Identifying optimal thermodynamic paths in Work and Heat Exchange Network Synthesis

Haoshui Yu[a], Chao Fu[b*], Matias Vikse[a], Chang He[c], Truls Gundersen[a]

[a] Department of Energy and Process Engineering, Norwegian University of Science and Technology, Kolbjoern Hejes v. 1A, NO-7491 Trondheim, Norway

[b] SINTEF Energy Research, Kolbjoern Hejes v. 1A, NO-7491 Trondheim, Norway

[c] School of Chemical Engineering and Technology, Sun Yat-sen University, 519082 Zhuhai, China

fuchao83@hotmail.com

Abstract: The Process Synthesis problem referred to as Work and Heat Exchange Networks (WHENs) is an extension of the classical HENs problem considering only temperature and heat. In WHENs, additional properties are pressure and work, and strong interactions exist between temperature, pressure, work and heat. The actual sequence of heating, cooling, compression and expansion for pressure changing streams will affect the shape of the Composite and Grand Composite Curves, the Pinch point, and the thermal utility demands. Even stream identities (hot or cold) will sometimes change. The identification of the optimal thermodynamic path from supply to target state for pressure changing streams becomes a primary and fundamental task in WHENs. An MINLP model has been developed based on an extension of the Duran-Grossmann model (that can handle variable temperatures) to also consider changing stream identities. Three reformulations of the extended Duran-Grossmann model have been developed and tested for two examples.

Keywords: Work and Heat Exchange Networks, thermodynamic path, Duran-Grossmann model, stream identity.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

Introduction

Heat integration in the process industry is a mature research area. Significant achievements and a considerable number of methodologies have been published since the 1970s. Two thorough reviews were presented by Gundersen and Naess[1] and Furman and Sahinidis[2]. Once the process stream conditions are known, heat integration can be performed by sequential or simultaneous methods. Heat integration has achieved great success in both grassroot design and retrofit of Heat Exchanger Networks (HENs). However, the pressure of a process stream is also important in most industrial processes, such as ammonia synthesis[3], methanol synthesis and natural gas liquefaction[4]. Pressure manipulation results in temperature change, especially for gaseous streams. Due to the interplay of pressure and temperature, it is clear that heat integration considering pressure change will result in better designs and considerable energy savings. Consequently, process synthesis considering temperature and pressure simultaneously gives rise to a new field of engineering, Work and Heat Exchange Network (WHEN) synthesis.

Townsend and Linnhoff [5] presented the Appropriate Placement of heat engines and heat pumps in a heat exchanger network during the early stages of Pinch Analysis. However, the pressures of process streams are constant in their study, which is the main difference from the WHENs problem discussed here. Aspelund et al.[6] proposed a graphical methodology referred to as Extended Pinch Analysis and Design (ExPAnD), where 10 heuristic rules on manipulating the pressure of process streams were proposed to utilize the pressure based exergy in process streams. In 2009, Gundersen et al.[7] addressed the rules to manipulate stream pressure and phase as well as the sequence of heating, cooling, compression and expansion. Based on ExPAnD, Aspelund and Gundersen[8] applied this systematic method to design an efficient energy chain for liquefaction, transportation and utilization of natural gas for power production with CO_2 capture and storage. Fu and Gundersen[9] presented a systematic graphical design procedure for integration of compressors into HENs above ambient temperature. They concluded that compression should be performed at pinch or ambient temperature to achieve minimum exergy consumption. Similarly, Fu and Gundersen[10] integrated compressors into heat exchanger networks below ambient temperature. Four theorems were proposed as the basis for the design methodology. Integrating expanders into heat exchanger networks above[11] and below[12] ambient temperature has been investigated as well. A systematic methodology was developed by Fu and Gundersen[13] to integrate both compressors and expanders into heat exchanger networks above ambient temperature. However, these above-mentioned studies are based on Pinch Analysis, which relies on Composite Curves (CC) and the Grand Composite Curve (GCC). The arguments regarding Pinch Analysis about providing insight at the cost of time consumption also apply to these studies. In addition, if multiple pressure changing streams, multiple utilities and multiple stages of pressure manipulation are considered, it will be extremely tedious or even prohibitive to apply this methodology.

Accordingly, there are many studies based on mathematical programming focusing on the WHENs problem. Wechsung et al.[14] presented a mathematical formulation to synthesize work and heat exchange networks. They assumed that hot streams go through one compressor and two expanders, and cold streams go through two compressors and one expander. Of course, such a predefined scheme may not be the optimal thermodynamic path. Based on the work by Wechsung et al.[14], Onishi et al.[15] proposed a mathematical model for the simultaneous synthesis of heat exchange and work exchange networks. A superstructure based on Yee and Grossmann[16] was proposed for Heat Exchanger Networks (HENs) considering work recovery. This model is formulated using generalized disjunctive programming (GDP) and reformulated as a mixed-integer nonlinear programming (MINLP) problem. Later, Onishi et al.[17] proposed another superstructure for Work Exchange Networks (WENs) considering heat integration. The proposed WENs superstructure is composed of several stages of compression or expansion for each pressure changing stream. However, they assumed heaters and coolers are only used

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

to reach the target temperature for high and low-pressure streams respectively. Huang and Karimi[18] argued that this assumption is not logical and proposed a similar superstructure consisting of two subnetworks. One network is exclusively for heat integration, and the other for work integration. The superstructure explicitly considers constant pressure streams for heat integration and enables optimal selection of end-heaters and end-coolers. Their approach yields a network with 3.1 % lower total annualized cost, 10.6 % more work exchange, and 81.0 % more heat exchange than the best solution obtained from the study by Onishi et al.[17]. However, they also assumed the low and high-pressure streams to be hot and cold streams respectively before entering the WEN. The purpose of this assumption is to boost the power recovery from high-pressure streams by increasing their temperature and to reduce the power consumption for low-pressure streams by decreasing their temperature. Unfortunately, this assumed superstructure may eliminate energy efficient heat integration schemes. Our case study shows that when considering work and heat simultaneously, it may not be optimal to decrease the temperature of low-pressure streams before compression. Recently, Nair et al.[19] proposed a framework for work and heat exchange network synthesis. A new stage-wise superstructure for WHENs incorporating single-shaft turbine-compressors (SSTCs), valves, heat exchangers, etc. is developed. The model also accommodates pressure manipulation of constant pressure streams. The objective function is Total Annualized Cost (TAC).

The above-mentioned superstructures may omit the optimal configuration of the system. However, rich superstructures for the WHENs problem are computationally challenging due to combinatorial and non-linear (non-convex) issues. If the superstructure is considering all possible thermodynamic paths and network configurations, the optimization problem will be very difficult or even impossible to solve. The largest challenge in WHENs compared with HENs is the unknown thermodynamic paths of pressure changing streams. Once the optimal thermodynamic paths are determined, the WHENs problem reduces to a HENs problem. To

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

the best of the authors' knowledge, a model to determine the thermodynamic paths in WHENs has not yet been reported in the literature.

In this study, a new method to determine optimal thermodynamic paths of pressure changing streams in WHENs is proposed. The MINLP optimization model is based on the Pinch location method presented by Duran and Grossmann[20], while allowing for unknown stream identities, stream splitting for optimal compression and expansion schemes, and equal supply and target temperatures for streams. Compared with previous studies, this work has several contributions to the WHENs problem: 1) the paper proposes a superstructure to determine the optimal thermodynamic path of pressure changing streams, 2) the Duran-Grossmann model is extended to WHENs, with unknown stream identities, 3) this extended model is reformulated into 3 mathematical expressions to facilitate the computation, and 4) the proposed model can be easily applied to multiple pressure changing streams. These features are distinct advantages when compared with the manual Pinch based method[13]. Future work will include consideration of multiple utilities (even with non-constant temperature) and multi-stage pressure manipulation.

Problem Statement

WHENs have numerous potential applications in the process industries. The configuration of refrigeration cycles[21], heat pump integration[22], and organic Rankine cycles recovering waste heat in HENs[23] are examples of WHEN problems, since they have pressure manipulations while considering heat recovery. It is necessary to define the WHENs problem in a general and systematic way to facilitate communication among researchers in the field and to promote industrial applications. A comprehensive definition of WHENs is provided in the following.

Temperature and pressure are two critical attributes to be considered for the streams involved in WHENs. Therefore, the stream definition is different from that in HENs, where there are only two kinds of streams, namely hot streams that release heat and cold streams that absorb heat. For WHENs, one more attribute (pressure) needs to be considered. Due to the interplay

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

between pressure and temperature changes, the supply and target temperatures cannot indicate the identity of a stream. The reason is that the identity of a process stream can temporarily change due to pressure manipulations. Unlike the definition of streams in HENs, there are more categories of streams in WHENs. A P-T diagram is proposed to define the streams in WHENs. Figure 1 shows the definition of streams according to the supply and target states. If both the pressure and temperature of the target state is greater than that of the supply state, this stream is called Low Pressure Cold stream (*LPC*) as the stream (0-1) shown in Figure 1. If the pressure or temperature is constant, one attribute is enough to reflect the changing state of a stream. Therefore, the stream 0-2 is defined as Low Pressure stream (*LP*).

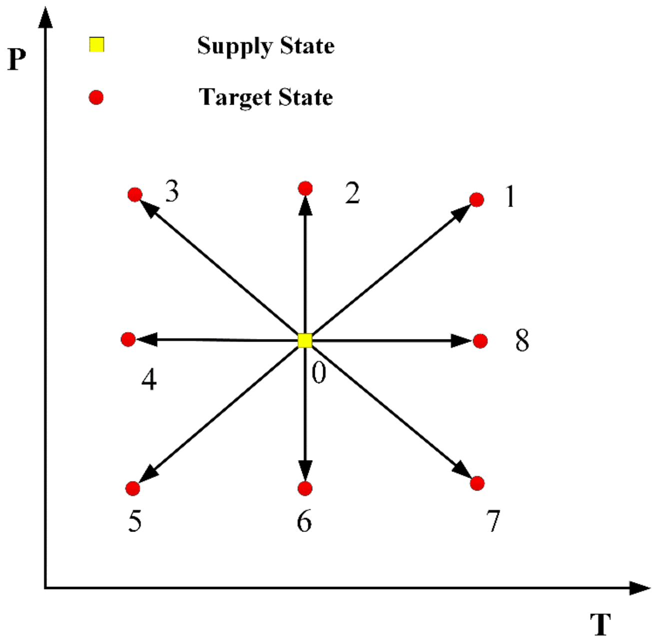

Figure 1. P-T diagram for stream definition in WHENs

By similar arguments, there are eight possible sets of streams in a WHENs problem:

1) The set of Low Pressure Cold streams $LPC = \{ s | P_{sup} < P_{tar}, T_{sup} < T_{tar} \}$

2) The set of Low Pressure Hot streams $LPH = \{ s | P_{sup} < P_{tar}, T_{sup} > T_{tar} \}$

3) The set of High Pressure Hot streams $HPH = \{ s | P_{sup} > P_{tar}, T_{sup} > T_{tar} \}$

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

4) The set of High Pressure Cold streams $HPC = \left\{ s \middle| P_{sup} > P_{tar}, T_{sup} < T_{tar} \right\}$

5) The set of Low Pressure streams $LP = \left\{ s \middle| P_{sup} < P_{tar}, T_{sup} = T_{tar} \right\}$

6) The set of High Pressure streams $HP = \left\{ s \middle| P_{sup} > P_{tar}, T_{sup} = T_{tar} \right\}$

7) The set of Cold streams $C = \left\{ s \middle| P_{sup} = P_{tar}, T_{sup} < T_{tar} \right\}$

8) The set of Hot streams $H = \left\{ s \middle| P_{sup} = P_{tar}, T_{sup} > T_{tar} \right\}$

The set of cold streams (*C*) and the set of hot streams (*H*) are the same as the cold and hot stream definitions in the HENs problem. However, it should be noted that 'hot' and 'cold' in the other sets of process streams in WHENs only indicate the relationship between supply and target temperatures and do not necessarily reflect the identities of the streams in heat integration. As an example, consider a low pressure cold stream (*LPC*). Even though the target temperature is higher than the supply temperature, the temperature after compression can be less than, greater than or equal to the target temperature. Then this stream can be cold, hot or even disappear in the heat integration. Since pressure change always causes a temperature change, especially for gas streams, the identities of streams in heat integration are not consistent with the literal meaning in the set definition. On the contrary, supply and target pressure always indicate the correct attribute of the stream (*HP* or *LP*). Streams whose target pressure is less than the supply pressure will always be expanded and generate work. Therefore, this kind of streams are called Work Source (*WSR*) streams and defined as $WSR = HP \cup HPH \cup HPC$. Similarly, Work Sink (*WSK*) streams are defined as $WSK = LP \cup LPH \cup LPC$. Then the union of *WSR* and *WSK* can be defined as the set of Pressure Changing streams (*PC*) as follows: $PC = WSR \cup WSK$. The set of constant pressure streams can be defined as Non-Pressure Changing streams (*NPC*): $NPC = H \cup C$. The WHENs problem can then be defined:

"*Given a set of process streams with supply and target state (temperature and pressure) as well as utilities for heating, cooling and power; design a Work and Heat Exchange Network* *consisting of heat transfer equipment such as heat exchangers, heaters and coolers, as well as pressure changing equipment such as compressors, expanders, pumps and valves, in a way that minimizes Exergy consumption or Total Annualized Cost*".

This paper mainly focuses on the determination of the thermodynamic path for the process streams. Once the thermodynamic paths of pressure changing streams are determined, the WHENs problem is reduced to a HENs problem. Any available heat exchanger network synthesis technique can be applied to synthesize the final network with any objective function. Determining the thermodynamic paths of pressure changing streams from supply to target state is challenging. For example, a low pressure cold stream needs to be compressed to target pressure. This stream can be compressed at the supply state directly. After compression, the temperature can be less than, equal to or greater than the target temperature of the stream depending on the compression ratio. Therefore, there are three possible thermodynamic paths for direct compression. Similarly, the stream can be heated or cooled before compression as shown in Figure 2. Three possible thermodynamic paths exist for each case. Thus, there are 9 unique thermodynamic paths for single stage compression, as well as any combination of these by stream splitting. If multiple compression stages (possibly with variable pressure ratios) and a combination of compression and expansion are considered, a larger number of possible thermodynamic paths exist. In addition, the relationship between pressure and temperature is nonlinear, which makes it more difficult to trace and understand the process from heuristic insights. Since a low-pressure stream can be heated or cooled before and after compression, the identity of the stream is unknown both before and after compression. This causes considerable challenges for traditional heat integration models.

If the stream is heated first, more work is consumed to compress the stream to target pressure, however, an increased compressor outlet temperature results in higher quality heat into the system. If the stream is cooled first, less work is consumed to compress the stream to the target

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

pressure. Accordingly, the temperature of the stream at the outlet of the compressor is reduced and the quality of the heat is lower. Therefore, it is hard to know which thermodynamic path is more efficient, especially when there are more than one pressure changing stream in the system.

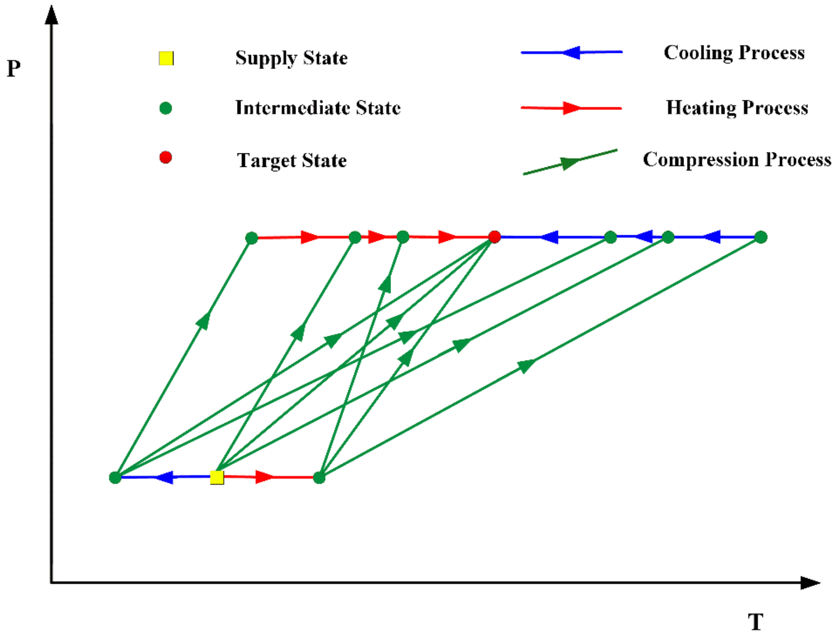

Figure 2. Possible thermodynamic paths for low pressure cold streams

The primary task of this research is to identify the optimal thermodynamic paths for the pressure changing streams to minimize exergy consumption. However, the identities of the streams are unknown and so are the intermediate temperatures of the streams. None of the current heat integration models can handle this case. The Duran-Grossmann model can handle heat integration problems with variable stream temperatures, but it requires a priori knowledge about the identities of the streams. Hence, the Duran-Grossmann model is extended to the WHENs problem, where the identity of some of the stream segments is unknown. With a rich superstructure, the optimal thermodynamic paths of the process streams can be determined.

Superstructure and Model Formulation

Superstructure for Pressure Changing Streams

Figure 2 indicates that a cold process stream to be compressed could be pre-heated, pre-cooled or compressed directly. After compression, unless the outlet temperature coincidently matches

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

the target temperature, additional heating or cooling will be required. When using the term cold stream here, it should be emphasized that this only reflects the fact that the target temperature is higher than the supply temperature. Using a similar analysis, a hot stream could also be pre-heated, pre-cooled or directly compressed. After compression, heat exchange is required to reach the target temperature. Thus, when developing a superstructure for a stream to be compressed, there is no difference between a hot and a cold stream.

The combination of thermodynamic paths indicated in Figure 2 is achieved by stream splitting. A logical approach would be to split the process streams (hot or cold) into three branches for pre-heating, pre-cooling or direct compression. Following the insight of Fu and Gundersen[13], however, direct compression is only a promising alternative if the supply temperature coincides with the Pinch or ambient temperature. In addition, the stream branches can be subject to any combination of heating and cooling, including heating only or cooling only.

In conclusion, all stream branches before and after compression have unknown identity. The next critical issue is the number of branches for each individual stream that is subject to compression. Based on experience from a number of case studies in previous work in our group, as well as to avoid too complex network structures, it was decided to use three stream branches in the superstructure. Identical arguments can be used for process streams that are subject to expansion. The resulting superstructures for streams to be compressed and expanded are shown in Figures 3 and 4. The superstructures take into account different heat manipulations and stream splits simultaneously. The number of stream branches can obviously be increased for individual streams with considerably larger heat capacity flowrates (FCp) than the other streams, however, it is believed that three branches represent a practical solution with near-optimal trade-off between energy cost and equipment cost. Since heat capacity flowrates, temperatures and even stream identities are variables, heat integration methods relying on

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

temperature intervals cannot be applied to the WHENs problem. In this study, the Duran-Grossmann model is extended to the case with unknown stream identities.

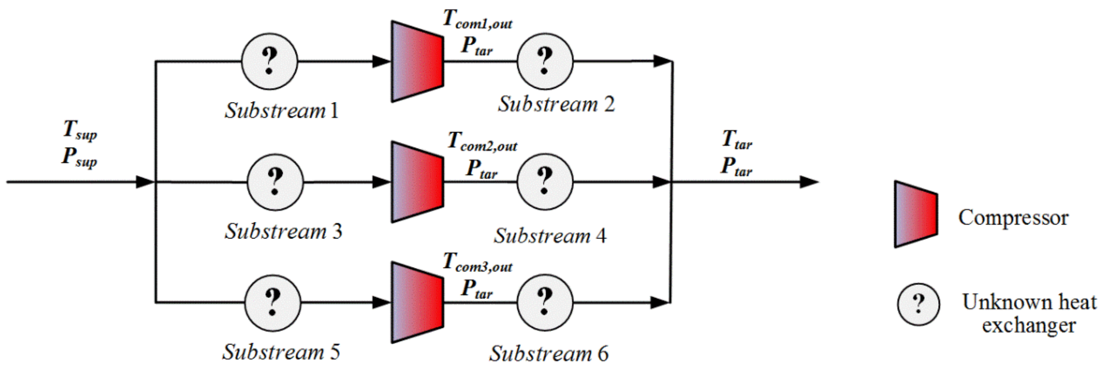

Figure 3. Superstructure for streams belonging to *WSK*

Extended Duran-Grossmann Model

For the superstructures in Figures 3 and 4, a proper mathematical model should be proposed to determine the optimal thermodynamic path of the pressure changing streams. It should be noted that isothermal mixing is assumed before reaching the target state (P_{tar}, T_{tar}). Duran and Grossmann[20] proposed a heat integration model with variable stream data. Their model performs simultaneous heat integration and process optimization, and has been successfully applied to process integration of organic Rankine cycles[24] and fuel cell systems[25]. The classical Duran-Grossmann model is as follows:

$$\min obj = F(\omega, x) + C_{hu}Q_{hu} + C_{cu}Q_{cu}$$

$$s.t.\ \ h(\omega, x) = 0 \quad \text{DG.1}$$

$$g(\omega, x) \le 0 \quad \text{DG.2}$$

$$T_i^p = T_i^{in} \quad i \in H \quad \text{DG.3}$$

$$T_j^p = T_j^{in} + HRAT \quad j \in C \quad \text{DG.4}$$

$$QSOA(x)^p = \sum_{i \in H} FCp_i \left[\max\left\{0, T_i^{in} - T^p\right\} - \max\left\{0, T_i^{out} - T^p\right\} \right] \quad \text{DG.5}$$

$$QSIA(x)^p = \sum_{j \in C} FCp_j \left[\max\left\{0, T_j^{out} - (T^p - HRAT)\right\} - \max\left\{0, T_j^{in} - (T^p - HRAT)\right\} \right] \quad \text{DG.6}$$

$$Z_H^p(x) = QSIA(x)^p - QSOA(x)^p \quad \text{DG.7}$$

$$Z_H^p(x) \le Q_{hu} \quad \text{DG.8}$$

$$\Omega(x) + Q_{hu} - Q_{cu} = 0 \quad \text{DG.9}$$

$$\Omega(x) = \sum_{i \in H} FCp_i (T_i^{in} - T_i^{out}) - \sum_{j \in C} FCp_j (T_j^{out} - T_j^{in}) \quad \text{DG.10}$$

$$Q_{hu} \ge 0, Q_{cu} \ge 0 \quad \text{DG.11}$$

It is obvious that in the original Duran-Grossmann model, different equations are formulated for the hot and cold stream sets respectively as shown by Eqs. DG.3-6. Only inlet temperatures are considered as Pinch candidates. The superscript $p \in P$ in the Duran-Grossmann model denotes potential Pinch candidates. For each Pinch candidate, *QSOA* and *QSIA* denote the heat load of hot and cold streams respectively above the Pinch candidate. $Z_H^p(x)$ is the heat deficit above Pinch candidate *p*. $\Omega(x)$ is the heat load difference between hot streams and cold streams.

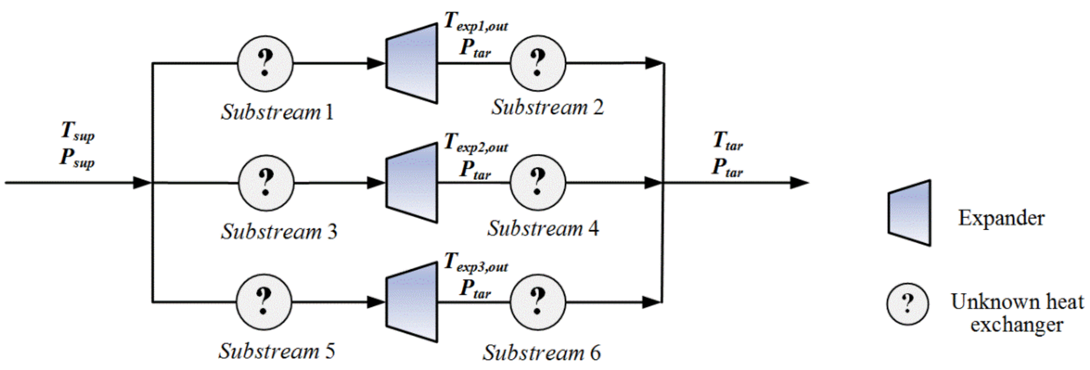

Figure 4. Superstructure for streams belonging to WSR

Since identities of the streams are unknown a priori in WHENs, the Duran-Grossmann model cannot be applied to WHENs directly and is therefore extended to a new model using binary

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

variables to denote the identity of streams. In the new version of the Duran-Grossmann model, the sets of hot and cold streams no longer exist. Binary variables are instead used to distinguish automatically between hot and cold streams in the model:

$$y_s = \begin{cases} 1 & \textit{if s is a cold stream} \\ 0 & \textit{otherwise} \end{cases}$$

The model can pick up the optimal identity for each stream. Pinch candidates of the system are the supply temperatures of all streams. The Pinch candidate temperature is the supply temperature for hot streams and the supply temperature plus the Heat Recovery Approach Temperature (HRAT) for cold streams. Eq. (1) can be used to define the set of Pinch candidate temperatures and replaces Eqs. DG.3-4 in the original Duran-Grossmann model.

$$T_s^p = T_s^{in} + y_s \cdot HRAT \tag{1}$$

For any stream, the heat load is calculated by Eq. (2). If the stream is a hot stream, then Q_s is positive, whereas Q_s is negative for cold streams. FCp_s denotes the heat capacity flowrate of stream *s*, which is assumed to be constant in this study. However, streams can be decomposed into stream segments to take into account non-constant heat capacity flowrates. The temperature-enthalpy relation of the original stream is then piece-wise linear. Correspondingly, the model size will be larger.

$$Q_s = FCp_s(T_s^{in} - T_s^{out}) \tag{2}$$

The heat load of hot streams above a Pinch candidate can be expressed by Eq. (3):

$$QSOA(x)^p = \sum_{s \in S}(1 - y_s)FCp_s \begin{bmatrix} \max\left\{0, T_s^{in} + y_s \cdot HRAT - T^p\right\} \\ -\max\left\{0, T_s^{out} + y_s \cdot HRAT - T^p\right\} \end{bmatrix} \tag{3}$$

The heat load of cold streams above a Pinch candidate can be expressed by Eq. (4):

$$QSIA(x)^p = \sum_{s \in S} y_s \cdot FCp_s \begin{bmatrix} \max\left\{0, T_s^{out} + y_s \cdot HRAT - T^p\right\} \\ -\max\left\{0, T_s^{in} + y_s \cdot HRAT - T^p\right\} \end{bmatrix} \tag{4}$$

The heat deficit above each Pinch candidate can be calculated by Eq. (5):

$$Z_H^p(x) = QSIA(x)^p - QSOA(x)^p \tag{5}$$

The hot utility can be calculated by Eq. (6):

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

$$Z_H^p(x) \le Q_{hu} \tag{6}$$

The energy difference between hot streams and cold streams is

$$\Omega(x) = \sum_{s \in S} \left(1 - y_s\right) FCp_s (T_s^{in} - T_s^{out}) - \sum_{s \in S} y_s \cdot FCp_s (T_s^{out} - T_s^{in}) \tag{7}$$

The cold utility can be calculated by Eq. (8):

$$Q_{cu} = \Omega(x) + Q_{hu} \tag{8}$$

Based on the superstructure proposed in this study as shown in Figures 3 and 4, a set of constraints for the WHENs problem can be derived. The following equations are used to assign the supply and target temperatures to the sub-streams and perform the mass balances in the superstructure.

$$T_{s,1}^{in} = T_s^{sup} \tag{9}$$
$$T_{s,3}^{in} = T_s^{sup} \tag{10}$$
$$T_{s,5}^{in} = T_s^{sup} \tag{11}$$
$$T_{s,2}^{out} = T_s^{tar} \tag{12}$$
$$T_{s,4}^{out} = T_s^{tar} \tag{13}$$
$$T_{s,6}^{out} = T_s^{tar} \tag{14}$$
$$FCp_s = FCp_{s,1} + FCp_{s,3} + FCp_{s,5} \tag{15}$$
$$FCp_{s,1} = FCp_{s,2} \tag{16}$$
$$FCp_{s,3} = FCp_{s,4} \tag{17}$$
$$FCp_{s,5} = FCp_{s,6} \tag{18}$$

The inlet temperature of sub-streams (2, 4 and 6) and the outlet temperature of sub-streams (1, 3 and 5) satisfy Eqs. (19)-(21), where γ is the heat capacity ratio.

$$T_{s,2}^{in} = T_{s,1}^{out} \left(P_s^{tar} / P_s^{sup}\right)^{(\gamma/\gamma-1)} \tag{19}$$
$$T_{s,4}^{in} = T_{s,3}^{out} \left(P_s^{tar} / P_s^{sup}\right)^{(\gamma/\gamma-1)} \tag{20}$$
$$T_{s,6}^{in} = T_{s,5}^{out} \left(P_s^{tar} / P_s^{sup}\right)^{(\gamma/\gamma-1)} \tag{21}$$

For each stream $s \in WSK$, Eqs. (22)-(25) are used to calculate the work consumption of each compressor and total work consumption.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

$$W_s^{com1} = FCp_{s,1}\left(T_{s,2}^{in} - T_{s,1}^{out}\right) \tag{22}$$

$$W_s^{com2} = FCp_{s,3}\left(T_{s,4}^{in} - T_{s,3}^{out}\right) \tag{23}$$

$$W_s^{com3} = FCp_{s,5}\left(T_{s,6}^{in} - T_{s,5}^{out}\right) \tag{24}$$

$$W_s = W_s^{com1} + W_s^{com2} + W_s^{com3} \tag{25}$$

Similarly, the following equations are applied to $s \in WSR$ in order to calculate the expansion work.

$$W_s^{exp1} = -FCp_{s,1}\left(T_{s,2}^{in} - T_{s,1}^{out}\right) \tag{26}$$

$$W_s^{exp2} = -FCp_{s,3}\left(T_{s,4}^{in} - T_{s,3}^{out}\right) \tag{27}$$

$$W_s^{exp3} = -FCp_{s,5}\left(T_{s,6}^{in} - T_{s,5}^{out}\right) \tag{28}$$

$$W_s = W_s^{exp1} + W_s^{exp2} + W_s^{exp3} \tag{29}$$

Logical constraints exist between heat loads and the identity of the streams. According to the definition of heat load for a process stream in Eq. (2), logical constraints as shown in Eqs. (30) and (31) can be derived, where M is a large enough number. To facilitate the solution, M is assigned as the upper bound of the heat load of streams.

$$Q_s \le (1 - y_s) \cdot M \tag{30}$$

$$Q_s \ge -y_s \cdot M \tag{31}$$

Objective Function

Since both heat and work are involved in WHENs, it is a challenge to trade off these two forms of energy. The purpose of the integration is to make full use of the thermal energy and pressure energy of the original process streams. Exergy can be a useful criterion to trade off different forms of energy. In the literature, exergy is decomposed into various forms. For WHENs, only thermo-mechanical (also referred to as physical) exergy is relevant, and this exergy form can be decomposed into temperature based and pressure based exergies[26]. Exergy consumption[10,12,13] and utility cost[27] have been adopted as objective functions in previous studies. To make a fair comparison of different energy forms, minimization of exergy consumption is also used as the objective function in this study. For processes above ambient temperature, the exergy of cold utility is neglected. Work is 100% exergy. For hot utility above

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

ambient temperature, the Carnot factor is used to calculate the exergy, and this gives an optimistic estimation for the exergy of heat. This problem can be mitigated by incorporating a correction factor η to the exergy calculation for hot utility as shown in Eq. (32). To be consistent and make a fair comparison with previous studies, this factor is assumed to be 1 ($\eta = 1$) in this study. However, η can be freely changed to other values in the proposed model to obtain more realistic results.

$$Exergy = Q \cdot (1 - T_0/T) \cdot \eta \tag{32}$$

Then the objective function can be formulated as follows.

$$Exergy_{total} = Exergy_{hu} + Exergy_{cu} - \sum_{s \in WSR} W_s + \sum_{s \in WSK} W_s$$

Compared with the original Duran-Grossmann model, the identities of streams are unknown and the pressure manipulation process is highly non-linear, thus resulting in a higher degree of complexity in the model. The model can be formulated as the following problem P_0:

$$\begin{aligned} &\text{Min } Exergy_{total} \\ &\quad s.t. \text{ Eqs. } (1) - (32) \end{aligned} \tag{P_0}$$

Model Reformulation

The new model incorporates max operators in Eqs. (3) and (4), which result in non-differential functions at T^p. Max operators represent a challenge for deterministic solvers and have to be removed. In this study, the max operators have been reformulated by different methods. The corresponding reformulations are provided in the following sections.

Smooth Approximation to Replace Max Operators

A smooth approximation method is proposed by Balakrishna and Biegler[28] to replace max operators. Yu et al.[29] applied this smooth approximation to design an organic Rankine cycle system recovering low-temperature waste heat, in which good results were obtained. The max operator is smoothed by the following approximation:

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

$$\max\{0,x\} \cong \frac{1}{2}(x+\sqrt{x^2+\varepsilon}) \tag{33}$$

ε is a small constant, typically between 10^{-3} and 10^{-6}. Then Eqs. (3) and (4) can be reformulated into Eqs. (34) and (35).

$$QSOA(x)^p = \frac{1}{2}\sum_{s\in S}(1-y_s)FCp_s\begin{bmatrix}(T_s^{in}+y_s\cdot HRAT-T^p+\sqrt{(T_s^{in}+y_s\cdot HRAT-T^p)^2+\varepsilon})\\-(T_s^{out}+y_s\cdot HRAT-T^p+\sqrt{(T_s^{out}+y_s\cdot HRAT-T^p)^2+\varepsilon})\end{bmatrix} \tag{34}$$

$$QSIA(x)^p = \frac{1}{2}\sum_{s\in S}-y_s\cdot FCp_s\begin{bmatrix}(T_s^{in}+y_s\cdot HRAT-T^p+\sqrt{(T_s^{in}+y_s\cdot HRAT-T^p)^2+\varepsilon})\\-(T_s^{out}+y_s\cdot HRAT-T^p+\sqrt{(T_s^{out}+y_s\cdot HRAT-T^p)^2+\varepsilon})\end{bmatrix} \tag{35}$$

Thus, problem P_0 can be reformulated as the following MINLP problem P_1:

$$\begin{aligned}&\text{Min } Exergy_{total}\\ &s.t.\ \text{Eqs. }(1),(2),(5)-(32),(34),(35)\end{aligned} \tag{P$_1$}$$

Explicit Disjunction to Replace Max Operators

Grossmann et al.[30] proposed a disjunctive formulation to eliminate the max operator in the Duran-Grossmann model. The key idea of the disjunctive formulation is the explicit treatment of three possibilities for process stream temperatures: a process stream is entirely above, entirely below or across the Pinch candidate. However, in the proposed model, the identities of the streams are also variables. Then the three possibilities mentioned above are illustrated by six cases as shown in Figure 5. Three Boolean variables are adopted to denote if the stream is above, across or below a certain Pinch candidate.

$$Y_1^{s,p}\begin{cases}True & if\ stream\ s\ is\ totally\ above\ Pinch\ candidate\ p\\ False & otherwise\end{cases}$$

$$Y_2^{s,p}\begin{cases}True & if\ stream\ s\ is\ across\ Pinch\ candidate\ p\\ False & otherwise\end{cases}$$

$$Y_3^{s,p}\begin{cases}True & if\ stream\ s\ is\ totally\ below\ Pinch\ candidate\ p\\ False & otherwise\end{cases}$$

Consider for example a hot stream: If both the inlet and outlet temperatures are above the temperature of the Pinch candidate ($T_s^{in} > T_s^{out} > T^p$), the heat load of the stream above Pinch is $FCp_s(T_s^{in}-T_s^{out})$. If the inlet temperature is above the temperature of the Pinch candidate and

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

the outlet temperature is below the temperature of the Pinch candidate ($T_s^{in} > T^p > T_s^{out}$), the heat load of the stream above Pinch is $FCp_s(T_s^{in} - T^p)$.

If both the inlet and outlet temperatures are below the temperature of the Pinch candidate ($T^p > T_s^{in} > T_s^{out}$), the heat load of the stream above Pinch is zero.

Based on the above observations, the disjunction in Eq. (36) can be derived for each stream to replace the max operators in P0. However, since the stream identities are unknown, new intermediate variables $\phi_s^{in,p}$ and $\phi_s^{out,p}$ are introduced to express the three possibilities for both hot and cold streams.

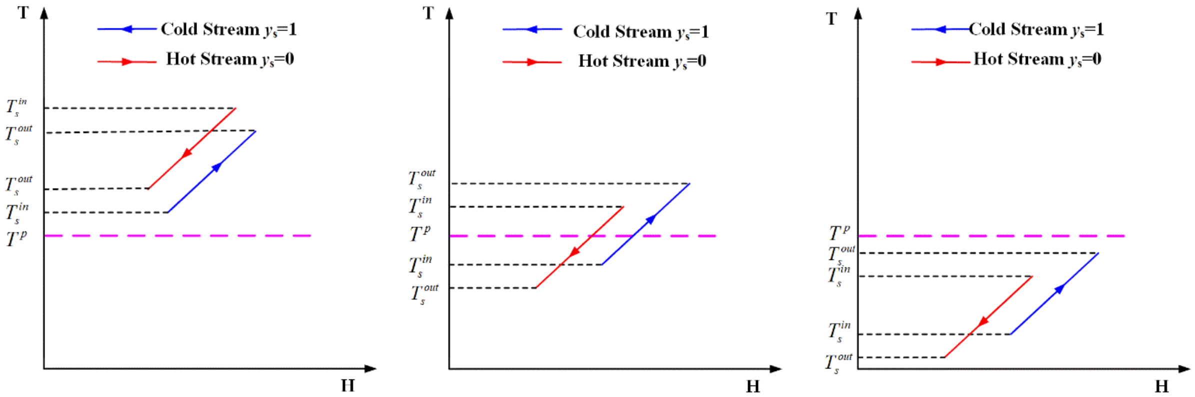

Figure 5. Relationships between a Pinch candidate and stream inlet/outlet temperatures

$$\begin{bmatrix} Y_1^{s,p} \\ T_s^{in} + y_s \cdot HRAT \geq T^p \\ T_s^{out} + y_s \cdot HRAT \geq T^p \\ \phi_s^{in,p} = T_s^{in} + y_s \cdot HRAT - T^p \\ \phi_s^{out,p} = T_s^{out} + y_s \cdot HRAT - T^p \end{bmatrix} \vee \begin{bmatrix} Y_2^{s,p} \\ T_s^{in} + y_s \cdot HRAT \geq T^p - y_s \cdot R \\ T_s^{out} + y_s \cdot HRAT \geq T^p - (1-y_s) \cdot R \\ T_s^{in} + y_s \cdot HRAT \leq T^p + (1-y_s) \cdot R \\ T_s^{out} + y_s \cdot HRAT \leq T^p + y_s \cdot R \\ \phi_s^{in,p} = (1-y_s) T_s^{in} - (1-y_s) T^p \\ \phi_s^{out,p} = y_s \cdot T_s^{out} + y_s \cdot HRAT - y_s \cdot T^p \end{bmatrix} \vee \begin{bmatrix} Y_3^{s,p} \\ T_s^{in} + y_s \cdot HRAT \leq T^p \\ T_s^{out} + y_s \cdot HRAT \leq T^p \\ \phi_s^{in,p} = 0 \\ \phi_s^{out,p} = 0 \end{bmatrix} \quad (36)$$

$$QSOA(x)^p = \sum_{s \in S} (1-y_s) FCp_s (\phi_s^{in,p} - \phi_s^{out,p})$$

$$QSIA(x)^p = \sum_{s \in S} -y_s \cdot FCp_s (\phi_s^{in,p} - \phi_s^{out,p})$$

Here, R is a sufficiently large number to relax the corresponding constraints in the disjunction.

Then problem P0 can be reformulated as the following disjunctive problem P2:

$$\begin{aligned} &\text{Min } Exergy_{total} \\ &\quad s.t. \text{ Eqs. } (1),(2),(5)-(32),(36) \end{aligned} \tag{P$_2$}$$

Direct Disjunction to Replace Max Operators

Recently, Quirante et al.[31] proposed a novel robust alternative disjunctive reformulation that shows reduced relaxation gap and reduced number of equations and variables. The max operator is directly replaced by a disjunction without physical insights. This reformulation has fewer Boolean variables compared with the previous disjunctive reformulation by Grossmann et al.[30]. The max operator is expressed as follows: $\varphi = \max(0, c^T x)$. To avoid using max operators and smooth approximations, the direct disjunctive model is proposed as follows:

$$\begin{bmatrix} Y \\ c^T x \geq 0 \\ \varphi = c^T x \\ x_{\text{lo}} \leq x \leq x_{\text{up}} \end{bmatrix} \vee \begin{bmatrix} \neg Y \\ c^T x \leq 0 \\ \varphi = 0 \\ x_{\text{lo}} \leq x \leq x_{\text{up}} \end{bmatrix}$$

$$Y \in \{True, False\}$$

Then the above disjunction is applied to Eqs. (3) and (4) in the model. The following disjunction can be derived as shown in Eq. (38).

$$\begin{gathered} \begin{bmatrix} Y_{in} \\ T_s^{in} + y_s \cdot HRAT - T^p \geq 0 \\ \phi_s^{in,p} = T_s^{in} + y_s \cdot HRAT - T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y_{in} \\ T_s^{in} + y_s \cdot HRAT - T^p \leq 0 \\ \phi_s^{in,p} = 0 \end{bmatrix} \\ \begin{bmatrix} Y_{out} \\ T_s^{out} + y_s \cdot HRAT - T^p \geq 0 \\ \phi_s^{out,p} = T_s^{out} + y_s \cdot HRAT - T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y_{out} \\ T_s^{out} + y_s \cdot HRAT - T^p \leq 0 \\ \phi_s^{out,p} = 0 \end{bmatrix} \\ QSOA(x)^p = \sum_{s \in S} (1 - y_s) FCp_s (\phi_s^{in,p} - \phi_s^{out,p}) \\ QSIA(x)^p = \sum_{s \in S} -y_s \cdot FCp_s (\phi_s^{in,p} - \phi_s^{out,p}) \end{gathered} \tag{37}$$

When Eqs. (3) and (4) are replaced by the disjunction in Eq. (37), the direct disjunction model (P$_3$) can be formulated as follows:

$$\begin{aligned} &\text{Min } Exergy_{total} \\ &\quad s.t. \text{ Eqs. } (1),(2),(5)-(32),(37) \end{aligned} \tag{P$_3$}$$

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

Computational Aspects

The proposed models are implemented in the GAMS[32] software. The proposed model is highly nonlinear and non-convex, which can result in a large number of local solutions. For the Smooth Approximation reformulation, the model was solved with BARON[33] or DICOPT[34]. BARON is based on a Branch-and-Bound method, which performs very well when the NLP sub-problems are small or when only some of the NLP sub-problems need to be solved[35]. The DICOPT solver is based on an extension of the outer approximation method[36]. The algorithm decomposes the MINLP into NLP and MILP sub-problems. The NLP problems are solved with CONOPT[37] and the MILP problems are solved with CPLEX[38]. For the disjunctive model, LogMIP[39] is adopted as the solver in this study. LogMIP is a specially designed program for disjunctive programming. The code is implemented in GAMS for solving disjunctive/hybrid programs. The new model proposed in this study is hybrid, since one part of the model is expressed in disjunctive form and the other part in mixed integer form. LogMIP complements the GAMS modeling framework by enabling the expression of discrete decisions in the form of disjunctions directly. LogMIP greatly facilitates the reformulation and solution of disjunctive models. Convex hull or Big-M reformulations can be selected through the LogMIP solver directly. The LogMIP solver reformulates the disjunctive model into an MINLP model and then calls the appropriate solver for the model. Still, BARON and DICOPT are adopted as the solvers for the MINLP model. For small size problems, BARON can solve the model to global optimum. However, BARON is computationally expensive for large scale problems. Due to the multiple start attributes of BARON, feasible initial points can be obtained. DICOPT is adopted to solve large-scale problems with the feasible initial point obtained from BARON. Even though SBB[40] is reported to outperform DICOPT in the study by Onishi et al.[15], SBB can not even get feasible solutions for the proposed model. All the models are solved using a

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

personal computer with 4 cores 2.8 GHz Intel i7 CUP and 32 GB of RAM running Windows 10 Ultimate with GAMS.

Case Studies

In this paper, two examples are presented to illustrate the effectiveness of the proposed superstructure and mathematical model. The objective of the case study is twofold: The first example aims at verifying the correctness of the model by comparing the solution provided by the proposed model with results from the previously published graphical design procedure[13]. The second example aims at extending the model to the case where there are multiple pressure changing streams and the GCC is unavailable, which is difficult to solve by the graphical design procedure.

Example 1

This case is adopted from the study by Fu and Gundersen[13]. The stream data are presented in Table 1. In this case, H1 is a high-pressure hot stream. H2 and H3 are hot streams without pressure change. C1 is a low-pressure cold stream. C2 is a cold stream without pressure change. The following assumptions are adopted in this paper to make a fair comparison with the study by Fu and Gundersen[13]. (1) The compressor and expander isentropic efficiencies are assumed to be 100%. (2) The heat recovery approach temperature (HRAT) is assumed to be 20℃. (3) The cold utility is supplied at ambient temperature (15℃), and the exergy of cold utility is zero. (4) The fluids to be compressed and expanded behave like ideal gas with constant specific heat capacity ratio $\gamma = 1.4$.

Table 1. Stream data for Example 1

Stream	T_{sup}(°C)	T_{tar}(°C)	FCp(kW/°C)	ΔH(kW)	P_{sup}(kPa)	P_{tar}(kPa)
H1	400	35	2	730	200	100
H2	320	160	4	640	-	-
H3	110	35	3	225	-	-
C1	15	380	3	1095	100	200

C2	190	250	10	600	-	-
Hot utility	400	400	-	-	-	-
Cold utility	15	15	-	-	-	-

The variable pressure streams H1 and C1 each result in 6 sub-streams according to the superstructure proposed in this study. Based on the corresponding model, the same results are obtained as in the study by Fu and Gundersen[13]. As shown in Figure 6, H1 should be split into two streams with branch heat capacity flowrates 2.66 kW/℃ and 0.34 kW/℃ respectively.

Table 2. Optimized results for Example 1

Stream	T_{sup} (°C)	T_{tar} (°C)	FCp(kW/°C)	ΔH (kW)	P_{sup} (kPa)	P_{tar} (kPa)
H1-S1	400	210	1.15	218.5	200	200
H1-S2	123.2	35	1.15	101.4	100	100
H1-S3	400	110	0.85	246.5	200	200
H1-S4	41.2	35	0.85	5.3	100	100
C1-S1	15	190	2.66	465.5	100	100
C1-S2	291.4	380	2.66	235.7	200	200
C1-S3	15	300	0.34	96.9	100	100
C1-S4	425.5	380	0.34	15.5	200	200

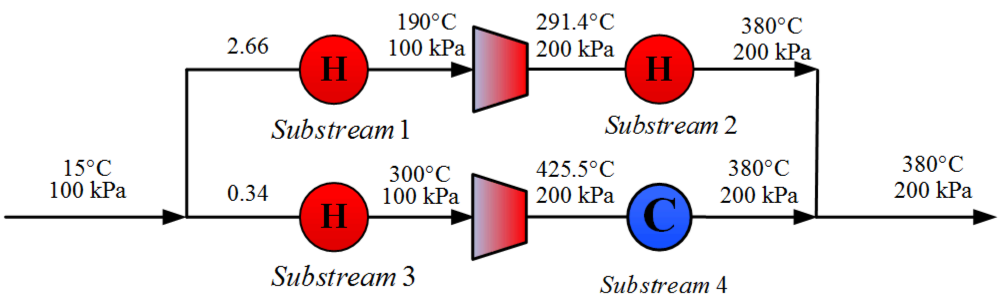

Figure 6. Optimized thermodynamic path for C1

Due to the non-convexity of the MINLP model, only small problems can be solved with global optimum solvers, such as BARON. For Example 1, the same results are obtained as presented by Fu and Gundersen[13]. Their results were proven mathematically to be the global optimal solution for the design, which verifies the effectiveness of the model proposed in this paper.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

Once the thermodynamic paths of the pressure changing streams are determined, the problem is reduced to a heat exchanger network synthesis problem. The final network configuration can be determined by mature heat exchanger network synthesis techniques, such as sequential or simultaneous methods[41]. More detailed information about the results and the final work and heat exchange network can be found in previous work by Fu and Gundersen[13].

Example 2

In Example 1, the results are consistent with those obtained from the graphical methodology proposed by Fu and Gundersen[13]. However, only one expanded stream and one compressed stream are considered. If more pressure-manipulated streams are introduced, the graphical design procedure that is based on the GCC to design a system with minimum exergy consumption is very tedious. In order to verify the effectiveness of our model for multiple pressure-manipulated streams, Example 1 is revised to a more challenging problem where all the streams are subject to pressure change. In addition, the supply and target temperatures are the same, thus there is no GCC in this case. The stream data for Example 2 are listed in Table 3. There is no heat load for the process streams at first sight since the target temperatures are equal to the supply temperatures for all streams. However, pressure change inevitably causes temperature change, which means that heat integration is an issue even for this example. Even without a GCC, the previously established theorems and corresponding graphical procedure can be applied, however, with five streams this will be very time consuming and possibly even prohibitive to solve.

Table 3. Stream data for Example 2

Stream	T_{sup} (°C)	T_{tar} (°C)	FCp(kW/°C)	ΔH (kW)	P_{sup} (kPa)	P_{tar} (kPa)
HP1	350	350	2	0	200	100
HP2	320	320	4	0	200	100
HP3	110	110	3	0	200	100
LP1	50	50	3	0	100	200

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

LP2	190	190	10	0	100	200
Hot utility	400	400	-	-	-	-
Cold utility	15	15	-	-	-	-

Table 4. Comparison of different reformulations for Example 2

Reformulations	obj.f. (kW)	hot utility (kW)	power consumed (kW)	power generated (kW)
Smooth Approximation	322.50	40	1127	827.24
Explicit Disjunction	332.34	40	1151	841.66
Direct Disjunction	366.41	237	1053	822.28

The optimal results are shown in Table 4 with different reformulations. Since the model is a highly non-convex and non-linear MINLP model, it is challenging to obtain the global optimum. In this case, there are five process streams, which results in 30 sub-streams in the proposed model. Therefore, it is impossible to find the global optimum with present global MINLP solvers. However, BARON was adopted as the solver to get an initial feasible solution due to its multi-start search attribute. Once an acceptable feasible solution is obtained, DICOPT is adopted as the solver for the final solution. Table 4 lists the model and solution statistics for the three different reformulations proposed in this study.

Table 5. Results for Example 2 with smooth approximation reformulation

Stream	T^{in} (°C)	T^{out} (°C)	FCp(kW/°C)	ΔH (kW)	P_{sup} (kPa)	P_{tar} (kPa)
HP1	**350**	**350**	**2**	**0**	**200**	**100**
HP1-S3	350	268.1	2	163.8	200	200
HP1-S4	170.8	350	2	-358.3	100	100
HP2	**320**	**320**	**4**	**0**	**200**	**100**
HP2-S6	213.4	320	4	-426.4	100	100
HP3	**110**	**110**	**3**	**0**	**200**	**100**
HP3-S6	41.1	110	3	-206.6	100	100
LP1	**50**	**50**	**3**	**0**	**100**	**200**
LP1-S1	50	35	3	45	100	100
LP1-S2	102.5	50	3	157.5	200	200
LP2	**190**	**190**	**10**	**0**	**100**	**200**
LP2-S1	190	35	3.67	569	100	100
LP2-S2	102.5	190	3.67	-321.3	200	200
LP2-S3	190	229.8	4	-159.4	100	100
LP2-S4	340	190	4	600	200	200

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

LP2-S6	291.4	190	2.33	236.2	200	200

It is notable that the smooth approximation reformulation gives the best results. The detailed results of the smooth approximation reformulation are listed in Table 5. The parent streams are highlighted in bold. It can be seen that stream LP2 is split into three sub-streams. The optimized thermodynamic path of LP2 is illustrated in Figure 7. However, it should be noted that this smooth approximation might suffer from numerical issues when isothermal streams or intermediate utilities are involved. Since isothermal streams are not considered in this study, smooth approximations should perform well. The GCC of the system is illustrated in Figure 8. There are three Pinch points in this system, which in itself indicates an energy efficient system. Once the thermodynamic paths of pressure changing streams are determined, the final heat and work exchange network can be synthesized based on a stage-wise superstructure[16]. However, the model is modified in the sense that the objective function minimizes the number of heat exchanger units, with the energy consumption fixed at the values predicted by the extended Duran-Grossman model. The minimum approach temperature is assumed to be 10°C while synthesizing the heat exchanger network. The motivation for using ΔT_{min} (10°C) < HRAT (20°C), while keeping utility consumption at the level corresponding to HRAT, is to provide additional degrees of freedom. In the network design phase this may reduce the number of units as well as stream splits, thus resulting in networks with reduced complexity[42]. One of the Work and Heat Exchange Networks (WHENs) featuring minimum exergy consumption is shown in Figure 9. One deficiency of the proposed model can be observed from the network in Figure 9. The match that cools LP2-S4 from 200°C to 190°C and heats LP2-S2 from 179.1°C to 190°C can be omitted, since the final mixer of stream LP2 will take care of this heating/cooling by direct heat transfer.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

Another comment could be made about the layout of Figure 9. While this version of the well-known grid diagram in Pinch Analysis clearly distinguishes the HEN and the WEN, it makes the HEN part more confusing since hot and cold stream segments are drawn both ways, i.e. from left to right and from right to left. This is why hot stream segments are drawn with red color, cold stream segments are drawn with blue color, and stream segments not participating in the HEN are drawn with black color.

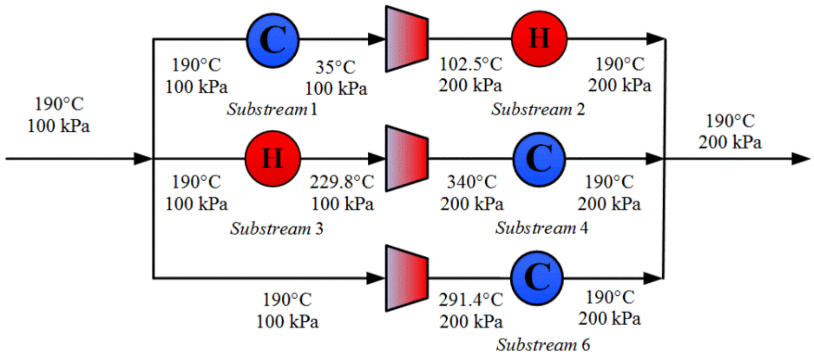

Figure 7. Optimal thermodynamic path for stream LP2

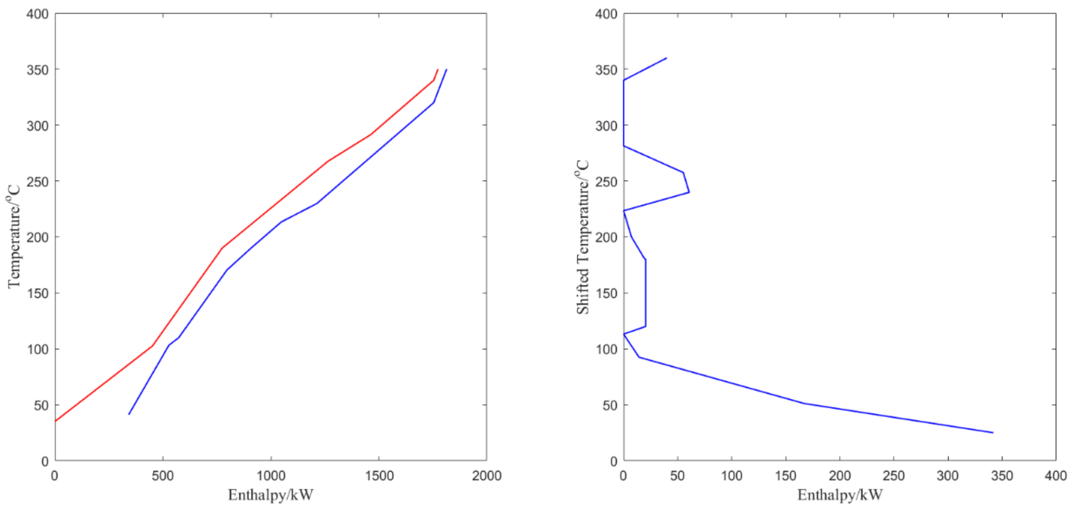

Figure 8. CCs and GCC for the system obtained from smooth approximations

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

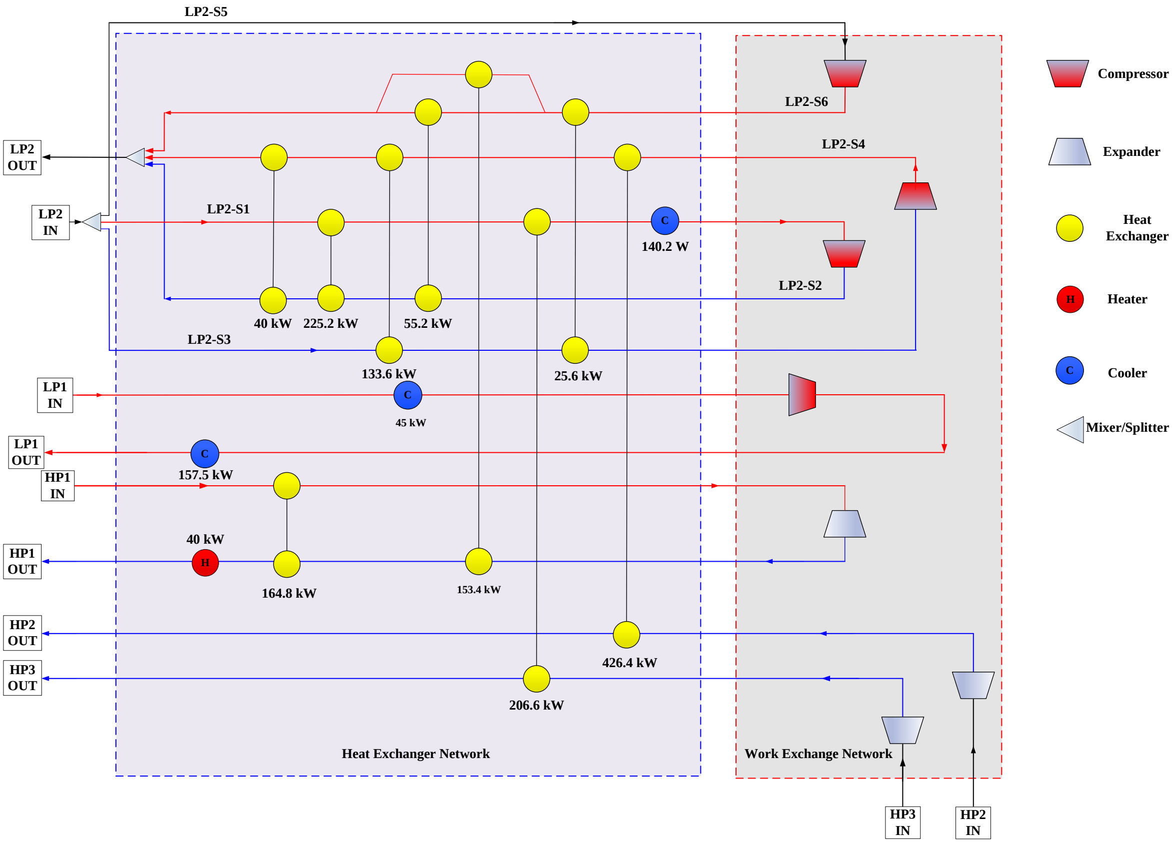

Figure 9. Final Work and Heat Exchange Network (WHEN) for Example 2

Conclusions and Future Work

A new mathematical model for Work and Heat Exchange Network (WHEN) synthesis is proposed, where the main objective is to determine the optimal thermodynamic paths of pressure changing streams that result in minimum exergy consumption. In WHEN problems, the identity of streams involved in heat integration is unknown a priori. The proposed model is an extension of the Duran-Grossmann model where the main new feature is that it can handle heat integration problems without knowing the identity of the streams. In order to avoid max operators, the extended model is reformulated into three different models, (1) smooth approximation, (2) explicit disjunction, and (3) direct disjunction. A comparison between these reformulations shows that, for the largest example, smooth approximation has a better performance than the other reformulations.

Each pressure changing stream has nine possible thermodynamic paths. A stream superstructure that contains all these alternatives is developed, and the proposed model can

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

handle multiple pressure changing streams. Once the optimal thermodynamic paths for pressure changing streams are determined, the WHENs problem reduces to a HENs problem that can be solved with existing heat integration technologies. The stage-wise superstructure model by Yee and Grossmann is adopted to synthesize the final heat exchanger network. The proposed WHEN synthesis model is used to solve two examples. The first example validates the correctness of the model by duplicating the results obtained by a manual and graphical procedure from an earlier paper where the global optimum is known. The second example illustrates the capability of the model to handle more complex cases where the manual procedure is too time consuming or even prohibitive to apply.

Future work should involve extensions to the capabilities of the model as well as improved solution strategies. The use of exergy to handle heat and work on a common basis should be improved by introducing a variable correction factor for the exergy of heat. Multi-stage compression and expansion is expected to be a straightforward extension of the model; however, it will introduce pressure ratios as additional optimization variables. A favorable property would be to allow a stream to undergo both compression and expansion. Multiple hot and/or cold utilities, possibly with gliding temperatures, represent more complicated extensions to the model. Finally, the ultimate goal is to handle phase change, both with gliding and constant temperature. Non-convexities in the model and binary variables used to handle the unknown identity (hot/cold) of streams result in a complex model where the global optimum cannot be guaranteed for medium or large-scale problems. Thus, a robust and efficient solution strategy should be investigated in future work.

Acknowledgments

This publication has been funded by HighEFF-Centre for an Energy Efficient and Competitive Industry for the Future. The authors gratefully acknowledge the financial support from the Research Council of Norway and user partners of HighEFF, an 8-year Research Centre under the FME-scheme (Centre for Environment-friendly Energy Research, 257632/E20). Thanks to John Eason at Carnegie Mellon University for his kind help with the GAMS code.

Notation

Abbreviations

DG	Duran-Grossmann model
GDP	General Disjunctive Programming
HRAT	Heat Recovery Approach Temperature
MINLP	Mixed Integer Nonlinear Programming
NLP	Nonlinear Programming

Sets

C	Cold streams
H	Hot streams
HPC	High Pressure Cold streams
HPH	High Pressure Hot streams
HP	High Pressure streams
LPC	Low Pressure Cold streams
LPH	Low Pressure Hot streams
LP	Low Pressure streams
NPC	Non-Pressure Changing streams
P	Pinch candidates
S	Streams involved in heat integration
WSK	Work Sink streams
WSR	Work Source streams

Binary and Boolean variables

y_s	Stream identity (1 for cold streams, 0 for hot streams)

Y	Boolean variable in the direct disjunction reformulation
$Y_1^{s,p}$	True if both the stream inlet and outlet temperatures are above the Pinch candidate for the explicit disjunction reformulation
$Y_2^{s,p}$	True if the stream inlet temperature is above the Pinch candidate and the outlet temperature is below the Pinch candidate for the explicit disjunction reformulation
$Y_3^{s,p}$	True if both the stream inlet and outlet temperatures are below the Pinch candidate for the explicit disjunction reformulation

Continuous variables and parameters

FCp	Heat capacity flowrate
M	Sufficiently large number used in Eqs. (31) and (32)
P	Pressure
$QSIA$	Heat load of cold streams above the Pinch candidate
$QSOA$	Heat load of hot streams above the Pinch candidate
R	Sufficiently large number used in Eq. (37)
T	Temperature

Greek letters

γ	Heat capacity ratio
ε	Small constant used in the smooth approximation
φ	Variable to denote the max operator in the direct disjunction reformulation
η	Correction factor to calculate the exergy of heat
ϕ	Temperature above Pinch candidates used in the explicit and direct disjunction reformulations
ω	Process variables in the original Duran-Grossmann model

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

ΔT	Minimum heat transfer approach temperature
Subscripts/ Superscripts	
cu	Cold utility
hu	Hot utility
s	Streams involved in heat integration
com	Compression/Compressor
exp	Expansion/Expander
in	Inlet
min	Minimum
out	Outlet
sup	Supply state
tar	Target state
total	Total exergy consumption

Literature Cited

1. Gundersen T, Naess L. The synthesis of cost optimal heat exchanger networks: an industrial review of the state of the art. Computers & Chemical Engineering. 1988;12(6):503-530.

2. Furman KC, Sahinidis NV. A critical review and annotated bibliography for heat exchanger network synthesis in the 20th century. Industrial & Engineering Chemistry Research. 2002;41(10):2335-2370.

3. Liu G, Zhou H, Shen R, Feng X. A graphical method for integrating work exchange network. Applied Energy. 2014;114:588-599.

4. Marmolejo-Correa D, Gundersen T. A new procedure for the design of LNG processes by combining Exergy and Pinch Analyses. Proceedings of ECOS. 2012.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

5. Townsend DW, Linnhoff B. Heat and Power Networks in Process Design. Part I: Criteria for Placement of Heat Engines and Heat Pumps in Process Networks. AIChE J. 1983;29(5):742-748.

6. Aspelund A, Berstad DO, Gundersen T. An Extended Pinch Analysis and Design procedure utilizing pressure based exergy for subambient cooling. Applied Thermal Engineering. 2007;27(16):2633-2649.

7. Gundersen T, Berstad DO, Aspelund A. Extending pinch analysis and process integration into pressure and fluid phase considerations. Chemical Engineering Transactions. 2009;18:33-38.

8. Aspelund A, Gundersen T. A liquefied energy chain for transport and utilization of natural gas for power production with CO2 capture and storage–Part 2: the offshore and the onshore processes. Applied Energy. 2009;86(6):793-804.

9. Fu C, Gundersen T. Integrating compressors into heat exchanger networks above ambient temperature. AIChE Journal. 2015;61(11):3770-3785.

10. Fu C, Gundersen T. Sub-ambient heat exchanger network design including compressors. Chemical Engineering Science. 2015;137:631-645.

11. Fu C, Gundersen T. Integrating expanders into heat exchanger networks above ambient temperature. AIChE Journal. 2015;61(10):3404-3422.

12. Fu C, Gundersen T. Sub-ambient heat exchanger network design including expanders. Chemical Engineering Science. 2015;138:712-729.

13. Fu C, Gundersen T. Correct integration of compressors and expanders in above ambient heat exchanger networks. Energy. 2016;116, Part 2:1282-1293.

14. Wechsung A, Aspelund A, Gundersen T, Barton PI. Synthesis of heat exchanger networks at subambient conditions with compression and expansion of process streams. AIChE Journal. 2011;57(8):2090-2108.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

15. Onishi VC, Ravagnani MASS, Caballero JA. Simultaneous synthesis of heat exchanger networks with pressure recovery: Optimal integration between heat and work. AIChE Journal. 2014;60(3):893-908.

16. Yee TF, Grossmann IE. Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis. Computers & Chemical Engineering. 1990;14(10):1165-1184.

17. Onishi VC, Ravagnani MASS, Caballero JA. Simultaneous synthesis of work exchange networks with heat integration. Chemical Engineering Science. 2014;112:87-107.

18. Huang K, Karimi IA. Work-heat exchanger network synthesis (WHENS). Energy. 2016;113:1006-1017.

19. Nair SK, Nagesh Rao H, Karimi IA. Framework for Work-Heat Exchange Network Synthesis (WHENS). AIChE Journal. 2018;64(7):2472-2485.

20. Duran MA, Grossmann IE. Simultaneous optimization and heat integration of chemical processes. AIChE Journal. 1986;32(1):123-138.

21. Dinh H, Zhang J, Xu Q. Process synthesis for cascade refrigeration system based on exergy analysis. AIChE Journal. 2015;61(8):2471-2488.

22. Fu C, Gundersen T. A Novel Sensible Heat Pump Scheme for Industrial Heat Recovery. Industrial & Engineering Chemistry Research. 2016;55(4):967-977.

23. Yu H, Feng X, Wang Y, Biegler LT, Eason J. A systematic method to customize an efficient organic Rankine cycle (ORC) to recover waste heat in refineries. Applied Energy. 2016;179:302-315.

24. Yu H, Eason J, Biegler LT, Feng X. Process integration and superstructure optimization of Organic Rankine Cycles (ORCs) with heat exchanger network synthesis. Computers & Chemical Engineering. 2017;107:257-270.

25. Marechal F, Palazzi F, Godat J, Favrat D. Thermo-Economic Modelling and Optimisation of Fuel Cell Systems. Fuel Cells. 2005;5(1):5-24.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

26. Marmolejo-Correa D, Gundersen T. New graphical representation of exergy applied to low temperature process design. Industrial & Engineering Chemistry Research. 2013;52(22):7145-7156.

27. Holiastos K, Manousiouthakis V. Minimum hot/cold/electric utility cost for heat exchange networks. Computers & Chemical Engineering. 2002;26(1):3-16.

28. Balakrishna S, Biegler LT. Targeting strategies for the synthesis and energy integration of nonisothermal reactor networks. Industrial & Engineering Chemistry Research. 1992;31(9):2152-2164.

29. Yu H, Eason J, Biegler LT, Feng X. Simultaneous heat integration and techno-economic optimization of Organic Rankine Cycle (ORC) for multiple waste heat stream recovery. Energy. 2017;119:322-333.

30. Grossmann IE, Yeomans H, Kravanja Z. A rigorous disjunctive optimization model for simultaneous flowsheet optimization and heat integration. Computers & Chemical Engineering. 1998;22:S157-S164.

31. Quirante N, Caballero JA, Grossmann IE. A novel disjunctive model for the simultaneous optimization and heat integration. Computers & Chemical Engineering. 2017;96:149-168.

32. McCarl BA, Meeraus A, van der Eijk P, et al. GAMS user guide: Citeseer; 2014.

33. Tawarmalani M, Sahinidis NV. A polyhedral branch-and-cut approach to global optimization. Mathematical Programming. 2005;103(2):225-249.

34. Grossmann IE, Viswanathan J, Vecchietti A, Raman R, Kalvelagen E. GAMS/DICOPT: A discrete continuous optimization package. GAMS Corporation Inc. 2002.

35. Grossmann IE. Review of nonlinear mixed-integer and disjunctive programming techniques. Optimization and engineering. 2002;3(3):227-252.

36. Duran MA, Grossmann IE. An outer-approximation algorithm for a class of mixed-integer nonlinear programs. Mathematical programming. 1986;36(3):307-339.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437

37. Drud A. GAMS/CONOPT. ARKI Consulting and Development, Bagsvaerd, Denmark. 1996.

38. Brooke A, Kendrick D, Meeraus A, Raman R. GAMS/CPLEX 7.0 user notes. GAMS Development Corp. 2000.

39. Vecchietti A, Grossmann I. Computational experience with LogMIP solving linear and nonlinear disjunctive programming problems. Paper presented at: Proc. of FOCAPD2004.

40. Rosenthal R. SBB Solver Manual—Gams: Washington, DC, USA: GAMS Development Corporation; 2010.

41. Biegler LT, Grossmann IE, Westerberg AW. Systematic methods for chemical process design: Prentice Hall, Old Tappan, NJ (United States); 1997.

42. Gundersen T, Traedal P, Hashemi-Ahmady A. Improved sequential strategy for the synthesis of near-optimal heat exchanger networks. Computers & Chemical Engineering. 1997;21:S59-S64.

This is the accepted version of an article published in AIChE Journal.
DOI: 10.1002/aic.16437