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Abstract

The extension from Heat Integration and design of Heat Exchanger Networks (HENs) to including heating, cooling and power 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 in Process Synthesis and PSE, and WHENs represent a considerably more complex design task than HENs. A key challenge is the fact that temperature changes and pressure changes of process streams are interacting. Changes in inlet temperature 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. The state-of-the-art of this new research area including insight, methodologies, tools, opportunities, challenges and literature is presented. Key aspects are illustrated by simple examples while smaller case studies indicate potentials for industrial applications.

Work and Heat Integration—A New Field in Process Synthesis and Process Systems Engineering

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The extension from heat integration and design of heat exchanger networks (HENs) to including heating, cooling, and power 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 in Process Synthesis and Process Systems Engineering, and WHENs represent a considerably more complex design task than HENs. A key challenge is the fact that temperature changes and pressure changes of process streams are interacting. Changes in inlet temperature 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. The state-of-the-art of this new research area including insight, methodologies, tools, opportunities, challenges, and literature is presented. Key aspects are illustrated by simple examples, whereas smaller case studies indicate potentials for industrial applications. © 2018 American Institute of Chemical Engineers *AIChE J*, 00: 000–000, 2018
Keywords: process integration, heat integration, work integration, expansion, compression, WHENs

Background

Improved energy efficiency is regarded by the International Energy Agency as well as the European Union to be in the front line of mitigating carbon emission from fossil fuels and thereby contribute toward more sustainable industrial processes and energy plants. A number of resource efficiencies represent important production goals and have therefore been used as key performance indicators (KPIs) for industrial processes. These KPIs relate to (1) raw materials, (2) energy, and (3) equipment, thus affecting both economic and environmental aspects of processing.

The field of designing such efficient processes in a systematic way has been referred to as Process Synthesis (Rudd et al., 1973).[1] Process Systems Engineering (PSE) considers modeling, simulation, optimization, control, and operation of production facilities, where the word system clearly indicates a holistic approach. More specifically related to efficiency, the field of process integration emerged during the 1980s. The word integration refers to the synergies obtained by matching needs of opposite kinds, such as heating/cooling and expansion/compression. Yet another example is byproducts from one process being used as raw materials in other processes. These efforts are referred to as heat integration, power integration, and chemical integration (industrial symbiosis), respectively. The key idea is to match sources with sinks. As an introduction to the topics in this article, Figure 1 attempts to put the different terms that are used into perspective. Only energy-related fields will be discussed, whereas material-related topics will only be briefly mentioned.

Heat integration and pinch analysis

This article is focusing on energy, and the field of heat integration represents a mature field that has been subject to large research efforts and extensive industrial applications during the last 35–40 years. Methodologies and tools developed have been based on thermodynamics, heuristics, and optimization, and they have had a nature of being manual or automatic. Of course, there has also been hybrid approaches. More specifically, pinch analysis (combining thermodynamics and heuristics), mathematical programming (deterministic optimization) and meta-heuristics (stochastic search) are established methodologies for heat integration.

The concept of a heat recovery pinch and graphical diagrams such as composite and grand composite curves (GCCs) form the core of the field of heat integration with early contributions from Hohmann (1971),[2] Huang and Elshout (1976),[3] Umeda et al. (1978),[4] and Linnhoff and Flower (1978).[5] Perhaps, the single most important insight based on the pinch concept is the decomposition of processes into a heat deficit region above pinch and a heat surplus region below pinch (Linnhoff et al., 1979).[6] This decomposition then provided

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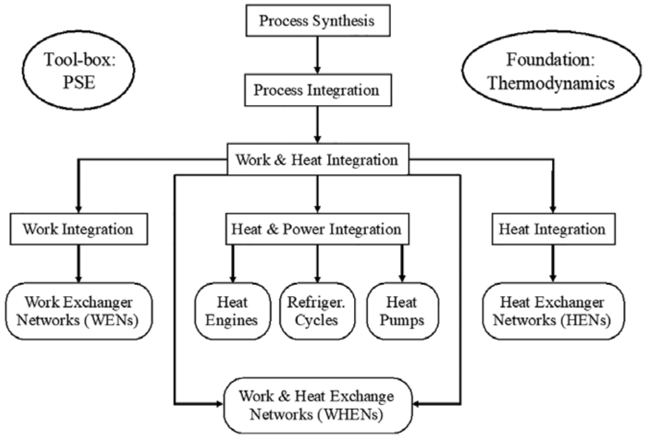

Figure 1. The perspective and hierarchy of energy related terms used in this article.

guidelines for design of heat exchanger networks (HENs) through the pinch design method (Linnhoff and Hindmarsh, 1983),[7] integration of distillation columns (Linnhoff et al., 1983),[8] and evaporators (Smith and Jones, 1990),[9] as well as appropriate placement of heat pumps and heat engines (Townsend and Linnhoff, 1983).[10] Glavič et al. (1988)[11] discussed the integration of chemical reactors; however, these are often operated at high temperatures for kinetic reasons, thus endothermic reactors (heat sinks) can normally not utilize available heat below pinch. Exothermic reactors (heat sources) can provide heat above pinch, but this is most commonly done in an indirect way using steam as the energy carrier.

The field of heat integration only considers heat and temperature, except for the work produced and consumed in heat engines and heat pumps. In the process industries, however, both pressure and temperature of process streams need to be considered and both heat and work are important energy forms. This is the main motivation for developing new methodologies that encapsulate these aspects of industrial processing. The result is a new emerging field of Process Synthesis and PSE referred to as work and heat exchange networks (WHENs).

Analogies to the heat pinch

Before introducing and defining WHENs, it is worth mentioning that a number of tools and methodologies have been developed by using analogies from heat integration and HENs. Concepts, representations, and graphical diagrams from HENs can be reused as important design tools in other areas. El-Halwagi and Manousiouthakis (1989)[12] discussed mass exchanger networks (MENs), whereas Wang and Smith (1994)[13] used similar ideas for wastewater minimization as a start of a new design field referred to as water networks. In addition to heat pinch, mass pinch, and water pinch, methodologies for hydrogen pinch (Alves and Towler, 2002),[14] oxygen pinch (Zhelev and Ntlhakana, 1999),[15] and carbon emission pinch (Tan and Foo, 2007)[16] have been developed.

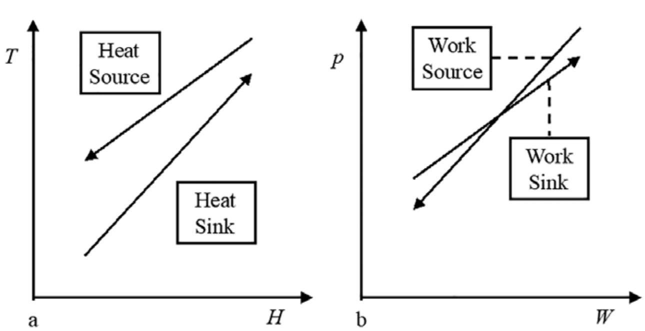

Figure 2. Source and sink profiles in heat exchanger networkss (a) and work exchange networkss (b).

Work Exchange Networks

In parallel, there have also been some efforts to develop systematic approaches to handle pressure and work in so-called work exchange networks (WENs). Work (or mechanical energy) typically comes in two forms; flow work and shaft work. Although flow work can be recovered (or exchanged) directly, shaft work is recovered directly (expansion and compression on a single shaft) or indirectly (using electricity generator and motor). Cheng et al. (1967)[17] introduced the flow work exchanger, and Huang and Fan (1996)[18] later defined the WENs problem as an analogy to HENs. Although the flow work exchanger is an interesting concept, pressure changing equipment in the process industries are more typically compressors, pumps, fans, expanders (turbines), and valves. Expanders can be used to run compressors and pumps, either directly by single shaft solutions or indirectly by generators and motors, as mentioned above.

The analogy between HENs and WENs is, however, not very strong. One example is temperature driving forces that are fundamental in HENs (see Figure 2a), although there are no driving force limitations related to pressure in WENs. In fact, the pressure profiles in a flow work exchanger show crossover as a necessary means to operate the unit (see Figure 2b). This lack of driving force requirements also applies to shaft work exchange, where, for example, an expander operating between 4 and 1 bar can be used to drive a compressor operating between 6 and 15 bar. This is the case both for direct (i.e., single-shaft-turbine-compressor—SSTC) and indirect (i.e., generator and motor) shaft work exchange. In conclusion, for WENs, there are no driving force requirements ($\Delta p \geq \Delta p_{\min}$), and thus no work recovery pinch. The obvious reason is that pressure-based energy is converted into mechanical energy (or power), which is then subsequently used to pressurize another process stream. Because the main focus of this review article is on WHENs dealing with pressure, temperature, work, and heat, methodologies for WENs without considering heat and temperature will only be briefly discussed here, with a few selected references that indicate the different schools of methods.

Brief literature review of WENs

As mentioned above, the WENs field was pioneered by Huang and Fan (1996)[18] who proposed necessary and sufficient conditions for stream matching in networks of flow work exchangers. The outlet pressure of the work source should be lower than the inlet pressure of the work sink, whereas the inlet pressure of the work source must be higher than the outlet pressure of the work sink, as shown in Figure 2b. Both thermodynamic- and optimization-based approaches have been proposed.

Zhou et al. (2011)[19] extended pinch analysis to WENs based on flow work exchangers by using the problem table algorithm to determine minimum work utility requirements. Chen and Feng (2012)[20] proposed a novel graphical method for constructing composite curves in a pressure–work diagram to determine the theoretical work target. Liu et al. (2014)[21] further developed this graphical integration method, where composite curves for work sources and sinks are drawn in an ln p vs. W diagram. They also proposed five rules for optimally matching work sources and sinks. Yet, another upgraded graphical method for the synthesis of direct WENs was proposed by Zhuang et al. (2017).[22] Finally, Amini-Rankouhi and Huang (2017)[23] proposed a thermodynamic modeling and analysis method for direct WENs to identify the maximum amount of recoverable work by using a matrix of pressure intervals.

Analysis and design of WENs have also been subject to the use of optimization. Razib et al. (2012)[24] developed a superstructure for WENs with a corresponding mixed integer nonlinear programming (MINLP) model that minimizes total annualized cost (TAC). This model can synthesize WENs while considering operational issues such as surging, choking, and shaft speed. Du et al. (2015)[25] developed an optimization model where compression and expansion ratios are regarded as variables. Their transshipment-based model is easy to solve because it is linear. Zhuang et al. (2015)[26] used a transshipment model to target minimum utility (work) consumption, whereas WEN synthesis was approached using a linear programming model assuming isothermal compression and expansion. Later, Zhuang et al. (2017)[27] used a stage-wise superstructure with and without stream splits to synthesize direct work exchanger networks with minimum TAC.

Introducing Work and Heat Exchange Networks

After introducing HENs and WENs, the combined case of WHENs will be thoroughly introduced, defined, and reviewed. It is important to realize that HENs and WENs should not be solved independently, because temperature changes and pressure changes of process streams are interacting. The inclusion of heating from compression and cooling from expansion in the heat recovery system is the key element that distinguishes WHENs from HENs and WENs. It also distinguishes WHENs from previous synthesis studies on heat and power systems, such as Townsend and Linnhoff (1983)[10] who presented criteria for appropriate placement of heat engines and heat pumps, Colmenares and Seider (1987)[28] who developed a nonlinear programming (NLP) model for heat and power integration, Yoon (1990)[29] who developed models for simultaneous synthesis of utility systems and HENs, Linnhoff and Dhole (1992)[30] who presented shaft work targets for heat and power integration, and Holiastos and Manousiouthakis (2002)[31] who developed models for minimizing hot, cold, and electric utility cost for the design of HENs including heat pumps and heat engines. In all these references to heat and power integration, it is only the working fluids of the thermodynamic cycles that change pressure.

Problem definition for WHENs

Because WHENs include energy forms with different quality (heat and work), exergy has been used as a common measure. Correspondingly, exergy efficiency is an adequate KPI for energy efficiency. Unfortunately, several exergy efficiencies have been proposed in the literature with varying ability to properly capture the essential features of the energy and exergy transfer processes in a plant (Marmolejo-Correa and Gundersen, 2012).[32]

The WHEN synthesis problem can be defined in the general situation as follows: *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 WHEN of heat transfer equipment such as heat exchangers, evaporators, and condensers, as well as pressure changing equipment such as compressors, expanders, pumps, and valves.* As a first step, with a focus on energy targeting while handling energy forms with different quality, minimum exergy consumption has been used as the objective function. Of course, the ultimate goal is to identify WHENs with minimum TAC. The fact that compressors and turbines (expanders) are significantly more expensive pieces of equipment than heat exchangers makes it even more important to move from energy/exergy to economy (cost).

Appropriate placement of compressors and expanders

In WHENs, the interaction between heat and temperature on one hand and work and pressure on the other hand can be described as follows: changes in inlet temperature 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. This is why identifying optimal inlet temperatures to compressors and expanders, also referred to as appropriate placement (or correct integration) of these units, is a key issue in WHENs. Although appropriate placement is straightforward for equipment such as chemical reactors, distillation columns, evaporators, heat pumps, and heat engines, it is considerably more complex for pressure changing equipment such as compressors and expanders. The appropriate placement concept is based on pinch decomposition; however, pressure changes result in temperature changes, especially for gas-phase streams. Changes in stream temperatures result in changes in the shape of the composite and GCCs, and thus possibly changes in pinch location as well as thermal utility requirements. This is the main complicating factor for WHENs that makes it much more challenging to solve as a design problem than HENs.

Developing insight based on thermodynamics

Insight related to appropriate placement of compressors and expanders has developed gradually. Aspelund et al. (2007)[33] realized that compressors provide heat and should thus be placed (operated) above pinch in the heat deficit region. Likewise, expanders provide cooling and should be placed below pinch in the heat surplus region. It should be noticed that these guidelines are in conflict with current industrial practice. This new insight was stated more firmly by Gundersen et al. (2009),[34] who suggested that compressors and expanders should be placed (i.e., have inlet temperatures) exactly at the pinch. As mentioned above, however, pressure changes may result in changes in pinch location, thus the appropriate placement concept becomes less obvious and more insight was required.

In a series of papers, Fu and Gundersen (2015)[35-38] proposed theorems that were based on thermodynamics and proven mathematically for integration of compressors and expanders above and below ambient temperature. The simplified case with only one hot and one cold constant temperature utility was considered, and the chosen objective function was minimum exergy consumption (or maximum exergy production) to properly account for the difference in energy quality between heat and work. The main result from these studies is that only a few inlet temperatures to these units are potential candidates for optimal integration. These are the hot and cold utility temperatures (T_{HU} and T_{CU}), pinch temperature(s) (T_{PI}), and ambient temperature (T_0), depending on whether the case is compression or expansion and whether the process is above or below ambient temperature.

This important insight will be illustrated by a simple example where a stream is to be expanded above ambient temperature, that is, the situation discussed by Fu and Gundersen (2015).[36] There are two important variables that determine the optimal inlet temperature for the expander; the cooling duty resulting from expansion if the stream in question is expanded at pinch temperature, $Q_{exp,PI}$, and the outlet temperature if expansion starts at hot utility temperature, $T_{exp,HU}$. Four cases are possible depending on the values of these two variables, and the minimum cooling requirement, $Q_{C,min}$ (the lumped variable *mCp* is the product of mass flow rate and specific heat capacity):

1. The simplest case is the rare situation when $T_{exp,HU} \leq T_0$. Then, expansion at hot utility temperature provides an amount of cooling below pinch, $mCp \times (T_{PI} - T_0)$, that is equal to or greater than any other expansions, while producing a maximum amount of work (Theorem 4).

2. A very common situation is when $T_{exp,HU} > T_0$ and $Q_{exp,PI} \leq Q_{C,min}$. Then, only pinch expansion should be used (Theorem 1).

3. If $T_{exp,HU} \geq T_{PI}$ and $Q_{exp,PI} > Q_{C,min}$, then pinch expansion should be used until external cooling requirements are satisfied. The remaining expansion could be done at T_{HU} or T_0. These alternatives are equal from an exergy point of view (Theorem 2).

4. The most complicated case is when $Q_{exp,PI} > Q_{C,min}$ and $T_0 < T_{exp,HU} < T_{PI}$. Expansion at hot utility temperature then becomes a strong competitor to pinch expansion, because it provides some cooling below pinch while producing more work than pinch expansion due to a higher inlet temperature to the expander. An iterative procedure is required where pinch expansion is reduced and expansion at hot utility temperature is increased (Theorem 3).

Cases 2 and 3 are, however, more complicated than indicated above. There are cases where expanding a part of the stream (Case 3) or the entire stream (Case 2) at pinch temperature will create a new pinch at a lower temperature. Then, the stream must be split, and a fraction of the stream should be expanded at this new pinch. Obviously, this situation may have to be repeated several times. The tool to identify the maximum cooling that can be utilized below pinch from expansion at pinch is the GCC, see Figure 3. A number of potential new pinch candidates exist; however, the new pinch can be identified as the point on the line from the pinch point with the steepest slope while touching but not intersecting with the GCC, that is, point *c* in Figure 3. By extending this line to the outlet temperature from pinch expansion, $T_{exp,PI}$, the maximum amount of cooling that can be utilized by pinch expansion, $Q_{exp,max}$, is identified. The corresponding maximum *mCp* that can be subject to pinch expansion is then found by the simple equation $mCp_{max} = Q_{exp,max}/(T'_{PI} - T'_{exp,PI})$. Here, T' indicates modified temperature that is used in the GCC to be able to represent hot and cold streams in the same diagram while satisfying ΔT_{min} requirements. The remaining *mCp* of the stream to be expanded is then routed to an expander operating at the new pinch temperature, and the procedure is repeated.

Interestingly, expansion below ambient as well as compression above and below ambient have the same four cases as mentioned above with considerable symmetry between the four situations of compression/expansion above/below ambient temperature. The essence of the 16 cases (four theorems for each of the four situations) is described in Table 1. A manual and iterative procedure has been developed for the four cases discussed above (expansion or compression above or below ambient temperature). As mentioned, the GCC is used to determine maximum expansion or compression as well as the identification of new pinch points that may occur as a result of pinch expansion or compression. Fu and Gundersen (2016)[39,40] also discussed the simultaneous use of compression and expansion below and above ambient temperature.

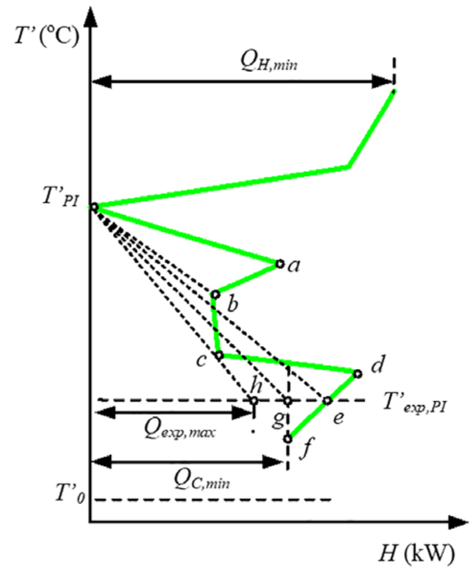

Figure 3. Maximum pinch expansion determined by the grand composite curve (Fu and Gundersen, 2015).[36]

[Color figure can be viewed at wileyonlinelibrary.com]

Appropriate placement of compressors and expanders—an illustrative example

Consider the simple example represented by the stream data provided in Table 2. Two streams are subject to pressure change. Hot stream H1 should be expanded from 3 to 1 bar, whereas cold stream C1 needs to be compressed from 1 to 2 bar. Ambient temperature and the reference temperature for exergy are assumed to be 288 K. Hot utility is assumed to be available at ambient temperature, thus its exergy value is zero. Polytropic efficiency for compression and expansion is assumed to be 1.0, whereas the minimum approach temperature (ΔT_{min}) for heat exchange is assumed to be 4 K. Ideal gas is assumed with constant heat capacity ratio $\kappa = c_p/c_v = 1.4$. The objective function is minimum exergy consumption.

Before considering pressure change in streams H1 and C1 (referred to as Case 0), minimum hot and cold utility requirements for the specified ΔT_{min} are $Q_{H,min} = 145$ kW and $Q_{C,min} = 112$ kW, whereas the pinch temperature is 200 K (in modified temperature; half of ΔT_{min} above the supply temperature of cold stream C2). Three different cases are considered: (1) compression at cold utility temperature (C1) and expansion at hot utility temperature (H1), (2) pinch compression and expansion, and (3) compression and expansion according to the manual design procedure suggested by Fu and Gundersen (2016).[39]

Table 1. Integrating Compressors and Expanders into Heat Exchanger Networks Above and Below Ambient

Theorem	Expansion Above T_0	Compression Above T_0	Expansion Below T_0	Compression Below T_0
1	If $Q_{exp,\,PI} \le Q_{C,\,min}$ and $T_{exp,\,HU} > T_0$, then use pinch expansion	If $Q_{comp,\,PI} \le Q_{H,\,min}$ and $T_{comp,\,0} < T_{HU}$, then use pinch compression	If $Q_{exp,\,PI} \le Q_{C,\,min}$ and $T_{exp,\,0} > T_{CU}$, then use pinch expansion	If $Q_{comp,\,PI} \le Q_{H,\,min}$ and $T_{comp,\,CU} < T_0$, then use pinch compression
2	If $Q_{exp,\,PI} > Q_{C,\,min}$ and $T_{exp,\,HU} \ge T_{PI}$, then split and maximize pinch expansion, remaining expansion at T_{HU} or T_0	If $Q_{comp,\,PI} > Q_{H,\,min}$ and $T_{comp,\,0} \le T_{PI}$, then split and maximize pinch compression, remaining compression at T_0	If $Q_{exp,\,PI} > Q_{C,\,min}$ and $T_{exp,\,0} \ge T_{PI}$, then split and maximize pinch expansion, remaining expansion at T_0	If $Q_{comp,\,PI} > Q_{H,\,min}$ and $T_{comp,\,CU} \le T_{PI}$, then split and maximize pinch compression, remaining compression at T_{CU} or T_0
3	If $Q_{exp,\,PI} > Q_{C,\,min}$ and $T_0 < T_{exp,\,HU} < T_{PI}$, then increase hot utility (HU) expansion and reduce pinch expansion	If $Q_{comp,\,PI} > Q_{H,\,min}$ and $T_{PI} < T_{comp,\,0} < T_{HU}$, then increase ambient compression and reduce pinch compression	If $Q_{exp,\,PI} > Q_{C,\,min}$ and $T_{CU} < T_{exp,\,0} < T_{PI}$, then increase ambient expansion and reduce pinch expansion	If $Q_{comp,\,PI} > Q_{H,\,min}$ and $T_{PI} < T_{comp,\,CU} < T_0$, then increase cool utility (CU) compression and reduce pinch compression
4	If $T_{exp,\,HU} \le T_0$, then use HU expansion	If $T_{comp,\,0} \ge T_{HU}$, then use ambient compression	If $T_{exp,\,0} \le T_{CU}$, then use ambient expansion	If $T_{comp,\,CU} \ge T_0$, then use CU compression

Table 2. Stream Data for a Small Illustrative Example (Fu and Gundersen, 2016)[39]

Stream	T_s (K)	T_t (K)	mCp (kW/K)	ΔH (kW)	P_s (bar)	P_t (bar)
H1	288	124	2	328	3	1
H2	252	168	4	336	–	–
C1	138	284	3	438	1	2
C2	198	235	7	259	–	–
Hot utility	288	288	–	–	–	–
Cold utility	120	120	–	–	–	–

The results shown in Table 3 clearly illustrate the advantage of compression and expansion at the pinch temperature (Case 2). Compared to Case 1 where stream H1 is expanded at ambient temperature (which is equal to the hot utility temperature) and stream C1 is compressed at cold utility temperature, hot utility requirements are reduced from 300.2 to 47.6 kW, whereas cold utility requirements are reduced from 193.6 to 36.0 kW. It should be noticed that Case 1 indeed is representative for current industrial practice. Compression work increases from 81.6 to 130.2 kW, whereas expansion work decreases from 155.2 to 108.8 kW. From a situation with net production of work (73.6 kW), the use of pinch expansion and compression results in a net consumption of work (21.4 kW). For this sub-ambient example, cold utility represents a considerable exergy consumption. Hot utility has zero exergy because its temperature is equal to the reference temperature (ambient) for exergy. Considering the arrangement as a refrigeration cycle, cold utility is reduced by 157.6 kW by investing in 95.0 kW of power. Thus, this "refrigeration cycle" has a COP (coefficient of performance) of 1.66. It should be noticed, however, that no new equipment is introduced, because according to the stream data in Table 2, streams H1 and C1 should be subject to pressure change. The essence of the scheme is that heat from compression and cooling from expansion are utilized to improve heat recovery. Of course, the sizes of the compressor and the expander will change. It should also be noticed that exergy consumption is reduced from 197.4 kW (Case 1—industrial practice) to 71.8 kW (Case 2—pinch compression and expansion), that is, a reduction of 63.6%.

Table 3. Main Results for the Small Illustrative Example (Fu and Gundersen, 2016)[39]

Cases	0	1	2	3
Hot utility demand (kW)	145	300.2	47.6	9.6
Cold utility demand (kW)	112	193.6	36.0	13.0
Pinch temperature(s) (K)	200	200	140	140; 200; 250
Compression work (kW)	–	81.6	130.2	135.5
Expansion work (kW)	–	155.2	108.8	99.1
Exergy consumption (kW)	–	197.4	71.8	54.6

By following the manual design procedure based on the new insight about appropriate placement of compressors and expanders, it is possible (Case 3) to reduce exergy consumption even further. This comes, however, at the expense of significantly increased network complexity and obviously a considerable increase in investment cost. Details about the required equipment for the three cases are provided in Table 4. The final WHEN for Case 2 with only pinch compression and expansion is shown in Figure 4. As indicated in this figure, the compression of C1 and expansion of H1 both start at the original pinch temperature of 200 K. As a result, however, the pinch temperature will change to 140 K.

The lesson to be learned from this small illustrative example is that pinch compression and expansion considerably improves the energy efficiency of the process. Although energy (and exergy) efficiency can be improved even further by following the mentioned manual design procedure when pinch points change, the savings in this case cannot justify the additional investment. At least, however, the manual design procedure provides a target for best performance from an energy/exergy point of view.

The special case when there is no further external heating and cooling demands to be satisfied and there are still streams

Table 4. Key Complexity Properties for the Small Illustrative Example

Property	Case 1	Case 2	Case 3
Exergy consumption (kW)	197.4	71.8	54.6
No. of pinch points	1	1	3
No. of compressors	1	1	2
No. of expanders	1	1	2
No. of heat exchangers	8	7	10
No. of stream splits	0	1	4

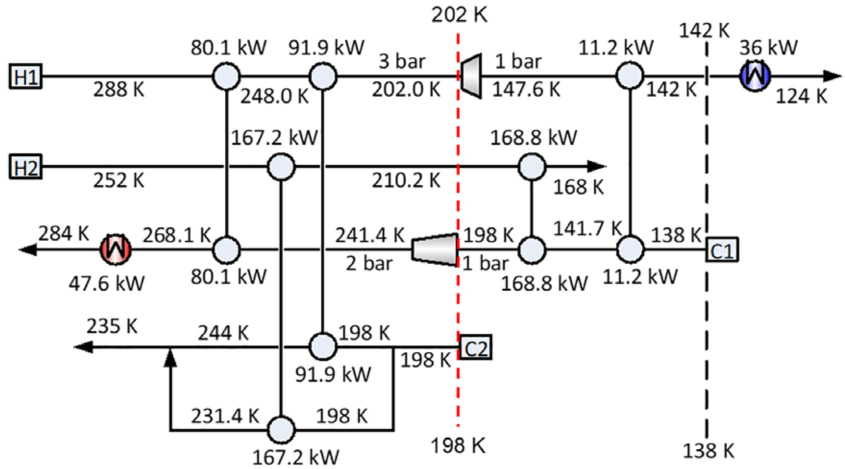

Figure 4. Work and heat exchange network for the small illustrative example when using pinch compression and expansion only (Case 2) (Fu and Gundersen, 2016).[39]
[Color figure can be viewed at wileyonlinelibrary.com]

to be compressed and/or expanded was analyzed by Fu and Gundersen (2016).[40] A remaining question is then whether compression or expansion should be done first, that is, the sequence problem. This problem is related to the following facts: (1) if compression is implemented before expansion, the heat from compression can be used to preheat the stream to be expanded so that expansion work can be increased, and (2) if expansion is implemented before compression, the cooling from expansion can be used to precool the stream to be compressed so that compression work can be reduced. An additional theorem was proposed for these cases, and it was concluded that minimum exergy consumption is achieved at ambient operation and is independent of the sequence of compression and expansion.

Another piece of insight was established by Fu et al. (2017),[41] based on a master thesis by Uv (2016).[42] The GCC that is used as a tool for the manual procedure mentioned above uses modified temperatures to be able to draw hot and cold streams in the same diagram. When discussing compression and expansion at pinch temperature, Fu and Gundersen (2015)[35-38] used the original identity of the streams to determine which pinch temperature (hot or cold) should be used. Because process streams in WHENs may change identity (hot or cold) due to pressure changes in the process between supply state and target state, Fu et al. (2017)[41] emphasized that it is the identity of the stream segment subject to compression or expansion that should be used to determine the right pinch temperature (hot or cold) at which compression or expansion should start, not the identity of the original (or parent) stream.

Optimal thermodynamic paths for process streams

Determining the presence and sequence of equipment for heating, cooling, compression, and expansion can be referred to as the problem of identifying the optimal thermodynamic path for a process stream from its supply state to its target state. In HENs, it makes sense to classify process streams into hot and cold streams. Likewise, in WENs, it makes sense to classify process streams into high pressure (HP) and low pressure (LP) streams. In WHENs, however, such classifications cannot be made. In the most general case, the thermodynamic path for a process stream from its supply state to its target state may involve all four operations of heating, cooling, compression, and expansion. As a result, process streams can temporarily be both hot and cold and they can be both HP and LP. Even a process stream with the same supply and target pressure could be considered compressed and expanded. In such cases, the process stream acts as a utility or a working fluid in a thermodynamic cycle generating power (heat engine), heating (heat pump), or cooling (refrigeration).

The pressure–temperature diagrams in Figure 5 are used to illustrate different thermodynamic paths for a process stream that has supply (s) and target (t) temperatures (T) and pressure (p) as follows: $T_t > T_s$ and $p_t > p_s$. For simplicity, only compression is considered for pressure manipulation in this case. Figure 5a shows the case when the stream is first compressed. Then, depending on the outlet temperature from the compressor, the stream must be heated (i), cooled (iii), or the target temperature could be reached by coincidence through the compression (ii). Similar situations may occur if the stream is

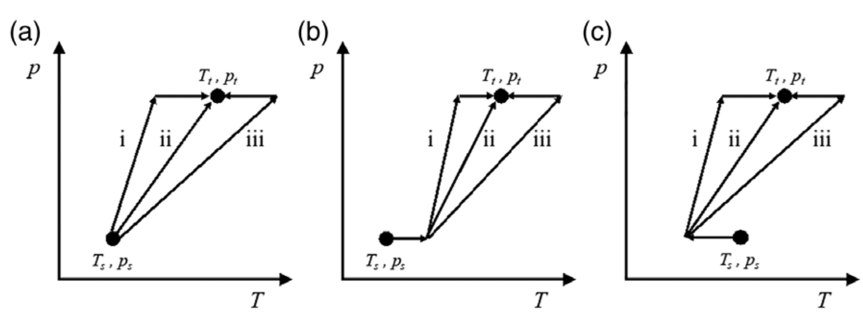

Figure 5. Alternative thermodynamic paths for process streams from supply to target state: (a) compress first, (b) heat and then compress, and (c) cool and then compress.

heated before compression (Figure 5b) or the stream is cooled before compression (Figure 5c). In total, even for this simple case with a process stream that is only subject to compression (no expansion), there are nine different thermodynamic paths. When adding expansion as well as multistage operation with interstage heating or cooling, it is obvious that the complexity of the design problem becomes unmanageable using a manual procedure.

The problem of identifying optimal thermodynamic paths for the process streams was therefore formulated as an optimization problem by Yu et al. (2018).[43] The optimization model is based on the superstructure in Figure 6, which illustrates a stream to be compressed. In fact, this superstructure represents all the nine possible thermodynamic paths shown in Figure 5. With the stream split arrangement, even combinations of the nine basic thermodynamic paths are possible. As a result, the different stream branches can be compressed at different temperatures, such as the original pinch and new pinch temperatures that may appear. The unknown heat exchangers before the compressors represent preheating or precooling before compression as well as direct compression (if the heat exchanger duty is zero). Likewise, the unknown heat exchangers after the compressors will adjust the stream temperature to reach the target. It is important to emphasize that for multiple hot and cold streams, the optimal inlet temperatures to pressure changing equipment are unknown and subject to optimization. As already discussed, the pinch point(s) will change as a result of compression and expansion, thus the appropriate placement concept cannot be used ahead of optimization to identify the inlet temperatures to the compressors in Figure 6.

This means that the identities of the six sub-streams indicated in Figure 6 are unknown; they can be both hot and cold independent of the identity of the parent stream that should be heated or cooled from T_s to T_t. Duran and Grossmann (1986)[44] developed a pinch location algorithm that was used for simultaneous process optimization and heat integration where the flow rates and temperatures are unknown. The problem described by the superstructure in Figure 6 has another complicating feature, because the stream identities are unknown. Yu et al. (2018)[45] extended the Duran–Grossmann model to allow for variable stream identities so that the model could be used to address WHENs problems. This was realized by adding binary variables to the model formulation. Both the original and the extended Duran–Grossmann algorithm use max operators to identify the pinch point, and this causes nonsmoothness in the model with corresponding problems for gradient-based optimization algorithms. Yu et al. (2018)[45] presented and compared three alternative reformulations to overcome this problem; smooth approximation, explicit disjunction, and direct disjunction. For the two last alternatives, both big-M and convex hull formulations were tested. Process stream identities have also been treated as variables in a recent study by Onishi et al. (2018).[46] Their study presents a multistage superstructure including several stages of heat and work integration. It is indicated that global optimality can be obtained based on robust and effective model formulations.

Of course, the superstructure in Figure 6 is far from representing all possible structural alternatives; however, this will be discussed in a later section where challenges and future work are outlined. At this point, it could be mentioned that both compression and expansion should be considered, and to be even more realistic, multistage compression and expansion with heating or cooling between the stages should be included in the superstructure. It is important to notice that independent of the richness of the superstructure, as soon as the thermodynamic path is identified for all process streams, the remaining problem to be solved is the classical HEN design and optimization problem, for which there are a large number of different methodologies and tools available. This two-stage approach for WHENs is similar to pinch analysis for HENs, where performance targets are established ahead of the design stage.

A Comprehensive Review of WHENs

Based on the previous sections, the new field of WHENs has been introduced, defined, and to some extent illustrated. More detailed illustrations will be provided in the next section where the potential of this new methodology is indicated through small industrial case studies. Similar to neighboring engineering fields, methodologies for WHENs are based on combined use of thermodynamics (pinch analysis), heuristics (rules of thumb), and optimization (mathematical programming or stochastic search algorithms). As discussed earlier, the complexity of the WHENs problem is considerably larger than the HENs problem. This means that even small literature problems with 4–6 streams become unmanageable using manual design procedures. As a result, some kind of optimization has to be applied, although thermodynamics and heuristics typically are used to narrow the scope, to assist in building adequate superstructures, and to guide the search for optimal solutions.

Because combined approaches are most common, it does not make sense to classify WHEN methodologies into groups. Thus, the following review will discuss the different contributions to the field in some kind of historical order. Focus will be on approaches used, representations, types of superstructures, model types, computing requirements, and application

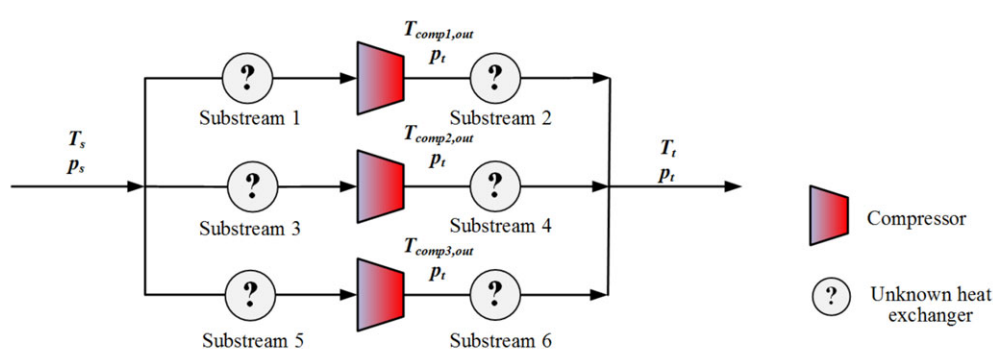

Figure 6. Superstructure for the simple case of compression only (Yu et al., 2018).[43]
[Color figure can be viewed at wileyonlinelibrary.com]

areas. The limitations of the various studies are also mentioned to indicate areas of further research. More details can be found in the section Challenges and Future Research.

Setting the stage—some early contributions

Aspelund et al. (2007)[33] proposed a graphical methodology referred to as the extended pinch analysis and design (ExPAnD) procedure, where traditional pinch analysis is extended with pressure considerations and exergy analysis. A set of 10 heuristic rules for manipulating the pressure of process streams were proposed to utilize pressure based energy (or exergy). They found that even the pressure of a stream with the same supply and target pressure can be manipulated to reduce total irreversibilities. This adds richness to the problem definition but complicates the design of WHENs significantly. The ExPAnD procedure was applied to develop a novel process for offshore liquefaction of natural gas (Aspelund and Gundersen, 2009).[47] Gundersen et al. (2009)[34] studied the integration of compression heat for a small heat recovery problem. By manipulating the inlet temperature to the compressor, they found in one case study that total exergy consumption was minimized when the inlet temperature to the compressor was exactly at the pinch temperature. In another case study, the same result was obtained; however, they also observed that the pinch temperature was changing as a result of compression at different temperatures. At the same time, Kansha et al. (2009)[48] developed the self-heat recuperation methodology that involves the use of compression and expansion to improve heat recovery. Without any thermodynamic arguments, they arrived at a design for a small case study where the compressor and the expander both have inlet temperatures equal to the pinch temperature.

Wechsung et al. (2011)[49] combined pinch analysis, exergy analysis, and mathematical programming to synthesize HENs below ambient temperature considering compression and expansion of process streams. A state space model incorporating a pinch operator (heat integration) and a pressure operator (work integration) was proposed. The pinch operator is based on the simultaneous heat integration and process optimization model proposed by Grossmann et al. (1998).[50] The resulting MINLP model was applied to the offshore liquefied natural gas (LNG) process studied by Aspelund and Gundersen (2009).[47] In contrast to the model for identification of an optimal thermodynamic path discussed earlier (Yu et al., 2018),[43] Wechsung et al. (2011)[49] applied a fixed thermodynamic route from supply to target state. Nevertheless, it was demonstrated that the optimization formulation was capable of generating reasonable designs for different objective functions and constraints. The optimization model was also able to reproduce the design obtained by Aspelund and Gundersen (2009).[47] The simplifying assumption of ideal gas behavior was made.

An emerging new research field—more recent contributions

Onishi et al. (2014)[51] proposed a mathematical model for the simultaneous synthesis of WHENs. The stage-wise superstructure of Yee and Grossmann (1990)[52] for HENs was adapted to synthesize HENs considering work recovery. This model used generalized disjunctive programming and was reformulated as an MINLP problem. The superstructure is based on the prefixed pressure manipulation route of expansion and compression proposed by Wechsung et al. (2011).[49] Onishi et al. (2014)[53] also proposed a multistage superstructure for HENs, wherein the pressure manipulation of process streams is used to enhance heat integration. It was shown that the integration of work and heat reduces the need for thermal utilities in HENs significantly.

Starting from a different angle, Onishi et al. (2014)[54] proposed another superstructure for WENs-considering heat integration. The proposed WEN superstructure is composed of several stages of compression or expansion for each pressure-changing stream. The HP streams only pass through pressure reduction equipment, whereas LP streams are only subject to compression. However, as shown by Aspelund and Gundersen (2009)[47] and Wechsung et al. (2011),[49] allowing both compression and expansion for streams may lead to lower irreversibilities in the system. Therefore, the monotonic nature is a limitation of the superstructure by Onishi et al. (2014).[54] Heat integration is performed between the compression and expansion stages of the WEN. Heaters and coolers were used to reach the target temperature for HP and LP streams, respectively. The inherent assumption that HP and LP streams after pressure change are considered to be cold and hot streams, respectively, is another limitation of this superstructure. As a result, some promising configurations will not be identified. Onishi et al. (2014)[55] also established an MINLP optimization model for WHEN synthesis with focus on how to arrange the rotating equipment. Their model allows the use of several SSTC units operating at different rotational speed, which is an obvious advantage compared to having all rotating equipment on the same shaft and with the same rotational speed.

The series of papers by Fu and Gundersen (2015)[35-38] was thoroughly discussed earlier, thus only highlights will be repeated here. New insight was established for the appropriate placement of compressors and expanders both above and below ambient temperature. The main outcome of their work is that optimal inlet temperatures to compressors and expanders, assumed to be part of the heat recovery problem, are limited to the following set of temperatures:

- Expansion above ambient: hot utility, pinch, or ambient temperature
- Compression above ambient: pinch or ambient temperature
- Expansion below ambient: pinch or ambient temperature
- Compression below ambient: cold utility, pinch, or ambient temperature

In these studies, it was assumed that ambient temperature acted as cold utility above ambient and hot utility below ambient. Only one hot and one cold utility were included, both assumed to be at constant temperature. This new insight was formulated as a set of four theorems and used to establish a manual and iterative design procedure with extensive use of the GCC (Fu and Gundersen, 2015).[56] The objective function was to minimize exergy consumption (or maximize exergy production). A small case study with five process streams, where two2 streams are subject to pressure change shows 38.5% reduction in exergy consumption by maximum utilization of pinch compression and expansion. A more thorough discussion about integration of compressors and expanders below and above ambient is provided by Fu and Gundersen (2016).[39,40] Although exergy is used to handle heat and work in a consistent way, it should be mentioned that cost does not always follow the second law of thermodynamics. This will be further discussed later. The mentioned manual design procedure was applied to three carbon capture processes (Fu and Gundersen, 2016).[57] Two of these are presented in some detail in the next section. A novel sensible heat pump was also developed where expander and compressor inlet temperatures are based on the manual design procedure (Fu and Gundersen, 2016).[58] The optimal compression ratio is determined by mathematical analysis while minimizing exergy consumption.

Marmolejo-Correa and Gundersen (2016)[59] proposed a new design method combining heuristic rules from the ExPAnD procedure and the above mentioned insight about appropriate placement of compressors and expanders. The resulting design methodology is particularly useful for processes operating below and across ambient temperature. The main novelty is that exergy analysis is performed at the conceptual stage of design, rather than being used as a post-design tool. An exergy cascade and a new exergy diagram are proposed to target the requirement, rejection, destruction, and recovery of exergy. The procedure only considers single-stage pressure manipulation, and the use of heuristic rules makes it difficult to apply to large-scale problems while guaranteeing optimal solutions.

Based on the study by Onishi et al. (2014),[54] Huang and Karimi (2016)[60] proposed a similar WHEN superstructure consisting of two distinct but interconnected networks. One network is exclusively for heat integration, and the other is for work integration. The main difference from the work of Onishi et al. (2014)[54] is the superstructure that allows for the flexibility of selecting heaters or coolers at the end of the HEN superstructure. Onishi et al. (2014)[54] had fixed heaters for HP streams (assumed to be cold streams) and coolers for LP streams. Huang and Karimi (2016)[60] compared their model with the one by Onishi et al. (2014)[54] and showed that their model has fewer variables, fewer and/or tighter constraints, tighter relaxations, fewer nonlinear terms, better numerical stability, faster solutions, and better objective function values. However, some unrealistic assumptions were made by Huang and Karimi (2016)[60] in their case studies, such as high and constant hot utility temperature of 680 K resulting in optimistic efficiencies for the turbines. In addition, their model had the same limitation regarding the assumption of HP/LP streams being cold/hot streams before entering the WEN stage. The purpose of this assumption is to boost the power generation from HP streams and to reduce the power consumption for LP streams. This is in line with the assumption that mechanical energy (work) is more valuable than thermal energy (heating/cooling), which is not always correct, especially in sub-ambient processes.

Onishi et al. (2015)[61] proposed a new mathematical model for the retrofit of HENs considering pressure recovery of process streams. The proposed multistage superstructure allows additional heat transfer area to existing heat exchangers, as well as the purchase of new heat exchangers and pressure manipulators. Later, Onishi et al. (2017)[62] proposed a new multi-objective mathematical model for optimal WHEN synthesis considering both environmental impacts and economic performance based on the superstructure proposed by Onishi et al. (2014).[54] The LCA (Life Cycle Assessment)-based Eco-indicator 99 methodology is chosen to evaluate the environmental effects. This mathematical model can determine a set of alternative Pareto-optimal solutions to support decision makers toward more environment-friendly and cost-effective WHENs. This article is the first study considering the conflicting environmental and economic objective functions in WHENs.

Uv (2016)[42] proposed a new model with and without using the thermodynamic insight for WHEN synthesis developed by Fu and Gundersen (2015).[35-38] By including this insight, it is possible to fix the inlet and outlet temperatures for pressure changing units at specific temperatures. As a result, the optimization model reduces to a simple LP model. However, the model is only suitable for targeting and cannot design optimal WHENs.

Vikse et al. (2017)[63] discussed and compared the three different optimization models for WHENs proposed by Wechsung et al. (2011),[49] Huang and Karimi (2016),[60] and Uv (2016).[42] They noticed that all three models share the common problem of having equations that are not differentiable everywhere, thus Vikse et al. (2017)[63] proposed to use recent nonsmooth algorithms to deal with these problems. These algorithms will be discussed later.

Zhuang et al. (2017)[64] proposed a step-wise WHEN synthesis methodology, combining mathematical programming, and heuristic rules. The method first synthesizes a direct WEN based on a transshipment model. To remove small load compressors and expanders and thereby reduce equipment cost, heat exchangers are introduced to substitute small load pressure change equipment and then adjust the load of direct work exchangers. Five rules and three strategies are proposed to integrate heat exchange equipment into direct WENs. With the heuristic and manual elements in the procedure, optimal network configuration cannot be guaranteed. In addition, the method appears to be rather complicated to implement.

Zhuang et al. (2018)[65] proposed a model for simultaneous synthesis of WHENs based on a superstructure considering thermodynamic and economic factors. First, a model to determine the hot or cold identity of process streams is developed based on exergy analysis. Then, an economic analysis is performed by formulating an MINLP model to optimize the sequence of work and heat integration (WHI), minimizing TAC.

Deng et al. (2017)[66] proposed a systematic method for synthesizing WHENs based on pinch analysis. A pressure pinch is proposed in a similar way as the temperature pinch. The method is applied to a rectisol process in the coal-water slurry gasification section of an ammonia plant. Unfortunately, this method can only deal with liquid streams, and because the temperature effect of pressure change is neglectable for liquid streams, the WEN has little effect on the HEN synthesis.

Based on a state space superstructure, Liao et al. (2017)[67] developed a process network design for effluent gas recovery at sub-ambient temperature. The superstructure contains operators for the HEN, pressure, and separation. To recover the effluent gas, the flashing temperature and pressure should be within certain ranges. Compressors and turbines are considered in the condensing block and the cryogenic separation block, respectively. To avoid rigorous thermodynamic calculations and still guarantee the accuracy, empirical correlations are adopted to calculate the thermodynamic properties of the effluent gas streams.

As an application of WHENs in industry, Zhang et al. (2018)[68] investigated the optimal design of the hydrogenation system in a refinery. They established an NLP model to determine the optimal inlet and outlet temperatures of compressors while simultaneously considering compression work and HEN utilities.

Nair et al. (2017)[69] proposed a generalized framework for WHENs based on a very rich superstructure and an MINLP model. A more detailed presentation of this approach is provided by Nair et al. (2018).[70] Streams are not pre-classified as hot/cold or HP/LP. Pressure change is allowed for nonpressure changing streams, and vapor–liquid phase change can be handled. This framework is applied successfully to a propane–propylene separation process and a simplified offshore natural gas liquefaction process. At present, this methodology appears to be the most advanced WHENs tool, and the developed superstructure is shown in Figure 7. The reported computing times for the mentioned case studies are considerable, primarily caused by a large number of binary variables. Based on this work, Nair and Karimi (2018)[71] investigated the synergy between work and heat for holistic energy integration. The advantage of treating stream identities as unknown variables was demonstrated.

The most recent contribution from Onishi et al. (2018)[46] was briefly mentioned earlier in the section on Optimal Thermodynamic Paths for Process Streams and the discussion about unknown stream identities. They used their previous HENs/WENs superstructure with TAC as objective function. The identities (hot or cold, HP or LP) of the streams are treated as variables. Stream splitting is not included in the superstructure. Yu et al. (2018)[43] illustrates that the performance of WHENs can be improved with compression (or expansion) of stream branches from different temperatures in their case studies.

Rademacher et al. (2018)[72] investigated the effect of electricity prices on the design of WHENs. The concept of reconfigurable design was introduced and demonstrated through a case study. They compared and analyzed the optimal configurations of WHENs during off-peak, mid-peak, and on-peak periods. The authors introduced the term WHEN "suprastructure" to indicate a reconfigurable flow sheet that can modify each optimal configuration in an ad hoc fashion to have more common equipment for the modified configurations. The objective is to minimize capital investment.

The work by Yu et al. (2018)[43,45] was thoroughly presented earlier and will not be detailed here. A superstructure was developed for identifying optimal thermodynamic paths for process streams, where the corresponding optimization model used an extension of the pinch location algorithm by Duran and Grossmann (1986),[44] capable of handling unknown stream identities.

As a continuation of Fu et al. (2017),[73] Yu et al. (2018)[74] discussed opportunities and challenges in WHENs, both from a methodology and an application point of view. Both pinch-based and mathematical programming–based methods are discussed. Applications of WHENs are illustrated by an offshore LNG process, a post-combustion carbon capture process, and a sensible heat pump for industrial heat recovery.

It should be noticed that the WHENs problem has been further extended to include mass exchange. Dong et al. (2014)[75] developed a state space model for the simultaneous integration of heat, mass, and pressure exchange networks. To optimize HENs, MENs and WENs simultaneously, exergoeconomic analysis was used as a unified criterion for the three different networks. The proposed state space model performed well for the synthesis of water distribution networks with integrated MENs, HENs, and WENs. However, because pressure change of water hardly causes temperature change, the HENs and WENs are weakly related and the interaction between them was neglected. Dong et al. (2015)[76] extended their previous study to hydrogen distribution networks considering pressure and heat recovery. It was shown that simultaneous integration of work and heat reduces energy consumption and cost significantly.

Finally, it should be mentioned that Yu and Gundersen (2017)[77] provided a brief review of the research contributions to WENs and WHENs, whereas Fu et al. (2018)[78] provided a comprehensive reference list when they described WHI as an emerging research area. The main motivation behind the current article has been to introduce WHI as a new field in Process Synthesis and PSE. Although the article has included most of the relevant literature, it should not be regarded as a regular review article. Thus, focus has been on describing established insight based on thermodynamics, discussing current limitations, and to illustrate opportunities for industrial applications.

Illustrative Examples

The emerging methodologies for WHENs are expected to find applications in a large number of processes where both thermal and mechanical energies are important. In particular, there is an expectation that the recent developments in this field will increase the use of process integration in subambient processes, and thereby enable the design of significantly more efficient low temperature processes. This does not mean that improvements cannot be made in processes operating above ambient temperature, and in fact, the two small industrial applications presented in this section are indeed above ambient processes. The manual design procedure

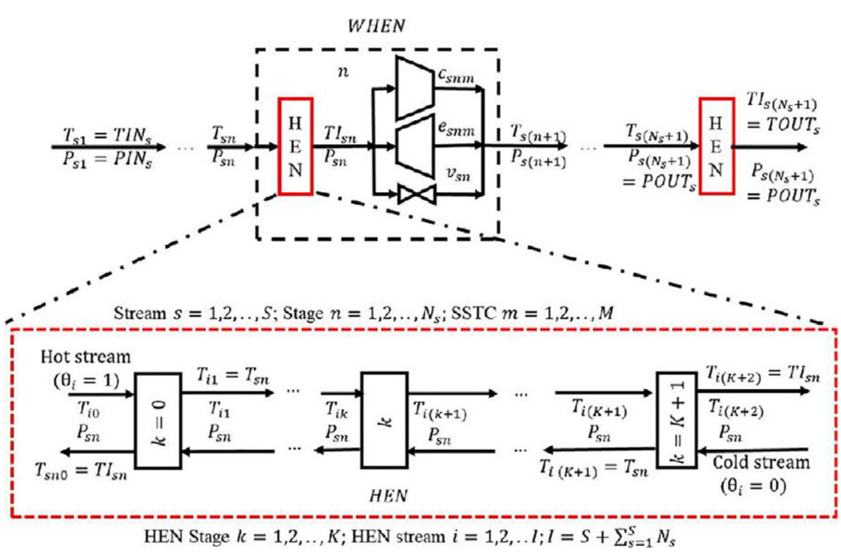

Figure 7. An advanced work and heat exchange network superstructure (Nair et al., 2018).[70]
[Color figure can be viewed at wileyonlinelibrary.com]

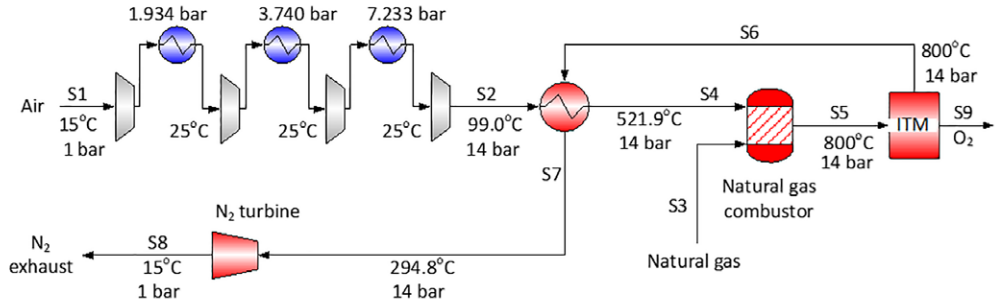

Figure 8. Original flow sheet for membrane separation of air (Fu and Gundersen, 2016)[57].
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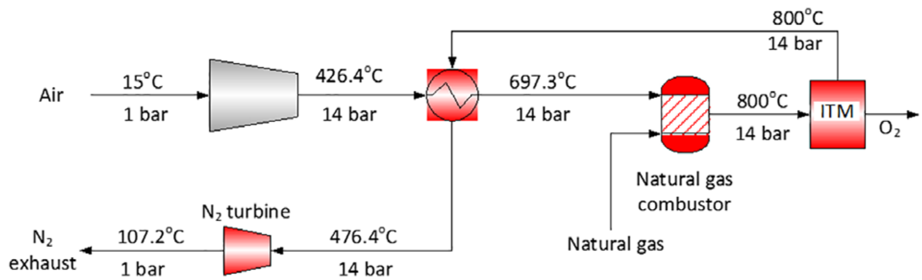

Figure 9. Improved flow sheet for membrane separation of air (Fu and Gundersen, 2016).[57]
[Color figure can be viewed at wileyonlinelibrary.com]

(Fu and Gundersen, 2016)[40] based on appropriate placement of compressors and expanders is used to derive the design solutions for the two case studies.

Membrane separation of air for oxy-combustion processes

This example illustrates the case where both compression and expansion are involved in heat integration, and the details are provided in Fu and Gundersen (2016).[57] Figure 8 shows the original process (referred to as Case A) as it is described in literature (DOE/NETL, 2008).[79] An ion transport membrane (ITM) operating at HP (14 bar) and high temperature (800°C) is used. Ambient air is compressed in four stages with interstage cooling to minimize compression work, then preheated by the effluent N_2 stream, before it reaches the required inlet temperature to the ITM (800°C) by a natural gas combustor. The thermal energy in the O_2 depleted N_2 stream is then recovered by preheating air, whereas the mechanical energy is recovered by expanding the stream to ambient pressure. The heat exchanger is specified in such a way that the outlet temperature from the expander exactly reaches ambient temperature (15°C) when expanding from 14 to 1 bar.

By using the earlier-mentioned manual design procedure that is based on the new insight about appropriate placement of compressors and expanded, with guidelines provided in Table 1, the improved process (from an energy point of view) shown in Figure 9 can be established (referred to as Case B). Near isothermal compression (four stages with intercooling) is replaced by adiabatic compression. As a result, heat at high temperature from compression can be recovered in the preheating process rather than being wasted to cooling water. In this case, the heat exchanger is specified by the need for a minimum approach temperature of 50°C. The two process alternatives are compared in Table 5.

The performance comparison in Table 5 between Cases A and B shows that network consumption increases by

Table 5. Key Results for the Air Separation Example (Fu and Gundersen, 2016)[57]

Property	Case A	Case B
Compression work (kW)	29,350	41,140
Expansion work (kW)	23,419	30,902
Network consumption (kW)	5931	10,238
Heating demand (kW)	27,815	10,275

4307 kW; however, the heating demand is reduced by 17,540 kW. Assuming that the thermal efficiency of a natural gas based power plant is 55%, the reduced heating demand in Case B (i.e., natural gas for the combustor) can be used to generate 9647 kW of work. This means that network consumption is reduced from 5931 kW to 591 kW (10,238 − 9647), that is, a 90% reduction. Thus, in this case, it was not necessary to use exergy arguments to demonstrate improved energy efficiency.

Two-stage membrane process for capturing CO_2

This example is related to post-combustion carbon capture in a power plant, where a two-stage membrane process is used to separate CO_2 from N_2 in the exhaust gas (Zhao et al., 2010).[80] As indicated in Figure 10, the permeate from the first stage (Mem1) is further separated in a second stage (Mem2). The feed to both stages are at 8 bar and 25°C. Interstage and after-stage coolers are not shown to keep the flow sheet simple. The retentates from both stages are expanded to 1 bar for work recovery. The process in Figure 10 without integration will be referred to as Case A. The work recovery can, however, be increased by preheating the retentate in the combustion air preheater. This design with integration will be referred to as Case B and is shown in Figure 11.

The results in Table 6 show that it is only expander Exp1 that is affected by the design modification. More work is produced in this expander due to integration of the retentate

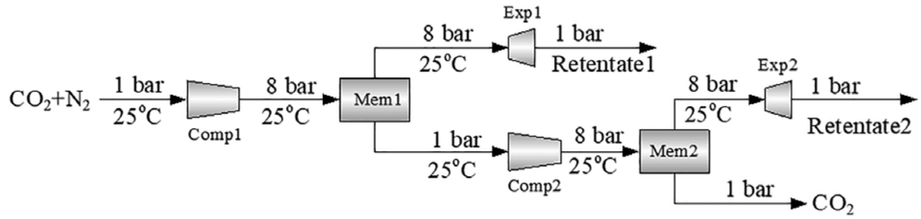

Figure 10. Original flow sheet for carbon capture by a two-stage membrane process (Fu and Gundersen, 2016).[57]

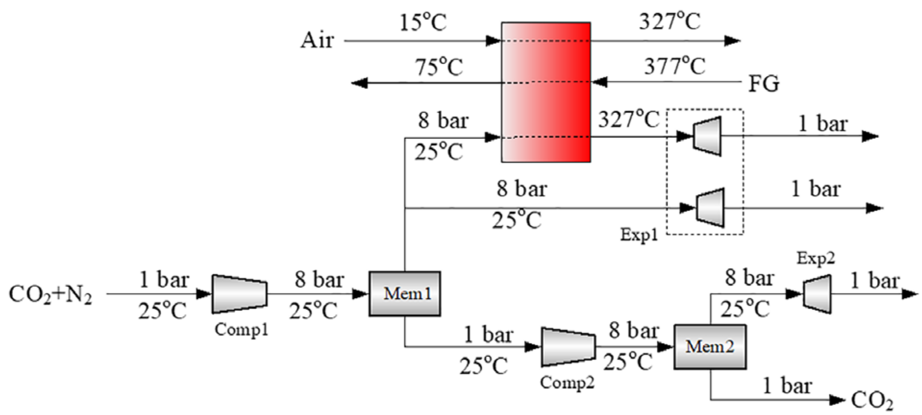

Figure 11. Improved flow sheet for carbon capture by a two-stage membrane process (Fu and Gundersen, 2016).[57]
[Color figure can be viewed at wileyonlinelibrary.com]

stream with flue gas in the air preheater. Notice that the retentate from the first membrane is split and expanded at two different temperatures. The improvement in specific energy consumption for the carbon capture process is 12.9%.

Challenges and Future Research

WHENs represent an emerging field within process integration with considerable promise for industrial applications, increased energy efficiency, and reduced environmental impact. A number of methodologies using different approaches have been proposed, and a few industrial applications have also been reported. Before these methods will reach deployment in industrial practice, however, a number of challenges still exist, and these must be addressed in future research in this field.

Industrial requirements

The current WHEN methodologies have varying but in general low realism when it comes to solving industrial problems. Ultimately, the approaches for WHENs must address as many as possible of the following issues: (1) multiple hot/cold utilities, (2) gliding temperature utilities such as flue gas, hot oil circuits, and so forth, (3) multistage compression and expansion, (4) variable pressure ratios for multistage operation, (5) phase change, (6) rigorous thermodynamic models, and (7) realistic efficiencies for compressors and expanders.

Focus may well be on energy efficiency; however, the ultimate objective should be to minimize TAC. It should be noticed that shifting focus from energy to economy will make the mathematical models considerably more complex. One example is the need for binary variables to represent cost equations with a fixed charge term. Another example is that economy of scale type cost laws introduces non-convexities. There are also other challenges such as sizing of equipment for cost calculations and all the uncertain factors in cost evaluations.

In addition, industrial requirements related to operability, controllability, maintainability, flexibility, and reliability must be considered when suggesting solutions that involve higher levels of process integration. One of the main insights from WHENs is to operate compressors at high (above pinch) temperature and expanders at low (below pinch) temperature. This is the opposite of current industrial practice, and practical issues related to operating rotating machinery in these temperature ranges must be addressed. This is, however, mainly a task for the vendors.

Finally, WHENs should of course be optimized together with the rest of the background process, because important interactions exist between the core process (reactors and separators), the work and heat recovery system, and the utility system for heating, cooling, and power.

Table 6. Key Results for the Carbon Capture Example (Fu and Gundersen, 2016)[57]

Property	Case A	Case B
Comp1 (kW)	8797	8797
Comp2 (kW)	2368	2368
Exp1 (kW)	3703	4601
Exp2 (kW)	595	595
Network consumption (kW)	6867	5969
Specific work consumption (kWh/kg CO_2)	0.372	0.324

Challenges in methodologies

Methodologies have been proposed for WHENs that are based on thermodynamics (pinch and exergy analyses), optimization (mathematical programming and stochastic search), and heuristics (rules of thumb). As argued in this article, the complexity of WHENs requires some use of mathematical optimization. The role of thermodynamics and heuristics is to narrow the scope, to assist in building adequate superstructures, and to guide the search for optimal solutions.

Based on thermodynamics, new insight has been developed related to the appropriate placement of compressors and expanders in heat recovery systems. Unfortunately, the proposed theorems and the corresponding manual and iterative design procedure are only applicable to rather simplified situations. Thus, a major challenge in WHENs is to extend this insight to more complex cases that are closer to industrial reality. With multistage operation of compressors and expanders, new degrees of freedom become available that can be used to reduce thermodynamic losses related to heat transfer. The total pressure ratio can be distributed among the stages in such a way that heating or cooling resulting from pressure manipulations will better match the requirements of the GCC.

When using optimization for WHENs, a number of challenges must be dealt with. As always in process synthesis and process integration, decisions related to selection and sequence of equipment result in the use of binary (0,1) variables. The problem size and the optimization search in a branch and bound tree grow exponentially with the number of binary variables. The other major challenge for these optimization formulations is the fact that the model equations are nonlinear and non-convex. This means that most optimization algorithms will fail to identify the global optimum and end up in local optima.

Irrespective of using thermodynamics or optimization, there are features in the HENs field that would be most valuable in WHENs. One such feature is the concept of establishing best performance targets ahead of design. Some of the proposed methodologies for WHENs are more related to targeting than actual design. Another issue is the fact that compressors and expanders are considerably more expensive and complex pieces of equipment than heat exchangers. Procedures should therefore be developed that enable the removal of low duty compressors and expanders by paying a penalty in thermal utilities and heat transfer area. This would be similar to the use of heat load loops and paths in pinch analysis for removing low duty heat exchangers.

As described earlier, the optimal thermodynamic paths for streams from supply state to target state may involve all four operations of heating, cooling, compression, and expansion. Thus, any future WHENs method must be able to handle unknown stream identities (hot/cold).

It should also be mentioned that as long as exergy is used to handle energy forms of different quality, such as heat and work, a challenge is to avoid using the Carnot equations to establish the exergy of heat. This means that reversible processes are assumed, and the value or quality of heat is overestimated. Thus, some kind of correction factor is required to better balance work and heat. Of course, this problem will disappear when moving to economy focused methods minimizing TAC.

Another important topic in the use of optimization for WHENs is the development of sufficiently rich but still efficient superstructures. The superstructure of Nair et al. (2018)[70] shown in Figure 7 is an example of a very rich superstructure, but the reported computing times even for fairly small problems indicate that it is not very efficient. Further research on superstructures is expected. One very recent and quite promising superstructure that may be applicable to WHENs is the one presented by Li et al. (2018).[81] A so-called block superstructure is used for Process Synthesis with automated flowsheet generation and optimization.

New paradigms for modeling and optimization

As mentioned above, the two main challenges in the use of mathematical optimization for design of WHENs are related to binary variables (combinatorial explosion) and non-convex models (local optima). There is a massive amount of research reported to address these issues, however, so far without any real breakthrough. One additional feature with models for WHENs that causes problems for gradient-based optimization methods is the presence of discontinuities in nature (e.g., when passing a phase boarder) and in models (e.g., the use of max operators). New developments in the area of non-smooth analysis may well form the basis for a new paradigm for modeling and optimization that may prove valuable in the field of WHENs. Two areas that may prove successful are the handling of discontinuities and the avoidance of using binary variables in the models.

As discussed several times in this article, methods for WHENs trying to utilize concepts from HENs often arrive at the point where thermal utilities must be obtained for the case with variable temperatures and even possibly unknown stream identities. This can be achieved by so-called pinch location algorithms. The model that obtains the best scaling in terms of the number of process streams is the NLP formulation by Duran and Grossmann (1986).[44] However, the formulation includes non-smooth elements (max operators) for locating the pinch point, resulting in a formulation that is not differentiable everywhere. Smooth approximations have frequently been used to deal with non-differentiabilities. However, the choice of parameters for smooth approximations is nontrivial and may affect both the condition and accuracy of the formulation (Grossmann et al., 1998).[50]

Alternatively, there are extensions to the concept of derivatives that are applicable to certain classes of non-smooth functions. One such generalized derivative is the Clarke generalized Jacobian for locally Lipschitz continuous functions (Clarke, 1990).[82] A difficulty with using elements of the Clarke Jacobian, however, is that these elements follow calculus rules (e.g., the chain rule) as inclusions rather than as equations. As a result, they are impractical to calculate for most composite functions. Another generalized derivative for functions that satisfy conditions for lexicographic (L-) smoothness as described by Nesterov (2005)[83] are lexicographic (L-) derivatives. The L-derivatives have been proven to be just as useful elements in non-smooth numerical methods as the Clarke generalized Jacobian (Khan and Barton, 2014).[84] The lexicographic directional (LD-) derivative is the equivalent extension of the directional derivative to that of L-smooth functions. The LD-derivatives are calculated by taking the higher order directional derivatives sequentially in directions indicated by the columns of the directions matrix **M**. Furthermore, LD-derivatives follow sharp calculus rules and can be calculated for composite functions using an automatic differentiation framework for L-smooth functions (Khan and Barton, 2015).[85] An extensive review on evaluating LD-derivatives and their applications is provided by Barton et al. (2017).[86]

Flow-sheet optimization using LD-derivatives for sensitivity calculations have already been applied to LNG processes. Liquefaction processes for natural gas exhibit strong resemblance to WHENs, in that they mainly consist of compressors and a liquefaction part. The large temperature span from ambient temperature to about −160°C along with small temperature differences in the heat exchangers make natural gas liquefaction processes challenging to analyze. Small driving forces are a result of heat exchange at very low temperatures where thermodynamic irreversibilities become large. In particular, conventional state-of-the-art process simulators lack rigorous checks to avoid temperature crossovers in multistream heat exchangers, and a feasible operating condition must therefore be determined through a manual iterative approach. Consequently, a simulation and optimization tool was developed using a non-smooth flow-sheeting strategy. The model includes a reformulation for preventing temperature crossovers (Watson et al., 2015)[87] when using the simultaneous optimization and heat integration algorithm by Duran and Grossmann (1986).[44] Additional non-smooth equations are included for correct phase detection of the process streams (Watson et al., 2017 and Watson and Barton, 2017).[88-90] The resulting simulation model was applied to single mixed refrigerant and dual mixed refrigerant processes (Vikse et al., 2018)[91,92] using a non-smooth Newton solver. Later, optimization was included using IPOPT (Raghunathan and Biegler, 2005).[93] Despite assumptions of twice differentiable objective functions and constraints, IPOPT provided good results when using LD-derivatives for sensitivity information, as long as the dual feasibility criterion is relaxed (Watson et al. 2018).[94]

Concluding Remarks

The field of WHENs has received considerable attention during the last 5 years. A total of 36 publications from the period 2014 to 2018 have been discussed in this article, whereas the number of publications before 2014 is only 4. To provide a relevant background for the emerging field of WHENs, some key publications from neighboring fields such as HENs, WENs, and heat and power systems have been included.

Because compressors and expanders are used in WHENs to reduce the use of thermal utilities, there are strong similarities to heat pumps and refrigeration cycles. However, methodologies for WHENs take a Process Systems Engineering approach, where heat pumps and refrigeration cycles are designed as an integral part of the process and its heat recovery system. In fact, the working fluids for heat pumps and refrigeration cycles may be regular process streams.

Although WHEN methodologies have considerable potential for industrial applications and even innovations, there are a number of challenges that must be addressed in future research. These challenges have been thoroughly outlined in this article, and they are related to both industrial realism and features of the design methodologies. Future use of the new paradigm for modeling and optimization based on non-smooth analysis is expected in the field of WHENs.

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