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Synthesis of Work and Heat Exchange Networks Considering Practical Operating Constraints

Leandro V. Pavão, Caliane B. B. Costa, Mauro A. S. S. Ravagnani*

Department of Chemical Engineering, State University of Maringá, Av. Colombo, 5790, Bloco D90, CEP 87020900, Maringá, PR, Brazil
massravagnani@uem.br

The synthesis of work and heat exchange networks (WHEN) has drawn much attention from process synthesis researchers in the present decade, arising as a promising field of study. The current literature has shown that simultaneously integrating heat and work may lead to substantial savings in utilities usage in highly energy-demanding processes. The problem, however, comprises highly nonlinear constraints and efficient solutions are difficult to obtain. Optimisation-based approaches have presented interesting solutions. However, in some cases, they may not be practical. When coupling several compressors and turbines via one single-shaft for work exchange, it may become technically difficult to maintain the same rotation speed. Moreover, discharge temperatures in compressors/turbines in some literature solutions may be considered impractically high/low. In order to address the first issue, the number of units that can be coupled via single-shaft was limited, and the use of multiple axes rotating at different speeds was considered. Such a new constraint is handled with a new stage coupled to a previous meta-heuristic method for solving the WHEN synthesis model. The method is able to identify optimal couplings respecting the constraints proposed for more mechanically practical designs. Regarding the discharge temperature issues, penalty functions were employed and the optimization approach was able to find solutions within practical operating range for compressors/turbines temperatures.

1. Introduction

Concurrently to the advances being achieved on heat integration by means of optimization procedures in the process synthesis literature, simultaneous work and heat integration has come forth as a subject of major interest of the community. Briefly, the simultaneous work/heat integration problem can be described as: given a set of process streams (which can be hot or cold to be expanded or compressed), it is necessary to find the optimal configuration of heat exchangers and pressure manipulators that lead those streams to their target conditions. That problem can be approached by merging a heat integration method, namely the synthesis of heat exchanger networks (HEN) to finding optimal pressure manipulation routes with compressors, turbines and valves. Work exchange may also be an option, either via single-shaft-turbine-compressor (SSTC) units or by direct work exchangers (also called flow work exchangers). In the case that both work and heat exchange are being considered, the work/heat integration case can be addressed to as a work and heat exchange network (WHEN) synthesis problem.

Simultaneously considering pressure and temperature manipulations entails several additional intricacies in comparison to the well-studied heat integration case. The main challenges to the area have been pointed out in the work of Fu et al. (2017) as (i) the resulting temperature changes from pressure manipulation procedures, which influences the heat integration procedure; (ii) work consumption/production varies as inlet temperature in pressure manipulators change; (iii) energy quality (exergy) is different for work and heat. As pointed out by Vikse et al. (2017), the use of approaches based on mathematical optimization arises as the most promising path, as a manual synthesis is only possible to perform efficiently for small cases.

Several process synthesis research groups are concentrating considerable effort on developing new frameworks on the matter. Some important contributions are worth mentioning here. In the framework of Onishi et al. (2014), the WHEN synthesis problem is modelled with streams passing sequentially through a heat recovery area and then through a pressure manipulation/work exchange region. The heat exchange stage was

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modelled with the stage-wise superstructure (SWS) (Yee and Grossmann, 1990). SSTC units were considered for work exchange. Huang and Karimi (2016) also presented a model with sequential passes through HEN and WEN stages, but considered both heaters or coolers at streams ends, used a different formulation for capital costs and presented a model with fewer variables and constraints than that developed by Onishi et al. (2014). Nair et al. (2017) presented a framework for WHEN synthesis that did not classify streams as hot or cold, neither low or high pressures, providing the model with some flexibility regarding equipment to be used. In the work of Zhuang et al. (2017), a method for work exchange networks (WEN) synthesis using direct work exchangers is presented as an analogy to HEN synthesis. Pavão et al. (2018a) presented a framework for WHEN synthesis that used a meta-heuristic as solution method to a pass-based model (similar to Onishi et al., 2014). That model used the enhanced SWS of Pavão et al. (2018b) in the heat recovery stage. The framework was later improved to handle extended pressure manipulation routes and larger-scale cases (Pavão et al., 2019). Furthermore, literature reviews have been conducted on the WEN and WHEN matter with clear definitions for the problem and challenges on the development of WHENs (Fu et al., 2018), and broad state-of-the-art analysis and opportunities on the field (Yu et al., 2018).

Note that this area of study is relatively recent in optimization. Therefore, in order for the solution approaches to be able to attain good, or even feasible solutions, some practical operating aspects may be simplified. Namely, in WHEN, some considerations often observed are (i) a single-shaft coupling several compressors and turbines and (ii) unconstrained inlet/outlet temperatures in turbines and compressors.

The first issue may lead to difficulties regarding the rotational speed of the unit or to transport concerns, since all work-exchanging streams must be transported to the SSTC unit. Coupling-related concerns already stated in the work of Onishi et al. (2014). Those authors were the first to allow multiple shafts in a WEN/WHEN model so that different rotational speed could be considered in further design stages. However, the number of couplings was not limited and a high number of units could be coupled (*e.g.*, 14 in one of the reported solutions). In the present work, more practical limits are imposed so that an optimal coupling configuration is found within practical boundaries.

The second issue regards operating temperature ranges that are imposed by manufacturers due to material limitations or to avoid condensing fluids in the units. According to Seider et al. (2017), specialized compressors may operate with temperatures as high as 600 °F (518 K). More widely employed units, however, have discharge temperatures limited by manufacturers to lower values. In general, these maximum values range from around 375 °F to 400 °F (463 K to 477 K). Therefore, as typically observed in the industry, especially in above-ambient processes, multiple compression stages with intercooling are necessary not only to reduce compression shaft-work, but also to avoid undesirable temperatures. However, in the WHEN literature considerably higher values are typically observed (e.g, 700 K assumed by Onishi et al., 2014, and 500 °C by Fu and Gundersen, 2016). Given that in above-ambient processes compression reaches high temperatures very easily, finding optimal, or even feasible solutions with a one-step MINLP optimization model is particularly difficult when such rigorous temperature bounds are imposed. Therefore, this work has as an objective to propose a method able to find solutions within more practical temperature boundaries.

Regarding solution approaches and model implementations, it is worth noting that most of the cited literature employs deterministic solution approaches, in general implemented in GAMS platform for solving WHEN case studies. The present work, on the other hand, uses a meta-heuristic solution approach. Even though meta-heuristics are stochastic methods and therefore global optimization cannot be assured, these approaches have drawn much attention from process engineering academia. They arise as interesting alternatives due to some advantages. For instance, being derivative-free methods, objective functions can be programmed in them as "black-boxes". In that manner, disjunctive operators can be implemented as simple condition statements within the program code, which in some cases is more intuitive than their algebraic implementation for platforms such as GAMS. Moreover, programming routines with simple heuristics may be implemented within the code to aid in maintaining solutions feasible. It has been demonstrated in the work of Pavão et al. (2019) that by using a simple matrix representation with discrete values a meta-heuristic that was originally developed for HEN synthesis (Simulated Annealing/Rocket Fireworks Optimization, SA-RFO, Pavão et al., 2017) could be adapted to handle WHEN synthesis as well. The results found in that work were promising and outperformed previous literature reports, which used deterministic methods.

2. Problem statement

This section complements the brief problem description given in the Introduction. A set of process streams is given. These may require either compression or expansion and/or heating or cooling.

In order for those streams to be compressed, compressor units can be used. These can either use a motor or be coupled via single-shaft to a turbine(s) for supplying their shaft work rate demand. In order for a stream to be expanded, turbine units can be used. These can be coupled either to a generator for converting mechanical energy into electric energy electric energy to be sold, or to compressor(s) via single-shaft for providing shaft-work. Compression and expansion are considered isentropic processes for ideal gases, with known isentropic efficiencies and polytropic exponents. Expansion by means of valves is considered isenthalpic with constant Joule-Thompson coefficient.

A stream can be heated by receiving heat from a hot utility or from another process stream, by means of heat exchangers. It can be cooled by exchanging heat with a cold utility or another process stream.

In this work, constraints are imposed to the problem so that its results are in accordance with industrial practice. A fixed number of units is allowed to be coupled via single-shaft in order to prevent stream transportation issues or mechanical difficulties in maintaining shaft rotational speed. Inlet/outlet temperatures in compressors/turbines are limited to values that are typically used in the industry. For instance, it is commonly observed that, for above-ambient conditions, compression is carried out in multiple stages with intercooling. Manufacturers typically establish stage compression ratios in a manner that temperatures are not raised to undesirably high values.

3. Computational implementation

3.1 Mathematical modeling

The mathematical model used here is based on concepts presented in previous studies by the present authors (Pavão et al., 2019, 2018a). The superstructure is tailored considering that a single stream can pass multiple times through a heat recovery region, and, between two passes, it may have its pressure changed. Figure 1 shows high- and low-pressure streams in the WHEN superstructure, as well as the multiple shafts proposal of this work. It should be noted that the model implementation is based on matrices/vectors with discrete values representing streams characteristics. These aspects include data such as its original identification (hot/cold) and the identification assumed at each pass, and streams numbers, and are illustrated in Figure 1c. Note that two numbering systems are used in the WHEN superstructure. The *i,j,k* system is used for match identification and HEN-related calculations in the heat recovery region. The system numbers hot streams with the *i* index, cold streams with the *j* index and stages with the *k* index. Note that the stage concept in HEN was established by Yee and Grossmann (1990). The modified SWS used here in the heat recovery region is that developed in Pavão et al. (2018b), which allows the use of utilities in intermediate stages. The *w* system basically numbers all stream passes sequentially. A binary vector ($IsLinked_w$) is used for identifying whether a stream pass is a continuation of the previous one, or a new stream.

In order to handle the use of multiple shafts a new matrix is created. In this matrix, each line represents a shaft, while each column is a “slot” in which a compressor/turbine can be placed. A shaft is only valid if at least one compressor and one turbine are coupled.

The mathematical model equations are similar to those presented in Pavão et al. (2019), with the addition of the temperature-related penalties and the multiple shaft modelling. Note that the objective function is programmed with a main “for” loop statement that runs with *w* as loop control variable. Within that loop, the penalties, which are later summed up and added to the WHEN total annual costs (TAC) are written in a generic form as follows:

$$TOutPen_w = PenA + PenB(Tout_w - TUB) \tag{1}$$

$$TInPen_w = PenA + PenB(TLB - Tin_w) \tag{2}$$

where *PenA* and *PenB* are penalty constants, *Tin* and *Tout* are respectively the inlet and outlet temperatures from a given pressure manipulator, *TUB* and *TLB* are the upper and lower temperature bounds (which may differ for compressors and turbines).

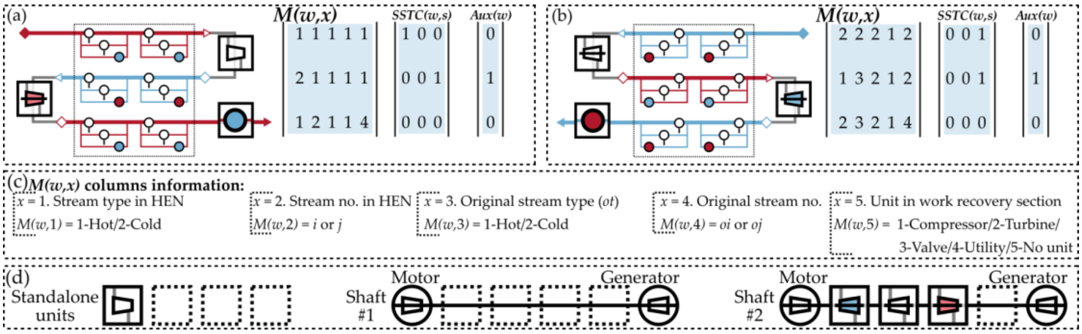

Figure 1: M, SSTC and Aux variables in (a) example of low-pressure stream with final cooling; (b) example of high-pressure stream with final heating; (c) M(w,x) columns data and standalone units and multiple shafts in (d).

The modelling concerning multiple shafts entails changes in the SSTC equations. The total shaft-work rate for compressors coupled to a shaft *s* is calculated in a "*for"* loop statement with *s* as loop control variable. That *s* loop is contained within the main *w* loop in the coded objective function.
If a given unit is a compressor ($M_{w,5}$ = 1), the following is applied:

$$\begin{cases} TotalCompWork_1 \leftarrow TotalCompWork_1 + Work_w, if\ SSTC_{w,s} = 0 \\ TotalCompWork_s \leftarrow TotalCompWork_s + Work_w, if\ SSTC_{w,s} = 1 \end{cases} \\ w \in NG \tag{3}$$

Or, if the unit is a turbine ($M_{w,5}$ = 2):

$$\begin{cases} TotalTurbWork_1 \leftarrow TotalTurbWork_1 + Work_w, if\ SSTC_{w,s} = 0 \\ TotalTurbWork_s \leftarrow TotalTurbWork_s + Work_w, if\ SSTC_{w,s} = 1 \end{cases} \\ w \in NG \tag{4}$$

Later, in capital cost calculations, costs for auxiliary motors/generators coupled to each shaft are calculated as:

$$MotCost_s = \max\,(0, BMot \cdot (TotalCompWork_s - TotalTurbWork_s)^{CMot}) \tag{5}$$

$$GenCost_s = \max\,(0, BGen \cdot (TotalTurbWork_s - TotalCompWork_s)^{CGen}) \tag{6}$$

3.2 Solution approach

The solution approach is based on the adapted version of SA-RFO for WHEN synthesis (Pavão et al., 2019). In short, SA-RFO is a two-level optimization method where SA is used to handle binary variables and RFO is employed to optimize continuous variables associated to the topology proposed by SA. The present implementation, however, has a new optimization step between each of the RFO applications. After RFO is applied, a simple SA-based algorithm is used to find optimal coupling configuration for the multiple shafts. At each iteration, the method may couple a standalone compressor/turbine to a slot on a shaft, set a couple unit as standalone or change shaft to which a unit is coupled. The method may also perform a correction move in case that a single unit is coupled to the shaft (i.e., add other random unit/remove the single unit from the coupling) or when there are only compressors or turbines in the shaft (i.e., add a random unit of the other type).
In order to increase the solution method efficiency, its initial solution should be feasible. When temperature bounds are not considered, a feasible configuration to be considered is the "trivial" solution. Such a trivial solution consists of a configuration where only auxiliary units are used. A hot/cold stream is totally cooled/heated by cold/hot utilities at the end of the stream. A high/low pressure stream is expanded/compressed by a turbine/compressor at the last possible pressure manipulator slot. An auxiliary pressure manipulator is enforced to reach the stream target pressure. However, with the practical temperature limitations considered in this work, such a configuration may be infeasible. For instance, carrying out a single-stage compression with the aforementioned auxiliary unit may lead a low-pressure stream to temperatures higher than those recommended by compressor manufacturers. In such cases, multi-stage compression should be considered.
Initializing the algorithm with an infeasible (and therefore penalized solution) may lead to premature stagnation at an invalid minimum. In that sense, a simple two-step strategy is proposed here:

(i) *HEN step.* A case with upper/lower bounds for pressure manipulator inlet/outlet temperatures is firstly optimized as a HEN, disregarding its pressure changes. Each of the HEN streams is a pass, as in the superstructure described in Section 3.1. However, none of the passes are linked, and in the end of each stream, a heater/cooler is placed for mandatory temperature correction. These corrections targets are manually set in order for the streams to reach temperatures that are in accordance with the proper operating range of pressure manipulators. For instance, if compressors discharge temperature should be below 450 K, a stream can have its temperature mandatorily corrected to a lower temperature (*e.g.*, 350 K) in the first step of the optimization procedure.

(ii) *WHEN step.* It is expected that such a HEN solution is promising for heat recovery. That configuration is used as input to the WHEN optimization procedure, in its heat recovery stage. It is evident that, with the temperature setup from step (i), that solution is a feasible WHEN configuration. However, now, the optimization is carried out regarding pressure manipulation as well, and streams inlet/outlet temperatures may be connected according to their passes. Costs for pressure manipulations are now considered as well.

4. Case study

The stream data for this case study was presented by Onishi et al. (2014), in the third case study of the referred work. It comprises four streams, being two low pressure and two high pressure streams. The target temperatures of the low-pressure streams are lower than their inlet ones, while the opposite happens in the high-pressure streams. By observing stream temperatures (all within a range of 350 to 600 K), it can be stated that this is an above-ambient process and that compression may lead to undesirably high temperatures. It is here assumed that compressors inlet/discharge temperature may not exceed 450 K, which is in conformity with common industrial practice (Seider et al., 2017). This consideration leads to an interesting situation: both low pressure streams are initially at 600 K, which means they are required to be cooled down upstream to the compressors, and it is very likely that multiple compression stages will be required. For turbine inlet temperatures, typically observed operating values can be as high as 800 K, and should not be an issue in the present case. A lower bound of 288 K is set, as proposed by Onishi et al. (2014) for this case. The WHEN superstructure is set up with three possible compression stages in low-pressure streams and two possible expansion stages in high-pressure streams. Regarding single-shaft couplings, it is imposed that only two units (namely, one compressor and one turbine) can be coupled per shaft. The addition of auxiliary motors/generators is possible. Seven hypothetical shafts are made available for the couplings. The capital costs formulation used is that from Pavão et al. (2019). Isentropic efficiency is considered with a value of 0.7 and polytropic exponent is assumed as 1.4. Heat transfer coefficient is 0.1 kW/(m^{2}K) for process streams and 1.0 kW/(m^{2}K) for utilities.

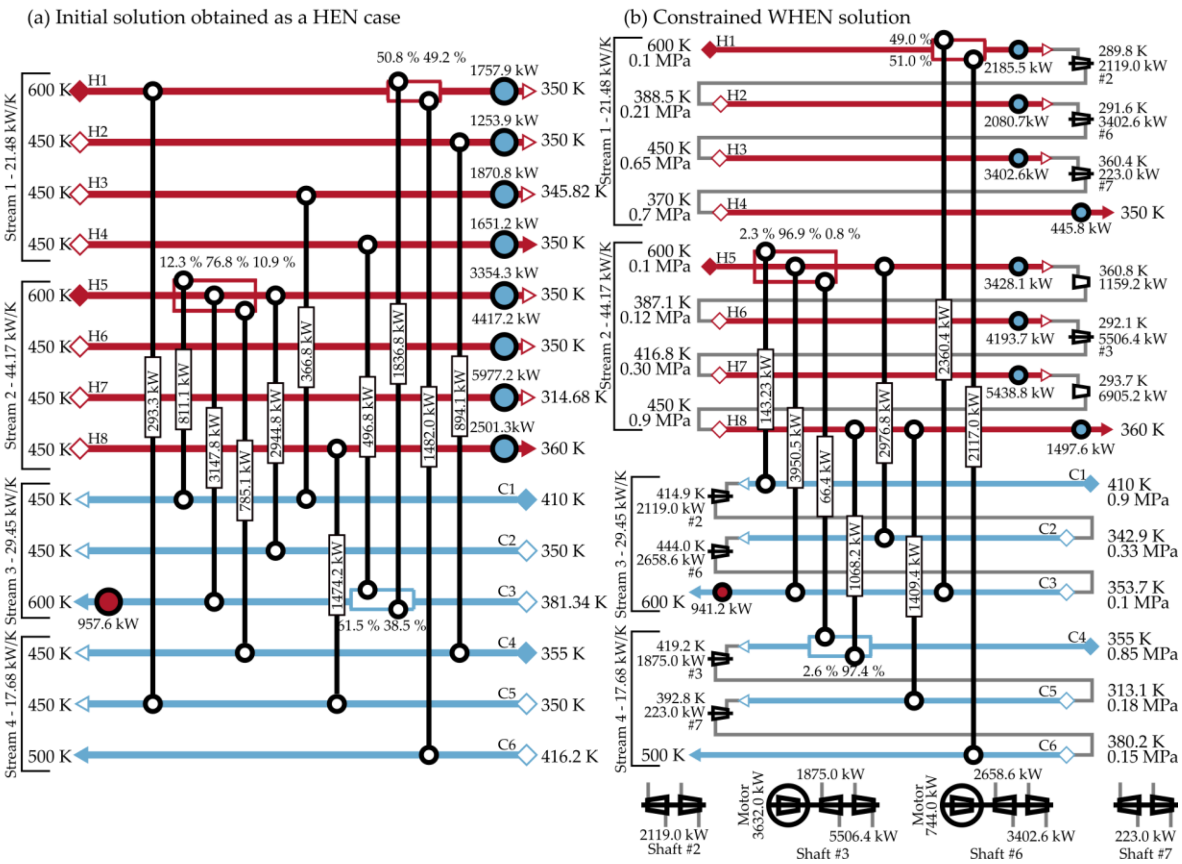

Figure 2: (a) solution for step 1 of the method; (b) final WHEN solution

For the first step of the optimization procedure (see Section 3.2), a HEN problem is proposed. The temperature operating range for compressors is assumed as 350 K to 450 K. Therefore, in the proposed HEN, hot streams should reach 350 K. Cold streams are set to reach 450 K prior to expansion for an increase in the shaft-work to be generated via turbines (note that turbines highest possible temperature is assumed as 800 K). The initial configuration obtained from this optimization run is illustrated in Figure 2a.

Note, for instance, that H3 outlet temperature is slightly lower than 350 K. That is due to the fact that, if the compression procedure is conducted with that stream until the compressor reaches 450 K, its discharge pressure would be lower than the required 0.7 MPa. This also applies to H7. In C3 and C6, inlet temperature is higher than 350 K because the target pressures were already obtained at those temperatures. If that configuration is input as WHEN solution (with compressors/turbines operating at the pre-fixed temperature ranges), its TAC is of 20.76 M\$/y, with total compression work of 21,345 kW, total expansion work of 7,332 kW, total heating requirement of 958 kW and total cooling requirement of 22,784 kW. Figure 2b presents the final

WHEN configuration, attained after optimization step (ii). The final TAC achieved is of 18.439 M$/y. The total energy-related requirements are of: 19,316 kW for compression, of which 6875 kW are provided from expansion work in turbines; 941 kW for heating and 21,196 kW for cooling. Four single-shaft couplings are performed, all within the allowed limit of two units per shaft. Two auxiliary motors are used, for shafts #3 and #6, while in shafts #2 and #7 the compressor work rate needs are fulfilled by the respective coupled turbines. Two standalone compressors are also present in this configuration. That demonstrates that the method was efficient in proposing a configuration that is practical regarding both the temperature thresholds and number of coupled units per shaft with reasonable costs. Optimization step 1 took nearly 15 minutes, while step 2 took nearly 35 minutes in a computer with an Intel® Core™ i5-4690 3.50 GHz processor and 8 GB of RAM.

5. Conclusions

A method for work and heat exchange network (WHEN) synthesis considering more practical operating temperature and couplings for compressors and turbines was presented. The former was included in the WHEN model as new penalization constraints, while the latter was modelled with a matrix representing the pressure manipulators and the shaft each one is coupled to. The solution approach developed is a step-wise method. In it, the WHEN is firstly treated as a HEN with fixed temperature ranges based on practical values. In the second step, the HEN configuration is used as initial solution in the WHEN synthesis model. The HEN solution was within practical temperature bounds, which made the meta-heuristic method more efficient in finding an improved feasible WHEN solution regarding the temperature-related constraints in the case studied. The new SA-based step was also efficient in finding an optimal coupling configuration considering the multiple available shafts and the limit imposed of two units per shaft.

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