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A Bilevel Decomposition Method for the Simultaneous Synthesis of Utility Systems, Rankine Cycles and Heat Exchanger Networks

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Abstract

This work tackles the simultaneous optimization of utility systems, Rankine cycles and heat exchanger networks (HEN). Thanks to the combination of two superstructures (Rankine cycle and HEN), all heat integration options between heat sources/sinks and Rankine cycle can be considered, and the trade-off between efficiency and plant costs is optimized. On the other hand, the resulting MINLP is extremely challenging due to its large number of binary variables and bilinear terms. We present an ad-hoc bilevel decomposition algorithm based on the McCormick relaxation with reinforcement constraints, piecewise linearization of the cost functions and "nested" integer cuts. The algorithm is applied to literature and real-world case studies to show its effectiveness compared to commercial MINLP solvers and metaheuristic algorithms.

Keywords: nonconvex MINLP, bilevel decomposition, McCormick relaxation, utility systems, Rankine cycle superstructure.

1. Introduction

The heat integration problem involves the design and synthesis of the Heat Exchanger Network (HEN) and the utility systems necessary to provide thermal, refrigeration, mechanical and electric power to the process units of energy systems and chemical processes. A key role is often played by steam cycles and, in general, Rankine Cycles, because of their capability of converting waste heat into useful mechanical power and/or achieving high efficiency by cogenerating heat/steam and power for the plant. Several authors, for instance (Papoulias & Grossmann, 1983; Bruno et al., 1998), proposed approaches to improve the design of steam cycles and steam networks. However, the optimization of the steam generator layout (pre-heating, evaporation and superheating) and of the possible integration options with the process heaters/coolers is not dealt with. Previous studies mainly focus either on the design of utility systems or on the synthesis of HEN, and the two problems are carried out sequentially. Only a few studies tackle both problems together: (Marechal & Kalitventzeff, 1998), (Mian et al. 2016), (Duran & Grossmann, 1986), (Hipólito-Valencia et al., 2013) and (Yu et al., 2017), adapted the sequential framework for HEN synthesis while, more recently, (Martelli et al. 2017) and (Elsido et al., 2017a) proposed a simultaneous approach.
In this work, we present an ad hoc bilevel decomposition to tackle the general model proposed by (Martelli et al., 2017) and extended by (Elsido et al., 2017a) for the

simultaneous optimization of utility systems, Rankine cycles and heat exchanger networks. The model enables the automated generation of Rankine cycles (e.g., Steam Cycles, Organic Rankine Cycles, Heat pump cycles), recovering heat from one or more heat sources, and the HEN of the overall heat integration (i.e., considering also the internal heat exchanger arrangement of the boilers).

2. Mathematical model

The problem of simultaneous optimization of utility systems, Rankine cycles and HEN can be stated as follows: “Given the set of hot and cold streams of the process (i.e., heat sources/sinks), the process needs of hot water/liquid and steam/vapor, the technical limitations (e.g., forbidden/forced matches, no stream splitting, etc.) and economic data (e.g., price of fuels, price of electricity, cost models of process units, etc.), determine the optimal configuration of the Rankine Cycle, the mass flow rates and the optimal HEN.”
The model is based on the SYNHEAT superstructure (Yee & Grossmann, 1990) for the optimal design of heat exchanger networks. The SYNHEAT model is extended to include the streams of the heat recovery cycle, with variable mass flow rate.
The thermodynamic cycles are modelled with a very general “*p*-*h* superstructure” (Elsido et al., 2017a, 2017b), capable of reproducing many configurations of Rankine cycles, both power cycles and inverse cycles (refrigeration cycles or heat pumps), steam cycles or Organic Rankine Cycles (ORC), with single or multiple pressure levels, as well as heat/steam distribution networks. A schematic representation of the Rankine cycle superstructure proposed to tackle the heat recovery steam cycle design problems proposed in this work is represented in Fig. 1. The steam cycle can be designed with up to three levels of pressure. Cycle pressures and temperatures are not optimized. All components have a binary activation variable (*y*). Economizers, evaporators, superheaters, reheaters, and condensers are also part of the HEN (i.e., they are streams with variable flow rates).

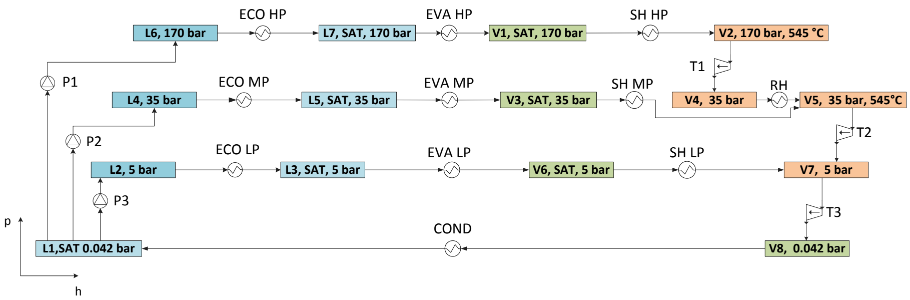

Figure 1: The steam cycle “*p*-*h* superstructure” with three levels of pressure used in this work.

The main constraints are: overall heat balance for each stream (Eq.1); heat balance for stage for non-isothermal streams (Eq.2); feasibility of temperatures (Eq.3); calculation of approach temperature differences (Eq.4); logical constraints such as upper bounds on heat loads, existence of components, no stream splitting, forced and forbidden matches; mass and energy balances on components (Eq.5 and Eq.6). The objective function is the Total Annual Cost (TAC) of the overall plant including HEN, utilities and Rankine cycle, minus revenues (Eq.7). The extended model is a challenging nonconvex Mixed Integer NonLinear Program (MINLP), because of the logarithmic mean temperature difference (LMTD) terms in the objective function (Eq.7) and the bilinear products in the energy balances of the streams with variable mass flow rate (Eq.2).

$$\left(Tin_i - Tout_i\right)\cdot F_i \cdot Cp_i = \sum_k \sum_j q_{ijk} + qcu_i, \forall i$$
$$\left(Tout_j - Tin_j\right)\cdot F_j \cdot Cp_j = \sum_k \sum_i q_{ijk} + qhu_j, \forall j \qquad (1)$$

$$\left(t_{i,k} - t_{i,k+1}\right)\cdot F_i \cdot Cp_i = \sum_j q_{ijk}, \forall i,k \quad \left(t_{j,k} - t_{j,k+1}\right)\cdot F_j \cdot Cp_j = \sum_i q_{ijk}, \forall j,k \qquad (2)$$

$$t_{i,k} \geq t_{i,k+1}, \forall i,k \qquad t_{j,k} \geq t_{j,k+1}, \forall j,k \qquad (3)$$

$$dt_{ijk} \leq t_{i,k} - t_{j,k} + \Delta T_{ij,\max}\left(1 - z_{ijk}\right), \forall i,j,k \qquad (4)$$

$$\sum_{in} F_{in} - \sum_{out} F_{out} = 0, \forall c \qquad (5)$$

$$\sum_{in} F_{in} h_{in} - \sum_{out} F_{out} h_{out} + Q_{in} - Q_{out} - P_{out} = 0, \forall c \qquad (6)$$

$$TAC = \sum_c FC_c y_c + \sum_{ijk} FC_{ij} z_{ijk} + \sum_c VC_c F_c^{\alpha} + \sum_{ijk} VC_{ij}\left(\frac{q_{ijk}}{U_{ij} LMTD_{ijk}}\right)^{\beta} - R \qquad (7)$$

3. Bilevel decomposition

While (Mistry & Misener, 2016) proposed an outer approximation algorithm for the global solution of a similar problem with bilinear terms and LMTD, this work proposes a bilevel decomposition. In the first stage (i.e., the “master” problem), a linearized and relaxed version of the original problem (MILP) is solved, then, in the second stage, for fixed binary variables, the continuous variables are re-optimized solving a nonconvex nonlinear program (NLP). Two nested loops of integer cuts allow exploring different system configurations very efficiently.

3.1. Master problem

The master problem includes all the linear constraints of the full MINLP problem while the bilinear terms ($F_i\, t_{i,j,k}$) in the energy balance constraints in Eq.2 (due to the variable mass flow rates of utility streams, F) are linearized with McCormick relaxations (McCormick, 1976), as shown in Eq.8. Since for each utility component the lower bound of F is zero when the component is not selected ($y = 0$) and F^L when it is selected ($y = 1$), the auxiliary variable θ is needed to replace the product between t and y.

$$Ft \geq Ft^L + F^L\vartheta - F^L yt^L \qquad Ft \geq F^U t + Ft^U - F^U t^U$$
$$Ft \leq Ft^U - F^L yt^U + F^L\vartheta \qquad Ft \leq F^U t + Ft^L - F^U t^L \qquad (8)$$
$$\vartheta \geq yt^L \qquad \vartheta \geq t + yt^U - t^U \qquad \vartheta \leq yt^U \qquad \vartheta \leq t + yt^L - t^L$$

Since the relaxation of the energy balance equations of temperature stages (Eq.2) overestimates the availability of high temperature heat, the heat cascade (Papoulias & Grossmann, 1983) constraints (i.e., the linear heat balance constraints for each temperature zone defined by the inlet temperature of streams) are included in the MILP.

These constraints guarantee heat transfer feasibility and tighten the relaxation. The nonlinear terms for the calculation of the areas of the heat exchangers, using Chen approximation (Chen, 1987) for the LMTD, are linearized with first order Taylor's series expansions. The exponential expression of the costs of components, such as heat exchangers and turbines, are linearized with piecewise linearization.

3.2. NLP subproblem

In the second stage, the binary variables from the solution of the master problem (i.e., the plant configuration and heat exchangers layout) are fixed. The continuous variables of the nonlinear subproblem are optimized with a nonlinear optimization algorithm, with the TAC as objective function. The solution of the subproblem yields a valid upper bound for the problem.

3.3. Nested integer cuts and termination criterion

In each iteration, the MILP master problem and the NLP subproblem are solved in sequence, and integer cuts are added to the master level at each iteration to exclude the binary solutions already evaluated. Fig. 2 shows the scheme of the algorithm. Two types of integer cuts are added in nested loops: the outer loop adds "utility cuts" on the binary selection variables of the utilities and Rankine cycle components (*y*), while the inner loop, for fixed utility selection/cycle configuration, adds "HEN cuts" on the selection of heat exchangers (*z*). "HEN cuts" are added at each iteration, while "utility cuts" are added after $N_{I,MAX}$ iterations without solution improvement. The algorithm stops after $N_{TOT,MAX}$ iterations without solution improvement.

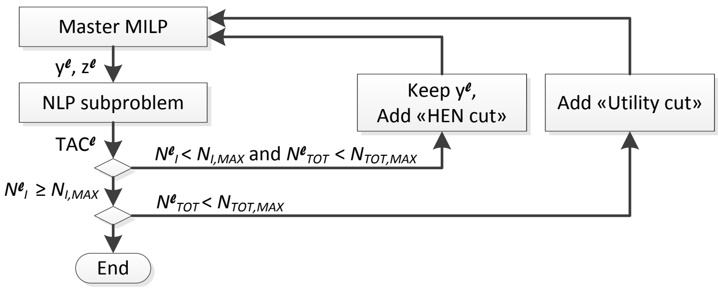

Figure 2: Scheme of the algorithm. For each iteration *l*, N^l_I and N^l_{TOT} count the number of iterations with no solution improvement respectively in the inner loop and overall.

4. Test cases

The methodology is used to optimize the design and the HEN of three different real-world test cases reported in literature.

- Design and HEN of a Heat Recovery Steam Cycle (HRSC) of a Combined Cycle (Martelli et al., 2017). The only hot process stream is the stream of flue gases of a gas turbine. The steam cycle superstructure is represented in Fig.1. The full MINLP problem has 2,060 variables (446 binaries) and 4,245 equations.
- Design and HEN of a geothermal Organic Rankine Cycle (ORC). The only hot process stream is represented by geothermal hot water. The ORC superstructure, with pentane as working fluid, and the data for the problem are described in (Elsido

et al., 2017b). The full MINLP problem has 1,231 variables (270 binaries) and 2,371 equations.

- Design of HRSC and HEN of an Integrated Gasification Combined Cycle (IGCC) plant (Martelli et al., 2017) with 9 hot process streams and 4 cold process streams in addition to the streams of the superstructure. The steam cycle superstructure is the same as for the Combine Cycle test case. The full MINLP problem has 8,608 variables (1,999 binaries) and 15,737 equations.

For all test cases, Rankine cycle pressures and temperatures have not been optimized. The proposed bilevel decomposition algorithm is solved using CPLEX as solver for the MILP master problem and the Sequential Quadratic Programming algorithm of SNOPT for the NLP subproblem. The results are compared with two alternative solution strategies: direct solution of the nonconvex MINLP problem with the global MINLP solver BARON (Tawarmalani & Sahinidis, 2005), and a meta-heuristic two-stage algorithm, consisting of the Variable Neighbourhood Search (VNS) in the first stage for the binary variables and SNOPT for the real variables, as described in (Martelli et al., 2017). Computational results are reported in Table 1.

Table 1. Computational results of the test problems.

	BARON	**Two-stage (Martelli et al. 2017)**	**Bilevel (this work)**
Combined Cycle			
Best solution found, M$/y	-37.0	-42.8	-42.8
Computational time, s	20,000 (limit)	6,000	120
Number of iterations		50,000	50
ORC			
Best solution found, M$/y	-0.277	-0.321	-0.357
Computational time, s	20,000 (limit)	4,000	41
Number of iterations		20,000	48
IGCC			
Best solution found, M$/y	No feasible sol.	-86.7	-88.5
Computational time, s	20,000 (limit)	6,000	2,000
Number of iterations		10,000	60

It should be noticed that a negative value of the objective function represents a revenue. In all cases, BARON has the worst performances in solving the challenging nonconvex MINLP problem among the three methods. Indeed, it reaches suboptimal solutions for the Combined Cycle and the ORC cases and not even finding a feasible solution for the IGCC test case. On the other hand, the bilevel decomposition method is very effective, finding the best solutions in all cases (16-29 % better objective values than BARON) with a computational time up to 2 orders of magnitude shorter than to the other two approaches.

5. Conclusions

We presented an ad-hoc bilevel decomposition method to solve complex optimization problems for the simultaneous design of utility systems, Rankine cycles and HEN. The literature and real-world case studies proved that the bilevel decomposition method, compared to commercial MINLP solver and meta-heuristic two-stage algorithm, is the most effective both in terms of computational time and quality of the solutions found.

Nomenclature

Indices
i, j hot/cold process or utility stream
k index for temperature stage
c component of Rankine cycle
in input, *out* output
L, U lower/upper bound
Parameters
Cp heat capacity
Tin, Tout inlet/outlet temperature
U heat transfer coefficient
$\Delta Tmax$ upper bound for temp. difference
h enthalpy
FC fixed cost for component/exchanger
VC flow/area cost coefficient
α, β exponent for component/area cost

Binary Variables
z existence of heat exchanger
y existence of utility/Rankine cycle component
Continuous variables
F mass flow rates of streams (fixed for process streams)
t temperature of streams at a stage
dt approach temperature difference
LMTD log mean temperature difference
q, qcu, qhu heat exchanged
Q thermal power
P electric power
R revenues from electricity selling
TAC Total Annual Cost
θ auxiliary variable for McCormick relaxations

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