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# 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 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 excellent numerical performance, even in large-scale models.

## 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 (Linnhoff and Flower, 1978a, 1978b; Umeda et al., 1978) and the Pinch Design Method (Linnhoff and Hindmarsh, 1983), for the design of heat exchanger networks (HEN). Since those seminal works, hundreds of papers have been published related to heat integration.

Significant advances have been developed over the last few decades. Papoulias and Grossmann (1983) presented a mathematical programming model 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). However, the vertical heat transfer area assumption can be problematic if the heat transfer coefficient is significantly different for the various stream matches. A rigorous model for dealing with such a case was presented by Manousiouthakis and Martin (2004). 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 been 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 and Kravanja, 2013). In El-Halwagi and Manousiouthakis (1989) 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

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## Nomenclature

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| | |
|---|---|
| $i$ | Hot stream |
| $j$ | Cold stream |
| $k$ | Unclassified process stream |
| $m$ | Non-differentiable ‘kink’ point in the hot and cold composite curve and its end points |
| $p$ | Process streams that are pinch candidates |
| $s$ | Process stream |

*Sets*

| | |
|---|---|
| $COLD$ | Set of all the cold streams $j$ |
| $HOT$ | Set of all the hot streams $i$ |
| $ISO$ | Set of all the isothermal streams |
| $M$ | Set of ‘kink’ points |
| $MCOLD$ | Set of ‘kink’ points corresponding to an inlet or outlet temperature of a cold stream |
| $MHOT$ | Set of ‘kink’ points corresponding to an inlet or outlet temperature of a hot stream |
| $STR$ | Set of all the process streams $s$ |
| $UNC$ | Set of unclassified process streams $k$ |

*Variables*

| | |
|---|---|
| $f^{iso}$ | Binary variable that takes the value ‘1’ if the isothermal stream $s$ is a hot stream and ‘−1’ if it is a cold stream |
| $F_i$ | Heat capacity flowrate of the hot stream $i$ |
| $f_j$ | Heat capacity flowrate of the cold stream $j$ |
| $H_m$ | Enthalpy value in each one of the points in the set $M$ |
| $m$ | Mass flowrate of a stream |
| $Q^{iso}$ | Heat content below a pinch candidate for isothermal streams |
| $Q_C$ | Heat removed by the cold utility |
| $Q_H$ | Heat provided by the hot utility |
| $Q_C^p$ | Cooling utilities required for each pinch candidate $p$ |
| $Q_H^p$ | Heating utilities required for each pinch candidate $p$ |
| $T^p$ | Pinch point temperature |
| $T_{C,k}^{in}$ | Disaggregated variable for actual inlet temperature of the cold streams |
| $T_{C,k}^{out}$ | Disaggregated variable for actual outlet temperature of the cold streams |
| $T_{H,k}^{in}$ | Disaggregated variable for actual inlet temperature of the hot streams |
| $T_{H,k}^{out}$ | Disaggregated variable for actual outlet temperature of the hot streams |
| $T_i^{in}$ | Actual inlet temperature for the hot stream $i$ |
| $T_i^{out}$ | Actual outlet temperature for the hot stream $i$ |
| $t_j^{in}$ | Actual inlet temperature for the cold stream $j$ |
| $t_j^{out}$ | Actual outlet temperature for the cold stream $j$ |
| $t_m$ | Cold composite curve temperature of the ‘kink’ point $m$ |
| $T_m$ | Hot composite curve temperature of the ‘kink’ point $m$ |
| $T_s^+$ | Variable that will take a positive value for hot streams |
| $T_s^-$ | Variable that will take a positive value for cold streams |
| $TS_{C,k}^{in}$ | Disaggregated variable for shifted inlet temperature of the cold streams |
| $TS_{C,k}^{out}$ | Disaggregated variable for shifted outlet temperature of the cold streams |
| $TS_{H,k}^{in}$ | Disaggregated variable for shifted inlet temperature of the hot streams |
| $TS_{H,k}^{out}$ | Disaggregated variable for shifted outlet temperature of the hot streams |
| $TS_i^{in}$ | Shifted inlet temperature for the hot stream $i$ |
| $TS_i^{out}$ | Shifted outlet temperature for the hot stream $i$ |
| $ts_j^{in}$ | Shifted inlet temperature for the cold stream $j$ |
| $ts_j^{out}$ | Shifted outlet temperature for the cold stream $j$ |
| $TS_p^{in}$ | Pinch candidate of all the inlet temperatures of all the streams |
| $wc$ | Binary variable that takes the value of ‘1′ if the stream $k$ is classified as cold |
| $wh$ | Binary variable that takes the value of ‘1′ if the stream $k$ is classified as hot |
| $WC$ | Boolean variable that takes the value of ‘True’ if the stream $k$ is classified as cold |
| $WH$ | Boolean variable that takes the value of ‘True’ if the stream $k$ is classified as hot |
| $y_{m,m'}$ | Binary variable that takes the value ‘1’ if the unordered enthalpy value that originally was in position $m$ is assigned to position $m$’ in the non-decreasing reordered enthalpies |
| $Y_{m,m'}$ | Boolean variable that 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 |
| $y_s^{iso}$ | Binary variable that takes the value of ‘1’ if the isothermal stream is located below the pinch |
| $Y_s^{iso}$ | Boolean variable that takes the value of ‘True’ if the isothermal stream is located below the pinch |
| $\lambda$ | Specific heat associated with the change of phase |
| $\Delta T_m^{LM}$ | Logarithmic mean temperature |
| $\Delta T_{min}$ | Minimum heat recovery approach temperature |

total site integration can be found in Raissi (1994) and Dhole and Linnhoff (1993). Holiastos and Manousiouthakis (2002) established the theoretical basis of power and heat integration by determining the best integration between heat exchangers, heat pumps and heat engines. They showed that the optimal placement rules (Linnhoff et al., 1982; Townsend and Linnhoff, 1983a, 1983b) of heat pumps across the pinch and heat engines entirely below or above the pinch can be violated in the optimal design. Wechsung et al. (2011) and Onishi et al. (2014b) extended the concept –they called it Work and Heat Exchanger Networks (WHEN)– and proposed superstructures for generating the optimal configuration.

One of the major limitations of the pinch technology applied to the design of heat exchanger networks is that it has 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 can produce larger benefits than a sequential approach (Biegler et al. (1997) presented an illustrative example).

Different alternatives have been proposed to deal with this problem. One interesting approach is the Infinite DimEnsionAl State-space (IDEAS) approach (Drake and Manousiouthakis, 2002; Martin and Manousiouthakis, 2003; Pichardo and Manousiouthakis, 2017). It allows consideration of all process networks employing a set of unit operations. For example, a distillation column (or sequence) can be described by a distribution network, a mass exchange network and a heat exchanger network. It has the advantage that