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Heuristics with performance guarantees for the minimum number of matches problem in heat recovery network design☆

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ABSTRACT

Heat exchanger network synthesis exploits excess heat by integrating process hot and cold streams and improves energy efficiency by reducing utility usage. Determining provably good solutions to the minimum number of matches is a bottleneck of designing a heat recovery network using the sequential method. This subproblem is an $\mathcal{NP}$-hard mixed-integer linear program exhibiting combinatorial explosion in the possible hot and cold stream configurations. We explore this challenging optimization problem from a graph theoretic perspective and correlate it with other special optimization problems such as cost flow network and packing problems. In the case of a single temperature interval, we develop a new optimization formulation without problematic big-M parameters. We develop heuristic methods with performance guarantees using three approaches: (i) relaxation rounding, (ii) water filling, and (iii) greedy packing. Numerical results from a collection of 51 instances substantiate the strength of the methods.

1. Introduction

Heat exchanger network synthesis (HENS) minimizes cost and improves energy recovery in chemical processes (Baliban et al., 2012; Biegler et al., 1997; Elia et al., 2010; Smith, 2000). HENS exploits excess heat by integrating process hot and cold streams and improves energy efficiency by reducing utility usage (Escobar and Trierweiler, 2013; Floudas and Grossmann, 1987; Furman and Sahinidis, 2002; Gundersen and Naess, 1988). Floudas et al. (2012) review the critical role of heat integration for energy systems producing liquid transportation fuels (Niziolek et al., 2015). Other important applications of HENS include: refrigeration systems (Shelton and Grossmann, 1986), batch semi-continuous processes (Castro et al., 2015; Zhao et al., 1998) and water utilization systems (Bagajewicz et al., 2002).

Heat exchanger network design is a mixed-integer nonlinear optimization (MINLP) problem (Ciric and Floudas, 1991; Hasan et al., 2010; Papalexandri and Pistikopoulos, 1994; Yee and Grossmann, 1990). Mistry and Misener (2016) recently showed that expressions incorporating logarithmic mean temperature difference, i.e. the nonlinear nature of heat exchange, may be reformulated to decrease the number of nonconvex nonlinear terms in the optimization problem. But HENS remains a difficult MINLP with many nonconvex nonlinearities. One way to generate good HENS solutions is to use the so-called *sequential method* (Furman and Sahinidis, 2002). The sequential method decomposes the original HENS MINLP into three tasks: (i) minimizing utility cost, (ii) minimizing the number of matches, and (iii) minimizing the investment cost. The method optimizes the three mathematical models sequentially with: (i) a linear program (LP) (Cerda et al., 1983; Papoulias and Grossmann, 1983), (ii) a mixed-integer linear program (MILP) (Cerda and Westerberg, 1983; Papoulias and Grossmann, 1983), and (iii) a nonlinear program (NLP) (Floudas et al., 1986). The sequential method may not return the global solution of the original MINLP, but solutions generated with the sequential method are practically useful.

This paper investigates the *minimum number of matches* problem (Floudas, 1995), the computational bottleneck of the sequential method. The minimum number of matches problem is a strongly $\mathcal{NP}$-hard MILP (Furman and Sahinidis, 2001). Mathematical symmetry in the problem structure combinatorially increases the possible stream configurations and deteriorates the performance of exact, tree-based algorithms (Kouyialis and Misener, 2017).

Because state-of-the-art approaches cannot solve the minimum number of matches problem to global optimality for moderately-

☆ This manuscript is dedicated, with deepest respect, to the memory of Professor C.A. Floudas. Professor Floudas showed that, given many provably-strong solutions to the minimum number of matches problem, he could design effective heat recovery networks. So the diverse solutions generated by this manuscript directly improve Professor Floudas' method for automatically generating heat exchanger network configurations.

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Table 1
Nomenclature.

Name	Description
Cardinalities	
n	Number of hot streams
m	Number of cold streams
k	Number of temperature intervals
v	Number of matches (objective value)
Indices	
$i \in H$	Hot stream
$j \in C$	Cold stream
$s,\ t,\ u \in T$	Temperature interval
$b \in B$	Bin (single temperature interval problem)
Sets	
$H,\ C$	Hot, cold streams
T	Temperature intervals
M	Set of matches (subset of $H \times C$)
$C_i(M),\ H_j(M)$	Cold, hot streams matched with $i \in H$, $j \in C$ in M
B	Bins (single temperature interval problem)
$A(M)$	Set of valid quadruples (i, s, j, t) with respect to a set M of matches
$A_u(M)$	Set of quadruples $(i, s, j, t) \in A(M)$ with $s \leq u < t$
$V^H(M)$	Set of pairs $(i, s) \in H \times T$ appearing in $A(M)$ (transportation vertices)
$V^C(M)$	Set of pairs $(j, t) \in C \times T$ appearing in $A(M)$ (transportation vertices)
$V^C_{i,s}(M)$	Set of pairs $(j, t) \in V^C(M)$ such that (i, s, j, t) belongs to $A(M)$
$V^H_{j,t}(M)$	Set of pairs $(i, s) \in V^H(M)$ such that (i, s, j, t) belongs to $A(M)$
Parameters	
h_i	Total heat supplied by hot stream i ($h_i = \sum_{s \in T} \sigma_{i,s}$)
$h_{\max}$	Maximum heat among all hot streams ($h_{\max} = \max_{i \in H}\{h_i\}$)
c_j	Total heat demanded by cold stream j ($c_j = \sum_{t \in T} \delta_{j,t}$)
$\sigma_{i,s}$	Heat supply of hot stream i in interval s
$\delta_{j,t}$	Heat demand of cold stream j in interval t
$\vec{\sigma}, \vec{\delta}$	Vectors of all heat supplies, demands
$\vec{\sigma}_t, \vec{\delta}_t$	Vectors of all heat supplies, demands in temperature interval t
R_t	Residual heat exiting temperature interval t
$U_{i,j}$	Upper bound (big-M parameter) on the heat exchanged via match (i, j)
$\lambda_{i,j}$	Fractional cost approximation of match (i, j) (Lagrangian relaxation)
$\vec{\lambda}$	Vector of all fractional cost approximations $\lambda_{i,j}$
Variables	
$y_{i,j}$	Binary variable indicating whether i and j are matched
$q_{i,j,t}$	Heat of hot stream i received by cold stream j in interval t
$q_{i,s,j,t}$	Heat exported by hot stream i in s and received by cold stream j in t
$\vec{y}, \vec{q}$	Vectors of binary, continuous variables
$r_{i,s}$	Heat residual of heat of hot stream i exiting s
x_b	Binary variable indicating whether bin b is used
$w_{i,b}$	Binary variable indicating whether hot stream i is placed in bin b
$z_{j,b}$	Binary variable indicating whether cold stream j is placed in bin b
Other	
N	Minimum cost flow network
G	Solution graph (single temperature interval problem)
$\phi(M)$	Filling ratio of a set M of matches
$\vec{y}^f, \vec{q}^f$	Optimal fractional solution
$\alpha_i,\ \beta_j$	Number of matches of hot stream i, cold stream j
$L_{i,j}$	Heat exchanged from hot stream i to cold stream j
I	Instance of the problem
r	Remaining heat of an algorithm

sized instances (Chen et al., 2015b), engineers develop experience-motivated heuristics (Cerda et al., 1983; Linnhoff and Hindmarsh, 1983). Linnhoff and Hindmarsh (1983) highlight the importance of generating good solutions quickly: a design engineer may want to actively interact with a good minimum number of matches solution and consider changing the utility usage as a result of the MILP outcome. Furman and Sahinidis (2004) propose a collection of approximation algorithms, i.e. heuristics with performance guarantees, for the minimum number of matches problem by exploiting the LP relaxation of an MILP formulation. Furman and Sahinidis (2004) present a unified worst-case analysis of their algorithms' performance guarantees and show a non-constant approximation ratio scaling with the number of temperature intervals. They also prove a constant performance guarantee for the single temperature interval problem.

The standard MILP formulations for the minimum number of matches contain big-M constraints, i.e. the on/off switches associated with weak continuous relaxations of MILP. Both optimization-based heuristics and exact state-of-the-art methods for solving minimum number of matches problem are highly affected by the big-M parameter. Trivial methods for computing the big-M parameters are typically adopted, but Gundersen et al. (1997) propose a tighter way of computing the big-M parameters.

This manuscript develops new heuristics and provably efficient approximation algorithms for the minimum number of matches problem. These methods have guaranteed solution quality and efficient run-time bounds. In the sequential method, many possible stream configurations are required to evaluate the minimum overall cost (Floudas, 1995), so a complementary contribution of this work is a heuristic methodology for producing multiple solutions efficiently. We classify the heuristics based on their algorithmic nature into three categories: (i) relaxation rounding, (ii) water filling, and (iii) greedy packing.

The relaxation rounding heuristics we consider are (i) Fractional LP Rounding (FLPR), (ii) Lagrangian Relaxation Rounding (LRR), and (iii) Covering Relaxation Rounding (CRR). The water-filling heuristics are (i) Water-Filling Greedy (WFG), and (ii) Water-Filling MILP (WFM). Finally, the greedy packing heuristics are (i) Largest Heat Match LP-based (LHM-LP), (ii) Largest Heat Match Greedy (LHM), (iii) Largest Fraction Match (LFM), and (iv) Shortest Stream (SS). Major ingredients of these heuristics are adaptations of single temperature interval algorithms and maximum heat computations with match restrictions. We propose (i) a novel MILP formulation, and (ii) an improved greedy approximation algorithm for the single temperature interval problem. Furthermore, we present (i) a greedy algorithm computing maximum heat between two streams and their corresponding big-M parameter, (ii) an LP computing the maximum heat in a single temperature interval using a subset of matches, and (iii) an extended maximum heat LP using a subset of matches on multiple temperature intervals.

The manuscript proceeds as follows: Section 2 formally defines the minimum number of matches problem and discusses mathematical models. Section 3 discusses computational complexity and approximation algorithms for the minimum number of matches problem. Section 4 focusses on the single temperature interval problem. Section 5 explores computing the maximum heat exchanged between the streams with match restrictions. Sections 6–8 present our heuristics for the minimum number of matches problem based on: (i) relaxation rounding, (ii) water filling, and (iii) greedy packing, respectively, as well as new theoretical performance guarantees. Section 9 evaluates experimentally the heuristics and discusses numerical results. Sections 10 and 11 discuss the manuscript contributions and conclude the paper.

2. Minimum number of matches for heat exchanger network synthesis

This section defines the minimum number of matches problem and presents the standard transportation and transshipment MILP models. Table 1 contains the notation.

2.1. Problem definition

Heat exchanger network design involves a set *HS* of *hot process streams* to be cooled and a set *CS* of *cold process streams* to be heated. Each hot stream i posits an initial temperature $T^{HS}_{\text{in},i}$