CHEMICAL ENGINEERING TRANSACTIONS

VOL. 81, 2020

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Qiuwang Wang, Min Zeng, Panos Seferlis, Ting Ma, Jiří J. Klemeš

ISBN 978-88-95608-79-2; **ISSN** 2283-9216

DOI: 10.3303/CET2081022

The importance of thermodynamic insight in Work and Heat Exchange Network Design

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Work and Heat Exchange Network (WHEN) design has been an emerging topic in the area of Process Synthesis and has attracted increasing research interest in the past few years. Not only temperature changes but also pressure changes of process streams have been taken into consideration in WHEN design. As a result, pressure changing equipment such as compressors, expanders, pumps, valves, etc., as well as traditional heat exchange equipment is included in WHEN design. Similar to HEN design problems, both graphical and mathematical optimization approaches have been under development for WHEN design. The graphical approaches utilize fundamental thermodynamic insight while mathematical optimization approaches enable dealing with large size problems. This paper focuses on a comparison between the graphical and mathematical optimization approaches for WHEN design. A case study is used to illustrate the importance of thermodynamic insight in WHEN design even in the case of using mathematical optimization approaches.

1. Introduction

The Heat Integration problem has been extended to the Work and Heat Integration (WHI) problem when changes in both temperature and pressure of process streams are taken into consideration simultaneously (Fu and Gundersen, 2016a). The design of Work and Heat Exchange Networks (WHENs) is the key topic of WHI problems. In addition to traditional heat exchange equipment, pressure changing equipment such as compressors, expanders, pumps, valves, etc., are included in WHEN design. The WHEN design problem is much more complex than the Heat Exchanger Network (HEN) design problem, mostly due to the fact that there are interactions between pressure changes and temperature changes of streams: (1) changing the pressure of a stream normally changes its temperature that influences the definition of the Heat Integration problem; (2) the amount of work consumed/produced will vary as a result of any change in the operating temperature of a stream before being compressed or expanded. Such changes in temperatures are resulting from Heat Integration.
The WHEN design has been an emerging topic in the area of Process Synthesis and attracted increasing research interest in the past few years. A special session entitled "Work and Heat Exchange Networks" (WHENs) was actually organized at the 20th Conference on Process Integration, Modelling and Optimization for Energy Saving and Pollution Reduction – PRES'17. The development and challenges in WHI and WHENs were addressed in one of the contributions from this session (Fu et al., 2017), which was further extended to a more comprehensive review paper (Fu et al., 2018). The WHI problem has actually been regarded as a new field in Process Synthesis and Process Systems Engineering (Yu et al., 2019).
Similar to HEN design problems, both graphical and mathematical optimization approaches have been under development for WHEN design. The graphical approaches utilize fundamental thermodynamic insight while mathematical optimization approaches enable dealing with large size problems. An introduction of the two approaches are presented in the following section. Historically, there was a competition between the graphical approach (i.e. the Pinch Design Method-PDM) and the mathematical optimization approach in HEN design, while the two approaches later were combined in the sense that insight from the PDM was used to simplify the mathematical models. However, the combination of the two approaches for WHEN design has been much less

Paper Received: 31/03/2020; Revised: 04/05/2020; Accepted: 13/05/2020
Please cite this article as: Fu C., Wang X., Gundersen T., 2020, The importance of thermodynamic insight in Work and Heat Exchange Network Design, Chemical Engineering Transactions, 81, 127-132 DOI:10.3303/CET2081022

investigated except for an initial study by Maurstad Uv (2016). This paper focuses on a comparison between the two approaches for WHEN design. A case study is performed to illustrate the importance of thermodynamic insight in WHEN design even in the case of using mathematical optimization approaches.

2. Approaches for WHEN design

WHEN design is a relatively new topic. Both graphical and mathematical approaches have been investigated and are under development. The graphical approach for WHEN design has been much less investigated in literature compared to the mathematical optimization approach. Most of the research related to this approach has actually been performed in a group at NTNU. The approach developed in the group originates from the concept of Appropriate Placement for pressure-changing equipment that determines the optimal inlet temperature to compressors and expanders. Glavič et al. (1988) suggested to place compressors above the Pinch temperature since they act like hot utilities. Aspelund et al. (2007) proposed the following heuristic rules: compression/expansion adds/removes heat to/from the system and should preferably be done above/below Pinch temperature. The rules were more explicitly stated by Gundersen et al. (2009): Both compression and expansion should start at the Pinch temperature. Kansha et al. (2009) developed a self-heat recuperation scheme where both compression and expansion were found to incidentally start at the Pinch temperature (Fu et al., 2018). Starting from the heuristic rules, a set of fundamental theorems has been proposed for integration of compressors and expanders in HENs (Fu and Gundersen, 2016b). It was concluded that compression and expansion should start at Pinch, ambient, or hot/cold utility temperatures depending on the actual design problem. On the basis of these theorems, systematic graphical design procedures have been developed for WHEN design. Exergy consumption has been used as the objective since both heat and work are involved. In these graphical design procedures, the Grand Composite Curve (GCC) has been used for identifying the maximum portions of streams that can utilize Pinch Compression/Expansion. Stream splitting is sometimes used to achieve the objective of minimum exergy consumption. There are limitations in using the graphical design procedure for WHEN design (Fu et al., 2017): (1) it is time-consuming even to solve very small problems and prohibitive to solve industrial size problems, and (2) exergy consumption might not properly reflect cost.

The mathematical optimization approaches for WHEN design have attracted more research interest. Wechsung et al. (2011) developed a superstructure and a corresponding MINLP problem formulation for WHENs using an approach where Heat Integration and pressure manipulations are assigned to a Pinch operator and a pressure operator. Onishi et al. (2014) conducted a total annualized cost (TAC) analysis using the same superstructure together with additional operators for the coupling of compressors and expanders. The authors (Onishi et al., 2018) further developed models to deal with unclassified streams (i.e. stream identity as hot or cold is unknown). A superstructure for TAC analysis of WHENs was proposed by Huang and Karimi (2016). Similar to Wechsung et al. (2011), the superstructure divides the problem into a HEN and a pressure manipulation part. The latter is formulated as a Work Exchange Network problem. A very rich superstructure has been developed by Nair et al. (2018). Pressure changes are allowed for streams with the same supply and target pressure. More recent developments on the mathematical optimization models can be found in a recent review study (Yu et al., 2020).

3. Case study

The importance of thermodynamic insight in WHEN design is illustrated by a case study for better understanding in this section. Due to limitations of the graphical approach in dealing with large size problems, a case study with only two process streams is selected. Onishi et al. (2018) used this case to illustrate the application of their mathematical optimization models developed for WHEN design. A key feature of the models is that a disjunctive-based modeling approach is proposed to deal with unclassified streams. This is an obvious advantage compared to previous models. The objective function is the minimization of TAC. Details about the models can be found in Onishi et al. (2018). The stream data are presented in Table 1, where T_s and T_t are supply and target temperatures, p_s and p_t are supply and target pressures, mc_p is heat capacity flowrate, and ΔH is enthalpy change. Assumptions made include: (1) isentropic efficiencies $\eta_{comp} = \eta_{exp} = 1$, (2) minimum approach temperature $\Delta T_{min} = 5$ K, (3) polytropic exponent κ = 1.352, and (4) ambient temperature $T_0 = 300$ K.

Table 1: Stream data for the case study

Stream	T_s, K	T_t, K	mc_p, kW/K	ΔH, kW	p_s, MPa	p_t, MPa
H1	650	370	3	840	0.1	0.5
C1	410	645	2	470	0.5	0.1
Hot utility (HU)	680	680	-	-	-	-
Cold utility (CU)	300	300	-	-	-	-

The WHEN design resulting from the model by Onishi et al. (2018) is presented in Figure 1(a). Notice that the grey box represents a simplification of the HEN design. It should not be regarded as a multi-pass heat exchanger. The HEN was excluded from the cost estimations in Onishi et al. (2018). Similar simplification of the HEN design has been applied in other WHEN designs of this study.
Since the number of streams in this case study is small, the graphical design procedure (Fu and Gundersen, 2016b) can be easily applied and compared with the mathematical optimization approach. A brief introduction about the graphical design procedure for this case study follows. Detailed description of the design procedure can be found in Fu and Gundersen (2016b) and is not presented in this paper due to space limitation.

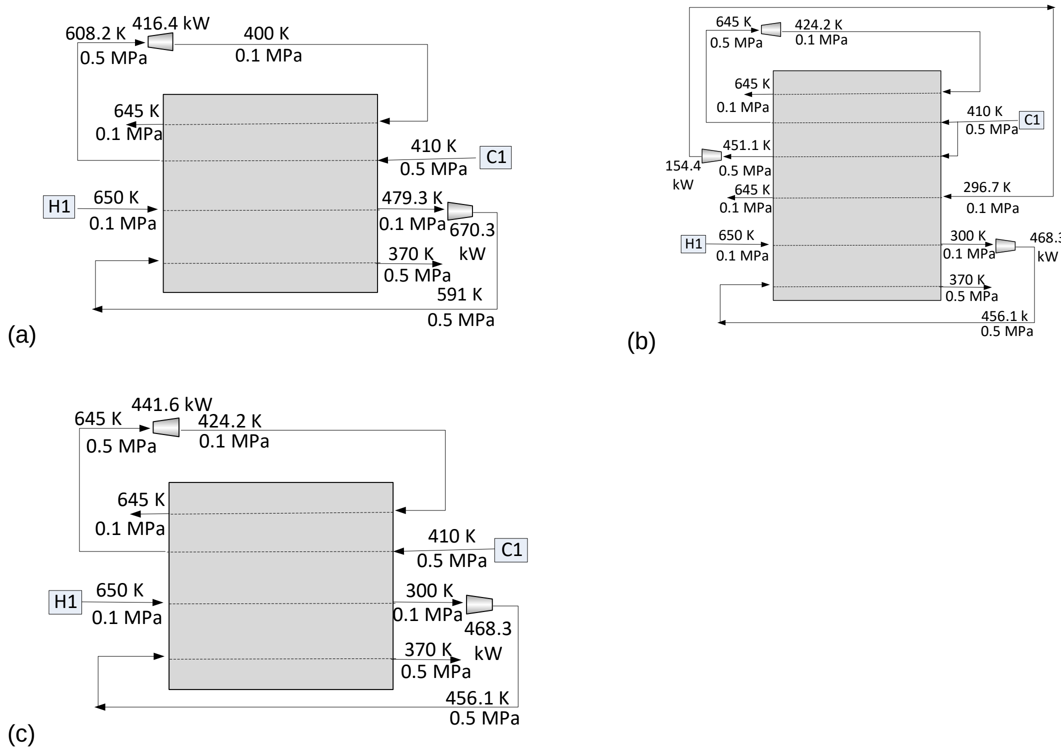

Figure 1: WHEN design: (a) Onishi et al. (2018), (b) The graphical design procedure, (c) Alternative design

<u>Step 1</u>: The GCC is drawn for streams without pressure manipulation as shown in Figure 2(a), which gives the following results: Q_{HU} = 0 kW, Q_{CU} = 370 kW, and Pinch temperature T'_{PI} = 647.5 K (a threshold problem). According to the theorems, expansion of C1 should be done at the (cold) Pinch temperature of 645 K. The outlet temperature from expansion is $T_{exp,PI} = 645 \times 0.2^{(1.352-1)/1.352}$ = 424.2 K. Stream C1 should be split and portion α is expanded at Pinch temperature after being heated from its supply temperature 410 K. The expansion work should exactly equal the required cooling duty at $T = T_{exp,PI}$ on the GCC, which means that $(mc_p)_\alpha$ = 1 kW/K. The optimal WHEN design identifies whether heating or cooling is required before pressure manipulation.
<u>Step 2</u>: The new stream data for Step 2 are presented in Table 2 and the corresponding GCC is presented in Figure 2(b). The results are Q_{HU} = 0 kW, Q_{CU} = 149.2 kW, T'_{PI} = 426.7 K. The remaining portion β should be expanded at the new Pinch temperature 424.2 K and $T_{exp,PI} = 424.2 \times 0.2^{(1.352-1)/1.352}$ = 279.0 K. The required cooling duty is larger than the expansion work when the portion β is expanded at the new Pinch, we can conclude that $(mc_p)_\beta$ = 1 kW/K.
<u>Step 3</u>: The new stream data for Step 3 are presented in Table 2 and the corresponding GCC is presented in Figure 2(c). The results are Q_{HU} = 0 kW, Q_{CU} = 4 kW, T'_{PI} = 412.5 K. The cooling demand is negligible and according to the theorems (Fu and Gundersen, 2016b), stream H1 should be compressed at T_{CU} = 300 K with an outlet temperature $T_{comp,CU} = 300 \times 5^{(1.352-1)/1.352}$ = 456.1 K. The outlet temperature is above the Pinch (426.7 K) from Step 2. The heat resulting from compression should be utilized to preheat the portion β before being expanded. The portion β can then be expanded at a higher temperature of 451.1 K rather than 424.2 K, and the outlet temperature is $T_{exp,\ 451.1\ K} = 451.1 \times 0.2^{(1.352-1)/1.352}$ = 296.7 K.
<u>Step 4</u>: The new stream data for Step 4 are presented in Table 2 and the corresponding GCC is presented in

Figure 2(d). The results are Q_{HU} = 0 kW, Q_{CU} = 463.2 kW, T'_{PI} = 453.6 K. Both compression and expansion have been implemented. The WHEN design is presented in Figure 1(b).

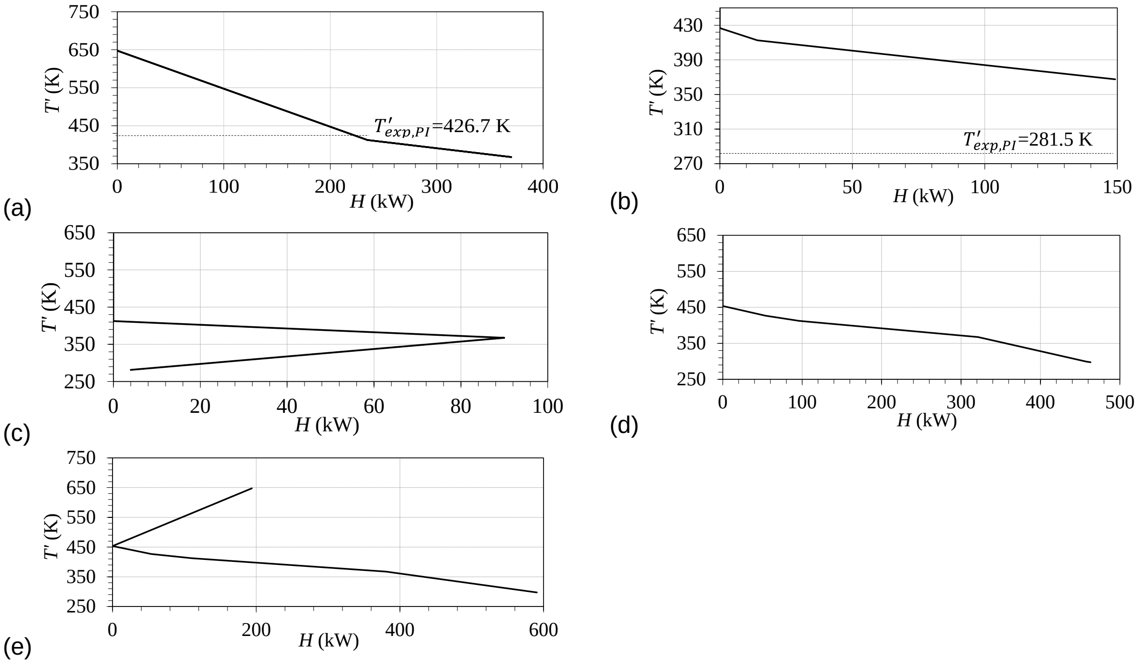

Figure 2: GCCs: (a) Step 1, (b) Step 2, (c) Step 3, (d) Step 4 in the graphical design, (e) alternative design

Table 2: Stream data for the graphical design procedure

Stream	T_s, K	T_t, K	mc_p, kW/K	ΔH, kW	p_s, MPa	p_t, MPa
Step 2						
H1	650	370	3	840	0.1	0.5
C1_α1	410	645	1	235	0.5	0.5
C1_α2	424.2	645	1	220.8	0.1	0.1
C1_β	410	645	1	235	0.5	0.1
Step 3						
H1	650	370	3	840	0.1	0.5
C1_α1	410	645	1	235	0.5	0.5
C1_α2	424.2	645	1	220.8	0.1	0.1
C1_β1	410	424.2	1	14.2	0.5	0.5
C1_β2	279	645	1	366	0.1	0.1
Step 4						
H1_1	650	300	3	1050	0.1	0.1
H1_2	456.1	370	3	258.3	0.5	0.5
C1_α1	410	645	1	235	0.5	0.5
C1_α2	424.2	645	1	220.8	0.1	0.1
C1_β1	410	451.1	1	41.1	0.5	0.5
C1_β2	296.7	645	1	348.3	0.1	0.1
Alternative design						
H1_1	650	300	3	1050	0.1	0.1
H1_2	456.1	370	3	258.3	0.5	0.5
C1_1	410	645	2	470	0.5	0.5
C1_2	424.2	645	2	441.6	0.1	0.1

The above design procedure aims to minimize exergy consumption and does not take cost into consideration. It is known that stream splitting increases the number of units and normally increases equipment cost. An alternative design is to eliminate the stream splitting. In this case, the entire stream C1 is expanded at the Pinch temperature 645 K (see Step 1 above), and stream H1 is compressed at T_{CU} = 300 K. The stream data are

presented in Table 2 and the GCC is presented in Figure 2(e). The results are Q_{HU} = 193.9 kW, Q_{CU} = 590.6 kW, T'_{PI} = 453.6 K. The WHEN design is presented in Figure 1(c). Compared to Onishi et al. (2018), C1 is expanded at a higher temperature and H1 is compressed at a lower temperature.
A comparison of the three designs is presented in Table 3. The exergy consumption for the design developed with the graphical procedure and the alternative design is much lower than the design from Onishi et al. (2018). Minimum exergy consumption is achieved by the graphical design procedure. However, one more expander is used. Following the estimation method presented in Onishi et al. (2018), a comparison of cost has also been performed, and the results are included in Table 3. The following annual utility cost data were used (in $/kW/y): electricity-850.51, HU-80, CU-20. Note that heat exchanger cost was excluded in Onishi et al. (2018) and is also excluded in this study. It can be found that both CAPEX and OPEX for the design in Onishi et al. (2018) are much higher than the values of the other two designs. A comparison of the results for the graphical design procedure and the alternative design is interesting in the sense that: (1) The CAPEX is almost the same for the two designs although stream splitting is avoided in the alternative design. The reason is that the equipment cost is simply correlated to the duty of the equipment. (2) The OPEX of the alternative design is even lower although the exergy consumption is higher. The reason is that the relative price between power and heat is much larger than the ratio between power and the exergy content of heat. The relative price between power and HU is 10.63. The exergy content of 1 kW HU is 0.559 kW. A relative price of less than 1.789 between power and HU is required if minimum exergy consumption is used as targeting e.g. in the graphical design procedure. According to the costing results, it is more valuable to focus on reducing power consumption than reducing heat consumption.

Table 3: Performance comparison

	Onishi et al. (2018)	The graphical design	Alternative design
Energy performance			
Compression power, kW	670.3	468.3	468.3
Expansion power, kW	416.4	375.2	441.6
Total power consumption, kW	253.9	93.1	26.7
HU consumption, kW	0	0	193.9
CU consumption, kW	623.9	463.1	590.6
Exergy consumption, kW	253.9	93.1	135.1
Number of compressors	1	1	1
Number of expanders	1	2	1
Cost performance			
CAPEX			
Compressor, k$-2017	660	532.3	532.3
Turbine α, k$-2017	89.6	53.6	94
Turbine β, k$-2017	0	40.1	0
Bare module factor	2	2	2
Total CAPEX, k$-2017	1,499.2	1,252.0	1,252.5
Annualized CAPEX, k$	388.9	324.7	324.9
OPEX			
Annual power cost, k$	216.0	79.2	22.7
Annual HU cost, k$	0	0	15.5
Annual CU cost, k$	12.5	9.3	11.8
Total annual OPEX, k$	228.5	88.5	50
Total annualized cost, k$	617.4	413.2	374.9

4. Discussion

The case study clearly illustrates that it is not an easy task to get optimal solutions using mathematical optimization models for WHEN design. This observation has also been found in other literature studies. When using Mathematical Programming to optimize Work and Heat Exchange Networks, there are three critical activities: (i) a sufficiently rich superstructure must be developed that includes the optimal topology, (ii) an efficient mathematical model must be developed based on the superstructure, and (iii) a robust solver must be selected or developed. Both process models and cost equations are non-convex, which means that it is extremely challenging to obtain the global rather than a local optimum. Future studies will include modeling approaches beyond Onishi et al. (2018), and the graphical design method will be compared with these mathematical optimization methods for selected case studies. The graphical design procedure based on thermodynamic insight can provide helpful guidelines for model development as well as the target for optimal solutions at least for small-size problems. Unfortunately, both approaches (graphical and mathematical) are under development and the two groups of methods have not yet been effectively combined.

5. Conclusions

Considerable progress has been achieved in both Pinch Analysis motivated graphical design procedures and mathematical optimization approaches for Work and Heat Exchange Network (WHEN) design. When solving non-linear and non-convex mathematical programming problems, despite significant progress in algorithms and solvers, identifying the global optimum is still a challenging task. A small case study illustrates that the graphical design procedure achieves better results in both energy consumption and cost than one of the published methods based on mathematical optimization. Thermodynamic insight and the graphical design approach can provide helpful guidelines for both mathematical model development and provide targets for the optimal solution. In contrast to the graphical design procedure, mathematical programming approaches can properly address the multiple trade-offs in WHEN design, and they can be used to solve industrial size problems. The two approaches are expected to be combined in the future.

Acknowledgements

The author Xiaoling Wang would like to acknowledge funding support by the Tianjin Municipal University Science and Technology Development Fund Project [Number 20140519].

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