SIMULTANEOUS OPTIMIZATION MODELS FOR
HEAT INTEGRATION—II. HEAT EXCHANGER
NETWORK SYNTHESIS

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(Received 28 June 1990; received for publication 6 July 1990)

Abstract—In this paper, a mixed integer nonlinear programming (MINLP) model is presented which can
generate networks where utility cost, exchanger areas and selection of matches are optimized simul-
taneously. The proposed model does not rely on the assumption of fixed temperature approaches (HRAT
or EMAT), nor on the prediction of the pinch point for the partitioning into subnetworks. The model
is based on the stage-wise representation introduced in Part I of this series of papers, where within each
stage, potential exchanges between each hot and cold stream can occur. The simplifying assumption on
isothermal mixing to calculate heat transfer area for stream splits allows the feasible space to be defined
by a set of linear constraints. As a result, the model is robust and can be solved with relative ease.
Constraints on the network design that simplify its structure, e.g. no stream splits, forbidden matches,
required and restricted matches as well as the handling of multiple utilities can be easily included in the
model. In addition, the model can consider matches between pairs of hot streams or pairs of
cold streams, as well as variable inlet and outlet temperatures. Several examples are presented to illustrate the
capabilities of the proposed simultaneous synthesis model. The results show that in many cases, heuristic
rules such as subnetwork partitioning, no placement of exchangers across the pinch, number of units, fail
to hold when the optimization is performed simultaneously.

INTRODUCTION

Most of the current synthesis methods for heat
exchanger networks rely on sequential or step-wise
procedures (Gundersen and Naess, 1988). In general,
the design problem is decomposed in order to pro-
gressively determine targets for synthesizing a net-
work. For example, the pinch design method by
Linnhoff and Hindmarsh (1983) first uses a cost
target to establish a minimum energy consumption,
thus fixing the utility requirement for the network
and the pinch location. The problem is then partition-
ted into subnetworks disallowing exchangers to be
placed across the pinch. Finally, each subnetwork is
evolved using guidelines and heuristics to synthesize
networks with minimum number of units.

Another example is the mathematical program-
ing approach built into the interactive program
MAGNETS (Floudas et al., 1986). The design prob-
lem is decomposed into three steps. The first two steps
involve the solution of the LP and MILP transship-
ment model of Papoulias and Grossmann (1983). For
a particular HRAT value, the LP model determines
the minimum utility requirement for the network.
With the utility consumption fixed at the LP solution,
the MILP model is solved to determine the minimum
number of matches and their corresponding heat
loads. Finally, in the third step, heat loads and
matches are fixed and the area cost is minimized by

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the solution of an NLP model (Floudas et al., 1986)
to determine the optimal network configuration.

The limitation of a sequential synthesis method is
that different costs associated with the design cannot
be optimized simultaneously. In other words, trade-
offs between the different costs, as shown in Fig. 1,
cannot be accounted for accurately. In general, early
decisions on HRAT (the level of energy recovery to
be achieved by the network) and whether or not to
partition the problem into subnetworks can have
negative effects on the latter decisions of number of
units and area requirement for the network configur-
ation. Sequential design methods, as a result, can	only lead to suboptimal networks.

Floudas and Ciric (1989) developed an MINLP
model to simultaneously optimize the selection of
process stream matches and the network configura-
tion for a fixed level of energy recovery (HRAT).
The formulation is based on a hyperstructure, which
is similar to the superstructure of Floudas et al.
(1986) that embeds all the possible matches. Optimiz-
ation of the model identifies which of the embedded
matches are needed to minimize the total investment
cost of the exchangers.

Dolan et al. (1987, 1989) and Yee and Grossmann
(1988) proposed methods to account for all types of
costs simultaneously. Dolan et al. proposed the
method of simulated annealing as a synthesis tech-
tique, whereas Yee and Grossmann formulated an
extensive MINLP model for retrofit design where the
piping layout is also considered. In both approaches,
operating cost and capital cost are considered simultaneously in the search of a least-cost network. Furthermore, one does not have to decide whether subnetworks must be partitioned or not, nor does one have to specify fixed temperature approaches (EMAT). Specifically, as shown in Fig. 1, trade-offs between utility cost, fixed charges for the number of units, and heat transfer area cost are determined simultaneously. The difficulty, however, as shown by the results of the two methods, is that it is not trivial to establish efficient computational schemes when accounting for all the trade-offs. In the case of the simulated annealing method by Dolan et al., a very large number of trials is required, while the MINLP model by Yee and Grossmann is very large in size and has a poor relaxation.

In this paper, the superstructure representation proposed in Part I of this series of papers (Yee et al., 1990) is applied to a synthesis model which accounts for all the costs simultaneously yet requiring very reasonable solution times. The costs include fixed charges and area costs for the exchangers, and the cost for the utilities. Based on the simplifying assumption for isothermal mixing of streams, it is shown that the problem can be formulated as an MINLP which has the desirable feature that all the constraints are linear. The solution scheme determines the network which exhibits least annual cost by optimizing simultaneously for utility requirement (HRAT), minimum approach temperature (EMAT), the number of units, the number of splits and heat transfer area. Constraints on matches, on the number of units and on stream splitting that simplify the network structure can be easily incorporated into the model, as well as the specification of inlet or outlet temperatures as inequalities. Furthermore, the model can consider the possibilities of matching pairs of streams of the same type, i.e. hot-to-hot and cold-to-cold as previously proposed by Grimes et al. (1982), Viswanathan and Evans (1987) and Dolan et al. (1987).

**PROBLEM STATEMENT**

The HEN synthesis problem addressed in this paper can be stated as follows:

Given are a set of hot process streams HP to be heated and a set of cold process streams CP to be cooled. Specified are also each hot and cold stream’s heat capacity flow rates and the initial and target temperatures stated as either exact values or inequalities. Given also are a set of hot utilities HU and a set of cold utilities CU and their corresponding temperatures. The objective then is to determine the heat exchanger network which exhibits the least annual cost. The solution defines the network by providing the following:

1. Utilities required.
2. Stream matches and the number of units.
3. Heat loads and operating temperatures of each exchanger.
4. Network configuration and flows for all branches.
5. Area of each exchanger.

As will be shown, constraints on stream matches, stream splits and number of units can also be specified. In the proposed method, no parameters are required to be fixed; i.e. level of energy recovery (HRAT), minimum approach temperature (EMAT), number of units and matches. Also, there is no need to perform partitioning into subnetworks, and the pinch point location(s) are not pre-determined but rather optimized simultaneously.

**REMARKS ON SUPERSTRUCTURE**

The proposed strategy involves the development of a stage-wise superstructure and its modeling and solution as an MINLP problem to obtain a cost-optimal network. The reader is referred to Part I of this series of papers for the detailed discussion of the superstructure.

A superstructure involving two hot and two cold streams along with hot and cold utilities is shown in Fig. 2. Similar assumptions as those used in Part I are imposed. The number of stages in the superstructure can be set for instance to the maximum number of hot or cold streams, i.e. \( \max\{N_H, N_C\} \). Also, as shown in Fig. 2, although in principle, each utility stream can be treated as a process stream with unknown flow rate, it will be assumed for simplicity that utility streams are placed at the extreme ends of the sequence of stages. Finally, the assumption of isothermal mixing of streams is imposed. As discussed in Part I, this simplification eliminates the requirement for nonlinear heat balances around each exchanger as well as nonlinear heat mixing equations. Instead, only an overall heat balance around each stage is needed. As a result, flow variables are no longer required in the model and the model size is reduced. More importantly, though, the feasible space of the problem can now be defined by strictly linear constraints. The only nonlinearities appear in the objective function which involves the cost terms for the heat exchanger areas, which are expressed in terms of stage temperatures. Therefore, the MINLP model is robust and can be solved very efficiently.
It should be noted that the simplifying assumption for isothermal mixing is rigorous for the case when the network to be synthesized does not involve stream splits. For structures where splits are present, however, the assumption may lead to an overestimation of the area cost since it will restrict trade-offs of area between the exchangers involved with split streams. Also, in some cases this assumption might exclude network structures which are only feasible with non-isothermal mixing. In order to partially overcome this limitation, the scheme shown in Fig. 3 is proposed. The idea is to use the MINLP model to determine an optimal structure. If this structure involves split streams, then an NLP suboptimization problem is formulated with the fixed configuration and variable flows and temperatures, and solved to determine optimal split flow rates and area distribution for the exchangers. The solution of the suboptimization is then considered as the final cost-optimal network.

Finally, it should be noted that there are certain alternatives in the network configuration which the proposed superstructure neglects. Specifically, the superstructure does not account for the case of a split stream going through two or more exchangers in series and the case of stream bypasses. For clarification, these structures are shown in Fig. 4. In general, disregarding stream bypasses is not a significant limitation since these are usually not required and more importantly, not favorable. In very particular cases, however, the use of bypasses may help to decrease the number of units, though at the expense of requiring more area (see Wood et al., 1985).
The more important configuration which the superstructure neglects is the case where a split stream goes through several exchangers in series. In small examples where there is not much flexibility in selecting structures, this limitation may cause the network to require larger areas. However, for larger problems, this restriction is less important since greater flexibility in matching and selection of configuration can usually ensure an equally good network without the particular split structure. This in fact will be demonstrated by an example later in the paper by synthesizing networks which are as good if not better than certain solutions in the literature where the reported optimal network involves split streams going through exchangers in series.

MODEL FORMULATION

In this section, the formulation for the MINLP synthesis model subject to the simplifying assumption for isothermal mixing of streams is presented. Binary variables are introduced to designate the existence of each potential heat exchanger in the superstructure, and to model fixed cost charges for the exchangers. Continuous variables are assigned to temperatures and heat loads. The general model involves overall heat balances for each stream, stream energy balances at each stage, assignment of known stage temperatures, calculation of hot and cold utility loads, logical constraints and calculation of approach temperatures. The MINLP model is solved to minimize the total annual cost comprising of utility cost, fixed charges for each exchanger and heat transfer area cost.

For simplicity in the presentation, utility exchangers are placed at the outlet of the superstructure and only one type of hot and one type of cold utility are assumed. These two assumptions can be easily relaxed to accommodate cases of multiple utilities with various temperatures.

In order to formulate the proposed MINLP model, similar definitions as in Part I (Yee et al., 1990) are necessary:

(i) Indices:
- \( i \) = hot process or utility stream,
- \( j \) = cold process or utility stream,
- \( k \) = index for stage \( 1, \ldots, NOK \) and temperature location \( 1, \ldots, NOK + 1 \);

(ii) Sets:
- \( HP \) = \{ \( i \) | \( i \) is a hot process stream\},
- \( CP \) = \{ \( j \) | \( j \) is a cold process stream\},
- \( HU \) = hot utility,
- \( CU \) = cold utility,
- \( ST \) = \{ \( k \) | \( k \) is a stage in the superstructure, \( k = 1, \ldots, NOK \)\};

(iii) Parameters:
- \( TIN \) = inlet temperature of stream,
- \( TOUT \) = outlet temperature of stream,
- \( F \) = heat capacity flow rate,
- \( U \) = overall heat transfer coefficient,
- \( CCU \) = per unit cost for cold utility,
- \( CHU \) = per unit cost for hot utility,
- \( CF \) = fixed charge for exchangers,
- \( C \) = area cost coefficient,
- \( B \) = exponent for area cost,
- \( NOK \) = total number of stages,
- \( \Omega \) = an upper bound for heat exchange,
- \( \Gamma \) = an upper bound for temperature difference;

(iv) Variables:
- \( dt_{i,k} \) = temperature approach for match \( (i,j) \) at temperature location \( k \),
- \( dcu_i \) = temperature approach for the match of hot stream \( i \) and cold utility,
- \( dhu_i \) = temperature approach for the match of cold stream \( j \) and hot utility,
- \( q_{i,k} \) = heat exchanged between hot process stream \( i \) and cold process stream \( j \) in stage \( k \),
- \( qcui \) = heat exchanged between hot stream \( i \) and cold utility,
- \( qhu_i \) = heat exchanged between hot utility and cold stream \( j \),
- \( t_{i,k} \) = temperature of hot stream \( i \) at hot end of stage \( k \),
- \( t_{j,k} \) = temperature of cold stream \( j \) at hot end of stage \( k \),
- \( z_{i,j,k} \) = binary variable to denote existence of match \( (i,j) \) in stage \( k \),
- \( zcu_i \) = binary variable to denote that cold utility exchanges heat with hot stream \( i \),
- \( zhu_i \) = binary variable to denote that hot utility exchanges heat with cold stream \( j \).

With these definitions, the formulation can now be presented. For completeness, the relevant equations, (1–5), which appeared in Part I (Yee et al., 1990) are restated without duplicating the discussion. Additional constraints for the synthesis model are then presented along with the modified objective function.

Overall heat balance for each stream

\[
(TIN_i - TOUT_i) F_i = \sum_{k \in ST} \sum_{j \in CP} q_{i,k} + qcu_i, \quad i \in HP, \quad (1)
\]

Heat balance at each stage

\[
(t_{i,k} - t_{i,k+1}) F_i = \sum_{j \in CP} q_{i,k}, \quad k \in ST, \quad i \in HP, \quad (2)
\]

\[
(t_{j,k} - t_{j,k+1}) F_j = \sum_{i \in HP} q_{i,k}, \quad k \in ST, \quad j \in CP.
\]

It should be noted that for cases where the inlet or target temperatures are defined by a range of values, the corresponding parameters can be substituted by variables in the constraints. The variables then would be bounded to reflect the given range.
Assignment of superstructure inlet temperatures

\[ TIN_i = t_{i,1}, \quad i \in HP, \]

\[ TIN_j = t_{i,NOK+1}, \quad j \in CP. \] (3)

Feasibility of temperatures

\[ t_{i,k} \geq t_{i,k+1}, \quad k \in ST, \quad i \in HP, \]

\[ t_{i,k} \geq t_{i,k+1}, \quad k \in ST, \quad i \in CP, \]

\[ TOUT_i \leq t_{i,NOK+1}, \quad i \in HP, \]

\[ TOUT_j \geq t_{j,1}, \quad j \in CP. \] (4)

Hot and cold utility load

\[ (t_{i,NOK+1} - TOUT_i)F_i = qcu_i, \quad i \in HP, \]

\[ (TOUT_j - t_{j,1})F_j = qhu_j, \quad j \in CP. \] (5)

Logical constraints

Logical constraints and binary variables are needed to determine the existence of process match \((i, j)\) in stage \(k\) and also any match invoking utility streams. The \(0-1\) binary variables are represented by \(z_{ij,k}\) for process stream matches, \(z_{cu}\) for matches involving cold utilities and \(z_{hu}\) for matches involving hot utilities. An integer value of one for any binary variable designates that the match is present in the optimal network. The constraints are then as follows:

\[ q_{ijk} - \Omega z_{ij,k} \leq 0, \quad i \in HP, \quad j \in CP, \quad k \in ST, \]

\[ q_{cu} - \Omega z_{cu} \leq 0, \quad i \in HP, \]

\[ q_{hu} - \Omega z_{hu} \leq 0, \quad j \in CP, \]

\[ z_{ij,k}, z_{cu}, z_{hu} = 0, 1, \] (6)

where the corresponding upper bound \(\Omega\) can be set to the smallest heat content of the two streams involved in the match.

Calculation of approach temperatures

The area requirement of each match will be incorporated in the objective function. Calculation of these areas requires that approach temperatures be determined. In the area targeting formulation presented in Part I, the approach temperatures were calculated explicitly in the objective function which required the use of max operators. Although these terms can be handled with the use of smooth approximations, the synthesis model can avoid their use completely through the introduction of approach temperature variables \(d_{t,j,k}\) coupled with the use of the binary variables. To ensure feasible driving forces for exchangers which are selected in the optimization procedure, the binary variables are used to activate or deactivate the following constraints for approach temperatures:

\[ dt_{ij,k} \leq t_{i,k} - t_{j,k} + \Gamma (1 - z_{ij,k}), \quad k \in ST, \quad i \in HP, \quad j \in CP, \]

\[ dt_{ij,k+1} \leq t_{i,k+1} - t_{j,k+1} + \Gamma (1 - z_{ij,k}), \quad k \in ST, \quad i \in HP, \quad j \in CP, \]

\[ dt_{cu} \leq t_{i,NOK+1} - TOUT_{cu} + \Gamma (1 - z_{cu}), \quad i \in HP, \]

\[ dt_{hu} \leq TOUT_{hu} - t_{j,1} + \Gamma (1 - z_{hu}), \quad j \in CP. \] (7)

Note that these constraints can be expressed as inequalities because the cost of the exchangers decreases with higher values for the temperature approaches \(dr\). Also, the role of the binary variables in the constraints in (7) is to ensure that nonnegative driving forces exist for an existing match. When a match \((i,j)\) occurs in stage \(k\), \(z_{ij,k}\) equals one and the constraint becomes active so that the approach temperature is properly calculated. However, when the match does not occur, \(z_{ij,k}\) equals zero, and the contribution of the upper bound \(\Gamma\) on the right-hand side deems the equation inactive. Similar constraints are used for utility exchangers when the outlet temperature of the utility stream, \(TOUT\), is not strictly higher (for hot utilities) or lower (for cold utilities) than the target temperature of the process stream. Also, in order to avoid infinite areas, small positive bounds are specified for the approach temperature variables \(dt\); that is:

\[ dt_{ij,k} \geq \epsilon, \] (8)

where \(\epsilon\) can be interpreted as the lowest allowable value of EMAT.

Objective function

Finally, the objective function can be defined as the annual cost for the network. The annual cost involves the combination of the utility cost, the fixed charges for exchangers, and the area cost for each exchanger. LMTD terms in the objective function are approximated using the Chen equation (1987):

\[
\begin{align*}
\text{min} & \quad \sum_{i \in HP} CCU_i q_{cu_i} + \sum_{j \in CP} CHU_j q_{hu_j} \\
& \quad + \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} CF_{ij,k} q_{ij,k} + \sum_{i \in HP} CF_{cu,k} q_{cu} \\
& \quad + \sum_{j \in CP} CF_{hu,k} q_{hu} \\
& \quad + \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} C_i[q_{ij,k} \\
& \quad / (U_i[(d_{t,j,k} + 1)(d_{t,j,k+1})/2]^{1/3})]^{b_i} \\
& \quad + \sum_{i \in HP} C_{cu,i} [q_{cu,i} / (U_i [d_{t,cu} (TOUT_i - TIN_{cu})] / 2)]^{b_{cu,i}} \\
& \quad + \sum_{j \in CP} C_{hu,j} [q_{hu,j} / (U_{hu,j} [d_{t,hu} (TIN_{hu} - TOUT_{hu})] / 2)]^{b_{hu,j}}. \\
\end{align*}
\] (9)

The proposed MINLP model for the HEN synthesis problem consists then of minimizing the
The attractive feature of the proposed MINLP model is that equations (1–8), which define the feasible space, are all linear. Therefore, there is no need to approximate the feasible region by any linearization scheme. This leads in general to a reasonable computational time for solving the MINLP problem. It should be noted, however, that the nonlinearities in the objective function (8) may lead to more than one local optimal solution due to their nonconvex nature.

In view of the nature of the MINLP model, the Combined Penalty Function and Outer-Approximation Method by Viswanathan and Grossmann (1990) can be applied to solve the proposed MINLP model. The solution scheme for the method is shown in Fig. 5. The initial step involves the solution of the relaxed NLP. If the solution of the relaxed NLP is integer, the algorithm stops. Otherwise, if the relaxed NLP is noninteger, an MILP master problem based on the linearization of the relaxed NLP solution is then formulated to predict a set of integer values for the binary variables. This master problem involves slack variables that allow the violation of linearizations of nonconvex functions and which are incorporated in an augmented penalty function. A sequence of NLP and MILP master problems is then solved in which the linear approximations are accumulated in the master problem. The cycle of major iterations is continued until there is no improvement between two successive feasible NLP subproblems. This method has proved to be effective in solving nonconvex MINLP problems and has shown to often lead to the global optimum. In general, it has been observed that an important factor leading to a globally optimal solution is that a good solution be obtained at the level of the relaxed NLP. As a result, even though the problem is very robust in nature, an initialization scheme can be used to increase the probability of obtaining the best relaxed solution. In addition to the simple procedure presented in Part I (Yee et al., 1990) of this series of papers, an alternative procedure which relies on an LP approximation of the MINLP is outlined in the Appendix. As shown by the examples in the next section, although none of the solutions obtained has been proven to be globally optimal, they are indeed very satisfactory in terms of minimizing the annual cost.

EXAMPLES

Example 1

Example 1 is from Linnhoff et al. (1982) involving two hot and two cold streams along with stream and...
cooling water as utilities. The problem data as well as the exchanger cost equations are presented in Table 1. Four networks are synthesized to account for cases of:

1. No network restrictions.
2. No stream splitting allowed.
3. Forbidden, required and restricted matches.
4. Target temperature as inequalities.

Results for cases 1 and 3 are presented in the MAGNETS User Guide (Grossmann, 1985), and therefore will be compared with the solutions from the simultaneous methodology.

Case 1—no network restrictions

In constructing the superstructure, the number of stages is fixed at two corresponding to \( \max \{ N_H, N_C \} \). Utility exchangers are placed at the two ends of the superstructure as shown in Fig. 2. The corresponding MINLP formulation involves 62 constraints and 50 variables of which nine are binary. Since the cost equation does not have an explicitly fixed charge, the binary variables are only needed to account for the approach temperatures [see equation (7)]. Since three of the utility matches do not require binary variables as feasibility of approach temperatures is always guaranteed, nine instead of 12 binary variables are needed. Also, the value of \( c \) in (8) was set to 0.1 as in the other examples. The model was solved by the package DICOPT++ (Viswanathan and Grossmann, 1990) via GAMS (Brooke et al., 1988) using MINOS5.2 (Murtagh and Saunders, 1985) and MPSX (IBM, 1979). Three major iterations were required using a total CPU time of 12.5 s on an IBM 3083. The network structure obtained did involve split streams. As a result, a suboptimization was performed to determine the proper split ratios and temperatures. The final optimal network is shown in Fig. 6. This network minimizes the utility to just $8000 yr\(^{-1}\) needing only cooling water. It is apparent that the cost data favor the trade-off of requiring more area to minimize the utility requirement. The total annual cost for the network is $80,274. The level of energy recovery corresponds to that of a threshold problem since only cooling utility is needed. However, an internal pinch (minimum approach temperature) exists according to the composite curves at 358.56-353 K. It is important to note that in the proposed network, three of the exchangers (2, 3, 4) are placed across this pinch and that the minimum approach temperature (EMAT at exchanger 3) is just 2.69 K.

The problem was also solved with MAGNETS with a fixed HRAT = 10 K. The solution obtained, which is the same as the one reported by Linnhoff et al. (1982), has an annual cost of $89,832 (see Fig. 7), which is 11% higher than the proposed network in Fig. 6. A drawback of the MAGNETS solution is that utility consumption or the level of energy recovery (HRAT) was fixed throughout the optimization procedure. Also, since in MAGNETS, the problem was decomposed into two subnetworks at the pinch (363-353 K), six units were required as compared to five for the simultaneous solution.

It is interesting to note that for HRAT = 10 K, the heuristic estimate of minimum number of units for this problem is seven (e.g. Linnhoff et al., 1982). However, for a level of energy recovery corresponding to the threshold case, the heuristic estimate is only four. In fact, a four-exchanger network can be obtained using MAGNETS if the HRAT is fixed at the threshold value of 5.56 K while the EMAT is allowed to be less than HRAT. This network is shown in Fig. 8 and has an EMAT at exchanger 2 of only 1.79 K. The annual cost is $80,000, which is about $300 less than the network derived by the simultaneous approach. However, a more complicated structure is required where a bypass at the outlet of exchanger 2 is needed. As mentioned previously, bypasses are undesirable since additional stream splitting is required making the network harder to operate. From a practical standpoint, it is hard to justify the added complexity to the network for a nominal savings of $300 yr\(^{-1}\). Interestingly, the MAGNETS network of Fig. 8 makes use of both of the structures (the bypass and the split stream going through exchangers 2 and 4 in series) which are not considered by the proposed superstructure. Even so, the network is less than 0.5% better in terms of cost. This result indicates that the simplicity of the proposed superstructure in Fig. 2 should in general not be a serious restriction for determining good networks.

Case 2—no stream splitting

As discussed in the preceding paragraph, the complexity of the network in regards to the number of

<table>
<thead>
<tr>
<th>Stream</th>
<th>TIN (K)</th>
<th>TOUT (K)</th>
<th>Fcp (kW K(^{-1}))</th>
<th>Cost ($ kW(^{-1}) yr(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>443</td>
<td>333</td>
<td>30</td>
<td>—</td>
</tr>
<tr>
<td>H2</td>
<td>423</td>
<td>303</td>
<td>15</td>
<td>—</td>
</tr>
<tr>
<td>C1</td>
<td>293</td>
<td>408</td>
<td>20</td>
<td>—</td>
</tr>
<tr>
<td>C2</td>
<td>353</td>
<td>413</td>
<td>40</td>
<td>—</td>
</tr>
<tr>
<td>S1</td>
<td>450</td>
<td>450</td>
<td>—</td>
<td>80</td>
</tr>
<tr>
<td>W1</td>
<td>293</td>
<td>313</td>
<td>—</td>
<td>20</td>
</tr>
</tbody>
</table>

\( U = 0.8 \) (kW m\(^{-2}\) K\(^{-1}\)) for all matches except ones involving steam.
\( U = 1.2 \) (kW m\(^{-2}\) K\(^{-1}\)) for matches involving steam.
Annual cost = 1000 x \([\text{area (m}^2\)](\text{)}\)\(^8\) for all exchangers except heaters.
Annual cost = 1200 x \([\text{area (m}^2\)](\text{)}\)\(^8\) for heaters.
stream splits is also a very important factor for HEN design. Although the proposed network of Fig. 6 is much better in terms of cost than the MAGNETS network of Fig. 7, stream splitting is required. Since a network with stream splitting is more difficult to operate, it may be desirable to design a network with no stream splits. As mentioned earlier in the paper, a no split network simply corresponds to selecting at most one unit for each stream in the superstructure.

When the model is constrained so that no stream splitting is allowed, it may be necessary to incorporate more stages in the superstructure in order to allow for more flexibility in the rematching of streams. To do so for Example 1, the number of stages is increased from two to three. Along with the no split constraints (10), the MINLP formulation involved 95 constraints and 66 variables of which 13 are binary. The optimal solution was obtained in four major iterations after 15 CPU s on the IBM 3083. The network is shown in Fig. 9 and has an annual cost of $80,909. As compared to the previous design with stream splitting, the annual cost is less than 1% higher, which is insignificant since the two stream splits are now unnecessary. Once again, only five units are required and exchangers 2 and 4 are placed across the internal pinch (358.56–353 K), and EMAT for exchanger 4 is just 2.65 K.

**Case 3 forbidden, required and restricted matches**

It may often be the case that when designing the HEN, certain restrictions on the network must be imposed for practical or safety reasons. One such example is presented in the MAGNETS manual for Example 1. The restriction forbids matching stream H2 with cooling water, requires stream H1 to exchange a minimum of 300 kW of heat with cooling water, and restricts match H1–C1 to a maximum of 300 kW. In the proposed formulation, these constraints can be easily incorporated into the model by setting bounds and adding constraints to regulate heat loads for the matches and fixing the values of the relevant binary variables. Using a two-stage superstructure, the restricted formulation required 63 constraints, 50 continuous variables and nine binary variables. The problem was solved in three major iterations using 16.25 CPU s on the IBM 3083. The

<table>
<thead>
<tr>
<th>Exch.</th>
<th>Heat Load (kW)</th>
<th>Area (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>628.8</td>
<td>22.8</td>
</tr>
<tr>
<td>2</td>
<td>271.2</td>
<td>19.3</td>
</tr>
<tr>
<td>3</td>
<td>2400</td>
<td>265.1</td>
</tr>
<tr>
<td>4</td>
<td>1400</td>
<td>179.0</td>
</tr>
<tr>
<td>5</td>
<td>400</td>
<td>38.3</td>
</tr>
</tbody>
</table>

Fig. 6. Example 1 — unrestricted case.
network, with five units and an annual cost of $87,225, is shown in Fig. 10. Again, the solution compares well with the one obtained from MAGNETS which requires, for HRAT = 10 K, an annual cost of $90,831 with six units. In both of the solutions, the same utility requirement is needed. It is interesting to note that the solution obtained using MAGNETS requires 59 m² less area. However, due to a different distribution of area in the exchangers and economy of scale (a 0.6 exponent on the area cost equation), the annual cost required by the MAGNETS solution is about 4% more. The results clearly show that the trade-off between the number of units and area must be considered. Once again, exchangers (1, 2, 4) are placed across the internal pinch and EMAT is 3.55 K.

Case 4—target temperatures as inequalities

As mentioned previously, in formulating the model, the temperatures for the stream data can be specified as inequalities. To illustrate this point, the target temperature for stream C2 in Example 1 is modified from the fixed value of 413 K to a range such that 373 K ≤ Tout_C2 ≤ 413 K. To represent this in the formulation, the parameter Tout_C2 is replaced by a new variable tout_C2. Specifically, the replacement appears in the overall heat balance for stream C2 and in the objective function term for calculating the area cost for the heater involving C2. Furthermore, tout_C2 is bounded to reflect the allowable range of outlet temperature.

With the modification in the formulation, a two-stage model involving 63 constraints and 41 continuous and nine binary variables was solved in 12.6 CPU s on the IBM 3083 using DICOPT++. As shown by the optimal network in Fig. 11, the solution did indeed take advantage of the range specification for the target temperature. The solution selected a minimum heat exchange for stream C2 with a network outlet temperature of 373 K. Note that unlike the other cases, the utility usage is not minimized since 2000 kW is needed from cooling water instead of the 400 kW of cooling water when the outlet temperature of 413 K is specified. The cost of cooling water appears to be sufficiently cheap so that the cost of capital is more significant. Hence, the network

![Fig. 7. MAGNETS solution for Example 1, HRAT fixed at 10 K.](image)
requires only four units and relatively little area, and the annual utility cost of $40,000 is more than the annual capital cost of $36,880. Total annual cost for the network is $76,880, which corresponds to a savings of about $3000 yr\(^{-1}\) as compared to the network of case 1 where the target temperature for C2 is fixed at 413 K.

**Example 2**

Example 2 is from Gundersen and Grossmann (1988) and was also analyzed by Colberg and Morari (1990). In both papers, no cost data are presented for utility streams and the level of energy recovery is fixed at HRAT = 20°C. As a result, for comparison purposes, the utility usage is fixed for the proposed method at HRAT = 20°C, so that the emphasis is placed on the trade-off between the number of units and area. The problem has the same number of streams as Example 1 although the cost equation for the exchangers involves an explicit fixed charge for each unit. The problem data are shown in Table 2.

Using the proposed method, a superstructure with two stages is constructed and the corresponding MINLP model is formulated. The formulation involves 67 constraints and 53 variables with 12 being binary. The solution procedure using DICOPT++ required three major iterations and 17.9 CPU s on the IBM 3083. The optimal network obtained is shown in Fig. 12. The total cost for the network is $715,970, which is roughly $13,000 less than the previously best reported solution of $729,000 by Gundersen and Grossmann (1988). In both of the previous papers, the reported network required six units and 2960 m\(^2\) of area. The optimal solution from the proposed method also requires six units, but the area requirement is 3045.5 m\(^2\), or about 85 m\(^2\) more. However, the total cost actually turns out to be less. One reason for the additional area requirement for the optimal network is the fact that one of the temperature approaches in exchanger 1 is relatively small, lying below 20°C, which leads to a small driving force and a large area requirement. The effect of the large area on cost, though, is compensated by the effect of economy of scale where the incremental area of an exchanger becomes progressively cheaper. Overall, it appears that the optimal network is able to fully take advantage of economy of scale so that, as compared to the previously reported solution, even though the area requirement is higher, the cost is lower. This result clearly illustrates that the minimization of area
does not necessarily go hand-in-hand with the minimization of cost, even when the same number of exchangers is considered.

In addition, it is important to note that in the network of Fig. 12, exchanger 5 is placed across the pinch at 90–70°C. It is also interesting to note that although the net total heat flow of the composite streams across the pinch is zero, there is heat transferred across the pinch within exchanger 5. It is easy to verify that across the temperatures 90–70°C, stream H1 transfers 213.5 kW which is absorbed by stream C1 below the pinch thus cancelling this extra heat flow. Also, note that the driving force is relatively high in this exchanger. This example clearly shows that not placing exchangers across the pinch is a heuristic which may not always hold.

Another heuristic that may not hold is the one for the minimum number of units. Using the heuristics for the case where the problem is decomposed into subnetworks, seven units are predicted. When the problem is not decomposed, five units are predicted. However, the optimal solution for the problem requires six units. Finally, it should be noted that the capital cost requirement for the optimal network corresponded very closely with the capital cost target for the problem established in Colberg and Morari (1990) of $716,000.

Example 3

Example 3 is from the MAGNETS User Manual. The main purpose of this example is to analyze the proposed method in the case where split streams are required. The problem involves five hot streams and one cold stream along with steam and cooling water. The problem data are shown in Table 3. Since only one large cold stream is present, it is likely that the final network will require many split streams, which is exactly the case for the solution obtained by MAGNETS shown in Fig. 13. In networks where several stream splits may be required, restriction on the type of split allowed in the model, where the outlet temperatures at each stage are assumed to be equal, may have significant impact on the optimal network generated.

The superstructure for the problem was set up with five stages. The MINLP formulation contains 222 constraints and 104 continuous and 31 binary variables. The solution was obtained in three major iterations using DICOPT++, which required 2.78 CPU min on the IBM 3083. The network ob-
Example 4

Example 4 is from Colberg and Morari (1990), a problem involving three hot and four cold streams along with steam and cooling water. The data are shown in Table 4. The interesting aspects of this example are that: (1) the streams have significantly different heat transfer coefficients; (2) the synthesized network for the fixed HRAT from Colberg and Morari (1990) requires a split stream going through exchangers in series as shown in Fig. 4a, a configuration the proposed superstructure does not consider. In order to synthesize a network for comparison, the level of energy recovery was fixed at HRAT = 20 K which leads to a pinch at 517-497 K. Also, since no cost equation was given, the exchanger cost equation from Example 2 of $8600 + 670 \times (\text{Area})^{0.8}$ was used.

The superstructure for the problem was constructed with four stages. The formulation involved 231 constraints and 151 continuous and 48 binary variables. Solution of the problem to optimality required three major iterations and 13.8 CPU min on the IBM 3083. Two split streams are required in the
solution, and therefore the NLP suboptimization is performed to determine the optimal split ratios. The final network is shown in Fig. 15. The cost for the network is $150,998. This compares well with the Colberg and Morari network which, using the same cost equation, is at $177,385, roughly 17.5% higher. However, the Colberg and Morari solution does achieve their objective of minimizing the total area. Their network requires 188.9 m² vs 217.8 m² for the network from the proposed approach. The trade-off, though, is that the Colberg and Morari network also requires three additional units and 10 additional split streams. One reason why the number of units is larger is that their problem was partitioned into subnetworks. Since the heat transfer coefficients are so different, certain cross-pinch exchanges may be desirable. In fact, the optimal solution derived from the simultaneous approach does indicate this and cross-pinch exchanges exist in exchangers 2 and 3. It is especially interesting to note that the exchange at unit 3 has an approach temperature on one side of a mere 0.88 K. However, the area for the unit is not large since the two streams involved have the largest heat transfer coefficients.

**Example 5**

This example involves the 4SP1 problem of Lee et al. (1970). The data are presented in Table 5 and involves two hot and two cold process streams along with steam and cooling water. The problem is used here to illustrate the incorporation of cold-to-cold or hot-to-hot matches in the proposed method. As discussed previously, several authors have noted that it may be desirable in certain cases to have heat exchange between two hot or two cold streams. Dolan et al. (1987) considered this type of matching when they analyzed the 4SP1 problem using simulated annealing for the case where a match between hot stream H1 and cold stream C1 is forbidden. For a minimum approach temperature (EMAT) of 18°F, they derived a network with a cold-to-cold exchanger which required a total annual cost of $13,800. They also compared their solutions with the one derived by Papoulias and Grossmann (1983) for the same restriction and EMAT, and where the objective was to minimize the number of units. In the Papoulias and Grossmann network, the use of cold-to-cold matches was not considered. As a result, more utility was
HRAT fixed at 20°C
Total Capital Cost = $715,970
Total Area = 3045.4 m²

<table>
<thead>
<tr>
<th>Exch.</th>
<th>Heat Load (kW)</th>
<th>Area (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1563.5</td>
<td>1210.3</td>
</tr>
<tr>
<td>2</td>
<td>436.5</td>
<td>225.7</td>
</tr>
<tr>
<td>3</td>
<td>400</td>
<td>160.0</td>
</tr>
<tr>
<td>4</td>
<td>686.5</td>
<td>150.95</td>
</tr>
<tr>
<td>5</td>
<td>1800</td>
<td>1174.1</td>
</tr>
<tr>
<td>6</td>
<td>388.5</td>
<td>124.4</td>
</tr>
</tbody>
</table>

Fig. 12. Optimal network for Example 2.

required and the network has a higher annual cost of $21,100.

In the proposed model, hot-to-hot or cold-to-cold matches can be embedded in the superstructure. As an example, consider the case of cold-to-cold matches for which the following modifications are required in the formulation:

1. Introduce new heat load variables for cold-to-cold matches, $q_{j\beta,k}$, to represent the heat transfer from cold stream $j$ to cold stream $\beta$, where $j \neq \beta$.

2. Relax the monotonic decrease of temperatures along the stages by removing the constraint in (4):

   \[ t_{j,k} \geq t_{j,k+1}, \quad k \in ST, \quad j \in CP. \quad (11) \]

3. Introduce the new variables into the overall and interval heat balances [equations (1) and (2)]:

   \[ (T_{OUT} - T_{IN})F_j = \sum_{k \in ST} \sum_{\beta \in CP} q_{j\beta,k} \]

   \[ - \sum_{k \in ST} \sum_{\beta \neq j} (q_{j\beta,k} - q_{\beta j,k}) + q_{h\beta,j}, \quad j \in CP, \]

   \[ (t_{j,k} - t_{j,k+1})F_j = \sum_{i \in HP} q_{i\beta,k} \]

   \[ - \sum_{\beta \in CP} (q_{j\beta,k} - q_{\beta j,k}), \quad k \in ST, \quad j \in CP. \quad (12) \]

4. Introduce new terms in the objective function to calculate the cost of the cold-to-cold exchangers.

With these modifications, the 4SP1 problem was formulated embedding cold-to-cold matches. A three-stage representation was used since the problem involves potentially three “hot” streams. For comparison with the results of Dolan et al. (1987), the minimum approach temperature is set to 18°F. The MINLP model involves 94 constraints and 70 continuous and 15 binary variables. Solution of the problem using DICOPT++ required 23.31 CPU s on the IBM 3083. The optimal solution derived is shown in Fig. 16. The solution obtained indeed requires a cold-to-cold match between streams C1 and C2, where C2 is considered the “hot” stream. The total annual cost for the network is $13,800, which is
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identical to the solution from Dolan et al. (1987). A comparison between the two networks shows that the configurations are the same and both networks achieve minimum energy requirement. The heat load distribution, however, is slightly different but not enough to significantly affect the capital cost.

A second network for the example was obtained for the case where the specification of minimum approach temperature is eliminated. The optimal network is shown in Fig. 17. Again, the same network configuration is obtained, with one cold-to-cold match involved in the network. The heat load distri-

Fig. 13. MAGNETS solution for Example 3.

### Table 3. Problem data for Example 3

<table>
<thead>
<tr>
<th>Stream</th>
<th>(T_{IN}) (K)</th>
<th>(T_{OUT}) (K)</th>
<th>(F_{cp}) (kW K(^{-1}))</th>
<th>Cost ($/kW K(^{-1}) yr(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>500</td>
<td>320</td>
<td>6</td>
<td>—</td>
</tr>
<tr>
<td>H2</td>
<td>480</td>
<td>380</td>
<td>4</td>
<td>—</td>
</tr>
<tr>
<td>H3</td>
<td>460</td>
<td>360</td>
<td>6</td>
<td>—</td>
</tr>
<tr>
<td>H4</td>
<td>380</td>
<td>320</td>
<td>20</td>
<td>—</td>
</tr>
<tr>
<td>H5</td>
<td>380</td>
<td>320</td>
<td>12</td>
<td>—</td>
</tr>
<tr>
<td>C1</td>
<td>290</td>
<td>660</td>
<td>18</td>
<td>—</td>
</tr>
<tr>
<td>S1</td>
<td>700</td>
<td>700</td>
<td>—</td>
<td>140</td>
</tr>
<tr>
<td>W1</td>
<td>300</td>
<td>320</td>
<td>—</td>
<td>10</td>
</tr>
</tbody>
</table>

\(U = 1\) (kW m\(^{-2}\) K\(^{-1}\)) for all matches.
Annual cost = 1200 \times [area (m\(^2\))]\(^{0.6}\) for all exchangers.
bution, however, is quite different than the previous network, with significant reduction in the utility requirement. The annual utility cost is reduced by about $3300. The optimal trade-off, though, requires an increase of over 50% in heat transfer area. Since area cost is relatively cheap, the annual capital cost increases by just $859 despite the fact that an EMAT of just 2.15°F exist at exchanger 2. The total annual cost for the network is $11,374, which is about 18% less as compared to the previous network where EMAT is fixed at 18°F.

**CONCLUSION**

In this paper, a systematic procedure has been proposed for the synthesis of heat exchanger net-

### Table 4. Problem data for Example 4

<table>
<thead>
<tr>
<th>Stream</th>
<th>TIN (K)</th>
<th>TOUT (K)</th>
<th>( Fcp ) (kW K(^{-1}))</th>
<th>( k ) (kW m(^{-2}) K(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>626</td>
<td>586</td>
<td>9.802</td>
<td>1.25</td>
</tr>
<tr>
<td>H2</td>
<td>420</td>
<td>519</td>
<td>2.931</td>
<td>0.05</td>
</tr>
<tr>
<td>H3</td>
<td>528</td>
<td>353</td>
<td>6.161</td>
<td>3.20</td>
</tr>
<tr>
<td>C1</td>
<td>497</td>
<td>513</td>
<td>7.179</td>
<td>0.65</td>
</tr>
<tr>
<td>C2</td>
<td>389</td>
<td>576</td>
<td>0.641</td>
<td>0.25</td>
</tr>
<tr>
<td>C3</td>
<td>326</td>
<td>386</td>
<td>7.627</td>
<td>0.33</td>
</tr>
<tr>
<td>C4</td>
<td>313</td>
<td>566</td>
<td>1.690</td>
<td>3.20</td>
</tr>
<tr>
<td>S1</td>
<td>650</td>
<td>650</td>
<td></td>
<td>3.50</td>
</tr>
<tr>
<td>W1</td>
<td>293</td>
<td>308</td>
<td></td>
<td>3.50</td>
</tr>
</tbody>
</table>

\( 1/U = (1/h_a + 1/h_b) \)

Cost = 8600 + 670 \times \text{area} (m^2)\(^{10} \) for all exchangers.
Simultaneous optimization models for heat integration—II

Fig. 15. Optimal network for Example 4.

Table 5. Problem data for Example 5

<table>
<thead>
<tr>
<th>Stream</th>
<th>TIN (°F)</th>
<th>TOUT (°F)</th>
<th>Fcp (B.t.u. °F⁻¹)</th>
<th>($1000 B.t.u. yr⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>320</td>
<td>200</td>
<td>16,666.8</td>
<td>—</td>
</tr>
<tr>
<td>H2</td>
<td>408</td>
<td>260</td>
<td>20,000</td>
<td>—</td>
</tr>
<tr>
<td>C1</td>
<td>131</td>
<td>220</td>
<td>14,450.1</td>
<td>—</td>
</tr>
<tr>
<td>C2</td>
<td>240</td>
<td>500</td>
<td>11,530</td>
<td>—</td>
</tr>
<tr>
<td>S1</td>
<td>540</td>
<td>540</td>
<td>12.76</td>
<td>—</td>
</tr>
<tr>
<td>W1</td>
<td>100</td>
<td>180</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

Pinch Location: 517-497K
HRAT fixed at 20 K
Total Cost = $150,998

works. Unlike previous methods, the proposed approach does not rely on a sequential decomposition of the problem since it accounts simultaneously for the trade-offs between energy cost, fixed charges for units and cost for exchanger area. The method involves the optimization of a stage-wise superstructure that is modeled as an MINLP problem. No account is made for pinch considerations, such as partitioning into subnetworks or not placing exchangers across the pinch. Energy recovery (HRAT), heat loads, minimum approach temperatures (EMAT) and stream matches are not fixed. The simplifying assumption on isothermal mixing in the superstructure eliminates flow variables and heat mixing equations which allows the feasible space for the model to be defined by linear constraints. Thus, the model can be solved more efficiently. Given the assumption of isothermal mixing of streams, a suboptimization is performed to determine optimal split ratios when the predicted network requires stream splits. A positive
No match allowed for H1-C1
EMAT = 18°F
Cold-to-cold matches allowed

Annual Utility Cost = $9,888
Annual Capital Cost = $3,817
Total Annual Cost = $13,800
Total Area = 832.9 ft²

Exch. | Heat Load (1000Btu) | Area(ft²)
---|---|---
1 | 438.1 | 38.5
2 | 1886.9 | 286.8
3 | 2113.1 | 167.1
4 | 1160.7 | 221.7
5 | 839.3 | 66.4
6 | 487.9 | 52.6

Fig. 16. Example 5—restricted case with EMAT = 18°F.

No match allowed for H1-C1
Cold-to-cold matches allowed

Annual Utility Cost = $5,698
Annual Capital Cost = $4,676
Total Annual Cost = $11,374
Total Area = 1295.4 ft²

Exch. | Heat Load (1000Btu) | Area(ft²)
---|---|---
1 | 255.4 | 25.4
2 | 1969.4 | 643.7
3 | 2030.6 | 170.4
4 | 1343.5 | 331.1
5 | 655.6 | 56.2
6 | 579.5 | 68.7

Fig. 17. Example 5—restricted case with no EMAT specification.
effect from the simplifying assumption is that the model will tend to favor structures with no stream splits.

The MINLP model can also easily accommodate constraints on stream matches, heat loads and stream splitting. In addition, the model can consider hot-to-hot or cold-to-cold matches. The limitation of the method lies in the fact that certain configurations are not explicitly included in the superstructure. Examples have shown, however, that the limitation is not severe in view of the combinatorial nature of the synthesis problem, where several alternative configurations may be very close to the global optimum. The MINLP model, which has been applied to problems involving up to seven process streams, may or course become more expensive to solve in larger problems.

The example problems presented have also shown that pinch considerations may not be relevant for synthesizing the network structure when all the trade-offs are accounted for simultaneously; this is true even for the case when heat transfer coefficients for the streams are the same. Considerations for the economy of scale for area cost and fixed charges for the number of units do not necessarily favor the minimization of area for which the pinch heuristics are based. Furthermore, as shown by the examples, optimal networks often involve exchangers that are placed across the pinch.

Acknowledgment—The authors would like to acknowledge financial support from the Department of Energy under Grant DE-FG-02-85ER13396.

REFERENCES


APPENDIX

Initialization Procedure for Solving the MINLP Models

As shown in Fig. 5, the first step of the Combined Penalty Function/Outer Approximation Method involves the solution of the relaxed NLP problem. Even though this NLP formulation is very robust in that it only has linear constraints, it is desirable to supply a "good" initial guess so one can increase the likelihood of obtaining the best solution in cases where multiple local optima may exist. In general, it has been observed that a good relaxed NLP solution will lead to the global optimum for the MINLP model.

Following is an initialization procedure that reduces the MINLP to an LP by assuming fixed temperature driving forces for each match:

1. Estimate a value of HRAT.
2. Estimate a driving force for each match by:
   (a) determining the $LMTD_n$ for each enthalpy interval $n$ using its corresponding temperatures;
   (b) using the following weighting equation to calculate an average driving force for each match $(i,j)$:

$$ALMTD_{ij} = \left( \frac{\sum \theta_i LMTD_{ij}}{\sum \theta_i} \right) / \sum \theta_i.$$
where $q_{ij}$ is the maximum heat transfer that can occur between hot stream $i$ and cold stream $j$ in enthalpy interval $n$.

3. For each match $i, j$ in different stages of the superstructure, set the driving forces in the objective function (8) with the fixed value of the average driving force $ALMTD_{ij}$, and replace the nonlinear cost term of the area by a linear approximation with a fixed charge. This reduced the MINLP in (1-8) to an MILP.

4. Solve the relaxed LP of the MILP in Step 3.

5. Use the LP solution along with the estimated driving forces ($ALMTD_{ij}$) as an initial guess for the relaxed NLP problem.