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Work and Heat Integration: An emerging research area

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Abstract

The extension from Heat Integration (HI) and design of Heat Exchanger Networks (HENs) to including heating and cooling effects from pressure changing equipment has been referred to as Work and Heat Integration and design of Work and Heat Exchange Networks (WHENs). This is an emerging research area of Process Synthesis, however, WHENs is a considerably more complex design task than HENs. A key challenge is the fact that temperature changes (related to heat) and pressure changes (related to work) of process streams are interacting. Changes in inlet temperatures to compressors and expanders resulting from heat integration will influence work consumption and production. Likewise, pressure changes by compression and expansion will change the temperatures of process streams, thus affecting heat integration.

As a result, Composite and Grand Composite Curves will change shape due to pressure changes in the process. The thermodynamic path of process streams from supply (pressure, temperature) to target state is not known and depends on the sequence of heating, cooling, compression and expansion. This paper introduces a definition and describes the development of WHENs. Future research challenges related to methodology development and industrial applications will be addressed. The potential of WHENs will be indicated through examples in literature.

Keywords: work and heat integration; work and heat exchange network; compressor; expander; exergy

1 Introduction

Industrial processes convert feed streams to products and byproducts through extensive consumption and production of thermal and mechanical energies in complex systems of reaction and/or separation. Energy efficiency is thus an important subject both for economic and environmental reasons. Energy efficiency can be addressed at various levels, such as phenomena (heat and mass transfer, pressure drop, etc.), equipment, processes, production sites and industrial clusters. The focus of this paper is energy efficiency measures at the systems level, i.e. processes, plants or sites. Process Integration is a methodology that can be defined as a way to combine (i.e. integrate) process needs of opposite types, such as heating and cooling or compression and expansion. Thus, energy efficiency measures at the systems level can be referred to as Work and Heat Integration (WHI), with subareas Heat Integration (HI) for thermal energy and Work Integration (WI) for mechanical energy. HI can be further broken down into subareas such as Correct Integration (also referred to as Appropriate Placement) of special equipment (e.g. distillation columns and evaporators) and design of Heat Exchanger Networks (HENs). WI means integration of compression and expansion either directly (by Single Shaft Turbine Compressors – SSTCs or Companders) or indirectly by electric generators and motors.

In the discussion of energy efficiency measures above, only separate considerations of thermal energy and mechanical energy have been made. There are also important combined considerations of mechanical energy (work) and thermal energy (heat) that can be made to improve energy efficiency in industry. Examples include combined heat and power production (e.g. gas turbines and extracting steam turbines),

thermodynamic cycles converting heat to power and vice versa (e.g. heat engines, heat pumps and refrigeration cycles), and Work and Heat Exchange Networks (WHENs). As the name indicates, WHENS is a combination of WI and HI, where the main new aspect is that heating and cooling resulting from compression and expansion is included in the HI problem and the design of HENs. WHENs represent an emerging engineering field that will be properly defined in this paper.

The main objective of this paper is to describe the current state-of-the-art in the field of WHENs while describing research in our group as well as contributions from other researchers working in the same field. The literature on WHENs as defined in this paper is still relatively sparse, thus the list of references is very close to complete. The paper will also discuss research challenges and potentials for industrial use. Towards the end, some suggestions will be provided for future research in this field. First, a brief introduction to the pioneering work in Process Integration will be provided, since this provides a basis for the more recent developments in WHENs.

Heat Integration (HI) is a well-developed research area that has enabled considerable energy savings in the process industry. The key research topic has been the design of Heat Exchanger Networks (HENs). Two well-defined methodologies have been developed. The first is the Pinch Design Method (PDM). The concept of a heat recovery Pinch was discovered independently by Hohmann [1], Huang and Elshout [2], Linnhoff et al. [3] and Umeda et al. [4]. The second is based on Mathematical Programming, which is more powerful in solving complex HEN design problems with large-size and the consideration of economic trade-offs. The pioneering work is the models developed by Papoulias and Grossmann [5]. More introductions to the development of HI can be found in an early review [6], an updated review [7] and a recent handbook [8].

The Pinch Design Method has been extended from HI to other applications such as Mass Integration. El-Halwagi and Manousiouthakis [9] developed design methods for Mass Exchange Networks (MENs), which mainly deal with mass exchange between rich and lean process streams. The MENs focus on the changes in concentration of process streams. Wang and Smith [10] introduced Water Pinch Analysis. Alves and Towler [11] developed the concept of Hydrogen Pinch. Tan and Foo [12] applied Pinch Analysis to carbon emission systems.

Analogous to the HEN and MEN problems, the Work Exchange Network (WEN) problem deals with matching of compressors and expanders. Huang and Fan [13] presented an analytical study of WEN design. Mathematical optimization models were later developed by Razib et al. [14]. Liu et al. [15] developed a graphical approach for the design of WENs. The graphical approach was updated by Zhuang et al. [16], and the same group developed a superstructure based MINLP model minimizing total annual cost [17] in a recent study. An analysis method for identifying the maximum recoverable mechanical energy of WENs was presented recently [18].

The combination of HENs, MENs and/or WENs has also been investigated in several studies. Bagajewicz and Manousiouthakis [19] studied HENs and MENs in distillation networks. The problem was further investigated using the state space approach [20]. Papalexandri and Pistikopoulos [21] studied the design of flexible HENs and MENs. A superstructure for HENs and MENs was modeled as a mixed integer non-linear program (MINLP) [22]. Jiménez-Gutiérrez et al. [23] investigated the integration of heat, mass and properties in water networks. Liu et al. [15] presented a graphical approach for synthesizing HENs and MENs. Huang and Karimi [24] developed MINLP models that enable simultaneous work and heat exchange, however, without accounting for heating and cooling from compression and expansion when designing the HEN. Dong et al. [25] developed optimization models for the integration of HENs, MENs and WENs using an exergoeconomic method.

Townsend and Linnhoff [26] presented criteria for Appropriate Placement of heat engines and heat pumps in the design of heat and power networks. Colmenares and Seider [27] developed nonlinear programming models for heat and power integration. Yoon [28] developed models for the simultaneous synthesis of utility systems and HENs using the term Heat and Work Integration. However, the problem addressed was the same as the one discussed by Townsend and Linnhoff [26], thus the study did not consider pressure changes for the process streams. Linnhoff and Dhole [29] presented shaftwork targets for heat and power integration.

Holiastos and Manousiouthakis [30] developed models for minimizing the hot/cold/electric utility cost for the design of HENs including heat pumps/engines. The models were used for heat and power integration in methane reforming based hydrogen production [31]. In all these references to heat and power integration, it is only the working fluids of the thermodynamic cycles that change pressure.

Pressure and temperature are equally important parameters in the process industry. HI only takes the temperature change of process streams into consideration. When pressure changes of streams are considered, the design problem becomes significantly more complex for a number of reasons: (1) As mentioned in the Abstract, the thermodynamic paths of the process streams between supply and target states are not known a priori, (2) the identity of the streams (hot/cold) may temporarily change, (3) even streams with the same supply and target pressure may be compressed and expanded, i.e. the streams act like thermal utilities, and (4) energy forms with different qualities (i.e. heat and work) are handled.

Although the concept of WHI and the corresponding WHENs problem have not yet been consistently defined in the available literature, increasing research activities related to these topics have been performed in recent years. A special session entitled "Work and Heat Exchange Networks" (WHENs) was organized at the 20th Conference on Process Integration, Modelling and Optimization for Energy Saving and Pollution Reduction – PRES'17 [66]. One of the contributions was a review of WENs and WHENs [32]. Based on another contribution to the special session [33], this work addresses the development and challenges in WHI and WHENs. A definition and literature review related to WHENs are introduced in the following sections. The challenges in both methodology development (Pinch Analysis and/or Mathematical Programming) and industrial applications are addressed in subsequent sections.

2 Problem statement

The fundamental insights and the definition of the WHENs problem were presented by Fu and Gundersen [34]. The problem is stated in the following way: "Given a set of process streams with supply and target states (temperature and pressure), as well as utilities for power, heating and cooling; design a work and heat exchange network of heat transfer equipment such as heat exchangers, evaporators and condensers, as well as pressure changing equipment such as compressors, expanders, pumps and valves, in such a way that the exergy consumption is minimized or the exergy production is maximized". Similar to HEN problems, the formulation can of course be extended to consider economic performance. This is, however, beyond the scope of this paper and would introduce a number of additional challenges. A non-convex MINLP model, possibly with a considerable number of binary variables would have to be solved if an accurate economic optimization is to be performed.

The differences in problem definition between HENs and WHENs are illustrated in Figure 1, where Q is heat, W is work, T is temperature, p is pressure, and subscripts "s" and "t" represent "supply" and "target", respectively. Compared to the HENs problem, not only temperature changes but also pressure manipulations of process streams are included in the WHENs problem. In addition, power utility and pressure changing equipment such as compressors and expanders are involved.

A distinct feature of WHENs is that work (pressure) and heat (temperature) are interacting. A stream to be compressed or expanded can be pre-heated or pre-cooled to change the inlet temperature of compression or expansion, so that the heating and cooling resulting from compression and expansion can be utilized in the HENs problem. The work related to compression and expansion will of course change. The following analyses for above-ambient cases can be used to illustrate the interaction between work and heat: (1) The compression work increases when a stream to be compressed is pre-heated, however, the temperature of the stream after compression also increases and more heat (at higher temperature) is available for heat integration. Less hot utility may thus be required. (2) The compression work decreases when a stream to be compressed is pre-cooled, however, the temperature of the stream after compression also decreases and less heat (at lower temperature) is available for heat integration. More hot utility may thus be required. (3) The expansion work increases when a stream to be expanded is pre-heated, however, more heat (at higher

temperature) will also be consumed for the pre-heating process. More hot utility may thus be required. (4) The expansion work decreases when a stream to be expanded is pre-cooled, however, more heat (at higher temperature) will be available for heat integration as a result of the pre-cooling process. Less hot utility may thus be required. The sub-ambient cases can be analyzed in a similar way.

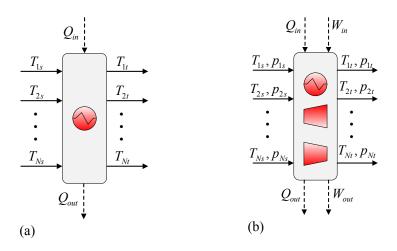


Figure 1 Illustration of HENs (a) and WHENs (b)

3 A literature review related to WHI

Quite a few studies related to WHENs are available in literature. The studies cover topics from fundamental thermodynamic insight to mathematical models. This section presents a literature review of this emerging field.

3.1 Fundamental thermodynamic insight

A key question in WHEN design is the optimal inlet temperature of pressure-changing equipment such as compressors and expanders, which is related to the concept of Appropriate Placement. Glavič et al. [35] briefly discussed the placement of compressors in reactor systems. Compressors were suggested to be placed above the Pinch temperature since they act like hot utilities. Aspelund et al. [36] proposed the following heuristic rules for the placement of compressors and expanders: compression/expansion adds/removes heat to/from the system and should preferably be done above/below Pinch temperature. Based on these heuristic rules, a design methodology called "ExPAnD" was developed for utilizing pressure based exergy in sub-ambient processes. The heuristic rules were further developed by Gundersen et al. [37] in the following way: Both compression and expansion should start at the Pinch temperature. This conclusion was observed from a sensitivity analysis on the inlet temperature of a compressor in a test example where one hot stream (with pressure manipulation) and two cold streams were involved. The sensitivity analysis showed that minimum exergy consumption is achieved when compression starts at the Pinch temperature. However, the heuristic rules were not strictly proven and it was not sufficiently explained why a minimum exergy consumption had been achieved. It was also observed in another test example that the Pinch temperature may change with changing inlet temperature to the compressor.

Kansha et al. [38] developed a self-heat recuperation scheme. The heating demand is satisfied by internal heat exchange and compression heat. External heat is not required. The following analysis shows that both compression and expansion incidentally start at the Pinch temperature. The scheme is illustrated in Figure 2. A feed stream 1 (a cold stream to be heated) undergoes a unit operation "X" (e.g. reaction) after being heated. Figure 2(a) presents one alternative where a feed-product heat exchanger and an external heater are

used to pre-heat feed stream 1 to the operating temperature of "X". Unless unit operation "X" is an exothermic reactor, heating must be used since the temperature of product stream 4 cannot heat feed stream 1 to the operating temperature $(T_3 = T_4)$ due to the requirement of a minimum temperature difference for heat transfer. Figure 2(b) presents the self-heat recuperation scheme as proposed in [38]. To avoid introducing external heating, the product stream is compressed to a temperature high enough so that the product stream can pre-heat stream 1 to the operating temperature of "X". The product stream is then expanded after cooling. The Grand Composite Curve (GCC) for the external heating scheme (Figure 2(a)) is shown in Figure 3. Note that although the temperatures of streams 3 and 4 are the same $(T_3 = T_4)$, the modified temperatures used in the GCC are different since stream 3 is cold and stream 4 is hot. According to the heuristic rules developed by Gundersen et al. [37], both compression and expansion should start at the Pinch temperature. Compression should be done at the higher Pinch temperature 4, i.e. the product stream from "X", and expansion should be done at the lower Pinch temperature 5, i.e. the product stream after being cooled in the feed-product heat exchanger. As can be seen in Figure 2(b), both the compressor and the expander in the self-heat recuperation scheme are placed at the right Pinch temperatures. The self-heat recuperation approach is also the basis for a more recent study of a heat circulation system for a continuous heating and cooling gas cycle process [39].

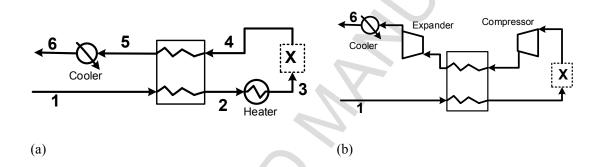


Figure 2 A thermal heating process (redrawn from [38]): (a) the external heating scheme, (b) the self-heat recuperation scheme

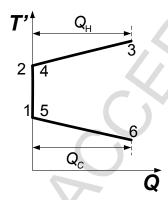


Figure 3 GCC for the external heating scheme

The heuristic rules developed in [37] are, however, not always applicable, e.g. compression of a stream at the Pinch temperature may produce more heat than required, thus stream splitting is needed. Based on strict thermodynamic and mathematical analyses, a set of fundamental theorems has been proposed for the integration of compressors [40] and expanders [41] in above ambient HENs. Considerable symmetry has been found for the integration of expanders [42] and compressors [43] in sub-ambient HENs. The objective

has been to minimize the consumption of exergy (or maximize the production of exergy). Dealing with both work and heat, exergy was used to measure the different qualities of these energy forms in the study. It was concluded that compression/expansion should start at Pinch, ambient, or cold/hot utility temperatures depending on the actual design problem. The conditions for operating at each of these temperatures are well defined in the theorems. The conclusion is obviously different from the heuristic rules presented in [37], which indicated that both compression and expansion should start at Pinch temperature. These theorems form the basis of a systematic graphical design procedure for WHENs [44]. The Grand Composite Curve (GCC) has been used for identifying the maximum portions of streams that can use Pinch Compression/Expansion. Stream splitting is used in order to achieve the objective of minimum exergy consumption. Exergy has thus been used as a pre-design tool, i.e. minimum exergy consumption can be achieved at an early stage of process design. Exergy analysis has in the past only been used as a post-design tool for identifying thermodynamic losses in many literature studies.

In the cases when there is no further external heating or cooling demands to be satisfied and there are some streams still to be compressed/expanded, a remaining question is whether compression or expansion should be implemented first. This problem is related to the following facts: (1) if compression is implemented before expansion, the heat from compression can be used to pre-heat a stream to be expanded so that the expansion work can be increased, and (2) if expansion is implemented before compression, the cooling from expansion can be used to pre-cool a stream to be compressed so that the compression work can be reduced. An additional theorem was proposed for these cases [45], and it was concluded that minimum exergy consumption is achieved at ambient operation and it is independent of the sequence of compression and expansion.

In the cases when there is no stream to be compressed/expanded, e.g. traditional heat integration problems without any pressure manipulation, a stream (either a process stream or any external stream) can still be compressed/expanded as long as it will be brought back to its supply pressure. The heating/cooling resulting from compression/expansion can then be included in the heat integration problem. A sensible heat pump can be realized [46] and the stream being compressed/expanded is used as the working fluid of the heat pump. An illustration is shown in Figure 4. In this heat pump, the working fluid is preheated to the Pinch temperature by receiving process heat below Pinch before being compressed. It is then cooled to the Pinch temperature by delivering heat to process streams above Pinch before being expanded. As a result, both the heating and cooling demands can be reduced. Note that the operation of this heat pump is different from the concept of appropriate placement of heat pumps in traditional Pinch Analysis [8], which indicates that heat should be taken from below Pinch (the evaporator) and delivered above Pinch (the condenser). In the sensible heat pump scheme as shown in Figure 4, there is no phase change and thus evaporator/condenser. The key issue is the placement of compressors and expanders, i.e. both compression and expansion should start at Pinch temperatures. In addition, the optimal amounts of compression heat and expansion cooling are determined following a graphical design procedure using the GCC [46].

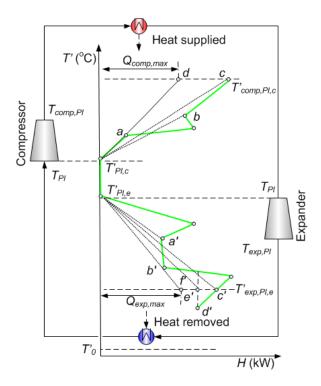


Figure 4 A novel sensible heat pump and the use of the GCC as described by Fu and Gundersen [46]

The term "sensible" indicates that there is no phase change in the heat pump. The heat transfer between the heat pump and process streams thus takes place at non-constant temperature; the irreversibilities are thus lower due to smaller temperature differences for heat transfer compared to normal heat pumps with phase changes often at constant or near-constant temperature. In addition, the heating/cooling resulting from compression/expansion can be utilized.

3.2 Superstructures used for optimization of WHENs

Despite its success, the Pinch Design Method suffers from significant limitations in HEN synthesis. In particular, the methodology can be time consuming when dealing with large size problems, and is rigid with respect to the supply and target temperatures. This is a challenge during simultaneous optimization and heat integration where stream temperatures are normally treated as variables in the model. Consequently, the Mathematical Programming approach is more competitive when solving such problems. Different simultaneous optimization and heat integration models exist in the literature, among them the well-known formulations by Duran and Grossmann [47] and Grossmann et al. [48]. In addition, a HEN synthesis model capable of handling variable stream temperatures has been developed by Yee and Grossmann [49] based on a superstructure where every hot and cold streams are allowed to exchange heat over a predefined number of stages. However, the models may still be very computationally expensive or even impossible to solve for large problems due to the often nonlinear, nonconvex and possibly disjunctive constraints involved. As a result, a hybrid approach combining Pinch Analysis and Mathematical Programming is frequently exploited to simplify the problems appropriately, making them easier to solve. As stated in the Introduction, WHENs is significantly more complex than HENs. Actually, design of WHENs using a Pinch based procedure is computationally difficult even for smaller sized problems with a single variable pressure stream (see examples in Fu and Gundersen [40-43]). Therefore, an optimization based approach (Mathematical Programming) is necessary to study larger and more industrially relevant processes. A superstructure provides the basis for the mathematical model, which must be rich enough to be applied to a variety of different applications for WHENs. However, the level of detail in the superstructure greatly affects the

solvability of the models. Furthermore, it is important that decisions made in the development of the superstructure do not eliminate the optimal solution from the search space. Consequently, superstructures for developing exergy efficient designs should take into account the obtained insights about the placement of compressors and expanders mentioned in Section 3.1. As a result of the growing interest in WHENs, several superstructures have been proposed in the literature.

Wechsung et al. [50] formulated the problem of WHENs using an approach where heat integration and pressure manipulations are assigned to a Pinch operator and a pressure operator, respectively. The Pinch operator can be regarded as a modified heat cascade from Pinch Analysis, however, with both fixed and variable hot and cold streams. The results from the Pinch operator include values for hot and cold utility requirements as well as outlet temperatures for the stream segments belonging to the set of variable process streams. The pressure operator consists of pressure changing units such as compressors and expanders. The results from the pressure operator include net amount of work produced or consumed as well as outlet temperatures for the streams that are subject to pressure manipulations. A third operator is used for the objective function, thus reducing the problem to that of simultaneous optimization and heat integration under varying pressure. Figure 5 provides a detailed illustration of the superstructure. Several objective functions have been considered during their studies of an offshore LNG process. Onishi et al. [51] conducted a total annual cost (TAC) analysis using the same superstructure together with additional operators for the coupling of compressors and expanders, and for selecting valves or turbines. The model was later expanded to retrofit analysis of WHENs at sub-ambient process conditions [52]. The authors also developed a superstructure for WENs that interacts with HENs [53].

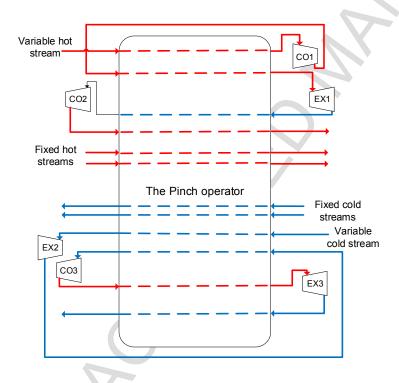


Figure 5 The WHEN superstructure developed by Wechsung et al. [50]

The process streams in the model by Wechsung et al. [50] are classified as fixed or variable pressure streams, where the fixed streams are kept at constant pressure and thus only interact with the Pinch operator. The variable pressure streams, on the other hand, are also connected to the pressure operator through an elaborate compression/expansion scheme. The pressure operator was developed based on the insight from

the ExPAnD methodology [36] with a focus on sub-ambient processes and Liquefied Natural Gas (LNG) in particular. In sub-ambient processes, cooling is the primary objective with exergetic values superseding that of work for significantly low temperatures (less than half of the ambient temperature). The proposed compression/expansion scheme (with three stages) is shown in Figure 5 and depends on whether the variable pressure streams are hot or cold streams. Hot streams are first cooled to Pinch temperature, where they are compressed. Then, the heat of compression is exploited in the HEN as the same stream is cooled back down again to Pinch temperature. From there, the stream is expanded to provide cooling in the network, before it is heated back to Pinch, compressed, and then cooled to the target temperature. In an analogous way, cold streams are heated to Pinch, expanded, heated, compressed, cooled, and then expanded again before they are heated to the target temperature.

Inlet temperatures to the compressors and expanders are variables in the resulting MINLP model. Even though the heuristics from ExPAnD [36] and a later publication by Gundersen et al. [37] stated that compression and expansion should start at the Pinch temperature, the Pinch may change with changes in pressure for the process streams. As a result, the inlet temperature to compressors and expanders are variables. Consequently, the Pinch operator employed in the model must be capable of handling variable supply/target temperatures. Wechsung et al. [50] used the simultaneous optimization and heat integration algorithm of Grossmann et al. [48] in their examples. The compression/expansion scheme is subject to stream identity changes in the model. For instance, the variable hot stream is temporarily a cold stream after expander EX1, before it changes back to a hot stream after the compressor CO2. In this case, the stream identity changes come as a result of the underlying heuristics applied in the development of the superstructure and are therefore known a priori. Consequently, no additional binary variables are required to account for these identity changes. This is in contrast to some of the emerging superstructures that will be discussed in Section 4.3 where the stream identities are not known a priori.

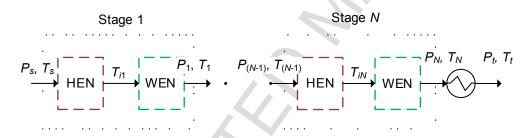


Figure 6 The multi-stage superstructure proposed by Huang and Karimi [23]

A superstructure for TAC analysis of WHENs was proposed by Huang and Karimi [24]. Similar to Wechsung et al. [50], the superstructure divides the problem into a HEN and a pressure manipulation part. The latter is formulated as a WEN problem, thus allowing for pressure recovery from using Single Shaft Turbine Compressor (SSTC) units. Multi-stage compression/expansion is included in the model, and variable pressure streams pass through successive stages of HEN/WEN as seen in Figure 6. The fixed pressure streams are not included in the WEN blocks and thus only affect the heat integration. The WEN superstructure is adapted from the work of Razib et al. [14] and includes SSTCs, stand-alone (utility) compressors/expanders, throttling valves and the possibility of bypassing the pressure stage. In addition, instead of the compression/expansion scheme proposed by Wechsung et al. [50], which distinguishes between hot and cold streams, the model divides the variable pressure streams into sets of high-pressure (HP) and low-pressure (LP) streams. The HP streams are expanded, whereas the LP streams are compressed. Details of the WEN blocks are found in Figure 7.

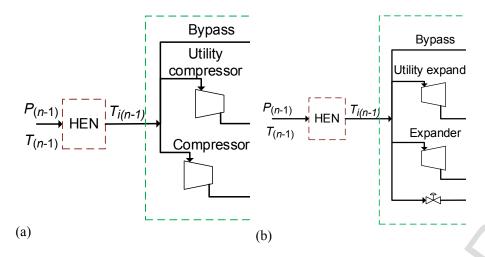


Figure 7 The WEN superstructure for pressure stage *n* in the model by Huang and Karimi [24]: a) for low-pressure streams, b) for high-pressure streams

The model by Huang and Karimi [24] does not rely on heuristics from the ExPAnD methodology or the fundamental insight developed by Fu and Gundersen (described in Section 3.1). Instead, the model increases the net power production through expansion at high temperatures and compression at low temperatures. HP and LP streams are thus treated as cold and hot streams respectively in the HEN. This means that their model is not able to identify solutions where compression is done at high temperatures (i.e. above Pinch) and expansion is done at low temperatures (i.e. below Pinch), which in many cases has proven to improve heat recovery and reduce total exergy consumption. These limitations have been removed in a more recent publication by Nair et al. [54] from the same research group, which is an extension of a paper submitted to the earlier mentioned special session at PRES 2017 [55]. In the extended paper [54], a very rich superstructure for WHEN synthesis is proposed that has been applied to a distillation column with vapor recompression and a simplified offshore LNG process. The optimization model developed by Onishi et al. [51] for TAC minimization applies the WEN superstructure proposed by Razib et al. [14]. The superstructure considers only pressure-changing gas streams, with a heater at the end of the HP streams and cooler at the end of the LP streams. Later, Onishi et al. [56] used the same superstructure in a multi-objective optimization model with the simultaneous minimization of TAC and environmental impact.

As previously explained, the temperature changes and pressure changes of process streams are interacting. Considerable energy savings can be obtained by not decomposing the problem into sub-problems for temperature changes and pressure changes. This fact motivates the research efforts of developing much more complex models that consider both pressure and temperature changes within the same task formulation.

A superstructure based on the theorems for appropriate placement of compressors and expanders (described in Section 3.1) has been proposed by Maurstad Uv [57]. Figure 8 presents a schematic of this WHEN superstructure, where the pressure-changing streams are split into *n* branches, each corresponding to a different compression/expansion temperature. Following the theorems, the inlet temperatures must be either at a Pinch temperature, a hot or cold utility temperature, or the ambient temperature to guarantee a solution for which exergy consumption is minimal. Moreover, two additional stream segments are used for each stream branch; one before and one after the pressure-changing unit. The stream segments interact with the HEN through the individual heat exchangers placed both upstream and downstream of the compressor/expanders. Furthermore, the supply temperature for each branch upstream of the pressure-changing unit is set equal to the supply temperature of the original stream, whereas the target temperature of the individual stream segments downstream of the compressor/expander will equal the target temperature of the process stream. This means that isothermal mixing is assumed, similar to the stage-wise HEN model by Yee and Grossmann [49]. The resulting model represents an automated version of the manual design procedure suggested by Fu and Gundersen [45], where stream branches are integrated successively using

the heat cascade to locate process Pinch point(s).

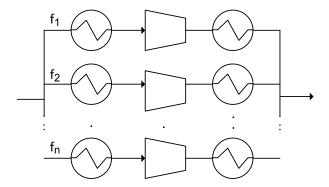


Figure 8 The superstructure by Maurstad Uv [57] for WHENs

4 Challenges in WHENs

The previous literature review clearly shows the increasing research interest and achievements in the area of WHENs. This section provides discussions about remaining problems and challenges in both methodology development and industrial applications.

4.1 Targeting

In Pinch Analysis, the targeting of energy consumption (heat/cooling) can be obtained using graphical diagrams (Composite and Grand Composite Curves) or numerical tools (Problem Table Algorithm or Heat Cascade) prior to detailed HEN design. Due to different energy qualities of heat and work, the targeting of energy consumption ahead of WHEN design is considerably more challenging. Exergy may be used to evaluate energy systems with both heat and work by determining the theoretical work content (exergy) of heat. Several studies have attempted to set minimum exergy targets when both heat and work are involved. Linnhoff and Dhole [29] introduced the Exergy Grand Composite Curve. Heat targeting was obtained using the GCC as in Pinch Analysis. The exergy content of heat was calculated using the Carnot factor. The sum of the exergy of heat and work was then used for exergy targeting. Rather than using the Carnot factor, Feng and Zhu [58] introduced the energy level, defined as the ratio between exergy and energy to set the exergy target. Marmolejo-Correa and Gundersen [59] developed a graphical approach for exergy targets based on the decomposition of thermo-mechanical (or physical) exergy into temperature and pressure based parts. However, none of these approaches for exergy targeting can be applied in WHEN problems since the interactions between temperature changes (related to heat) and pressure changes (related to work) of streams have not been considered. The graphical methodology for WHEN design developed by Fu and Gundersen [45] does not set the minimum exergy target ahead of process design. The minimum exergy consumption is rather a result that is obtained after process design following the insight-based theorems mentioned in Section 3.1.

The concept of targeting (i.e. identifying best performance indicators) ahead of design is fundamental in Pinch Analysis. Such targets (energy, heat exchange units and heat transfer area) provide an indication of how far a specific design is from what can be achieved. An additional important benefit is that fundamental insight on how to design for these targets is obtained as a result of the targeting exercise. Examples of such insight in the Pinch Design Method are (i) Pinch decomposition for minimum energy consumption, (ii) the tick-off rule for reducing the number of units, and (iii) vertical heat transfer for reducing total heat transfer area. Such targets would be even more valuable for WHENs, where an exergy target would include energy

targets for heating, cooling and power. A target for minimum number of units (in line with the exergy target) would account for compressors, expanders and heat exchangers, thus important elements in economic considerations of the design. These targets would also be helpful in identifying optimal solutions of the mathematical models used in optimization approaches. Methodologies for such targeting have not yet been developed. Further research on this topic is required and expected. The main difficulty is that heat and work are interacting with each other in WHEN problems.

4.2 Fundamental thermodynamic insights

There are a number of limitations when applying the fundamental theorems developed by Fu and Gundersen (described in Section 3.1):

- (1) The theorems have been developed for and mainly apply to rather simplified cases, such as only one stream being compressed/expanded and only one hot/cold utility available at constant temperature. When multiple pressure-changing streams are involved, a challenging question is about the integration sequence of streams being compressed/expanded, i.e. which stream should first be integrated with the HEN. In a WHENs problem, since the pressure ratios and thermodynamic properties of the pressure-changing streams may be different, the heating/cooling demands (described by temperatures and heat capacity flowrates) resulting from pressure manipulation can be different. The profiles of driving forces for heat transfer (temperature differences) between the streams with pressure changes and other process streams may thus vary for different integration sequences. As a result, the thermodynamic losses related to heat transfer can be different.
- (2) Only single stage has been assumed for compression/expansion. In practice, multiple stages can and should be used in cases of large pressure ratios. A challenging question is then related to the splitting of pressure ratios in addition to the issue of integration sequence. The total pressure ratio can be distributed among the multiple stages in such a way that the heating or cooling resulting from pressure manipulation matches the GCC in order to reduce thermodynamic losses related to heat transfer (note that cost is not considered here).
- (3) The temperatures of hot/cold utilities have been assumed to be constant at given levels. In the case of non-constant temperature utilities such as flue gas and hot oil circuits, the theorems are no longer applicable, and further investigation is needed. When multiple-utilities such as steam/refrigeration at different temperature levels are used, utility Pinches may be created at some intermediate temperature levels. The theorems should be modified for application to such cases.
- (4) Exergy has been used to account for the different energy qualities of work and heat. However, the exergy of heat is calculated as the maximum amount of work that can be obtained if this heat is used to run a heat engine that operates as a Carnot cycle. Thus, the maximum amount of work corresponding to a given amount of heat can only be obtained in reversible processes. The work obtained from heat in real processes is always less than its exergy content. The quality of heat is thus over-estimated. A factor that reflects the relative value between work and heat in practice should be identified.

Further research is expected to overcome these limitations so that the fundamental insights become more general and can be applied to larger and more complex cases. These insights are also helpful when developing Mathematical Programming models.

It is valuable to point out that a number of graphical diagrams and other representations, such as the Composite and Grand Composite Curves, the Heat Cascade, and the Grid Diagram, acted as catalysts for understanding and further development of the methodology in Pinch Analysis and Heat Exchanger Network Synthesis. Work and Heat Integration is an emerging and complex research area. An appropriate representation of WHEN models can be very helpful for understanding the models. Further research work on such representations are expected.

4.3 Superstructures and optimization of WHENs

Fu and Gundersen developed a graphical design procedure for WHENs (see Section 3.1), which uses the GCC and theorems for appropriate integration of compressors and expanders in HENs. However, the methodology is tediously iterative, to the extent of being prohibitive for large-scale applications. In addition, the developed insight has a number of limitations when it comes to industrial applications, as indicated in Section 4.2. Even if new insight is developed in the future, optimization approaches such as Mathematical Programming will be required for studying and solving industrial size WHEN problems. The key challenge is to develop models that are capable of considering both pressure changes and temperature changes within the same task formulation.

Different superstructures for the design and optimization of WHENs were presented in Section 3.2. The superstructures by Huang and Karimi [24] and Onishi et al. [51] were developed with TAC analysis in mind, whereas the models by Wechsung et al. [50] and Maurstad Uv [57] use exergy consumption as the objective. Adhering to the WHEN problem statement, the superstructures should avoid conflicting with the insight based theorems discussed in Section 3.1 in order to obtain optimal results. Wechsung et al. [50] utilized the heuristic ExPAnD methodology in developing the compression and expansion scheme for the superstructure, which states that pressure-changing equipment should be integrated at the Pinch. However, the main new result from the research by Fu and Gundersen presented in Section 3.1 is that Pinch compression/expansion is not always optimal and that stream splitting in order to compress/expand at different temperatures is sometimes necessary to match the surplus or deficit of heat in the GCC at given temperature levels. Consequently, rather than compressing/expanding from the Pinch temperature, the theorems propose an alternative integration strategy where the variable pressure streams should be compressed/expanded from either a Pinch temperature, hot or cold utility temperature or the ambient temperature. As a result, not accounting for stream splitting in the superstructure may lead to suboptimal results.

The model by Huang and Karimi [24] uses stream splits for utility compressors or expanders, and Single Shaft Turbine Compressor (SSTC) arrangements. In addition, they included the possibility to bypass a pressure stage and added valves for the HP streams. However, interaction with the HEN module occurs upstream of the stream splits, and as a consequence, the inlet temperatures to the pressure changing units are the same. As a result, the WEN superstructure maximizes the net power production by increasing the inlet temperature before expansion, and reducing the temperature before compression. Thus, the heating/cooling from compression/expansion is not utilized in the HEN modules. In a more recent work by Nair et al. [54], a very rich superstructure is proposed that can handle (i) unknown stream identities, (ii) pressure changes even for streams with the same supply and target pressure, (iii) liquid-vapor phase changes, and (iv) phase-based property correlations. Unfortunately, this richness in the superstructure results in very large computing times. This is related to an extensive use of binary variables. As an example, the corresponding MINLP model for a C3-splitter involves 196 binary variables, 482 continuous variables, 1,704 constraints, and it takes 19,787 seconds (5.5 hours) to solve using Baron to a relative gap of 0.5%.

Vikse et al. [60] discussed the various superstructures that have been proposed with focus on the ones that are applicable for WHENs. Challenges related to modeling, such as non-convexity and non-smoothness, were also discussed since these are of extreme importance in optimization formulations. The complexity of the mathematical models is expected to be considerably reduced with the utilization of fundamental thermodynamic insights. The models developed by Maurstad Uv [57] show that the problem can be simplified to a Linear Programming (LP) model by using the theorems by Fu and Gundersen for compression above Pinch [40], expansion above Pinch [41], expansion below Pinch [42], and compression below Pinch [43]. The study also added to the fundamental insights in the following way: In the mentioned studies by Fu and Gundersen, the GCC was used to identify the maximum portions of streams for Pinch Compression/Expansion. For simplicity, however, the Pinch identity (hot or cold) was not considered when using the GCC. Slightly improved solutions can be achieved if the Pinch identity is taken into consideration. The following new insight has been formulated by Maurstad Uv [57] and Fu et al. [61] for the selection of the true Pinch temperature: The Pinch identity (hot or cold) should be the same as the identity of the stream segment at the inlet of compression/expansion, not the identity of the original ("parent") stream.

The superstructure by Maurstad Uv [57] was developed based on the graphical design procedure for WHENs with stream splits and inlet temperatures to the pressure-changing units as variables in the model. Pinch points are located using the heat cascade prior to optimization. The algorithm is sequential, with stream temperatures calculated prior to optimization and re-iterated in case additional Pinch points are created after integrating the pressure changing streams. Although a sequential approach has a clear advantage in that it results in an LP model, this strategy also has several disadvantages. Integration of several compressors/expanders sequentially can result in suboptimal solutions as the integration sequence might influence the set of Pinch points and thus the number of stream branches in the network. In such cases, the sequential approach reduces to an enumeration problem for which all possible integration sequences must be evaluated to ensure global optimality. Another issue with the sequential approach is the creation of additional Pinch points due to integration of pressure-changing streams. In such cases, additional stream branches are required, and the procedure must be repeated until reaching an appropriate number of stream branches in the superstructure. Alternatively, a simultaneous optimization approach for heat and power integration similar to the models by Wechsung et al. [50] and Huang and Karimi [24] can be employed. In that case, the issue with the integration sequence of compressors and expanders is avoided, though it also requires the simple LP formulation to be replaced by a nonconvex NLP or MINLP model. In addition, a superstructure having stream branches for every Pinch point will be difficult with a simultaneous approach, as new Pinch points may occur when integrating variable pressure streams in the HEN. As a result, the number of branches and thus stream segments also change during optimization causing the sets of variable hot and cold streams to be dynamic.

Unknown stream identities represent an additional challenge for optimization of WHENs. Unlike heat integration where stream identities remain fixed during optimization, the stream segments in the superstructure by Maurstad Uv [57] change identity depending on the location of the Pinch point(s). Yu et al. [62] developed an optimization model based on the superstructure by Maurstad Uv [57], where the stream identities are unknown variables. With binary variables used to identify the stream identities, the resulting model is a non-convex MINLP with corresponding problems related to local optima. In addition, due to the current limitations of the fundamental thermodynamic insights mentioned in Section 4.2, combining an optimization approach (Mathematical Programming) with fundamental insights for the design of WHENs is restricted to small size problems. Further developments of both insights and the mathematical models are therefore required to be able to deal with large scale problems.

4.4 Industrial applications

WHENs is expected to have considerable scope for industrial applications. Quite a few studies related to application of WHENs have been published. It was reported that energy savings of 14.5% can be achieved in the azeotropic distillation process for a mixture of ethanol and water with application of the Self-Heat Recuperation scheme [63]. In an oxy-combustion coal-based power plant with CO₂ capture, the boiler feedwater of a regenerative steam Rankine cycle can be partly pre-heated by the compression heat from an air separation unit. The overall plant thermal efficiency is improved by 0.5-0.6% points according to a mathematical modeling study [64]. Aspelund et al. [36] applied the ExPAnD design methodology to LNG processes using liquid CO₂ and liquid N₂ as cold carriers. The exergy efficiency was reported to be increased from 49.7% to 85.7% compared to a design based on using standard Pinch Analysis. Fu and Gundersen [34] presented the applications of WHENs in three CO₂ capture processes: (1) In an oxy-combustion coal-based power plant, an N₂ Brayton cycle was developed by integrating the N₂ expansion process with the flue gas cooling process. As a result, the work consumption for the air separation unit is reduced by 10.1%. (2) In a post-combustion coal-based power plant using a membrane for separation of CO₂ and N₂, the specific work consumption for CO₂ separation is reduced by 12.9% through integration of the expansion process of the retentate gases from the membrane with the flue gas cooling process. (3) In an ion transport membrane separation process for O2 production, adiabatic compression of the air feed is suggested so that the

compression heat can be utilized. The net consumption of work is reduced by 90% with proper work and heat integration. Despite the successful applications described above, there are a number of remaining challenges related to industrial use of the emerging WHENs methodology, and those issues will be discussed in this section.

The compressors will be operated at temperatures above ambient when the results from using the WHENs methodology is implemented. For example, in a case where Pinch compression is preferred and the Pinch temperature is above ambient, a stream needs to be pre-heated to the Pinch temperature and then compressed. However, very few compressors in industry operates at temperatures significantly above ambient temperature. The elevated operating temperature is a considerable challenge for industrial compressors. The materials of construction are potential limiting factors. Nevertheless, the considerable energy saving potential is an attractive driving force for the development of advanced compressors/expanders. For example, the Ramgen compressor [65] has been developed in industry for compressing CO₂ in a single stage with a pressure ratio up to 10, so that the compression heat can be utilized.

It should also be noted that the variation of compressor/expander efficiency with operating temperature has not been considered in detail in the developed theorems and insight mentioned in Section 3.1. More precise energy saving potentials can be obtained if the variation of efficiencies with temperature is considered. However, such knowledge is normally limited to the manufacturers and not publicly available.

Economics has to be taken into consideration for industrial applications. Of course, it is helpful to eliminate the less promising WHENs at an early stage of process design so that detailed economic analysis is avoided. The complexity and the cost of pressure changing equipment (e.g. compressors and expanders) are normally higher compared to heat exchangers. The number of compressors/expanders, that results from the splitting of streams to be compressed/expanded, should thus be reduced unless their investment cost can be justified by the savings in operating cost. Similar to the Pinch Design Method, heuristic rules for the removal of small units are expected to be developed for WHEN design.

The relative value of work and heat should be evaluated in specific case studies. As explained in Section 4.1, the true value (or quality) of heat is less than its exergy value. The reason is that the exergy of heat is obtained from the Carnot equations using the assumption of reversible (ideal) processes. In addition, the relative prices of hot/cold utilities and work (power) are determined by a number of factors. Heat may even be more expansive than work in some special cases. A common relative value between work and heat can hardly be specified for all industrial applications. Methodologies for establishing such relative values are expected to be developed through different case studies.

Finally, the integration of work and heat may increase the process complexity and thus reduce the process operability, flexibility and reliability in many cases. The size, layout and controllability of the plants should also be considered when it comes to industrial applications.

5 Conclusions

The Heat Integration problem deals with process streams that only change temperature. The problem has to be extended from Heat Integration to Work and Heat Integration when pressure changes of streams are included. This topic is an emerging research area that has already attracted considerable interest in both thermodynamic (fundamental insight) and mathematical modeling studies in recent years. The interaction between the temperature change (related to heat) and pressure change (related to work) of streams represents a considerable challenge for the new problem. In addition, with energy forms of different quality involved (i.e. heat and work), exergy has been used as a performance indicator. Exergy has actually been successfully used as a pre-design tool in a graphical design procedure developed for WHENs. Preliminary conceptual design studies show that the energy savings are quite promising for industrial applications.

Despite the increasing achievements in the new area of Work and Heat Integration, there are still quite a number of limitations and remaining challenges to be studied in both fundamental methodology development and industrial applications, such as (1) targeting for exergy, energy and units ahead of process

design has not yet been achieved for the more general case; (2) the fundamental theorems as well as the graphical design procedure developed in literature can only deal with small size problems. The single hot/cold utilities were assumed to be at constant temperature levels. The pressure manipulations were assumed to be achieved in a single compression/expansion stage; (3) the Mathematical Programming models available are complex to solve and are expected to be simplified in combination with the development of fundamental thermodynamic insights; and (4) many other factors such as economic issues, operating temperatures, process operability, controllability, flexibility and reliability should be considered when it comes to practical industrial applications.

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Highlights

- Simultaneous Work and Heat Integration is a new research area in Process Synthesis
- A literature review/overview related to Work and Heat Integration is performed
- Combined use of Thermodynamic insight and Mathematical Programming
- Challenges in methodologies and industrial applications are discussed
- Heat Exchanger Networks is extended with stream pressures and work/power