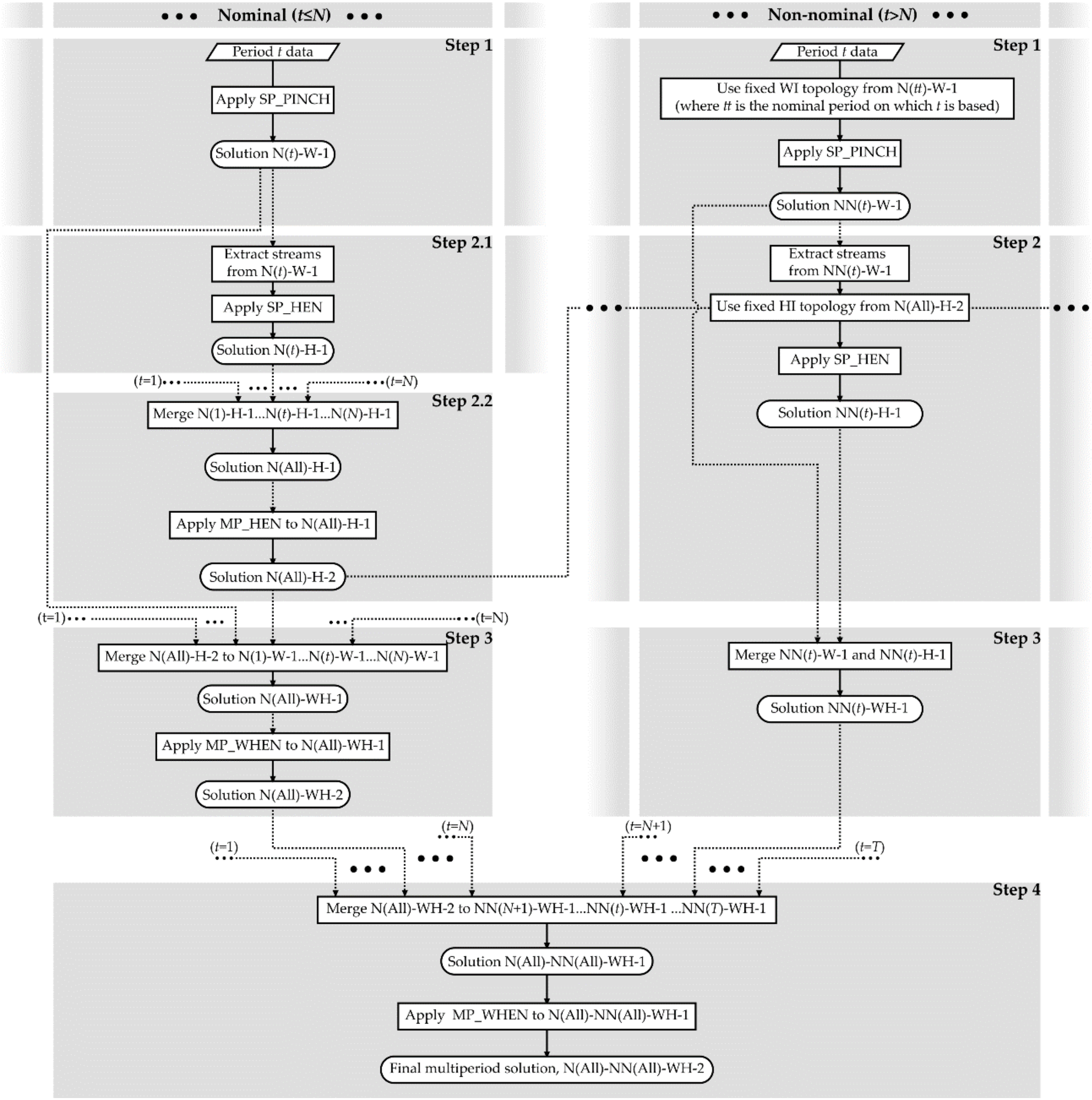

Figure 2. Flow diagram for the multiperiod WHEN synthesis methodology

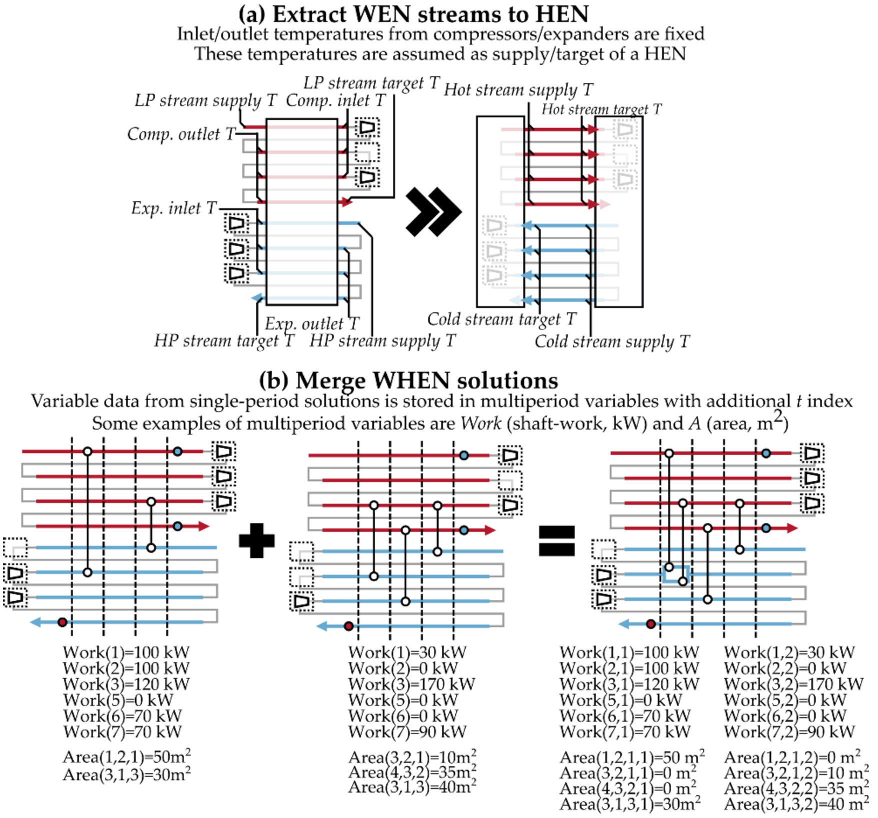

Figure 3. Extraction and merging procedures that are carried out in the methodology

2.4 *Implementation and solution methods*

All models were coded in a non-algebraic programming language (C++ in Microsoft Visual Studio 2019), which means that some implementations presented in the previous sub-section (e.g., max operators in Eqs. (5) and (6)) are made with simple *for*/*while*/*if* loops and condition statements. Hence, note that if the model were to be reproduced in algebraic environments such as GAMS it may require some adaptation.

The solution approaches are different for each model. However, they are mostly bi-level combinations of the Simulated Annealing (SA) [43] and Particle Swarm Optimization (PSO) [44] metaheuristics. The hybridization of meta-heuristics with other meta-heuristics or deterministic methods as bi-level approaches has been proven efficient in solving HEN synthesis problems since the late 1990’s [45]. These bi-level hybrid methods have evolved further throughout the 2000’s [46] and 2010’s [42] and demonstrated increasing capacity for solving HEN and WHEN synthesis problems to near-optimal solutions as computer technology also evolved. The main advantage of a bi-level hybrid approach for HEN/WHEN synthesis is the readiness in handling binary variables and continuous variables separately, each with an approach that is more efficient to that respective end. While a combinatorial optimization meta-heuristic can be used for the binary “outer” level, a continuous optimization meta-heuristic or a deterministic method can be used in the “inner” level for continuous variables.

For solving SP_PINCH, SA is used to repeatedly activate/deactivate compressors/turbines between stream passes. For each new combination proposed by the SA scheme, inlet/outlet temperature levels from pressure manipulation units as well as the *HRAT* variable for the heat exchange stage of the model are altered by multiple PSO applications. The SA/multi-PSO method was presented for solving the Pinch-based WHEN model in Ref. [33]. SP_HEN and MP_HEN use the Simulated Annealing – Rocket Fireworks Optimization (SA-RFO) method. In this method, SA proposes new topologies to an initial HEN structure (in general, as initial solution an “empty” structure is used, i.e., one with no heat exchange matches, but only hot/cold utilities at stream ends). The structure is changed at each SA iteration by addition of a random heat exchanger. RFO finds optimal heat loads for heat exchangers, as well as optimal stream split fractions in the structure. When a heat exchanger has null heat load in the configuration optimized by RFO, that unit is removed from the topology. RFO consists of an adaptation of SA for continuous spaces (continuous SA, CSA), which finds a single promising solution that is later incorporated into a random particle swarm for PSO application, providing the latter with a promising solution and enhancing its performance. The SA-RFO method was first presented in Ref. [42] for single-period HEN synthesis, and later adapted for multiperiod HEN in Ref. [13]. SA-RFO was later revamped for handling decision variables related to pressure manipulation units in work/heat exchange frameworks [30,32]. The methodology is used for solving the SP_WHEN model. In this work, it was adapted to handle multiple periods. SA and RFO moves were adapted for changing values in all periods under consideration.

The respective optimization procedures were applied five times to each model. The best solution among the five ones found for each model was considered. All optimization runs were carried out on a computer with an Intel® Core™ i7-8750H CPU @ 2.20GHz CPU and 8.00 GB of RAM.

3 Numerical example

In order to illustrate the present methodology, streams from the largest case study from the work of Onishi et al. [27] are taken as example. In its nominal case, it comprises two LP and three HP streams (Nominal Period 1 in Table 2). In all streams, supply and target temperatures are equal. However, the compression/expansion processes considered alter not only pressure, but temperatures as well, giving rise to heat recovery opportunities.

Table 2. Stream data for the numerical example

Nominal period 1							
Stream	Type	Tsupply (K)	Ttarget (K)	psupply (MPa)	ptarget (MPa)	CP (kW/K)	h (kW/(m^2·K))

1	LP	390	390	0.1	0.7	25.776	0.1
2	LP	420	420	0.1	0.9	36.810	0.1
3	HP	350	350	0.9	0.1	36.810	0.1
4	HP	350	350	0.85	0.15	14.730	0.1
5	HP	400	400	0.7	0.2	21.480	0.1
Nominal period 2							
1	LP	400	390	0.1	1.0	19.332	0.1
2	LP	440	420	0.1	0.6	18.405	0.1
3	HP	320	350	1.2	0.1	55.215	0.1
4	HP	320	350	1.0	0.1	14.730	0.1
5	Absent	-	-	-	-	0.0	-
	HU	680	680	-	-		1.0
	CU	300	300	-	-		1.0

Cel = 455.04 \$/kWy; Rel = 400.00 \$/kWy; Chu = 337.00 \$/kWy; Ccu = 100.00 \$/kWy;
$\eta_c = \eta_t = 0.7$; $\kappa = 1.4$; $\mu = 1.961$ K/MPa

The example is considered here as two cases. In the first, the streams as in the original example are considered as the nominal period. Six critical situations are considered as non-nominal scenarios, as shown in Table 3.

Table 3. Stream supply variations in critical scenarios

Scenario	LP-Tsupply	HP-Tsupply	LP-CP	HP-CP	LP-psupply	HP-psupply
Nominal						
Minimum expansion		–		–		–
Maximum compression	–		+		–	
Maximum hot utility		–		+		+
Maximum cold utility	+		+		–	
Maximum area	+	–	+	+	–	+
Maximum total pressure manipulation units capacity	–	+	+	+	–	+

Minus/plus signs mean 5 % increase/decrease of a given property (supply temperature/pressure, heat capacity flowrate). Note that this approach is inspired on that of Marselle et al. [38], which comprised, besides nominal HEN conditions, three critical scenarios, which are assumed as non-nominal periods, yielding four total periods. In the WHEN case, scenarios from Table 3 yield a multiperiod design case with seven total periods. The nominal period is assumed with a 90 % yearly duration, while the other six have equal durations within the remaining 10 % (1.67 % each). In the second case, the example is considered with two nominal periods (Table 2). The plant is expected to operate under each of these periods half of the total operating time. For WHEN resiliency, we use the conditions of Table 3 for critical scenarios for each period. Using the same nominal/non-nominal period duration assumption as in the first case (90 %/10 %) yields 45 % duration for each nominal period. There is a total of 12 non-nominal periods, evenly distributed within the remaining 10 % (0.83 % for each), which yields a problem with a total of 14 periods.

It is worth noting that in most multiperiod HEN cases seen in literature, the number of periods is around three or four, which demonstrates the considerable additional difficulty in solving this case for WHEN (which inherently has more decision variables due to pressure changes).

For a better grasping of the method, the methodology steps are presented in detail for Case 1. Figure 2 can be followed during the application. In Step 1, SP_PINCH is applied to the data presented for the nominal period (Nominal period 1 in Table 2). Pinch-based prediction values for total annual costs, total compression, expansion, thermal utilities and total heat exchange area are presented in Table 4. The topology of that solution is then used for the non-nominal periods 2-7. Results for those solutions are presented in Table 4 as well. The pressure manipulation routes obtained are presented in Figure 4. Bar charts of period capacity data are placed in the background for illustrating capacity usage. Maximum capacity bars are highlighted.

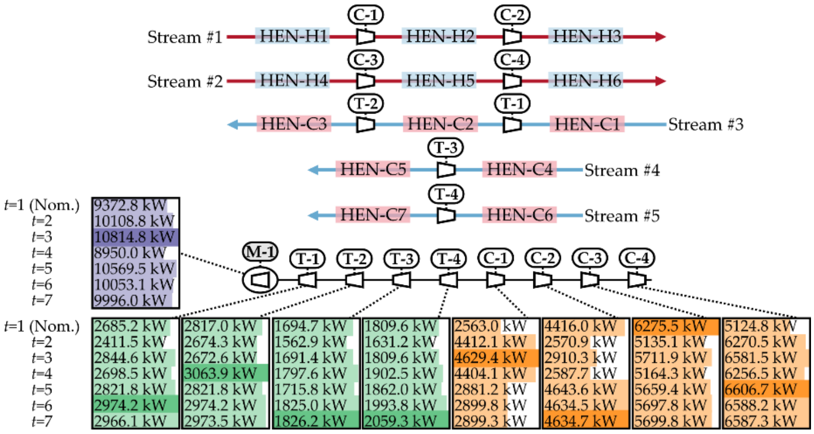

Figure 4. Work integration solution topology, resulting HEN streams and all compressors/turbines/motor power requirement/production in each period solution after Step 1 in Case 1

Figure 4 presents labels to parts of the streams that become streams for heat integration (e.g., Stream #1 becomes HEN-H1, HEN-H2 and HEN-H3). Compressors labeled from C-1 to C-4, turbines from T-1 to T-4, the motor M-1, as well as the shaft-work demanded/produced by these units at each period are also presented. The maximum values are highlighted. Evidently, if these highlighted values were used for sizing the pressure manipulation units, also considering the inlet/discharge temperatures obtained in the solutions, the work integration would be feasibly performed in the nominal and critical periods.

With the extraction of inlet/discharge temperatures and conversion into a HEN synthesis case (see Figure 3a), the SP_HEN model is then applied. Given that in Case 1 there is only one nominal period, Step 2.2 from Figure 2 is ignored, and the topology of Solution N(1)-H-1 is fixed for use in non-nominal periods. The solutions obtained in Step 2 are presented in Table 4. The topology for these solutions is shown in Figure 5. Stream supply and target temperatures are also presented. As in Figure 4, the main design variable (in this case, area) is shown for each period, with respective capacity bar charts in the background. If those individual HEN solutions were merged, a multiperiod solution with heat exchanger areas equal to the highlighted values would be obtained.

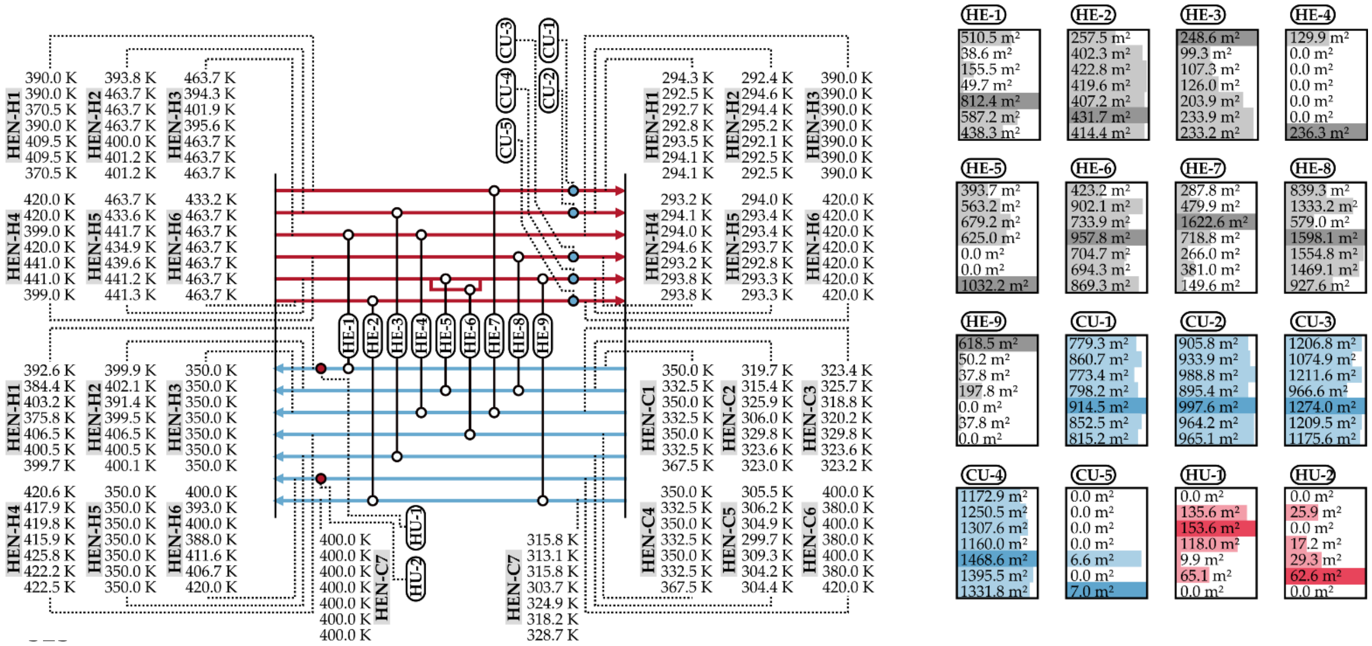

Figure 5. HEN topology, supply/target temperatures for extracted heat integration case and heat exchanger areas for each period solution (Step 2) in Case 1

In the third step, for the nominal period, the heat integration and the work integration solutions (N(1)-H-1 and N(1)-W-1) are merged into a work and heat integration configuration (solution N(1)-WH-1). Note that N(1)-WH-1 is a single-period solution. Hence, the application of MP_WHEN for refinement in Step 3, with one period only, is the same as applying SP_WHEN. The application of either one leads to N(1)-WH-2. The MP_WHEN model was solved considering a maximum of three coupled turbine/compressors per shaft (with the possibility of an additional auxiliary motor or generator) and eight total shafts. The solution is presented in Figure 6, and some summarized design aspects are shown in Table 4. For non-nominal periods, solutions work (NN(*t*)-W-1) and heat integration (NN(*t*)-H-1) are simply merged.

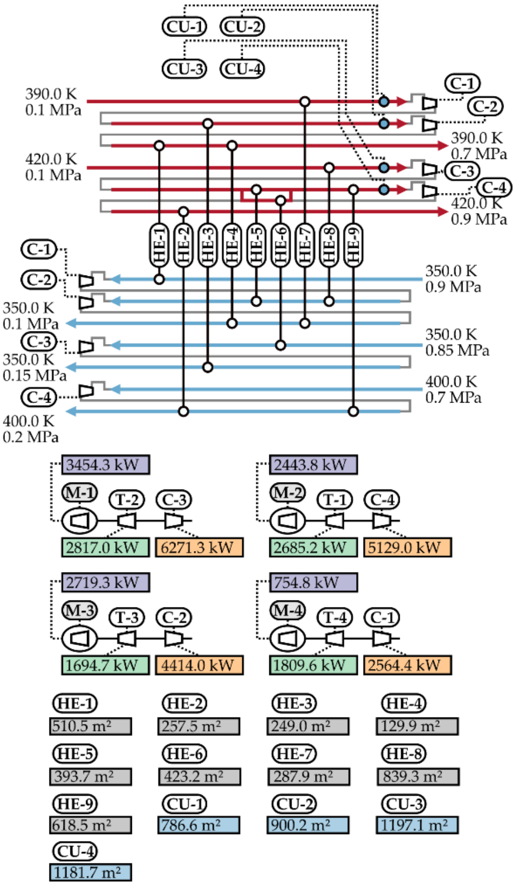

Figure 6. Solution N(1)-WH-2 for Case 1

Table 4. Single-period solutions found for Case 1

Step 1	Obj. Fun. ($/y)	Comp. (kW)	Exp. (kW)	HU (kW)	CU (kW)	Area (m^2)
N(1)-W-1	13,962,157	18,379	9,006	0	9,373	7,687
NN(2)-W-1	14,218,258	18,389	8,280	0	8,844	7,802
NN(3)-W-1	14,980,082	19,833	9,018	0	9,475	7,796
NN(4)-W-1	13,697,784	18,413	9,462	0	7,552	8,080
NN(5)-W-1	15,201,433	19,791	9,221	0	11,909	8,329
NN(6)-W-1	14,885,780	19,820	9,767	0	9,994	8,784
NN(7)-W-1	14,708,371	19,821	9,825	0	10,055	7,675
Step 2						
N(1)-H-1	13,999,579	18,379	9,006	0	9,373	7,774
NN(2)-H-1	14,870,201	18,389	8,280	1,968	10,812	8,150
NN(3)-H-1	14,859,311	19,833	9,018	1,636	11,111	8,773
NN(4)-H-1	14,695,568	18,413	9,462	1,711	9,262	8,648
NN(5)-H-1	14,516,908	19,791	9,221	334	12,243	8,650
NN(6)-H-1	14,683,547	19,820	9,767	1,235	11,229	8,384
NN(7)-H-1	14,178,426	19,821	9,825	0	10,055	8,596
Step 3						
N(1)-WH-2	13,975,807	18,379	9,006	0	9,372	7,775

Finally, work/heat integration solutions obtained in the previous step are merged in Step 4, yielding solution N(1)-NN(All)-WH-1, whose TAC is 15,679,303 $/y. After the final application of MP_WHEN (with the constraint of three maximum units per shaft with an additional auxiliary motor/generator), N(1)-NN(All)-WH-2 is obtained with TAC of 15,165,455 $/y. This solution is presented in Figure 7. It also has two valves. The design values shown for valves are heat capacity flowrates through such pieces of equipment. More detailed design data such as heat loads and stream split fractions in heat exchangers are presented in Tables S.1-S.4, in the Supplementary material.

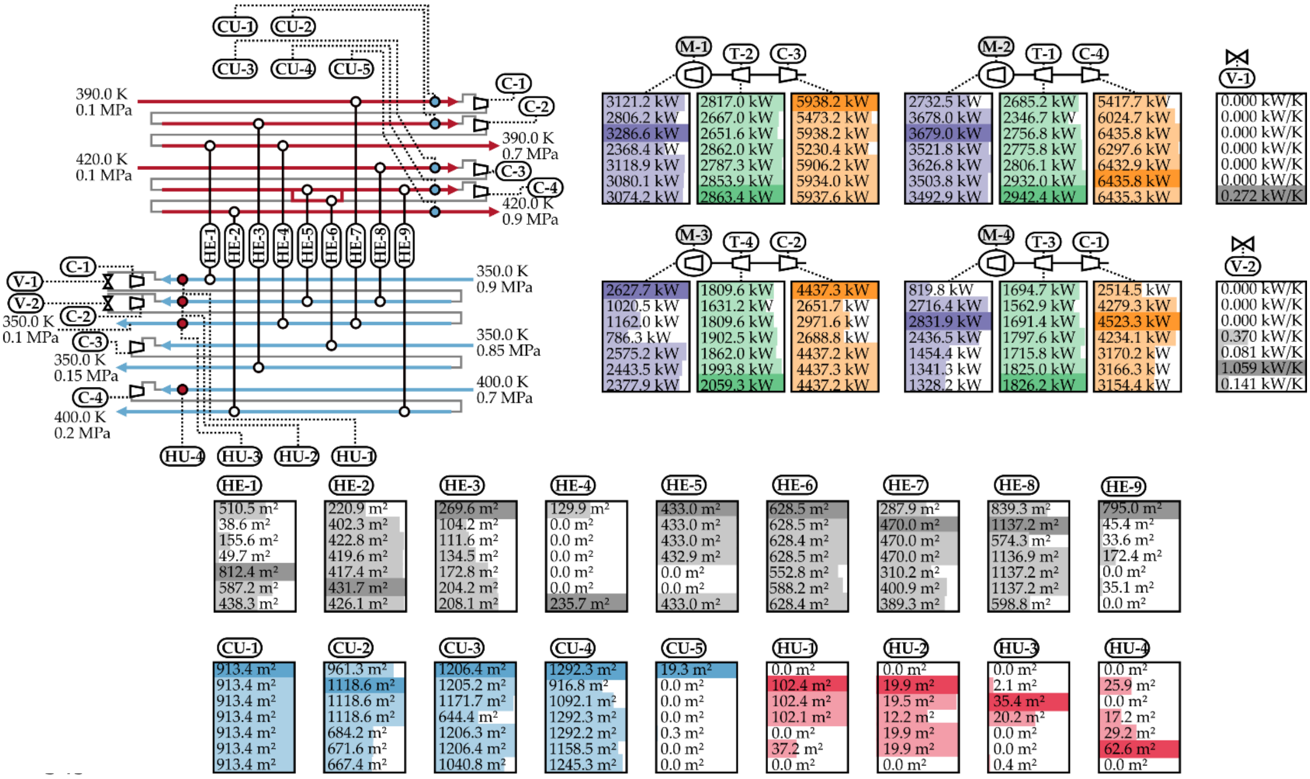

Figure 7. Solution N(1)-N(All)-WH-2 for Case 1

Table 5 presents design aspects of some solutions for better putting the present methodology into perspective regarding additional capital investments for enabling the WHEN for operating feasibly in critical conditions. The solution N(1)-WH-1 was obtained by the simple merging of the work integration and the heat integration solutions of the nominal period 1 (see Step 3 for nominal solutions, Figure 2). If merged to other single-period WHI solutions for non-nominal periods, a multiperiod WHEN is obtained which is able to operate in all critical scenarios previously described. We label this solution N(1)-NN(All)-WH-0 (“-0” suffix is used to distinguish it from solutions used in the methodology, in Step 4, which use “-1” and “-2” suffixes). That is the most straightforward method one can use to obtain a multiperiod WHEN solution, which is basically merging feasible solutions obtained for each period individually and considering maximum unit sizes for capital costs calculation. It should be noted that this straightforward merging leads to a solution with a simple coupling configuration for the SSTC units. All units are coupled via a single shaft, which may be complex to implement. The refined solution N(1)-NN(All)-WH-2 has a more realistic configuration with maximum of three units coupled and one possible motor/generator per shaft.

Given that multiperiod has not yet been approached in the literature for WHEN synthesis, we may compare our novel method to this aforementioned simple approach. The final solution obtained by the present method has capital costs of 9,895,681 \$/y. That yields an additional investment of 1,149,816 \$/y for the WHEN to be able to perform in all critical scenarios considering the durations described for Case 1, in comparison to the WHEN obtained by simple merging for the nominal scenario (N(1)-WH-1). Furthermore, for the multiperiod WHEN obtained with the simple merging strategy (N(1)-NN(All)-WH-0) this additional investment is of 1,646,326 \$/y (i.e., the additional capital investment in the refined solution is 496.510 \$/y, or 30.2 %, lower). The refined solution has considerably lower heat exchange area, and smaller compressors and turbines as well. Regarding the total required to total available capacity ratio, it can be noted that these values are higher in N(1)-NN(All)-WH-2 for all types of units except for motors. This is probably due to the fact that in the refined solution, a detailed work integration structure is designed, with three separate motors providing auxiliary power for three couplings. In the straightforwardly merged solution, that structure is simplified with a single motor providing auxiliary power. This demonstrates that the method can find designs that use most of the capacity of the equipment set, mitigating the necessity for overdesigning these units.

Table 5. Capital costs and design aspects related to capital cost increases for Case 1

	N(1)-WH-1	N(1)-WH-2	N(1)-NN(All)-WH-0*	N(1)-NN(All)-WH-2
HI-related CC (\$/y)	1,213,587	1,213,734	1,879,892	1,575,275
WI-related CC (\$/y)	7,532,278	7,560,044	8,512,299	8,320,406
Total CC (\$/y)	8,745,865	8,773,778	10,392,191	9,895,681
Total OC (\$/y)	5,202,365	5,202,029	5,287,409	5,269,774
TAC (\$/y)	13,948,230	13,975,807	15,679,600	15,165,455
Area (m^2)	7,774	7,775	11,670	9,964
Total Available Comp. (kW)	18,379	18,379	22,146	21,335
Total Available Exp. (kW)	9,006	9,006	9,924	9,691
Average HU (kW)	0	0	115	120
Average CU (kW)	9,373	9,372	9,514	9,475
Area CR	-	-	60.2 %	84.7 %
Comp. CR	-	-	83.4 %	86.3 %
Turb. CR	-	-	91.1 %	93.1 %
Motor CR	-	-	87.3 %	75.6 %

*N(1)-NN(All)-WH-0 is a solution obtained from merging N(1)-WH-1, NN(2)-WH-1… NN(*T*)-WH-1. It is never rendered in the methodology (N(1)-WH-1 is refined via MP_WHEN prior to merging), but it serves for comparison purposes: merging single-period WHEN solutions is the simplest way to obtain a multiperiod WHEN solution.

As already mentioned, the second case is more complex, comprising 14 total periods. The solution of this case differs slightly from the previous one in Step 2. In Step 2.1, for each nominal period

(1 and 2), SP_HEN is applied to streams extracted from Step 1 solutions. A HEN solution for each of these periods is obtained (N(1)-H-1 and N(2)-H-1). These two solutions are merged into a single multiperiod HEN solution (N(All)-H-1) in Step 2.2. That solution is refined and the solution presented in Figure 8 is obtained (N(All)-H-2). Note in the referred figure that supply and target temperatures for HEN cold streams #7 and #8 are equal. That is because these streams precede turbines, although no heating is required prior to their inlet, as found by the SP_PINCH model. In that case, the solution is extracted with these streams, but they are, evidently, never used for heat exchange. That 12-heat-exchanger topology is then transferred to all non-nominal periods, which use it for obtaining single-period HENs.

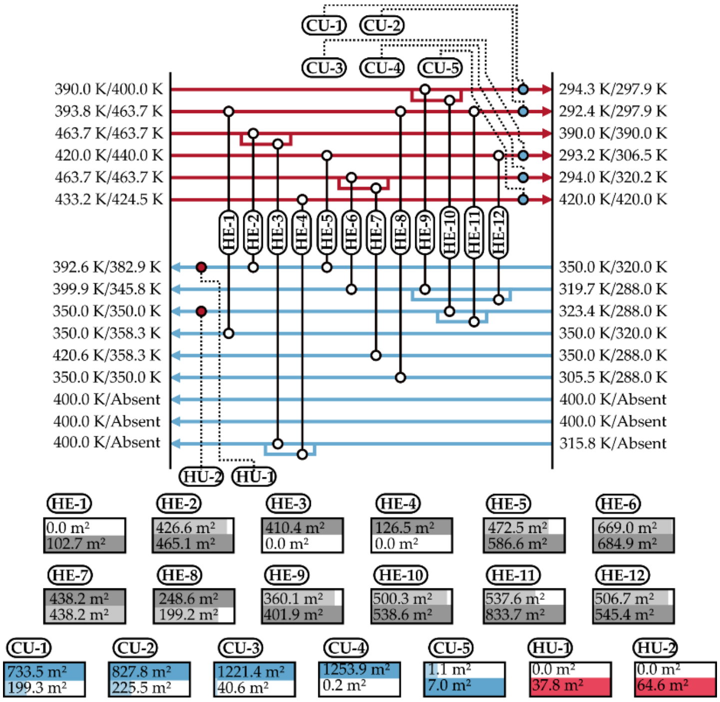

Figure 8. Two-period HEN considering the two nominal periods of Case 2

From that step on, the solution approach remains the same. The final solution (N(All)-NN(All)-WH-2) is presented in Figure 9. Given the large volume of design data, we included only the maximum variable values. The complete data set for all 14 periods with power for compressors/turbines/motors/generators, heat capacity flowrates for valves and areas for heat exchangers (as well as heat loads and stream split fractions) are presented in Tables S.5-S.8 in the Supplementary Material. The TAC for the multiperiod WHEN obtained for the two nominal periods (N(All)-WH-2) is 12,542,190 $/y. The 14-period solution (N(All)-NN(All)-WH-2) has TAC of 13,541,906 $/y. Design aspects, additional investments and capacity ratios are presented in Table 6. The two-period solution N(All)-WH-2 refines the one obtained from merging solutions for single-periods 1 and 2 (N(All)-WH-1). Capital investment is lowered from 9,617,558 $/y to 9,422,363 $/y (2.0 %) with such a refinement.

Consider as basis the merged solution for nominal stages N(All)-WH-1, disregarding the one obtained with the refining model. The solution obtained by merging the single-period WHEN for the 14 periods, N(All)-NN(All)-WH-0, requires additional 2,003,258 $/y capital investment for being able to operate in critical scenarios. The refined 14-period solution requires additional 837,522 $/y (58.2 % lower than the straightforwardly merged one). Regarding overdesign, it is possible to notice that the issue is greatly reduced. Capacity ratios are greater for all unit types in N(All)-NN(All)-WH-2 (generators are not present in N(All)-NN(All)-WH-0). Particularly, it is worth stressing out the 85.2 % greater use of available area in that solution in comparison to N(All)-NN(All)-WH-0.

Some interesting design aspects of the final WHEN solution is that several valves are present. It can also be noted that some couplings require a motor in some periods due to power shortage from turbines, and a generator in others due to power surplus.

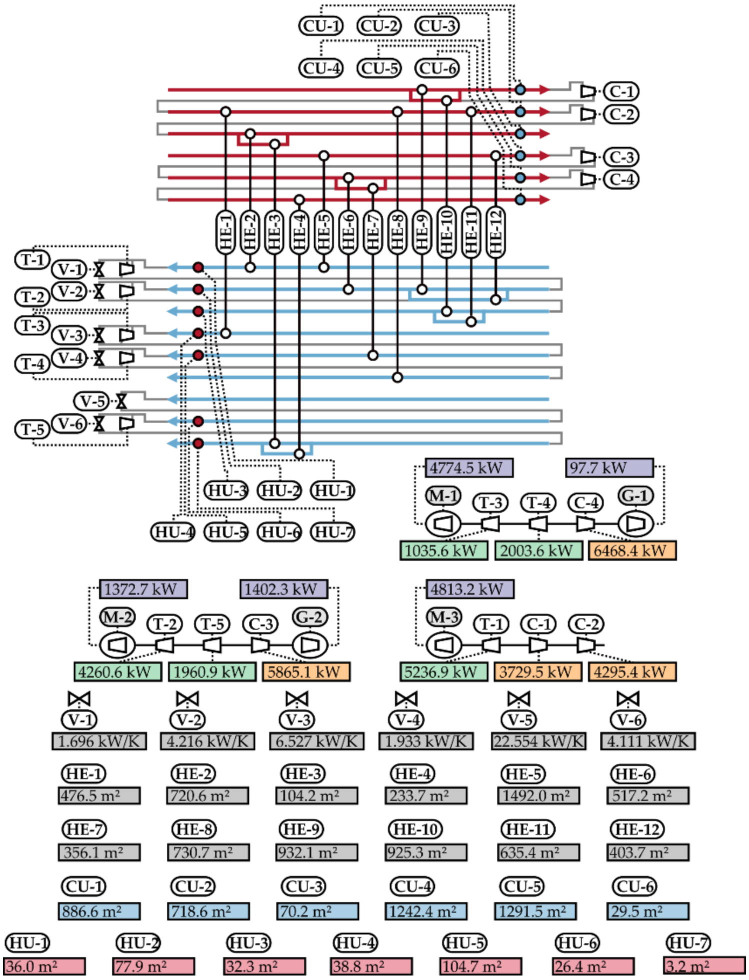

Figure 9. Final WHEN for Case 2 showing maximum power/area/heat capacity flowrate values

Table 6. Capital costs and design aspects related to capital cost increases for Case 2

	N(All)-WH-1	N(All)-WH-2	N(All)-NN(All)-WH-0*	N(All)-NN(All)-WH-2
HI-related CC ($/y)	1,526,889	1,475,666	2,577,000	1,948,238

WI-related CC (\$/y)	8,090,669	7,946,696	9,043,816	8,506,842
Total CC (\$/y)	9,617,558	9,422,362	11,620,816	10,455,080
Total OC (\$/y)	3,171,928	3,119,828	3,470,794	3,086,826
TAC (\$/y)	12,789,486	12,542,190	15,091,610	13,541,906
Area (m^2)	9,529	9,200	16,660	12,086
Total Available Comp. (kW)	19,021	18,560	22,155	20,358
Total Available Exp. (kW)	12,972	12,613	16,073	14,498
Average HU (kW)	670	519	712	498
Average CU (kW)	4946	5049	4996	4850
Area CR	-	-	42.80 %	79.30 %
Comp. CR	-	-	67.10 %	79.50 %
Turb. CR	-	-	60.90 %	66.60 %
Motor CR	-	-	47.10 %	48.80 %
Gen. CR	-	-	-	11.80 %

*N(All)-NN(All)-WH-0 is a solution obtained from merging N(1)-WH-1, N(2)-WH-1… NN(*T*)-WH-1. It is never rendered in the methodology (N(All)-WH-1 is refined via MP_WHEN prior to merging), but it serves for comparison purposes: merging single-period WHEN solutions is the simplest way to obtain a multiperiod WHEN solution.

4 Conclusions

A stepwise methodology for multiperiod work and heat integration was proposed. The scheme was based on the sequential application of a Pinch-based model for pressure manipulation routes determination, single and multiperiod heat integration models for determining the matches in the heat exchanger network, a single-period model for work and heat integration and a novel multiperiod work and heat integration model in order to achieve final work and heat exchange network configurations. A multiperiod study proposal was presented considering seven periods, being one nominal and other six non-nominal that account for critical operating conditions. In case that the plant must be able to operate under two or more well-defined conditions (i.e., more than one nominal period), six additional non-nominal critical periods are included for each period. A large-scale single-period WHEN synthesis literature example was approached for testing the methodology. The example was extended with multiperiod considerations, being approached under two cases. In the first, one nominal, and therefore six additional non-nominal periods are considered. The second one comprised two nominal and twelve additional non-nominal periods. The framework was able to find feasible solutions in both cases. Final results were compared to the straightforward approach of searching for minimum-TAC WHENs individually for each period and then considering maximum design variables (e.g., heat exchanger areas, compressor/turbine power, etc.). Additional capital investments were considerably smaller (30.2 % in Case 1 and 58.2 % in Case 2) with the optimization-strategies presented here. The novel WHEN multiperiod model was able to find more efficient designs, with units that use most of their capacities throughout all operating periods. In comparison to the aforementioned straightforward individual solution merging designs, the total required to total available capacity ratios were greatly reduced for most unit types in both cases. It is thus demonstrated that the method is reliable for the synthesis of multiperiod WHEN, even with the large number of periods considered. The presented method applies to early design stages, where a macro analysis of the process streams regarding energy integration must be performed. Pressure/temperature interactions are not intuitive to observe given the large number of streams in these cases. These synergies become even more complex when multi-period interactions occur. The proposed method can present a preliminary near-optimal design under a cost-minimization objective. Given this is an early design model, specific phenomena in the pressure/temperature manipulation units of the model are not included, such as fluid phase-changes, rotor velocity maintenance and possible controllability issues. These issues, as well as more rigorous thermal-hydraulic design equations and fluid property correlations could be included in further works. Exergy analysis may be included as well, given that the present model is solely based on costs reduction.

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6 Appendix A

This appendix presents all calculation steps for cooler/compressor and heater/turbine blocks in the multiperiod work and heat integration model. Note that index *w* is an index used for all streams. The matrix-based approach developed in our previous work [30] is used for connecting such an index to the *i,j* indexes for hot/cold streams in the heat integration section of the model. The referred matrix also contains information regarding stream passes and block types. The calculations presented here are executed within a loop that uses *w* as loop control variable. At each *w* update ($w \leftarrow w+1$), equations are run according to the block type and stream information retrieved from the aforementioned matrix. Note that this model format cannot be directly implemented in algebraic optimization platforms (e.g., GAMS) and should require some adaptation. This is more evident, for instance, on updating equations such as (A-9) (A-10), (A-12), (A-13), (A-20), (A-21), (A-24) and (A-25).

Details of these aspects can be found in detail in Refs. [30,32]. Details on the heat integration section of the superstructure can be found in Ref. [13].

Cooler/compressor (Block 1)

$$Qpre_{w,t} = CP_{w,t}\left(Tprein_{w,t} - Tpreout_{w,t}\right), w \in NG, t \in NP \qquad \text{(A-1)}$$

If $(Tprein_{w,t} - Tcuout_n) \neq (Tpreout_{w,t} - Tcuin_n)$:

$$LMTDpre_{w,t} = \frac{\left(Tprein_{w,t} - Tcuout_n\right) - \left(Tpreout_{w,t} - Tcuin_n\right)}{\ln\left(\frac{Tprein_{w,t} - Tcuout_n}{Tpreout_{w,t} - Tcuin_n}\right)} \quad w \in NG, n \in NCU, t \in NP \tag{A-2}$$

Otherwise, note that *LMTDpre_{w,t}* tends to either aforementioned values between parentheses. Hence, for avoiding numerical issues ($ln(1) = 0$ in the denominator):

$$LMTDpre_{w,t} = Tprein_{w,t} - Tcuout_n \quad w \in NG, n \in NCU, t \in NP \tag{A-3}$$

$$Ucu_{i,n} = \frac{1}{\frac{1}{hh_i} + \frac{1}{hcu_n}} \quad i \in NH, n \in NCU \tag{A-4}$$

$$Apre_{w,t} = \frac{Qpre_{w,t}}{Ucu_{i,n} LMTDpre_{w,t}} \quad w \in NG, i \in NH, n \in NCU, t \in NP \tag{A-5}$$

$$Work_{w,t} = CP_{w,t}(Tout_{w,t} - Tin_{w,t}), w \in NG, t \in NP \tag{A-6}$$

$$Trevout_{w,t} = \eta_c \cdot \left(Tout_{w,t} - Tin_{w,t}\right) + Tin_{w,t}, w \in NG, t \in NP \tag{A-7}$$

$$pout_{w,t} = \exp\left(ln\left(pin_{w,t}\right) - \kappa \cdot \frac{\left(ln\left(Tin_{w,t}\right) - ln\left(Trevout_{w,t}\right)\right)}{\kappa - 1}\right), w \in NG, t \in NP \tag{A-8}$$

If the number of parallel units in this block (*Par_w*) is equal to one (i.e., there is only one cooler and one single compressor):

$$ComWork_{s,t} \leftarrow ComWork_{s,t} + Work_{w,t}, if\ SSTC_{w,f} = s, w \in NG, s \in NSh, f \in NF, t \in N \tag{A-9}$$

$$SACompWork_t \leftarrow SACompWork_t + Work_{w,t}, if\ SSTC_{w,f} = 0, w \in NG, f \in NF, t \in NP \tag{A-10}$$

Otherwise, if $Par_w > 1$ (i.e., there are Par_w parallel compressors):

$$ParWork_{w,f,t} = Fw_{w,f,t} \cdot CP_{w,t}(Tout_{w,t} - Tin_{w,t}), w \in NG, f \in NF, t \in NP \tag{A-11}$$

$$ComWork_{s,t} \leftarrow ComWork_{s,t} + ParWork_{w,f,t}, if\ SSTC_{w,f} = s, w \in NG, s \in NSh, f \in NF, t \in NP \quad \text{(A-12)}$$

$$SACompWork_{t} \leftarrow SACompWork_{t} + ParWork_{w,f,t}, if\ SSTC_{w,f} = 0, w \in NG, f \in NF, t \in NP \quad \text{(A-13)}$$

Heater/turbine (Block 2):

$$Qpre_{w,t} = CP_{w,t}(Tpreout_{w,t} - Tprein_{w,t}), w \in NG, t \in NP \quad \text{(A-14)}$$

If ($Thuin_m - Tpreout_{w,t}$) ≠ ($Thuout_m - Tprein_{w,t}$):

$$LMTDpre_{w,t} = \frac{\left(Thuin_m - Tpreout_{w,t}\right) - \left(Thuout_m - Tprein_{w,t}\right)}{\ln\left(\frac{Thuin_m - Tpreout_{w,t}}{Thuout_m - Tprein_{w,t}}\right)} \quad w \in NG, m \in NHU, t \in NP \quad \text{(A-15)}$$

Otherwise:

$$LMTDpre_{w,t} = Thuin_m - Tpreout_{w,t} \quad w \in NG, m \in NHU, t \in NP \quad \text{(A-16)}$$

$$Uhu_{i,m} = \frac{1}{\frac{1}{hh_i} + \frac{1}{hhu_m}} \quad i \in NH, m \in NHU \quad \text{(A-17)}$$

$$Work_{w,t} = CP_{w,t}(Tin_{w,t} - Tout_{w,t}), w \in NG, t \in NP \quad \text{(A-18)}$$

$$Trevout_{w,t} = Tin_{w,t} - \frac{Tin_{w,t} - Tout_{w,t}}{\eta_t}, w \in NG, t \in NP \quad \text{(A-19)}$$

If the number of parallel units in this block (Par_w) is equal to one (i.e., there is only one heater and one single turbine):

$$TurWork_{s,t} \leftarrow TurWork_{s,t} + Work_{w,t}, if\ SSTC_{w,f} = s, s \in NSh, f \in NF, t \in NP \quad \text{(A-20)}$$

$$SATurbWork_{t} \leftarrow SATurbWork_{t} + Work_{w,t}, if\ SSTC_{w,f} = 0, f \in NF, t \in NP \quad \text{(A-21)}$$

Otherwise, if $Par_w > 1$ (i.e., there are one heater, $Par_w - 1$ turbines and one valve in parallel):

$$ParWork_{w,f,t} = Fw_{w,f,t} \cdot CP_{w,t}\left(Tin_{w,t} - TurTout_{w,t}\right), w \in NG, f \in NF, t \in NP \quad \text{(A-22)}$$

$$Trevout_{w,t} = Tin_{w,t} - \frac{Tin_{w,t} - TurTout_{w,t}}{\eta_t}, w \in NG, t \in NP \tag{A-23}$$

$$TurWork_{s,t} \leftarrow TurWork_{s,t} + ParWork_{w,f,t}, if\ SSTC_{w,f,t} = s, w \in NG, s \in NSh, f \in NF, t \in NP \tag{A-24}$$

$$SATurbWork_t \leftarrow SATurbWork_t + ParWork_{w,f,t}, if\ SSTC_{w,f} = 0, w \in NG, f \in NF, t \in NP \tag{A-25}$$

$$ValTout_{w,t} = Tin_{w,t} - \mu\left(pin_{w,t} - pout_{w,t}\right), w \in NG, t \in NP \tag{A-26}$$

$$Tout_{w,t} = \sum_{f<Par_w} Fw_{w,f,t} \cdot TurTout_{w,t} + Fw_{w,Par(w),t} \cdot ValTout_{w,t}, w \in NG, f \in NF, t \in NP \tag{A-27}$$

7 Nomenclature

Variables

A	Heat exchanger area [m^2]
Acu	Final cooler area [m^2]
Ahu	Final heater area [m^2]
Apre	Pre-heater/pre-cooler area [m^2]
AreaCC	Area-related capital costs [$/y]
Cap	Illustrative capacity variable for generic unit [-]
Comp	Binary variable denoting compression block existence [-]
ComWork	Total compression shaft-work at a given shaft [kW]
Exp	Binary variable denoting expansion block existence [-]
Fw	Stream split fraction in parallel compression/expansion stage [-]
LMTDpre	Logarithmic mean temperature difference in pre-heaters/pre-coolers [K]
ParWork	Shaft-work in parallel compressor/turbine [kW]
Pin	Pressure manipulation unit inlet pressure [MPa]
Pout	Pressure manipulation unit outlet pressure [MPa]
Qcu	Available heat at the end of an original hot stream [kW]
Qhu	Required heat at the end of an original cold stream [kW]
Qpre	Heat load in pre-heater/pre-cooler [kW]
SSTC	Matrix for unit shaft identification of compressor/turbine [-]
SACompWork	Total standalone compressor work [kW]
SATurbWork	Total standalone turbine work [kW]
TAC	Total annual cost [$/yr]

Tin	Pressure manipulation unit inlet temperature [K]
Tout	Pressure manipulation unit outlet temperature [K]
Tprein	Process stream inlet temperature in pre-heater/pre-cooler [K]
Tpreout	Process stream outlet temperature in pre-heater/pre-cooler [K]
Trevout	Outlet temperature in reversible process [K]
TurTout	Outlet temperature from parallel turbines [K]
TurWork	Total expansion shaft-work at a shaft [kW]
UtilOC	Thermal utility-related operating costs [$/y]
ValTout	Outlet temperature from parallel valve [K]
Work	Work rate produced/required in a turbine/compressor or energy loss in valves [kW]
WorkCC	Work-related capital costs [$/y]
WorkOC	Work-related operating costs [$/y]
Parameters	
Ccu	Cold utility cost [$/(kWy)]
Cel	Electricity cost [$/kWy]
Chu	Hot utility cost [$/(kWy)]
CP	General process stream total heat capacity flowrate [kW/K or kW/°C]
D	Relative period duration [-]
F	Number of stream branches in WI blocks [-]
H	General heat transfer coefficient [kW/(m^2K)]
Hcu	Cold utility heat transfer coefficient [kW/(m^2K)]
Hh	Hot stream heat transfer coefficient [kW/(m^2K)]
N	Total number of nominal periods [-]
Par	Vector containing information on parallel unit numbers per stream [-]
Psupply	Stream supply pressure [MPa]
Ptarget	Stream target pressure [MPa]
Rel	Electricity revenue price [$/kWy]
T	Total number of periods [-]
Tcuin	Cold utility inlet temperature [K]
Tcuout	Cold utility outlet temperature [K]
Thuin	Hot utility inlet temperature [K]
Thuout	Hot utility outlet temperature [K]
Tsupply	Stream supply temperature [K]
Ttarget	Stream target temperature [K]
Ucu	Cooler global heat transfer coefficient [kW/(m^2K)]
Uhu	Heater global heat transfer coefficient [kW/(m^2K)]
η_c	Isentropic efficiency for compressors [-]
η_t	Isentropic efficiency for turbines [-]
κ	Polytropic exponent [-]
μ	Joule-Thompson coefficient [K/MPa]

Functions	
AreaCost	Calculates the heat transfer device cost as a function of its area [$/y]
ComCost	Calculates compressor capital cost [$/y]
TurCost	Calculates turbine capital cost [$/y]
ValCost	Calculates valve capital cost [$/y]
MotCost	Calculates auxiliary motor capital cost [$/y]
GenCost	Calculates auxiliary generator capital cost [$/y]
Indexes:	
F	Stream fraction at pressure manipulation stage [-]
I	Hot stream [-]
J	Cold stream [-]
K	Stage [-]
M	Hot utility type [-]
N	Cold utility type [-]
Oi	Original hot stream [-]
Oj	Original cold stream [-]
S	Shaft [-]
T	Period [-]
Tt	Auxiliary period index [-]
W	General stream [-]
X	Generic unit index [-]
Models	
SP_PINCH	Single-period pinch-based model
SP_HEN	Single-period heat exchanger network synthesis model
MP_HEN	Multi-period heat exchanger network synthesis model
SP_WHEN	Single-period work and heat exchanger network synthesis model
MP_WHEN	Multi-period work and heat exchanger network synthesis model
Sets:	
NC	Cold streams [-]
NCU	Cold utility type [-]
NF	Stream split fractions in WEN blocks [-]
NG	General streams [-]
NH	Hot streams [-]
NHU	Hot utility type [-]
NOC	Original cold streams [-]
NOH	Original hot streams [-]
NP	Periods [-]
NS	Stages [-]
NSh	Shafts [-]
NX	Illustrative generic unit set [-]
Acronyms	

CC	Capital costs
CR	Capacity ratio (total required to total available)
CU	Cold utility
HEN	Heat exchanger network
HP	High-pressure
HU	Hot utility
LP	Low-pressure
MINLP	Mixed-integer nonlinear programming
OC	Operating costs
PSO	Particle swarm optimization
RFO	Rocket fireworks optimization
SA	Simulated annealing
SSTC	Single-shaft-turbine-compressor
SWS	Stagewise superstructure
TAC	Total annual costs
WEN	Work exchange network
WHEN	Work and heat exchange network

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