Computers and Chemical Engineering 82 (2015) 68–83

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Computational strategies for large-scale MILP transshipment models for heat exchanger network synthesis

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ARTICLE INFO

Article history:
Received 7 November 2014
Received in revised form 14 May 2015
Accepted 17 May 2015
Available online 27 May 2015

Keywords:
Heat exchanger network synthesis (HENS)
Transshipment model
Mixed-integer linear programming
Computational strategies
Model reformulation

ABSTRACT

Determining the minimum number of units is an important step in heat exchanger network synthesis (HENS). The MILP transshipment model (Papoulias and Grossmann, 1983) and transportation model (Cerda and Westerberg, 1983) were developed for this purpose. However, they are computationally expensive when solving for large-scale problems. Several approaches are studied in this paper to enable the fast solution of large-scale MILP transshipment models. Model reformulation techniques are developed for tighter formulations with reduced LP relaxation gaps. Solution strategies are also proposed for improving the efficiency of the branch and bound method. Both approaches aim at finding the exact global optimal solution with reduced solution times. Several approximation approaches are also developed for finding good approximate solutions in relatively short times. Case study results show that the MILP transshipment model can be solved for relatively large-scale problems in reasonable times by applying the approaches proposed in this paper.

1. Introduction

Heat exchanger network synthesis (HENS) has been an important topic in power, refining and chemical industries for several decades due to its crucial role in energy savings and cost reduction. Recently it is also of increased interest in broader areas, including carbon capture and storage (CCS), water treatment and energy polygeneration. HENS has been extensively studied in process systems engineering research, and a number of methodologies have been developed. Linnhoff and Hindmarsh (1983) proposed the pinch design method, which is based on physical insight for the maximum heat recovery in heat exchanger networks. Mathematical programming based approaches were developed by Papoulias and Grossmann (1983), Cerda et al. (1983) and Cerda and Westerberg (1983). Both methods are now widely used in grassroots design and retrofit of heat exchanger networks. Detailed reviews on developments of HENS methods can be found in Gundersen and Naess (1988), Furman and Sahinidis (2002), Morar and Agachi (2010) and Klemeš and Kravanja (2013).

Two different types of HENS approaches have been studied: sequential and simultaneous. In the sequential approach the HENS problem is solved in three steps (Biegler et al., 1997): first, the utility cost (or consumption) is minimized with a linear programming (LP) model (Papoulias and Grossmann, 1983; Cerda et al., 1983); second, the number of heat exchangers is minimized with a mixed-integer linear programming (MILP) model to determine the optimal stream matches (Papoulias and Grossmann, 1983; Cerda and Westerberg, 1983); finally, the total investment cost is minimized with a nonlinear programming (NLP) model, and the optimal heat exchanger network structure is derived (Floudas et al., 1986). In contrast to the target-based sequential approach, the simultaneous synthesis approach optimizes energy, number of units and total heat exchanger area simultaneously in a mixed-integer nonlinear programming (MINLP) model (Yee and Grossmann, 1990; Ciric and Floudas, 1991). Due to its computational complexity, the simultaneous approach usually can only solve problems with small to medium sizes. The sequential approach, on the other hand, decomposes the HENS problem into several smaller subproblems that are much easier to solve, and hence is still considered the most practical way to solve industrial-scale HENS problems.

In the sequential approach, minimization of the number of heat exchangers is a key step to determine the optimal structure and the minimum fixed cost of heat exchanger networks. The MILP transhipment and MILP transportation models are basic tools to

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http://dx.doi.org/10.1016/j.compchemeng.2015.05.015

calculate the minimum number of units. The major difference between the two is that the former uses a heat cascade while the latter uses direct matches, which makes the size of the former model significantly smaller. These models have been further developed during the last 20 years. A vertical MILP transshipment model was proposed by Gundersen and Grossmann (1990) and Gundersen et al. (1996), in which non-vertical heat transfer (i.e., criss-crossing) was minimized and the optimal solution with smallest heat exchange area could be identified. Floudas and Grossmann (1986) extended the MILP transshipment model for multiperiod operations. The MILP transshipment/transportation models were also incorporated into the simultaneous approach for heat exchanger network design (Shethna et al., 2000; Barbaro and Bagajewicz, 2005) and retrofit (Nguyen et al., 2010). In process synthesis, the MILP transshipment model has been applied to the optimal design of heat exchanger networks in a wide range of systems and processes, such as refrigeration systems (Shelton and Grossmann, 1986), batch/semi-continuous processes (Zhao et al., 1998), water utilization systems (Bagajewicz et al., 2002) and hybrid transportation fuel production processes (Elia et al., 2010).

Despite significant advances in MILP solvers (e.g., CPLEX, GUROBI, XPRESS) and application of the MILP transhipment/transportation models, solving the MILP itself is still quite challenging. Furman and Sahinidis (2001) proved that the minimum number of matches problem is $\mathcal{NP}$-hard in the strong sense due to its combinatorial nature. So far the MILP transshipment/transportation models are quite difficult to solve for large-scale problems, as will be shown later, rendering the minimum number of units problem as the major bottleneck in the HENS procedure. Only a few papers have investigated efficient solution approaches for large-scale MILP transshipment/transportation models. Gundersen et al. (1997) developed a MILP transshipment formulation with tighter heat transfer upper bounds and indicated that the gap between the MILP solution and its LP relaxation could be reduced by using the tighter formulation. Anantharaman et al. (2010) systematically studied approaches for improving the solution performance for the MILP transshipment model. The authors proposed three major approaches: pre-processing to reduce model size using insight and heuristics, model modification/reformulation, and improving efficiency of the branch and bound method. Several ideas for model modification and reformulation were investigated in this article, including decreasing the upper bound, adding integer cuts and reformulating the original model to set-partitioning formulations. The authors tested these ideas for several cases with the size of up to 22 process streams, and showed that the LP relaxation was significantly tightened. However, the above two papers did not present the effect on solution times. Hence, the actual computational performance of these model reformulations is unknown. Pettersson (2005) developed an approximate approach, which includes match set reduction and grouping, and solved the minimum number of matches problem with up to 39 process streams in reasonable times. The minimum number of units problem was also solved by evolutionary methods (Mocsny and Govind, 1984; Shethna and Jezowski, 2006). These approximate approaches, however, cannot guarantee the global optimal solution and also cannot indicate how far the obtained solution is with respect to the global optimum.

This paper investigates several rigorous and approximate approaches for reducing the computational time required to solve large-scale MILP transshipment models. Both LP relaxation and solution time results are presented. The remaining part of this paper is organized as follows. Section 2 presents solution times of MILP transshipment models for a variety of cases with small to large sizes, discusses reasons for the slow computation, and then shows results for weighted matches. Section 3 proposes several reformulations, including model disaggregation and addition of integer cuts, and then compares their results with the original model. Several solution strategies, e.g., branching priority, strong branching, parallel computing, are discussed in Section 4. Finally, Section 5 describes several approximation approaches, including using a relative optimality gap, a combined model, a reduced MILP model and a NLP reformulation. The paper is concluded in Section 6.

2. Preliminary results

2.1. MILP transshipment model – case study and results

The MILP transshipment model is usually difficult to solve for the full heat exchanger network due to its computational complexity. Instead, the full network is partitioned into several subnetworks defined by the pinch points, and then the MILP transshipment model is solved for each subnetwork. This is a reasonable procedure because stream matches across the pinch are usually avoided (for exceptions see Wood et al. (1985)).

Before solving the MILP transshipment model, the following LP transshipment model (Papoulias and Grossmann, 1983) is solved, which provides the minimum utility consumption and the location of pinch points that partition the full network into subnetworks:

$$
\begin{aligned}
&\min Z = \sum_{m\in S} c_m Q_m^S + \sum_{n\in W} c_n Q_n^W \\
&\text{s.t. } R_{ik} - R_{i,k-1} + \sum_{j\in C_k} Q_{ijk} + \sum_{n\in W_k} Q_{ink} = Q_{ik}^H \quad \forall i\in H'_k \quad \forall k\in K \\
&R_{mk} - R_{m,k-1} + \sum_{j\in C_k} Q_{mjk} - Q_m^S = 0 \quad \forall m\in S'_k \quad \forall k\in K \\
&\sum_{i\in H_k} Q_{ijk} + \sum_{m\in S_k} Q_{mjk} = Q_{jk}^C \quad \forall j\in C_k \quad \forall k\in K \\
&\sum_{i\in H_k} Q_{ink} - Q_n^W = 0 \quad \forall n\in W_k \quad \forall k\in K \\
&R_{ik},\ R_{mk},\ Q_{ijk},\ Q_{mjk},\ Q_{ink},\ Q_m^S,\ Q_n^W \ge 0 \\
&R_{i0} = R_{iK} = 0
\end{aligned}
\tag{M0}
$$

where K is the index set for all temperature intervals; c_m and c_n are the unit cost of hot utility m and cold utility n, which are known parameters; Q_{ik}^H and Q_{jk}^C are the heat content of hot process stream i and cold process stream j at temperature interval k, which are known parameters; Q_m^S and Q_n^W are the heat load of hot utility m and cold utility n; Q_{ijk}, Q_{mjk}, and Q_{ink} are the amount of heat exchanged between hot stream i and cold stream j, hot utility m and cold stream j, and hot stream i and cold utility n at interval k; R_{ik} and R_{mk} are the heat residual of hot stream i and hot utility m exiting interval k. Pinch points are identified by those temperature intervals for which all the heat residuals are zero. The index sets are defined below:

$H_k = \{i|\text{hot stream } i \text{ supplies heat to interval } k\}$

$H'_k = \{i|\text{hot stream } i \text{ is present at interval } k \text{ or at a higher interval}\}$

$C_k = \{j|\text{cold stream } j \text{ demands heat from interval } k\}$

$S_k = \{m|\text{hot utility } m \text{ supplies heat to interval } k\}$

$S'_k = \{m|\text{hot utility } m \text{ is present at interval } k \text{ or at a higher interval}\}$

$W_k = \{n|\text{cold utility } n \text{ extracts heat from interval } k\}$

Next, the MILP transshipment model is solved for each subnetwork, obtaining the minimum number of units and one set of matches between hot and cold streams that achieve the minimum number of units. In this model, the heat loads of hot and cold utilities are fixed