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Modelling and Optimization of Multistream Heat Exchanger with Area Targeting

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In this work, a new multi-objective mixed integer nonlinear programming (MINLP) model based on Pinch Technology principles is presented. The proposed framework is able to simultaneously maximize the heat recovery, minimize the total heat exchange surface while guaranteeing the heat transfer feasibility. The formulation adopted for the heat integration problem significantly reduces the number of binary variables when dealing with variable temperatures and flowrates, thus enhancing the solution efficiency. The model is then augmented with the introduction of a novel approach for the total area estimation not requiring heavy disjunctions nor complex tailor-made algorithms. A study on the optimization of an air separation unit (ASU) is finally performed to show the potential and effectiveness of the proposed framework.

1. Introduction

The systematic application of Multistream Heat Exchangers (MHEXs) to recover heat among process streams, is widely documented in energy-intensive processes (Klemeš et al., 2015). Their compact structure and high recovery efficiency have made MHEXs unsurprisingly appealing for cryogenic applications including air separation plants and liquified natural gas productions among others. However, in spite of a successful industrial implementation, the development of a comprehensive, reliable and efficient model for such process units is still being investigated by many researchers. Hasan et al. (2009) adopted a superstructure approach where the system is assimilated to a two-streams Heat Exchanger Network (HEN), and the heat recovery is optimized by means of a MINLP model. Such approach can however result highly computational demanding, thus hindering the numerical efficiency of the method itself. Kamath et al. (2012) proposed a nonlinear programming (NLP) equation-oriented model based on the pinch location method proposed by Duran and Grossmann (1986), treating the system as a particular case of a HEN featuring no external utilities. Despite the merit of handling phase-changing streams, the method makes use of a smoothing approximation (Balakrishna and Biegler, 1992) to handle the 'max' operator, thereby introducing numerical inefficiencies. Moreover, the total heat exchange surface of the unit is not considered and nor is its impact in the total costs optimization. Finally, Watson et al. (2015) developed a nonlinear model for the design and simulation of MHEXs, allowing one to calculate up to three unknown variables. Their major contribution was the introduction of an algorithm able to embed the simultaneous estimation of the area in the system of equations, and they later broadened the scope of their work to embrace phase-changing streams (Watson and Barton, 2016). However, the final problem consists in solving a nonlinear system of equations, and no optimization is intended nor achieved. It is therefore clear that, despite the recent efforts, the modelling and optimization of MHEXs still face major challenges, and thus require further improvement. The aim of the present work is the development of a MINLP model for the optimization of counter current MHEXs, able to maximize the heat recovery and simultaneously minimize the total area for problems featuring variables stream data. A novel, simple and yet reliable method for the evaluation of the heat exchange surface is introduced and successfully

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implemented. Finally, the framework is tested on an industrial case study (ASU) to show also the ability of our model to handle phase changing streams when the inlet and outlet phases are known.

2. Methodology

The proposed approach for the modelling of MHEXs takes the form of an optimization problem based on the Pinch Analysis principles, and the system will be accordingly treated as an HEN not requiring any external utilities. In particular, the general framework for the Pinch location method with variable stream data presented by Duran and Grossmann (1986) is inherited and implemented using the Multi-M formulation by Hui (2014). The obtained model will be completed with a new approach for the estimation of the heat exchange surface.

2.1 Pinch location method

A Multi-M formulation is here used to tackle the optimization problem. Its name stems from the fact that, instead of a single Big-M parameter (Grossmann et al., 1998), different tailor-defined M parameters are used within each disjunctive constraint. The size of such parameters is therefore reduced if compared to the Big-M, with great benefits to the model's efficiency (Hui, 2014). In addition, the mutual position of two streams (above, below or overlapping) is defined solely considering their inlet temperatures, and since the use of binary variable is required whenever an overlapping is present, this definition allows considerably reducing their number, again enhancing the performance of the model (Hui, 1999). Having these aspects considered, the MHEXs model for heat recovery maximization and simultaneous area minimization takes the following form:

$$\max\ Q_{tot} = \sum_{i \in H} W_i \cdot Cp_i (T_i^{in} - T_i^{out}) \tag{1}$$

$$\min\ A_{tot} \tag{2}$$

s.t.

$$\sum_{i \in H} W_i \cdot Cp_i \left(T_i^{in} - T_i^{out}\right) = \sum_{j \in C} W_j \cdot Cp_j \left(T_j^{out} - T_j^{in}\right) \tag{3}$$

$$QSIA_k(x) - QSOA_k(x) \le 0 \quad \forall k \in ST \tag{4}$$

$$QSIA_k(x) = \sum_{j \in C} W_j \cdot Cp_j \left(T_{j,k}^{out} - T_{j,k}^{in}\right) \quad \forall k \in ST \tag{5}$$

$$QSOA_k(x) = \sum_{i \in H} W_i \cdot Cp_i \left(T_{i,k}^{in} - T_{i,k}^{out}\right) \quad \forall k \in ST \tag{6}$$

$$T_k^p = T_i^{in} \ \ if \ \ k = i \in H; \quad T_k^p = T_j^{in} + \Delta T_{min} \ \ if \ \ k = j \in C \tag{7}$$

$$T_{i,k}^{in} = T_i^{in} \quad \forall i \in H; \forall k \in ST \quad if \ \ 'i' \text{ above } 'k' \tag{8}$$

$$T_{i,k}^{in} = T_k^p \quad \forall i \in H; \forall k \in ST \quad if \ \ 'i' \text{ below } 'k' \tag{9}$$

$$T_{i,k}^{in} \le T_i^{in} + M_{i,k}\left(1 - Y_{i,k}\right) \quad \forall i \in H; \forall k \in ST \quad if \ \ 'i' \text{ overlaps } 'k' \tag{10}$$

$$T_{i,k}^{in} \le T_k^p + M_{i,k} Y_{i,k} \quad \forall i \in H; \forall k \in ST \quad if \ \ 'i' \text{ overlaps } 'k' \tag{11}$$

$$T_{i,k}^{out} \ge T_i^{out} \quad \forall i \in H; \forall k \in ST \tag{12}$$

$$T_{i,k}^{out} \ge T_k^P \quad \forall i \in H; \forall k \in ST \tag{13}$$

$$T_{j,k}^{in} = T_j^{in} \quad \forall j \in C; \forall k \in ST \quad if \ \ 'j' \text{ above } 'k' \tag{14}$$

$$T_{j,k}^{in} = T_k^p - \Delta T_{min} \quad \forall j \in C; \forall k \in ST \quad if \ \ 'j' \text{ below } 'k' \tag{15}$$

$$T_{j,k}^{in} \le T_j^{in} + M_{j,k}\left(1 - Y_{j,k}\right) \quad \forall j \in C; \forall k \in ST \quad if \ \ 'j' \text{ overlaps } 'k' \tag{16}$$

$$T_{j,k}^{in} \le T_k^p - \Delta T_{min} + M_{j,k} Y_{j,k} \quad \forall j \in C; \forall k \in ST \quad if \ \ 'j' \text{ overlaps } 'k' \tag{17}$$

$$T_{j,k}^{out} \ge T_j^{out} \quad \forall j \in C; \forall k \in ST \tag{18}$$

$$T_{j,k}^{out} \ge T_k^P - \Delta T_{min} \quad \forall j \in C; \forall k \in ST \tag{19}$$

$$h(x,w) = 0; \quad g(x,w) \le 0 \tag{20}$$

In the system of constraints presented above ST, H, C are the sets for all the process streams, the hot streams and the cold streams respectively, with k, i, and j being their respective indexes. W and Cp are the flowrates and specific heat capacities used to evaluate the heat content of the streams having T^{in}/T^{out} as inlet/outlet temperatures. Eq(3) represents the energy balance for the system in absence of external utilities, while Eq(5) and Eq(6) respectively evaluate the heat sink ($QSIA_k$) and source ($QSOA_k$) above the pinch candidate k using the definition of the so called "pseudo-temperatures" $T_{i,k}^{in}/T_{i,k}^{out}$ and $T_{j,k}^{in}/T_{j,k}^{out}$ in Eq(8) to Eq(19) (Hui, 2014). The variables $Y_{i,k}/Y_{j,k}$ present in these equations are binary variables used to identify the position of stream i/j with respect to the pinch candidate k, while $M_{i,k}/M_{j,k}$ correspond to the aforementioned M parameters, and are defined as in Hui (1999). Finally, Eq(20) describes other equality and inequality constraints possibly related to the process (e.g. material balances, governing equations, etc.). The set of equations Eq(3) to Eq(19) needs to be solved in order to maximize the energy recovery Q_{tot} at a fixed heat recovery approach temperature ΔT_{min}. For MHEXs, this coincides with the maximization of the heat content either of the hot (as shown here in Eq(1)) or the cold streams.

2.2 New approach for area targeting

The novel technique proposed in this section for the evaluation of the MHEX's surface, only requires the knowledge of the total heat exchanged across the system (Q_{tot}), of the heat recovery approach temperature (ΔT_{min}), and of the area comprised between the Balanced Composite Curves (A_{CC}) (Figure 1a). Once such quantities are known, the system is simplified and represented using an auxiliary trapezoid of area A_{CC} having ΔT_{min} as a smaller base and Q_{tot} as height, as shown in Figure 1b. It is then possible to calculate the larger base of the trapezoid (ΔT_{end}), which can be regarded as a mean final temperature difference for the simplified system. Finally, a logarithmic mean temperature difference can be calculated with ΔT_{min} and ΔT_{end}, and its value can be used for the estimation of the total area in case of known and constant overall heat transfer coefficient U.

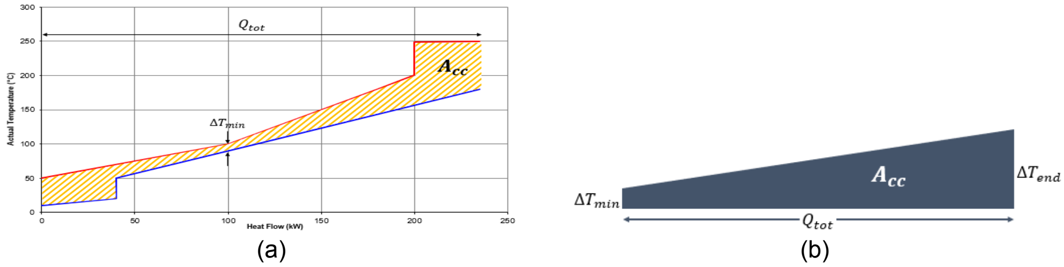
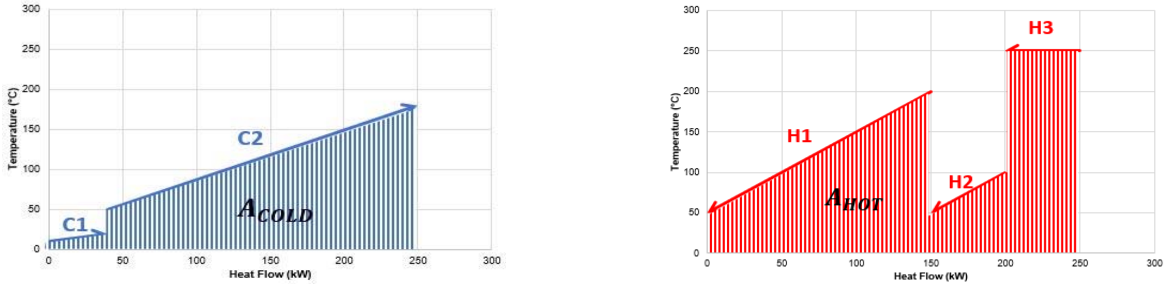


Figure 1: Graphical representation of the main parameters required for the area estimation (a), and auxiliary trapezoid for log mean temperature difference calculation (b).

The main difficulty within this framework is the estimation of the area enclosed in between the Balanced Composite Curves A_{CC}. However, it is possible to demonstrate that this area equals the difference of the areas lying below the individual hot (A_{HOT}) and cold (A_{COLD}) streams before their arrangement in the Composite Curves as stated in Eq(23). Using the same dataset as that of Figure 1a reported in Table 1, the corresponding A_{COLD} and A_{HOT} are shown in Figure 2a and 2b respectively.

Table 1: Dataset adopted in Figure 1a and Figure 2

Stream	Inlet T (°C)	Outlet T (°C)	W (kW/°C)
H1	200.0	50.0	1.0
H2	100.0	50.0	1.0
H3	250.0	249.0	50.0
C1	10.0	20.0	4.0
C2	50.0	180.0	1.615



(a) (b)

Figure 2: Area below cold (a) and hot (b) streams before their arrangement in the Composite Curves

$$A_{COLD} = \frac{1}{2}\sum_{j\in C} W_j \cdot Cp_j\left(T_j^{out^2} - T_j^{in^2}\right) \tag{21}$$

$$A_{HOT} = \frac{1}{2}\sum_{i\in H} W_i \cdot Cp_i\left(T_i^{in^2} - T_i^{out^2}\right) \tag{22}$$

$$A_{cc} = A_{HOT} - A_{COLD} \tag{23}$$

$$\Delta T_{end} = \frac{2 \cdot A_{cc}}{Q_{tot}} - \Delta T_{min} \tag{24}$$

$$\Delta T_{lm} = \left(\Delta T_{min}\Delta T_{end} \cdot \frac{\Delta T_{min} + \Delta T_{end}}{2}\right)^{\frac{1}{3}} \tag{25}$$

$$A_{tot} = \frac{Q_{tot}}{U \cdot \Delta T_{lm}} \tag{26}$$

Eq(21) and Eq(22) are necessary for the evaluation of the area of the graph lying below the individual cold and hot streams, represented by the coloured dashed area of Figure 2a and 2b. Moreover, since they involve the difference between square temperature's values, the adoption of Kelvin as unit of measurement is highly preferable, and it becomes necessary when dealing with temperatures lower than 0°C. Eq(24) represents the calculation of the larger base of the auxiliary trapezoid, needed to estimate the log mean ΔT in Eq(25). It is worth remarking that the expression of the ΔT_{lm} used in Eq(25) is an approximation introduced by Chen (1987) to prevent the result from being undefined when the two ΔT are equal. Furthermore, it yields a slightly lower value than the one obtained with the standard definition, thus making the estimation of the total area in Eq(26) more conservative. Eq(21) to Eq(26) can be easily implemented in the optimization procedure described in the previous paragraph. In this way, among all the feasible solutions able to guarantee the maximum heat recovery, it is possible to identify the one which ensures the minimization of the total surface.

3. Case study

The proposed model is tested on an industrial MHEX belonging to an air separation unit, whose simplified flowsheet is shown in Figure 3. The problem features three hot streams and three cold streams with variable stream temperatures and/or flowrates. On the other hand, the compositions and pressures of each stream are fixed, and the phase changes undergone across the MHEX are assumed to be known a priori. Labels 'g', 'm' and 'l' between brackets will be used to identify the gas, mixed and liquid phase of the streams respectively. Dew point and bubble points for phase-changing streams are calculated using the Soave-Redlich-Kwong (SRK) equation of state, while the heat capacities are estimated with the use of Aspen Plus® and are considered to be constant for each phase. The data for the proposed case study are reported in Table 2 along with the variables' boundaries. The problem is solved considering a minimum ΔT inside the MHEX of 3 K, a fixed air feed flowrate (P1) of 0.8 kmol/s and a constant overall heat transfer coefficient U of 1 kW/m^2K. The simulation was carried out in GAMS using BARON (Sahinidis, 1996) as the MINLP solver, with a computer featuring a 2.50 GHz Intel® Core™ i7-6500U Processor and 6 GB of RAM.

Table 2: Process streams' data for MHEX in Figure 1

Stream	Inlet T (K)	Outlet T (K)	W (kmol/s)	Cp (kJ/kmol·K)	P (kPa)	N_2 mol%	O_2 mol%
H1 (g)	293.15-303.15	100.57	0.05-0.30	30.51	610	78.85	21.15
H1 (m)	100.57	98.55	0.05-0.30	2536.20	610	78.85	21.15
H2 (g)	298.15	143.65-200.0	0.10-0.60	44.26	6,350	78.85	21.15
H2 (l)	143.65	95.0-110.0	0.10-0.60	73.40	6,350	78.85	21.15
H3 (g)	298.15	133.31-180.0	0.10-0.60	42.78	4,000	78.85	21.15
C1 (g)	102.48	102.48-298.15	0.04	31.94	590	65.27	34.73
C2 (g)	89.15	100.0-298.15	0.62	29.18	130	96.00	4.00
C3 (l)	80.0-100.0	168.40	0.14	70.01	8,500	1.00	99.00
C3 (g)	168.40	168.40-298.15	0.14	82.46	8,500	1.00	99.00

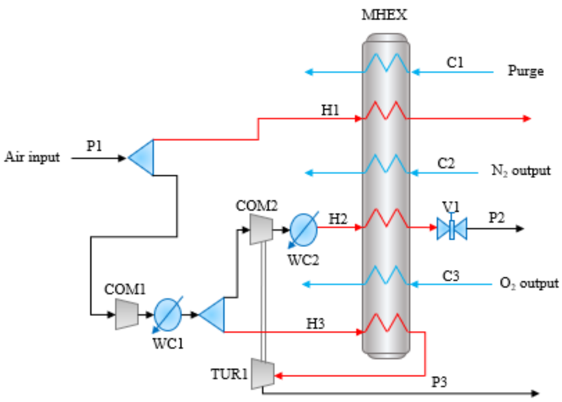


Figure 3: Simplified flowsheet for MHEX under study

Results for the case study are obtained in two different scenarios: (I) the heat recovery is maximized inside the MHEX without considering the contribution of the heat exchange surface; (II) having fixed the recovery to its maximum value, the problem is solved again to minimize the total area of the process unit. The main results and the performance of the models are reported in Tables 3 and 4, with the extensive solution being provided only for the second of the mentioned scenarios. The error ε reported in Table 3 represents the relative error with sign between the area estimated using the proposed approach, and the minimum area evaluated with the well-known framework proposed by Linnhoff and Ahmad (1990):

$$\epsilon = \frac{A_{tot} - A_{min}}{A_{min}} \cdot 100 \quad (27)$$

Table 3: Final results and performance of the model

Case	Recovery (kW)	Atot (m^2)	Amin (m^2)	ε	CPU time (s)	N° of Eq	N° of Var	N° of Bin Var
I	6,312.385	781.233	750.038	4.16%	17.532	294	226	8
II	6,312.385	724.431	730.780	-0.87%	25.106	298	230	8

Table 4: Complete results for the case study (II)

Stream	Inlet T (K)	Outlet T (K)	W (kmol/s)
H1 (g)	303.15	100.57	0.063
H1 (m)	100.57	98.55	0.063
H2 (g)	298.15	143.65	0.186
H2 (l)	143.65	110.0	0.186
H3 (g)	298.15	134.069	0.551
C1 (g)	102.48	295.463	0.04
C2 (g)	89.15	295.463	0.62
C3 (l)	80.0	168.40	0.14
C3 (g)	168.40	295.463	0.14

4. Results and discussion

In this work, a novel approach for the modelling and optimization of MHEXs with variable stream data has been introduced. This new method is based on the Multi-M formulation for heat integration problems proposed by Hui (2014) and it has been successfully implemented for the optimization of an industrial MHEX. Moreover, an original area targeting method has been developed and embedded within the optimization framework, for the minimization of the total surface. The maximum heat recovery for the system was found to be equal to 6312.385 kW. Including the simultaneous minimization of the total surface, the minimum heat transfer area is reduced from 750.04 to 730.78 m^2, thus leading to lower capital investments. The heat recovery problem featuring 294 equations and 226 variables was solved in less than 20 seconds whereas the area minimization, with 4 equations and 4 variables more, just took few seconds longer. In addition, the use of an appropriate thermodynamic package allows the modelling of phase changing streams when the phases are known a priori at the inlet and outlet sections of the unit. This is accomplished by splitting the stream into sub-streams (one for every phase traversed) each with constant heat capacity. Future studies will focus on broadening the scope of the proposed framework to embrace the modelling of unclassified and isothermal process streams.

5. Conclusions

A challenging case study has been tackled to prove the effectiveness of the overall framework. Not only it is worth remarking that the number of binary variables in the model is very small (just 8), but also that the proposed method for the area estimation does not require the introduction of any others, with great benefits to the model's numerical performance. Despite its simplicity, this new approach has proved to be highly reliable, with small values of the percentage error for both the scenarios (4.16 % and - 0.87 %), and given its complete novelty, a great deal of room is present for further improvement. It is finally evident how the proposed methodology could lead to important savings in both the energy and capital expenses of an industrial plant.

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