A Novel Disjunctive Model for the Simultaneous Optimization and Heat Integration

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Abstract

This paper introduces a new disjunctive formulation for the simultaneous optimization and heat integration of systems with variable inlet and outlet temperatures in process streams as well as the possibility of selecting and using different utilities. The starting point is the original compact formulation of the Pinch Location Method, however, instead of approximating the "maximum" operator with smooth, but non-convex functions, these operators are modeled by means of a disjunction. The new formulation has shown to have equal or lower relaxation gap than the best alternative reformulation, thus reducing computational time and numerical problems related to non-convex approximations.

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

1. Introduction

An important factor in determining the optimal design of a chemical process is heat integration because energy consumption contributes significantly to the total cost of a process. Therefore, minimizing energy consumption, minimizing energy losses, and increasing the energy efficiency increases the efficiency and the economic benefits of a chemical plant.

The most important technique to decrease energy consumption is through the implementation of heat exchanger networks. The concept of heat integration making the concept of pinch analysis was introduced in 1978 by Linnhoff and Flower (1978). The idea was based on determining the minimum utility requirements of a process, and identifying the maximum possible grade of heat recovery as a function of the minimum temperature difference inside the heat exchanger network. In 1983, Linhoff and Hindmarsh (1983) showed that it is possible to save a significant part of the energy required by a plant.

A detailed review of heat integration and heat integration alternatives is out of the scope of this paper. A simple search using the Scopus Database (SCOPUS Database, 2016) using the keywords «Heat Integration» yields more than 5400 results in just the last 5 years, and more than 1100 in the specific area of Chemical Engineering. Comprehensive information about the initial advances after the pinch introduction can be found in the reviews by Gundersen and Naess (1988) or Jezowski (1994a, 1994b). A comprehensive review with annotated bibliography that covers all the advances in the 20th century was due to Furman and Sahinidis (2002). A general overview of the state of the art at the end of 20th century in process engineering including heat integration can be found in the work by Grossmann et al. (1999) or Dunn and El-Halwagi (2003). More recent reviews including the most relevant advances in the last years are those by Morar and Agachi (2010), and Klemeš and Kravanja (2013). With the focus on heat exchanger networks retrofit, the recent review by Sreepathi and Rangaiah (2014) is also interesting. The importance of process integration in general and the combination of Heat Integration with some particular subsystems has also received considerable attention. For example, Ahmetovic reviewed the literature for water and energy integration (Ahmetović et al., 2015; Ahmetović & Kravanja, 2013). Wechsung et al. (2011) and Onishi et al. (2014a) introduced the concept of heat and mechanical power integration. Fernández et al. (2012) presented a comprehensive review of energy integration in batch processes, Quirante and Caballero

(2016) proposed the simultaneous optimization, heat integration, and life cycle assessment (LCA) for the optimization of a very large scale sour water stripping plant.

A heat integrated flowsheet can be obtained using mainly two different approaches: Sequential or simultaneous strategy. In the first stage of the sequential strategy, the process configuration and the operating conditions are optimized assuming that all heating and cooling needs are supplied by utilities. In the second stage, with the information of the optimal stream conditions, heat integration is performed and the heat exchanger network (HEN) is designed (Ahmad et al., 1990; Linhoff & Hindmarsh, 1983; Linnhoff, 1993; Linnhoff & Ahmad, 1990).

In the simultaneous strategy, the heat integration and the flowsheet synthesis are performed simultaneously. Some works have demonstrated that the simultaneous optimization and heat integration can achieve important savings in the total cost of a process, compared to the sequential strategy (Duran & Grossmann, 1986; Lang et al., 1988). In problems with specific characteristics like some subsystems or in small or medium size problems (Caballero & Grossmann, 2006; Onishi et al., 2014b) it is possible to use a superstructure (Yee & Grossmann, 1990; Yee et al., 1990) and simultaneously obtaining the optimal operating conditions and the heat exchanger network. However, in large problems the size of the model is so large that usually it cannot be solved with the state of the art NLP/MINLP solvers. However, in many cases, the energy costs dominate the investment costs or we expect that for a given minimum energy consumption target, the investment in the different alternatives do not have an important influence in the optimal operating conditions of the optimized flowsheet. In other words, we simultaneously optimize the operating conditions and the energy consumption but without considering the actual structure of the heat exchanger network. The information required to predict the minimum energy target for a given set of hot and cold streams can be obtained from the “Problem Table” (Linnhoff, 1993) or using the transshipment model (Papoulias & Grossmann, 1983). In both approaches, it is necessary to introduce the concept of «Temperature intervals». This is adequate for ‘a posteriori’ heat integration or if the optimization is performed using a derivative-free solver (Corbetta et al., 2016). However, the state of the art gradient based NLP/MINLP solvers require smooth functions. If the process stream temperatures are not constant some temperature intervals can disappear or other news can appear, which mathematically translates into discontinuities, and therefore into points of non-differentiability.

To overcome the numerical difficulties related to the temperature intervals, Duran and Grossmann (1986) presented the «Pinch Location Method» (PLM). The next section presents an overview of PLM. Even though the PLM does not rely on the temperature interval concept, the final model includes the “maximum” operator that introduces non-differentiabilities. In the original work, Duran and Grossmann proposed to approximate the max operator with smooth functions. This approach avoids the non-differentiability problem, and reduces the problem into an NLP. However, the smooth approximation is non-convex and its numerical behavior depends on parameters in the approximation function. Later, Grossmann et al. (1998) presented a disjunctive model that overcomes all previous limitations at the cost of introducing integer variables. Alternatively, Navarro-Amorós et al. (2013) presented an MI(N)LP model that maintains the concept of temperature interval. They assumed a maximum number of temperature intervals and dynamically assign process temperatures to each interval. The numerical test presented by the authors showed that the numerical performance is similar to the disjunctive formulation of the PLM. However, the number of constraints and binary variables can be orders of magnitude larger.

In the rest of the paper we first present and overview of the Pinch Location Method. Then we introduce a novel disjunctive reformulation that has better relaxation gap than the disjunctive model presented by Grossmann et al. (1998) and a similar number of variables and equations. A set of numerical test illustrates the performance of the novel approach in examples with different complexity. Finally, we finish with some conclusions.

2. The pinch location method. Overview

In the following paragraphs, we present an overview of the Pinch Location Method. It does not pretend to be a comprehensive description. Notwithstanding, the novel disjunctive formulation is based on it and we consider of interest to introduce the more relevant aspects. For further details, the interested reader is referred to the original work (Duran & Grossmann, 1986).

The pinch analysis assumes that the heat flow of a process stream can be considered constant. If this is not the case in the entire range of temperatures then it is possible to approximate the process streams by different streams with constant heat flows (piecewise linear approximation). Under these conditions, the pinch point occurs always at the inlet temperature of a process stream. Duran and Grossmann (1986) observed that for a given Heat Recovery Approach Temperature (HRAT or ΔT_{min}), if we check all the candidate to pinch point temperatures, the correct one is the temperature with the largest heating and cooling utilities among all the candidates. Fig. 1 with data from Table 1 shows an illustrative example.

Table 1. Stream data for example.

Streams	Tin (ºC)	Tout (ºC)	F (kW/ºC)
H1 (hot)	170	70	3.0
H2 (hot)	150	70	1.5
C1 (cold)	80	140	4.0
C2 (cold)	60	170	2.0

ΔT_{min} = 20 ºC

<Insert Fig. 1>

Fig. 1. Utilities needed for different pinch stream candidates (—— Hot - - - Cold). (a) Pinch candidate H1. (b) Pinch candidate H2. (c) Pinch candidate C1. (d) Pinch candidate C2.

Mathematically, the previous result can be written as follows:

$$\begin{aligned} Q_H &= \max_{p \in P}\left(Q_H^p\right) \\ Q_C &= \max_{p \in P}\left(Q_C^p\right) \end{aligned} \qquad (1)$$

Where P is the index set of all the hot and cold process streams (pinch candidates). $i = 1 \ldots n_H$, $j = 1 \ldots n_C$; and Q_H^p, Q_C^p are the heating and cooling utilities required from each pinch candidate. Using an energy balance, Eq. (1) can be written in terms only of heating (or cooling) utilities:

$$Q_C = \Omega + Q_H \qquad (2)$$

Where Ω is the total heat surplus.

$$\Omega = \sum_{i \in Hot} F_i\left(T_i^{in} - T_i^{out}\right) - \sum_{j \in Cold} f_j\left(t_j^{out} - t_j^{in}\right) \qquad (3)$$

At this point is very important to note that all the temperatures are “shifted temperatures”:

$$\left.\begin{aligned} T_i^{in} &= Tin_i - \frac{\Delta T_{min}}{2} \\ T_i^{out} &= Tout_i - \frac{\Delta T_{min}}{2} \end{aligned}\right\} \; i \text{ is a hot stream}$$
$$\left.\begin{aligned} t_j^{in} &= tin_j + \frac{\Delta T_{min}}{2} \\ t_j^{out} &= tout_j + \frac{\Delta T_{min}}{2} \end{aligned}\right\} \; j \text{ is a cold stream} \qquad (4)$$

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

where *Tin*, *Tout*, *tin*, *tout* are the actual stream process temperatures. Note that T^p is also referred to the shifted scale.

From Eq. (1) and (2), the criterion for the pinch location reduces to:

$$Q_H = \max_{p \in P} \left(Q_H^p \right) \qquad Q_C = \Omega + Q_H \tag{5}$$

It is still necessary to get an explicit equation to calculate the term Q_H^p for each pinch candidate in terms of heat flows and temperatures.

Duran and Grossmann (1986) noted that in order to calculate Q_H^p it is necessary to take into account only the process streams above the pinch because there is not net heat transfer across the pinch. Therefore, considering an energy balance above the pinch we can write:

$$Q_H^p = QA_C^p - QA_H^p \tag{6}$$

where QA_C^p and QA_H^p are the total cold and heat content, respectively, above the pinch of the process.

To calculate QA_H^p (or QA_C^p) in terms of heat flows and temperatures, we only need to calculate the contribution of each hot (or cold) stream above the pinch.

For example, for a hot stream *i*:

- If the inlet and outlet temperatures are greater than the inlet temperature of the pinch candidate *p* $\left(T_i^{in} \geq T_i^{out} \geq T^p\right)$ then the heat content above the pinch is $F_i\left(T_i^{in} - T_i^{out}\right)$.
- If the stream crosses the pinch $\left(T_i^{in} \geq T^p \geq T_i^{out}\right)$ then the heat content above the pinch is $F_i\left(T_i^{in} - T^p\right)$.
- If the stream is below the pinch $\left(T^p \geq T_i^{in} \geq T_i^{out}\right)$ then there is no heat content above the pinch.

Duran and Grossmann (1986) showed that the following expression captures the three cases:

$$QA_i^p = F_i\left[\max\left(0, T_i^{in} - T^p\right) - \max\left(0, T_i^{out} - T^p\right)\right] \tag{7}$$

Following a similar approach, the heat content above the pinch for a cold stream *j* can be calculated by the following expression:

$$QA_j^p = f_j\left[\max\left(0, t_j^{out} - T^p\right) - \max\left(0, t_j^{in} - T^p\right)\right] \tag{8}$$

Note that lower case letters are used for cold streams and capital letters for hot streams.

The final model for the simultaneous optimization and heat integration can then be written as follows:

$$\begin{aligned} \min \ & f(x) + C_H Q_H + C_C Q_C \\ s.t. \ & h(x) = 0 \\ & g(x) \leq 0 \\ & Q_H \geq \sum_{j \in Cold} f_j\left[\max\left(0, t_j^{out} - T^p\right) - \max\left(0, t_j^{in} - T^p\right)\right] \\ & \qquad - \sum_{i \in Hot} F_i\left[\max\left(0, T_i^{in} - T^p\right) - \max\left(0, T_i^{out} - T^p\right)\right] \qquad p \in P \\ & Q_C = Q_H + \sum_{i \in Hot} F_i\left(T_i^{in} - T_i^{out}\right) - \sum_{j \in Cold} f_j\left(t_j^{out} - t_j^{in}\right) \end{aligned} \tag{9}$$

$$Q_H, Q_C, F_i, f_j \geq 0$$

3. Pinch location method. Disjunctive formulation

The formulation in Eq. (9) has the difficulty of the presence of 'max' operators that are non-differentiable. Duran and Grossmann (1986) proposed to use a smooth approximation (see also (Balakrishna & Biegler, 1992)). In that case, the model can be solved using state-of-the-art NLP solvers. The major problem with this approach is that the smooth approximations are highly non-convex and depend on at least one small parameter, which must be fixed by the user, and eventually can also introduce numerical conditioning problems.

To solve all the previous drawbacks, Grossmann et al. (1998) proposed a disjunctive formulation.

The basic idea is to explicitly take into account for each combination of process stream with pinch candidate the three possibilities: the stream is above the pinch, it crosses the pinch or it is below the pinch. The model also takes explicitly into account isothermal streams. The model was solved as an MI(N)LP model using a big-M reformulation. If the stream heat flows (F_i, f_j) are constant, the resulting model (at least the part related with the heat integration) is linear and can be easily added to any flowsheet model.

In this paper, instead of explicitly dealing with the positions of the different streams in relation to the pinch, we use a disjunction to deal directly with the 'max' operators in the model. Let us first consider the disjunctive model of the following expression and its reformulation to an MILP model using the hull reformulation:

$$\phi = \max(0, c^T x) \tag{10}$$

In Eq. (10) $\boldsymbol{c}$ is a vector of known coefficients and $\boldsymbol{x}$ is a vector of variables. An equivalent disjunctive formulation for the previous equation can be written as follows:

$$\begin{bmatrix} Y \\ c^T x \geq 0 \\ \phi = c^T x \\ \underline{x} \leq x \leq \overline{x} \end{bmatrix} \underline{\vee} \begin{bmatrix} \neg Y \\ c^T x \leq 0 \\ \phi = 0 \\ \underline{x} \leq x \leq \overline{x} \end{bmatrix} \tag{11}$$

$$Y \in \{True, False\}$$

If the Boolean variable takes the value «True» the first term in the disjunction is enforced and ϕ must be positive, otherwise ϕ is equal to zero.

The hull reformulation (Grossmann & Trespalacios, 2013) of the previous model –Eq. (11)- is as follows:

$$\begin{aligned} & x = x_1 + x_2 \\ & \phi = \phi_1 + \phi_2 \\ & c^T x_1 \geq 0 \qquad\qquad c^T x_2 \leq 0 \\ & \phi_1 = c^T x_1 \qquad\qquad \phi_2 = 0 \\ & y\underline{x} \leq x_1 \leq y\overline{x} \qquad (1-y)\underline{x} \leq x_2 \leq (1-y)\overline{x} \end{aligned} \tag{12}$$

The model in Eq. (12) introduces new variables and equations. However, this formulation can be simplified taking into account that:

- Variable ϕ_2 is fixed to zero and, therefore, it can be removed.
- The particular value of the x_2 variables is not relevant to the problem (they are not used in the model). It is possible then to lump the term $c^T x_2$ in a single variable:

$$s = -c^T x_2; \qquad s \geq 0 \tag{13}$$

The minus sign is only to force the variable s to be non-negative.

- It is possible to write the model given in Eq. (12) in terms of the original variables *x* and the new variable *s*, without defining new variables. To that end, we multiply the first equation in Eq. (12) by the coefficients *c* and remove variables x_1 and x_2:

$$x = x_1 + x_2 \quad \rightarrow \quad c^T x = c^T x_1 + c^T x_2 \quad \rightarrow \quad c^T x = c^T x_1 - s \quad \rightarrow \quad c^T x_1 = c^T x + s \tag{14}$$

- The last equations in Eq. (12) that force the variables to be zero if the binaries are zero, can be written in terms of the original *x* and *s* variables.

The final hull reformulation can then be written as follows:

$$\begin{aligned} &\phi = c^T x + s \\ &y\phi^{LO} \le \phi \le y\phi^{UP} \\ &(1-y)s^{LO} \le s \le (1-y)s^{UP} \\ &s \ge 0; \;\; \phi \ge 0 \end{aligned} \tag{15}$$

Note that good upper and lower bounds for the *s* and ϕ variables can be easily obtained from the bounds of *x* variables and *c* values.

It is interesting to note that the Eq. (15) can also be obtained from the "max" operator formulated as an optimization problem with complementarity constrains (Biegler, 2010), and re-writing the complementarity constraint as a disjunction (or in terms of binary variables).

$$\phi = \max(0, c^T x) \Rightarrow \begin{cases} \phi = c^T x + s \\ 0 \le \phi \perp s \ge 0 \end{cases} \Rightarrow \begin{gathered} \phi = c^T x + s \\ \begin{bmatrix} Y \\ s = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y \\ \phi = 0 \end{bmatrix} \\ s \ge 0; \quad \phi \ge 0 \end{gathered} \tag{16}$$

The hull reformulation of the disjunctive model in Eq. (16) yields the equations in Eq. (15).

Taking all the previous equations into account, the final model for the simultaneous optimization and heat integration can be written as follows:

$$
\begin{aligned}
\min\ & f(x) + C_H Q_H + C_C Q_C \\
s.t.\ & h(x) = 0 \\
& g(x) \le 0 \\
& Q_C = Q_H + \sum_{i \in Hot} F_i \left(T_i^{in} - T_i^{out}\right) - \sum_{j \in Cold} f_j \left(t_j^{out} - t_j^{in}\right) \\
& Q_H \ge \sum_{j \in Cold} f_j \left[\phi t_{j,p}^{out} - \phi t_{j,p}^{in}\right] - \sum_{i \in Hot} F_i \left[\phi T_{i,p}^{in} - \phi T_{i,p}^{out}\right] \qquad p \in P \\
& \phi t_{j,p}^{out} = t_j^{out} - T^p + st_{j,p}^{out} \qquad j \in Cold;\ \ p \epsilon P \\
& \phi t_{j,p}^{in} = t_j^{in} - T^p + st_{j,p}^{in} \qquad j \in Cold;\ \ p \epsilon P \\
& \phi T_{i,p}^{in} = T_i^{in} - T^p + sT_{i,p}^{in} \qquad i \in Hot;\ \ p \epsilon P \\
& \phi T_{i,p}^{out} = T_i^{out} - T^p + sT_{i,p}^{out} \qquad i \in Hot;\ \ p \epsilon P \\
& st_{j,p}^{in} \le \max\left(0, -\underline{t_j^{in}} + \overline{T^p}\right)\left(1 - yc_j^{in}\right) \\
& \phi t_{j,p}^{in} \le \max\left(0, \overline{t_j^{in}} - \underline{T^p}\right) yc_j^{in} \\
& st_{j,p}^{out} \le \max\left(0, -\underline{t_j^{out}} + \overline{T^p}\right)\left(1 - yc_j^{out}\right) \\
& \phi t_{j,p}^{out} \le \max\left(0, \overline{t_j^{out}} - \underline{T^p}\right) yc_j^{out} \\
& sT_{i,p}^{in} \le \max\left(0, -\underline{T_i^{in}} + \overline{T^p}\right)\left(1 - yh_i^{in}\right) \\
& \phi T_{i,p}^{in} \le \max\left(0, \overline{T_i^{in}} - \underline{T^p}\right) yh_i^{in} \\
& sT_{i,p}^{out} \le \max\left(0, -\underline{T_i^{out}} + \overline{T^p}\right)\left(1 - yh_i^{out}\right) \\
& \phi T_{i,p}^{out} \le \max\left(0, \overline{T_i^{out}} - \underline{T^p}\right) yh_i^{out} \\
& Q_H, Q_C \ge 0 \\
& F_i, \phi T_{i,p}^{in}, \phi T_{i,p}^{out}, sT_{i,p}^{in}, sT_{i,p}^{out} \ge 0 \qquad i \in Hot;\ \ p \in P \\
& f_j, \phi t_{j,p}^{in}, \phi t_{j,p}^{out}, st_{j,p}^{in}, st_{j,p}^{out} \ge 0 \qquad j \in Cold;\ \ p \in P \\
& yc_j^{in}, yc_j^{out} \in \{0,1\}\ \ j \in Cold;\ \ p \in P \\
& yh_i^{in}, yh_i^{out} \in \{0,1\}\ \ i \in Hot;\ \ p \in P
\end{aligned}
\tag{17}
$$

In the previous model, the set *Hot* makes reference to the hot streams, the set *Cold* to the cold streams. The variables *st*, *sT* are equivalent to the '*s*' variable in Eq. (15) and ϕt, ϕT are equivalent to the ϕ variable in Eq. (15). The lower bound of a variable is indicated by a line under that variable, and an upper bound by a line over the variable. Variables *yc* and *yh* are binary variables related to each one of the max operators in the model.

Some final remarks: Based on the bounds of *st*, *sT* and ϕt, ϕT variables, it is possible to fix a priori some variables. For example if:

$$-\underline{t_j^{in}} + \overline{T^p} \le 0 \ \text{ then } \ st_{j,p}^{in} = 0 \ \text{ and } \ yc_j^{in} = 1$$

The novel disjunctive reformulation has fewer Boolean (binary) variables that the disjunctive version presented by Grossmann et al. (1998). The disjunctive formulation proposed by Grossmann et al. (1998) introduces 3 Boolean variables for each combination of hot or cold streams and pinch candidate (the stream is above, crosses or is under the pinch candidate). In contrast, in the present model only two binary variables are needed for each process stream pinch candidate. The total number of binary variables is then:

$$\begin{aligned} &\#Binaries\ (Grossmann\ et\ al.(1998)) = (3n_H + 3n_C)(n_H + n_C) = 3(n_H + n_C)^2 \\ &\#Binaries\ (Present\ work) = (2n_H + 2n_C)(n_H + n_C) = 2(n_H + n_C)^2 \end{aligned} \tag{18}$$

However, the total number of variables is larger, because we must add the 's' variables. But, the total number of constraints is also lower in the new formulation.

Notwithstanding, the most relevant aspect is that the numerical test shows that the new formulation has always smaller relaxation gaps than the original Grossmann et al. (1998) model.

3.1. Extension to isothermal streams and multiple utilities

The inclusion in the model of isothermal streams can be done with at least two different approaches. The first one consists of using a fictitious 1 ºC of variation and calculating the equivalent heat flow assuming that 'dummy' temperature variation. In the second one, we maintain the isothermal condition of the stream. Then the heat added or removed to or from the system can be calculated as:

$$Q_{isothermal} = \lambda m \tag{19}$$

where λ is the specific heat associated with the change of phase, and m is the mass flow rate of the stream. An isothermal stream cannot cross the pinch, therefore to calculate the heat content above the pinch (QA) of the isothermal stream, we can use the following disjunction:

$$\begin{bmatrix} Y^{iso} \\ QA^{iso} = \lambda m \\ T^{iso} \geq T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y^{iso} \\ QA^{iso} = 0 \end{bmatrix} \tag{20}$$

where Y^{iso} is a Boolean variable that takes the value of True if the temperature of the isothermal stream is greater than the pinch candidate temperature. The hull reformulation of the previous disjunction is as follows:

$$\begin{aligned} &QA^{iso} = \lambda m \cdot y^{iso} \\ &T^p - T^{iso} \leq \left(\overline{T^p} - \underline{T^{iso}}\right) y^{iso} \end{aligned} \tag{21}$$

The final model considering isothermal streams can be written as follows:

$$\begin{aligned} \min\ & f(x) + C_H Q_H + C_C Q_C \\ s.t.\ & h(x) = 0 \\ & g(x) \leq 0 \\ & Q_C = Q_H + \sum_{i \in Hot} F_i \left(T_i^{in} - T_i^{out}\right) + \sum_{i \in Hiso} \lambda_i m_i - \sum_{j \in Cold} f_j \left(t_j^{out} - t_j^{in}\right) - \sum_{j \in Ciso} \lambda_j m_j \\ & Q_H \geq \sum_{j \in Cold} f_j \left[\phi t_{j,p}^{out} - \phi t_{j,p}^{in}\right] + \sum_{j \in Ciso} \lambda_j m_j y c_j^{iso} \\ & \qquad - \sum_{i \in Hot} F_i \left[\phi T_{i,p}^{in} - \phi T_{i,p}^{out}\right] - \sum_{i \in Hiso} \lambda_i m_i y h_i^{iso} \qquad p \in P \\ & T^p - T_i^{iso} \leq \left(\overline{T^p} - \underline{T_i^{iso}}\right) y h_i^{iso} \qquad p \in P;\ i \in Hiso \\ & T^p - t_j^{iso} \leq \left(\overline{T^p} - \underline{t_j^{iso}}\right) y c_j^{iso} \qquad p \in P;\ j \in Ciso \\ & \phi t_{j,p}^{out} = t_j^{out} - T^p + s t_{j,p}^{out} \qquad j \in Cold;\ p \epsilon P \\ & \phi t_{j,p}^{in} = t_j^{in} - T^p + s t_{j,p}^{in} \qquad j \in Cold;\ p \epsilon P \end{aligned} \tag{22}$$

$$\phi T_{i,p}^{in} = T_i^{in} - T^p + sT_{i,p}^{in} \qquad i \in Hot;\ \ p \epsilon P$$

$$\phi T_{i,p}^{out} = T_i^{out} - T^p + sT_{i,p}^{out} \qquad i \in Hot;\ \ p \epsilon P$$

$$st_{j,p}^{in} \le \max\left(0, -\underline{t_j^{in}} + \overline{T^p}\right)\left(1 - yc_j^{in}\right)$$

$$\phi t_{j,p}^{in} \le \max\left(0, \overline{t_j^{in}} - \underline{T^p}\right) yc_j^{in}$$

$$st_{j,p}^{out} \le \max\left(0, -\underline{t_j^{out}} + \overline{T^p}\right)\left(1 - yc_j^{out}\right)$$

$$\phi t_{j,p}^{out} \le \max\left(0, \overline{t_j^{out}} - \underline{T^p}\right) yc_j^{out}$$

$$sT_{i,p}^{in} \le \max\left(0, -\underline{T_i^{in}} + \overline{T^p}\right)\left(1 - yh_i^{in}\right)$$

$$\phi T_{i,p}^{in} \le \max\left(0, \overline{T_i^{in}} - \underline{T^p}\right) yh_i^{in}$$

$$sT_{i,p}^{out} \le \max\left(0, -\underline{T_i^{out}} + \overline{T^p}\right)\left(1 - yh_i^{out}\right)$$

$$\phi T_{i,p}^{out} \le \max\left(0, \overline{T_i^{out}} - \underline{T^p}\right) yh_i^{out}$$

$$Q_H, Q_C \ge 0$$

$$F_i, \phi T_{i,p}^{in}, \phi T_{i,p}^{out}, sT_{i,p}^{in}, sT_{i,p}^{out} \ge 0 \qquad i \in Hot;\ \ p \in P$$

$$f_j, \phi t_{j,p}^{in}, \phi t_{j,p}^{out}, st_{j,p}^{in}, st_{j,p}^{out} \ge 0 \qquad j \in Cold;\ \ p \in P$$

$$yc_j^{in}, yc_j^{out} \in \{0,1\}\ \ j \in Cold;\ \ p \in P$$

$$yh_i^{in}, yh_i^{out} \in \{0,1\}\ \ i \in Hot;\ \ p \in P$$

Note that in Eq. (22) the sets *Hot* and *Cold* make reference to the non-isothermal process streams, and the sets *Hiso* and *Ciso* refer to the hot and cold isothermal streams.

The introduction of multiple utilities is straightforward. In this case, the inlet and outlet temperatures are known and the variable is the heat flow (*f* or *F*) in non-isothermal streams and the mass flowrate in the case of isothermal streams.

4. Case studies: Heat integration examples

In this paper, a series of examples are presented to illustrate the performance of the method. Examples include: fixed and variable stream temperatures (MILP); variable stream temperatures with a penalty function that simulates the behavior of a system; simultaneous process optimization and heat integration using a hybrid simulation-optimization approach, where the flowsheet is solved by a commercial process simulator, and the heat integration model is in equation form; and variable stream temperatures with addition of multiple utilities.

Calculations of fixed and variable stream temperature problems were carried out in GAMS (Rosenthal, 2012). Calculations of the simultaneous process optimization and heat integration problem were performed in TOMLAB-MATLAB (Holmström, 1999) and the simulations were performed on Aspen HYSYS v.8.4. (Hyprotech, 1995 - 2011). The computations were performed in a computer with a 3.60 GHz Intel® Core™ i7 Processor and 8 GB of RAM under Windows 7.

All the problems were solved for a minimum heat recovery approach temperature (ΔT_{min}) of 10ºC.

4.1. Case study 1: Process with fixed stream conditions (MILP)

The first example solved (test problem 1) consists of a problem in which heat flow rates, and inlet and outlet temperatures are known and constant. The objective consists of determining the minimum utility costs. This problem has to be solved as a mixed integer linear problem (MILP) because it includes continuous and binary variables and all the model equations are linear. Data corresponding to test problem 1 are shown in Table 2.

Table 2. Data for test problem 1 (fixed temperatures).

Test problem 1: 6 hot and 6 cold streams							
Hot stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)	Cold stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)
H1	1.00	280	100	C1	0.50	30	200
H2	3.00	200	80	C2	1.50	60	90
H3	1.00	220	150	C3	2.00	70	170
H4	2.00	210	90	C4	3.00	110	230
H5	1.00	250	180	C5	1.50	90	140
H6	2.00	270	120	C6	4.00	120	250

Price of steam: $80 kg/kW.
Price of cooling water: $20 kg/kW.

To validate the model (see Eq.(17)), our results are compared with the results obtained by the pinch location method, in its disjunctive version, proposed by Grossmann et al. (1998) and the results obtained according to the method proposed by Navarro-Amorós et al. (2013).

The solution of this example is shown in Table 3.

Table 3. Computational statistics and solution of test problem 1 (fixed temperatures).

Results test problem 1			
	Present work	GYK model	Navarro-Amorós et al.
No equations	890	1622	6059
No variables	886	614	1169
No binary variables	288	432	900
CPU time (s)[a]	0.20	0.27	0.35
Heating requirements (kW/kg)	80.00	80.00	80.00
Cooling requirements (kW/kg)	15.00	15.00	15.00
Optimal solution ($)	6700.00	6700.00	6700.00
Solution of relaxed problem	6700.00	5200.00	0.00

[a]Intel Core i7-4790 3.60GHz, using CPLEX 12.4.6 for MILP.

The results show that the number of continuous and binary variables and total equations is lower in the proposed model versus the other methods, even though the total number of variables is larger than in the original disjunctive PLM. The optimal solution ($6700) is exactly the same in all cases. Regarding the solution of the relaxed problem, the proposed model obtains the best possible solution.

4.2. Case study 2: Process with variable stream conditions (MILP)

In the following examples, inlet and outlet temperatures for hot and cold streams are variables. For these examples, we have assumed that temperature variation does not affect the rest of the process. To validate our model (see Eq.(17)), these test problems are also compared with results obtained by the pinch location method (Grossmann et al., 1998) and the method proposed by Navarro-Amorós et al. (2013).

As in the preceding case, the objective function consists of minimizing the utility cost, remaining the heat flow rates as constant values.

Data for different test problems are shown in Table 4.

Table 4. Data for test problem 2-5 (variable temperatures).

Hot stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)	Cold stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)
Test problem 2: 3 hot and 3 cold streams							
H1	0.15	180 - 260	30 - 50	C1	0.20	15 - 135	170 - 190
H2	0.50	120 - 220	75 - 95	C2	0.30	110 - 190	225 - 235
H3	0.10	110 - 155	90 - 100	C3	0.15	70 - 130	140 - 150
Test problem 3: 4 hot and 4 cold streams							
H1	0.15	230 - 260	30 - 50	C1	0.20	10 - 40	170 - 190
H2	0.50	135 - 155	110 - 150	C2	0.30	90 - 110	180 - 225
H3	0.25	80 - 100	20 - 30	C3	0.15	125 - 160	225 - 235
H4	0.30	110 - 120	80 - 100	C4	0.40	130 - 150	250 - 280
Test problem 4: 16 hot and 12 cold streams							
H1	30.00	210 - 255	65 - 90	C1	40.00	25 - 60	160 - 195
H2	45.00	170 - 210	30 - 45	C2	60.00	125 - 160	250 - 295
H3	0.10	95 - 120	35 - 60	C3	0.10	160 - 190	245 - 300
H4	0.10	105 - 135	30 - 60	C4	0.10	155 - 200	240 - 280
H5	0.10	100 - 120	20 - 50	C5	0.10	160 - 195	250 - 290
H6	0.10	100 - 125	40 - 50	C6	0.10	145 - 175	255 - 295
H7	0.10	105 - 130	45 - 60	C7	0.10	160 - 205	235 - 280
H8	0.10	90 - 115	40 - 75	C8	0.10	160 - 190	245 - 300
H9	0.10	95 - 120	35 - 60	C9	0.10	155 - 200	240 - 280
H10	0.10	105 - 135	30 - 60	C10	0.10	160 - 195	250 - 290
H11	0.10	100 - 120	20 - 50	C11	0.10	145 - 175	255 - 295
H12	0.10	100 - 125	40 - 50	C12	0.10	160 - 205	235 - 280
H13	0.10	105 - 130	45 - 60				
H14	0.10	85 - 115	30 - 75				
H15	0.10	105 - 135	40 - 55				
H16	0.10	100 - 125	35 - 65				
Test problem 5: 20 hot and 20 cold streams							
H1	6.00	360 - 440	108 - 132	C1	14.00	144 - 176	360 - 440
H2	2.00	306 - 374	108 - 132	C2	3.00	90 - 110	225 - 275
H3	0.50	342 - 418	135 - 165	C3	0.40	45 - 55	270 - 330
H4	8.00	270 - 330	90 - 110	C4	2.50	180 - 220	342 - 418
H5	3.00	378 - 462	144 - 176	C5	2.00	135 - 165	405 - 495
H6	4.00	351 - 429	99 - 121	C6	6.00	90 - 110	162 - 198
H7	0.20	324 - 396	180 - 220	C7	1.50	180 - 220	315 - 385
H8	0.60	252 - 275	117 - 143	C8	0.20	108 - 132	297 - 363
H9	1.50	225 - 275	72 - 88	C9	5.50	99 - 121	198 - 242
H10	4.00	297 - 363	153 - 187	C10	3.00	171 - 209	324 - 396
H11	12.00	387 - 473	270 - 330	C11	8.00	234 - 286	378 - 462
H12	8.00	180 - 220	90 - 110	C12	12.00	72 - 88	162 - 198
H13	5.00	135 - 165	63 - 77	C13	0.30	117 - 143	351 - 429
H14	0.06	297 - 363	162 - 198	C14	4.50	162 - 198	234 - 286
H15	0.30	333 - 407	103 - 127	C15	1.00	139 - 170	328 - 401
H16	6.00	319 - 391	94 - 115	C16	0.10	85 - 104	432 - 528
H17	0.90	279 - 341	117 - 143	C17	7.00	157 - 192	346 - 423
H18	3.00	234 - 286	81 - 99	C18	2.00	117 - 143	261 - 319
H19	1.00	270 - 330	103 - 127	C19	0.50	189 - 231	387 - 473
H20	0.30	238 - 291	171 - 209	C20	1.70	207 - 253	333 - 407

Price of steam: \$80 kg/kW.
Price of cooling water: \$20 kg/kW.

In Table 5 and Table 6 we can see the results obtained and some relevant parameters of the test problems.

Table 5. Results of test problem 2-5 (variable temperatures).

Hot stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)	Cold stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)
Test problem 2: 3 hot and 3 cold streams							
H1	0.15	260.00	50.00	C1	0.20	15.00	190.00
H2	0.50	210.00	95.00	C2	0.30	110.00	225.00
H3	0.10	110.00	100.00	C3	0.15	70.00	150.00
Test problem 3: 4 hot and 4 cold streams							
H1	0.15	260.00	50.00	C1	0.20	10.00	170.00
H2	0.50	155.00	120.50	C2	0.30	90.00	180.00
H3	0.25	80.00	30.00	C3	0.15	160.00	225.00
H4	0.30	110.00	100.00	C4	0.40	150.00	250.00
Test problem 4: 16 hot and 12 cold streams							
H1	30.00	255.00	90.00	C1	40.00	25.00	160.00
H2	45.00	210.00	45.00	C2	60.00	136.32	250.00
H3	0.10	95.00	60.00	C3	0.10	190.00	245.00
H4	0.10	105.00	60.00	C4	0.10	200.00	240.00
H5	0.10	100.00	50.00	C5	0.10	195.00	250.00
H6	0.10	100.00	50.00	C6	0.10	175.00	255.00
H7	0.10	105.00	60.00	C7	0.10	205.00	235.00
H8	0.10	90.00	75.00	C8	0.10	190.00	245.00
H9	0.10	95.00	60.00	C9	0.10	200.00	240.00
H10	0.10	105.00	60.00	C10	0.10	195.00	250.00
H11	0.10	100.00	50.00	C11	0.10	175.00	255.00
H12	0.10	100.00	50.00	C12	0.10	205.00	235.00
H13	0.10	105.00	60.00				
H14	0.10	85.00	75.00				
H15	0.10	105.00	55.00				
H16	0.10	100.00	65.00				
Test problem 5: 20 hot and 20 cold streams							
H1	6.00	423.00	127.00	C1	14.00	149.00	365.00
H2	2.00	337.00	127.00	C2	3.00	95.00	270.00
H3	0.50	337.00	149.00	C3	0.40	50.00	335.00
H4	8.00	325.00	105.00	C4	2.50	225.00	423.00
H5	3.00	437.00	149.00	C5	2.00	140.00	437.00
H6	4.00	365.00	116.00	C6	6.00	95.00	182.00
H7	0.20	365.00	175.00	C7	1.50	225.00	365.00
H8	0.60	286.00	138.00	C8	0.20	113.00	365.00
H9	1.50	270.00	83.00	C9	5.50	104.00	247.00
H10	4.00	337.00	182.00	C10	3.00	214.00	401.00
H11	12.00	423.00	270.00	C11	8.00	286.00	383.00
H12	8.00	182.00	105.00	C12	12.00	77.00	203.00
H13	5.00	130.00	72.00	C13	0.30	122.00	423.00
H14	0.06	337.00	162.00	C14	4.50	167.00	291.00
H15	0.30	401.00	122.00	C15	1.00	144.00	406.00
H16	6.00	365.00	110.00	C16	0.10	90.00	437.00
H17	0.90	336.00	138.00	C17	7.00	162.00	365.00
H18	3.00	236.00	94.00	C18	2.00	122.00	286.00
H19	1.00	325.00	122.00	C19	0.50	236.00	401.00
H20	0.30	286.00	167.00	C20	1.70	236.00	338.00

Table 6. Computational statistics and solution of test problem 2-5 (variable temperatures).

	No equations	No variables	No binary variables	CPU time (s)[a]	Heating requirements (kW/kg)	Cooling requirements (kW/kg)	Optimal solution ($)	Solution of relaxed problem
Test problem 2								
Present work	230	237	42	0.03	0.0	8.5	170.0	0.00
GYK model	416	171	108	0.45	0.0	8.5	170.0	0.00
Navarro-Amorós	3047	1247	216	0.75	0.0	8.5	170.0	0.00
Test problem 3								
Present work	402	411	26	0.02	49.5	5.0	4060.0	3282.73
GYK model	730	291	192	0.11	49.5	5.0	4060.0	620.00
Navarro-Amorós	5375	2125	307	0.22	49.5	5.0	4060.0	3124.02
Test problem 4								
Present work	4762	4791	364	0.14	1694.0	1852.2	172564.0	84768.34
GYK model	8710	3251	2352	0.42	1694.0	1852.2	172564.0	0.00
Navarro-Amorós	44719	5857	4763	1000.05	1694.0	1852.2	172564.0	0.00
Test problem 5								
Present work	9682	9723	704	0.36	0.0	116.3	2326.0	0.00
GYK model	17722	6563	4800	37.74	0.0	116.3	2326.0	0.00
Navarro-Amorós	109799	11725	9683	1161.33	0.0	116.3	2326.0	0.00

[a]Intel Core i7-4790 3.60GHz, using CPLEX 12.4.6 for MILP.

As it is shown in Table 6, for test problem 2, the optimal solution is $170 for all cases, and the relaxation gap for all methods is bad because the solution to the relaxed problem is equal to zero.

The optimal solution to test problem 3 is $4060 and the relaxation gap of the proposed model is much better than the relaxation gap obtained by the other methods (19 % in the novel model, 84 % in the Grossmann Disjunctive model and 23 % in the model by Navarro-Amorós et al. (2013)).

The same behavior occurs on test problem 4. The optimal solution to test problem 4 is $172564 and the relaxation gap is better than the gap obtained by the others models. It is the only model with relaxation different from zero.

Regarding the test problem 5, the optimal solution and the relaxation gap is the same for all cases. However, it is interesting to remark the CPU time difference between the models. Indubitably, our model is much faster than the other methods, allowing to solve problems with a high number of hot and cold streams.

4.3. Case study 3: Process with variable stream conditions with penalty function (MINLP)

In previous examples, we assumed that the operating conditions do not affect the heat integration and, therefore, basically the optimal solution select the temperatures that allow the maximum heat integration. In order to simulate the behavior of an actual system, we propose an example in which the temperatures for the optimal operating conditions without heat integration are known and any deviation of those values carries out a penalty in the total cost.

In this case study (test problem 6), the objective function consists of two parts; the first one concerns the cost of utilities, and the second term penalizes the deviation of temperature from a given set value:

$$\min\ (cost_H Q_H + cost_C Q_C) +\ w \cdot \sum_{k \in ST} \left(T_k^{in} - TM_k^{in}\right)^2 + (T_k^{out} - TM_k^{out})^2 \qquad (23)$$

where *w* is the penalization factor and *TM* are the optimal temperatures of the non-heat integrated process (we have assumed that the optimal temperatures are the mean values between the upper and lower bounds).

Data used in this case are shown in Table 7.

Table 7. Data for test problem 6 (non-linear, variable temperatures).

Test problem 6 (non-linear): 3 hot and 3 cold streams							
Hot stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)	Cold stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)
H1	0.15	180 - 260	30 - 50	C1	0.20	15 - 25	170 - 190
H2	0.50	120 - 140	75 - 95	C2	0.30	110 - 140	225 - 235
H3	0.10	110 - 155	90 - 100	C3	0.15	70 - 100	140 - 150

Price of steam: $80 kg/kW.
Price of cooling water: $20 kg/kW.

In this case, the model is a non-convex MINLP problem. The optimal solution achieved with our model ($2900.5) is better than the solution obtained by the other models (the same initial point was used in all the cases). Furthermore, the relaxation gap is considerably reduced compared to the other models. For this case, the results and the other relevant parameters are shown in Table 8 and Table 9, respectively.

Table 8. Results of test problem 6 (non-lineal, variable temperatures).

Test problem 6 (non-linear): 3 hot and 3 cold streams							
Hot stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)	Cold stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)
H1	0.15	260.00	50.00	C1	0.20	15.00	190.00
H2	0.50	210.00	95.00	C2	0.30	110.00	225.00
H3	0.10	110.00	100.00	C3	0.15	70.00	150.00

Table 9. Computational statistics and solution of test problem 5 (non-linear, variable temperatures).

Test problem 6			
	Present work	GYK model	Navarro-Amorós et al.
No equations	230	416	3047
No variables	237	171	1247
No binary variables	17	108	216
CPU time (s)[a]	0.02	0.68	3.33
Heating requirements (kW/kg)	29.25	28.90	29.25
Cooling requirements (kW/kg)	10.80	12.76	11.11
Optimal solution ($)	2900.50	2918.63	2903.63
Solution of relaxed problem	2002.62	767.00	1904.73

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

Optimization has been performed with different weights of the penalization factor *w* (see Eq. (23)). The optimal results are shown in Fig. 2.

<Insert Fig. 2>

Fig. 2. Optimal solutions to test problem 6 for different penalization factors.

The results show that when the penalty factor is lower than two, the optimal solution is mainly affected by the utility costs. However, when the penalty factor increases, the term that penalizes the deviation of temperature from the central values between the upper and lower bounds is the most important factor, making the optimal solution constant (around $3300).

4.4. Case study 4: Hybrid simulation-optimization process (MINLP)

Another case study performed was a hybrid simulation-optimization problem, in which the heat integration in the form of explicit equations is combined with the simulation of a chemical process. The process was simulated in Aspen HYSYS v.8.4. (Hyprotech, 1995 - 2011). As MINLP solver, we use an in-house implementation (Caballero et al., 2014) of a basic Branch and Bound algorithm interfaced with TOMLAB-MATLAB (Holmström, 1999).

The following case study corresponds to the design of a natural gas plant (Seider et al., 1999). Consider that we want to obtain a gaseous product with at least 4500 kmol/h of nC_4 and lighter species, with a combined mole percentage of at least 99.5 % and at 2026 kPa. The liquid product is required to be at least 1034 kPa, with at least 30 kmol/h of nC_5 and nC_6 and a combined mole percentage of at least 65 %. Data for the problem are shown in Table 10.

Table 10. Feed data to natural gas flowsheet.

Feed stream		
Molar flow	5000.0	kmol/h
Composition (molar flows)		
C_1	4138.0	kmol/h
C_2	435.5	kmol/h
C_3	205.5	kmol/h
nC_4	70.5	kmol/h
nC_5	28.5	kmol/h
nC_6	16.5	kmol/h
N_2	105.5	kmol/h
Temperature	20.0	ºC
Pressure	1013.0	kPa
Thermodynamics (fluid package)	Peng-Robinson	

The flowsheet for the process is shown in Fig. 3. The feed is compressed to 2280 kPa, and is cooled before entering the flash unit, at 2103 kPa. The flash products are heated. The liquid product enters in the second flash vessel, at 2068 kPa. Its liquid product is fed to the distillation column, where most of the propane is removed by overhead. The column has 12 theoretical trays, and the feed enters to the fourth tray from the top. The column recovers 99 % of C_3 in the distillate and 99 % of nC_5 in the bottoms.

<Insert Fig. 3>

Fig. 3. Process flow diagram for natural gas synthesis.

We assume that the cost of the process are not considerably affected (the TAC of the system is around $3.039 million/year, without the heat and cooling requirements). As a result, it is not taken into account, but changes in temperatures modified the operating conditions and the purity constraints must be met. Therefore, the objective of this problem consists of minimizing the heat supplied by the hot and the cold utilities. The streams affected by the heat integration were all inlet and outlet streams of the heat exchangers, and the streams of the condenser (the reboiler was not taken into account because, by the temperature differences, it cannot be heat integrated). The temperature bounds for all streams, the main constraints, and the optimal solution are shown in Table 11.

Table 11. Data and optimal solution to natural gas flowsheet.

	Streams	Temperature range (ºC)	Solution temperature (ºC)
H1	In HE1	88.82 – 88.82	88.82
	Out HE1	-30.00 – -20.00	-20.00
H2	In HE2	-30.00 – -20.00	-20.00
	Out HE2	0.00 – 60.00	60.00
H3	In HE3	-30.00 – -20.00	-20.00
	Out HE3	0.00 – 60.00	60.00
Restrictions	Range	Optimal value	
Molar flow light product (kmol/h)	≥ 4500	4950.3521	
Molar frac. (nC4 + lighter) in light product	≥ 0.995	0.9977	
Molar flow heavy product (kmol/h)	≥ 30	49.6479	
Molar frac. (nC5 + nC6) in heavy product	≥ 0.65	0.6755	
Solution parameters			
Number of equations	111		
Number of variables	78		
Number of binary variables	32		
Optimal solution			
Heating requirements (kW)	0.000		
Cooling requirements (kW)	2,465.904		
Optimal solution ($)	12,329.520		
Total Annualized Cost ($/year)	3,051,293.981		

Table 11 shows that the optimal solution satisfies all the constraints. Furthermore, the heat integration of the system eliminates the need for hot utility (except the hot utility needed in the reboiler, which does not affect the heat exchanger network); only cold utilities are needed to satisfy the requirements of the process. The heat exchanger network is shown in Fig. 4.

<Insert Fig. 4>

Fig. 4. Heat exchanger network for natural gas process.

This case study shows that the proposed model can be implemented to optimize hybrid simulation-optimization problems, in which the process simulation is combined with the heat integration in the form of explicit equations.

4.5. Case study 5: Extension of the method to multiple utilities (MILP)

As a final point, the method has been extended to the case of multiple utilities. In the next examples, all inlet and outlet streams are variables.

The first example (test problem 7) corresponds to a problem with four hot streams and six cold streams. We have considered the possibility of adding a new hot utility ($TH_{MP} = 254°C,$). The objective function consists of minimizing the utility costs ($C_{HP}Q_{HP} + C_{MP}Q_{MP} + C_C Q_C$).

The second example (test problem 8) corresponds to a problem with two hot streams and one cold stream. We have consider the possibility of adding two new hot utilities, ($TH_{MP} = 160°C$) and ($TH_{LP} = 130ºC$). The objective function consists of minimizing the utility costs ($C_{HP}Q_{HP} + C_{MP}Q_{MP} + C_{LP}Q_{LP} + C_C Q_C$).

Data used in this case study are shown in Table 12.

Table 12. Data for case study 5 (non-linear, variable temperatures).

Hot stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)	Cold stream	FCp (kW/ºC)	Inlet T (ºC)	Outlet T (ºC)
Test problem 7: 4 hot and 6 cold streams							
H1	0.100	315 - 327	20 - 30	C1	0.200	85 - 110	290 - 330
H2	0.250	210 - 220	140 - 160	C2	0.070	25 - 55	160 - 185
H3	0.020	200 - 220	50 - 60	C3	0.175	70 - 95	120 - 140
H4	0.340	155 - 160	40 - 45	C4	0.060	55 - 70	150 - 185
				C5	0.200	135 - 150	270 - 320
				C6	0.300	8 - 30	42 - 75
Test problem 8: 2 hot and 1 cold stream							
H1	10.000	95 - 115	15 - 35	C1	7.500	15 - 35	175 - 195
H2	5.000	175 - 195	25 - 45				

Price of HP steam: $160 kg/kW.
Price of MP steam: $110 kg/kW.
Price of LP steam: $50 kg/kW.
Price of cooling water: $10 kg/kW.

Results have been compared with the same process, but taking into account only single utilities, where the objective function consist of minimizing the utility costs ($C_H Q_H + C_C Q_C$).

For test problem 7, the optimal solution achieved is $2533.0, while the optimal solution obtained taking into account only single utilities is $3168.0. Regarding the solution obtained for test problem 8, the optimal solution achieved adding two utilities is $16875.0, while the optimal solution obtained taking into account only one hot utility is $24750.0.

The results obtained and other relevant parameters of case study 5 are shown in Table 13 and Table 14, respectively.

Table 13. Computational statistics and solution of test problem 7 (variable temperatures).

	Test problem 7 (single utilities)	Test problem 7 (multiple utilities)
No equations	622	749
No variables	633	547
No binary variables	29	29
CPU time (s)[a]	0.11	0.86
Heating requirements (kW/kg)		
HP steam	19.80	7.10
MP steam	-	12.70
Cooling requirements (kW/kg)	0.00	0.0
Optimal solution ($)	3168.00	2533.00
Solution of relaxed problem	2912.00	2357.00

[a]Intel Core i7-4790 3.60GHz, using CPLEX 12.4.6 for MILP.

Table 14. Computational statistics and solution of test problem 8 (variable temperatures).

	Test problem 8 (single utilities)	Test problem 8 (multiple utilities)
No equations	62	160
No variables	66	120
No binary variables	6	6
CPU time (s)[a]	0.08	0.52
Heating requirements (kW/kg)		
HP steam	125.00	12.50
MP steam	-	75.00
LP steam	-	37.50
Cooling requirements (kW/kg)	475.00	475.00
Optimal solution ($)	24750.00	16875.00
Solution of relaxed problem	7750.00	16375.00

[a]Intel Core i7-4790 3.60GHz, using CPLEX 12.4.6 for MILP.

In addition, as it is shown in Table 13 and Table 14, the relaxation gap is reasonable.

5. Conclusions

We have proposed a new MILP model based on disjunctive programming for the simultaneous optimization and energy integration of systems with variable input and output process stream temperatures. This model allows us to obtain a robust alternative to the disjunctive model for the simultaneous flowsheet optimization and heat integration proposed by Grossmann et al. (1998).

The results show that our model is very competitive from the point of view of CPU time, includes fewer binary variables and equations, although the number of total variables is slightly larger than the original disjunctive formulation. Furthermore, the proposed model improves the relaxation gap, compared to two different methods.

Different test problems have shown that the model is robust and reliable. One of the main characteristics of the novel model is that it can be ‘added’ to any model with almost no modifications of the existing model and, therefore, its implementation is straightforward. If the heat flows in the original model are not affected by the temperature then the new equations are all linear, with some integer variables, and therefore we do not expect a significant increase in the complexity of the original model.

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Nomenclature

C_C	Cost of the cold utility
C_H	Cost of the heat utility
F_i	Heat capacity flowrate of hot stream *i*
f_j	Heat capacity flowrate of cold stream *j*
i	Hot stream
j	Cold stream
m	Mass flow rate of a stream
n_c	Number of cold streams

n_h Number of hot streams
P Index set of all the hot and cold process streams (pinch candidates)
Q_C Heat removed by the cold utility
Q_H Heat provided by the hot utility
Q_C^p Cooling utilities required form each pinch candidate
Q_H^p Heating utilities required form each pinch candidate
QA_C^p Total cool content above the pinch
QA_H^p Total heat content above the pinch
T^p Pinch point temperature
T_i^{in} Inlet temperature for the hot stream *i*
T_i^{out} Outlet temperature for the hot stream *i*
t_j^{in} Inlet temperature for the cold stream *j*
t_j^{out} Outlet temperature for the cold stream *j*
Tin_i Actual inlet temperature for the hot stream *i*
tin_j Actual inlet temperature for the cold stream *j*
$Tout_i$ Actual outlet temperature for the hot stream *i*
$tout_j$ Actual inlet temperature for the cold stream *j*
TM Optimal temperatures of the non-heat integrated process
w Penalization factor
Y^{iso} Boolean variable that takes the "True" value if the temperature of the isothermal stream is greater than the pinch candidate temperature
yc Binary variable related to the max operator that represents the cold streams
yh Binary variable related to the max operator that represents the hot streams
ΔT_{min} Minimum heat recovery approach temperature
λ Specific heat associated with the charge of phase
Ω Total heat surplus

References

Ahmad S, Linnhoff B, Smith R. Cost optimum heat exchanger networks—2. targets and design for detailed capital cost models. Comput Chem Eng 1990; 14:751-767.
Ahmetović E, Ibrić N, Kravanja Z, Grossmann IE. Water and energy integration: A comprehensive literature review of non-isothermal water network synthesis. Comput Chem Eng 2015; 82:144-171.
Ahmetović E, Kravanja Z. Simultaneous synthesis of process water and heat exchanger networks. Energy 2013; 57:236-250.
Balakrishna S, Biegler LT. Targeting strategies for the synthesis and energy integration of nonisothermal reactor networks. Ind Eng Chem Prod DD 1992; 31:2152.
Biegler LT. Nonlinear Programming. Concepts, Algorithms, and Applications to Chemical Processes. SIAM. Society for Industrial and Applied Mathematics; 2010.
Caballero JA, Grossmann IE. Structural considerations and modeling in the synthesis of heat-integrated-thermally coupled distillation sequences. Ind Eng Chem Res 2006; 45:8454-8474.
Caballero JA, Navarro MA, Ruiz-Femenia R, Grossmann IE. Integration of different models in the design of chemical processes: Application to the design of a power plant. Appl Energy 2014; 124:256-273.
Corbetta M, Grossmann IE, Manenti F. Process simulator-based optimization of biorefinery downstream processes under the Generalized Disjunctive Programming framework. Comput Chem Eng 2016; 88:73-85.
Dunn RF, El-Halwagi MM. Process integration technology review: background and applications in the chemical process industry. J Chem Technol Biotechnol 2003; 78:1011-1021.

Duran MA, Grossmann IE. Simultaneous optimization and heat integration of chemical processes. AIChE J 1986; 32:123-138.

Fernández I, Renedo CJ, Pérez SF, Ortiz A, Mañana M. A review: Energy recovery in batch processes. Renew Sust Energ Rev 2012; 16:2260-2277.

Furman KC, Sahinidis NV. A critical review and annotated bibliography for heat exchanger network synthesis in the 20th Century. Ind Eng Chem Res 2002; 41:2335-2370.

Grossmann IE, Caballero JA, Yeomans H. Mathematical programming approaches to the synthesis of chemical process systems. Korean J Chem Eng 1999; 16:407-426.

Grossmann IE, Trespalacios F. Systematic modeling of discrete-continuous optimization models through generalized disjunctive programming. AIChE J 2013; 59:3276-3295.

Grossmann IE, Yeomans H, Kravanja Z. A rigorous disjunctive optimization model for simultaneous flowsheet optimization and heat integration. Comput Chem Eng 1998; 22:A157-A164.

Gundersen T, Naess L. The synthesis of cost optimal heat exchanger networks. Comput Chem Eng 1988; 12:503-530.

Holmström K. The TOMLAB optimization environment in Matlab. Adv Model Optim 1999; 1:47-69.

Hyprotech, Ltd. HYSYS. Hyprotech Ltd. 1995 - 2011.

Jezowski J. Exchanger Network Grassroot and Retrofit Design. The Review of the State-of-the-Art: Part II. Heat Exchanger Network Synthesis by Mathematical Methods and Approaches for Retrofit Design. Hung J Ind Chem 1994a; 22:295-308.

Jezowski J. Heat Exchanger Network Grassroot and Retrofit Design. The Review of the State-of-the-Art: Part I. Heat Exchanger Network Targeting and Insight Based Methods of Synthesis. Hung J Ind Chem 1994b; 22:279-294.

Klemeš JJ, Kravanja Z. Forty years of Heat Integration: Pinch Analysis (PA) and Mathematical Programming (MP). Curr Opin Chem Eng 2013; 2:461-474.

Lang YD, Biegler LT, Grossmann IE. Simultaneous optimization and heat integration with process simulators. Comput Chem Eng 1988; 12:311-327.

Linhoff B, Hindmarsh E. The pinch design method for heat exchange network. Chem Eng Sci 1983; 38:745-763.

Linnhoff B. Pinch analysis - a state-of-the-art overview. Chem Eng Res Des 1993; 71:503-522.

Linnhoff B, Ahmad S. Cost optimum heat exchanger networks—1. Minimum energy and capital using simple models for capital cost. Comput Chem Eng 1990; 14:729-750.

Linnhoff B, Flower JR. Synthesis of heat exchanger networks: I. Systematic generation of energy optimal networks. AIChE J 1978; 24:633-642.

Morar M, Agachi PS. Review: Important contributions in development and improvement of the heat integration techniques. Comput Chem Eng 2010; 34:1171-1179.

Navarro-Amorós MA, Caballero JA, Ruiz-Femenia R, Grossmann IE. An alternative disjunctive optimization model for heat integration with variable temperatures. Comput Chem Eng 2013; 56:12-26.

Onishi VC, Ravagnani MASS, Caballero JA. Simultaneous synthesis of heat exchanger networks with pressure recovery: Optimal integration between heat and work. AIChE J 2014a; 60:893-908.

Onishi VC, Ravagnani MASS, Caballero JA. Simultaneous synthesis of work exchange networks with heat integration. Chem Eng Sci 2014b; 112:87-107.

Papoulias SA, Grossmann IE. A structural optimization approach in process synthesis. Part II: Heat recovery networks. Comput Chem Eng 1983; 7:707-721.

Quirante N, Caballero JA. Large scale optimization of a sour water stripping plant using surrogate models. Comput Chem Eng 2016; 92:143-162.

Rosenthal RE. GAMS - A user's guide. Washington, DC: GAMS Development Corporation; 2012.

SCOPUS Database. Scopus Database. 2016.

Seider WD, Seader JD, Lewin DR. Process Design Principles: Synthesis, Analysis, and Evaluation. Wiley; 1999.

Sreepathi BK, Rangaiah GP. Review of heat exchanger network retrofitting methodologies and their applications. Ind Eng Chem Res 2014; 53:11205-11220.

Wechsung A, Aspelund A, Gundepsen T, Barton PI. Synthesis of Heat Exchanger Networks at Subambient Conditions with Compression and Expansion of Process Streams. AIChE J 2011; 57:2090-2108.

Yee TF, Grossmann IE. Simulatneous optimization models for heat integration II. Heat exchanger network synthesis. Comput Chem Eng 1990; 14:1165-1184.

Yee TF, Grossmann IE, Kravanja Z. Simultaneous optimization models for heat integration III. Process and heat exchanger network optimization. Comput Chem Eng 1990; 14:1185-1200.

Figure(s)

Figure captions

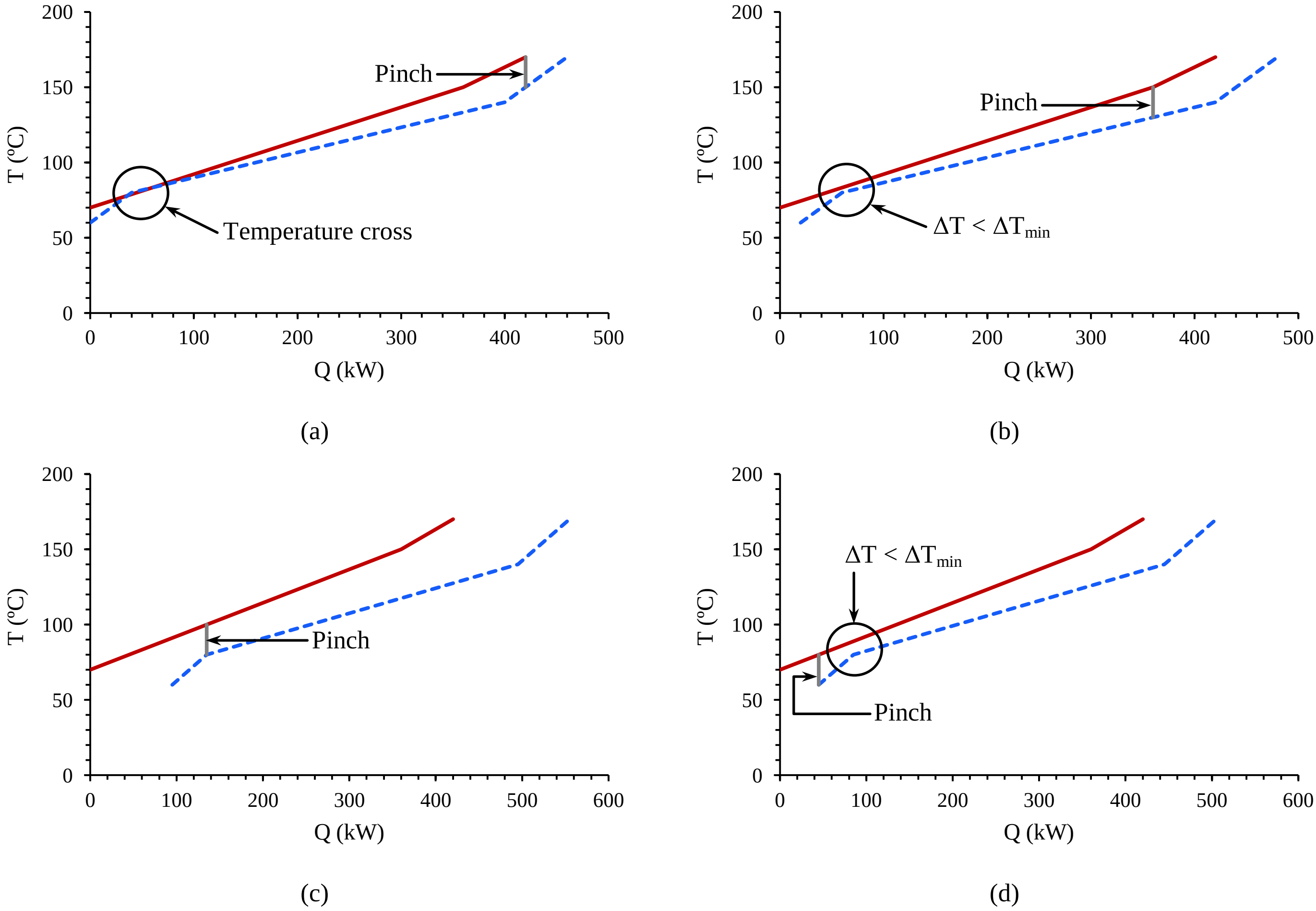
Fig. 1. Utilities needed for different pinch stream candidates (—— Hot - - - Cold). (a) Pinch candidate H1. (b) Pinch candidate H2. (c) Pinch candidate C1. (d) Pinch candidate C2.

Fig. 2. Optimal solutions to test problem 6 for different penalization factors.

Fig. 3. Process flow diagram for natural gas synthesis.

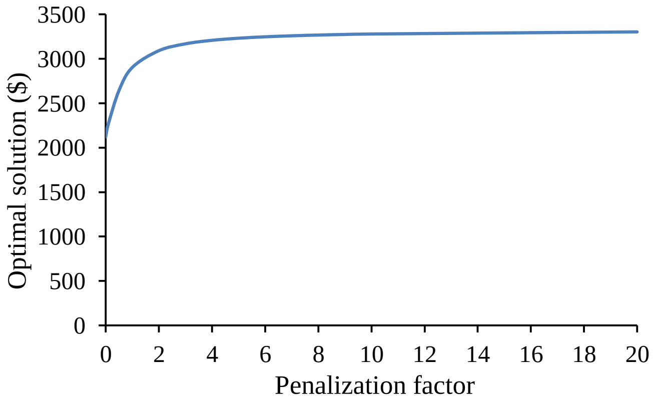
Fig. 4. Heat exchanger network for natural gas process.

Figure(s)



200
150
100
50
0
T (ºC)
0
100
200
300
400
500
600
Q (kW)
Pinch
Temperature cross
ΔT < ΔTmin
(a)
(b)
(c)
(d)

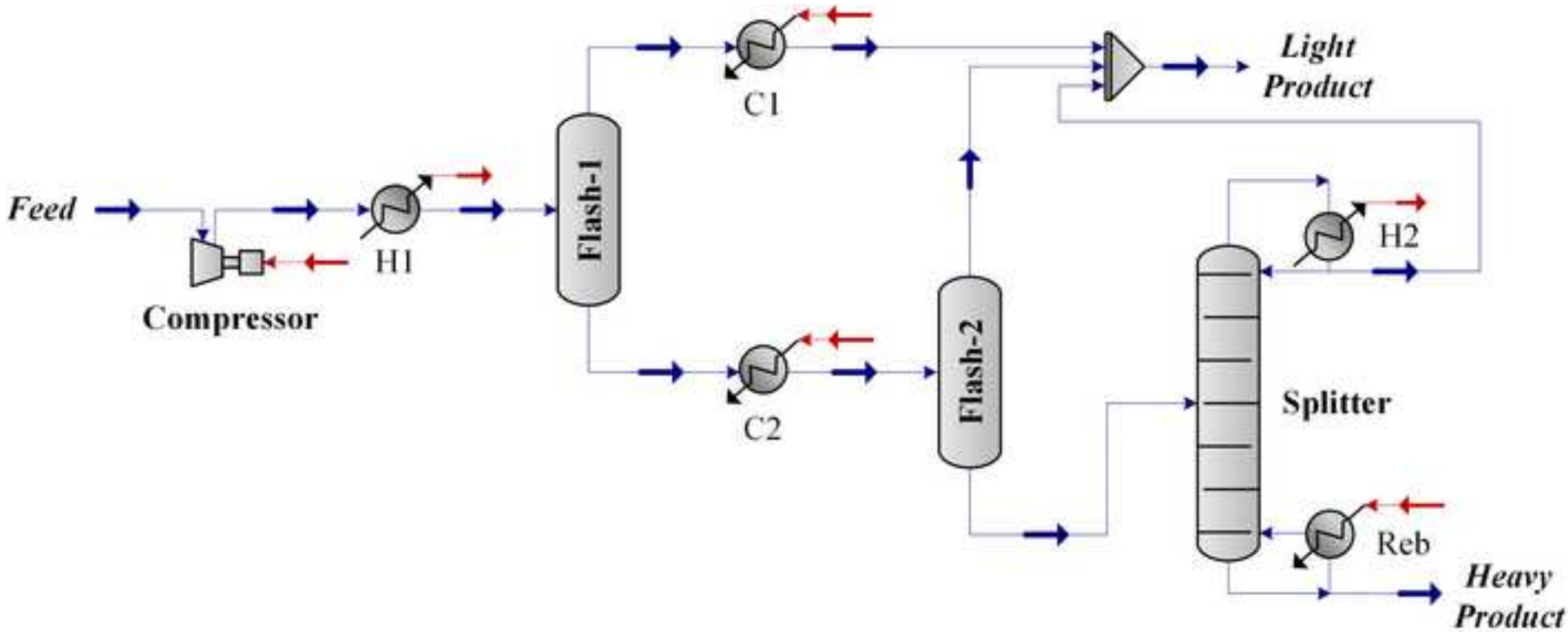
Figure(s)

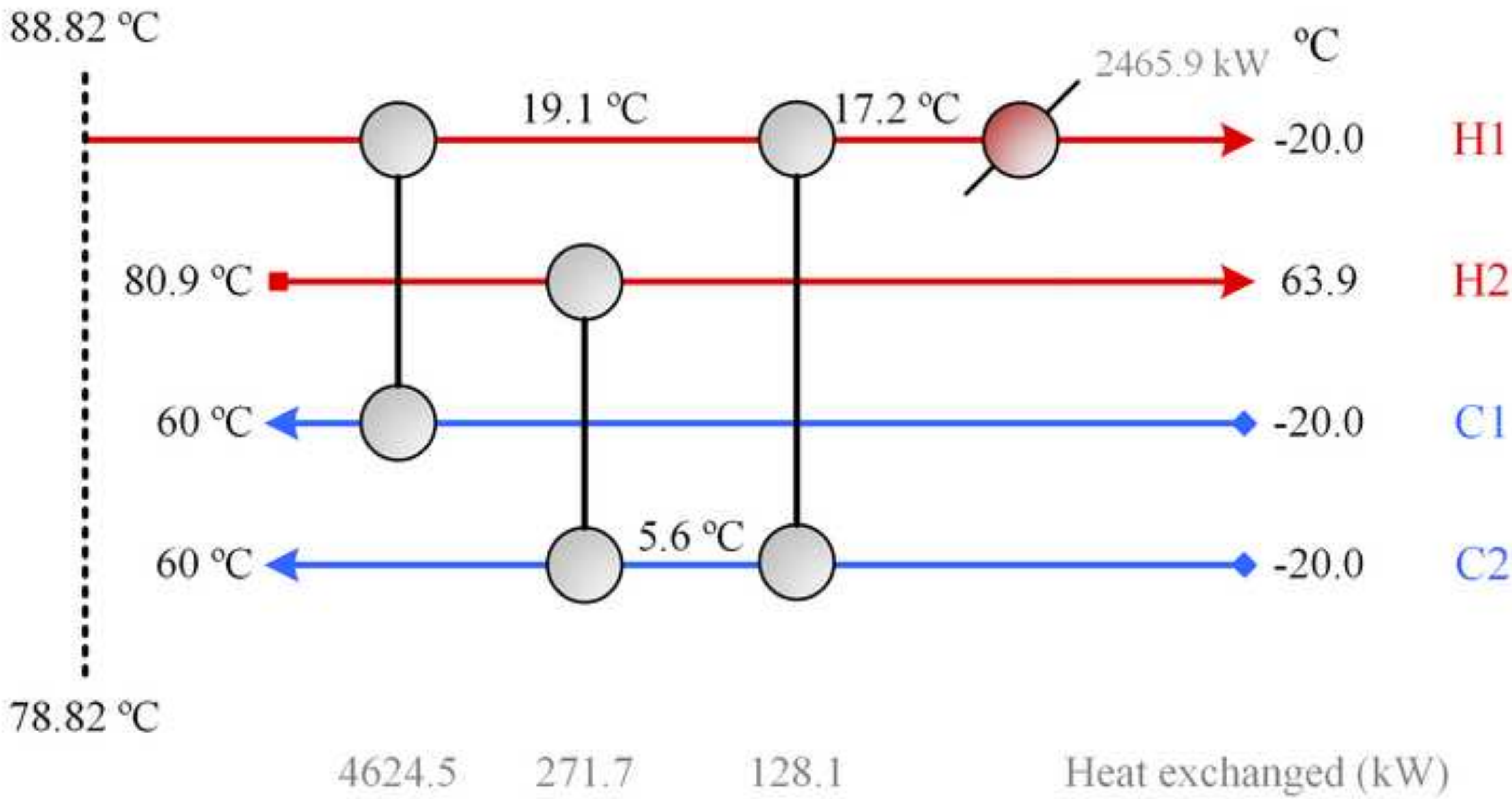


3500
3000
2500
2000
1500
1000
500
0
Optimal solution ($)
0
2
4
6
8
10
12
14
16
18
20
Penalization factor

Figure(s)

Click here to download high resolution image




88.82 °C
78.82 °C
19.1 °C
17.2 °C
2465.9 kW
°C
-20.0
H1
80.9 °C
63.9
H2
60 °C
-20.0
C1
5.6 °C
60 °C
-20.0
C2
4624.5
271.7
128.1
Heat exchanged (kW)