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WORK AND HEAT EXCHANGER NETWORK SYNTHESIS: A NEW SUPERSTRUCTURE AND DEGREES OF FREEDOM ANALYSIS OF DERIVED MODEL

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Abstract – In the context of achieving higher efficiencies in industrial process, work and heat exchanger network (WHEN) can play an important role since it improves energy recovery. One way to make WHEN synthesis, which is a topic of current research interest, is via superstructure-based mathematical optimization. Although superstructure-based mathematical optimization has shown its value in WHEN synthesis in the past few years, its optimization results deeply depend on the quality of the superstructure and its derived model. Degrees of freedom analysis is an interesting technique to evaluate a model, quantify the number of decision variables to be manipulated and measure the size of the search space. In this work, we present a new superstructure and a new model for WHEN synthesis that incorporates the new concept of stream pseudo-identity and considering non-isothermal mixing to extend the search space. A degrees of freedom analysis is performed, and the model is compared to previous models reported in the literature.

Keywords: Superstructure; Work and heat network synthesis; Degrees of freedom analysis.

Introduction

In industrial processes, the seek for higher energy efficiencies, less environmental impacts, and lower costs led researchers to work increasingly in developing more effective process integration. Fu and Gundersen [1] defined process integration as a methodology that combines (i.e. integrates) process needs of opposite types, such as compression and expansion (in case of work integration), and heating and cooling (in case of heat integration). Once some process needs are satisfied with the recovery of process resources, less external supply is required; therefore, less usage of external energy, higher energy efficiency, less environmental impacts, and lower costs are obtained.

Heat and work are two forms of energy frequently available in industrial plants. Thus, work and heat integration (WHI) is deeply important in order to diminish process costs and it is achieved by means of a work and heat exchanger network (WHEN). This network is a set of heat exchangers, heaters, coolers, turbines, compressors, single-shaft-turbine-compressors (SSTCs) [2], valves, helper motors, and electric generators that are allocated in process streams so they exchange heat and work with each other as well as with hot and cold utilities, and by means of electricity to go from an initial state to a target one.

In the past few years, much progress has been achieved in WHEN synthesis using superstructure-based mathematical optimization [2-6]. Superstructure is a structure that contains different topology options for process synthesis and can guide the search for the best process structure. A superstructure may be formulated as a series of equal stages repeatedly. When that happens, it is called stage-wise superstructure. Chronologically, the first revolutionary publication regarding stage-wise superstructure was the one from Yee and Grossmann [7]. Tackling heat exchanger network (HEN) synthesis, they came up with a superstructure for mathematical optimization that led to interesting results. This superstructure consisted of dividing all process streams into K stages, in which each hot (cold) stream can exchange heat with every cold (hot) stream

parallelly. One major simplification of their model was isothermal mixing, which implies that every piece of a stream that exchanges heat in stage k must be at the same temperature when mixed. After stage K for hot streams one cooler is allocated in each stream to adjust to the final temperature. The same is true for a cold stream after stage 1 where a heater is allocated in each stream

Wechsung et al. [3] presented a stage-wise superstructure for WHEN synthesis in which there are fixed and variable pressure streams. The former can only exchange heat with other process streams or utilities. The latter is submitted to routes of possible compressions, expansions, heating, and cooling. A hot, variable pressure stream in a three-staged superstructure can be cooled, compressed, cooled, expanded, heated, compressed, and cooled. On the other hand, a cold, variable pressure stream can be heated, expanded, heated, compressed, cooled, expanded, and heated. This is illustrated in Fig. 1. Regarding pressure manipulator placement, those authors considered a heuristic rule in which inlet temperature for compression and expansion should be above and below the pinch, respectively; however, both pressure manipulations should preferably start at the pinch temperature.

Figure 1 – Superstructure for hot and cold, fixed and variable pressure streams [3].

Differently from above-mentioned authors, Razib et al. [2] proposed a multi-staged superstructure that classifies streams as high pressure (HP) and low pressure (LP). In each stage the former can be heated up (with hot utility) and then expanded and the latter can be cooled down (with cold utility) and then compressed (see Fig. 2-a). For each stage, after heating up, a HP stream can either expand parallelly (sub-streams) in a valve, in a utility turbine, or in several SSTCs, or by pass entirely (see Fig. 2-c). Clearly, all these sub-streams must have the same pressure to be merged after pressure manipulation, but they may have different temperatures. For a LP stream it is similar to the HP stream except that coolers replace heaters, compressors replace turbines, and no valve exists (see Fig. 2-b). After stage K_s , it does not matter a stream identity because a heater or a cooler is placed in the stream depending on its needs (decrease or increase temperature).

Figure 2 – Multi-staged superstructure [2]. a) multi-stage-one-stream superstructure. WEN superstructure for b) low-pressure stream, c) high-pressure stream.

Onishi et al. [4] developed a superstructure relying on fixed routes depending on streams identities, as in Wechsung et al. [3], but with some novelties. A major difference is that no heuristic rule is used for appropriate placement of pressure manipulators. In other words, the inlet temperature of a pressure manipulator does not rely on heuristic rules but is an unknown variable to be calculated. Therefore, the former pinch operator was substituted by the well-known superstructure of Yee and Grossman [7] for HEN. This is illustrated in Fig. 3 for one hot and one cold stream.

Figure 3 – Superstructure for one hot and one cold stream [4].

Huang and Karimi [5] based their stage-wise superstructure on Razib et al. [2]. The main difference between these two superstructures is that instead of having a cooler before compression units, a LP stream can be cooled exchanging heat with HP process streams as well as cold utility accordingly with Yee and Grossmann [7], see Fig. 4-c. Similarly, a HP process stream is treated as cold stream in a HEN superstructure [7] and then is directed to expansion units (see Fig. 4-b). A stream can also simply be hot or cold, with fixed pressure; therefore, only interacts with the problem in the HEN. Finally, their superstructure is composed by K_s stages of HEN + work exchanger network (WEN) and a final heater or cooler (see Fig. 4-a).

Figure 4 – Superstructure overview [5]. a) multi-stage-one-stream superstructure. WEN superstructure for b) high-pressure stream, c) low-pressure stream.

Nair et al. [6] introduced to the superstructure of Huang and Karimi [5] the very important idea of unclassified streams. This means that they did not pre-classify streams as neither hot or cold, nor stream with fixed or variable pressure. It allowed streams with no net pressure to change pressure in cycles. Also, it permitted streams to heat up or cool down before expanding or compressing, i.e. without a fixed logic like before

(heating + expanding or cooling + compressing). This superstructure is illustrated in Fig. 5.

Figure 5 – One-stream superstructure [6].

In the present paper, a new superstructure is proposed, and a new model for work and heat exchanger network synthesis, which contains more possible solutions than all above mentioned models, is derived. It is proposed the concept of pseudo-hot and pseudo-cold streams. This concept showed to be a powerful tool to deal with unclassified streams, and to allow for one stream in an intermediary temperature to supply and receive energy via heat transfer. Another improvement is the consideration of non-isothermal mixing that gives more freedom for the appropriated placement of heat exchangers.

Superstructure and Derived Model

Given a set of S streams ($s=1,2,...,S$) with known initial state ($Tin(s)$ & $Pin(s)$), and target state ($Tout(s)$ & $Pout(s)$), the main objective is to find a network of temperature and pressure manipulating devices, in a way that this network performs the above-mentioned state changes. For temperature changes, this model considers two-stream heat exchangers between process streams, heaters with hot utility, and coolers with cold utility. Likewise, for pressure changes, this model allows for SSTCs, valves, helper motors, and electric generators. The proposed superstructure is presented in Fig. 6.

As shown in Fig. 6, a stream s in a horizontal stage n can be initially divided into two: s,n -pseudo-hot and s,n -pseudo-cold streams. The former is treated as a hot stream in a HEN superstructure similar, but not equal, to the one of Yee and Grossmann [7] because isothermal mixing is not considered anymore. In other words, this stream can exchange heat with every pseudo-cold stream parallelly once for each stage $k \in [2, K-1]$. Also, in the last stage K , this stream can be cooled down in a cooler with cold utility. The latter is exactly the opposite from $k=K-1$ to $k=2$, and with a heater in $k=1$.

After leaving stage $k=K$ for pseudo-hot and $k=1$ for pseudo-cold stream, these two pseudo streams are mixed back together, which implies the model to compute mass and energy balances in this mixing point. Then, the stream s goes to the WEN, in which it can be expanded in a turbine, compressed in a compressor, expanded in a valve, or simply bypass these pressure change devices. All those temperature and pressure changes correspond to a complete horizontal stage n , which is repeated N_s-1 times.

Finally, the last horizontal stage $n=N_s$ allows only temperature manipulation, once the stream pressure must be already at its target value.

For simplicity, some assumptions are considered in conformity with previous works [2-6]:

- Steady-state operation;

- Every turbine and compressor are connected in a same shaft. A possible lack of work is supplied by a helper motor using electricity, or an excess of work is transformed into electricity in a generator;
- Compressions in compressors and expansions in turbines are isentropic;
- Expansions through valves are isenthalpic with a constant Joule-Thompson coefficient;
- All streams are considered ideal gases;
- Heat capacities and heat transfer coefficients are constant;
- Pressure drops and heat losses in thermal devices are neglected;

Figure 6 – Proposed superstructure for one stream.

Mathematical formulation

For clarity, the mathematical formulation was divided into 7 sections and the main equations are presented:

1) Mass and energy balance in pre-HEN stream splitter:

for $s \in [1, S]$, $n \in [1, N_s]$:

$$FH(s, n) = d(s, n) \cdot CP(s) \quad (1)$$

$$FC(s, n) = CP(s) - FH(s, n) \quad (2)$$

$$TH(s, n, k) = T(s, n) \quad 1 \leq k \leq 2 \quad (3)$$

$$TC(s, n, k) = T(s, n) \quad K - 1 \leq k \leq K \quad (4)$$

Given that $d(s, n)$ is the portion of the stream s in stage n that goes to s, n -pseudo-hot stream, it varies from 0 to 1. It is worth mentioning that for $n=1$, the value of $T(s, 1)$ and $P(s, 1)$ for every stream is equal to the value of initial state ($T_{in}(s)$ and $P_{in}(s)$). Also, when $n=N_s$, a stream is either hot or cold depending on if it needs to be cooled down or heated up. Then, $d(s, N_s)$ is either 1 (hot stream) or 0 (cold stream).

2) Mass and energy balance in stream splitters of each stage k of the HEN:

for $s \in [1, S]$, $ss \in [1, S]$, $n \in [1, N_s]$, $nn \in [1, N_s]$, $k \in [2, K - 1]$:

$$FH_{in}(s, n, ss, nn, k) = dh(s, n, ss, nn, k) \cdot FH(s, n) \quad (5)$$

$$FC_{in}(s, n, ss, nn, k) = dc(s, n, ss, nn, k) \cdot FC(ss, nn) \quad (6)$$

$$TH_{in}(s, n, ss, nn, k) = TH(s, n, k) \quad (7)$$

$$TC_{in}(s, n, ss, nn, K - k + 1) = TC(ss, nn, K - k) \quad (8)$$

Now, an important definition is the indexing (s,n,ss,nn,k) . It stands for the heat exchanger between s,n -pseudo-hot and ss,nn -pseudo-cold streams in stage k . Thus, $dh(s,n,ss,nn,k)$ is the portion of s,n -pseudo-hot stream ($FH(s,n)$) that exchanges heat with ss,nn -pseudo-cold stream in stage k . Similarly, $dc(s,n,ss,nn,k)$ is the portion of ss,nn -pseudo-cold stream ($FC(ss,nn)$) that exchanges heat with s,n -pseudo-hot stream in stage k .

3) Energy balance in heat exchanger between process streams:
for $s \in [1, S]$, $ss \in [1, S]$, $n \in [1, N_s]$, $nn \in [1, N_s]$, $k \in [2, K - 1]$:

$$THout(s, n, ss, nn, k) = THin(s, n, ss, nn, k) - \frac{y(s, n, ss, nn, k).Q(s, n, ss, nn, k)}{FHin(s, n, ss, nn, k)} \quad (9)$$

$$TCout(s, n, ss, nn, K - k + 1) = TCin(s, n, ss, nn, K - k + 1) + \frac{y(s, n, ss, nn, K - k + 1).Q(s, n, ss, nn, K - k + 1)}{FCin(s, n, ss, nn, K - k + 1)} \quad (10)$$

The binary variable $y(s, n, ss, nn, k)$ dictates whether the heat exchanger between s,n -pseudo-hot stream and ss,nn -pseudo-cold stream exists in stage k (1 if it exists or 0 if not).

4) Energy balance in mixer after each stage k :
for $s \in [1, S]$, $n \in [1, N_s]$, $k \in [2, K - 1]$:

$$TH(s, n, k) = TH(s, n, k - 1) - \frac{\sum_{ss=1}^S \sum_{nn=1}^{N_s} y(s, n, ss, nn, k-1).Q(s, n, ss, nn, k-1)}{FH(s, n)} \quad (11)$$

$$TC(s, n, K + 1 - k) = TC(s, n, K - k) + \frac{\sum_{ss=1}^S \sum_{nn=1}^{N_s} y(ss, nn, s, n, k).Q(ss, nn, s, n, k)}{FC(s, n)} \quad (12)$$

5) Energy balance in heat exchanger between process streams and utilities:
for $s \in [1, S]$, $n \in [1, N_s]$:

$$TH(s, n, K) = TH(s, n, K - 1) - \frac{y_w(s, n).Q_w(s, n)}{FH(s, n)} \quad (13)$$

$$TC(s, n, 0) = TC(s, n, 1) + \frac{y_s(s, n).Q_s(s, n)}{FC(s, n)} \quad (14)$$

Also, the binary variables $y_w(s, n)$ and $y_s(s, n)$ stand for the existence or not of coolers and heaters, respectively. In the horizontal stage $n=N_s$, the final temperature (*i.e.* target temperature) is known; therefore, instead of calculating TH and TC at this point, Q_w and Q_s are calculated.

6) Energy balance in mixers before WEN:
for $s \in [1, S]$, $n \in [1, N_s]$:

$$TI(s, n) = d(s, n).TH(s, n, K) + (1 - d(s, n)).TC(s, n, 0) \quad (15)$$

7) Energy balance due to pressure manipulation:
for $s \in [1, S]$, $n \in [1, N_s - 1]$:

$$T(s, n + 1) =$$

$$TI(s, n) + c(s, n). \frac{1}{\eta_c} \cdot \left(\left(\frac{P(s, n+1)}{P(s, n)} \right)^{1-\frac{1}{\kappa}} - 1 \right) + e(s, n). \eta_e \cdot \left(\left(\frac{P(s, n+1)}{P(s, n)} \right)^{1-\frac{1}{\kappa}} - 1 \right) + v(s, n). \mu_s (P(s, n + 1) - P(s, n)) \quad (16)$$

$$WC(s, n) = c(s, n).CP(s). (T(s, n + 1) - TI(s, n)) \quad (17)$$

$$WE(s, n) = e(s, n).CP(s). (TI(s, n) - T(s, n + 1)) \quad (18)$$

$$WM = h. \sum_{s=1}^S \sum_{n=1}^{N_s} (WC(s, n) - WE(s, n)) , \text{ if } (WM < 0), \text{ then: } h = 0 \quad (19)$$

$$WG = g. \sum_{s=1}^S \sum_{n=1}^{N_s} (WE(s, n) - WC(s, n)) , \text{ if } (WG < 0), \text{ then: } g = 0 \quad (20)$$

Now, 5 new binary variables are introduced. They are $c(s, n)$, $e(s, n)$, $v(s, n)$, h , and g that indicate whether there is a compressor, a turbine, a valve, a helper motor, or an electric generator, respectively. The energy of compression (WC), and energy of expansion (WE) are calculated based on ideal gas definition of no enthalpy change due to pressure variation, but only to temperature change. Additionally, if the SSTC presents a lack of energy, then a helper motor is placed ($h=1$) with work duty of WM . Oppositely,

if the SSTC presents an excess of energy, then an electric generator is placed ($g=I$) with work duty of WG .

Degrees of Freedom Analysis

In order to use a model in mathematical optimization, it is deeply recommended to make a degrees of freedom analysis, which is the difference between the number of unknown variables and the number of independent equations. This analysis is necessary to determine the flexibility for optimization, since some degree of freedom is required. Then, a degrees of freedom analysis of the proposed model follows:

- 1) Mass and energy balance in pre-HEN stream splitter:

Unknown variables (d, FH, FC, TH, TC): 5 for each $s \in [1, S], n \in [1, N_s - 1] = 5 \cdot S \cdot (N_s - 1)$.

Independent equations: 4 for each $s \in [1, S], n \in [1, N_s - 1] = 4 \cdot S \cdot (N_s - 1)$.

Degrees of freedom = $1 \cdot S \cdot (N_s - 1)$.

This result shows that whenever d, FH , or FC is assigned with values independently, the other 2 variables are totally defined. Consequently, either d, FH , or FC is a decision variable of a possible optimization. These degrees of freedom are due to the new concept of stream pseudo-identity that adds new possibilities to the superstructure when compared to previous works [2-6].

- 2) Mass and energy balances in stream splitters for all stages of HEN:

Unknown variables ($FH_{in}, FC_{in}, dh, dc, TH_{in}, TC_{in}$): 6 for each $s \in [1, S], n \in [1, N_s], ss \in [1, S], nn \in [1, N_s], k \in [2, K - 1] = 6 \cdot S^2 \cdot N_s^2 \cdot (K - 2)$.

Independent equations: 4 for each $s \in [1, S], n \in [1, N_s], ss \in [1, S], nn \in [1, N_s], k \in [2, K - 1] = 4 \cdot S^2 \cdot N_s^2 \cdot (K - 2)$.

Degrees of freedom = $2 \cdot S^2 \cdot N_s^2 \cdot (K - 2)$.

Here, it is not any pair of these unknown variables that can be chosen as decision variables. It must be those that appear in the equations that has degree of freedom (Eq. 5 and Eq. 6). Thus, one must be FH_{in} or dh , and the other FC_{in} or dc . These degrees of freedom are due to non-isothermal mixing, which also adds new possibilities to the superstructure compared to [2-6].

- 3) Energy balance in heat exchanger between process streams:

Unknown variables (TH_{out}, TC_{out}, y, Q): 4 for each $s \in [1, S], n \in [1, N_s], ss \in [1, S], nn \in [1, N_s], k \in [2, K - 1] = 4 \cdot S^2 \cdot N_s^2 \cdot (K - 2)$

Independent equations: 2 for each $s \in [1, S], n \in [1, N_s], ss \in [1, S], nn \in [1, N_s], k \in [2, K - 1] = 2 \cdot S^2 \cdot N_s^2 \cdot (K - 2)$.

Degrees of freedom = $2 \cdot S^2 \cdot N_s^2 \cdot (K - 2)$.

These degrees of freedom are also due to non-isothermal mixing.

- 4) Energy balance in mixer after each stage k :

Unknown variables (TH, TC): 2 for each $s \in [1, S], n \in [1, N_s] = 2 \cdot S \cdot N_s$

Independent equations: 2 for each $s \in [1, S], n \in [1, N_s] = 2 \cdot S \cdot N_s$

Degrees of freedom = 0

- 5) Energy balance in heat exchanger between process streams and utilities:

Unknown variables ($TH, TC, y_w, y_s, Q_w, Q_s$): 6 for each $s \in [1, S], n \in [1, N_s - 1] = 6 \cdot S \cdot (N_s - 1)$

Independent equations: 2 for each $s \in [1, S], n \in [1, N_s - 1] = 2 \cdot S \cdot (N_s - 1)$

Degrees of freedom = $4 \cdot S \cdot (N_s - 1)$

- 6) Energy balance in mixer before WEN:

Unknown variables (TI): 1 for each $s \in [1, S], n \in [1, N_s] = 1 \cdot S \cdot N_s$

Independent equations: 1 for each $s \in [1, S], n \in [1, N_s] = 1 \cdot S \cdot N_s$

Degrees of freedom = 0

- 7) Energy balance after pressure manipulation:

Unknown variables (T, c, e, v, P, WC, WE) : 7 for each $s \in [1, S]$, $n \in [1, N_s - 2] + 3$ for each $s \in [1, S] = 7.S.(N_s - 2) + 3.S$

Independent equations: 2 for each $s \in [1, S]$, $n \in [1, N_s - 1] = 3.S.(N_s - 1)$

Degrees of freedom = $4.S.(N_s - 2)$.

Finally, the total number of degrees of freedom is $9.S.(N_s-1) - 4.S + 4.S^2.N_s^2.(K-2)$. For a simple example of $S=4$, $N_s=3$, and $K=5$, its total degrees of freedom is 1784. Then, 1784 binary and continuous variables must be assigned with values for the problem to be computed. This number increases very fast, for example a problem with $S=5$, $N_s=4$, and $K=6$ has its total degrees of freedom of 6515.

Increasing degrees of freedom of a model means enlarging the search space of solutions. That leads to a two-sided analysis. On one hand, the superstructure covers more possible solutions, among which it may be included one with better evaluation function (usually total annualized cost) than all other solutions that were covered by previous superstructures. On the other hand, increasing the degrees of freedom of a model enlarges the mathematical problem and hinders finding the optimum solution.

Conclusion

The new model for WHEN synthesis allows for more possible solutions than previous ones [2-6]. A reason for that is regarding the new concept of stream pseudo-identity. This allows a stream to be treated partially as hot and partially as cold streams in the same stage n . Mathematically, this introduced $1.S.(N_s-1)$ degrees of freedom which can be fulfilled by a decision variable like $d(s,n)$. Another reason for increasing possible solution space was the non-isothermal mixing consideration. This introduced $4.S^2.N_s^2.(K-2)$ degrees of freedom that can be fulfilled by some decision variables like $dh(s,n,ss,nn,k)$, $dc(s,n,ss,nn,k)$, $y(s,n,ss,nn,k)$, and $Q(s,n,ss,nn,k)$. Finally, this model with increased degrees of freedom may lead to reveal a solution that was not considered in previous works, at the expense of making the mathematical problem larger.

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References

1. C. Fu, M. Viske, T. Gundersen. Work and heat integration: An emerging research area. *Energy*. 2018, 158, 796-806.
2. M.S. Razib, M.M.F. Hasan, I.A. Karimi. Preliminary synthesis of work exchange networks. *Computers and Chemical Engineering*. 2012, 37, 262-277.
3. A. Wechsung, A. Aspelund, T. Gundersen, P.I. Barton. Synthesis of heat exchanger networks at subambient conditions with compression and expansion of process streams. *AIChE Journal*. 2011, 57, 2090-2108.
4. V.C. Onishi, M.A.S.S. Ravagnani, J.A. Caballero. Simultaneous synthesis of heat exchanger networks with pressure recovery: Optimal integration between heat and work. *AIChE Journal*. 2014, 60, 893-908.
5. K. Huang, I.A. Karimi. Work-heat exchanger network synthesis (WHENS). *Energy*. 2016, 113, 1006 – 1017.
6. S.K. Nair, H.N. Rao, I.A. Karimi. Framework for work-heat exchange network synthesis (WHENS). *AIChE Journal*. 2018, 64, 2472-2485.
7. T.F. Yee, I.E. Grossmann. Simultaneous optimization models for heat integration-II. Heat exchanger network synthesis. *Computers and Chemical Engineering*. 1990, 14, 1165-1184.