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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.

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, reducing energy losses, and maximizing the energy efficiency, increase 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 pinch analysis in heat integration was introduced in 1978 by Bodo 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. 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 and 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

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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 for each pinch candidate
Q_H^p	Heating utilities required for 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	Penalty 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

and the heat exchanger network (HEN) is designed (Ahmad et al., 1990; Linhoff and Hindmarsh, 1983; Linnhoff, 1993; Linnhoff and 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 and Grossmann, 1986; Lang et al., 1988). In problems with specific characteristics like some subsystems or in small or medium size problems (Caballero and Grossmann, 2006; Onishi et al., 2014b) it is possible to use a superstructure (Yee and 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 Nonlinear Programming/Mixed Integer Nonlinear Programming (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 does 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 and 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