Chemical Engineering Science 147 (2016) 30–46

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Global optimization of heat exchanger networks using a new generalized superstructure

Sung Young Kim, Miguel Bagajewicz *

School of Chemical Engineering and Material Science, University of Oklahoma, 100 East Boyd Street, T-335, Norman, OK 73019-0628, USA

HIGHLIGHTS

- We extend the general HEN superstructure proposed by Floudas et al., 1986.
- we compare two different reformulations, and we solve the problem globally.
- We introduce a new feature to RYSIA, the global optimizer we developed recently, called lifting partitioning.
- Among results, we obtain structures that cannot be obtained using other models (stages, etc.).

ARTICLE INFO

Article history:
Received 9 July 2015
Received in revised form
7 January 2016
Accepted 2 February 2016
Available online 9 February 2016

Keywords:
Heat exchanger networks
Global optimization
RYSIA
Generalized superstructure

ABSTRACT

We present an extension of a previously presented superstructure (Floudas et al., 1986) for heat exchanger network grassroots design. This extension is such that it includes several matches between two streams, activates splitting control and allows for mixing temperature control. We solve this model globally using RYSIA, a recently developed method bound contraction procedure (Faria and Bagajewicz, 2011a, 2011b, 2011c; Faria et al., 2015). We also add a new RYSIA feature called Lifting Partitioning. Results show structures that cannot be obtained using the stages model (Yee and Grossmann, 1990) or other similar restrictive models.

1. Introduction

The problem of designing heat exchanger networks is perhaps the oldest problem in the discipline of Process Synthesis/Process Systems Engineering. Many articles were published and continue to be published because, arguably, the problem continues to challenge academia and practitioners.

The latest good review is an annotated bibliography by Furman and Sahinidis (2002). Of all this work, we specifically point to a general superstructure for HEN design was presented by Floudas et al. (1986), which is the starting point of our work. It consisted of a model that included one heat exchanger between every hot and cold stream, with connections made such that every possible flowsheet is represented in the superstructure. The model, however, was not used in practice for a variety of reasons. First, the MINLP solvers of the time, and many of them today, do not have good enough feasibility steps that would guarantee at least one local minimum (the model is non-convex) and without good initial points it usually turns infeasible. This discouraged researchers and practitioners. Second, the model would render some impractical answers, product of several splitting and mixing (we illustrate this later in this article). Third, many systems that exhibit heat transfer bottlenecks (i.e. pinches), require that some pairs of streams exchange heat in more than one exchanger, typically two (one exchanger on each side of the pinch, not consecutively, of course).

As a response to the aforementioned difficulties, a model more amenable to MINLP solvers was proposed (Yee and Grossmann, 1990), which makes a series of assumptions: it assumes isothermal mixing and presents several stages where more than one match between streams takes place. What made the model attractive is that the only nonlinearity could be confined to the objective function. The model became very popular, to the point that some other studies followed not assuming isothermal mixing (Björk and Weterlund, 2002) and allowing some different configurations (Huang and Karimi, 2013). All these efforts were not able to capture some alternative structures, like several exchangers in series on each branch of each stage. Thus, the only model that is still capable of capturing important and useful alternatives is a

* Corresponding author. Tel.: +1 405 325 5458.
E-mail address: bagajewicz@ou.edu (M. Bagajewicz).

http://dx.doi.org/10.1016/j.ces.2016.02.002
0009-2509/

generalized superstructure where several exchangers between two streams can be used.

As stated, the major difficulty of all the aforementioned models is the high level of non-convexity of the MINLP models, which not only leads to local optima, but may also fail to produce a feasible answer if it is not provided with good initial points. The only alternative to these models is the use of global optimization.

The academic efforts and the available commercial software were reviewed in our previous article (Faria et al., 2015). We only highlight what are the options we pursue in this article: all HEN models contain bilinear terms consisting of flowrates multiplied by temperatures. In addition, for HEN models, the heat transfer equations relating heat transferred with LMTD values are nonconvex. If one uses some rational approximations (Paterson, 1984; Chen, 1987), one can make appropriate substitutions (Manousiouthakis and Sourlas, 1992), to reformulate the problem using as one containing purely quadratic/bilinear models.

In this article, we explore the use of our bound contraction procedure for global optimization (Faria and Bagajewicz, 2011a). In our lower bound, we follow the direct partitioning procedure 1 (DPP1) strategy for the relaxation of bilinear terms and we exploit the univariate nature of the LMTD terms (or their rational equivalents), to build relaxations that do not require the addition of new variables (Faria et al., 2015). Finally, we also use a new concept of partitioning additional variables that help "lift" the value of the lower bound. We call the technique Lifting Partitioning.

The paper is organized as follows: we present the revised superstructure model first, including mixing and splitting control constraints. We follow with the lower bound model. We discuss the bound contraction strategy next, including the lifting partitioning and the uneven interval size bound contraction procedure. We then present results.

2. Generalized superstructure

The HEN design model of the heat exchanger network uses the superstructure model developed by Floudas et al. (1986). In order to describe how the HEN design model can be developed, we address a simple network, which has one hot stream and two cold streams in Fig. 1. Without loss of generality, we assume there are two heat exchangers per hot/cold stream match and they are not necessarily contiguous or in series. Fig. 1 illustrates the nature of the superstructure for just one hot stream and two cold streams and two exchangers per pair of streams, although the model can have many exchangers.

In the original formulation by Floudas et al. (1986) the feasible space is defined by nonlinear constraints, many of which are bilinear, and other purely nonconvex functions. Bilinear functions are included in the heat balances equations of heat exchangers and mixers. Nonconvex functions are the part of heat exchanger area calculations. The non-convex and bilinear MINLP model presented in this paper differs slightly from the original formulation.

We first introduce the nomenclature for streams. They are depicted in Fig. 2. Index i refers to hot stream and j to cold stream. Each exchanger k has their inlet and outlet temperatures and flowrates denoted by $Th^{i,j,k}_{hx-in}, Th^{i,j,k}_{hx-out}, Fh^{i,j,k}_{hx-in}$ and $Fh^{i,j,k}_{hx-out}$, respectively. These inlet temperatures and flowrates are a product of mixing a portion of the feed $Fh^{i,j,k}_{in}$ with streams from other exchangers (i,jj,kk), $fh^{i,jj,j}_{kk,k}$. The variable $fh^{i,j,jj}_{k,kk}$ represents the hot stream from the heat exchanger (i,j,k) to split to the heat exchanger (i,jj,kk). If kk is greater than k, there is no stream from the heat exchanger (i,j,k) to (i,jj,kk).

We now present the equations of the model:

- *Mass balances for splitters*

$$F_i - \sum_j \sum_k Fh^{i,j,k}_{in} = 0 \quad \forall i \tag{1}$$

$$F_j - \sum_i \sum_k Fc^{i,j,k}_{in} = 0 \quad \forall j \tag{2}$$

$$Fh^{i,j,k}_{hx-out} - \left(\sum_{jj} \sum_{kk} fh^{i,j,jj}_{k,kk} + Fh^{i,j,k}_{out} \right) = 0 \quad (k \le kk) \quad \forall i,j,k \tag{3}$$

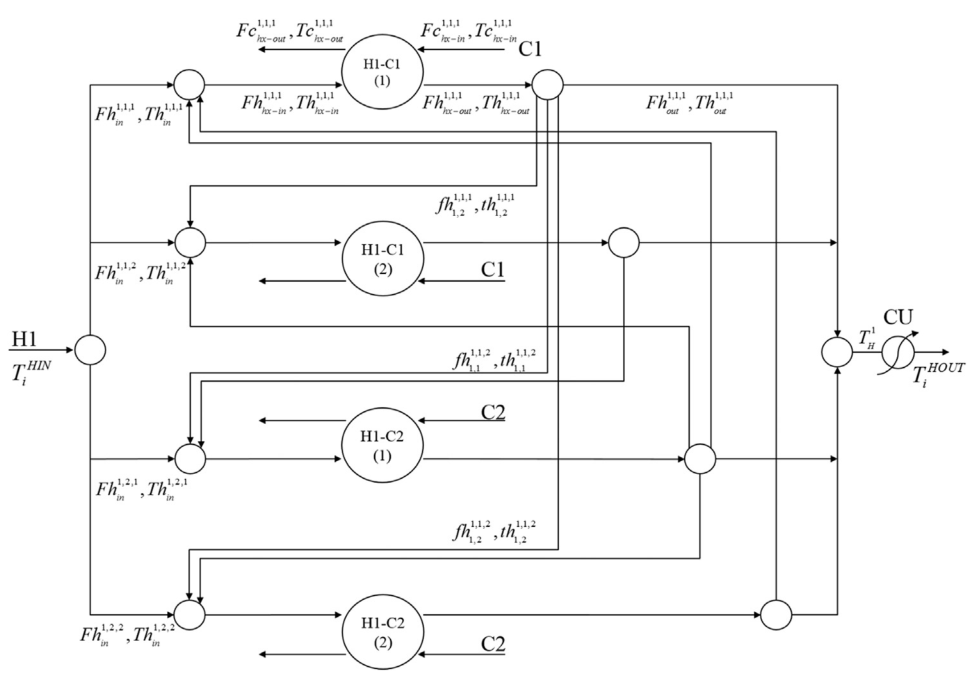

Fig. 1. Heat exchanger network superstructure; two exchangers per match.