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Enhanced Superstructure-based Model for Synthesis of Sub-ambient Heat Exchanger Networks with Expansion Process

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Work and heat are two significant forms of energy in chemical industries, and complex relationship exists in these strongly interacting properties (heat, work, temperature and pressure). Therefore, the research on the simultaneous integration of work and heat has a significant impact on the overall energy-efficiency improvement of the process. In this paper, a mixed-integer nonlinear programming (MINLP) model aiming at the minimum exergy consumption is formulated to obtain the optimal network configuration, which reveals the interactive mechanism between the expanders/valves placement and the heat exchanger networks synthesis. An enhanced stage-wise superstructure that involves pressure manipulation both in stages and between stages along with heat integration for each pressure-change sub-stream in stages is proposed in this paper. These sub-streams from one stream must concurrently perform pressure manipulation in the same stage and then return to their parent state at the end of the stage by adopting non-isothermal mixing. It is quite essential for the expanded streams to optimise the selection of end-heaters and end-coolers to meet their desired temperature targets. In addition, the multi-stream expansion problem can also be solved using the proposed method. A case study from the literature is used to demonstrate the proposed method. The results are consistent with the literature solutions. Moreover, the proposed method can successfully perform another case study with multi-stream expansion, which is not solved using the GCC-based graphical approach.

1. Introduction

The heat exchanger networks (HEN) and the work exchanger networks (WEN) are used for heat and work recovery, respectively. The temperature will be changed after compression and/or expansion, whilst the amount of work transfer should also be affected by temperature variation. Therefore, it is a challenging problem in the field of work and heat integration to optimise the compressor, expander and valve placement in HEN. Gundersen et al. (2009) proposed heuristic rules that both compression and expansion should start at the pinch temperature. Based on this, a set of thermodynamic viewpoints were provided to appropriately integrate compressors and/or expanders into HEN on the basis of the grand composite curves (GCC) aiming at the minimum exergy consumption (Fu and Gundersen, 2015b). Further, Fu et al. (2017) presented the novel insight on how to select the correct pinch temperature for compression/ expansion. The same group explored the potential application of the work and heat integration in the CO_2 capture process, in which the energy consumption of oxy-combustion process and post-combustion process was reduced by 10.1% and 12.9% respectively through the integration of expansion process and HEN (Fu and Gundersen, 2016).
In recent years, more research has been conducted on the integration of work and heat based on mathematical programming. Zhuang et al. (2017) proposed a step-wise method for direct WEN and HEN synthesis. Huang and Karimi (2016) proposed a more flexible and effective model for work and heat exchanger networks (WHEN) synthesis, considering constant-pressure streams for heat integration and performing an optimised selection of end-heaters and end-coolers for pressure-change streams. To address the issue of WHEN synthesis with thermal identity changes of process streams, Nair et al. (2018) proposed a generalized framework for integrating heat and work simultaneously based on the strategies that do not pre-classify streams identity. Currently，

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Onishi et al. (2018) introduced a new optimization model for work and heat integration without classified process streams in terms of mathematical programming model combined with pinch location method. However, the current mathematical model for work and heat integration considers HEN and WEN modules separately, which leads to local optimal solutions.

This paper presents an enhanced stage-wise superstructure that involves pressure manipulation both in stages and between stages along with HEN synthesis, to achieve the optimal coupling of heat integration and expansion equipment (expanders and valves) placement on the specified pressure-change sub-streams. In addition, the proposed method can optimise the selection of expanders/valves and successfully solve the problem of multi-stream expansion. Two case studies are conducted to illustrate the feasibility and efficacy of the proposed method.

2. Problem statement

The HEN synthesis with appropriate expansion equipment (expanders and valves) placement is achieved by coupling the expansion optimization and heat exchange identification for each sub-stream in an enhanced superstructure-based model aiming at minimum exergy consumption. Given a set of process streams with known supply state (pressure, temperature) and target state (pressure, temperature). In addition, heat capacity, temperature of heating and cooling utility and the minimum approach temperature (ΔT_{min}) are also known. This article only considers sub-ambient condition which the temperature of all streams is lower than the ambient temperature. The assumptions in Huang and Karimi (2016) are adopted in order to simplify the synthesis procedure.

3. Model formulations

3.1 Equations

The enhanced stage-wise superstructure that combines HEN synthesis with expansion optimization is based on the traditional HEN superstructure (Yee and Grossmann, 1990), which has been widely used in literature. Therefore, more details are mainly devoted to addressing model additions and modifications due to expansion manipulation. The overall energy balance for high-pressure streams ($i \in PH$) is expressed by Eq. (1), which contains the work produced by expanders before $\left(We_{i,j,k}^{before}\right)$ and after $\left(We_{i,j,k}^{after}\right)$ heat exchangers on each sub-stream.

$$\left(TIN_i - TOUT_i\right)F_i = \sum_{k \in KN}\sum_{j \in C} q_{ijk} + qcu_i + \sum_{k \in KN}\sum_{j \in C} We_{i,j,k}^{after} + \sum_{k \in KN}\sum_{j \in C} We_{i,j,k}^{before} - qhu_i, i \in PH \tag{1}$$

Eq. (2) represents the work produced by expanders before heat exchangers on each sub-stream, and the stream which expanded by valves do not produce any work. Similarly, the work formula after heat exchangers can also be derived that is not listed in this paper. The high-pressure streams may expand through expanders/valves or not expand at this stage, the corresponding heat capacity flowrates are $Fe_{H,i,j,k}^{before}, Fv_{H,i,j,k}^{before}, F_{H,i,j,k}^{before}$, so the relationship between the heat capacity flowrates of all sub-streams is shown in Eq. (3). Similarly, the sub-stream temperature and pressure can be calculated by Eqs. (4) and (5), $Pe_{i,j,k}^{before}, Pv_{i,j,k}^{before}$ $\left(te_{H,i,j,k}^{before}, tv_{H,i,j,k}^{before}\right)$ denote the outlet pressure (temperature) of expanders and valves. In addition, $yv_{ijk}^{before}, ye_{ijk}^{before}$ are binary variables to model the existence of valves and expanders before heat exchangers on each sub-stream.

$$We_{i,j,k}^{before} = Fe_{H,i,j,k}^{before} t_{i,k}\left[1 - \left(\frac{Pe_{i,j,k}^{before}}{P_{i,k}}\right)^{\frac{n_e - 1}{n_e}}\right], i \in PH, j \in C, k \in KN \tag{2}$$

$$F_{H,i,j,k} = Fv_{H,i,j,k}^{before} yv_{ijk}^{before} + Fe_{H,i,j,k}^{before} ye_{ijk}^{before} + F_{H,i,j,k}^{before}\left(1 - yv_{ijk}^{before} - ye_{ijk}^{before}\right), i \in PH, j \in C, k \in KN \tag{3}$$

$$P_{i,j,k} = Pv_{i,j,k}^{before} yv_{ijk}^{before} + Pe_{i,j,k}^{before} ye_{ijk}^{before} + P_{i,j,k}^{before}\left(1 - yv_{ijk}^{before} - ye_{ijk}^{before}\right), i \in PH, j \in C, k \in KN \tag{4}$$

$$t\,\mathrm{in}_{H,i,j,k} = te_{H,i,j,k}^{before} ye_{ijk}^{before} + tv_{H,i,j,k}^{before} yv_{ijk}^{before} + t_{i,k}\left(1 - ye_{ijk}^{before} - yv_{ijk}^{before}\right), i \in PH, j \in C, k \in KN \tag{5}$$

Eq. (6) represents the energy balance of the expanded stream in each stage.

$$\left(t_{i,k}-t_{i,k+1}\right)F_i=\sum_{j\in C}q_{i,j,k}+\sum_{j\in C}We_{i,j,k}^{before}+\sum_{j\in C}We_{i,j,k}^{after},i\in PH,k\in KN \tag{6}$$

Eqs. (7) and (8) are the relations for inlet $\left(t_{i,k}\right)$ and outlet temperature $\left(tv_{H,i,j,k}^{before},te_{H,i,j,k}^{before}\right)$ of the expanded stream through valves and expanders, respectively. Where, μ_s is the average Joule-Thomson coefficient.

$$tv_{H,i,j,k}^{before}=t_{i,k}+\mu_s\left(Pv_{i,j,k}^{before}-P_{i,k}\right),i\in PH,j\in C,k\in KN \tag{7}$$

$$te_{H,i,j,k}^{before}=t_{i,k}\left[\left(\frac{Pe_{i,j,k}^{before}}{P_{i,k}}\right)^{\frac{n_e-1}{n_e}}\right],i\in PH,j\in C,k\in KN \tag{8}$$

The thermal identity of pressure-change streams may change due to pressure manipulation, so the optimised selection of end-heaters and end-coolers should be performed to achieve the target temperature. It is expressed by Eq. (9), where, qcu_i,qhu_i are the amount of heat exchanged by end-cooler and end-heater, and Eq. (10) that the end-heater (zhu) and end-cooler (zcu) cannot exist simultaneously.

$$\left(t_{i,N_k+1}-TOUT_i\right)F_i=qcu_i-qhu_i,i\in PH \tag{9}$$

$$zhu_i+zcu_i\le 1,i\in PH \tag{10}$$

In addition, Eqs. (11) and (12) are added to the model to ensure single-stage expansion of streams.

$$ye_{ijk}^{after}+ye_{ijk}^{before}+yv_{ijk}^{after}+yv_{ijk}^{before}=ye_{ij'k}^{after}+ye_{ij'k}^{before}+yv_{ij'k}^{after}+yv_{ij'k}^{before},i\in PH,j\in C,j'\in C,k\in KN \tag{11}$$

$$\sum_{k\in KN}\left(ye_{ijk}^{after}+ye_{ijk}^{before}+yv_{ijk}^{after}+yv_{ijk}^{before}\right)=1,i\in PH,j\in C \tag{12}$$

This article aims at minimising exergy consumption (or maximizing exergy production) to trade-off two different qualities of energy (work and heat), because HEN synthesis and expansion optimization are considered simultaneously, as shown in Eq. (15). The relationship between expansion work as well as heating/cooling utility and exergy consumption is expressed by Eqs. (13) and (14). The temperature of heating utility is equal to the ambient temperature at sub-ambient condition, so the exergy content of heating utility is negligible.

$$E_W=\sum_{k\in KN}\sum_{j\in C}We_{i,j,k}^{before}+\sum_{k\in KN}\sum_{j\in C}We_{i,j,k}^{after},i\in PH \tag{13}$$

$$Eqcu=\sum_{i\in H}qcu_i\left(\frac{T_0}{T_{CU}}-1\right) \tag{14}$$

$$E=\min\left\{Eqcu-E_W\right\} \tag{15}$$

3.2 Enhanced stage-wise superstructure

Compared with the current mathematical model for work and heat integration exclusively performed in two distinct networks (HEN and WEN) (Huang and Karimi, 2016), an enhanced stage-wise superstructure is established that involves synchronous optimization of expansion equipment (expanders and valves) placement and heat integration for each pressure-change sub-stream in stages, as shown in Figure 1. The superstructure is established based on the following ideas:

(1) In each stage ($k\in KN$), the streams are split into a number of sub-streams equal to the number of possible heat exchange, and then the sub-streams return to their parent state at the end of the stage by adopting non-isothermal mixing.
(2) Note that the expander and valve in each sub-stream may exist before or after the heat exchanger. Expanders and valves for each sub-stream at the same stage cannot coexist. The pressure manipulation

devices in the stages can be merged into one under certain circumstances. Therefore, our proposed superstructure involves both intra-stage expansion and inter-stage expansion along with HEN synthesis.

(3) It is assumed that the sub-streams from one stream must concurrently perform pressure manipulation in the same stage to ensure the stability of the operation. Moreover, this paper only considers single stage expansion through expanders.

(4) The superstructure enables an optimised selection of end-heaters and end-coolers for the expanded streams to meet target temperatures, due to the fact that the thermal identity may change after expansion.

(5) Different from the HEN synthesis with compression process, the synthesis of sub-ambient HEN with expansion process considers the optimal selection of valves/expanders and makes the superstructure more complex, because both valves and expanders have an effect on pressure reduction. The difference is that the stream is expanded by the expander to generate work (power) and the temperature of the stream is decreased, while the temperature of the stream that undergoes expansion through valves is basically unchanged and the work (power) is completely lost.

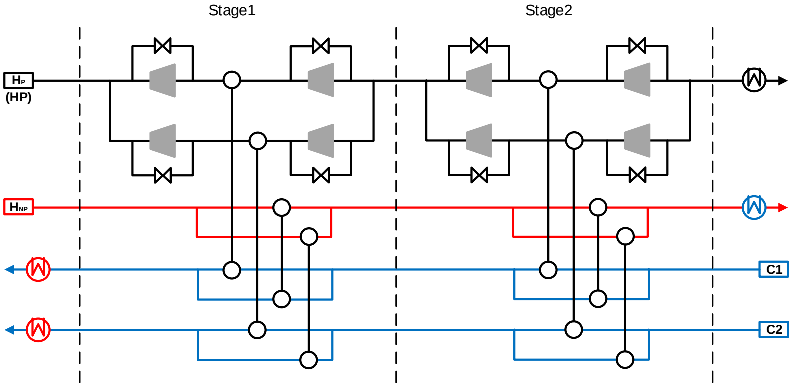

Figure 1: Stage-wise superstructure for Integrating expansion process into sub-ambient heat exchanger networks

4. Case studies

In this section, the feasibility and efficacy of the proposed method is illustrated by two case studies. Case study 1 is taken from Fu and Gundersen (2015a), and detailed stream data can be referred to the literature. The temperature of all streams is lower than ambient temperature and a hot stream H1 is expanded from 3bar to 1bar. The following assumptions are made: $\Delta T_{min}=4\ K$, ambient temperature $T_0=288\ K$, polytropic efficiency for expanders $\eta_{\infty,exp}=1$, specific heat ratio $\kappa=1.4$, the average Joule-Thomson coefficient $\mu_s=1.961\ K/MPa$, and heating and cooling utilities are 288 K and 120 K, respectively.

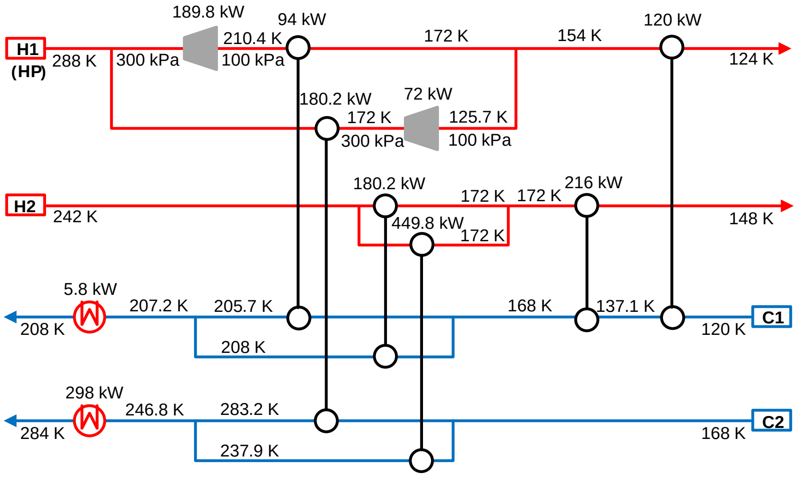

Figure 2: Optimal network configuration for case study 1

Figure 2 displays the optimal HEN configuration with appropriate expanders placement for case study 1. It is clear that two expanders are respectively expanded at different temperatures to minimise the exergy consumption.

The results obtained by the proposed mathematical programming method and the solutions obtained from the literature using the graphical approach are listed in Table 1. The amount of heating and cooling utility, expansion work and exergy consumption are close. In addition, the total number of devices and network configuration of the results obtained in this article are consistent with those obtained by Fu and Gundersen (2015a). The graphical design procedure to solve this problem is based on Grand Composite Curve (GCC), which has to undergo a tediously iterative solution process. However, our proposed enhanced superstructure-based model is more general and easier to derive optimal solutions in a reasonable CPU time which did not exceed 10 min. This case study fully proves the feasibility and superiority of our proposed method.

Table 1: Solution comparison of our model with those of Fu and Gundersen (2015a) for case study 1

Case	This work	Fu and Gundersen (2015a)
Exergy consumption, kW	-261.79	-261.3
Heating Utility demand, kW	303.8	303.6
Cooling Utility demand, kW	0	0
Expansion work, kW	261.79	261.3

Case study 2 contains two high-pressure streams (H1, H2) to illustrate the effective application of our model to cope with multi-stream expansion. The assumptions are the same as those in case study 1 and the detailed stream data is listed in Table 2.

Table 2: Stream data for case study 2

Stream	T_s (K)	T_t (K)	mc_p (kW·K^{-1})	p_s (kPa)	p_t (kPa)
H1	288	124	4	300	100
H2	288	154	3	500	100
H3	256	148	8	---	---
C1	120	213	7	---	---
C2	171	284	7	---	---

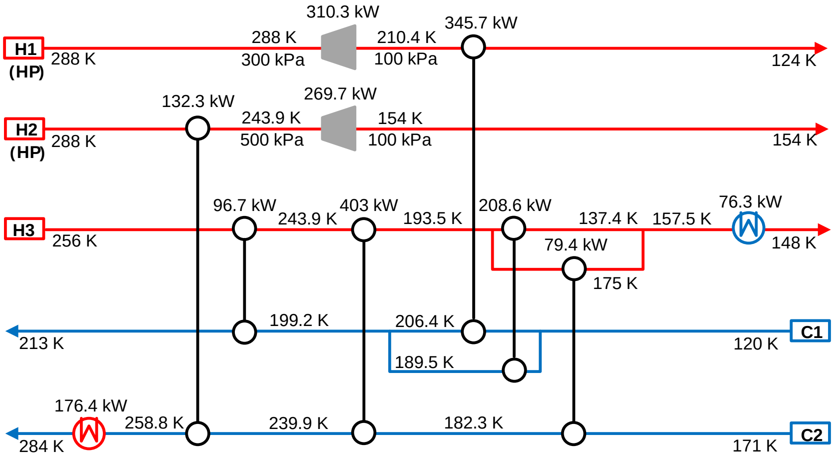

Figure 3: Optimal network configuration for case study 2

The optimal network configuration with the objective of minimising exergy consumption is shown in Figure 3. Both pressure-change streams are expanded by an expander. It can be seen from the figure that the stream may expand directly or expand after heat exchange, which reveals the different interactions between appropriate placement of expanders/valves and HEN design. The results of case study 2 calculated by the proposed mathematical programming method are listed in Table 3. As for the graphical approach proposed by Fu and Gundersen (2015a), it does not solve the multi-stream expansion problem. This is because the graphical approach should first find the pinch point and then determine the portion of pinch expansion by drawing the GCC in a tediously iterative manner. However, the pressure manipulation my change GCC shape and even generate multiple pinches, and thus the GCC needs to be redrawn. In other words, the pinch points are difficult to be determined during expansion optimization. In contrast, our model gives a more feasible network structure with better thermodynamic performances.

Table 3: Solution for case study 2

Case	This work
Exergy consumption, kW	-473.26
heating Utility demand, kW	176.4
Cooling Utility demand, kW	76.3
Expansion work, kW	580.07

5. Conclusions

In this article, a MINLP model aiming at the minimum exergy consumption is formulated to simultaneous optimization of expanders/valves placement and sub-ambient HEN synthesis based on an enhanced stage-wise superstructure. Heat exchangers and expansion equipment are simultaneously considered on the pressure-change sub-streams of the enhanced superstructure, which increases the diversity of the stream matching and is independent of rigorously determined thermodynamic route based on pinch location method. In case study 2, the proposed method successfully solves the problem of synchronous synthesis of multi-stream expansion and HEN design that cannot be solved by the graphical method and also surpasses the limitation that a graphical design approach is tediously iterative and can only cope with small-scale problems. Further, the synthesis of heat integration with expansion process considers the optimal selection of valves and expanders, because both valves and expanders have an effect on pressure reduction. However, the two case studies in this article do not reflect the use of the valve. The reason is that only thermodynamic analysis (minimum exergy consumption) is considered. When the pressure-change stream is expanded by the expander, it will generate work (power) and reduce exergy consumption, while the exergy of the stream that goes through valves is completely lost. However, when the economic analysis is considered, the valves may be needed, because the price of valves can be ignored compared with the expanders. Therefore, the comprehensive objectives including economic and environmental aspects should be investigated by using the presented methodology. This work is already in process.

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