Disjunctive Model for the Simultaneous Optimization and Heat Integration with Unclassified Streams and Area Estimation

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Abstract

In this paper, we propose a disjunctive formulation for the simultaneous chemical process optimization and heat integration with unclassified process streams –streams that cannot be classified a priori as hot or cold streams and whose final classification depend on the process operating conditions–, variable inlet and outlet temperatures, variable flow rates, isothermal process streams, and the possibility of using different utilities. The model is based on the original formulation of the Pinch Location Method (PLM), but in this case, the 'max' operators are represented by means of a disjunction.

The paper also presents an extension to allow area estimation assuming vertical heat transfer. The model takes advantage of the disjunctive formulation of the 'max' operator to explicitly determine all the 'kink' points on the hot and cold balanced composite curves and uses an implicit ordering for determining adjacent points in the balanced composite curves for area estimation.

The numerical performance of the proposed approach is illustrated with four case studies. Results show that the novel disjunctive model of the pinch location method has an excellent numerical performance, even in large-scale models.

Keywords: simultaneous optimization, heat integration, variable temperatures, disjunctive model, unclassified streams.

Nomenclature

1. Introduction

One of the greatest advances in chemical process engineering was the discovery by Hohmann (1971) in his PhD thesis that it is possible to calculate the least amount of hot and cold utilities required for a process without knowing the heat exchanger network. This advance motivated the introduction of the pinch concept (Bodo Linnhoff & Flower, 1978a, 1978b; Umeda et al., 1978) and the Pinch Design Method (B. Linnhoff & Hindmarsh, 1983), for the design of heat exchanger networks (HEN). Since that, seminal works has been published thousands of papers related to heat integration.

Without the intention of doing a comprehensive review, significant advances were developed in the decades of 1980-90 of the last century. Papoulias and Grossmann (1983) presented a mathematical programming that takes the form of a transshipment problem that allows calculating the minimum utilities and the minimum number of matches (an alternative version that used a transportation model was presented by Cerda et al. (1983). The first one to use the vertical heat transfer concept that allows estimating the heat transfer area without knowing the explicit design of a heat exchanger network was Jones in 1987 (Jones, 1987). The first automated HEN design, relying on a sequential approach –minimum utilities calculation, followed by a minimum number of heat exchangers and then the detailed network– was developed by Floudas et al. (1986). Later, Ciric and Floudas (1991), Floudas and Ciric (1989, 1990), Yee and Grossmann (1990), and Yuan et al. (1989) proposed different alternatives for the simultaneous design of the HEN, all of them based on mathematical programming approaches. Comprehensive reviews of the advances in HEN in the 20th century can be found in Gundersen and Naess (1988), Jezowski (1994a, 1994b), and Furman and Sahinidis (2002). More recent reviews can be found in Morar and Agachi (2010) and Klemeš and Kravanja (2013).

Pinch analysis has extended to almost all branches of chemical process engineering, for example, Ahmetović presented a review of the literature for water and energy integration (Ahmetović et al., 2015; Ahmetović & Kravanja, 2013). In El-Halwagi (2012) we can find the extension of the pinch analysis to mass exchange networks and process integration. Tan and Foo (2007) extended the pinch analysis to carbon-constrained energy sector planning. The cogeneration and total site integration can be found in Raissi (1994) and Dhole and Linnhoff (1993). Wechsung et al. (2011) and Onishi et al. (2014b) introduced the concept of work exchanger networks and the integration of work and heat exchanger networks (WHEN).

One of the major limitations of the pinch technology applied to the design of heat exchanger networks is that it had to be used once the chemical process has already been designed and all the flows and temperatures fixed. However, the simultaneous design and optimization of the process and the heat integration strategy could eventually produce larger benefits than a sequential approach (Biegler et al. (1997) presented an illustrative example).

In a mathematical programming-based approach for the design of chemical processes, one straightforward possibility to overcome this problem consists of extending the superstructure of the process with that of the heat exchanger network. Nevertheless, the problem rapidly becomes intractable due to the large number of variables (both continuous and integer) and equations. Despite this problem, different researchers have solved relatively complex problems following this approach (de la Cruz et al., 2014; Martelli et al.; Oliva et al., 2011; Onishi et al., 2014a; Vázquez-Ojeda et al., 2013; Yee et al., 1990). To alleviate that problem, an alternative consists of considering only the thermal effects (heat integration) without the design of a specific network; in other words, including in the optimization only the utilities and their nature (e.g., low, medium or high pressure steam) but not the investment costs in the heat exchangers network. The underlying idea is that energy costs have much larger impact than investment costs and could have an important effect when optimizing with the rest of the process. However, differences in the investment of two heat exchanger networks with similar utilities and the same streams involved are not expected to be significant at least when compares with the energy effects.

Under some conditions, it is possible to solve the Pinch Tableau problem at each iteration of the optimization or explicitly include in the model the equations of the transshipment (or extended transshipment) problem (Corbetta et al., 2016). For example, some of the superstructure-based approaches for the design of chemical processes include those equations as a part of the model (Ciric & Floudas, 1991). However, this approach relies on the concept of temperature interval. While the temperature intervals are maintained in all the optimization, this is likely the best alternative for dealing with the simultaneous optimization and heat integration problem, but if inlet (outlet) temperatures can change, the number of temperature intervals and the streams present in each interval change during the optimization. Mathematically this is equivalent to introduce discontinuities and non-differentiabilities, and consequently, the complete optimization can fail.

To overcome the previous problem Duran and Grossmann developed the Pinch Location Method (PLM) (Duran & Grossmann, 1986). The idea was to develop a mathematical approach that does not rely on the concept of temperature interval and, as a consequence, does not suffer from the drawbacks of previous approaches. The major drawback of the original model presented by Duran and Grossmann (1986) is that in their model appear the «max» operator. They proposed to use a smooth approximation. However, the smooth approximation is non-convex and its numerical behavior depends on parameters in the approximation function.

To avoid the non-differentiability introduced in the model of Duran and Grossmann (1986), several approaches have employed binary variables to locate pinch temperatures. In fact, Grossmann et al. (1998) presented a disjunctive formulation that explicitly takes into account the location of a stream –above, across or below– potential pinch candidate. Navarro-Amorós et al. (2013) presented an alternative MI(N)LP model that uses the concept of temperature intervals and the transshipment problem for heat integration with variable temperatures. Quirante et al. (2017) proposed a novel disjunctive model for the simultaneous optimization and heat integration of systems with variable inlet and outlet temperatures, based on the formulation of the pinch location method, modeling the 'max' operators by means of a disjunction. Kong et al. (2017) proposed an extension of the Navarro-Amorós et al. (2013) model for the simultaneous chemical process synthesis and heat integration considering also unclassified process streams.

A common situation that appears when the temperatures are not fixed is that a priori it is not possible to decide if a process stream is a hot (it requires cooling) or a cold (it requires heating) stream (Kong et al., 2017). The objective of this paper is to extend the research made in our last work (Quirante et al., 2017) to the case in which there are unclassified process streams. The proposed model has the advantage of reducing the number of equations and binary variables compared to existing alternatives, which allows to reduce the CPU time when solving the problems.

Besides, in a chemical process, usually more than a single hot and/or cold utility are present and it is important to deal with the selection of the best set of utilities among all those available, and some streams can suffer phase changes. In this paper, we will show how we can extend the pinch location method to deal with all these cases.

A drawback of the PLM is that we ignore the contribution of the area to the total cost of the heat exchanger network. Even though in most situations this is not a major problem because, as commented above, the effect of the area can be ignored without affecting to the final solution, this is not necessarily always the case. We will show that for problems of medium size it is possible to simultaneously estimate the area of the HEN and consequently its investment cost.

The rest of the paper is structured as follows. In the two following sections, we present an overview of the pinch location method. Then, we present the disjunctive model for solving problems with unclassified streams and the extension to isothermal process streams and multiple utilities. In section 4, we present how it is possible to include area estimation in the model using the vertical heat transfer problem. In section 5, we present some case studies to illustrate the performance of the proposed approach. Finally, we provide some conclusions obtained from this work.

2. The Pinch Location Method. Overview

In a system in which all the heat flows are constant, the pinch point is always in the inlet temperature of some of the process streams. Duran and Grossmann (1986) showed that for a fixed minimum approach temperature (ΔT_{min}) between the hot and cold composite curves, if we systematically calculate all the hot and cold utilities for all the pinch candidates (all the inlet temperatures of the process streams), the correct answer corresponds to the candidate with the largest heating and cooling utilities. Mathematically this result can be written as follows:

$$Q_H = \max_{p \in STR}(Q_H^p); \quad Q_C = \max_{p \in STR}(Q_C^p); \tag{1}$$

where *STR* is a set of all the process streams that are pinch candidates. Q_H, Q_C are the heating and cooling utilities for a given ΔT_{min} and Q_H^p, Q_C^p are the heating and cooling utilities for each one of the pinch candidates *p*.

In order to take into account that the hot and cold composite curves must be separated at least by the minimum approach temperature, we must work with shifted temperatures.

Defining the following index sets:

$HOT =$ [i | i is a hot stream] $\left(HOT \subseteq STR\right)$

$COLD =$ [j | j is a cold stream] $\left(COLD \subseteq STR\right)$

The shifted temperatures can be defined as follows:

$$\left.\begin{aligned} TS_i^{in} &= T_i^{in} - \frac{\Delta T_{\min}}{2} \\ TS_i^{out} &= T_i^{out} - \frac{\Delta T_{\min}}{2} \end{aligned}\right\} i \in HOT$$
$$\left.\begin{aligned} ts_j^{in} &= t_j^{in} + \frac{\Delta T_{\min}}{2} \\ ts_j^{out} &= t_j^{out} + \frac{\Delta T_{\min}}{2} \end{aligned}\right\} j \in COLD \tag{2}$$

where T_i^{in}, T_i^{out}, t_j^{in}, t_j^{out} are the actual inlet and outlet stream process temperatures.

From a total heat balance, we obtain the following equation:

$$Q_C = Q_H + \sum_{i \in Hot} F_i\left(T_i^{in} - T_i^{out}\right) - \sum_{j \in Cold} f_j\left(t_j^{out} - t_j^{in}\right) \tag{3}$$

where F_i is the heat capacity flowrate of the hot stream *i* and f_j is the heat capacity flowrate of the cold stream *j*.

Taking into account that the pinch point divides the problem into two heat balanced parts, to calculate the hot utility requirements we need to study only the streams above the pinch and the cold utilities can be calculated from the energy balance presented in Eq.(3) or vice versa, we can calculate the cold utilities from the energy content of the streams below the pinch and the hot utilities from the energy balance.

The problem consists of determining the energy content of the streams above (below) the pinch for each of the pinch candidates. To that end, Duran and Grossmann (1986) showed that it is necessary to explicitly take into account the following three situations: The stream is above the pinch, crosses the pinch or it is below the pinch. For the case in which we study the situations of the streams below the pinch for each pinch candidate, the following equation captures the three situations:

$$\begin{aligned} Q_C^p = & \sum_{j \in COLD} f_j \left[\max\left(0,\, T^p - ts_j^{out}\right) - \max\left(0,\, T^p - ts_j^{in}\right) \right] - \\ & \sum_{i \in HOT} F_i \left[\max\left(0,\, T^p - TS_i^{in}\right) - \max\left(0,\, T^p - TS_i^{out}\right) \right] \qquad \forall p \in STR \end{aligned} \tag{4}$$

where T^p is the shifted inlet temperature of all the streams.

$$T^p \begin{Bmatrix} T_i^{in} - \dfrac{\Delta T_{\min}}{2} & \textit{if } p \textit{ is a hot stream } i \\ t_j^{in} + \dfrac{\Delta T_{\min}}{2} & \textit{if } p \textit{ is a cold stream } j \end{Bmatrix} \tag{5}$$

Therefore, the simultaneous optimization and heat integration model can be written as follows:

$$\begin{aligned} & \min\ f(x) + C_H Q_H + C_C Q_C \\ & s.t.\ h(x) = 0 \\ & \quad g(x) \le 0 \\ & \quad Q_C \ge \sum_{j \in Cold} f_j \left[\max\left(0, T^p - ts_j^{out}\right) - \max\left(0, T^p - ts_j^{in}\right) \right] - \\ & \qquad \sum_{i \in Hot} F_i \left[\max\left(0,\, T^p - TS_i^{in}\right) - \max\left(0,\, T^p - TS_i^{out}\right) \right] \qquad p \in STR \\ & \quad Q_C = Q_H + \sum_{i \in Hot} F_i \left(T_i^{in} - T_i^{out}\right) - \sum_{j \in Cold} f_j \left(t_j^{out} - t_j^{in}\right) \\ & \quad Q_C,\ Q_H,\ F_i,\ f_j \ge 0 \end{aligned} \tag{6}$$

where *f(x)* refers to the effects of the rest of the process (everything but heat integration) in the objective function, *h(x)* is the set of equations defining the process, *g(x)* are constraints added to the process.

3. The Pinch Location Method with Unclassified Process Streams

In this section, we present a disjunctive model for the simultaneous optimization and heat integration that also takes into account the possibility of including unclassified process streams. These streams could behave as hot or cold streams depending on the operating conditions of the rest of the process and, therefore, cannot be classified *a priori*. The model is based on the pinch location in which the 'max' operators are replaced by disjunctions following the procedure presented by Quirante et al. (2017).

To formally introduce the model let us define the following index sets:

STR = [s | s is a process stream]
HOT = [i | i is a hot stream] $\left(HOT \subseteq STR\right)$
$COLD$ = [j | j is a cold stream] $\left(COLD \subseteq STR\right)$
UNC = [k | k is an unclassified stream] $\left(UNC \subseteq STR\right)$

Note that $HOT \cup COLD \cup UNC = STR$

Classification constrains

Here we follow the approach presented by Kong et al. (2017).

$$\begin{aligned} & T_s^{in} - T_s^{out} = T_s^{+} - T_s^{-} \qquad s \in STR \\ & T_s^{-} = 0 \qquad \forall s \in HOT \\ & T_s^{+} = 0 \qquad \forall s \in COLD \end{aligned} \tag{7}$$

In Eq.(7), we have introduced the variables T_s^{+}, T_s^{-}. The first one (T_s^{+}) will take a positive value for hot streams, and the second one (T_s^{-}) for the cold streams. The correct classification of the unclassified streams can be forced by the following disjunction:

$$\begin{bmatrix} WH_k \\ T_k^{+} \geq 0 \\ T_k^{-} = 0 \end{bmatrix} \veebar \begin{bmatrix} WC_s \\ T_k^{-} \geq 0 \\ T_k^{+} = 0 \end{bmatrix} \quad \forall k \in UNC \tag{8}$$

where *WH* and *WC* are Boolean variables that take the value of "True" if the stream '*k*' is classified as hot or cold respectively. This disjunction can be reformulated in terms of binary variables using the hull reformulation (Trespalacios & Grossmann, 2014):

$$\left.\begin{array}{l} wh_k + wc_k = 1 \\ T_k^+ \le \overline{T_k^+} \cdot wh_k \\ T_k^- \le \overline{T_k^-} \cdot wc_k \end{array}\right\} \quad \forall k \in UNC \qquad (9)$$

where *wh* and *wc* are now binary variables that take the value 1 if the stream is classified as hot or cold respectively, and 0 otherwise.

Definition of shifted temperatures

For the hot and cold streams, shifted temperatures are equivalent to those presented above Eq.(2) (we rewrite them here for the sake of clarity):

$$\begin{array}{l} \left.\begin{array}{l} TS_i^{in} = T_i^{in} - \dfrac{\Delta T_{\min}}{2} \\ TS_i^{out} = T_i^{out} - \dfrac{\Delta T_{\min}}{2} \end{array}\right\} \ \mathrm{i} \in HOT \\ \left.\begin{array}{l} TS_j^{in} = t_j^{in} + \dfrac{\Delta T_{\min}}{2} \\ TS_j^{out} = t_j^{out} + \dfrac{\Delta T_{\min}}{2} \end{array}\right\} \ \mathrm{j} \in COLD \end{array} \qquad (10)$$

The correct displacement of the unclassified streams can be forced with the following disjunction:

$$\begin{bmatrix} WH_k \\ TS_k^{in} = T_k^{in} - \dfrac{\Delta T_{\min}}{2} \\ TS_k^{out} = T_k^{out} - \dfrac{\Delta T_{\min}}{2} \end{bmatrix} \veebar \begin{bmatrix} WC_k \\ TS_k^{in} = T_k^{in} + \dfrac{\Delta T_{\min}}{2} \\ TS_k^{out} = T_k^{out} + \dfrac{\Delta T_{\min}}{2} \end{bmatrix} \quad \forall k \in UNC \qquad (11)$$

The previous disjunction can be written in terms of binary variables using the hull reformulation as follows:

$$\left.\begin{array}{ll} \multicolumn{2}{c}{wh_k + wc_k = 1} \\ TS_k^{in} = TS_{H,k}^{in} + TS_{C,k}^{in} & TS_k^{out} = TS_{H,k}^{out} + TS_{C,k}^{out} \\ T_k^{in} = T_{H,k}^{in} + T_{C,k}^{in} & T_k^{out} = T_{H,k}^{out} + T_{C,k}^{out} \\ TS_{H,k}^{in} = T_{H,k}^{in} - \dfrac{\Delta T_{\min}}{2} wh_k & TS_{H,k}^{out} = T_{H,k}^{out} - \dfrac{\Delta T_{\min}}{2} wh_k \\ TS_{C,k}^{in} = T_{C,k}^{in} + \dfrac{\Delta T_{\min}}{2} wc_k & TS_{C,k}^{out} = T_{C,k}^{out} + \dfrac{\Delta T_{\min}}{2} wc_k \\ T_{H,k}^{in} \le \overline{T_{H,k}^{in}} \cdot wh_k & T_{H,k}^{out} \le \overline{T_{H,k}^{out}} \cdot wh_k \\ TS_{H,k}^{in} \le \overline{TS_{H,k}^{in}} \cdot wh_k & TS_{H,k}^{out} \le \overline{TS_{H,k}^{out}} \cdot wh_k \\ T_{C,k}^{in} \le \overline{T_{C,k}^{in}} \cdot wc_k & T_{C,k}^{out} \le \overline{T_{C,k}^{out}} \cdot wc_k \\ TS_{C,k}^{in} \le \overline{TS_{C,k}^{in}} \cdot wc_k & TS_{C,k}^{out} \le \overline{TS_{k}^{out}} \cdot wc_k \end{array}\right\} \quad \forall k \in UNC \qquad (12)$$

The new variables $TS_{H,k}^{in}$, $TS_{C,k}^{in}$, $TS_{H,k}^{out}$, $TS_{C,k}^{out}$, $T_{H,k}^{in}$, $T_{C,k}^{in}$, $T_{H,k}^{out}$, $T_{C,k}^{out}$ in Eq.(12) correspond to the disaggregated variables needed in the hull reformulation.

Pinch Candidates

$$T^p = TS_p^{in} \qquad p \in STR \tag{13}$$

As previously commented, the pinch candidates are all the inlet temperatures of all the streams. For clarity in notation, we introduce the variable T^p.

Minimum utilities.

In order to calculate the utilities, we must introduce the unclassified streams in the Pinch Location Method. To that end, let us reordered the Eq.(4) as follows:

$$\begin{aligned} Q_C^p = &\sum_{j \in COLD} f_j \left[\max\left(0,\, T^p - ts_j^{out}\right)\right] + \sum_{i \in HOT} F_i \left[\max\left(0,\, T^p - TS_i^{out}\right)\right] - \\ &\sum_{j \in COLD} f_j \left[\max\left(0,\, T^p - ts_j^{in}\right)\right] - \sum_{i \in HOT} F_i \left[\max\left(0,\, T^p - TS_i^{in}\right)\right] \qquad \forall p \in STR \end{aligned} \tag{14}$$

In previous equation, the "max" terms related to the output temperatures on the right side of the equation are additive and those related to the input temperatures have a negative sign. The introduction of the unclassified streams is then straightforward.

$$\begin{aligned} Q_C^p = &\sum_{j \in COLD} f_j \left[\max\left(0,\, T^p - ts_j^{out}\right)\right] + \sum_{i \in HOT} F_i \left[\max\left(0,\, T^p - TS_i^{out}\right)\right] + \sum_{k \in UNC} F_k \left[\max\left(0,\, T^p - TS_k^{out}\right)\right] - \\ &\sum_{j \in COLD} f_j \left[\max\left(0,\, T^p - ts_j^{in}\right)\right] - \sum_{i \in HOT} F_i \left[\max\left(0,\, T^p - TS_i^{in}\right)\right] - \sum_{k \in UNC} F_k \left[\max\left(0,\, T^p - TS_k^{in}\right)\right] \\ &\forall p \in STR \end{aligned} \tag{15}$$

In Eq.(15), we are introducing the summation over hot, cold and unclassified streams (the complete set of process streams). Therefore, it is not necessary to maintain the differentiation between hot, cold or unclassified streams, and Eq.(15) can be written in the more compact form using a single index for all the process streams.

$$Q_C^p = \sum_{s \in STR} F_s \left[\max\left(0,\, T^p - TS_s^{out}\right) - \max\left(0,\, T^p - TS_s^{in}\right)\right] \quad \forall p \in STR \tag{16}$$

The 'max' operator has the drawback that it is non-differentiable and, therefore, cannot be directly included in an optimization model. In the original paper, Duran and Grossmann (1986) try to overcome that problem by using a smooth approximation. The major problem with this approach is that these kind of smooth approximations are non-convex, depend on parameters that must be adjusted to accurately approximate the ‘max’ operator and, at the same time, avoid numerical conditioning problems (Balakrishna & Biegler, 1992).

In 1998, Grossmann et al. (1998) proposed a disjunctive formulation for calculating the energy content of a stream above (below) the pinch (Q_H^p, Q_C^p) that explicitly take into account, for each pinch candidate, the three alternatives: the stream is above the pinch, the stream crosses it or it is below the pinch. This disjunctive model was reformulated as an MI(N)LP model using a big-M approach. If the heat flows of all the streams are constant –which is a good approximation in most cases– the resulting model is linear and can be easily added to any process model.

Quirante et al. (2017) presented an alternative disjunctive model in which they deal directly with the ‘max’ operator:

$$\phi = \max[0, c^T x] \quad \Rightarrow \quad \begin{bmatrix} Y \\ c^T x \geq 0 \\ \phi = c^T x \\ \underline{x} \leq x \leq \bar{x} \end{bmatrix} \underline{\vee} \begin{bmatrix} \neg Y \\ c^T x \leq 0 \\ \phi = 0 \\ \underline{x} \leq x \leq \bar{x} \end{bmatrix} \quad Y \in \{True, False\} \tag{17}$$

Quirante et al. (2017) showed that the hull reformulation of the disjunction of Eq.(17) can be written as follows:

$$\begin{gathered} \phi = c^T x + s \\ y\phi^{LO} \leq \phi \leq y\phi^{UP} \\ (1-y)s^{LO} \leq s \leq (1-y)s^{UP} \\ s \geq 0; \qquad \phi \geq 0 \end{gathered} \tag{18}$$

They also showed that previous reformulation requires a lower number of binary variables and equations and has better relaxation gap than the disjunctive model presented by Grossmann et al. (1998). In Appendix A, the interested reader can find a derivation of the previous formulation as well as tight bounds for ϕ and s. In this paper, we have followed this approach.

The complete disjunctive model for the simultaneous optimization and heat integration considering unclassified streams can be written as follows:

$$
\begin{array}{ll}
\min\ f(x) + C_H Q_H + C_C Q_C & \\
s.t.\quad \left.\begin{array}{l} h(x) = 0 \\ g(x) \le 0 \end{array}\right\} & \textit{Process Constraints} \\
\left.\begin{array}{l}
T_s^{in} - T_s^{out} = T_s^{+} - T_s^{-} \qquad s \in STR \\
T_s^{-} = 0 \qquad \forall s \in HOT \\
T_s^{+} = 0 \qquad \forall s \in COLD \\
\begin{bmatrix} WH_k \\ T_k^{+} \ge 0 \\ T_k^{-} = 0 \end{bmatrix} \underline{\vee} \begin{bmatrix} WC_k \\ T_k^{-} \ge 0 \\ T_k^{+} = 0 \end{bmatrix} \quad \forall k \in UNC
\end{array}\right\} & \textit{Classification Constraints} \\
\left.\begin{array}{l}
\left.\begin{array}{l} TS_i^{in} = T_i^{in} - \dfrac{\Delta T_{\min}}{2} \\ TS_i^{out} = T_i^{out} - \dfrac{\Delta T_{\min}}{2} \end{array}\right\} \ \mathrm{i} \in HOT \\
\left.\begin{array}{l} TS_j^{in} = t_j^{in} + \dfrac{\Delta T_{\min}}{2} \\ TS_j^{out} = t_j^{out} + \dfrac{\Delta T_{\min}}{2} \end{array}\right\} \ \mathrm{j} \in COLD \\
\begin{bmatrix} WH_k \\ TS_k^{in} = T_k^{in} - \dfrac{\Delta T_{\min}}{2} \\ TS_k^{out} = T_k^{out} - \dfrac{\Delta T_{\min}}{2} \end{bmatrix} \underline{\vee} \begin{bmatrix} WC_k \\ TS_k^{in} = T_k^{in} + \dfrac{\Delta T_{\min}}{2} \\ TS_k^{out} = T_k^{out} + \dfrac{\Delta T_{\min}}{2} \end{bmatrix} \quad \forall k \in UNC
\end{array}\right\} & \textit{Shifted Temperatures} \\
\left.T^{p} = TS_p^{in} \qquad p \in STR\right\} & \textit{Pinch Candidates} \\
\left.\left.\begin{array}{l}
\phi_{s,p}^{out} = T^{p} - TS_s^{out} + S_{s,p}^{out} \\
\begin{bmatrix} Y_{s,p}^{out} \\ S_{s,p}^{out} = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y_{s,p}^{out} \\ \phi_{s,p}^{out} = 0 \end{bmatrix} \\
\phi_{s,p}^{in} = T^{p} - TS_s^{in} + S_{s,p}^{in} \\
\begin{bmatrix} Y_{s,p}^{in} \\ S_{s,p}^{in} = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y_{s,p}^{in} \\ \phi_{s,p}^{in} = 0 \end{bmatrix}
\end{array}\right\} p, s \in STR\right\} & \max\ \textit{operator disjunctive formulation} \\
\left.Q_C \ge \sum_{s \in STR} F_s \left[\phi_{s,p}^{out} - \phi_{s,p}^{in}\right] \quad \forall p \in STR\right\} & \textit{Streams heat content below the pinch} \\
\left.Q_C = Q_H + \sum_{s \in STR} F_s \left(T_s^{+} - T_s^{-}\right)\right\} & \textit{Overall heat balance} \\
Q_C, Q_H, F_s, T_s^{+}, T_s^{-}, \phi_{s,p}^{out}, \phi_{s,p}^{in}, S_{s,p}^{out}, S_{s,p}^{in} \ge 0 & \\
WH_k, WC_k, Y_{s,p}^{out}, Y_{s,p}^{in} \in \left(True, False\right) & \\
\underline{T_s^{in}} \le T_s^{in} \le \overline{T_s^{in}};\ \underline{T_s^{out}} \le T_s^{out} \le \overline{T_s^{out}} & \\
\underline{\phi_{s,p}^{in}} \le \phi_{s,p}^{in} \le \overline{\phi_{s,p}^{in}};\ \underline{\phi_{s,p}^{out}} \le \phi_{s,p}^{out} \le \overline{\phi_{s,p}^{out}} & \\
\underline{S_{s,p}^{out}} \le S_{s,p}^{out} \le \overline{S_{s,p}^{out}};\ \underline{S_{s,p}^{in}} \le S_{s,p}^{in} \le \overline{S_{s,p}^{in}} &
\end{array}
\tag{19}
$$

Note that previous model is linear if the heat flows (*F*) are constant.

4. Extension to Isothermal Streams and Multiple Utilities

In the case of an isothermal process stream (for example, a pure component that suffers a phase change at constant pressure), we cannot use the Eq.(16) because all terms cancel each other. However, the heat content below a pinch candidate can be easily calculated by the following disjunction:

$$\begin{bmatrix} Y_{s,p}^{Iso} \\ T_s^{Iso} \le T^p \\ Q_{C,s}^{Iso} = m_s \lambda_s \end{bmatrix} \underline{\vee} \begin{bmatrix} \neg Y_{s,p}^{Iso} \\ T_s^{Iso} > T^p \\ Q_{C,s}^{Iso} = 0 \end{bmatrix} \forall s \in ISO,\ p \in STR \tag{20}$$

where *ISO* is an index set that makes reference to the isothermal streams ($ISO \subseteq STR$). λ is the specific heat for the change of phase and *m* the flowrate. Y_s^{Iso} is a Boolean variable that takes the value of '*True*' if the isothermal stream is located below the pinch and '*False*' otherwise.

The hull reformulation of the previous disjunction can be written as follows:

$$\left. \begin{array}{l} Q_{C\,s,p}^{Iso} = m_s \lambda_s \, y_{s,p}^{Iso} \\ Tp - T_s^{Iso} \le \left(\overline{T^p} - \underline{T_s^{Iso}} \right) y_{s,p}^{Iso} \end{array} \right\} s \in ISO,\ p \in STR \tag{21}$$

When there are isothermal streams, the streams heat content below the pinch must be modified as follows:

$$Q_C \ge \sum_{s \in STR|_{STR \ne ISO}} F_s \left[\phi_{s,p}^{out} - \phi_{s,p}^{in} \right] + \sum_{s \in ISO} Q_{C\ s,p}^{ISO} \quad \forall p \in STR \tag{22}$$

Note that the isothermal stream can also be either a hot or a cold stream and we must take this fact into account in the overall heat balance. Using the parameter f^{Iso} that takes value '1' if the isothermal stream *s* is a hot stream and "-1" if it is a cold stream, the energy balance becomes in:

$$Q_C = Q_H + \sum_{s \in STR|_{STR \ne ISO}} F_s \left(T_s^{+} - T_s^{-} \right) + \sum_{s \in ISO} f^{Iso}\, m_s \lambda_s \tag{23}$$

The inclusion of multiple utilities is straightforward. In the case of the utilities, we know the inlet and outlet temperatures but the heat flowrate is unknown, but from the point of view of modeling, except for the fact that we must include their costs in the objective function, the extra utilities are completely equivalent to process streams.

Note that if for the utilities, the inlet and outlet temperatures are constant, the model continues to be linear.

4.1. Area Estimation

In most of the chemical processes, the energy savings have an important economic (and environmental) impact. While the investment costs could eventually be also important, as a general rule, we would not expect important differences in investment costs between two different heat exchanger network designs for the same process in comparison with the energy impact. As a consequence, the simultaneous optimization of the process and the energy integration with a posteriori design of the heat exchanger network guarantees a good design. However, in some situations (i.e., expensive materials) the estimation of the area (and therefore of the cost) together with the energy savings could be of interest.

The area estimation can be done assuming a vertical heat transfer between the hot and cold balanced composite curves (Jones, 1987) (Smith, 2016). To that end, let us define the new index sets:

M =	[m | m is a non-differentiable (kink) point in the hot and cold composite curve and its end points] $\lvert K \rvert = 2\left(\lvert HOT \rvert + \lvert COLD \rvert\right)$
$MHOT$ =	[the 'kink' point m corresponds to an inlet or outlet temperature of a hot stream]
$MCOLD$ =	[the 'kink' point m corresponds to an inlet or outlet temperature of a cold stream]

According to Watson and Barton (2016); Watson et al. (2015), if we denote as H_m the enthalpy value in each one of the points in the set M, we can create a set of triples (H_m, T_m, t_m) ordered by non-decreasing enthalpy values. T_m makes reference to the hot composite curve temperature and t_m to the cold composite curve temperature, both at H_m.

Two adjacent pairs of triples demarcate a zone for the vertical heat transfer area between the hot and cold composite curves:

$$UA_m = \frac{H_{m+1} - H_m}{\Delta T_m^{ML}} \quad m \in M \,\big|_{m \neq |M|} \tag{24}$$

The difficulty is to calculate all the triples from an arbitrarily ordered set of hot and cold streams in which inlet and outlet temperatures are also unknown. Watson et al. (2015) and Watson and Barton (2016) showed that the enthalpy values for each of the 'kink' points can be calculated by the following expressions:

$$\begin{aligned} H_m &= \sum_{i \in HOT} F_i \left[\max\left(0,\, T^L - T_i^{out}\right) - \max\left(0,\, T^L - T_i^{in}\right) \right];\; T^L \in T_i^{in} \cup T_i^{out} : m \in MHOT \\ H_m &= \sum_{j \in COLD} f_j \left[\max\left(0,\, t^L - t_j^{in}\right) - \max\left(0,\, t^L - t_j^{out}\right) \right]; \quad t^L \in t_j^{in} \cup t_j^{out} : m \in MCOLD \end{aligned} \tag{25}$$

With previous equations, we can calculate all the enthalpy values and the corresponding temperatures of the 'kink' points for the hot and cold balanced composite curves. However, we still need to calculate the temperature values of hot streams for the 'kink' points of the cold composite curve and the temperatures of cold streams for the 'kink' points of the hot composite curve. In other words, there is one unknown temperature in each triple:

$$\begin{aligned} &\left(H_m,\, T_m,\, ?\right) \quad m \in MHOT \\ &\left(H_m,\, ?,\, t_m\right) \quad m \in MCOLD \end{aligned} \tag{26}$$

Watson et al. (2015) and Watson and Barton (2016) showed that if we know the enthalpies, the following expressions allow calculating the unknown temperatures (T_m, t_m):

$$\begin{aligned} H_m &= \sum_{i \in HOT} F_i \left[\max\left(0,\, T_m - T_i^{out}\right) - \max\left(0,\, T^L - T_i^{in}\right) \right]; \quad m \in MCOLD \\ H_m &= \sum_{j \in COLD} f_j \left[\max\left(0,\, t_m - t_j^{in}\right) - \max\left(0,\, t^L - t_j^{out}\right) \right]; \quad m \in MHOT \end{aligned} \tag{27}$$

At this point, it is worth mentioning that in Eq.(27) the 'max' operator can be formulated as a disjunction following the procedure presented by Quirante et al. (2017). Note also that the terms in Eq.(27) in which T^L (or t^L) correspond to inlet temperatures have already been included in the model because these temperatures are also the pinch candidates (T^p) in Eq.(16).

Unfortunately, the values of enthalpy (H_m) and, therefore, the temperatures of the hot and cold balanced composite curves, are unordered. To calculate the area, we must know which triplet is adjacent each other. This can be done using the following disjunctive model:

$$\underset{m \in M}{\veebar} \begin{bmatrix} Y_{m,m'} \\ H_{m'}^{Ord} = H_m \\ T_{m'}^{Ord} = T_m \\ t_{m'}^{Ord} = t_m \end{bmatrix} \quad \forall m' \in M$$

$$\underset{m' \in M}{\veebar} Y_{m,m'} \qquad \forall m \in M \tag{28}$$

$$\left. \begin{array}{l} H_m^{Ord} \le H_{j+1}^{Ord} \\ T_m^{Ord} \le T_{m+1}^{Ord} \\ t_m^{Ord} \le t_{m+1}^{Ord} \end{array} \right\} \quad \forall m \in M \mid m \ne \left| M \right|$$

where the Boolean variable $Y_{m,m'}$ takes the value 'True' if the unordered enthalpy value that originally was in position *m* is assigned to position *m'* in the non-decreasing reordered enthalpies and 'False' otherwise. The subscript '*ord*' makes reference to the ordered variables.

Disjunctions in Eq.(28) can be reformulated as a linear problem in terms of binary variables using either a big-M or a convex hull reformulation (Trespalacios & Grossmann, 2014). However, in this case, numerical tests have shown that the Big-M have better numerical performance due to in the convex hull reformulation a large number of new variables is not compensated by the better relaxation.

An estimation of the area can be obtained from:

$$UA = \sum_{m \in M|_{m \ne |M|}} \frac{H_{m+1}^{ord} - H_m^{ord}}{\Delta T_m^{LM}} \tag{29}$$

where ΔT_m^{LM} is the logarithmic mean temperature in the interval formed by two consecutive triples. To avoid eventual numerical problems when the difference of temperatures is the same at both ends of the interval, we substitute the logarithmic mean temperature by the Chen's approximation (Chen, 1987).

$$\Delta T_m^{LM} \approx \left[\theta_m \theta_{m+1} \frac{\left(\theta_m + \theta_{m+1} \right)}{2} \right]^{\frac{1}{3}} \quad \forall m \in M \; |_{m \ne |M|} \tag{30}$$

where:

$$\theta_m = T_m - t_m \quad \forall m \in M \tag{31}$$

Then the final model is formed by all the equations of the pinch location method and Eq.(25) and Eqs.(27)-(31).

The previous model allows the simultaneous optimization and heat integration considering the effect of the investment in the heat exchanger network. Not only the energy, ordering equations and the inherent non-convexities in the model constrain it into small or medium size problems, but the complexity of the problem depend also on the bounds on inlet and outlet temperatures and on the number of 'real' alternatives for ordering temperatures and enthalpies.

It is possible to increase the numerical performance by fixing *a priori* some $Y_{m,m'}$ variables. In other words, a point *m* in the balanced hot/cold composite curve cannot be assigned to any *m'* position. It is constrained to a subset of *m'* positions depending on the bounds of its inlet/outlet temperatures and the bounds of the inlet/outlet temperatures of the rest of streams. For example, if all the inlet/outlet temperatures are fixed, all $Y_{m,m'}$ variables can be fixed *a priori*, and if all bounds of the inlet/outlet temperatures are equal, we *a priori* cannot fix any $Y_{m,m'}$.

Navarro-Amorós et al. (2013) and Kong et al. (2017) proposed, in the context of implicitly ordering, a set of values in a mathematical programming model algorithms that allow to reduce the ordering alternatives. These algorithms can also be used for this particular problem.

Alternatively, it is also possible to reduce the reordering alternatives by solving a sequence of MILP problems. Note that if the heat flow values of the process streams are constant and the inlet and outlet temperatures of the utilities are fixed, all the reformulations in terms of binary variables of the equations of pinch location method, and the equation for interpolation and reordering in the area estimation are linear. Therefore, if we search for the highest (lowest) position in which the point *m* could be reordered in the non-decreasing sequence of enthalpy values, we can fix to '0' those values of the binary $y_{m,m'}$ outside of those limits. This can be done by solving, for each point *m*, the following MILP:

$$
\begin{aligned}
& Y_m^{LO} = \arg\min \left(m' Y_{m,m'} \right) \,/\, Y_m^{UP} = \arg\max \left(m' Y_{m,m'} \right) \\
& s.t. \;\; Eqs: 16,\, 25,\, 27,28 \\
& \qquad \underline{T_s^{in}} \le T_s^{in} \le \overline{T_s^{in}} \\
& \qquad \underline{T_s^{out}} \le T_s^{out} \le \overline{T_s^{out}}
\end{aligned}
\tag{32}
$$

Then:

$$
\begin{aligned}
& y_{m,m'} = 0 \;\; \forall m' < Y_m^{LO}, \forall m \in M \\
& y_{m,m'} = 0 \;\; \forall m' > Y_m^{UP} \;\; \forall m \in M \\
& y_{m,m'} = 1 \;\; \forall m' / Y_m^{LO} = Y_m^{UP} \; \forall m \in M
\end{aligned}
\tag{33}
$$

where *m'* makes reference to the position that the point *m'* occupies in the ordered set *M*.

If the heat flow values are not constant, then we still can solve the problem of Eq.(32) by using the corresponding upper/lower bounds for the heat flows.

5. Case Studies

In this paper, we present four case studies to illustrate and discuss the performance of the PLM with unclassified streams, multiple utilities isothermal streams and area estimation. As commented above, the area estimation is constrained to medium size problems, therefore, in the first three examples that deals with a large number of process streams, we consider only the heat integration and in the fourth example, we introduce the area (investment) cost estimation.

The first example integrated unclassified multiple utilities and isothermal process streams. In the second example, we introduce a large-scale problem and we show the excellent numerical performance of the proposed approach. To study the performance of the proposed approach without the interference of external factors, these two first examples deals only with the heat integration without taking into account the rest of the process, but in the third one, we simultaneously consider the process synthesis and heat integration. Finally, in the last example, we introduce the area estimation and illustrate the effect of the pre-processing in the numerical behavior of the model.

Problem calculations were carried out in GAMS (Rosenthal, 2012), using BARON (Sahinidis, 1996) as a solver. The computations were performed in a computer with a 3.60 GHz Intel® CoreTM i7 Processor and 8 GB of RAM under Windows 10.

5.1. Case Study 1

The first example includes six process streams: two hot streams, two cold streams, and two unclassified streams. All relevant data for this first case study is in Table 1.

Table 1. Data for case study 1.

Stream	Type	Inlet T (ºC)	Outlet T (ºC)	FCp (MW/ºC)
1	Hot	400 – 440	110 – 130	1
2	Hot (isothermal)	340 – 380	340 – 380	100
3	Cold	160 – 180	415 – 425	3 – 4
4	Cold	100 – 120	250 – 260	3 – 4
5	Unclassified	130 – 240	150 – 300	1
6	Unclassified	180 – 430	210 – 300	2
				Cost ($/kW year)
Hot Utility 1		500	500	80
Hot Utility 2		380	380	60
Cold Utility		20	30	20

ΔT_{min} = 20 ºC

We consider that the stream 2 is an isothermal stream, while the other streams are non-isothermal. We assume that a second hot utility is available at 380 ºC with a unit cost of $60/kW·year. The objective function consists of minimizing the utility costs. The results obtained and some relevant parameters for the case study are presented in Table 2 and Table 3.

Table 2. Stream temperatures, flow rates, and heat loads for the optimal solution of case study 1.

Stream	Type	Inlet T (ºC)	Outlet T (ºC)	FCp (MW/ºC)
1	Hot	440	130	1
2	Hot	341	341	100
3	Cold	180	415	3
4	Cold	120	250	3
5	Hot	240	150	1
6	Hot	430	210	2
				Q (MW)
Hot Utility 1		500	500	5
Hot Utility 2		380	380	160
Cold Utility		20	30	10

The optimal solution was $10.2 million/year. Both unclassified streams were correctly classified as hot streams. After heat integration, the process requires 10 MW of cooling duty, which is satisfied by the cold utility, and 165 MW of heating duty, which is satisfied by the hot utility (5 MW) and the intermediate hot utility (160 MW). It is worth remarking the model is solved very efficiently in a fraction second of CPU time.

Table 3. Computational statistics and solution of case study 1.

No equations	602
No variables	435
No binary variables	46
CPU time (s)[a]	0.326
Optimal solution (MM$/y)	10.20

5.2. Case Study 2

In the second example, we apply the methodology to a large-scale problem. This second example includes 17 process streams: six hot streams, seven cold streams, and four unclassified streams. Temperature and flow rate bounds are shown in Table 4. This problem was originally proposed by Kong et al. (2017). We use it as a means to validate the model –as far as we know, the work by Kong et al. (2017) is the only one that deals with unclassified stream– and show the performance of the proposed approach.

Table 4. Stream specifications for case study 2.

Stream	Type	Inlet T (ºC)	Outlet T (ºC)	FCp (MW/ºC)
1	Hot	400 – 440	110 – 130	1
2	Hot (isothermal)	340 – 380	340 – 380	100
3	Cold	160 – 180	415 – 425	3 – 4
4	Cold	100 – 120	250 – 260	3 – 4
5	Unclassified	130 – 240	150 – 300	1
6	Unclassified	180 – 430	210 – 300	2
7	Hot	280	140	1.5 – 2
8	Hot	355	190 – 200	1.1 – 1.3
9	Cold	360 – 410	411	3.3 – 4
10	Cold	230	320	3 – 3.5
11	Cold	390	460	0.9
12	Unclassified	150 – 160	120 – 180	3
13	Hot	220	170 – 180	0.5 – 1
14	Cold	300	400 – 408	1.6
15	Cold	170	440 – 450	3.5
16	Hot	480	440 – 460	1.8
17	Unclassified	170 – 190	180	3.2 – 4
				Cost ($/kW year)
Hot Utility		500	500	80
Hot Utility		380	380	60
Cold Utility		20	30	20

ΔT_{min} = 20 ºC

In this second case, the stream 2 is a hot isothermal stream, while the rest of streams are not isothermal. We have also two hot utilities. The heat flow rate of some of the streams is not constant with becomes the problem in non-linear and non-convex due to the bilinear term that appears in energy balances. Under these conditions, the resulting problem is an MINLP that is solved to global optimality using the deterministic global solver BARON (Sahinidis, 1996).

The objective function consists of minimizing the utility cost. The results obtained and some relevant parameters for the case study are presented in Table 5 and Table 6.

Table 5. Stream temperatures, flow rates, and heat loads for the optimal solution of case study 2.

Stream	Type	Inlet T (°C)	Outlet T (°C)	FCp (MW/°C)
1	Hot	440	130	1
2	Hot	380	380	100
3	Cold	180	415	3
4	Cold	100	250	3
5	Hot	240	190	1
6	Hot	430	210	2
7	Hot	280	140	2
8	Hot	355	190	1.3
9	Cold	410	411	3.3
10	Cold	230	320	3
11	Cold	390	460	0.9
12	Hot	150	140	3
13	Hot	220	170	1
14	Cold	300	400	1.6
15	Cold	170	440	3.5
16	Hot	480	440	1.8
17	Hot	180	180	3.6
				Q (MW)
Hot Utility 1		500	500	190.3
Hot Utility 2		380	380	859.5
Cold Utility		20	30	0.0

Table 6. Computational statistics and solution of case study 2.

	Present work	Kong et al. (2017)
No equations	3901	9714
No variables	2681	5801
No binary variables	163	2083
CPU time (s)[a]	2.947	13275
Heating requirements (MW)		
Hot utility	190.3	190.3
Intermediate hot utility	859.5	859.5
Cooling requirements (MW)	0.0	0.0
Optimal solution (MM$/y)	66.794	66.8

[a] Intel Core i7-4790 3.60 GHz, using BARON 14.4.0 for MINLP.

The optimal solution achieved with our model is $66.794 million/year. After heat integration, the process requires 1049.8 MW of heating duty, which is satisfied by the hot utility (190.3 MW) and the intermediate hot utility (859.5 MW), and no cooling is required.

The results show that the number of continuous and binary variables and the total number of equations is much lower in the proposed model in comparison to the model developed by Kong et al. (2017).

The model is solved in around three seconds of CPU time. Even though the model in this work and that presented by Kong et al. (2017) have been solved in different computers and therefore we cannot do a direct comparison, the four orders of magnitude reduction in CPU time and the lower number of variables (specially the number of binaries) and constraints show the potential applicability of the new approach.

5.3. Case Study 3

The following case study corresponds to an example of simultaneous process synthesis and heat integration. This case study is adapted from the work by Kong et al. (2017). Unfortunately, in the original paper some data are missing and consequently, both models cannot be compared.

The superstructure for the chemical process is shown in Fig. 1.

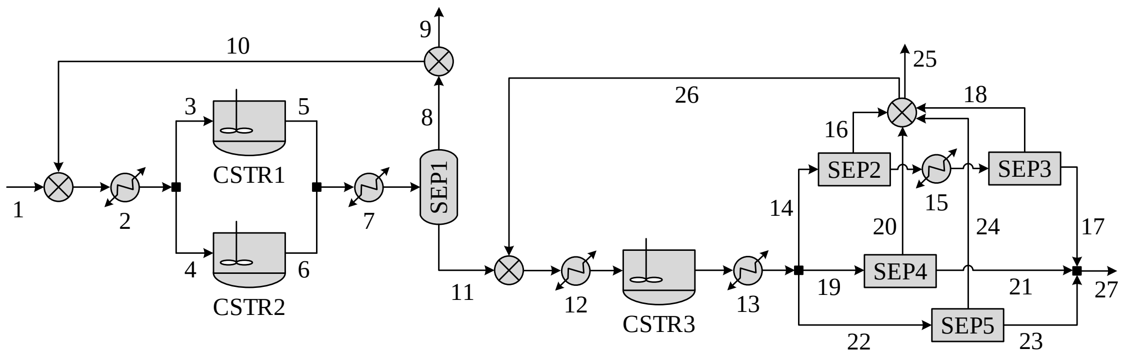

Fig. 1. Superstructure for the chemical process considered in case study 3.

Four components (A, B, C, and D) are taken into account in the process. The raw materials (components A and B) are used to produce the intermediate product C (Eq.(34)). The reaction can be carried out in two alternative isothermal continuous stirred-tank reactors (CSTR1 and CSTR2) that work with different conditions.

$$A + B \rightarrow C \tag{34}$$

The outlet stream from the reactor is sent to a flash unit in order to separate unreacted A and B from intermediate C. Unreacted A and B are separated by the top and recycled, while C is separated by the bottom. Pure component C is sent to another isothermal stirred-tan reactor

(CSTR3) to produce final product D. This second reaction Eq.(35) is assumed to be an equilibrium reaction, and the equilibrium constant (Kc) is a function of the reactor temperature.

$$C \leftrightarrow D \tag{35}$$

$$K_c = K_c^o \cdot \exp\left(-\frac{\Delta H^o}{R}\left(\frac{1}{T(K)} - \frac{1}{298}\right)\right) \tag{36}$$

where $K_c^o = 0.4$ is the equilibrium constant at standard state (298 K, 1 bar), $\Delta H^o = 8\ kJ/mol$ is the heat of reaction at standard state, R is the universal gas constant, and T is the temperature (in Kelvin) of the CSTR3.

For simplicity, we assume ideal behavior:

$$K_c = \frac{[D]}{[C]} \tag{37}$$

where [C] and [D] are the concentration of component C and D in stream 13, respectively. Reactor CSTR requires heating because the reaction is assumed endothermic. Finally, unreacted C is separated from D in one of the alternative separation technologies before recycled back to CSTR3. Table 7 summarizes the unit specifications for the superstructure.

Table 7. Unit specifications for the superstructure of case study 3.

Reactors	**RXN**	**Temperature (°C)**	**Conversion[a]**	**Unit cost pre-factor[b], *k* (\$/kmol$^{0.6}$·year$^{0.4}$)**
CSTR1	$A+B \rightarrow C$	227	0.9	0.90
CSTR2	$A+B \rightarrow C$	127	0.8	0.85
CSTR3	$C \leftrightarrow D$	57 – 127	variable	1.00
Separators	**Top/Bottom**			
SEP1	AB/C	157		1.00
SEP2	C/D[c]	107		1.10
SEP3	C/D	67		1.10
SEP4	C/D	87		0.90
SEP5	C/D	77		0.80

[a] The conversion is with respect to the limiting component B.

[b] Cost pre-factor relates the total molar flow at the inlet to the annualized cost: $k = k_i\left(F_i^T\right)^{0.6}$

[c] The split fractions in SEP2 are 0.6 and 0 for component C and D, respectively. The remaining separations are assumed sharp.

It is assumed that the feed stream (stream 1) flow rates are 2 kmol/s of A and 1 kmol/s of B, with a raw material cost of \$0.02/kmol A and \$0.01/kmol B, respectively. We are selling the final product D at a price of \$0.17/kmol. The objective is to maximize the profit, which takes into account the revenue, cost of raw materials, unit capital cost, and utility cost.

The case study contains four process streams that require heating or cooling (streams 2, 7, 12, and 13) which are unknown a priori, one process stream that requires cooling (stream 15) and two isothermal streams that represent the heat duties of SEP1 and CSTR3.

We assume that a hot utility is available at 500 ºC with a unit cost of \$80/kW·year, and the cold utility enters at 20 ºC and exists at 30 ºC with a cost of \$20/kW·year. All the problems were solved for a minimum heat recovery temperature (ΔT_{min}) of 20 ºC.

The resulting model consists of 651 variables (95 binary variables) and 917 equations. It was solved in 390 seconds with an objective of \$2.829 million/year. CSRT1 is selected for the first reaction, where the reaction takes place at 227 ºC with a 0.9 conversion of reactant B. Intermediate C is converted to D in CSTR3 at 115.14 ºC. Finally, the product D is sent to SEP5, where is separated at a rate of 0.930 kmol/s. The optimal stream conditions are shown in Table 8 and the optimal solution for streams in the heat integration are shown in Table 9. After the heat integration, the process requires 81.006 MW of heating utility and 2.505 MW of cooling water.

Table 8. Optimal solution for streams in the chemical process.

	Component molar flow rates (kmol/s)			
Stream	**A**	**B**	**C**	**D**
1	2.000	1.000	-	-
2	2.512	1.033	-	-
3	2.512	1.033	-	-
4	-	-	-	-
5	1.582	0.103	0.930	-
6	-	-	-	-
7	1.582	0.103	0.930	-
8	1.582	0.103	-	-
9	1.070	0.070	-	-
10	0.512	0.033	-	-
11	-	-	0.930	-
12	-	-	1.951	-
13	-	-	1.021	0.930
14	-	-	-	-
15	-	-	-	-
16	-	-	-	-
17	-	-	-	-
18	-	-	-	-
19	-	-	-	-
20	-	-	-	-
21	-	-	-	-
22	-	-	1.021	0.930
23	-	-	-	0.930
24	-	-	1.021	-
25	-	-	-	-
26	-	-	1.021	-
27	-	-	-	0.930

Table 9. Unit specifications for the superstructure of case study 3.

Stream	Tin (ºC)	Tout (ºC)	FCp (MW/ºC)	Type
2	47.00	227.00	4.050	Cold
7	227.00	157.00	143.835	Hot
12	115.14	127.00	303.707	Cold
13	127.00	77.00	4.910	Hot
15	107.00	67.00	0.000	Hot
SEP1	157.00	157.00	706.309	Cold
CSTR3	127.00	127.00	5356.113	Cold

The optimal superstructure obtained through the simultaneous optimization and heat integration is shown in Fig. 2.

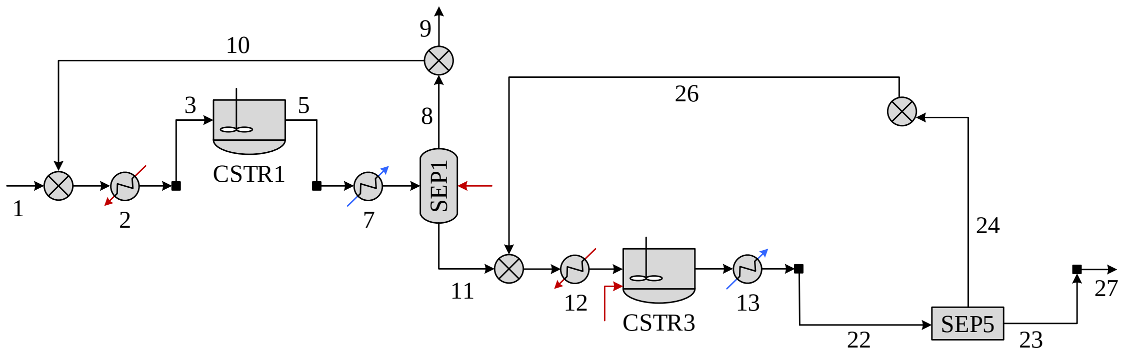

Fig. 2. Optimal superstructure for the chemical process of case study 3.

5.4. Case Study 4

In this last case study, we introduce the equations for area estimation together with those of the pinch location method. However, as commented in previous sections, the numerical performance of the model is very dependent on the number of process streams and on the bounds of the inlet and outlet temperatures. As a general rule, the model is constrained to medium size problems mainly due to the bad behavior of the implicit reordering equations. In any case, it could be useful in models in which the investment is as important as energy savings.

It is worth noting that although for large-scale problems we cannot ensure a globally optimal solution, it is always possible to get a good solution even though we cannot prove it is the best one.

Table 10 shows the data for this problem. Costs of utilities were obtained from Turton et al. (2013). The investment costs were also correlated from shell and tube heat exchangers also from Turton et al. (2013) and updated to 2017 using the Chemical Engineering Plant Cost Index (CEPCI).

Table 10. Data for case study 4.

Stream	Type	Inlet T (ºC)	Outlet T (ºC)	FCp (MW/ºC)
1	*Hot*	230 – 260	30 – 50	0.15
2	*Hot*	135 -155	110 – 125	0.50
3	*Hot*	80 – 100	20 – 30	0.25
4	Hot	110 – 120	80 – 100	0.30
5	Cold	10 – 40	170 – 190	0.20
6	Cold	90 – 110	180 – 225	0.30
7	Cold	125 – 160	225 – 235	0.15
8	Cold	130 - 150	200 - 240	0.40
				Cost (k$/MW year)
Hot Utility		250	250	408.96
Cold Utility		10	20	10.19
ΔT_{min} = 10 ºC				
U = 0.002 MW/m^2 ºC				
Area Cost (k$/year) = 47.65 + 0.7313 Area (m^2)				

The objective in this problem consists of minimizing the Total Annualized Cost (*TAC*). We will use the following objective:

$$TAC(k\$ / y) = 408.96\, Q_{Hot} + 10.19 Q_{Cold} + 0.7313 Area + 47.65 \tag{38}$$

The problem of determining which minimum utility consumption are required can be very efficiently solved by using the PLM. This problem was solved in 0.06 seconds of CPU time. The minimum hot utility consumption was 49.5 MW and the minimum cold utility consumption was 5 MW. In these conditions, it is possible to estimate the area of the heat exchanger network using the vertical heat transfer approach either by solving the MINLP model in which we fix all the temperatures or using the classical approach using a spreadsheet of even manually (Smith, 2016). If we fix all the inlet and outlet temperatures to the values obtained when solved the PLM method, BARON (Sahinidis, 1996) is able of solving this MINLP problem in less than 10 seconds of CPU time. The area estimation yields 2013 m^2, with a total annualized cost of 21814 k$/year. This relatively short CPU time shows that the proposed interpolation approach, using the 'max' operator for calculating the missing points in each triple is very efficient. Table 11 shows the optimal results with the *a posteriori* area estimation.

Table 11. Solution for case study 4.

		A posteriori area estimation		Simultaneous area estimation	
Stream	**Type**	**Inlet T (ºC)**	**Outlet T (ºC)**	**Inlet T (ºC)**	**Outlet T (ºC)**
1	*Hot*	260	50	260	50
2	*Hot*	155	120.5	155	120.91
3	*Hot*	80	30	80	30
4	Hot	110	100	118.62	100
5	Cold	10	170	10	170
6	Cold	90	180	100	180
7	Cold	160	225	160	225
8	Cold	150	250	150	250
Hot Utility (MW)		49.5		49.5	
Cold Utility (MW)		5		10.37	
Area (m^2)		1213		1712	
TAC (k$/year)		21814		21649	

However, if we include the equations of area estimation, without any pretreatment, the solver BARON is not even able of finding a feasible solution in 500 s of CPU time.

If we solve the pretreatment MILPs, then we can significantly reduce the number of alternatives to be considered in the implicit reordering (see Table 12). Even though BARON is not able to guarantee the global optimal solution in 500 s of CPU time, we get a good solution with just a relative gap of 5.3%.

The obtained solution shows just a marginal improvement in TAC (21649 k$/year) around a 0.8 %, which is in agreement with the assumption that, in general, neglecting the effect of area cost in the preliminary design of a heat exchanger network does not significantly affect the final result. The area is reduced from 2013 to 1712 m^2, (~ 15 %) but this reduction is only around a 1 % of the TAC, and we must take into account also the fact that the cold utility consumption increases from 5 to 10.3 MW.

Table 12. Feasible intervals for each inlet/outlet temperatures after pretreatment.

Stream		Type	Lower Position**	Upper position**
1	Inlet	Hot	12	15
1	Outlet	Hot	1	5
2	Inlet	Hot	10	13
2	Outlet	Hot	8	10
3	Inlet	Hot	4	8
3	Outlet	Hot	1	4
4	Inlet	Hot	8	10
4	Outlet	Hot	4	8
Hot Utility	Inlet	Hot	16	20
Hot Utility	Outlet	Hot	13	16
5	Inlet	Cold	1	7
5	Outlet	Cold	14	18
6	Inlet	Cold	6	11
6	Outlet	Cold	16	19
7	Inlet	Cold	11	15
7	Outlet	Cold	17	19
8	Inlet	Cold	11	15
8	Outlet	Cold	19	20
Cold Utility	Inlet	Cold	1	4
Cold Utility	Outlet	Cold	3	7

**It refers to the lower/upper position that the inlet/outlet enthalpy point of a given stream could be placed when ordered in non-decreasing enthalpy values.

Table 13. Computational statistics and solution of case study 4.

	PLM with area estimation
Nº equations	6439
No variables	2917
No binary variables	234(1124)[(a)]
Pre-processing time (s)	23.9
CPU time (s)	500[(b)]
Best solution found	21648.9

(a) Number of binary variables after the preprocessing and before (into brackets) preprocessing.
(b) Fixed a maximum CPU time in 500 s.

6. Conclusions

We have proposed a disjunctive model for the simultaneous process optimization and heat integration of systems that include variable temperatures, streams that cannot be classified as hot or cold streams *a priori* and whose classification as hot or cold stream depends on the operating conditions, isothermal streams and multiple utilities. The idea underlying the proposed approach is that the energy-related costs have a much larger impact than investment cost. The model is based on the disjunctive approach of the pinch location method proposed by Quirante et al. (2017) and the treatment of the unclassified streams presented by Kong et al. (2017).

The proposed formulation has proved to be numerically very efficient. The total number of variables and equations is lower than alternative formulations for dealing with the same problem proposed by Navarro-Amorós et al. (2013) for problems without unclassified streams or the extension proposed by Kong et al. (2017) that also considers unclassified streams and the CPU time is reduced by 3-4 orders of magnitude.

The model has also been extended to allow estimating the area of the heat exchanger network. Following the assumption of vertical heat transfer, it is possible to get an area estimation with an error small error –usually lower than 10 %– (Smith, 2016). To that end, it is necessary to calculate for each 'kink' point in the hot and cold balanced composite curves (all the inlet and outlet temperatures) the triples (H_m, T_m, t_m) and order those triples by non-decreasing enthalpy values. The first part (calculate the triples) can be efficiently done using the approach presented by Watson et al. (2015) and Watson and Barton (2016) that relies also on the 'max' operator and, therefore, can be efficiently reformulated as a disjunction following the procedure presented by Quirante et al. (2017). The advantage of this approach, in particular, the part related to the interpolation, is that for constant heat flow values it preserves the linearity and it has shown to be numerically efficient. The second part –determining adjacent triples– requires an implicit ordering that significantly complicates the model. However, in some situations, it is possible to reduce the combinatorial difficulties related to the ordering by reducing *a priori* the 'positions' that a given point could reach when sorted.

The proposed disjunctive model with unclassified and isothermal process streams and multiple utilities has proved to be robust and numerically very efficient in large-scale problems. The performance of the model extended with the area estimation depends on the problem characteristics –how large are the bounds on the inlet and outlet temperatures and the degree of overlap between those bounds–. However, even in the case where we cannot prove the global optimality, we are able of getting good solutions with a relatively low gap for medium size problems.

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Appendix A. Hull Reformulation of the «max[0, $c^T x$]» operator

In this Appendix A, we present the disjunctive reformulation of the 'max' operator following the approach presented by Quirante et al. (2017). We also show how to obtain good lower and upper bounds for the variables.

Consider the following expression:

$$\phi = \max\left(0, \mathbf{c}^T \mathbf{x}\right) \tag{A.1}$$

where *c* is a vector of known coefficients and *x* is a vector of variables. An equivalent disjunctive formulation of Eq.(A.1) is as follows:

$$\begin{pmatrix} Y \\ \mathbf{c}^T \mathbf{x} \geq 0 \\ \phi = \mathbf{c}^T \mathbf{x} \\ \mathbf{x}^{LO} \leq \mathbf{x} \leq \mathbf{x}^{UP} \end{pmatrix} \underline{\vee} \begin{pmatrix} \neg Y \\ \mathbf{c}^T \mathbf{x} \leq 0 \\ \phi = 0 \\ \mathbf{x}^{LO} \leq \mathbf{x} \leq \mathbf{x}^{UP} \end{pmatrix}$$
$$Y \in \left[True,\ False\right] \tag{A.2}$$

In disjunction from Eq.(A.2), if the Boolean variable takes the value 'True' the first term is enforced and ϕ must be positive, otherwise, it is equal to zero. The hull reformulation of Eq.(A.2) is as follows:

$$\begin{array}{ll} \multicolumn{2}{c}{\mathbf{x} = \mathbf{x}_1 + \mathbf{x}_2} \\ \multicolumn{2}{c}{\phi = \phi_1 + \phi_2} \\ \mathbf{c}^T \mathbf{x}_1 \geq 0 & \mathbf{c}^T \mathbf{x}_2 \leq 0 \\ \phi_1 = \mathbf{c}^T \mathbf{x}_1 & \phi_2 = 0 \\ y \cdot \mathbf{x}^{LO} \leq \mathbf{x}_1 \leq y \cdot \mathbf{x}^{UP} & (1-y) \cdot \mathbf{x}^{LO} \leq \mathbf{x}_2 \leq (1-y) \cdot \mathbf{x}^{UP} \\ \multicolumn{2}{c}{y \in (0,\ 1)} \end{array} \tag{A.3}$$

where the superscripts *LO* and *UP* make reference to the lower and upper bounds respectively.

The model in Eq.(A.3) introduces new variables and equations. However, Quirante et al. (2017) showed that this formulation can be simplified taking into account that variable ϕ_2 is fixed to zero and it does not have much sense to add a new variable and then fix it to zero. Therefore, it can be removed.

The particular values of variables x_2 are not relevant to the problem because they are not used in the model. It is possible to lump the term $c^T x_2$ in a single variable as follows:

$$\mathbf{x} = \mathbf{x}_1 + \mathbf{x}_2 \rightarrow \mathbf{c}^T\mathbf{x} = \mathbf{c}^T\mathbf{x}_1 + \mathbf{c}^T\mathbf{x}_2 \rightarrow \mathbf{c}^T\mathbf{x} = \mathbf{c}^T\mathbf{x}_1 - s \rightarrow \mathbf{c}^T\mathbf{x}_1 = \mathbf{c}^T\mathbf{x} + s \qquad \text{(A.4)}$$

Consequently, we can rewrite the hull reformulation in terms of the original x variables and the new variable s:

$$\begin{aligned} &\phi = \mathbf{c}^T\mathbf{x} + s \\ &y\phi^{LO} \le \phi \le \phi^{UP} \\ &(1-y)s^{LO} \le s \le (1-y)s^{UP} \\ &s \ge 0;\ \phi \ge 0;\ y \in (0,1) \end{aligned} \qquad \text{(A.5)}$$

Good lower and upper bounds for ϕ and s variables can be obtained from the bounds of x and c values.

It is worth remarking that Eq.(A.5) can be obtained directly from the hull reformulation of the disjunctive reformulation of the 'max' operator formulated as an optimization problem with complementarity constraints (Biegler, 2010).

$$\phi = \max\left(0, c^T x\right) \Rightarrow \begin{cases} \phi = c^T x + s \\ 0 \le \phi \perp s \le 0 \end{cases} \Rightarrow \begin{cases} \phi = c^T x + s \\ \begin{bmatrix} Y \\ s = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y \\ \phi = 0 \end{bmatrix} \\ s \ge 0; \quad \phi \ge 0 \end{cases} \qquad \text{(A.6)}$$

Note that the hull reformulation of the disjunction in Eq.(A.6) is the set of equations shown in Eq.(A.5).

As an example consider one of the terms that appear in the PLM:

$$\phi_{j,p} = \max\left\{0, t_j^{out} - T^p\right\}$$

$$\begin{aligned}
&\phi_{j,p} = t_j^{out} - T^p + s_{j,p}^{out} \\
&y_{j,p}^{out}\left(\phi_{j,p}^{out}\right)^{LO} \le \phi_{j,p}^{out} \le y_{j,p}^{out}\left(\phi_{j,p}^{out}\right)^{UP} \\
&\left(1 - y_{j,p}^{out}\right)\left(s_{j,p}^{out}\right)^{LO} \le s_{j,p}^{out} \le \left(1 - y_{j,p}^{out}\right)\left(s_{j,p}^{out}\right)^{UP} \\
&s_{j,p}^{out} \ge 0;\ \phi_{j,p}^{out} \ge 0
\end{aligned} \qquad \text{(A.7)}$$

The upper and lower bounds can be inferred from the bounds on temperatures as follows:

$$\begin{aligned}
&\left(\phi_{j,p}^{oup}\right)^{LO} = \max\left\{0,\ \left(t_j^{out}\right)^{LO} - \left(T^p\right)^{UP}\right\} \\
&\left(\phi_{j,p}^{oup}\right)^{UP} = \max\left\{0,\ \left(t_j^{out}\right)^{UP} - \left(T^p\right)^{LO}\right\} \\
&\left(s_{j,p}^{oup}\right)^{LO} = \max\left\{0,\ \left(T^p\right)^{LO} - \left(t_j^{out}\right)^{UP}\right\} \\
&\left(s_{j,p}^{oup}\right)^{UP} = \max\left\{0,\ \left(T^p\right)^{UP} - \left(t_j^{out}\right)^{LO}\right\}
\end{aligned} \qquad \text{(A.8)}$$

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