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A global MINLP optimization algorithm for the synthesis of heat exchanger networks with no stream splits

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Abstract

In this paper a global optimization algorithm is presented to rigorously solve the MINLP model by Yee and Grossmann (1990) for the synthesis of heat exchanger networks under the simplifying assumptions of linear area cost, arithmetic mean temperature difference driving forces and no stream splitting. The proposed approach relies on the use of two new different sets of convex underestimators for the heat transfer area. A thermodynamic analysis is used to derive the first set of analytical linear and nonlinear convex underestimators as well as variable bounds and bounds contraction relationships. The second set of convex underestimators is generated by a relaxation of the heat transport equation through the introduction of a new variable, and an inequality that contains a nonconvex term that is subsequently replaced by its concave envelope. Based on these new underestimator functions, the original nonconvex MINLP is replaced by a convex MINLP that predicts tight lower bounds to the global optimum, and which is used in a hybrid branch and bound/outer-approximation search method. Application of the proposed ideas, and the algorithm are illustrated with several numerical examples.

Keywords: Synthesis of heat exchanger networks; Mixed integer programming; Global optimization; Branch and bound; Outer approximation

1. Introduction

In the synthesis of heat exchanger networks (see Gundersen and Naess, 1988, for a review) the mathematical programming approach, which involves the simultaneous optimization of energy consumption, area and matches, requires the solution of nonconvex mixed integer nonlinear programming (MINLP) models (Yee and Grossmann, 1990; Ciric and Floudas, 1991). A MINLP model is nonconvex if the relaxation of the integrality condition yields a nonconvex nonlinear programming (NLP) problem. Current techniques for the solution of MINLP models include generalized Benders decomposition (Geoffrion, 1972), the branch and bound method (Gupta and Ravindran, 1985), outer approximation (Duran and Grossmann, 1986), the LP/NLP based branch and bound technique (Quesada and Grossmann, 1992), and the extended cutting plane method (Westerlund and Pettersson, 1992). A brief description of these techniques, and extensive references on the subject, can be found in Grossmann and Kravanja (1995). It is well known that, when applied to nonconvex MINLP models, these techniques might get trapped at suboptimal solutions, or even worse they may fail to obtain a feasible point. Although heuristic strategies have been used to try to reduce the effect of nonconvexities (see e.g. Viswanathan and Grossmann, 1990), none of the above techniques can guarantee global optimum solutions when solving nonconvex MINLP problems.

Assuming linear area cost functions, arithmetic mean driving force temperature differences, and no stream splitting on the MINLP model by Yee and Grossmann (1990), the only nonconvex terms in the model for the synthesis of heat exchanger networks (HEN) arise in the area equations. In this paper we propose a global optimization algorithm for the solution of this MINLP model, which in fact provides a lower bound to networks with no stream splits but which obey the logarithmic mean temperature difference (LMTD). Aside from the fact that solving to globality nonconvex MINLP problems remains an open question, a major complication is that straightforward extension of global methods for nonconvex NLP (Horst and Tuy, 1993; Horst and Pardalos, 1995; Grossmann, 1996) to MINLP problems

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yield poor bounds. Hence there is a need to develop effective methods that can exploit the structure of these problems.

The paper is organized as follows. We first present the detailed MINLP model. In section 3 we briefly review the work of Quesada and Grossmann (1993) on the global optimization of heat exchanger networks with fixed topology. Their linear and nonlinear estimators for bilinear and linear fractional terms are incorporated in the convex MINLP to obtain lower bounds on the global minimum cost of heat exchanger networks. In section 4 we analyze a single unit heat exchanger system, and develop new thermodynamics based underestimators for the approximation of heat exchangers. In section 5 we transform the heat transfer equation to generate a second set of underestimators for the area of heat exchangers. The two sets of estimators are proved to be convex, and conditions under which the approximation they provide is exact are established. The two sets of estimators are also shown to be nonredundant with respect to each other. Section 6 describes a strategy to bound the global minimum of the total annual cost of heat exchanger networks. A convex MINLP program that integrates the proposed estimators, as well as the previous ones from literature, are used to obtain tight lower bounds for the global minimum. In section 7 we present a hybrid branch and bound/outer-approximation global optimization algorithm for the synthesis of heat exchanger networks. The application of this algorithm to the synthesis of two heat exchanger networks demonstrates the tightness of the convex relaxation that we use, as well as the effectiveness of the proposed technique. Finally, in section 8 we draw the conclusions.

2. Problem statement

Yee and Grossmann superstructure for the synthesis of HEN

Yee and Grossmann (1990) proposed a stagewise superstructure representation for the simultaneous HEN synthesis problem. Figure 1 shows a three stage superstructure for a two hot–two cold stream synthesis problem. At each stage, hot and cold streams are split to allow the potential existence of a heat exchanger to match any hot–cold pair of streams. This concept enables the implicit inclusion of a large number of system topologies. Before a stream enters a new stage its streams of the preceding stage are remixed isothermally. Extreme utilities are assumed to be placed at the outlets of the superstructure. It should be noted that it is in principle possible to handle utility streams as process streams with which multiple utilities and their arbitrary placement in the superstructure can be handled. Generally, the number of stages in the superstructure is set equal to the maximum cardinality of the hot and cold sets of streams, although sometimes it is necessary to increase the number of stages to allow designs with minimum energy consumption (see Daichendt and Grossmann, 1994). These authors also proposed a preliminary screening procedure for selecting the number of stages, and eliminating units in the superstructure so as to guarantee that maximum recovery networks are embedded.

The MINLP model of Yee and Grossmann superstructure, allows nonvertical heat transfer, and stream rematches, assumes no heat recovery approach temperature (HRAT), and also simultaneously optimizes capital and operating costs. The isothermal mixing assumption, reduces the mathematical representation of the feasible region to be linearly constrained. Besides the isothermal mixing assumption, Yee and Grossmann model considers: constant heat capacity flowrates, constant film heat transfer coefficients, and countercurrent heat exchangers. Nonconvexities in the continuous space of variables are introduced to the MINLP objective function by the concave area cost function and the heat transfer equation, which fixes the area required for a specific heat load to take place. Due to the nonconvexities present in the model, current MINLP solvers (e.g. Viswanathan and Grossmann, 1990) often get trapped in poor solutions or cut off the global optimal solution converging to suboptimal network structures.

Simplifying assumptions and problem statement

In order to induce special structure in the MINLP model by Yee and Grossmann (1990) with which a

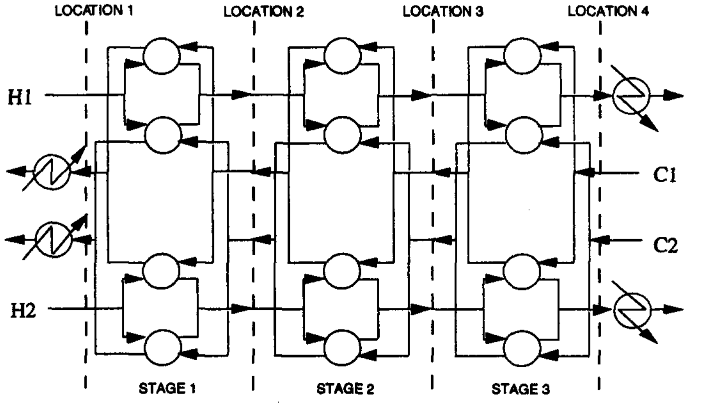


Fig. 1. Heat exchanger network superstructure

globally optimum solution for the synthesis of HEN can be determined rigorously, we impose three simplifying assumptions: i) Linear area cost functions; ii) Arithmetic mean driving force temperature differences; and iii) No stream splitting. Under these conditions, the problem addressed in this paper can be formally stated as follows:

Given

- A set of hot process streams to be cooled, and a set of cold process streams to be heated, with their corresponding heat capacity flowrates, film heat transfer coefficients, and stream supply and target temperatures.
- A set of hot and cold utilities, with film heat transfer coefficients, and input and output temperatures.
- Information on utilities and capital costs for heat exchangers.

Determine

- A globally optimal HEN structure with no stream splitting, and with its associated specifications and operating conditions such that the network exhibits the least total annual cost.

Nonconvex MINLP model (P)

Using the above assumptions, the model by Yee and Grossmann (1990) for the synthesis of heat exchanger networks can be modified to yield the MINLP model (P). This paper addresses the global optimization of model (P), which is nonconvex in the space of continuous variables due to the presence of linear fractional terms in the objective function.

Model (P)

Indices:
i=hot process stream
j=cold process stream
k=index for stage, and temperature location
cu=cold utility
hu=hot utility
in=inlet
out=outlet

Sets
$I=\{i: i$ is a hot process stream$\}$
$J=\{j: j$ is a cold process stream$\}$
$K=\{k: k$ is a stage in the superstructure, $|K|=NOK\}$

Parameters
$T_{i,in}$, $T_{i,out}$, $T_{j,in}$, $T_{j,out}$=inlet and outlet temperatures
ΔT_{mapp}=minimum approach temperature difference (EMAT)
F_i, F_j=heat capacity flowrates
h_i, h_j, h_{cu}, h_{hu}=film heat transfer coefficients
$U_{i,j}$, $U_{i,cu}$, $U_{j,hu}$=overall heat transfer coefficients
CCU=per unit cost of cold utility
CHU=per unit cost of hot utility
CF_{ij}, $CF_{i,cu}$, $CF_{j,hu}$=fixed charges for exchangers
C_{ij}, $C_{i,cu}$, $C_{j,hu}$=area cost coefficient
NOK=total number of stages
Ω=an upper bound for heat exchange
Γ=an upper bound for temperature difference

Positive, continuous variables
$t_{i,k}$=temperature of hot stream i at hot end of stage k
$t_{j,k}$=temperature of cold stream j at hot end of stage k
dt_{ijk}=temperature approach for match (i,j) at temperature location k
$dtcu_i$=temperature approach for the match of hot stream i and cold utility
$dthu_j$=temperature approach for the match of cold stream j and hot utility
q_{ijk}=heat exchanged between hot process stream i and cold process stream j in stage k
qcu_i=heat exchanged between hot stream i and cold utility
qhu_j=heat exchanged between cold stream j and hot utility
$AMTD_{i,j,k}$, $AMTD_{i,cu}$, $AMTD_{j,hu}$=heat transfer driving forces

Binary variables
z_{ijk}=existence of unit for match (i,j) in stage k
zcu_i=existence of unit for match (i,cu)
zhu_j=existence of unit for match (j,hu)

Objective function

minimize

$$\begin{aligned}&\sum_{i\in I}\sum_{j\in J}\sum_{k\in K} CF_{ij}z_{ijk}+\sum_{i\in I} CF_{i,cu}zcu_i+\sum_{j\in J} CF_{j,hu}zhu_j\\&+\sum_{i\in I}\sum_{j\in J}\sum_{k\in K} C_{ij}[q_{ijk}/(U_{i,j}\,AMTD_{i,j,k})]\\&+\sum_{i\in I} C_{i,cu}[qcu_i/(U_{i,cu}\,AMTD_{i,cu})]\\&+\sum_{j\in J} C_{j,hu}[qhu_j/(U_{j,hu}\,AMTD_{j,hu})]\\&+\sum_{i\in I} CCU\,qcu_i+\sum_{j\in J} CHU\,qhu_j\end{aligned}\tag{2-1}$$

where

$$\begin{aligned}U_{i,j}&=[1/h_i+1/h_j]^{-1}\\U_{i,cu}&=[1/h_i+1/h_{cu}]^{-1}\\U_{j,hu}&=[1/h_j+1/h_{hu}]^{-1}\end{aligned}\tag{2-2}$$

and

$$\begin{aligned}AMTD_{i,j,k}&=(dt_{ijk}+dt_{ijk+1})/2\\AMTD_{i,cu}&=(dtcu_i+T_{i,out}-T_{cu,in})/2\\AMTD_{j,hu}&=(dthu_j+T_{hu,in}-T_{j,out})/2\end{aligned}\tag{2-3}$$

Overall heat balance for each stream

$$\begin{aligned}&\sum_{j\in J}\sum_{k\in K} q_{ijk}+qcu_i=F_i(T_{i,in}-T_{i,out}) \quad i\in I\\&\sum_{i\in I}\sum_{k\in K} q_{ijk}+qhu_j=F_j(T_{j,out}-T_{j,in}) \quad j\in J\end{aligned}\tag{2-4}$$

Heat balance at each stage

$$\begin{aligned}&\sum_{j\in J} q_{ijk}=F_i(t_{i,k}-t_{i,k+1}) \quad i\in I,\ k\in K\\&\sum_{i\in I} q_{ijk}=F_j(t_{j,k}-t_{j,k+1}) \quad j\in J,\ k\in K\end{aligned}\tag{2-5}$$

Assignment of superstructure inlet temperatures

$$\begin{aligned}t_{i,1}&=T_{i,in} \quad i\in I\\t_{j,NOK+1}&=T_{j,in} \quad j\in J\end{aligned}\tag{2-6}$$

Monotonic decrease in temperatures

$$\begin{array}{ll} t_{i,k}\geq t_{i,k+1} & i\in \mathrm{I},\ k\in \mathrm{K} \\ t_{i,NOK+1}\geq \mathrm{T}_{i,out} & i\in \mathrm{I} \\ t_{j,k}\geq t_{j,k+1} & j\in \mathrm{J},\ k\in \mathrm{K} \\ T_{j,out}\geq t_{j,1} & j\in \mathrm{J} \end{array} \tag{2-7}$$

Hot and cold utilities load

$$\begin{array}{ll} qcu_i=\mathrm{F}_i(t_{i,NOK+1}-\mathrm{T}_{i,out}) & i\in \mathrm{I} \\ qhu_j=\mathrm{F}_j(\mathrm{T}_{j,out}-t_{j,1}) & j\in \mathrm{J} \end{array} \tag{2-8}$$

Minimum approach temperature constraints

$$\begin{array}{ll} dt_{ijk}\geq \Delta\mathrm{T}_{\mathrm{mapp}} & i\in \mathrm{I},\ j\in \mathrm{J},\ k\in \mathrm{K}\cup\{NOK+1\} \\ dtcu_i\geq \Delta\mathrm{T}_{\mathrm{mapp}} & i\in \mathrm{I}, \\ dthu_j\geq \Delta\mathrm{T}_{\mathrm{mapp}} & j\in \mathrm{J} \end{array} \tag{2-9}$$

Logical constraints

$$\begin{array}{ll} q_{ijk}\leq \Omega z_{ijk} & i\in \mathrm{I},\ j\in \mathrm{J},\ k\in \mathrm{K} \\ qcu_i\leq \Omega zcu_i & i\in \mathrm{I} \\ qhu_j\leq \Omega zhu_j & j\in \mathrm{J} \\ dt_{ijk}\leq t_{i,k}-t_{j,k}+\Gamma(1-z_{ijk}) & i\in \mathrm{I}, j\in \mathrm{J}, k\in \mathrm{K} \\ dt_{ijk+1}\leq t_{i,k+1}-t_{j,k+1}+\Gamma(1-z_{ijk}) & i\in \mathrm{I}, j\in \mathrm{J}, k\in \mathrm{K} \\ dtcu_i\leq t_{i,NOK+1}-\mathrm{T}_{cu,out}+\Gamma(1-zcu_i) & i\in \mathrm{I} \\ dthu_j\leq \mathrm{T}_{hu,out}-t_{j,1}+\Gamma(1-zhu_j) & j\in \mathrm{J} \end{array} \tag{2-10}$$

No stream splitting constraints

$$\begin{array}{ll} \sum_{j\in \mathrm{J}} z_{ijk}\leq 1 & i\in \mathrm{I},\ k\in \mathrm{K} \\ \sum_{i\in \mathrm{I}} z_{ijk}\leq 1 & j\in \mathrm{J},\ k\in \mathrm{K} \end{array} \tag{2-11}$$

Integrality conditions

$$z_{ijk},\ zcu_i,\ zhu_j=0,1 \quad i\in \mathrm{I}, j\in \mathrm{J}, k\in \mathrm{K} \tag{2-12}$$

Bounds

$$\begin{array}{l} \mathrm{T}_{i,out}\leq t_{i,k}\leq \mathrm{T}_{i,\epsilon} \quad i\in \mathrm{I} \\ \mathrm{T}_{j,in}\leq t_{j,k}\leq \mathrm{T}_{j,out} \quad j\in \mathrm{J} \\ q_{ijk}, qcu_i, qhu_i\geq 0 \quad i\in \mathrm{I}, j\in \mathrm{J}, k\in \mathrm{K} \\ \mathrm{AMTD}_{i,j,k},\ \mathrm{AMTD}_{i,cu},\ \mathrm{AMTD}_{j,hu}\geq \Delta\mathrm{T}_{\mathrm{mapp}} \quad i\in \mathrm{I},\ j\in \mathrm{J},\ k\in \mathrm{K} \end{array} \tag{2-13}$$

REMARK

Note that (2-11) replaces the isothermal mixing assumption of Yee and Grossmann (1990) by the more stringent no stream splitting assumption of this paper. If (2-11) is deleted from model (P), the original isothermal mixing model structure by Yee and Grossmann is recovered.

3. Previous work in global optimization

Quesada and Grossmann (1993) proposed a branch and bound algorithm for the global optimization of heat exchanger networks with fixed topology. Under the assumptions of fixed topology, linear area cost, arithmetic mean driving force temperature differences and isothermal mixing, a nonconvex nonlinear model that exhibits linear fractional terms in the objective function, and a feasible region defined by linear constraints is obtained. With the introduction of the area variable, A_{ijk}, into the model, a nonlinear reformulation that includes bilinear terms in the heat transfer equations is generated. Using McCormick's (1976, 1983) results for the development of convex and concave approximations of factorable functions, Quesada and Grossmann developed relationships that define the following non redundant inequalities,

$$\mathrm{A}_{ijk}\,\mathrm{AMTD}_{ijk}\leq Min[\mathrm{A}^L_{ijk}\,\mathrm{AMTD}_{ijk}+\mathrm{AMTD}^U_{ijk}\,\mathrm{A}_{ijk}-\mathrm{A}^L_{ijk}\,\mathrm{AMTD}^U_{ijk}, \tag{3-1}$$
$$\mathrm{A}^U_{ijk}\,\mathrm{AMTD}_{ijk}+\mathrm{AMTD}^L_{ijk}\,\mathrm{A}_{ijk}-\mathrm{A}^U_{ijk}\,\mathrm{AMTD}^L_{ijk}]$$

$$\mathrm{U}_{ij}\,\mathrm{A}_{ijk}\geq Max\left[\frac{q_{ijk}}{\mathrm{AMTD}^U_{ijk}}+q^L_{ijk}\left(\frac{1}{\mathrm{AMTD}_{ijk}}-\frac{1}{\mathrm{AMTD}^U_{ijk}}\right),\ \frac{q_{ijk}}{\mathrm{AMTD}^L_{ijk}}+q^U_{ijk}\left(\frac{1}{\mathrm{AMTD}_{ijk}}-\frac{1}{\mathrm{AMTD}^L_{ijk}}\right)\right] \tag{3-2}$$

Note that (3-1), and (3-2) hold as equalities in the case in which $\mathrm{A}_{ijk}=\mathrm{A}^L_{ijk},\mathrm{A}^U_{ijk}$ or $\mathrm{AMTD}_{ijk}=\mathrm{AMTD}^L_{ijk},\mathrm{AMTD}^U_{ijk}$, and $\mathrm{A}_{ijk}=\mathrm{A}^L_{ijk},\mathrm{A}^U_{ijk}$ or $q_{ijk}=q^L_{ijk},q^U_{ijk}$, respectively. It is not difficult to prove that the function on the right hand side of (3-1) is the concave envelope of the bilinear product on the left (see e.g. Al-Khayyal, 1990). Quesada and Grossmann also used the notion of Benders cuts (Geoffrion, 1972) to propose a procedure based on LP subproblems to generate a projected bounding function between the heat load and the arithmetic mean temperature difference of a heat exchanger. Although the proposed procedure does not always lead to a non-trivial relation, when it does, it provides a linear functional upper (or lower) bound for the driving force as a function of the heat load. Quesada and Grossmann used the projected relationships in conjunction with (3-2) to obtain a tighter approximation of the linear fractional terms of the original nonconvex model. In their branch and bound algorithm, a convex NLP relaxation is used which includes (3-1), (3-2), and the nonlinear projected convex underestimators. These authors applied their method to seven HEN problems obtaining very encouraging results in terms of times and quality of lower bounds.

It is important to mention that although the estimators used by Quesada and Grossmann have proved to be successful for fixed topology global optimization problems, the situation in the simultaneous synthesis (MINLP) problem is quite different. Firstly, the tight bounds that are obtained in problems with fixed structure, and that allow having good approximations of the nonconvex terms, are no longer obtained in the synthesis problems. The reason is that the variable bounds become very loose since the presence or non existence of each heat exchanger must be determined. Secondly, the procedure to generate the projected underestimators of Quesada and Grossmann cannot be effectively extended to the MINLP case. Finally, we must also consider the combinatorial nature introduced by the binary variables in the MINLP synthesis model.

4. Thermodynamics based approximation of heat exchangers

Analysis for a general heat exchanger

Consider streams i and j, which have ($T_{i,in}$, $T_{i,out}$), and ($T_{j,in}$, $T_{j,out}$) as supply and target temperatures, respectively. Also, assume that this hot–cold pair of streams is to be matched at stage k, with a heat load equal to q_{ijk}. The area required to perform the specified heat transfer operation at stage k can be minimized by taking the highest possible driving force in the system. In other words, if streams i and j have no interactions in other stages of the superstructure, they should enter the k-th stage with temperatures $t_{i,k}=T_{i,in}$ and $t_{j,k+1}=T_{j,in}$. In this way, stream i will undergo a change in temperature from $t_{i,k}=T_{i,in}$ at temperature level k to $t_{i,k+1}=T_{i,in}-q_{ijk}/F_i$ at temperature level $k+1$. Similarly, cold stream j will go from $t_{j,k+1}=T_{j,in}$ at temperature level $k+1$ to $t_{j,k}=T_{j,in}+q_{ijk}/F_j$ at temperature level k. As a consequence of this reasoning, we obtain the following bounding expression for the driving force:

$$AMTD_{i,j,k}\leq AMTD^{U}_{i,j,k}=T_{i,in}-T_{j,in}-q_{ijk}(1/F_i+1/F_j)/2 \quad (4\text{-}1)$$

Furthermore, in the case in which tighter upper and lower bounds are available, that is, $t_{i,k}\leq t^{U}_{i,k}\leq T_{i,in}$, and $t_{j,k+1}\geq t^{L}_{j,k+1}\geq T_{j,in}$, (4-1) can be refined to obtain a tighter representation for the driving force of each heat exchanger in the superstructure:

$$AMTD_{i,j,k}\leq AMTD^{U}_{i,j,k}=t^{U}_{i,k}-t^{L}_{j,k+1}-q_{ijk}(1/F_i+1/F_j)/2 \quad (4\text{-}2)$$

This representation of the upper bound for the driving force is especially useful in the reduction step performed after the branching operation of the global optimization algorithm, in which new temperature bounds are generated at some points in the network. The analytical relationship in (4-2), which has the same functional form as the projections obtained numerically in the work by Quesada and Grossmann (1993), can be used, along with the heat transfer equation, to generate the following new class of thermodynamics based linear fractional underestimators for the area of heat exchangers:

$$A_{i,j,k}\geq\frac{q_{ijk}}{U_{i,j}[t^{U}_{i,k}-t^{L}_{j,k+1}-q_{ijk}(1/F_i+1/F_j)/2]} \quad (4\text{-}3)$$

The significance of Eq. (4-3) is that it provides an analytical relationship that explains the physical nature of the projections that are obtained numerically by Quesada and Grossmann through the solution of a set of linear programming subproblems. As shown below, the approximation given in (4-3) is convex. This approximation is also exact when the inlet temperatures, the heat capacities flowrates, and the global heat transfer coefficient are known.

Theorem 1

The thermodynamics based estimator (4-3) is convex, underestimates the area of heat exchangers, and provides an exact representation when the hot and cold stream input temperatures are $t_{i,k}=t^{U}_{i,k}$, and $t_{j,k+1}=t^{L}_{j,k+1}$, respectively.

Proof: see Appendix 1.

Analysis for coolers and heaters

In the context of the previous section, a cooler is a heat exchanger with known temperatures for the outlet of the hot stream, and the inlet and outlet of the cooling utility. The specification of three temperatures in a cooler reduces the number of degrees of freedom of the heat exchanger representation. For this type of heat exchangers, the inlet temperature of the hot stream is the only unknown temperature in the system, and can be represented exactly as a linear function of qcu_i: $t_{i,NOK+1}=T_{i,out}+qcu_i/F_i$. Using this expression, $AMTD_{i,cu}$ can be written as a function of qcu_i, and the following underestimator for the area of a cooler can be obtained directly from the heat transfer equation:

$$A_{i,cu}\geq\frac{qcu_i}{U_{i,cu}[(2T_{i,out}-T_{cu,in}-T_{cu,out}+qcu_i/F_i)/2]} \quad (4\text{-}4)$$

Following a similar argument as in Theorem 1, it can be easily proved that (4-4) is convex if $T_{i,out}\leq(T_{cu,in}+T_{cu,out})/2$, and concave otherwise. Surprisingly, in the convex case, (4-4) exhibits a monotonic decrease in the area as the inlet temperature of the hot stream to the cooler increases. This effect is produced by a dominant increase of the driving force over the increase of the heat duty. A similar, but non monotonic effect, can also be observed in coolers calculated with the LMTD. Also interesting is the fact that, due to the AMTD assumption, if $T_{i,out}=(T_{cu,in}+T_{cu,out})/2$ the area requirement remains constant, $A_{i,cu}=2F_i/U_{i,cu}$, regardless of the heat load in the heat exchanger. It should be noted, however, that the more common case is when $T_{i,out}\geq(T_{cu,in}+T_{cu,out})/2$. To approximate coolers for which $T_{i,out}\geq(T_{cu,in}+T_{cu,out})/2$, we use the convex envelope of (4-4), which in this case is a straight line that exactly approximates the area at the lower and upper bounds of qcu_i.

A similar analysis can be performed for heaters, for which the following inequality can be obtained:

$$A_{j,hu}\geq\frac{qhu_j}{U_{j,hu}[(T_{hu,in}+T_{hu,out}-2T_{j,out}+qhu_j/F_j)/2]} \quad (4\text{-}5)$$

In this case the estimator is convex if $T_{j,out}\geq(T_{hu,in}+T_{hu,out})/2$, otherwise it is concave. The heat transfer area is constant, $A_{j,hu}=2F_j/U_{j,hu}$, when $T_{j,out}=(T_{hu,in}+T_{hu,out})/2$. Again, the common case is the nonconvex case in which $T_{j,out}\leq(T_{hu,in}+T_{hu,out})/2$, especially if $T_{hu,in}=T_{hu,out}$.

Example 1

To illustrate the advantages of the estimators proposed in this section, consider the task of underestimating the minimum cost of the heat exchanger network shown in Fig. 2 by solving one single convex underestimating problem. The stream heat capacity flowrates, temperatures, overall heat transfer coefficients and cost information for this problem are given in Table 1. Note that the outlet temperatures of the hot streams are not

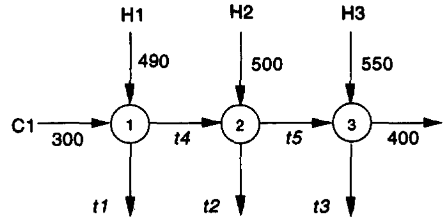


Fig. 2. Heat exchanger network for example 1

specified. A nonlinear programming model that can be formulated for the minimization of the cost of this network includes a linear objective function, linear energy balances and nonconvex heat transfer equations:

$$\text{Minimize } 1000(A_1+A_2+A_3) \qquad \text{(EX1-a)}$$

$$q_1=10(t_4-300)$$

$$q_1=10(490-t_1)$$

$$q_2=10(t_5-t_4)$$

$$q_2=10(500-t_2)$$

$$q_3=10(400-t_5)$$

$$q_3=10(550-t_3)$$

$$A_1\geq \frac{2q_1}{(t_1-t_4+190)}$$

$$A_2\geq \frac{2q_2}{(t_2-t_4-t_5+500)}$$

$$A_3\geq \frac{2q_3}{(t_3-t_5+150)}$$

$$q_1,q_2,q_3,A_1,A_2,A_3\geq 0;\ 300\leq t_4\leq t_5\leq 400$$

To generate a convex relaxation for this model, we must first develop convex underestimators for the area of each one of the three heat exchangers. The stream inlet temperatures for heat exchanger 1 are known. Therefore, the inequality in (4-3) provides an exact representation of its heat transfer area:

$$A_1\geq \frac{q_1}{190-0{\cdot}1q_1} \qquad \text{(EX1-b)}$$

Although the inlet temperature of the cold stream in the second heat exchanger is unknown, it is possible to design a reasonably good lower bounding approximation for this unit by using the lowest value for temperature t_4, that is 300 K, in (4-3). This yields,

$$A_2\geq \frac{q_2}{200-0{\cdot}1q_2} \qquad \text{(EX1-c)}$$

For the third heat exchanger, we need to take into account that, besides having a fixed input temperature for the hot stream, the outlet of the cold stream is also specified. This requires a particular analysis, similar to the ones performed for coolers and heaters. The convex underestimator obtained in this case is also exact and it is given by

$$A_3\geq \frac{q_3}{150} \qquad \text{(EX1-d)}$$

By solving the convex nonlinear programming problem defined by the objective function, the energy balances, and the three underestimators in (EX1-b), (EX1-c), and (EX1-d), a lower bound of \$6,269.93 is obtained for the global minimum cost of the heat exchanger network. The areas of the exchangers are $A_1=1{\cdot}26\ m^2$, $A_2=1{\cdot}55\ m^2$, and $A_3=3{\cdot}47\ m^2$. Quesada and Grossmann (1993) obtained the same result by solving a nonlinear program that, besides the objective function and the energy balances, includes their proposed linear, nonlinear, and projected underestimators. In addition, to obtain the bounds for the variables, and the information required by the estimators and to generate projections, these authors had to solve 18 linear programming problems.

Table 1. Data for example 1

Stream	F ($kW\ K^{-1}$)	Tin (K)	Tout (K)
C1	10	300	400
H1	10	490	
H2	10	500	
H3	10	550	

$U=1\ kW\ K^{-1}\ m^{-2}$ for all mataches.
Area cost coefficient $C=\$1000/m^2$.
No fixed charge.

5. A Second Convex Relaxation of the Heat Transfer Equation

Since the MINLP model can lead to loose lower bounds with the estimators in (3-1), (3-2), (4-3), (4-4), and (4-5), it is desirable to consider additional underestimators which preferably rely less on the variable bounds. To develop a second set of convex underestimators for the approximation of the area of heat exchangers, consider again that a hot stream i is matched with a cold stream j at stage k. In this case, let us also assume that the amount of heat, q_{ijk}, to be transferred belongs to the interval $[q^L_{ijk},q^U_{ijk}]$. Due to our interest in generating a HEN that exhibits minimum overall total annual cost, we can focus our attention on the following relaxed version of the heat transfer equation:

$$A_{i,j,k}\geq \frac{q_{ijk}}{U_{i,j}\,AMTD_{i,j,k}} \qquad (5\text{-}1)$$

Introducing the new variable $\Theta\equiv\sqrt{q_{ijk}}$ into (5-1) yields the following inequality:

$$A_{i,j,k}\geq \frac{\Theta^2}{U_{i,j}\,AMTD_{i,j,k}} \qquad (5\text{-}2)$$

The defining relationship for Θ is given by means of two inequalities:

$$\Theta^2\leq q_{ijk} \qquad (5\text{-}3a)$$

$$\Theta^2 \geq q_{ijk} \tag{5-3b}$$

The second inequality, a nonconvex expression, can be convexified by substituting the quadratic term by its concave envelope,

$$q_{ijk}^L + (\sqrt{q_{ijk}^L} + \sqrt{q_{ijk}^U})(\Theta - \sqrt{q_{ijk}^L}) \geq q_{ijk} \tag{5-4}$$

Solving for Θ we obtain,

$$\Theta \geq \frac{q_{ijk} + \sqrt{q_{ijk}^L q_{ijk}^U}}{\sqrt{q_{ijk}^L} + \sqrt{q_{ijk}^U}} \tag{5-5}$$

Finally, by using (5-5) in (5-2) we generate a second set of quadratic/linear underestimators for the heat transfer area of heat exchangers, which will be shown later to be convex:

$$A_{i,j,k} \geq \frac{1}{U_{i,j}\,\mathrm{AMTD}_{i,j,k}} \left(\frac{q_{ijk} + \sqrt{q_{ijk}^L q_{ijk}^U}}{\sqrt{q_{ijk}^L} + \sqrt{q_{ijk}^U}} \right)^2 \tag{5-6}$$

Note that only bounds for the heat load are required in the application of (5-6). For obvious reasons, q_{ijk}^L is set to zero in synthesis problems. From the second law of thermodynamics, and the maximum heat load allowed by supply and target temperatures in each stage we obtain an upper bound for the heat load q_{ijk},

$$q_{ijk}^U \leq Min[F_i(t_{i,k}^U - t_{i,k+1}^L),\ F_j(t_{j,k}^U - t_{j,k+1}^L),\ Min(F_i, F_j)(t_{i,k}^U - t_{j,k+1}^L - \Delta T_{\mathrm{mapp}})] \tag{5-7}$$

For coolers and heaters,

$$F_i(t_{i,NOK+1}^L - T_{i,out}) \leq q_{cu,i} \leq F_i(t_{i,NOK+1}^U - T_{i,out}) \tag{5-8}$$
$$F_j(T_{j,out} - t_{j,1}^U) \leq q_{hu,j} \leq F_j(T_{j,out} - t_{j,1}^L)$$

Theorem 2. The quadratic/linear fractional inequality in (5-6) is convex, underestimates the area of heat exchangers in the interval $q_{ijk} \in [q_{ijk}^L, q_{ijk}^U]$, and provides an exact representation when $q_{ijk} = q_{ijk}^L$ or $q_{ijk} = q_{ijk}^U$.

Proof: see Appendix 1.

Example 2

Consider example 1, but now, instead of using (EX1-c), we use (5-6) to underestimate the area of the second heat exchanger (recall that EX1-b and EX1-d provide an exact representation of exchangers 1 and 3). To use the inequality in (5-6), we require to have valid lower and upper bounds on the heat load for exchanger 2. A simple analysis of the heat exchanger system, yields $q_2^L = 0$ and $q_2^U = 1000$, which substituted in (5-6) produces

$$A_2 \geq \frac{(q_2)^2}{500(500 + t_2 - t_4 - t_5)} \tag{EX2-a}$$

When (EX2-a) is used, along with the objective function, energy balances, and (EX1-b) and (EX1-d), a lower bound of \$4,946.53 is obtained for the minimum cost of the heat exchanger network. The areas of the exchangers are $A_1 = 0{\cdot}52\ \mathrm{m}^2$, $A_2 = 1{\cdot}25\ \mathrm{m}^2$, and $A_3 = 3{\cdot}18\ \mathrm{m}^2$. The lower bound obtained here lies below the \$6,269.93 obtained in Example 1, when (EX1-c) is used. We conclude that, in this case, the thermodynamics based estimator is better than the new quadratic/linear estimator.

Example 3

Again, consider the same case as in Examples 1 and 2, but now, assume that the outlet temperature of the cold stream is 500 K, instead of 400 K. Also, assume that a minimum approach temperature of 10 K is to be enforced. Underestimation with the first set of estimators used in example 1 gives in this case a lower bound of \$20,993.59. To generate the quadratic/linear estimator for the second heat exchanger, bounds of $q_2^L = 0$ and $q_2^U = 1900$ are used. Solution of the lower bounding problem with the second estimator in (5-6) produces a lower bound of \$22,119.60, indicating that, in this case, the quadratic/linear estimator outperforms the thermodynamics based. Furthermore, when the two types of underestimators are used in conjunction, an even better lower bound, \$22,484.44, is obtained. This result proves that *neither of the two underestimators is dominant*, and therefore, it is desirable to use both of them.

6. Strategy for Bounding the Global Minimum of the Total Annual Cost

Lower bounding operation

The hybrid algorithm for the global optimization of model (P), which will be described in section 7, belongs to the family of branch and bound algorithms (see e.g. Horst and Tuy, 1993). A spatial search is performed in the space of the continuous variables, and at each node s, lower and upper bounds, β_s and α_s, for the global minimum of the total annual cost of the heat exchanger network are obtained. When the difference between these bounds is greater than a specified tolerance, ε, in order to obtain an improved approximation of the heat transfer areas, a partition of the feasible region is performed through a branching operation that imposes new bounds on a given temperature at a certain point in the superstructure. When the global lower bound, β, is within an ε-value of the global upper bound, α, the search process is stopped. The solution corresponding to the best upper bound is guaranteed to be an ε-global minimizer. To perform the lower bounding operation at each node we propose the following convex MINLP underestimating model:

Model (C)

Objective function

minimize

$$\sum_{i\in I}\sum_{j\in J}\sum_{k\in K} CF_{ij} z_{ijk} + \sum_{i\in I} CF_{i,cu} zcu_i + \sum_{j\in J} CF_{j,hu} zhu_j \tag{6-1}$$
$$+ \sum_{i\in I}\sum_{j\in J}\sum_{k\in K} C_{ij} A_{ijk} + \sum_{i\in I} C_{i,cu} A_{i,cu} + \sum_{j\in J} C_{j,hu} A_{j,hu}$$
$$+ \sum_{i\in I} CCUqcu_i + \sum_{j\in J} CHUqhu_j$$

Basic definitions, constraints, and specifications

$$\text{Equations } (2-2)-(2-13) \tag{6-2}$$

Thermodynamics based estimators

$$A_{ijk}\geq\frac{q_{ijk}}{U_{ij}[t_{i,k}^{s,U}-t_{j,k+1}^{s,L}-q_{ijk}(1/F_i+1/F_j)/2]}-\Lambda(1-z_{ijk})\quad i\in I, j\in J, k\in K$$

$$A_{i,cu}\geq\frac{qcu_i}{U_{i,cu}[(2T_{i,out}-T_{cu,in}-T_{cu,out}+qcu_i/F_i)/2]}-\Lambda(1-zcu_i)\quad i\in I$$

$$A_{j,hu}\geq\frac{qhu_j}{U_{j,hu}[(T_{hu,in}+T_{hu,out}-2T_{j,out}+qhu_j/F_j)/2]}-\Lambda(1-zhu_j)\quad j\in J \tag{6-3}$$

if r.h.s. of estimator is concave its convex envelope is used instead (coolers and heaters)

Quadratic/linear estimators

$$A_{ijk}\geq\frac{1}{U_{ij}\,\mathrm{AMTD}_{ijk}}\left(\frac{q_{ijk}+\sqrt{q_{ijk}^{s,L}q_{ijk}^{s,U}}}{\sqrt{q_{ijk}^{s,L}}+\sqrt{q_{ijk}^{s,U}}}\right)^2-\Lambda(1-z_{ijk})\quad i\in I, j\in J, k\in K \tag{6-4}$$

Nonlinear Estimators (Quesada and Grossmann, 1993)

$$U_{ij}A_{ijk}\geq\frac{q_{ijk}}{\mathrm{AMTD}_{ijk}^{s,U}}+q_{ijk}^{s,L}\left(\frac{1}{\mathrm{AMTD}_{ijk}}-\frac{1}{\mathrm{AMTD}_{ijk}^{s,U}}\right)-\Lambda(1-z_{ijk}) \tag{6-5}$$

$$U_{ij}A_{ijk}\geq\frac{q_{ijk}}{\mathrm{AMTD}_{ijk}^{s,L}}+q_{ijk}^{s,U}\left(\frac{1}{\mathrm{AMTD}_{ijk}}-\frac{1}{\mathrm{AMTD}_{ijk}^{s,L}}\right)-\Lambda(1-z_{ijk})\quad i\in I, j\in J, k\in K$$

Linear Estimators (Al-Khayyal, 1990; Quesada and Grossmann, 1993)

$$q_{ijk}\leq U_{ij}(A_{ijk}^{s,L}\,\mathrm{AMTD}_{ijk}+\mathrm{AMTD}_{ijk}^{s,U}A_{ijk}-A_{ijk}^{s,L}\,\mathrm{AMTD}_{ijk}^{s,U})+\Lambda(1-z_{ijk}) \tag{6-6}$$

$$q_{ijk}\leq U_{ij}(A_{ijk}^{s,U}\,\mathrm{AMTD}_{ijk}+\mathrm{AMTD}_{ijk}^{s,L}A_{ijk}-A_{ijk}^{s,U}\,\mathrm{AMTD}_{ijk}^{s,L})+\Lambda(1-z_{ijk})\quad i\in I, j\in J, k\in K$$

Bounds on variables

$$(T,q,\mathrm{AMTD},A)\in\Omega_s \tag{6-7}$$

where

$\Omega_s=\{(T,q,AMTD,A):T^{s,L}\leq T\leq T^{s,U},q^{s,L}\leq q\leq q^{s,U},$
$AMTD^{s,L}\leq AMTD\leq AMTD^{s,U},\ A^{s,L}\leq A\leq A^{s,U}\},$

$T=(t_{i,k},t_{j,k})$, $q=(q_{ijk},qcu_i,qhu_j)$, $\mathrm{AMTD}=(\mathrm{AMTD}_{ijk},\mathrm{AMTD}_{i,cu},\mathrm{AMTD}_{j,hu})$, and

$A=(A_{ijk},A_{i,cu},A_{j,hu})$.

The dimension of each of the vectors q, AMTD, and A is equal to |L|, which is the total number of exchangers, coolers and heaters in the superstructure. Note that in order to incorporate the underestimators developed in sections 4 and 5, as well as the ones from previous work, we express them in the form of disjunctions in (6-3)–(6-6) by including an extra logical term with a large parameter Λ. This extra term in the estimators renders the constraints inactive when a heat exchanger is not selected ($z_{ijk}=0$), and enforces the corresponding constraints when the heat exchanger is selected ($z_{ijk}=1$). All binary variables are also incorporated into a single vector $z=(z_{ijk}, zcu_i, zhu_j)$. M_0 denotes the feasible region defined by (6-2)–(6-7) at the branch and bound root node.

To obtain lower bounds for the global minimum of the total annual cost of HENs, the convex MINLP model (C) is solved at node s with the Outer Approximation Algorithm (Duran and Grossmann, 1986) by using the convex option in the code DICOPT++ (Viswanathan and Grossmann, 1990). Within this technique, lower bounds, $\lambda^{s,p}$ $p=\{1,2,\ldots p_s\}$, for the solution of model (C) are obtained by solving a Mixed Integer Linear Programming (MILP) master problem. This master problem is constructed by accumulating linearizations of the nonlinear terms in the model constraints, and the objective function. A binary vector, $z^{s,p}$, obtained from the solution of the master problem, is used to reduce the MINLP model to a convex NLP subproblem that is solved to obtain upper bounds, $\beta^{s,p}$, for the optimum solution of the underestimating model (C). The successive solution of the MILP master and NLP problems generates a composite sequence, $S_{oa}^{s}=\{s_{oa}^{s,p}\}$, $p\in OA_s=\{1,2,\ldots p_s\}$, that contains a sequence of binary vectors, $z^{s,p}$, a sequence of upper bounds with associated feasible solutions, $\beta^{s,p}$, and a nondecreasing sequence of lower bounds, $\lambda^{s,p}$, for the solution of the convex MINLP model. The iterative process stops when the value of the best available upper bound for (P) is exceeded by the value of a lower bound. Since model (C) is a convex relaxation of the nonconvex model (P) considered over Ω_s, its solution (best upper bound found by the outer approximation algorithm) provides a valid lower bound for the global minimum of the total annual cost of the heat exchanger network at node s.

Nonconvex upper bounding operation

To obtain upper bounds, $\alpha^{s,p}$, for the global minimum of the total annual cost of the heat exchanger network, the structures associated with the binary vectors generated by the outer approximation algorithm for problem (C) are analyzed. Firstly, by considering the fixed values of each of the binary vectors in the model (P), a set of nonconvex NLP problems, $Pl(z^{s,p})$ $p\in OA_s$, is generated. Starting from the corresponding upper bounding solution in the OA algorithm, these NLP problems are solved over Ω_s with the local optimizer MINOS 5·4 (Murtagh and Saunders, 1983). The best upper bound from the solution of these problems might improve the incumbent solution, $\{z^*, \alpha, T^*, q^*, \mathrm{AMTD}, A\}$, of the nonconvex MINLP model. It is important to mention that the local solution of the nonconvex NLP problems is intended to provide a fast mechanism for obtaining good upper bounds, and therefore, has no consequence on the convergence properties of the proposed global optimization algorithm.

Global upper bounding operation

In a second upper bounding operation, an attempt is made to find better solutions of the nonconvex NLP problems described above. These problems can be solved to global optimality by a specialized global NLP algorithm (see for example Quesada and Grossmann, 1993; Floudas and Visweswaran, 1990; Swaney, 1990; Ryoo and Sahinidis, 1995). In this paper a branch and bound algorithm is applied. Lower bounds for the solution of the nonconvex NLP problems are obtained from the solution of the convex NLP model (NLPC) generated when the integer part of model (C) is fixed. In the preprocessing stage of this algorithm, the input temperatures to the heat exchangers of the configuration that is analyzed, except the stream supply temperatures, are included in a set of *key temperature variables*. An LP model whose feasible region is defined by all the linear constraints in the model (NLPC) is used to compute lower and upper bounds for the *key temperature variables*. These new bounds are then used to compute tighter bounds on heat loads, driving forces, and areas through the bounding expressions in (4-2) to (4-5), (5-7), (5-8), and the ones given in Appendix 2. The node selection, the refining, and the pruning operations of the global NLP algorithm are similar to the ones described in the next section for the hybrid global MINLP optimization algorithm. Results from the first (local) upper bounding operation can reduce computing times considerably. The possibility of using the best upper bound available through all the global NLP searches often allows termination of these optimization subproblems at a very early stage. On the other hand, once the HEN designs associated with the corresponding binary vectors are globally optimized, integer cuts are added to the MINLP models to prevent the repetition of solutions previously analyzed.

7. A hybrid global optimization algorithm

A brief description of the algorithm

The proposed global optimization algorithm starts with an initialization stage, in which the bounding relationships presented in sections 4 and 5, and appendix 2, are used to compute the bounds required to initialize the convex estimators, and the hyperrectangle Ω_0. In this stage, the overall bounds, branch and bound list of open nodes, and the convergence tolerance parameter are also initialized. In the main stage of the algorithm, besides the bounding operations described in section 6, node selection, refining, and pruning operations are included. The selection operation is bound improving (see e.g. Horst and Tuy, 1993). In the beginning of the main stage of the algorithm, a node with a lower bound equal to the overall lower bound is removed from the branch and bound list to be analyzed. After the bounding operations are performed, and if convergence is not yet been achieved, the refining operation proceeds to create a partition of the hyperrectangle Ω_s by bisecting over the domain of a temperature level in the superstructure. To select the branching variable, the solution obtained in the lower bounding operation is considered. Firstly, the heat exchanger unit which gives rise to the largest approximation error in the heat transfer areas is identified. Secondly, for this heat exchanger, the relative distances between the upper bound and the actual value of the input temperature of the hot stream, and the actual value and the lower bound of the input temperature of the cold stream are computed. The temperature of the input stream which is further away from its corresponding bound is selected as branching variable. The two new hyperrectangles Ω_{s1}, and Ω_{s2}, are first reduced by propagating the temperature bounds imposed by the bisection operation to the other temperature levels in the superstructure. A further reduction is achieved by using the bounding relationships given in sections 4 and 5, and in Appendix 2. Once reduced, Ω_{s1}, and Ω_{s2} are used in conjunction with Ψ_s, a subset of the |L| dimensional binary vector space that excludes the vectors associated with the network structures already analyzed, to define the new branch and bound nodes. Finally, after the pruning operation is performed, the main stage is restarted.

The hybrid global MINLP optimization algorithm

The elements of the branch and bound algorithm for solving problem (P) are described in this section. Specific notation that will be used is as follows: the set $\mathscr{L}$ contains a list of elements (s,β_s) specifying the active subsets (s) pending to be analyzed as well as the corresponding lower bounds (β_s). C_s contains the set of integer vectors for which integer cuts are added; $B^{|L|}$ is the |L| dimensional binary vector space, and e is a vector with all unit entries.

Algorithm

Initialization

1.0 Compute initial bounds $T^{f,L}\le T\le T^{f,U}$, $q^{f,L}\le q\le q^{f,U}$, $AMTD^{f,L}\le AMTD\le AMTD^{f,U}$, and $A^{f,L}\le A\le A^{f,U}$ (see sections 4 and 5 and Appendix 2).

2.0 Set $\beta_0:=-\infty$, and $\Omega_0:=\{(T,q,AMTD,A)$: $T^{0,L}\le T\le T^{0,U}$, $q^{0,L}\le q\le q^{0,U}$, $AMTD^{0,L}\le AMTD\le AMTD^{0,U}$, $A^{0,L}\le A\le A^{0,U}\}$, where $T^{0,L}:=T^{f,L}$, $T^{0,U}:=T^{f,U}$, $q^{0,L}:=q^{f,L}$, $q^{0,U}:=q^{f,U}$, $AMTD^{0,L}:=AMTD^{f,L}$, $AMTD^{0,U}:=AMTD^{f,U}$, $A^{0,L}:=A^{f,L}$, $A^{0,U}:=A^{f,U}$.

3.0 Set $\mathscr{L}:=\{(0,\beta_0)\}$.

4.0 Set $\alpha:=\infty$, $\beta:=-\infty$, and $\varepsilon\ge 0$.

Main stage

1.0 Select from $\mathscr{L}$ an active node s with $\beta_s:=\beta$, set $\mathscr{L}:=\mathscr{L}\backslash(s,\beta_s)$ and $C_s:=\{\varnothing\}$.

2.0 Convex MINLP lower bounding operation.

2.1 Use OA to solve (C) over M_s. Generate the finite sequence $S^s_{oa}=\{s^{s,p}_{oa}\}$, where $s^{s,p}_{oa}=\{z^{s,p},\lambda^{s,p},\beta^{s,p},T^{s,p,R}, q^{s,p,R},AMTD^{s,p,R},A^{s,p,R}\}$, $p\in OA_s=\{1,2,\ldots p_s\}$. At any point, if $\lambda^{s,p}\ge\alpha-\varepsilon$ set $\beta^{s,p}:=\lambda^{s,p}$ and stop OA iterations.

2.2 Order the elements of S^s_{oa} by increasing value in $\beta^{s,p}$, then renumber the sequence elements starting from 1.

2.3 Set $\beta_s:=\beta^{s,1}$, and $\beta:=\min\{\beta_r, \beta_s\}\forall\in\mathscr{L}\ (r,\beta_r)\in\mathscr{L}$.

2.4 If $\alpha-\beta\le\varepsilon$, stop. Current best solution is a solution to (P).

2.5 If $\alpha-\beta_s\le\varepsilon$, restart main stage.

3.0 Nonconvex NLP upper bounding operation

3.1 Set $\alpha_s = \infty$.
3.2 For $p = 1, 2, \ldots p_s$
- If $\beta^{s,p} < \alpha - \varepsilon$, solve $P1(z^{s,p})$ over Ω_s starting from $\{T^{s,p,R}, q^{s,p,R}, AMTD^{s,p,R}, A^{s,p,R}\}$.
- If $\alpha^{s,p} < \alpha_s$, set $\alpha_s = Min(\alpha_s, \alpha^{s,p})$, and update $\{z_s, \alpha_s, T_s, q_s, AMTD_s, A_s\} := \{z^{s,p}, \alpha^{s,p}, T^{s,p}, q^{s,p}, AMTD^{s,p}, A^{s,p}\}$

3.3 - If $\alpha_s < \alpha$ update current best solution $\{z^*, \alpha, T^*, q^*, AMTD^*, A^*\} := \{z_s, \alpha_s, T_s, q_s, AMTD_s, A_s\}$.
4.0 Global NLP upper bounding operation.
4.1 For $p = 1, 2, \ldots p_s$
- Set $C_s := C_s \cup \{z^{s,p}\}$.
- If $\beta^{s,p} < \alpha - \varepsilon$, try to improve current best solution by solving $P1(z^{s,p})$ to global optimality over Ω_s.

If $\alpha - \beta \leq \varepsilon$, stop. Current best solution is a solution to (P).
5.0 Refining Operation.
5.1 Consider the solution $\{z^{s,l}, \lambda^{s,l}, \beta^{s,l}, T^{s,l,R}, q^{s,l,R}, AMTD^{s,l,R}, A^{s,l,R}\}$. Determine γ such that $\dfrac{q_\gamma^{s,l,R}}{U_\gamma\, AMTD_\gamma^{s,l,R}} - A_\gamma^{s,p,R} \geq \dfrac{q_r^{s,l,R}}{U_r\, AMTD_r^{s,l,R}} - A_r^{s,p,R}, \forall r \in L$.
Also, through indices *ijk*, identify input streams associated with the heat exchanger, cooler or heater γ.
5.2 If γ is associated with a heat exchanger *ijk*, compute $\delta_1 = (T_{i,k}^{s,U} - T_{i,k}^{s,l,R})/(T_{i,k}^{f,U} - T_{i,k}^{f,L})$, and $\delta_2 = (T_{j,k+1}^{s,l,R} - T_{j,k+1}^{s,L})/(T_{j,k+1}^{f,U}/T_{j,k+1}^{f,L})$. If $\delta_1 \geq \delta_2$ Define $\Omega_{s1} = \Omega_s \cap \{T_{i,k} \leq 0.5\, (T_{i,k}^{s,L} + T_{i,k}^{s,U})\}$ and $\Omega_{s2} = \Omega_s \cap \{T_{i,k} \geq 0.5\, (T_{i,k}^{s,L} + T_{i,k}^{s,U})\}$. Otherwise, define $\Omega_{s1} = \Omega_s \cap \{T_{j,k+1} \leq 0.5 (T_{j,k+1}^{s,L} + T_{j,k+1}^{s,U})\}$ and $\Omega_{s2} = \Omega_s \cap \{T_{j,k+1} \geq 0.5\, (T_{j,k+1}^{s,L} + T_{j,k+1}^{s,U})\backslash\}$.

5.3 If γ is associated with a cooler i, define $\Omega_{s1} = \Omega_s \cap \{T_{i,NOK+1} \leq 0.5\, (T_{i,NOK+1}^{s,L} + T_{i,NOK+1}^{s,U})\}$, and $\Omega_{s2} = \Omega_s \cap \{T_{i,NOK+1} \geq 0.5\, (T_{i,NOK+1}^{s,L} + T_{i,NOK+1}^{s,U})\}$.

5.4 If γ is associated with a heater j, define $\Omega_{s1} = \Omega_s \cap \{T_{j,1} \leq 0.5\, (T_{j,1}^{s,L} + T_{j,1}^{s,U})\}$ and $\Omega_{s2} = \Omega_s \cap \{T_{j,1} \geq 0.5\, (T_{j,1}^{s,L} + T_{j,1}^{s,U})\backslash\}$.

5.5 Use bounding relations to reduce Ω_{s1} and Ω_{s2}.

5.6 Define $M_{s1} = M_s \cap \Psi_s \cap \Omega_{s1}$ and $M_{s2} = M_s \cap \Psi_s \cap \Omega_{s2}$, where $\Psi_s = \{z \in B^{|L|}: (2z^{s,p} - e)^T z \leq \|z^{s,p}\|^2 - 1, \forall z^{s,p} \in C_s\}$.

5.7 Set $\beta_{s1} := \beta_s$, $\beta_{s2} := \beta_s$, and $\mathcal{L} := \mathcal{L} \cup (s1, \beta_{s1}) \cup (s2, \beta_{s2})$.
6.0 Delete from $\mathcal{L}$ all (r, β_r) such that $\beta_r \geq \alpha - \varepsilon$. Restart main stage.

Remarks

It should be noted that in the above algorithm convergence can be guaranteed with ε tolerance. The major bottleneck is the solution of the convex MINLP at each node. However, the number of nodes that need to be enumerated can be expected to be modest in most cases.

Example 4

To illustrate the application of the proposed algorithm, consider a problem involving two cold, and two hot streams, steam and cooling water. Table 2 presents the problem data, along with the heat exchanger area, and utilities cost information. The superstructure used for this problem consists of three stages (see Fig. 1), with 12 heat exchangers, two coolers, and two heaters. For this problem an absolute tolerance $\varepsilon = 1$ is used. The convex MINLP model (C) includes 245 equations with 121 continuous, and 16 binary variables. Table 3 shows the results obtained for the analysis of the first branch and bound node. OA performs three iterations to solve model (C), and a lower bound β_0 equal to \$70,483.7 yr^{-1} is obtained for the global minimum of the total annual cost of the heat exchanger network. To obtain this bound, the first OA master problem predicts a network structure with five heat exchangers, and provides a lower bound $\lambda^{0,1}$ equal to \$47,138.3 yr^{-1} for the solution of the convex MINLP problem. The first NLP subproblem then provides the corresponding upper bound, $\beta^{0,1}$ = \$70,483.7 yr^{-1}. OA stops iterating after only three

Table 2. Problem data for example 4
(Stream data from Linnhoff *et al.* 1982, Yea and Grossmann, 1990)

Stream	Tin (K)	Tout (K)	F (kW K^{-1})	Cost (\$ kW^{-1} yr^{-1})
H1	443	333	30	
H2	423	303	15	
C1	293	408	20	
C2	353	413	40	
S1	450	450		80
W1	293	313		20

U=0.8 (kW m^{-2} K^{-1}) for all matches except ones involving stream.
U=1.2 (kW m^{-2} K^{-1}) for matches involving steam.
Cost of Heat Exchangers and Coolers (\$ yr^{-1})=6250+83.26 [Area (m^2)].
Cost of Heaters (\$ yr^{-1})=6250+99.91 [Area (m^2)].

Table 3.

Iteration p	Exchangers in network	MINLP (C) $\lambda^{0,p}$	MINLP (C) $\beta^{0,p}$	Local and global NLP $\alpha^{0,p}$
1	(1, 1, 1), (1, 1, 3), (1, 2, 2), (2, 1, 2), (CU-2)	47,138.3	70,483.7	74.708.8
2	(1, 1, 2), (1, 2, 1), (2, 1, 1), (2, 1, 3), (2, 2, 2), (CU-2)	68,288.9	73,637.1	83.093.4
3	(1, 1, 2), (1, 2, 1), (2, 1, 1), (2, 1, 3), (2, 2, 2), (CU-2), (HU-1)	71,348.6	78,347.0	

major iterations, when $\lambda^{0,3}=\$71,348.6\ yr^{-1}$ exceeds the value of the best upper bound $\beta^{0,1}$.

In the upper bounding operations $\beta^{0,1}$, $\beta^{0,2}$, and $\beta^{0,3}$ become valid lower bounds for the global minimum cost of the three network structures that are provided by the lower bounding operation. The *local* optimization of the

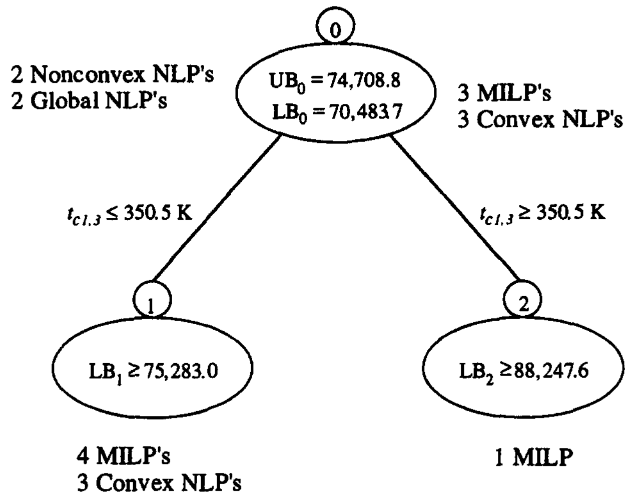
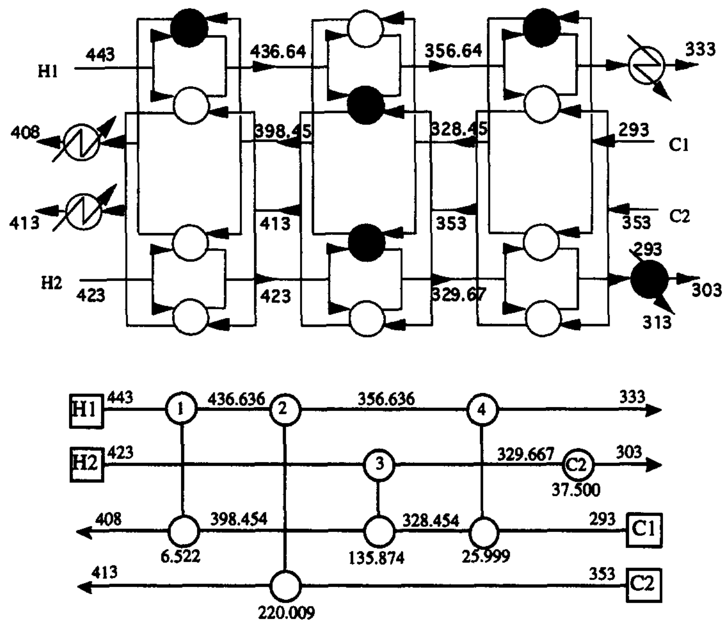
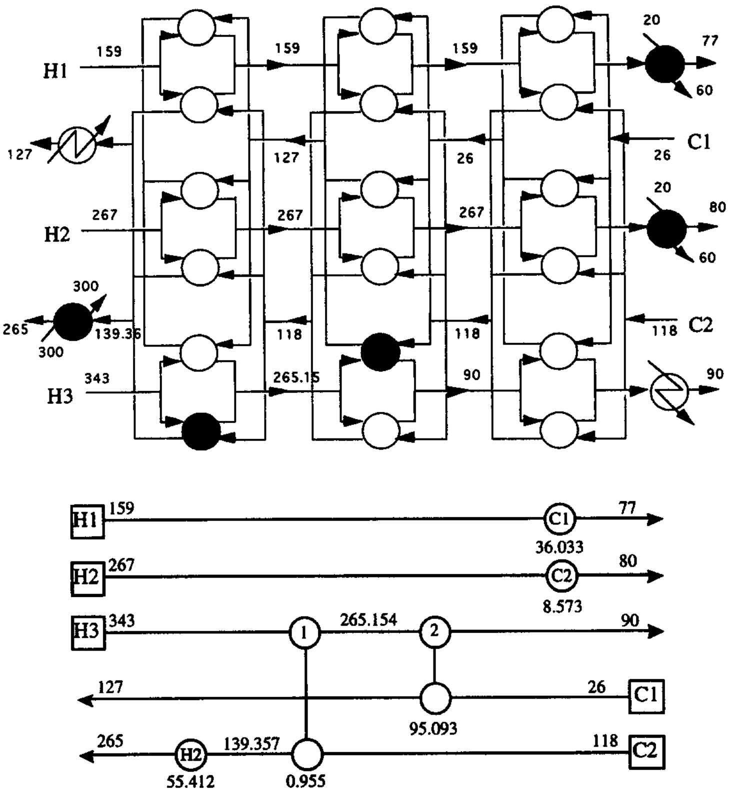


Fig. 3. Branch and bound tree for Example 4



Exchanger	Heat load (kW)	AMTD Area (m^2)	LMTD Area (m^2)
1-1-1	190.93	6.52	6.53
1-1-3	709.07	26.00	26.26
1-2-2	2400.00	220.01	280.79
2-1-2	1400.00	135.87	225.56
CU-2	400.00	37.50	38.31

Fig. 4. Global optimum solution of Example 4



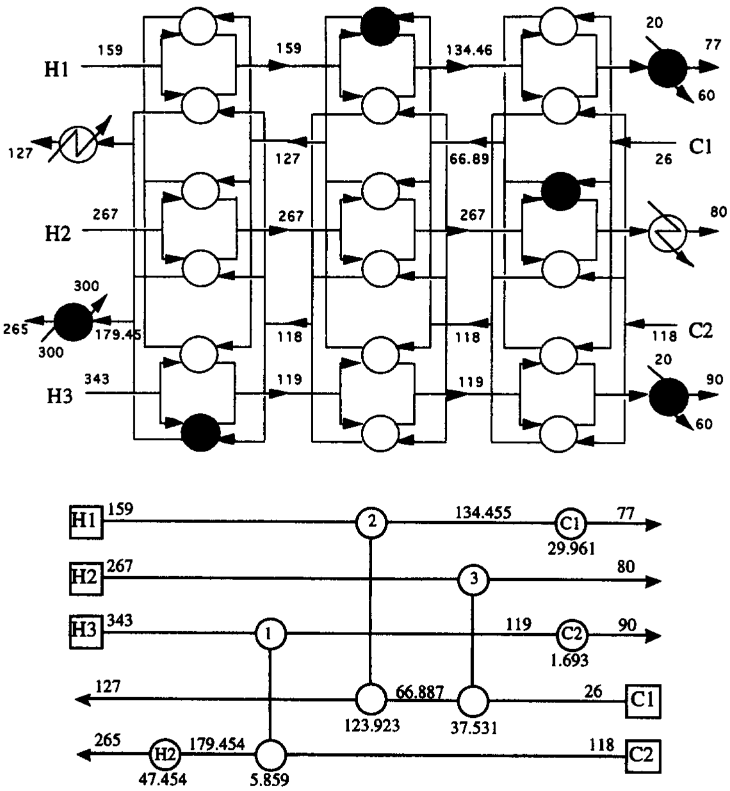
Exchanger	Heat Load (kW)	AMTD Area (m^2)	LMTD Area (m^2)
3-1-2	94.23	95.09	99.74
3-2-1	41.88	0.96	0.96
CU-1	187.37	36.03	36.94
CU-2	38.15	8.57	9.64
HU-2	246.39	55.41	65.47

Fig. 5. Global optimum solution of Example 5

nonconvex NLP problems $P1(z^{0,1})$, and $P2(z^{0,2})$ produce upper bounds with values $\alpha^{0,1}=\$74,708.8\ yr^{-1}$, and $\alpha^{0,2}=\$83,093.4\ yr^{-1}$ for the first two networks, respectively. $P1(z^{0,3})$ need not be solved since $\beta^{0,3}=\$78,347.2\ yr^{-1}\geq\alpha=\alpha^{0,1}$. The *global* optimization of $P1(z^{0,1})$ required a total of ten linear, and five nonlinear programming problems yielding also the value of \$74,708.8 yr^{-1} as the local search. The *global* optimization of problem $P2(z^{0,2})$ is terminated when $\beta^{0,2}$ takes a value of \$82,391.1 yr^{-1}, exceeding the value of the best available upper bound (\$74,708.8 yr^{-1}). This required the solution of 14 linear and one nonlinear programming problems.

In the refining step, the heat exchanger involving hot stream 2 and cold stream 1 in stage 2, exchanger (2-1-2), exhibits the largest error in the approximation of the heat transfer area, and $t_{c1,3}$ is selected as branching variable. After bisecting Ω_0 over $t_{c1,3}$, two hyperrectangles, $\Omega_{0,1}$ and $\Omega_{0,2}$, are created (see Fig. 3). These new sets are reduced, and used, along with Ω_0 and Ψ_0, to create the branch and bound nodes 1 and 2. The first iteration of the global optimization algorithm is then ended with overall lower, and upper bounds $\beta=\$70,483.7\ yr^{-1}$ and $\alpha=\$74,708.8\ yr^{-1}$, respectively. This accounts for a 5.65% approximation gap.

When OA is applied to the MINLP in node 1, a lower bound $\lambda^{1,4}$ equal to \$75,283.0 yr^{-1} is obtained after four major iterations. Since this value lies above the current overall upper bound, OA iterations are interrupted, and node 1 is eliminated. A similar situation arises when node 2 is analyzed. In this case $\lambda^{2,1}=\$88,247.6\ yr^{-1}$ is obtained after one master problem is solved. Note that in both cases integer cuts are used, which explains why lower bounds with higher values than the best available upper bound are obtained for nodes 1 and 2. In this way, the global optimization algorithm stops after only three nodes are analyzed, and the solution shown in Fig. 4, which corresponds to $\alpha=\$74,708.8\ yr^{-1}$, is found to be the global minimizer. The computations performed to solve Example 4 required approximately 156 CPU



Exchanger	Heat Load (kW)	AMTD Area (m^2)	LMTD Area (m^2)
1-1-2	56.08	123.92	129.64
2-1-3	38.15	37.53	42.75
3-2-1	120.51	5.86	15.12
CU-1	131.29	29.96	30.14
CU-3	15.60	1.69	1.70
HU-2	167.76	47.45	53.35

Fig. 6. Suboptimal solution of Example 5

seconds of an IBM RISC/6000 workstation. The summary of computations is shown in Table 4. In Fig. 4 we also show the corresponding areas calculated with the LMTD. The LMTD network has a total annual cost of $87,326.2. When this last network is locally optimized a total annual cost of $85,967.9 is obtained.

In order to provide some insight on the performance of the various bounding approximations, the effect of using 15 different versions of the MINLP model (C) for the calculation of the lower bound for the total annual cost of this example at node 0 is reported in Table 5. The models in this Table are ordered according to increasing value of their computed lower bounds. The first column in Table 5 shows that the lower bounds obtained from the NLP/LP relaxations of the corresponding version of model (C) are very weak for all 15 models. The second and third columns indicate that the lower bounds improve considerably for the solution of the first MILP master problem and the solution of the MINLP. Also, note that the model that includes only the quadratic/linear estimators (model 8) outperforms all models built up with the linear, the nonlinear, and the thermody-

Table 4. Summary of computations for example 4

Branch and bound nodes:	3
Convex MINLP's:	3 (8 MILP's+6 Convex NLP's)
Nonconvex (local) NLP's:	2 (24 LP's+6 Convex NLP's)
Total CPU time:	156 CPU seconds, IBM RISC/6000 workstation

Table 5. Lower bounds computed for node 0 of example 4

Model	Estimators included	Relaxed NLP/LP	First MILP	MINLP
1	A	22,752	47,138	
2	B	22,752	44,464	51,017
3	AB	22,752	47,138	55,552
4	C	23,038	42,372	58,607
5	AC	23,038	47,138	58,859
6	BC	23,038	46,892	61,550
7	ABC	23,038	47,138	62,709
8	D	22,752	39,250	64,839
9	BD	22,752	44,464	67,958
10	CD	23,038	42,372	68,116
11	BCD	23,038	46,892	70,386
12	ABCD	23,038	47,138	70,484
13	ABD	22,752	47,138	70,484
14	ACD	23,038	47,138	70,484
15	AD	22,752	47,138	70,484

A—Al-Khayyal's linear estimators in (6-6)
B—Quesada-Grossmann's nonlinear estimators in (6-5)
C—Thermodynamics based estimators in (6-3)
D—Quadratic/linear estimators in (6-4)

namics based estimators (models 1–7). Results also indicate that the quadratic/linear estimators in (6-4), and Al-Khayyal's linear estimators in (6-6) are the binding constraints for the best computed bound in this case. Although a general conclusion can not be drawn from the results for this particular example, it is worth stressing the remarkable improvement in the values of the lower bounds obtained when the estimators developed in this work are included.

Example 5

As a second example of the application of the proposed algorithm, consider the synthesis of a heat exchanger network for a problem with 3 hot, and 2 cold streams, steam, and cooling water. Problem data and cost information are provided in Table 6. A HEN superstructure consisting of 3 stages, with 18 heat exchangers, 3 coolers and 2 heaters is used this time.

Table 7 shows the results obtained for the solution of this problem. The first column shows the order in which the branch and bound nodes are analyzed, and the second column gives the corresponding immediate parent node. In the third column we show the variable selected for branching after the corresponding node is analyzed. The fourth and fifth columns present the bounds obtained when OA is applied to the lower bounding model (C), and the sixth gives the bound provided by the upper bounding operations (i.e. nonconvex and global NLP's). Note that only one, either $\lambda^{s,p}$ or β_s, is shown at a time. $\lambda^{s,p}$ is shown when its value goes above the current best solution, and OA iterations are interrupted. The last two columns of Table 7 show the overall lower and upper bounds obtained for this problem as the branch and bound algorithm proceeds analyzing nodes. From Table 7, we see that the computed lower bounds are very tight. The solution of this problem required the analysis of 17 nodes, and the

Table 6. Problem Data for example 5
(Stream data taken from Ahmad 1985, Rev and Fonyo 1991, Zhu *et al.* 1995)

Stream	T_{in} (°C)	T_{out} (°C)	F (kW C^{-1})	h (kW m^{-2} C^{-1})	Cost (\$ kW^{-1} yr^{-1})
H1	159	77	2.285	0.10	—
H2	267	80	0.204	0.04	—
H3	343	90	0.538	0.50	—
C1	26	127	0.933	0.01	—
C2	118	265	1.961	0.50	—
S1	300	300	—	0.05	110
W1	20	60	—	0.20	10

Cost of heat exchangers (\$ yr^{-1})=7400+80 [Area(m^2)]

Table 7. Results for example 5

node s	parent node	variable to branch	MINLP (C) $\lambda^{s,p}$	β_s	NLP's α_s	OA major iter p	global NLP probs	β	α
0		$t_{h3,2}$		77,268.3	82,151.5	10	3	77,268.3	82,151.5
1	0	$t_{c1,3}$		78,511.6	84,035.6	4	2	78,484.0	82,151.5
2	0	$t_{c1,3}$		78,484.0	84,035.6	5	2	78,484.0	82,151.5
3	2	$t_{c1,2}$		80,559.4	82,042.9	12	3	78,484.0	82,042.9
4	2	$t_{c2,1}$		81,606.6	82,042.9	6	0	78,511.6	82,042.9
5	1	$t_{c1,3}$		79,529.0	84,035.6	8	2	78,511.6	82,042.9
6	1		82,300.2			3	0	79,529.0	82,042.9
7	5	$t_{c2,1}$		81,208.2	83,596.3	7	1	79,529.0	82,042.9
8	5	$t_{h3,2}$		81,095.6	84,035.6	5	1	80,559.4	82,042.9
9	3		82,113.2			4	0	80,559.4	82,042.9
10	3			82,212.7		11	0	81,095.6	82,042.9
11	8		82,347.1			5	0	81,095.6	82,042.9
12	8		82,976.9			6	0	81,208.2	82,042.9
13	7		82,195.0			2	0	81,208.2	82,042.9
14	7		82,661.1			2	0	81,606.6	82,042.9
15	4		82,401.4			2	0	81,606.6	82,042.9
16	4		83,030.3			2	0	83,030.3	82,042.9

branching operation was performed eight times. Also, it can be seen that the process of solving eight MINLP convex underestimating problems was stopped before convergence, and the second upper bounding operation carried out the global optimization of 14 NLP problems.

The global optimum solution of this problem, which has a total annual cost equal to \$82,042.9 yr^{-1}, is found when the analysis of the fourth branch and bound node is performed. Figure 5 shows the corresponding heat exchanger network, and operating conditions. This problem required approximately 6 hours of CPU time. The summary of the computations, which were carried out on an IBM RISC/6000 workstation, is shown in Table 8. The LMTD network in Fig. 5 has a total annual cost of \$83,400.0. The same annual cost is obtained when the LMTD network is locally optimized.

The nonconvex problem (P) associated with this example was also solved with DICOPT++. This software was started from several different points, among which we have the GAMS default starting point (Brooke *et al.*, 1992), and the middle point of the hyperrectangle Ω_0. In all cases, a suboptimal network structure containing heat exchangers (1-1-2), (2-1-3), (3-2-1), (CU-1), (CU-3), and (HU-2), or an equivalent configuration, was obtained. This is a good example of how the global optimum might be cut off by the master problem when a nonconvex MINLP problem is solved by a local optimizer. Figure 6 shows the suboptimal network. Note that although the suboptimal network consumes less energy than the global optimal solution in Fig. 5 (167.8 kW *vs* 246.4 kW heating utilities; 146.9 kW *vs* 225.5 kW cooling utilities), the former requires an extra unit (6 *vs* 5), and a higher total heat transfer area (246.4 m^2 *vs* 196.1 m^2). The cost of the extra unit, and the increment in the total area required to perform the heat transfer operations renders the system in Fig. 6 more expensive than the global optimal solution (\$84,035.0 yr^{-1} *vs* \$82,042.9 yr^{-1}). The LMTD network associated with the suboptimal solution shown in Fig. 6 has a total annual cost of \$86,137.4. After being locally optimized this network yields a total annual cost equal to \$86,029.2.

8. Conclusions

A hybrid branch and bound/outer-approximation global optimization algorithm for the synthesis of heat exchanger networks has been presented in this paper. As shown, the solution of the proposed convex MINLP model, that incorporates the two new sets of convex underestimators for the area of heat exchangers, provides very good bounds for the global minimum of the total annual cost of HENs. It is important to note that although arithmetic mean temperature difference driving forces have been used in this paper, results obtained with the proposed algorithm will provide a valid lower bound to the total annual cost for the case with logarithmic mean temperature difference driving force (assuming no stream splits). The significance of this work is that it

Table 8. Summary of computations for example 5

Branch and bound nodes:	17
Convex MINLP's:	17 (94 MILPs+86 Convex NLP's)
Nonconvex (local) NLP's	23
Global NLP's:	14 (114 LP's+14 Convex NLP's)
Total CPU time:	6 CPU hours, IBM RISC/6000 workstation

provides an effective solution method to the global optimization of the simultaneous synthesis model for heat exchanger networks. Extensions for the case with logarithmic mean temperature difference, and concave cost functions are currently under investigation. Finally, we believe that the proposed bounding strategy can be also useful in the solution of other types of nonconvex MINLP models.

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Appendix 1

Proofs of Theorems 1 and 2

Theorem 1. The thermodynamics based estimator

$$A_{i,j,k} \geq \frac{q_{ijk}}{U_{i,j}[t^U_{i,k} - t^L_{j,k+1} - q_{ijk}(1/F_i + 1/F_j)/2]} \qquad \text{(A1-1)}$$

is convex, underestimates the area of heat exchangers, and provides an exact representation when $t_{i,k} = t^U_{i,k}$, and $t_{j,k+1} = t^L_{j,k+1}$.

Proof.

The r.h.s. of (A1-1), which is a function of q_{ijk} only, has a second derivative given by

$$\frac{(t^U_{i,k}-t^L_{j,k+1})(1/F_i+1/F_j)}{U_{i,j}[t^U_{i,k}-t^L_{j,k+1}-q_{ijk}(1/F_i+1/F_j)/2]^3}=\frac{(t^U_{i,k}-t^L_{j,k+1})(1/F_i+1/F_j)}{U_{i,j}[\mathrm{AMTD}^U_{i,j,k}]^3}$$

in which the upper bound for the driving force in (4-2) has been substituted in the denominator. For any match allowed by the second law of thermodynamics this quantity is greater than or equal to zero. Therefore, the r.h.s. of (A-1-1) is convex. Convexity of the inequality in (A1-1) follows from the fact that the sum of convex functions is convex. On the other hand, the approximation error of (A1-1) is given by Δ^1_{ijk}, where

$$\Delta^1_{ijk}=\frac{q_{ijk}}{U_{i,j}\,\mathrm{AMTD}_{i,j,k}}-\frac{q_{ijk}}{U_{i,j}[t^U_{i,k}-t^L_{j,k+1}-q_{ijk}(1/F_i+1/F_j)/2]} \tag{A1-2}$$

$$=\frac{q_{ijk}[t^U_{i,k}-t_{i,k}+t_{j,k+1}-t^L_{j,k+1}]}{U_{i,j}\,\mathrm{AMTD}_{i,j,k}[t^U_{i,k}-t^L_{j,k+1}-q_{ijk}(1/F_i+1/F_j)/2]}$$

Since $t_{i,k}\le t^U_{i,k}$, and $t_{j,k+1}\ge t^L_{j,k+1}$, the approximation error is always nonnegative, which implies that (A1-1) underestimates the area of heat exchangers. Also from (A1-2), it is obvious that Δ^1_{ijk} is equal to zero if $t_{i,k}=t^U_{i,k}$, and $t_{j,k+1}=t^L_{j,k+1}$.

Theorem 2. The quadratic/linear fractional inequality

$$A_{i,j,k}\ge\frac{1}{U_{i,j}\,\mathrm{AMTD}_{i,j,k}}\left(\frac{q_{ijk}+\sqrt{q^L_{ijk}q^U_{ijk}}}{\sqrt{q^L_{ijk}}+\sqrt{q^U_{ijk}}}\right)^2 \tag{A1-3}$$

is convex, underestimates the area of heat exchangers in the domain $q_{ijk}\in[q^L_{ijk},q^U_{ijk}]$, and provides an exact representation when $q_{ijk}=q^L_{ijk}$ or $q_{ijk}=q^U_{ijk}$.

Proof.

The Hessian matrix of the r.h.s. of (A1-3) is given by,

$$H=\begin{bmatrix}\dfrac{2}{U_{i,j}\,\mathrm{AMTD}_{i,j,k}(\sqrt{q^L_{ijk}}+\sqrt{q^U_{ijk}})^2} & \dfrac{-2(q_{ijk}+\sqrt{q^L_{ijk}q^U_{ijk}})}{U_{i,j}(\mathrm{AMTD}_{i,j,k})^2(\sqrt{q^L_{ijk}}+\sqrt{q^U_{ijk}})^2}\\ \dfrac{-2(q_{ijk}+\sqrt{q^L_{ijk}q^U_{ijk}})}{U_{i,j}(\mathrm{AMTD}_{i,j,k})^2(\sqrt{q^L_{ijk}}+\sqrt{q^U_{ijk}})^2} & \dfrac{2(q_{ijk}+\sqrt{q^L_{ijk}q^U_{ijk}})^2}{U_{i,j}(\mathrm{AMTD}_{i,j,k})^3(\sqrt{q^L_{ijk}}+\sqrt{q^U_{ijk}})^2}\end{bmatrix}$$

The two eigenvalues of H are

$$\lambda_1=0$$

$$\lambda_2=\frac{2(\mathrm{AMTD}_{i,j,k})^2+2(q_{ijk}+\sqrt{q^L_{ijk}q^U_{ijk}})^2}{U_{i,j}(\mathrm{AMTD}_{i,j,k})^3(\sqrt{q^L_{ijk}}+\sqrt{q^U_{ijk}})^2}$$

Since both eigenvalues of H are nonnegative, H is positive semidefinite (Bazaraa and Sheety, 1979). Therefore, the r.h.s. of (A1-3) is convex. Convexity of the inequality in (A1-3) follows from the fact that the sum of convex functions is convex. On the other hand, the approximation error of (A1-3) is given by

$$\Delta^2_{ijk}=\frac{q_{ijk}}{U_{i,j}\,\mathrm{AMTD}_{i,j,k}}-\frac{1}{U_{i,j}\,\mathrm{AMTD}_{i,j,k}}\left(\frac{q_{ijk}+\sqrt{q^L_{ijk}q^U_{ijk}}}{\sqrt{q^L_{ijk}}+\sqrt{q^U_{ijk}}}\right)^2 \tag{A1-4}$$

$$=\frac{(q_{ijk}-q^L_{ijk})(q^U_{ijk}-q_{ijk})}{U_{i,j}\,\mathrm{AMTD}_{i,j,k}(\sqrt{q^L_{ijk}}+\sqrt{q^U_{ijk}})^2}$$

Since $q^L_{ijk}\le q_{ijk}\le q^U_{ijk}$, Δ^2_{ijk} is greater than or equal to zero. Hence, (A1-3) underestimates the heat transfer area. Furthermore, and also from (A1-4), it is clear that the approximation error is zero when $q_{ijk}=q^L_{ijk}$ or $q_{ijk}=q^U_{ijk}$.

Appendix 2

Other Bounding Relationships

In order to use (3-1) and (3-2), bounds for the driving forces and areas are required. In this appendix we present bounding relationships that are used to initialize these estimators. Furthermore, all these expressions are also incorporated in the reduction step that follows the branching operation of the proposed global optimization algorithm.

Computation of bounds for the AMTD

For developing a lower bounding expression for the AMTD, consider again the case in which streams i, and j are matched in stage k with a heat load equal to q_{ijk}. In order to determine the minimum driving force that can allow this heat transfer operation, we propose the following minimization problem:

$$\mathrm{AMTD}^L_{ijk}\ge\mathrm{Min}\,\frac{1}{2}\,[t_{i,k}+t_{i,k+1}-t_{j,k}-t_{j,k+1}] \tag{A2-1}$$

s.t.

$$q_{ijk}=F_i(t_{i,k}-t_{i,k+1})$$

$$q_{ijk}=F_j(t_{j,k}-t_{j,k+1})$$

$$t_{i,k}-t_{j,k}\ge\mathrm{Max}[\Delta T_{mapp},\,t^L_{i,k}-t^U_{j,k},\,t^L_{i,k+1}-t^U_{j,k}+q_{ijk}/F_i]$$

$$t_{i,k+1}-t_{j,k+1}\ge\mathrm{Max}[\Delta T_{mapp},\,t^L_{i,k+1}-t^U_{j,k+1},\,t^L_{i,k+1}-t^U_{j,k}+q_{ijk}/F_j]$$

$$t_{i,k}\ge t_{i,k+1}$$

$$t_{j,k}\ge t_{j,k+1}$$

$$T_{i,out}\le t^L_{i,k}\le t_{i,k}\le t^U_{i,k}\le T_{i,in}$$

$$T_{i,out}\le t^L_{i,k+1}\le t_{i,k+1}\le t^U_{i,k+1}\le T_{i,in}$$

$$T_{j,in}\le t^L_{j,k}\le t_{j,k}\le t^U_{j,k}\le T_{j,out}$$

$$T_{j,in}\le t^L_{j,k+1}\le t_{j,k+1}\le t^U_{j,k+1}\le T_{j,out}$$

The energy balances are used to solve for $(t_{i,k}-t_{j,k})$, yielding

$$t_{i,k}-t_{j,k}=t_{i,k+1}-t_{j,k+1}+q_{ijk}(1/F_i-1/F_j)$$

Introducing this equality in the original problem reduces (A2-1) to

$$\mathrm{AMTD}^L_{ijk}\ge\mathrm{Min}(t_{i,k+1}-t_{j,k+1})+\frac{1}{2}\,q_{ijk}(1/F_i-1/F_j) \tag{A2-2}$$

s.t.

$$\begin{aligned}t_{i,k+1}-t_{j,k+1}\ge\mathrm{Max}[&\Delta T_{mapp},\,\Delta T_{mapp}-q_{ijk}(1/F_i-1/F_j),\\&t^L_{i,k}-t^U_{j,k}-q_{ijk}(1/F_i-1/F_j),\\&t^L_{i,k+1}-t^U_{j,k}+q_{ijk}/F_j,\\&t^L_{i,k+1}-t^U_{j,k+1}]\end{aligned}$$

$$T_{i,out}\le t^L_{i,k+1}\le t_{i,k+1}\le t^U_{i,k+1}\le T_{i,in}$$

$$T_{j,in}\le t^L_{j,k+1}\le t_{j,k+1}\le t^U_{j,k+1}\le T_{j,out}$$

From here we obtain

$$\mathrm{AMTD}^L_{ijk}\ge\Phi(q_{ijk})\equiv\mathrm{Max}[\Delta T_{mapp}+\frac{1}{2}\,q_{ijk}(1/F_i-1/F_j), \tag{A2-3}$$

$$\Delta T_{\mathrm{mapp}} - \frac{1}{2} q_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j}),$$

$$t^{L}_{i,k} - t^{U}_{j,k} - \frac{1}{2} q_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j}),$$

$$t^{L}_{i,k+1} - t^{U}_{j,k} + \frac{1}{2} q_{ijk}(1/\mathrm{F_i} + 1/\mathrm{F_j}),$$

$$t^{L}_{i,k+1} - t^{U}_{j,k+1} + \frac{1}{2} q_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j})]$$

Finally, exploiting monotonicity properties of (A2-3), a lower bound for the case in which $\mathrm{F}_i \geq \mathrm{F}_j$ is derived

$$\mathrm{AMTD}^{L}_{ijk} = \mathrm{Max}[\Delta T_{\mathrm{mapp}} + \frac{1}{2} q^{U}_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j}), \quad \text{(A2-4)}$$

$$\Delta T_{\mathrm{mapp}} - \frac{1}{2} q^{L}_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j}),$$

$$t^{L}_{i,k} - t^{U}_{j,k} - \frac{1}{2} q^{L}_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j}),$$

$$t^{L}_{i,k+1} - t^{U}_{j,k} + \frac{1}{2} q^{L}_{ijk}(1/\mathrm{F_i} + 1/\mathrm{F_j}),$$

$$t^{L}_{i,k+1} - t^{U}_{j,k+1} + \frac{1}{2} q^{U}_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j})]$$

Similarly, for the case in which $\mathrm{F}_i \leq \mathrm{F}_j$, the following bounding expression is obtained

$$\mathrm{AMTD}^{L}_{ijk} \geq \mathrm{Max}[\Delta T_{\mathrm{mapp}} + \frac{1}{2} q^{L}_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j}), \quad \text{(A2-5)}$$

$$\Delta T_{\mathrm{mapp}} - \frac{1}{2} q^{U}_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j}),$$

$$t^{L}_{i,k} - t^{U}_{j,k} - \frac{1}{2} q^{U}_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j}),$$

$$t^{L}_{i,k+1} - t^{U}_{j,k} + \frac{1}{2} q^{U}_{ijk}(1/\mathrm{F_i} + 1/\mathrm{F_j}),$$

$$t^{L}_{i,k+1} - t^{U}_{j,k+1} + q^{L}_{ijk}(1/\mathrm{F_i} - 1/\mathrm{F_j})]$$

Upper bounds for the AMTD are calculated with the following expressions

$$\mathrm{AMTD}^{U}_{ijk} \leq \mathrm{Min}[(t^{U}_{i,k} + t^{U}_{i,k+1} - t^{L}_{j,k} - t^{L}_{j,k+1})/2, \quad \text{(A2-6)}$$

$$(t^{U}_{i,k} + t^{U}_{i,k+1} - 2t^{L}_{j,k+1} - q^{L}_{ijk}/\mathrm{F_j})/2,$$

$$(2t^{U}_{i,k} - t^{L}_{j,k} - t^{L}_{j,k+1} - q^{L}_{ijk}/\mathrm{F_i})/2,$$

$$t^{U}_{i,k} - t^{L}_{j,k+1} - q^{L}_{ijk}(1/\mathrm{F_i} + 1/\mathrm{F_j})/2]$$

$$\mathrm{AMTD}^{U}_{ij1} \leq \mathrm{Min}[\mathrm{AMTD}^{U}_{ij1}, (t^{U}_{i,1} + t^{U}_{i,2} - 2t^{L}_{j,2} - (t^{U}_{i,1} - t^{U}_{i,2})\mathrm{F}_i/\mathrm{F_j})/2]$$

$$\mathrm{AMTD}^{U}_{ijNOK} \leq \mathrm{Min}[\mathrm{AMTD}^{U}_{ijNOK}, (2t^{U}_{i,NOK} - t^{L}_{j,NOK} - t^{L}_{j,NOK+1}$$

$$- (t^{L}_{j,NOK} - t^{L}_{j,NOK+1})\mathrm{F}_j/Fi)/2]$$

A simpler analysis for coolers and heaters produces

$$\mathrm{AMTD}^{L}_{i,cu} \geq \frac{1}{2}(\mathrm{Max}[\Delta T_{\mathrm{mapp}}, t^{L}_{i,NOK+1} - T_{cu,out}] + T_{i,out} - T_{cu,in}) \quad \text{(A2-7)}$$

$$\mathrm{AMTD}^{U}_{i,cu} \leq \frac{1}{2}(\mathrm{Max}[\Delta T_{\mathrm{mapp}}, t^{U}_{i,NOK+1} - T_{cu,out}] + T_{i,out} - T_{cu,in})$$

$$\mathrm{AMTD}^{L}_{j,hu} \geq \frac{1}{2}(\mathrm{Max}[\Delta T_{mapp}, T_{hu,out} - t^{U}_{j,1}] + T_{hu,in} \geqslant T_{j,out})$$

$$\mathrm{AMTD}^{U}_{j,hu} \leq \frac{1}{2}(\mathrm{Max}[\Delta T_{\mathrm{mapp}}, T_{hu,out} - t^{L}_{j,1}] + T_{hu,in} - T_{j,out})$$

Bounds for the heat transfer area

Initial lower bounds for the areas of heat exchangers are set equal to zero. Upper bounds for the areas are calculated with the following relationship

$$A^{U}_{ijk} \leq \mathrm{Min}\left[\frac{q^{U}_{ijk}}{U_{ij}\,\mathrm{AMTD}^{L}_{ijk}}, \mathrm{Max}\left[\frac{q^{L}_{ijk}}{U_{ij}\,\Phi(q^{L}_{ijk})}, \frac{q^{U}_{ijk}}{U_{ij}\,\Phi(q^{U}_{ijk})}\right]\right] \quad \text{(A2-8)}$$