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Heat and Work Integration Using a Meta-Heuristic Approach for Heat Exchanger Networks with Pressure Recovery

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

Heat integration by means of Heat Exchanger Network (HEN) synthesis is fundamental in Process Engineering. There are aspects and design options that so far have been scarcely explored in this area. That is the case of heat and work integration. Recent literature shows that the simultaneous optimization of HEN with pressure recovery units can yield substantial gains. Superstructure based mathematical models for HEN synthesis are usually extended for dealing with heat and work integration formulations. Those models are complex to solve, containing nonlinearities and non-convexities that need to be overcome with simplifying assumptions (e.g., isothermal mixing after stream splitting or limiting the structural possibilities) and efficient solution approaches. An important trend in the heat integration literature is the use of meta-heuristic methods. These have arisen as an interesting alternative to the deterministic approaches. Meta-heuristics are attractive since they do not require advanced derivative-based concepts and can treat objective functions as "black-boxes". Those strategies have been used for solving several industrial problems, including HEN synthesis. Promising solutions have been achieved in several benchmark case studies, often with formulations less simplified than those used when deterministic solvers are employed. This work aimed to fill a literature gap by applying a meta-heuristic approach to an enhanced stage-wise superstructure for HEN synthesis extended to handle streams with pressure recovery. The aforementioned superstructure-based model comprises more options than usually found in the literature, such as utilities allocation prior to units that perform heat exchange between two process streams. For achieving its goal, the model entailed several new variables related to pressure recovery, which had to be included to the meta-heuristic scheme. In order to test the methodology, it was applied to a case study taken from the literature. The strategy here used was able to outperform the solution previously reported in the literature, demonstrating that meta-heuristics can be efficiently applied to a heat/work integration model derived from a superstructure more complex than that employed in previous investigations.

1. Introduction

Energy recovery is fundamental in the industry for reducing operating costs as well as mitigating greenhouse gas emissions. Among the forms of energy present in industrial plants, heat is that whose efficient use and integration have attracted most efforts from Process Systems Engineering researchers. Under that scope, a core subject is the synthesis of heat exchanger networks (HEN), a widely investigated matter. HENs are responsible for transferring energy in that form among process streams that need heating or cooling, decreasing the requirements of hot and cold utilities.

Several approaches for HEN synthesis based on mathematical programming have been proposed. Within that sphere, a seminal contribution is the stage-wise superstructure of Yee and Grossmann (1990), which comprises all possible stream matches in different stages and gives rise to a Mixed Integer Nonlinear Programming (MINLP) formulation problem. A comprehensive comparison among other superstructure-based optimization models for HEN synthesis as well as among approximations for logarithmic mean temperature difference can be found in the work of Fraser et al. (2016).

Work recovery is important in processes with intense compression and expansion, such as the production of liquefied natural gas (LNG). For that reason, much of the community attention has been driven recently to the heat and work integration topic by means of work and heat exchange networks (WHEN). In WHEN, energy

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integration aims at reaching goal temperatures and pressures with minimal utilities and electricity requirements. Analogously to temperature manipulation in heaters, coolers and heat exchangers, pressure changes are handled with compressors and turbines, which can be also coupled by a single shaft, saving electricity.

As the subject can be treated as an optimization problem of cost minimization, mathematical models have been presented in the literature. Some noteworthy recent examples are based on such techniques. The models developed by Wechsung et al. (2011) coupled pinch analysis concepts and mathematical programming to solve problems with pressure manipulation routes defined with the plus-minus principle. Onishi et al. (2014a) improved the model of Wechsung et al. (2011) by replacing the pinch analysis stage for the HEN synthesis with the SWS model (Yee and Grossmann, 1990). Onishi et al. (2014b) developed a new superstructure with several options for pressure manipulation, including parallel units. Huang and Karimi (2016) introduced a model comprising sequential temperature and pressure manipulation stages. The model of Nair et al. (2017) did not classify stream pressures as high or low, allowing compression or expansion in all streams. That work was extended (Nair et al., 2018) and, besides not classifying stream pressures, streams were not classified regarding their temperatures (as hot/cold). Furthermore, the manipulation of pressure did not rely on the net pressure change, liquid-vapor phase change was considered and property correlations based on the phases were used. A broader literature review on Work Exchanger Networks (WEN) and WHEN topics has been presented by Yu and Gundersen (2017). Those authors pointed out that the main challenges to WHEN research regards the development of models able to handle real industrial problems and find solutions with minimal costs. In that sense, this work aims to contribute to the area by employing a meta-heuristic solution approach that has already achieved promising results for HEN synthesis.

It is worth noting that meta-heuristic methods are currently an important alternative to deterministic solution schemes, having outperformed those in various benchmark case studies. However, to the best of the authors' knowledge, no meta-heuristic scheme was yet applied to WHEN synthesis. The Simulated Annealing/Rocket Fireworks Optimization (SA-RFO) method employed here is a revamped version of that presented by Pavão et al. (2017b), which demonstrated potential not only for solving large-scale HEN synthesis problems regarding costs, but also regarding other features. For instance, Pavão et al. (2017a) proposed an adaptation for SA-RFO to perform the bi-criteria optimization of costs and environmental impacts based on the ε-constraint method. Later, the method was improved, becoming able to find more efficient solutions to larger-scale problems (Pavão et al., 2017c). The superstructure developed here takes as basis insights presented by Wechsung et al. (2011) and Onishi et al. (2014a), replacing their HEN synthesis stage by the enhanced SWS of Pavão et al. (2018).

2. Problem statement

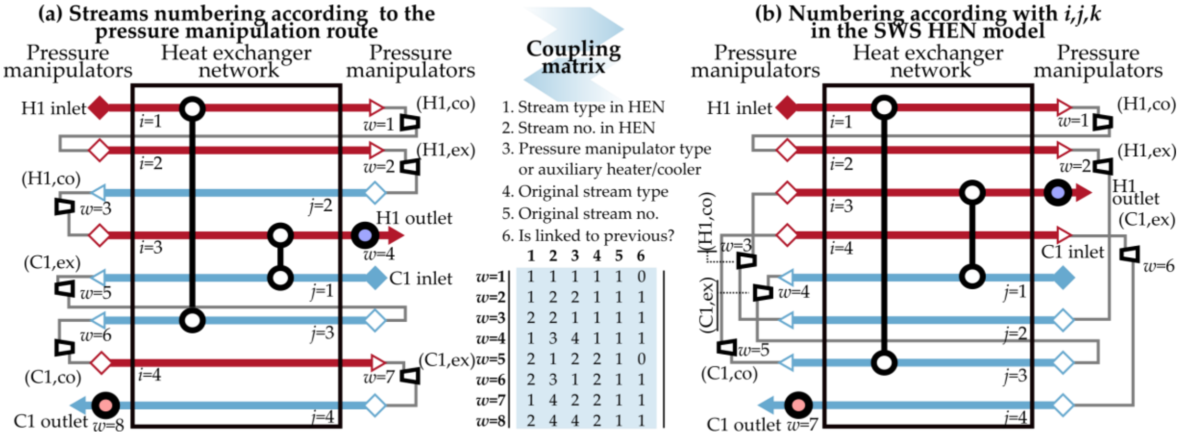
A set of hot and cold process streams is given. Their inlet and outlet temperatures and pressures, heat capacities and heat transfer coefficients are known. All streams must reach their outlet temperatures and pressures. For reaching the target outlet temperatures, heat can be exchanged among the streams in a heat exchanger or using auxiliary heating/cooling from utilities. Compressors are used to raise streams' pressure, while turbines and valves can be used for the opposite situation. Moreover, compressors and turbines might be coupled via single shaft, performing work exchange and thus providing electricity savings within the process. Some additional considerations are: (i) isentropic compression/expansion in compressors and turbines; (ii) adiabatic and irreversible expansion in valves; (iii) ideal gas behaviour. The required isentropic efficiencies, Joule-Thomson coefficient and polythropic exponents are known.

3. Formulation and computational implementation

The model developed here for WHEN synthesis is inspired by that presented by Onishi et al. (2014a), which uses predefined pressure manipulation routes. For the HEN synthesis, those authors used a model based on the SWS of Yee and Grossmann (1990), considering the isothermal mixing simplification. Here the enhanced SWS of Pavão et al. (2018) is used. Evidently, the model differs from that for HEN synthesis in the fact that there are inlet and outlet stream temperatures that are variable, which is a major difficulty in WHEN synthesis. Moreover, the derived model for HEN does not consider the isothermal mixing, which adds nonlinearity to the problem. Furthermore, in the present model, a single stream may undergo several pressure changes. That means a single stream becomes several others in the HEN synthesis model, entailing some HEN stream properties to be interconnected (*e.g.*, the inlet temperature of a given stream is equal to the outlet of another). Thus, the HEN model must be properly coupled to the pressure manipulation equations. In order to do so, a calculation order is pre-defined and followed accordingly.

Figure 1 illustrates a case with one hot and one cold stream. The hot stream route comprises the following: HEN (i=1), compression (w=1), HEN (i = 2), expansion (w = 2), HEN (j = 2), compression (w = 3), HEN (i = 3), cooling (w = 4). The cold stream follows the exact opposite route: HEN (j = 1), expansion (w = 5), HEN (j = 3), compression (w = 6), HEN (i = 4), expansion (w = 7), HEN (j = 4), heating (w = 8). That two-stream example thus becomes one with eight streams.

In Figure 1 (a), the representation is based on the calculation routes. However, it can be noticed that such order is different from the traditional "*i,j,k*" matrices usually employed for HEN data storage with the SWS model, which is represented in Figure 1 (b). For that reason, a "translation" scheme is used so that the data that is interconnected among streams because of the pressure manipulating routes is handled properly. This connection consists basically of using the aid of a "coupling matrix" (C) containing information such as: the order the program must use to calculate temperatures and pressures; the original stream number and if it is originally hot or cold; the i or j index of each of those streams. With such information, it is possible to associate pressure manipulators to the correct streams in the SWS and process the data properly. More information regarding the coupling matrix will be presented along with the equations that require it.



1. Stream type in HEN
2. Stream no. in HEN
3. Pressure manipulator type or auxiliary heater/cooler
4. Original stream type
5. Original stream no.
6. Is linked to previous?

	1	2	3	4	5	6
w=1	1	1	1	1	1	0
w=2	1	2	2	1	1	1
w=3	2	2	1	1	1	1
w=4	1	3	4	1	1	1
w=5	2	1	2	2	1	0
w=6	2	3	1	2	1	1
w=7	1	4	2	2	1	1
w=8	2	4	4	2	1	1

Figure 1: Representation of how data is sorted and stored for calculations related to (a) work or (b) heat

The model here developed aims to minimize total annual costs (TAC), which is a sum of capital and operating costs. In a simplified form, the equation as follows:

$$TAC = \left(EL \cdot TotalW + \sum_{m \in HU} Chu_m \cdot TotalQhu_m + \sum_{n \in CU} Ccu_n \cdot TotalQcu_n \right) + f \cdot \left(HEAreaC + HAreaC + CAreaC + ComC + TurC + ValC \right) \tag{1}$$

where EL represents electricity costs, $TotalW$ is the total power required by the compressors, Chu are hot utility costs and $TotalQhu$ is the total hot utility requirement. Ccu and $TotalQcu$ are parameters and variables for cold utilities that are analogous to previous ones. The indexes (m and n) associated to utility variables represent the hot or cold utility type. The f parameter is the annualization factor, and the terms between the parentheses that follow it are capital costs for heat exchanger areas, heaters, coolers, compressors, turbines and valves.

A more detailed description of TAC calculation can be found in the work of Onishi et al. (2014a).

The following presents the set of equations used for calculations related to pressure manipulators and details on how they are coupled to the HEN synthesis model of Pavão et al. (2018).

The inlet temperatures of pressure manipulators are:

$$\left(\begin{array}{c} C_{w,1} = 1 \\ Twin_w = Tmixh_{C(w,2),K} \end{array} \right) \underline{\vee} \left(\begin{array}{c} C_{w,1} = 2 \\ Twin_w = Tmixc_{C(w,2),1} \end{array} \right) \tag{2}$$

where C is the aforementioned coupling matrix, which has two indexes. The w index is the general number of the stream being evaluated, as in the representation of Figure 1(a). Note that such number is presented at pressure manipulation sections in that figure. That is, the terms presented in this section with a w index are related to property/design calculations for equipment placed at those positions. The index that follows w in the coupling matrix regards streams' information: 1 is for the stream type (as in the SWS); 2 stores stream number (i or j values in the SWS). $Twin_w$ is the inlet temperature of a pressure manipulator (*i.e.*, the outlet temperature of that stream from the HEN section). $Tmixh_{c(w,2),K}$ represents the last mixer's outlet temperature in hot stream

C(w,2). Note that *(w,2)* are indexes of *C*, which store the *i* or *j* index of a stream in the SWS. Those are not represented as subscripts in $Tmixh_{c(w,2),K}$ because sub-subscripts visualization would not be satisfactory.
Outlet temperatures of pressure manipulator:

$$\begin{pmatrix} C_{w,3} = 1 \\ Twout_w = Twin_w + Work_w / CP_{C(w,4),C(w,5)} \\ Trevwout_w = Twin_w + \eta_v (Twout_w - Twin_w) \end{pmatrix} \underline{\vee} \tag{3}$$

$$\begin{pmatrix} C_{w,3} = 2 \\ Twout_w = Twin_w - Work_w / CP_{C(w,4),C(w,5)} \\ Trevwout_w = Twin_w + \eta_t (Twout_w - Twin_w) \end{pmatrix} \underline{\vee} \begin{pmatrix} C_{w,3} = 3 \\ Twout_w = Twin_w - \mu (pwin_w - pwout_w) \end{pmatrix}$$

where the (*w*,3) position in the coupling matrix (*C*) stores a number that represents the pressure manipulator type: 1 for compressors, 2 for turbines and 3 for valves. If that number is 4, there is no pressure manipulator in that position, but an auxiliary one for temperature (*i.e.*, a heater/cooler is used to achieve the target temperature). A programming routine checks the value of $C_{w,3}$ and calculates properties/design according to the presented disjunction. $Twout_w$ are outlet temperatures from a given manipulator. $Work_w$ is the power input/output of compressors/expanders. $CP_{c(w,4),c(w,5)}$ is the heat capacity of a given original stream: in the *C* matrix, the *(w,4)* position stores the stream original classification (1 for hot, 2 for cold), while *(w,5)* stores its original number. $Trevwout_w$ are outlet temperatures for a reversible process. Efficiencies for compressors and turbines are represented by η_v and η_t. Inlet and outlet pressures of a given manipulator are represented by $pwin_w$ and $pwout_w$. Valves are considered only for pressure release. Thus, in case that $C_{w,3} = 3$, $pwout_w$ is always assumed as the final stream pressure. Other pressure calculations are performed with the equations that follow.
Outlet pressures (compressors and turbines):

$$pwin_w = pwout_{w-1} \tag{4}$$

$$pwout_w = \exp\left(\ln(pwin_w) - \frac{\kappa}{(\kappa - 1)} (\ln(Twin_w) - \ln(Trevout_w)) \right) \tag{5}$$

where κ is the polythropic coefficient.
Temperature coupling to the HEN synthesis model:

$$\begin{pmatrix} C_{w,1} = 1 \\ Th^0{}_{C(w,1)} = Twout_{w-1} \end{pmatrix} \underline{\vee} \begin{pmatrix} C_{w,1} = 2 \\ Tc^0{}_{C(w,1)} = Twout_{w-1} \end{pmatrix} \tag{6}$$

where $Th^0_{C(w,2)}$ and $Tc^0_{C(w,2)}$ are supply temperatures of hot and cold streams. Evidently, for a first stream inlet towards the HEN, $Th^0_{C(w,2)}$ and $Tc^0_{C(w,2)}$ are set to the values provided in the problem, instead of being linked to data of another stream. The *(w,6)* position in the *C* matrix is a binary value which indicates whether the present stream is linked to the previous or not. Mathematically, that would yield an extra disjunction which is here omitted for simplicity.

It is worth noting that the implementation of all the disjunctions presented in the model would be difficult in traditional platforms, such as GAMS, and would require some mathematical rearrangement in order to work properly. The sub-subscripts might be an issue as well. On the other hand, an objective function can be programmed as a "black box" in meta-heuristics. That means several nested *if* and *else* statements can be present, which is very intuitive and eases the treatment of problems containing several disjunctions, as in the present model. Although not as mathematically "elegant" as deterministic methods, meta-heuristics are able to handle non-differentiable models and have achieved interesting results for HEN synthesis. Attempts of applications to WHEN might lead to results with important improvements.

4. Example

This is the first example reported in Onishi et al. (2014a). It comprises one hot and one cold stream. The hot stream temperature is 650 K, and must achieve 370 K. That stream must be compressed from 0.1 MPa to 0.5 MPa. The cold stream must be heated from 410 K to 650 K and expanded from 0.5 MPa to 0.1 MPa. The authors proposed that the hot stream undergoes compression, expansion and compression, passing through heat recovery between those stages. The cold stream path is analogous, but with expansion, compression and expansion. More stream details can be found therein. The first two variations of the case proposed by the authors are implemented here and optimized with the proposed model.

As previously stated, the solution approach is an improved version of the SA-RFO method (Pavão et al., 2017b). The implementation was performed in C++ language in Microsoft Visual Studio 2017, which can be obtained free of charges for academic use, in an Intel® Core™ i5 3.50 GHz with 8.00 GB of RAM. SA-RFO is a two-level optimization scheme. Simulated Annealing (SA) is used in the “outer level”, proposing the addition of new random heat exchangers, compressors, turbines and valves to vacant positions in the superstructure (*i.e.*, manipulating binary variables). Rocket Fireworks Optimization (RFO) is then used to optimize the continuous variables associated to the proposed topology. That scheme consists of two coupled strategies: a continuous variation of Simulated Annealing (CSA) followed by an application of Particle Swarm Optimization. The former is able to find a promising solution, which is then incorporated to the swarm of initial solutions in the latter. With an initial good position, as provided by CSA, the performance of PSO improves considerably.

In the first problem variation (case 1), the aforementioned pressure manipulation paths are followed strictly, with no work exchange by means of single shaft equipment. In the second problem variation (case 2), work exchange via single shaft is allowed. The WHEN features achieved by the methodology are presented in Figure 2. Notice that some of the streams have no pressure or temperature manipulators. However, for elucidative purposes, all the possible streams that arise from the possible pressure manipulation route suggested by Onishi et al. (2014a) are present in that figure. The configurations achieved by Onishi et al. (2014a) for the two studied situations had TAC of 1.207 M$/y and 1.081 M$/y. The configurations found for both cases in this study are similar between themselves but dissimilar to those identified by Onishi et al. (2014a). TAC was 1.024 M$/y and 895.8 k$/y (15.2% and 17.1% lower than in the aforementioned work). It is worth noting that the present solutions use only one heat exchanger (versus four in the solutions reported in the cited literature). Both solutions obtained in this study were achieved using initially an “empty” solution (*i.e.*, both heat and work recovery stages had no units) and no variables were initialized *a priori* or had set lower/upper bounds (besides the thermodynamic constraints). For that reason, finding a nearly equal configuration for both cases demonstrates the reliability of the method.

The processing times required to obtain the best solutions were of 1.3 s and 2.4 s for the first and second cases, respectively. Commonly, meta-heuristics’ processing times are longer than those taken by deterministic methods. In this case, though, the times are competitive with the literature: Onishi et al. (2014a) took around 20 s with SBB solver in GAMS in an Intel® Core™ 2 Duo 2.40 GHz processor and 3.00 GB of RAM.

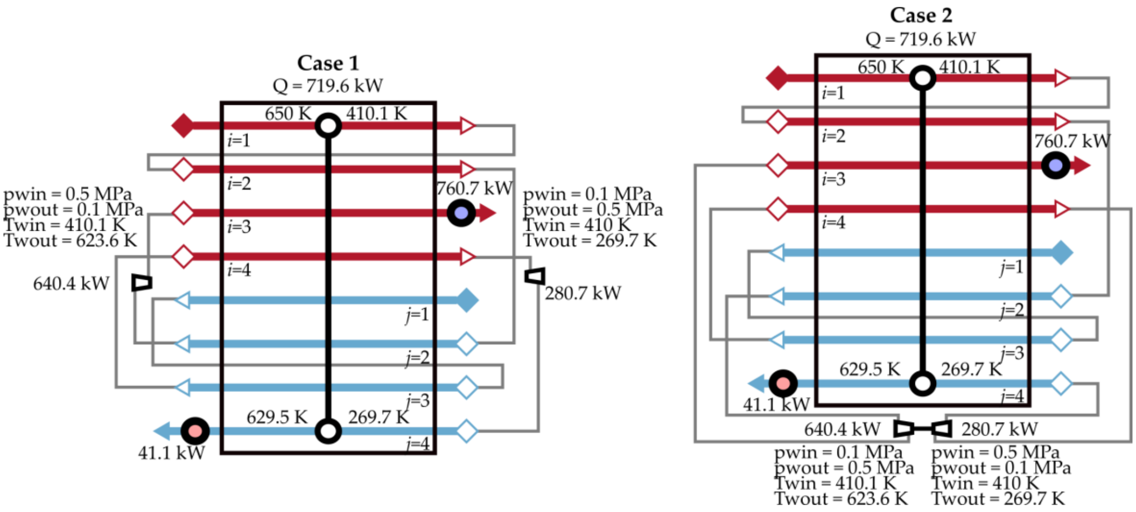


Figure 2: Synthesized WHEN for the case 1 and case 2

5. Conclusions

A new framework for simultaneous heat and work integration has been developed. The presented model differs from others in the sense that it has been developed for a meta-heuristic method. A coupling-matrix scheme was developed to couple the pressure manipulator variables to the HEN superstructure. Some of the features that such scheme yields, *e.g.*, disjunctions and nested subscripts, can be straightforwardly implemented in programming environments when coding the method. Those would be difficult to deal with in deterministic solvers. The methodology was applied to a literature case study under two variations: without and with compressor/expander single-shaft coupling. Evidently, the TAC achieved for the latter was lower, since much of the compressor required energy is supplied by the turbine. The method was able to achieve results remarkably lower (up to 17.1%) than those reported in the literature, which were obtained with a deterministic method. Structurally, the solutions obtained were also simpler regarding the number of units. It can be thus concluded that meta-heuristic methods, which have achieved considerable success in HEN synthesis, might be as well promising to handle WHEN synthesis problems.

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