Automatic Synthesis of Optimum Heat Exchanger Network Configurations

This paper addresses the problem of automatically generating heat exchanger network configurations that feature minimum investment cost subject to minimum utility cost and fewest number of units. Based on the linear programming and the mixed-integer linear programming (MILP) transshipment models for heat integration, a superstructure that has embedded many alternative configurations is proposed. This superstructure, which has as units the matches predicted by the MILP transshipment model, includes options for series and parallel matching, as well as stream splitting, mixing, and bypassing. Many of the implied stream connections in the superstructure are reduced to zero flow with a nonlinear programming formulation that leads to realistic and practical designs. Theoretical properties as well as the implementation aspects of the proposed procedure for the automatic generation of networks are presented. The method is illustrated with three example problems.

C. A. FLOUDAS, A. R. CIRIC and I. E. GROSSMANN

Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA, 15213

SCOPE

One of the major components in a chemical processing system is the heat exchanger network, because it determines to a large extent the energy efficiency of the process. The heat exchanger network has the task of integrating the hot and the cold process streams in a process in order to reduce the amount of heating and cooling utilities that are required. The problem of synthesizing optimal network configurations has received considerable attention in the literature, and an extensive review of the previous work can be found in Nishida et al. (1981). One of the most important insights that has been developed to overcome the combinatorial nature of this problem is the prediction of the minimum utility target (Hohmann, 1971; Linnhoff and Flower, 1978), which can be performed prior to developing the network structure. The number of network configurations satisfying the minimum utility target is often much smaller than the total number of possible configurations, and furthermore this target insures that the lowest utility cost will be obtained for a given minimum temperature approach. As is well known, networks featuring minimum utility cost and fewest number of units yield near-optimal network structures. However, the derivation of the network structure based on these two targets is often a nontrivial task which may require tedious trial and error effort when this is done manually. Thus, there is a clear incentive for developing synthesis tools that can automatically generate network structures of good quality.

Papoulias and Grossmann (1983) formulated models for the minimum utility cost target and the minimum number of units target—linear programming (LP) and mixed-integer linear programming (MILP) transshipment models, respectively. The LP transshipment model, which can handle unrestricted and restricted matches, predicts the consumption of utilities as well as the location of the pinch points that limit maximum heat integration. The solution of the MILP transshipment model determines the stream matches that should take place, and the corresponding heat that is exchanged at each match. Although these models provide valuable information on the required network structure at the level of matches, they do not provide information on the stream interconnections for the automatic synthesis of the network configuration. Furthermore, since in most cases different alternative interconnections will exist, it is clearly desirable to identify the one that leads to minimum investment cost.

Therefore, a major problem that remains in the synthesis of heat exchanger networks is how to automatically generate network structures that in fact not only satisfy the minimum utility target, but that also feature minimum investment cost as well as fewest number of units. Although a number of methods have been proposed for the automatic generation of the network structures (see Introduction section), they either do not satisfy the two additional criteria cited above, or they cannot handle all types of network configurations.

In this paper a procedure is presented for the automatic generation of optimal configurations for heat exchanger networks. The proposed networks feature minimum investment cost subject to having minimum utility cost and fewest number of units. The networks may involve stream splitting, mixing, and bypassing. As will be shown, an efficient automatic procedure based on a mathematical programming approach can be developed to solve this problem. In particular, the approach relies on the LP and MILP transshipment models for predicting the minimum utility cost and the fewest number of units. This information is then used within a nonlinear programming formulation of a proposed superstructure to generate an optimal network configuration. Theoretical properties of the method are discussed as well as its implementation in the computer program MAGNETS, which is used to illustrate three example problems.

Correspondence concerning this paper should be addressed to I. E. Grossmann.

CONCLUSIONS AND SIGNIFICANCE

The synthesis problem of automatically generating heat exchanger network structures has been considered. A procedure has been proposed that is based on a superstructure which includes alternatives for splitting, mixing, and bypassing of streams. Optimizing this superstructure through a nonlinear programming formulation, heat exchanger network configurations are derived automatically that feature minimum investment cost subject to the targets of minimum utility cost and fewest number of units. The optimization of the minimum temperature approach can easily be performed in an outer loop of the suggested synthesis method.

The proposed procedure features two important properties. First, the superstructure has embedded network configurations that have as many heat exchanger units as the minimum number of matches predicted by the MILP transshipment model. The existence of feasible network structures in which there is this one-to-one correspondence of matches and units has been proved. Therefore there is no need to delete or merge superfluous heat exchangers as is done in other methods. Second, it has been proved that the method has the property that it leads to realistic and practical network structures, since many of the implied stream connections in the proposed superstructure are reduced to zero flow and therefore are deleted.

The significance of the method presented in this paper is that it is an efficient synthesis tool based entirely on mathematical programming techniques for the full automatic generation of optimal network structures. This method has been implemented in the computer code MAGNETS, and its performance has been illustrated with three example problems. The computer implementation and the examples clearly show that the development of high quality automatic synthesis tools is indeed feasible.

INTRODUCTION

A very large number of synthesis procedures for heat exchanger networks has been published in the literature (Nishida et al., 1981). However, only a relatively modest number can be implemented as computer tools for the full automatic generation of network configurations. The suggested procedures for the automatic synthesis of networks can be classified into the following three categories:

1. Acyclic networks without stream splitting.
2. Cyclic networks without stream splitting.
3. Networks with stream splitting.

A selected sample of previous methods for automatic generation of these type of networks is given below.

In the first category, Lee et al. (1970) proposed a branch and bound procedure for the generation of acyclic heat exchanger networks which result from matching successively the hot and the cold streams, starting with their inlet temperatures. Since the streams exchange as much heat as possible, each pair of streams can only be matched once. Pho and Lapidus (1973) presented an alternate method based on a decision tree in which the nodes contain a compact matrix representation for acyclic networks. Enumeration of the entire tree is performed using a depth-first search procedure. When a complete enumeration is not feasible, a heuristic partial enumeration method is used.

In the second category, Ponton and Donaldson (1974) proposed a fast heuristic method for the synthesis of cyclic heat exchanger networks obtained by countercurrent matches of the hot and cold process streams. This method is based on the heuristic of matching successively the hottest inlet of the hot streams with the hottest outlet of the cold streams. In this method the network configurations may involve several matches for the same pair of streams. Grossmann and Sargent (1978) considered the optimum design of cyclic heat exchanger networks in two stages. In the first stage, they used an implicit enumeration algorithm to determine the optimum sequence for countercurrent matches of the process streams. In the second stage, the structure found in the first stage is optimized by a nonlinear program.

The main shortcoming of the methods cited above is that they cannot guarantee minimum utility consumption for the networks that are generated, since this may require splitting of streams (Linnhoff and Flower, 1978). A method for unsplit networks that does satisfy the minimum utility target is the thermodynamic combinatorial method of Flower and Linnhoff (1980). In this method only those networks that satisfy the criterion of minimum utility consumption are enumerated. However, since only unsplit networks can be considered with this enumeration method, no feasible heat exchanger network structure may be found with this procedure.

In the third category Nishida et al. (1977) proposed evolutionary rules for the derivation of network configurations that involve stream splitting. This method, however, does not guarantee minimum utility consumption nor the fewest number of units. Su and Motard (1984) proposed an algorithmic-evolutionary approach based on searching and breaking loops in an initial network structure derived from the TI method (Linnhoff and Flower, 1978). This approach incorporates some of the evolutionary rules proposed by Nishida et al. (1977) and produces in most cases networks that feature minimum numbers of units. Grimes et al. (1981) proposed an evolutionary approach based on special matching rules for synthesizing networks that feature stream splitting and minimum number of units. This procedure may produce networks where the minimum utility cost is not achieved. Finally, Hama (1984) has recently proposed a three-step iterative approach for the generation of optimal heat exchanger networks. This approach is based on the use of a T-H diagram to determine the minimum utility consumption and to derive the basic matches in the network that may involve stream splitting. The sizes of the exchangers and the split fractions are then optimized with a nonlinear optimization procedure. The network configurations generated by this method do not necessarily involve the minimum number of units.

As can be seen from this brief review, none of the methods cited above can automatically generate network configurations involving possible splitting, mixing, and bypassing of streams, and at the same time featuring minimum utility cost, fewest number of units, and minimum investment cost. It should be pointed out that although these three design objectives are not necessarily equivalent to the minimum total annual cost, they provide a very good approximation to this problem as well as a practical approach to the synthesis problem.

In this paper, a procedure based on a mathematical programming approach is presented for the automatic generation of network configurations. The basic idea in the proposed procedure is to derive a superstructure that has embedded heat exchanger network configurations that satisfy the criterion of the minimum utility cost and that contain as units the minimum number of matches predicted by the mixed integer linear programming (MILP) transshipment model proposed by Papoulias and Grossmann (1983). As will be shown, it is always possible to obtain a feasible network configuration with the proposed superstructure. The network configuration is generated automatically by minimizing the investment cost of the superstructure through a nonlinear programming (NLP) formulation for the proposed superstructure. The implementation of this systematic procedure in the computer program MAGNETS is discussed, and its application is illustrated with three example problems.

PROBLEM STATEMENT

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

A set of hot streams H that must be cooled and a set of cold streams C that must be heated are given. Fixed heat capacity flow rates and inlet and outlet temperatures are specified for these streams. Auxiliary heating and cooling are available from a set of hot utilities, HU, and a set of cold utilities, CU. The problem then is to derive automatically a heat exchanger network configuration that minimizes the investment cost of the heat exchangers while satisfying the criteria of:

a) Minimum utility cost.

b) Minimum number of heat exchanger units.

The potential configurations that are considered can involve series and/or parallel arrangements, as well as stream splitting, mixing, and bypassing.

The basic assumptions that will be made for this synthesis problem are that the enthalpy of the process streams is a linear function of temperature, and that the heat exchangers are of the countercurrent type. Also, it will be assumed that the objective of minimum number of units will be applied to each of the subnetworks defined by the pinch points (Papoulias and Grossmann, 1983), rather than applying this objective to the overall network (Wood et al., 1985). Finally, for the sake of simplicity in the presentation it will be assumed that a fixed minimum temperature approach is specified by the design engineer. As will be shown in the third example problem, this assumption can be relaxed with the proposed method.

OUTLINE OF SYNTHESIS STRATEGY

The basic idea behind the proposed synthesis strategy is to decompose the problem so as to insure first, minimum utility cost; second, fewest number of units for this utility target; and third, minimum investment cost for the first two objectives. As indicated in Figure 1, the suggested procedure for the automatic generation of network configurations involves the following steps:

1. The minimum utility cost and the location of the pinch points are predicted via the LP transshipment model. The location of the pinch points is used to divide the temperature range of the streams into subnetworks.

2. The fewest number of matches for each subnetwork is predicted with the MILP transshipment model. The solution to this problem will also provide information on the set of matches that must take place and the amount of heat that must be exchanged at each match.

3. A superstructure is derived for each subnetwork which has as units those matches predicted by the MILP transshipment model. This superstructure will contain unknown stream connections which may define series and/or parallel arrangements, as well as stream splitting and bypassing.

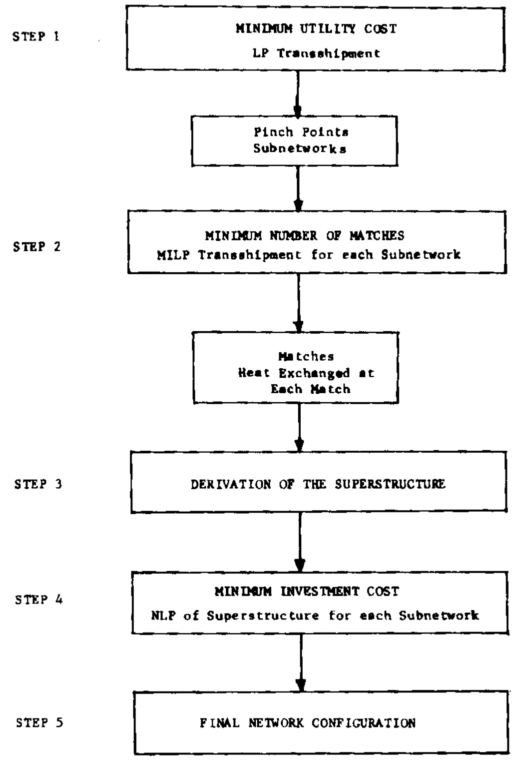

Figure 1. Outline of synthesis strategy.

4. The superstructure for each subnetwork is formulated as a nonlinear programming problem which has as its objective the minimization of the investment cost of heat exchangers. The solution to this problem will automatically provide for each subnetwork a heat exchanger network configuration with the appropriate stream connections for the exchangers, as well as their flowrates and temperatures.

5. The final configuration is obtained by simply adding the configurations of each subnetwork.

The detailed description of steps 1 and 2, which involve the solution of the transshipment models, will be omitted in this paper because it is presented in the work of Papoulias and Grossmann (1983). The original contribution of the present paper will be the development and theoretical justification of steps 3 and 4. In particular, it will be shown that there is a one-to-one correspondence of the matches predicted by the MILP transshipment model and the units of a feasible network configuration that is embedded in the superstructure. Also, it will be shown that many streams in the superstructure will have the tendency of being deleted. The significance of these results is that they allow the complete automation of the synthesis of heat exchanger networks.

DERIVATION OF SUPERSTRUCTURE

In order to derive a superstructure for the heat exchanger network, advantage can be taken of the information provided by the LP and MILP transshipment models. From the solution of the LP transshipment model the heat loads of the utilities that lead to minimum utility cost are determined, as well as the location of the pinch points. These pinch points are used to decompose the problem into subnetworks that represent temperature ranges for streams located between successive pinch points (Grimes et al., 1981). Solving the MILP transshipment model for each subnetwork, the minimum number of matches and the heat exchanged at each match are determined. Each of these matches with the corresponding heat exchange will be associated to heat exchanger units in the proposed superstructure, where the stream interconnections for the final network configuration are treated as unknowns.

An important feature in the proposed superstructure is that for each stream an independent superstructure can be developed. The stream superstructures can then be combined into one overall superstructure which has embedded all configurations of interest for each subnetwork. Each stream superstructure is derived in such a way so as to include alternatives on stream splits, bypasses, matches in series, matches in parallel, matches in series-parallel, matches in parallel-series, etc.

In order to demonstrate how such a superstructure can be developed, suppose that there is one cold stream *C1* that exchanges heat with three hot streams *H1, H2, H3,* in the three matches *C1-H1, C1-H2, C1-H3.* These matches and the heat exchanged in them would have been provided by the solution of the MILP transshipment model. One can then postulate stream superstructures as shown in Figure 2, where the exchangers correspond to the matches predicted by the MILP transshipment model. The heat load in each exchanger is the predicted heat exchange for each match.

The basic elements in the derivation of the stream superstructure for *C1* consist of the following (Figure 2):

1. Split the inlet of *C1* into three streams directed to the inlet of the three matches with the hot streams. That is, *C1* is split into streams *1, 2,* and *3.*

2. Split the output of *C1* at each match into: (a) One stream that goes to the outlet stream of *C1* in this subnetwork. (b) Two recycle streams that are mixed with the inlet streams of the two other matches.

As an example for step 2 consider the match *H1-C1.* The output of this match is split into streams *4, 5,* and *6.* Stream *4* goes to the outlet of *C1.* The recycle stream *5* is mixed with the inlet of the match *H2-C1,* while the recycle stream *6* is mixed with the inlet of the match *H3-C1.*

In the case of the hot streams *H1, H2, H3,* each stream superstructure is reduced to a single exchanger as shown in Figure 2,

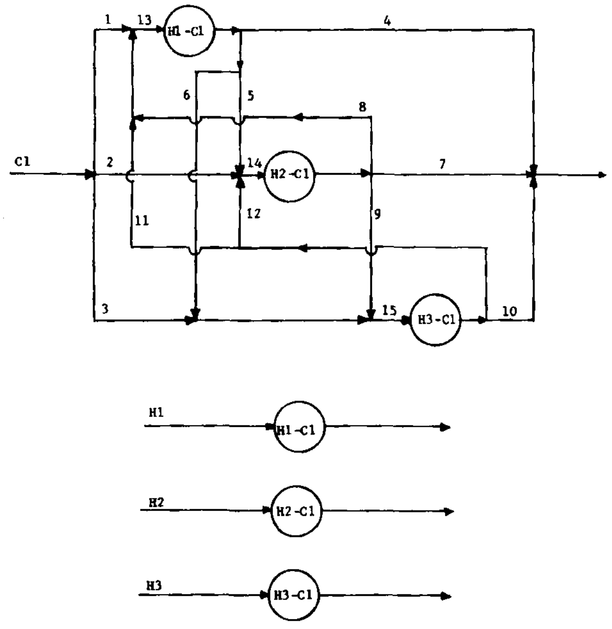

Figure 2. Stream superstructures of *C1, H1, H2, H3.*

since in this case there is no option of splitting the hot streams to another match.

From the superstructure for *C1* shown in Figure 2, the existence of many alternative configurations can be verified by setting the flow rates of some of the internal streams to zero values; for instance, following are several alternatives:

1. The sequence in parallel, *H1-C1, H2-C1, H3-C1,* results from setting $F5 = F6 = F8 = F9 = F11 = F12 = 0$, as shown in Figure 3a.

2. The sequence in series, *H1-C1, H2-C1, H3-C1,* results from setting $F2 = F3 = F4 = F6 = F7 = F8 = F11 = F12 = 0$, as shown in Figure 3b.

3. The mixed sequence of *H1-C1, H2-C1* in parallel and *H3-C1* in series, results from setting $F3 = F4 = F5 = F7 = F8 = F11 = F12 = 0$, as shown in Figure 3c.

4. The mixed sequence of *H1-C1* in series with *H2-C1, H3-C1* in parallel, results from setting $F2 = F3 = F4 = F8 = F9 = F11 = F12 = 0$, as shown in Figure 3d.

5. The previous sequence with a bypass, results from setting $F2 = F3 = F4 = F8 = F11 = F12 = 0$, as shown in Figure 3e.

It is interesting to note that this latter configuration may be required to achieve the objective of minimum number of units as indicated by Wood et al. (1985).

Therefore, it is clear from the above example that the proposed stream superstructures include all possible configurations for the matches and heat loads determined from the MILP transshipment model. Furthermore, this superstructure for process streams can readily be generalized for any number of matches. In particular, each stream superstructure consists of:

1. An initial splitting point for the inlet stream.
2. Splitters at the outlet of each exchanger that are directed to the inlets of other exchangers.
3. Mixers at the inlet of each exchanger.
4. A final mixing point for the outlet stream.

To derive a stream superstructure of a given hot or cold utility stream, it is more convenient to represent a utility stream by a number of separate streams that is equal to the number of matches in which the original utility stream participates. For example, if stream S matches with the cold streams *C1* and *C2*, then S can be decomposed into two streams: *S1* for the match with *C1*, and *S2* for the match with C2. Thus, a stream superstructure of a utility will simply be that of one match where the utility stream will have the heat load predicted for this match by the MILP transshipment model, with inlet and outlet temperatures of the given utility. The basic motivation behind this representation is that utility streams involved in several matches must be split anyhow; furthermore, this scheme provides a much simpler representation of the stream superstructure for each utility.

In summary, the procedure for the derivation of the total superstructure for the given set of matches in a particular subnetwork is as follows:

1. Derive for each process stream a process stream superstructure according to the following rules:

(a) Split each process stream into a number of streams equal to the number of matches in which this process stream participates. Each split branch contains an exchanger related to the given match.

(b) Split the output stream of a match (i.e., exchanger) into recycle streams that are fed to the mixers before the remaining matches, and into one additional stream that is fed to the final mixer for the outlet stream.

2. Derive for each utility stream a utility stream superstructure that consists of one match where the inlet and outlet temperatures of the utility stream are those provided by the initial data.

3. Define as the total superstructure for the particular sub-

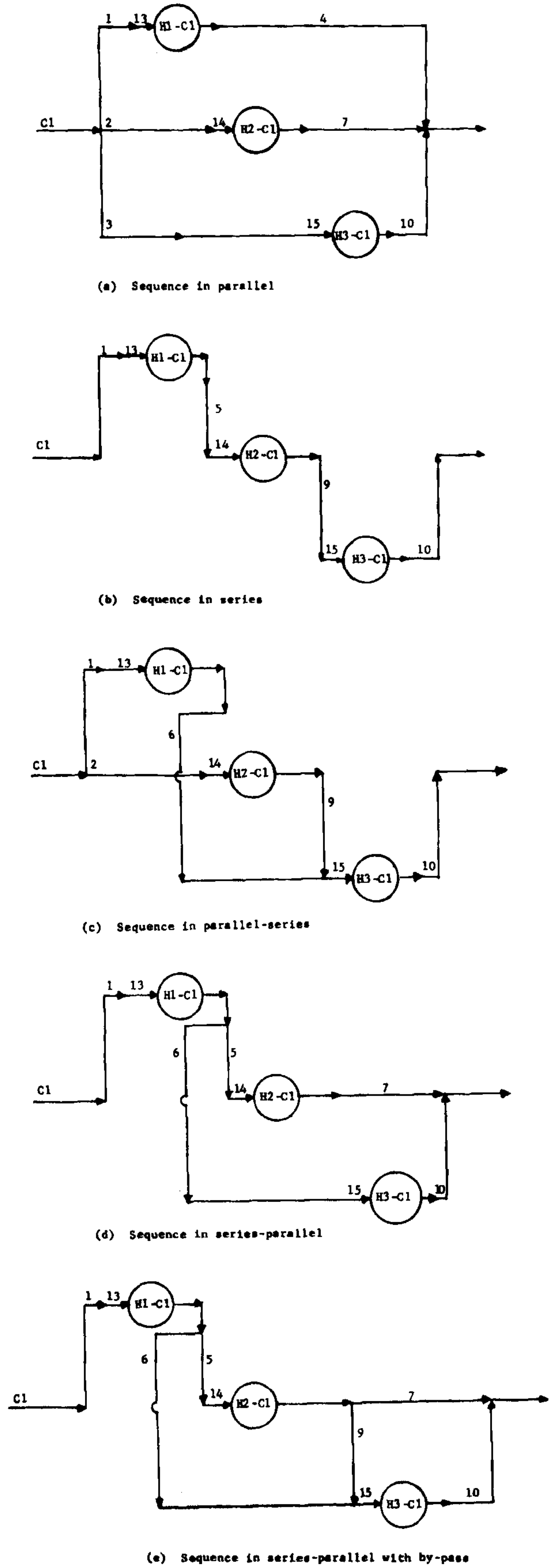

Figure 3. Alternative sequences in the superstructure of C1.

network the aggregate of all process stream and utility stream superstructures. The heat loads in the exchangers of this superstructure are given by the heat exchange predicted for each match by the MILP transshipment model.

It is interesting to note that the proposed superstructure can be interpreted as a "restricted" superstructure in which the exchangers correspond to the matches predicted by the MILP transshipment model, while the stream interconnections are treated as unknowns. In principle the superstructure could be postulated so as to have also the exchangers (matches) as unknown. However, such a general superstructure would result in a problem of very large size. As will be shown, the major advantage of the superstructure proposed in this paper is that it can be formulated as a nonlinear programming problem of manageable size for extracting a network configuration with minimum investment cost. Furthermore, as will be discussed later in the paper, a feasible network structure can always be derived with this procedure.

NONLINEAR PROGRAMMING FORMULATION

Having addressed the problem of deriving a superstructure that has embedded the different configurations for each subnetwork, a nonlinear programming (NLP) formulation is presented for the automatic generation of network structures with minimum investment cost. To simplify the notation in this paper no index will be assigned for identifying the subnetworks.

The available information to derive the NLP formulation for each subnetwork comes from solving the LP and MILP transshipment models, and involves the following items:

Stream Data. For every hot process stream $i \in H$ and cold process stream $j \in C$, the flowrates are given. The inlet and outlet temperatures are defined by the temperature range of the subnetworks. The flow rates and the temperatures will be denoted as F_i, T_i^{IN}, T_i^{OUT} for the hot streams, and F_j, T_j^{IN}, T_j^{OUT} for the cold streams.

Utility Data. For every hot utility $i \in HU$ and cold utility $j \in CU$ that is originally postulated, the solution of the LP transshipment model provides the corresponding heat duties. As discussed in the section on the superstructure, individual utility streams are defined from the utility matches predicted by the MILP transshipment model. These utility streams will be denoted for each subnetwork by the index sets HU' (hot utilities) and CU' (cold utilities). Inlet and outlet temperatures for these utilities will be denoted as T_i^{HIN}, T_i^{HOUT}, $i \in HU'$ and T_j^{CIN}, T_j^{COUT}, $j \in CU'$, while the change of specific enthalpies for these utilities will be denoted ΔH_i^H, $i \in HU'$, ΔH_j^C, $j \in CU'$.

Matches. The solution of the MILP transshipment model at a given subnetwork will provide information on the matches that take place for the process streams and utilities. The set of matches will be denoted as:

$$MA = \{(i,j) | \text{hot stream/utility } i \text{ exchanges heat with cold stream/utility } j,\ i \in HT, j \in CT\} \quad (1)$$

where $HT = (H) \cup (HU')$ and $CT = (C) \cup (CU')$. Also, from the MILP transshipment model, information is available on the heat exchanged, Q_{ij}, for each match $(i,j) \in MA$.

Using the above information, a total superstructure is derived for each subnetwork. As discussed in the previous section, this involves the derivation of stream superstructures for each hot stream/utility $i \in HT$, and for each cold stream/tuility $j \in CT$.

In order to derive the mathematical formulation of the nonlinear programming formulation, the following index sets will be defined for characterizing the topology of the superstructure for a particular subnetwork. First, all hot and cold streams, either process streams or utilities, will be denoted by the common index set,

$$HCT = (HT) \cup (CT) = \{k\} \quad (2)$$

The superstructure for each stream $k \in HCT$ involves a set of streams ℓ that will be denoted by the index set $N_k = \{\ell\}$. Each of these streams ℓ, will have associated as variables the heat capacity flowrate f^k_ℓ and the temperature t^k_ℓ.

Also, the superstructure of each stream k, will involve splitters and mixers that will be denoted by the index sets $S_k = \{s\}$, $M_k = \{m\}$ respectively. The splitter $s^\circ \in S_k$ will stand for the initial splitting point in the stream superstructure k, while $m^\circ \in M_k$ will stand for the final mixing point in that stream superstructure. The relation of the sets of splitters and mixers with the internal input and output streams in the stream superstructure k are given by:

$$\left.\begin{array}{l} S^{IN}_k(s) = \{\ell | \ell \in N_k \text{ is an inlet to splitter } s\} \\ S^{OUT}_k(s) = \{\ell | \ell \in N_k \text{ is an outlet from splitter } s\} \end{array}\right\} s \in S_k$$
$$\left.\begin{array}{l} M^{IN}_k(m) = \{m | m \in N_k \text{ is an inlet to mixer } m\} \\ M^{OUT}_k(m) = \{m | m \in N_k \text{ is an outlet from mixer } m\} \end{array}\right\} m \in M_k \quad (3)$$

The set of exchangers that are postulated corresponds to the predicted matches given by the index set MA defined previously. The inlet and outlet streams to each of the postulated exchangers for the matches MA are given by:

$$E^{HIN}_{ij} = \{n | n \in N_i \text{ is the inlet of hot stream } i \text{ to unit } (i,j) \in MA\}$$
$$E^{HOUT}_{ij} = \{p | p \in N_i \text{ is the outlet of hot stream } i \text{ from unit } (i,j) \in MA\}$$
$$E^{CIN}_{ij} = \{q | q \in N_j \text{ is the inlet of cold stream } j \text{ to unit } (i,j) \in MA\}$$
$$E^{COUT}_{ij} = \{r | r \in N_j \text{ is the outlet of cold stream } j \text{ from unit } (i,j) \in MA\} \quad (4)$$

Having defined the index sets and variables that describe the total superstructure for a given subnetwork, the constraints that apply are the following:

Mass Balances for Splitters

$$\sum_{\ell \in S^{IN}_k(s)} f^k_\ell - \sum_{\ell \in S^{OUT}_k(s)} f^k_\ell = 0 \quad s \in S_k \quad k \in HCT \quad (5)$$

Mass Balances for Mixers

$$\sum_{\ell \in M^{IN}_k(m)} f^k_\ell - \sum_{\ell \in M^{OUT}_k(m)} f^k_\ell = 0 \quad m \in M_k \quad k \in HCT \quad (6)$$

Heat Balances for Mixers

$$\sum_{\ell \in M^{IN}_k(m)} f^k_\ell t^k_\ell - \sum_{\ell \in M^{OUT}_k(m)} f^k_\ell t^k_\ell = 0 \quad m \in M_k \quad k \in HCT \quad (7)$$

Heat Balances for Exchangers

$$\left.\begin{array}{l} Q_{ij} - f^i_\ell(t^i_n - t^i_p) = 0 \\ \qquad n \in E^{HIN}_{ij} \quad p \in E^{HOUT}_{ij} \quad i \notin HU' \\ Q_{ij} - f^i_\ell \Delta H^H_i = 0 \\ \qquad n \in E^{HIN}_{ij} \quad p \in E^{HOUT}_{ij} \quad i \in HU' \\ Q_{ij} - f^j_\ell(t^j_q - t^j_r) = 0 \\ \qquad q \in E^{COUT}_{ij} \quad r \in E^{CIN}_{ij} \quad j \notin CU' \\ Q_{ij} - f^j_\ell \Delta H^C_j = 0 \\ \qquad q \in E^{COUT}_{ij} \quad r \in E^{CIN}_{ij} \quad j \in CU' \end{array}\right\} (i,j) \in MA \quad (8)$$

Minimum Temperature Approach Constraints

$$\left.\begin{array}{l} t^i_n - t^j_q \geq \Delta T_{min} \quad n \in E^{HIN}_{ij} \quad q \in E^{COUT}_{ij} \\ t^i_p - t^j_r \geq \Delta T_{min} \quad p \in E^{HOUT}_{ij} \quad r \in E_{ij}{}^{CIN} \end{array}\right\} (i,j) \in MA \quad (9)$$

Specifications for Inlet Heat Capacity Flow Rates

$$f^k_\ell = F_k \quad \ell \in S^{IN}_k(s^\circ) \quad k \in (H) \cup (C) \quad (10)$$

where

$$F_k = \{F_i, i \in H, F_j, j \in C\}$$

Specifications for Inlet and Outlet Temperatures

$$\left.\begin{array}{l} t^k_\ell = T^{IN}_k \quad \ell \in S^{IN}_k(s^\circ) \\ t^k_\ell = T^{OUT}_k \quad \ell \in M^{OUT}_k(m^\circ) \end{array}\right\} k \in HCT \quad (11)$$

where

$$T^{IN}_k = \{T^{IN}_i, i \in H, T^{IN}_j, j \in C, T^{HIN}_i, i \in HU', T^{CIN}_j, j \in CU'\}$$
$$T^{OUT}_k = \{T^{OUT}_i, i \in H, T^{OUT}_j, j \in C, T^{HOUT}_i, i \in HU', T^{COUT}_j, j \in CU'\}$$

Equality of Temperatures for Inlets and Outlets of Splits

$$t^k_\ell = t^k_p \quad \ell \in S^{IN}_k(s), \quad p \in S^{OUT}_k(s) \quad s \in S_k \quad k \in HCT \quad (12)$$

Nonnegativity Constraints

$$f^k_\ell \geq 0 \quad \ell \in N_k \quad k \in HCT \quad (13)$$

Finally, the areas of each exchanger can be expressed in terms of the given heat loads Q_{ij} and the temperatures of the streams, that is

$$A_{ij} = Q_{ij} U^{-1}_{ij} (LMTD)^{-1}_{ij} \quad (14)$$

where U_{ij} is the overall heat transfer coefficient for the match $(i,j) \in MA$ and $(LMTD)_{ij}$ is the log mean temperature difference for the match (i,j).

Thus, the objective function for minimizing the investment cost is given by:

$$\min \sum_{(i,j) \in MA} c_{ij} A^{b_{ij}}_{ij} \quad (15)$$

where c_{ij} and b_{ij} are cost coefficients, and the areas A_{ij} as given by Eq. 14, can be expressed explicitly in terms of temperatures.

In this way, the objective function in Eq. 15 subject to the constraints in Eqs. 5 to 13 defines a nonlinear programming problem in which the variables to be optimized are the heat capacity flow rates f^k_ℓ and the temperatures t^k_ℓ. It is important to note that the heat loads Q_{ij} in Eqs. 8 and 14 are treated as fixed parameter values provided by the solution of the MILP transshipment model. The numerical solution to the NLP problem can be obtained with standard algorithms.

By determining the optimal solution to the NLP problem, the heat exchanger network configuration with minimum investment cost will be obtained automatically for the given subnetwork. The particular configuration will simply be defined by the nonzero flows, which will indicate the required stream interconnections for the heat exchanger units.

REMARKS ON THE NLP FORMULATION

There are two major questions that arise on the validity of the NLP formulation presented in the previous section.

The first question is whether it is always possible to extract from the superstructure a feasible network configuration which has as exchangers the minimum number of matches predicted by the MILP transshipment model. As shown in Appendix A, it is indeed possible to prove the existence of a one-to-one correspondence between the matches predicted by the MILP transshipment model and the units of a feasible network embedded in the proposed superstructure. Hence, the proposed formulation of the NLP problem for the superstructure is always guaranteed to have a feasible solution. This property is extremely important because it provides a sound theoretical basis to the proposed procedure.

The second question that arises is whether enough streams will be deleted in the superstructure to yield a practical network configuration. Clearly, if most of the postulated streams are not deleted (i.e., their flows set to zero), the networks would be rather complicated and of questionable practical value. However, the recycle streams that are directed to the mixing points at the inlet of each exchanger and come from the outlets of other exchangers, will have the tendency to take zero values. More specifically, as shown in Appendix B, increasing the flow in the recycle streams (Figure B1) results in an increase in the objective function. This implies that due to the minimization of the objective function, their flows will be set to zero, unless heat load or temperature constraints prevent this from happening. Therefore, the main implication of this proof is that relatively simple network structures can be expected with this procedure (e.g., series or parallel). This property is clearly very important from a practical point of view.

An important remark on the NLP formulation is that due to the bilinearities of flows and temperatures that are present in the constraints of Eqs. 7 and 8, the problem is in general nonconvex. This implies that the existence of a unique optimal solution cannot be guaranteed. Thus, the solution that is obtained can only be considered as local minimum for the investment cost. This however, should not be a major drawback in practical applications since it is well known that investment cost functions are rather flat (Fisher et al., 1984).

It is important to note that the assumption about the fixed minimum temperature approach can be relaxed by calculating its optimum value. This can be achieved by optimizing the total cost (utility cost and investment cost of the heat exchangers) vs. the minimum temperature approach in an outer loop of the proposed synthesis procedure. This procedure then allows establishing the proper trade-off between investment and utility cost for the class of networks considered in this paper. It should be noted that since the network configuration may change for different values of the minimum temperature approach, the total cost function will in general be nondifferentiable, and hence a direct search procedure (e.g., golden section search) should be used for this optimization. The computational expense for optimizing the minimum temperature approach with this procedure is not very high, as will be shown in example 3.

It must also be pointed out that the assumption of a fixed minimum temperature approach, and fixed heat loads for each match as predicted from the MILP transshipment model, can easily be relaxed in the proposed superstructure. That is, in Eq. 9 of the NLP formulation lower minimum temperature approaches can be specified for each exchanger (even zero values), while the heat loads in Eq. 8 can be treated as variables with the addition of linear constraints to account for the heat content of each stream.

As for the matches predicted for the minimum number of units by the MILP transshipment model, these are not necessarily unique for a given network problem (Papoulias and Grossmann, 1983). However, alternative sets of matches can be generated by either imposing restricted matches in the MILP, or otherwise by successively adding integer constraints to exclude previous sets of matches found by the MILP problem. Different network structures can therefore be generated automatically by solving for each alternative set of matches the corresponding NLP problem.

Finally, to avoid difficulties in the numerical solution of the NLP problem, it is convenient to replace the logarithmic term in Eq. 14 with the approximation proposed by Paterson (1984). Also, when using infeasible path optimization techniques the power function in Eq. 15 can be redefined as a linear function for areas that become smaller than a given tolerance. This linear function must match the nonlinear cost function at the specified tolerance. Since the successful convergence of NLP algorithms is dependent on the starting points, it is obviously desirable to have a good initialization procedure for the variables in the NLP. The initialization procedure presented in the next section usually provides a good initial point in the superstructure.

INITIALIZATION

For the numerical solution of the NLP formulation described in the previous section, it would clearly be desirable to start with a "good" initial guess for deriving the network configuration. This section will describe an initialization procedure for this purpose.

For each subnetwork, the solution of the MILP transshipment model provides the set of matches MA, and the heat exchanged at each match Q_{ij}, $(i,j) \in MA$. Furthermore, for each match it is also known over which temperature intervals each match takes place. Based on this information, the initialization procedure is as follows:

Step 1. For each match $(i,j) \in MA$

(a) Determine the temperature ranges ΔT_i, ΔT_j over which the match takes place for the given pair of streams. These ranges are given by the difference of inlet and outlet temperatures of the streams in those intervals where the heat exchange takes place.

(b) Calculate

$\Phi_i^j = Q_{ij}\, \Delta T_i^{-1}$

$\Phi_j^i = Q_{ij}\, \Delta T_j^{-1}$

(c) If at either end of the match there is a minimum temperature approach $\Delta T_{\min}$, this implies a "limiting match" $(i,j) \in L$. Otherwise, the match corresponds to a "nonlimiting match" $(i,j) \in NL$.

Step 2. Check the following conditions for each hot stream $i \in HT$ and each cold stream $j \in CT$.

(a) If $\sum_{(i,k) \in MA} \Phi_i^k = F_i$, use parallel configuration for stream $i \in HT$.

(b) If $\sum_{(k,j) \in MA} \Phi_j^k = F_j$, use parallel configuration for stream $j \in CT$.

Step 3. For streams $i \in HT$, $j \in CT$ that were not assigned a parallel configuration in step 2, their summation in each stream is greater than the heat capacity flow rate F_i or F_j. This indicates that a bypass stream is needed. For these streams proceed as follows:

(a) For the limiting matches $(i,j) \in L$, use the flow rates Φ_i^j, Φ_j^i calculated in step 1b.

(b) For the remaining nonlimiting matches $(i,j) \in NL$, assign for each match as inlet and outlet temperatures those determined in step 1a and assign at the mixing and splitting points values for the flow rates so as to satisfy the mass balances.

It should be noted that the above initialization procedure might not necessarily yield an initial feasible configuration. However, the described procedure will provide, in general, a good initial point for the numerical solution of the nonlinear programming problem.

COMPUTER IMPLEMENTATION

The automatic synthesis procedure outlined in Figure 1 has been implemented in the computer package MAGNETS (*MA*thematical *G*eneration of heat exchanger *NET*work *S*tructures). This package creates and solves the LP and MILP transshipment models for both the unrestricted and restricted matches, as well as the NLP problem for the superstructure described in this paper. Both the LP and MILP models are solved with the computer code LINDO (Scharge, 1981); to expedite the solution of the MILP problem, a bound that overestimates the minimum number of units is added. The NLP problem is solved with the computer code MINOS (Murtagh and Saunders, 1981) by using analytical derivatives.

The organization of the package MAGNETS, which has been implemented on a DEC-20 system, is shown in Figure 4. A sequence of subprograms written in PASCAL reads the input data, prepares automatically the mathematical formulations of the LP, MILP, and NLP problems, and reports the utility consumption, pinch points, matches, and the final network configuration. This set of PASCAL subprograms communicates with the LINDO and MINOS codes through files in MPS format. In the case of the MINOS code, FORTRAN routines are used for the nonlinear terms in the objective function and the constraints. The coordination for execution of the PASCAL subprograms and of the codes LINDO and MINOS, is performed with a macroprogram written in the command language PCL. With this, the user does not need to be concerned with the transfer of information and execution between subprograms since this is done automatically.

MAGNETS accepts input data interactively, or with free format data files. The user can investigate different networks since the program has several options such as performing minimum utility calculations for different temperature approaches, imposing restricted matches, or having heat exchanger network configurations derived automatically.

In order to illustrate the use of MAGNETS, and in particular the NLP method described in this paper for automatic generation of network configurations, three examples will be considered.

EXAMPLE 1

The first example deals with a small problem to show that the method has the capability of handling unusual cases. The problem consists of one hot stream, two cold streams, one hot and one cold utility. The data are shown in Table 1. Assuming a minimum temperature approach of 10 K and solving the LP transshipment model for the minimum utility cost with MAGNETS, it is found that neither hot or cold utilities are required and that there is no pinch point. Solving the MILP transshipment model for the minimum number of matches results in the two matches shown in Table 2.

In the next step, the stream superstructures are derived automatically with MAGNETS; they are shown in Figure 5. The overall heat transfer coefficients and cost data for the two exchangers are shown in Table 3; the resulting nonlinear problem has twelve variables, five nonlinear constraints, and nine linear constraints. The total CPU time (DEC-20), for solving the LP and MILP models, deriving the overall superstructure, and solving the nonlinear optimization problem with MAGNETS was 6.5 s.

The results of the optimization problem provide the minimum cost configuration shown in Figure 6. This structure features an investment cost of 42,180 \$/yr, and the corresponding areas of the heat exchangers are shown in Table 3. Notice that this structure involves a special bypass from the outlet of the exchanger *H1-C1* to the inlet of the exchanger *H1-C2*. The reason this bypass was introduced is that there is no feasible network with only two units if the conventional arrangements are used; namely, matches in sequence with no splitting, or when *H1* is split into two parallel branches. Therefore, this example shows that the proposed method can automatically generate these unusual structures with bypass if this is required for a feasible network. This is an important capability which is currently not available in other automatic synthesis methods.

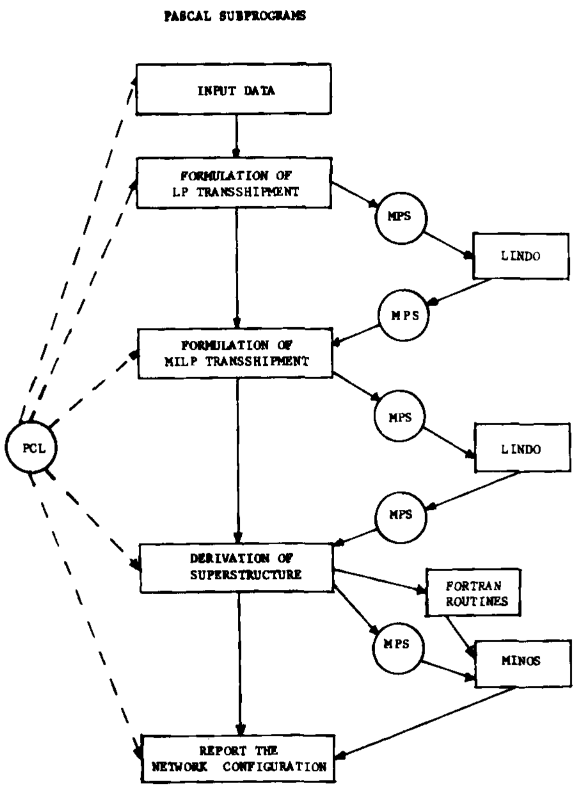

Figure 4. Structure of the computer program MAGNETS.

EXAMPLE 2

This example problem, which is taken from Duran and Grossmann (1986), consists of three hot streams, three cold streams, one hot and one cold utility. The problem data are shown in Table 4. According to the suggested systematic procedure, the temperature range is partitioned into temperature intervals using the inlet temperatures of the streams and a minimum temperature approach of 15 K. Solving the LP transshipment

TABLE 1. DATA FOR EXAMPLE 1

Stream	Fc_p, kW/K	T_{in}, K	T_{out}, K
H1	22	440	350
C1	20	349	430
C2	7.5	320	368
CW		300	320
S		500	500

TABLE 2. MATCHES AND HEAT EXCHANGED FOR EXAMPLE 1

Match *H1-C1*, $Q11 = 1{,}620$ kW
Match *H1-C2*, $Q12 = 360$ kW

TABLE 3. OVERALL HEAT TRANSFER COEFFICIENTS AND COST DATA FOR EXAMPLE 1

Match	U_{ij}, kW/m²·K	A_{ij}, m²
H1-C1	1.0	162
H1-C2	0.5	56.717

$C_{ij} = 1{,}300 A_{ij}^{0.6}$ \$/yr; $A = m^2$.

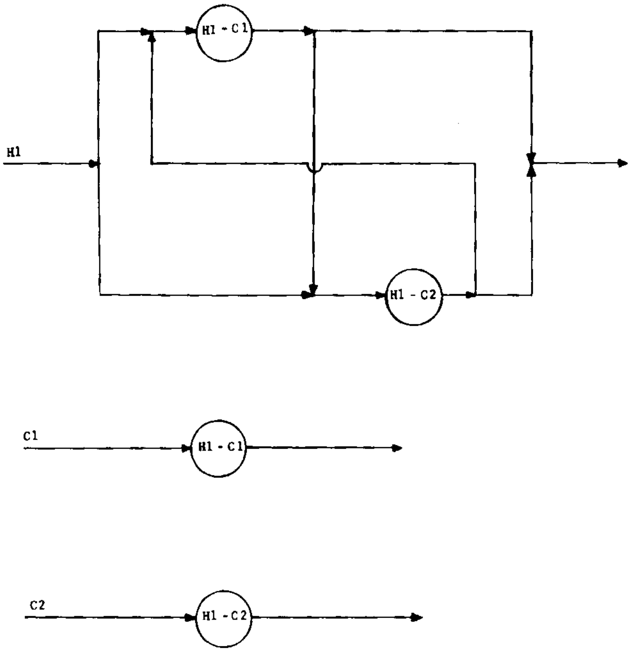

Figure 5. Stream superstructures for example 1.

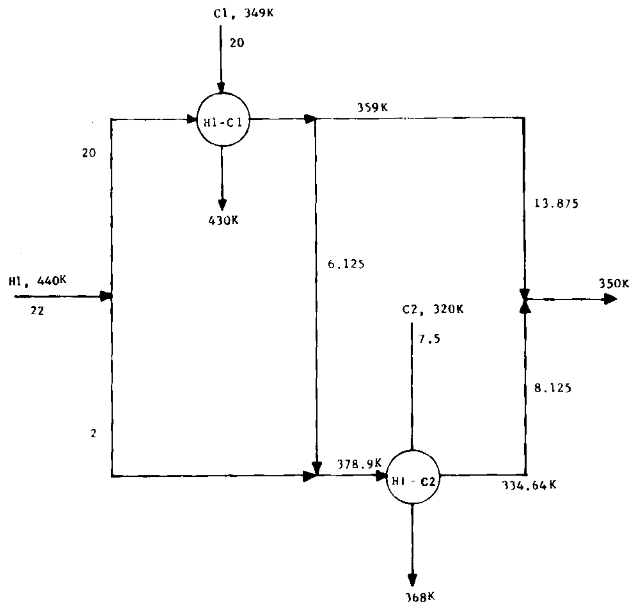

Figure 6. Network structure for example 1.

TABLE 4. DATA FOR EXAMPLE 2

Stream	Fc_p, kW/K	T_{in}, K	T_{out}, K
H1	111.844	502.65	347.41
H2	367.577	347.41	320.00
H3	29.7341	405.48	310.00
C1	9.236	320.00	670.00
C2	112.994	368.72	450.00
C3	107.698	320.00	402.76
CW		295.00	325.00
F		700.00	700.00

problem for the minimum utility cost with MAGNETS, the following results are obtained:

- QS = 1,684.19 kW
- QW = 10,631.3 kW
- Pinch at 502.65 – 487.65 K
- Pinch at 383.72 – 368.72 K

Since there are two pinch points, the synthesis problem is decomposed into three subnetworks, one above the first pinch, one between the two pinch points, and one below the second pinch, that is:

- Subnetwork 1: above the first pinch at 502.65 – 487.65 K
- Subnetwork 2: between the two pinch points
- Subnetwork 3: below the second pinch at 383.72 – 368.72 K

Solving the MILP transshipment problem for each subnetwork with MAGNETS yields the ten matches shown in Table 5. At this point information about the matches and the heat which is exchanged at each match is available. Note that for subnet-

TABLE 5. MATCHES AND HEAT EXCHANGED AT EACH SUBNETWORK FOR EXAMPLE 2

Subnetwork 1:	Match *F-C1*, $QF1$ = 1,684.19 kW
Subnetwork 2:	Match *H1-C1*, $Q11$ = 1,098.437 kW
	Match *H1-C2*, $Q12$ = 8,537.148 kW
	Match *H1-C3*, $Q13$ = 3,666.04 kW
	Match *H3-C2*, $Q32$ = 647.011 kW
Subnetwork 3:	Match *H1-C3*, $Q13$ = 4,061.055 kW
	Match *H2-C3*, $Q23$ = 1,185.991 kW
	Match *H3-C1*, $Q31$ = 449.978 kW
	Match *H2-CW*, $Q2W$ = 8,889.3 kW
	Match *H3-CW*, $Q3W$ = 1,742 kW

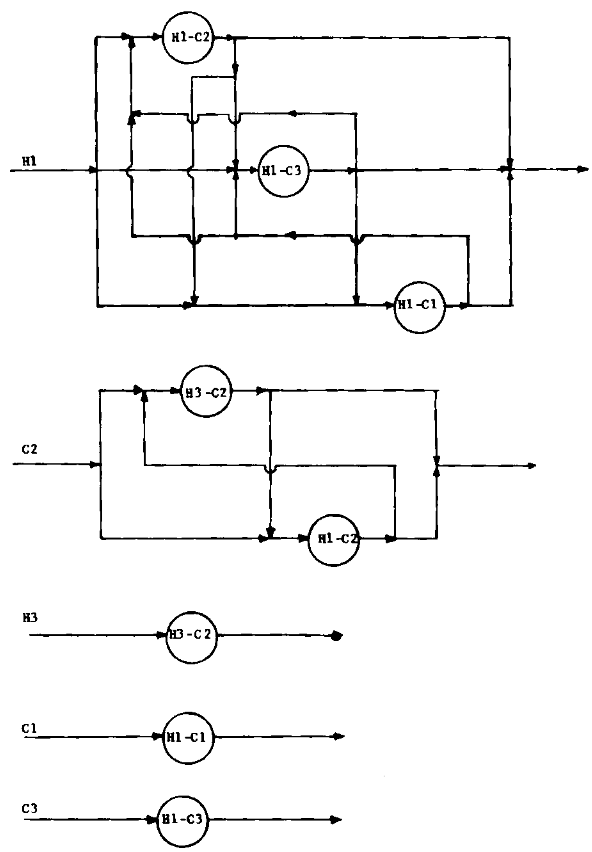

Figure 7. Stream superstructures of subnetwork 2 for example 2.

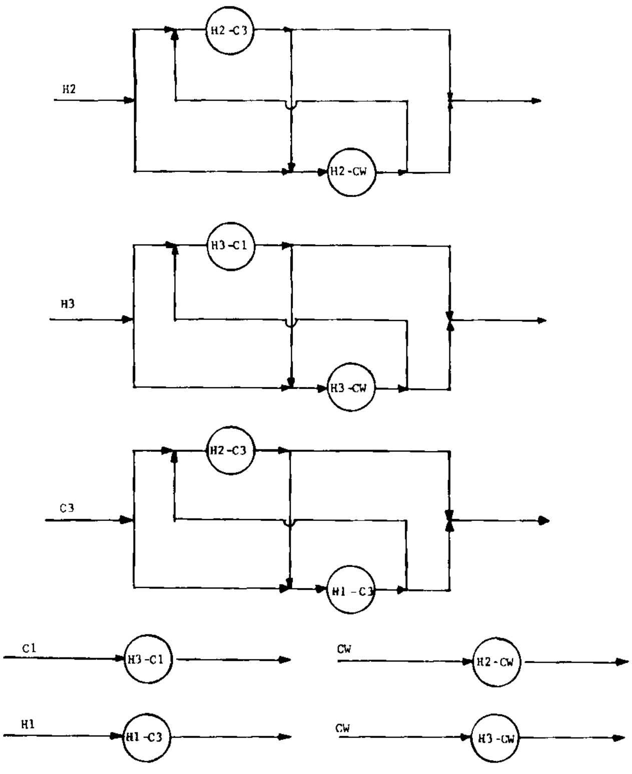

Figure 8. Stream superstructures of subnetwork 3 for example 2.

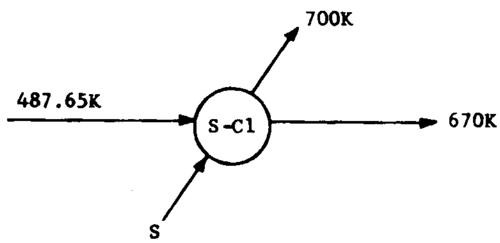

Figure 9. Structure of subnetwork 1 for example 2.

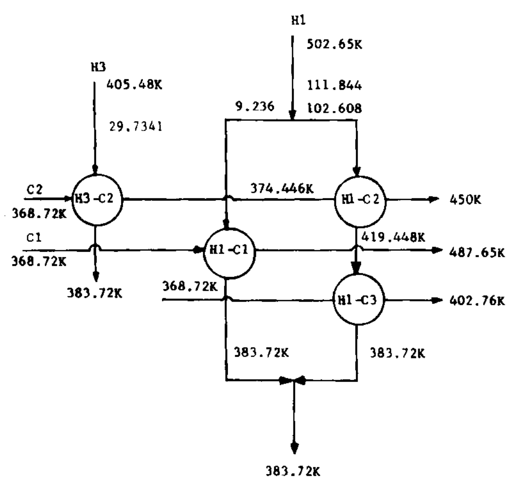

Figure 10. Structure of subnetwork 2 for example 2.

work 1 there is only one match. In the next step the stream superstructures of subnetworks 2 and 3 are derived; they are shown in Figures 7 and 8, respectively. Having obtained the stream superstructures for each subnetwork, mass balances, energy balances, and feasibility constraints, as well as specification constraints are applied to derive the nonlinear programming problem. Using the values for the overall heat transfer coefficients and the cost data shown in Table 6, the resulting nonlinear minimization problem is then solved for each subnetwork. Since subnetwork 1 has only one match, there is no need to solve the NLP problem. The NLP problem for subnetwork 2 has 33 variables, 12 nonlinear constraints, and 14 linear constraints. The NLP problem for subnetwork 3 consists of 36 variables, 15 nonlinear constraints, and 15 linear constraints. The total CPU time (DEC-20), for solving the LP and MILP transshipment models, deriving the overall superstructure, and solving the nonlinear optimization problems for subnetworks 2 and 3 was 35 s.

The results of the optimization problems provide the configurations shown in Figures 9, 10, and 11. By simply combining the configurations of the three subnetworks, a minimum investment cost configuration for the heat exchanger network is obtained as shown in Figure 12. This configuration features a minimum investment cost of 377,900 \$/yr and minimum utility cost of 347,800 \$/yr. The required areas of the heat exchangers are shown in Table 6.

As can be seen with this example problem, the proposed procedure has the capability of automatically synthesizing network configurations that involve stream splitting and multiple pinch points. It is interesting to note that networks involving multiple pinches are often difficult to derive manually. The reason is that the temperatures of matches in the intermediate subnetworks (which exhibit pinches at both ends of the temperature range) must be greatly constrained to avoid minimum temperature approach violations.

EXAMPLE 3

This example problem, which is taken from Papoulias and Grossmann (1983), consists of six hot streams, one cold stream, one hot and one cold utility. The problem data are shown in Table 7. In this example a network configuration featuring the optimum minimum temperature approach was automatically synthesized.

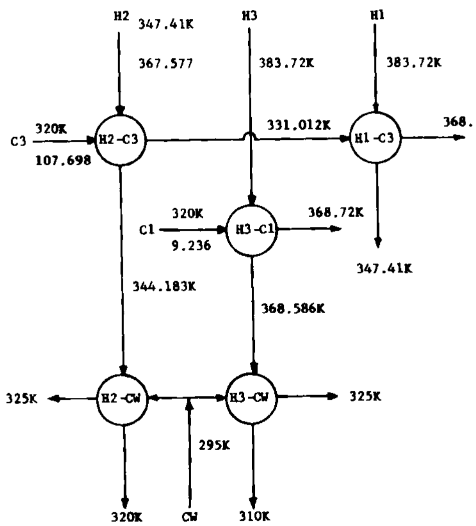

Figure 11. Structure of subnetwork 3 for example 2.

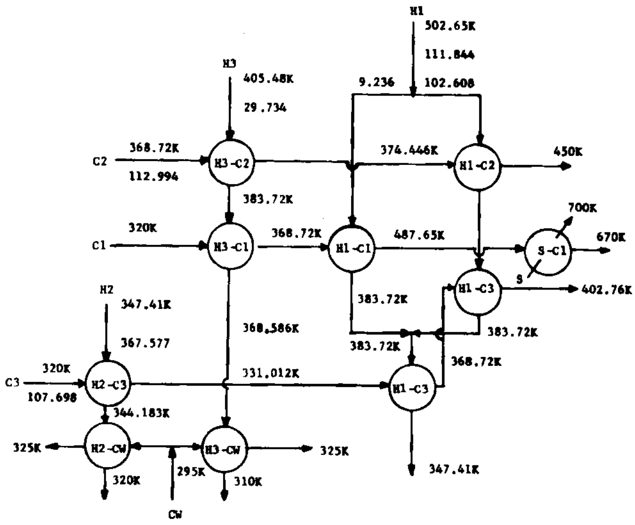

Figure 12. Network structure of example 2.

TABLE 6. OVERALL HEAT TRANSFER COEFFICIENTS AND COST DATA FOR EXAMPLE 2

Match	U_{ij}[(kW)/(m²)(K)]	A_{ij}[m²]
F-C1	—	—
H1-C1	0.22714	322.5
H1-C2	0.27256	643.5
H1-C3	0.3975	583.
H3-C2	0.22714	129.15
H1-C3	0.3975	651.25
H2-C3	0.51106	77.45
H3-C1	0.1947	80.86
H2-CW	0.75714	407.87
H3-CW	0.37856	171.715

Cost of furnace = $0.45754Q^{0.7}$ \$/yr, Q = W
$C_{ij} = 1{,}300A_{ij}^{0.6}$ \$/yr, A = m²
Fuel cost = 174.022 \$/kWyr
Cooling water cost = 5.149 \$/kWyr

TABLE 7. DATA FOR EXAMPLE 3

Stream	Fc_p, kW/K	T_{in}, K	T_{out}, K
C1	24.795	288.888	650.000
H1	7.913	630.555	338.888
H2	5.803	583.333	505.555
H3	2.374	555.555	319.444
H4	31.652	494.444	447.222
H5	6.3305	477.777	311.111
H6	65.943	422.222	383.333
CW	—	300.000	333.333
F	—	700.000	700.000

The optimization of the minimum temperature approach was performed applying the golden section search method in an outer loop of the proposed synthesis procedure. For every iteration in which a value for the minimum temperature approach was assumed, a LP, MILP, and NLP calculation was performed with MAGNETS. In a total of eight iterations the optimum minimum temperature approach was found to be 6.38 K, as indicated in Table 8. For each of these iterations the same network configuration was obtained. Note that in this problem the total annual cost is not very sensitive to the minimum temperature approach as shown in Table 8. The total CPU time (DEC-20) required for this optimization was 240 s.

TABLE 8. OPTIMIZATION OF ΔT_{min} FOR EXAMPLE 3

ΔT_{min} K	Utility Cost \$/yr	Investment Cost \$/yr	Total Cost \$/yr
11.11	436,900	217,650	654,550
8.88	427,000	223,300	650,300
7.77	422,100	226,300	648,400
6.94	418,400	229,150	647,550
6.66	417,200	230,100	647,300
6.38	415,950	231,100	647,050
6.11	414,730	233,020	647,750
5.55	412,270	241,130	653,400

TABLE 9. MATCHES AND HEAT EXCHANGED AT EACH SUBNETWORK FOR EXAMPLE 3

Subnetwork 1:	Match *F-C1*, $QF1$ = 2,341.84 kW
	Match *H1-C1*, $Q11$ = 1,077.07 kW
	Match *H2-C1*, $Q21$ = 451.34 kW
	Match *H3-C1*, $Q31$ = 145.07 kW
Subnetwork 2:	Match *H6-C1*, $Q61$ = 2,564.45 kW
	Match *H1-C1*, $Q11$ = 463.65 kW
	Match *H3-C1*, $Q31$ = 415.44 kW
	Match *H4-C1*, $Q41$ = 1,494.7 kW
	Match *H1-CW*, $Q1W$ = 767.28 kW
	Match *H5-CW*, $Q5W$ = 1,055.08 kW

For the optimum minimum temperature approach (6.38 K) the solution of the LP transshipment model provided the following results for the minimum utility cost:

- QS = 2,341.84 kW
- QW = 1,822.36 kW
- Pinch at 494.44–488.06 K

Since there is a pinch point, the synthesis problem was decomposed into two subnetworks, one above and one below the pinch:

- Subnetwork 1: above the pinch at 494.44–488.06 K
- Subnetwork 2: below the pinch at 494.44–488.06 K

Solving the MILP transshipment problem for each subnetwork yields the ten matches shown in Table 9. The stream superstructures of subnetworks 1 and 2 for the predicted matches in this table are shown in Figures 13 and 14 respectively. The values of the overall heat transfer coefficients and the cost data are shown in Table 10. The nonlinear minimization problem that was solved with MAGNETS provided the configuration shown in Figure 15. This configuration features a total annual cost of 647,050 \$/yr (utility cost 415,950 \$/yr, investment cost 231,100 \$/yr). The areas of the exchangers are shown in Table 10.

This example shows that due to the efficiency of the proposed automatic synthesis procedure, it is possible to perform the rigorous optimization of the minimum temperature approach with reasonable computational effort.

ACKNOWLEDGMENT

The authors would like to acknowledge financial support from the National Science Foundation under grant CPE-8315237, and from Dravo Corporation.

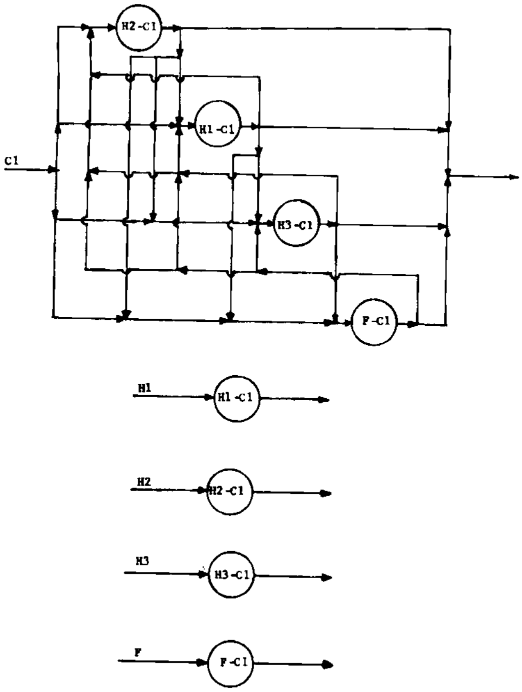

Figure 13. Stream superstructures of subnetwork 1 for example 3.

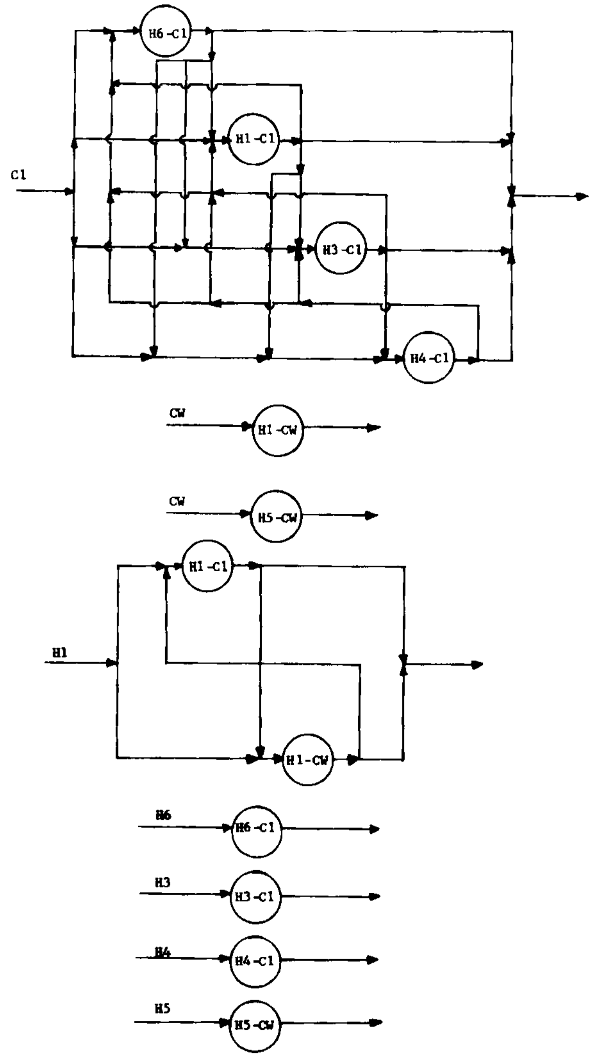

Figure 14. Stream superstructures of subnetwork 2 for example 3.

TABLE 10. OVERALL HEAT TRANSFER COEFFICIENTS AND COST DATA FOR EXAMPLE 3

Match	U_{ij}, kW/m²K	A_{ij}, m²
H1-C1	0.567	56.8
H2-C1	0.397	36.2
H3-C1	0.341	23.5
H6-C1	0.312	183.6
H1-C1	0.567	11.4
H3-C1	0.341	27.8
H4-C1	0.398	195.4
H1-CW	0.454	27.4
H5-CW	0.227	89.2

Cost of furnace = $0.4574Q^{0.7}$ \$/yr, Q = W
$C_{ij} = 1{,}300A_{ij}^{0.6}$ \$/yr, A = m²
Fuel cost = 174.022 \$/kWyr
Cooling water cost = 4.634 \$/kWyr

NOTATION

A_{ij} = area of heat exchanger
b_{ij} = cost exponent
c_{ij} = cost coefficient
C = set of cold process streams
CU = set of cold utilities
CT = set of cold process streams and cold utilities
E_{ij} = index set of exchangers
f = variable heat capacity flow rate
F = heat capacity flow rate
H = set of hot process streams
HU = set of hot utilities
HT = set of hot process streams and hot utilities
HCT = set of all streams and utilities
i = index for hot process stream
j = index for cold process stream
k = index for stream superstructure
ℓ = index for streams
L = set of limiting matches
$LMTD$ = log mean temperature difference
m = index for a mixer
M_k = index set of mixers
MA = set of matches (i, j)
n = index for inlet of hot stream
N_k = set of streams which belong to a stream superstructure
NL = set of nonlimiting matches
p = index for outlet of hot stream
q = index for inlet of cold stream
Q_{ij} = heat exchanged between hot i and cold j
QS = hot utility requirement
QW = cold utility requirement
r = index for outlet of cold stream
s = index for a splitter
S_k = index set of splitters
t = variable temperature
T = temperature
U_{ij} = overall heat transfer coefficient

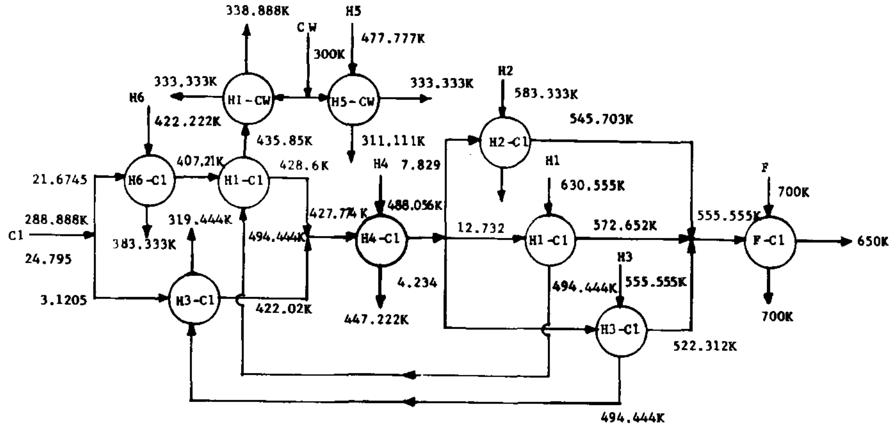

Figure 15. Network structure of example 3.

Greek Letters

ΔH^H = specific enthalpy of hot utility
ΔH^C = specific enthalpy of cold utility
ΔT_{min} = minimum temperature approach

APPENDIX A

Proposition 1. The minimum set of matches predicted by the MILP transshipment model for a given set of hot and cold process streams corresponds to a feasible heat exchanger network in the proposed superstructure.

Proof. Assume that there is no feasible network in which the characteristic of number of units is equal to the number of the predicted matches. This implies that there exists at least one match with temperature violations in one unit of the proposed superstructure. This, in turn, would imply that this match requires two or more units for feasible heat exchange.

Suppose that two units are needed for a given match that requires a fixed amount of heat exchange. The corresponding temperatures of the hot and the cold streams range within ($T1$, $T2$), and ($t1$, $t2$), respectively, while their flowrates are given by F and f, respectively. The superstructures of the hot and cold stream, which include the possible alternatives, are shown in Figure A1. Since heat exchange in this configuration is feasible, the following set of minimum temperature approach constraints are satisfied:

$$\text{HE1: } T1'' - t1' \geq \Delta T_{min} \Rightarrow T1'' - t1' = \Delta T_{min} + x,\ x \geq 0 \quad \text{(A1)}$$

$$T1' - t1'' \geq \Delta T_{min} \Rightarrow T1' - t1'' = \Delta T_{min} + y,\ y \geq 0 \quad \text{(A2)}$$

$$\text{HE2: } T2'' - t2' \geq \Delta T_{min} \Rightarrow T2'' - t2' = \Delta T_{min} + w,\ w \geq 0 \quad \text{(A3)}$$

$$T2' - t2'' \geq \Delta T_{min} \Rightarrow T2' - t2'' = \Delta T_{min} + z,\ z \geq 0 \quad \text{(A4)}$$

Also, from Figure A1 it is clear that the following constraints are satisfied.

$$\text{HE1: } \quad t1'' \geq t1 \Rightarrow t1'' = t1 + x_1,\ x_1 \geq 0 \quad \text{(A5)}$$

$$\text{HE2: } \quad t2'' \geq t1 \Rightarrow t2'' = t1 + x_2,\ x_2 \geq 0 \quad \text{(A6)}$$

At the final mixing points of the superstructure of the hot and cold stream the following heat balances are applied:

$$f3t1' + f4t2' = ft2 \quad \text{(A7)}$$

$$F3T1' + F4T2' = FT2 \quad \text{(A8)}$$

where

$$f = f3 + f4$$

and

$$F = F3 + F4$$

Using $T2$ from Eq. A8, the difference $T2 - t1$ is:

$$T2 - t1 = \frac{F3}{F}T1' + \frac{F4}{F}T2' - t1$$

Then using the Eqs. A2, A4, A5, and A6, and after algebraic manipulation

$$T2 - t1 = \Delta T_{min} + \frac{F3y + F4z}{F} + \frac{F3x1 + F4x2}{F} \quad \text{(A9)}$$

Since the two ratios on the righthand side of (A9) are positive, this implies that:

$$T2 - t1 \geq \Delta T_{min} \quad \text{(A10)}$$

Using a similar reasoning it can be established that:

$$T1 - t2 \geq \Delta T_{min} \quad \text{(A11)}$$

But Eqs. A10 and A11 imply that the match can take place in one single unit without violating temperature constraints.

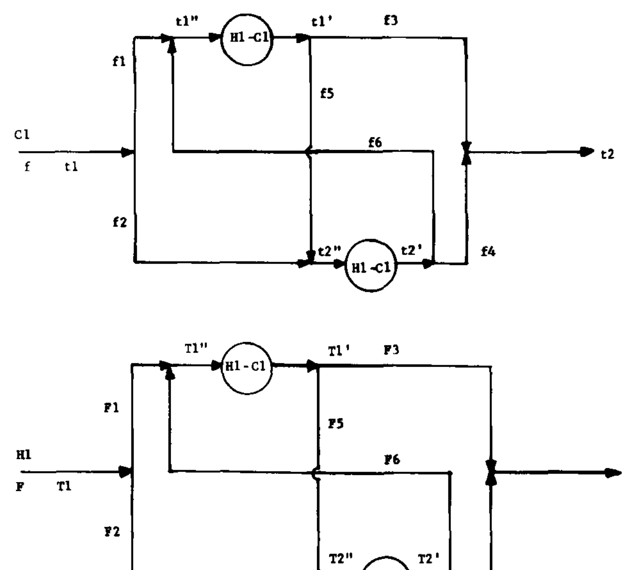

Figure A1. Stream superstructures of *C1, H1*.

Thus, this contradicts the assumption that two units are required for this match, and therefore it also contradicts the assumption that there is no feasible network with the characteristic of minimum number of units equal to the predicted number of matches.

APPENDIX B

In this appendix it will be shown that there exist a wide range of nonzero flows in the recycle streams of the stream superstructures that will result in larger exchanger areas and hence larger investment cost. The proof will be restricted to a stream superstructure of one cold stream and two hot streams as shown in Figure B1. In this figure, fractions denoted as α, β_1, β_2, have been assigned to each splitting point and the recycle streams are indicated as F_1^R, F_2^R for heat exchangers 1 and 2, respectively.

Proposition 2. There exists a finite range for the split fraction, α, shown in Figure B1, for which the areas increase monotonically with any increase of the split fractions β_1, β_2 in the range [0, 1].

Proof. To prove the above proposition it is sufficient to prove that any increase in β_1 or β_2 will imply a decrease in the log mean temperature difference of heat exchanger 1, $(LMTD)_1$, for a finite range of the split fraction α. To express this statement mathematically, it has to be proved that:

$$\frac{\partial(LMTD)_1}{\partial\beta_1} < 0 \tag{B1}$$

$$\frac{\partial(LMTD)_1}{\partial\beta_2} < 0 \tag{B2}$$

$$\text{for } \beta_1, \beta_2 \in [0, 1].$$

For the superstructure of *C1*, shown in Figure B1, the following mass balances are applied at the splitting and mixing points:

$$\begin{aligned} F_1 &= \alpha F_0 \qquad 0 \le \alpha \le 1 \\ F_2 &= (1-\alpha)F_0 \\ F_1^R &= \beta_1 F_1^e \quad 0 \le \beta_1 \le 1 \\ F_2^R &= \beta_2 F_2^e \quad 0 \le \beta_2 \le 1 \end{aligned} \tag{B3}$$

$$\begin{aligned} F_1^e &= \alpha F_0 + \beta_2 F_2^e \\ F_2^e &= (1-\alpha)F_0 + \beta_1 F_1^e \end{aligned} \tag{B4}$$

where F_0 is the total flow rate of *C1* and F_1^e, F_2^e are the flow rates of exchangers 1 and 2, respectively. Solving the system of Eq. B4 for F_1^e, F_2^e, the following expressions are obtained:

$$\begin{aligned} F_1^e &= \frac{\alpha + \beta_2(1-\alpha)}{1-\beta_1\beta_2} F_0 \\ F_2^e &= \frac{\beta_1\alpha + (1-\alpha)}{1-\beta_1\beta_2} F_0 \end{aligned} \tag{B5}$$

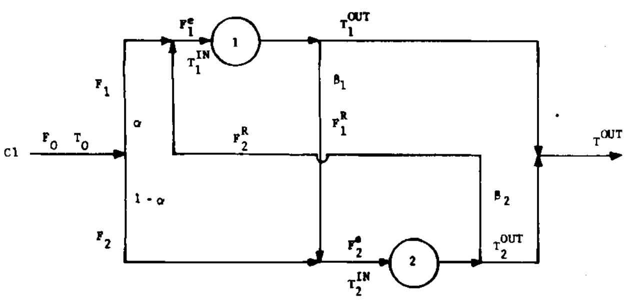

Figure B1. Stream superstructure of *C1*.

Applying energy balances at the heat exchangers as well as at the two mixing points before the heat exchangers, the following equations are derived:

$$\begin{aligned} Q_1 &= F_1^e(T_1^{out} - T_1^{in}) \\ Q_2 &= F_2^e(T_2^{out} - T_2^{in}) \\ F_1^e T_1^{in} &= \alpha F_0 T_0 + \beta_2 F_2^e T_2^{out} \\ F_2^e T_2^{in} &= (1-\alpha)F_0 T_0 + \beta_1 F_1^e T_1^{out} \end{aligned} \tag{B6}$$

where T_1^{out}, T_1^{in} stand for the outlet and inlet temperature of heat exchanger 1, while T_2^{out}, T_2^{in} represent the outlet and inlet temperature of heat exchanger 2. Q_1, Q_2 are the loads of exchangers 1 and 2, respectively. Substituting in Eq. B6 the expressions of Eq. B5 for F_1^e, F_2^e and solving for T_1^{out}, T_1^{in}, expressions of T_1^{out}, T_1^{in} are obtained as functions of F_0, T_0, Q_1, Q_2, α, β_1, β_2 as follows:

$$\begin{aligned} T_1^{out} &= T_0 + \frac{Q_1 + \beta_2 Q_2}{F_0[\alpha + \beta_2(1-\alpha)]} \\ T_1^{in} &= T_0 + \frac{\beta_2(\beta_1 Q_1 + Q_2)}{F_0[\alpha + \beta_2(1-\alpha)]} \end{aligned} \tag{B7}$$

Assuming that the temperature differences at both ends of the heat exchangers satisfy the ΔT_{min} criterion, the log mean temperature difference at exchanger 1 can be expressed as:

$$\begin{aligned} (LMTD)_1 &= \frac{A1\text{-}B1}{C} \\ A1 &= A - T_1^{out} \\ B1 &= B - T_1^{in} \\ C &= \ln(A1/B1) \end{aligned} \tag{B8}$$

where *A*, *B* stand for the inlet and outlet temperature of the hot stream in exchanger 1.

Substituting Eqs. B7 and B8 in Eq. B1 implies the following inequality:

$$\omega\{\ln\phi - (\phi - 1)\} < 0 \tag{B9}$$

where

$$\omega = \frac{\beta_2 Q_1}{F_0[\alpha + \beta_2(1-\alpha)]}$$

and

$$\phi = A1/B1$$

If the inequality in Eq. B9 holds, this implies that:

$$f(\phi) = \ln\phi - (\phi - 1) < 0 \tag{B10}$$

Since

$$f(1) = 0 \tag{B11}$$

$$f'(1) = 0 \tag{B12}$$

$$f''(1) < 0 \tag{B13}$$

Eqs. B11–B13 imply that the function $f(\phi)$ has a maximum of zero at $\phi = 1$. Therefore, Eq. B10 holds for every value of ϕ, and hence Eq. B1 holds for every value of $\alpha, \beta_1, \beta_2 \in [0, 1]$.

To prove the inequality in Eq. B2, consider that Eqs. B7 and B8 are substituted in Eq. B2. After some algebraic manipulation the following inequality must hold:

$$f(\phi) = \omega_1 \ln\phi - \omega_2\left[\frac{1}{\phi} - 1\right] - \omega_3(\phi - 1) < 0 \tag{B14}$$

where

$$\omega_1 = Q_1[\beta_1\alpha + (1-\alpha)]$$

$$\omega_2 = \alpha(Q_1 + Q_2) - Q_1$$

$$\omega_3 = \alpha(\beta_1 Q_1 + Q_2)$$

The function $f(\phi)$ exhibits a stationary point at $\phi = 1$, since

$$f(1) = 0 \quad \text{(B15)}$$

$$f'(1) = 0 \quad \text{(B16)}$$

$$f''(1) = -\alpha[(1 + \beta_1)Q_1 + 2Q_2] + Q_1 \quad \text{(B17)}$$

Thus, in order to satisfy Eq. B14, the inequality

$$f''(1) < 0 \quad \text{(B19)}$$

must hold. This implies that:

$$\frac{Q_1}{(1 + \beta_1)Q_1 + 2Q_2} < \alpha < 1 \quad \text{(B20)}$$

Therefore, the inequality in Eq. B2 is satisfied for the finite range of α, given by Eq. B20 and for every $\beta_1, \beta_2 \in [0, 1]$.

In the above proposition it has been shown that for every α, $\beta_2 \in [0, 1]$, any increase of $\beta_1 \in [0, 1]$ (recycle F_1^R) results in a decrease of the $(LMTD)_1$, and hence an increase of the area of exchanger 1, which means an increase of the investment cost. Also, it has been shown that for every $\beta_1 \in [0, 1]$ there is a finite range of the split fraction α for which any increase of $\beta_2 \in [0, 1]$ (recycle F_2^R) results in a decrease of the $(LMTD)_1$ and so an increase of the investment cost. However, as will be shown below, one can expect that the inequality in Eq. B20 will be satisfied for most cases. Rearranging Eq. B20, the following inequality is obtained:

$$Q_1 < \alpha[(1 + \beta_1)Q_1 + 2Q_2] \quad \text{(B21)}$$

Multiplying both sides of Eq. B21 by F_0/F_1F_0 and using Eq. B3 results in:

$$\frac{Q_1}{F_1} < \frac{Q_1 + Q_2}{F_0} + \frac{\beta_1 Q_1 + Q_2}{F_0} \quad \text{(B22)}$$

Notice that since

$$\frac{Q_1}{F_1} = T_1^{out} - T_0$$

$$\frac{Q_1 + Q_2}{F_0} = T^{out} - T_0 \quad \text{(B23)}$$

where T^{out} is the final outlet temperature of *C1*, Eq. B22 can be expressed as:

$$T_1^{out} < T^{out} + \frac{\beta_1 Q_1 + Q_2}{F_0} \quad \text{(B24)}$$

Then, there are two cases:

Case 1. If $T_1^{out} \leq T^{out}$, which can be expected to be the most frequent case, then Eq. B24 holds, and hence Eq. B2 holds for every value of $\alpha, \beta_1, \beta_2 \in [0, 1]$.

Case 2. If $T_1^{out} > T^{out}$, which implies that the outlet of the cold stream of exchanger 1 is overheated, it is not clear whether the term on the right side compensates for the overheating of the outlet of cold stream for exchanger 1. However, Eq. B24 indicates that whenever overheating takes place, in order to obtain minimum investment cost configurations an increase of the split fraction β_1 might be necessary.

REFERENCES

Duran, M. A., and I. E. Grossmann, "Simultaneous Optimization and Heat Integration of Chemical Processes," *AIChE J.* **32,** 123 (1986).

Fisher, W. R., and M. F. Doherty, and J. M. Douglas, "An Evolutionary and Hierarchical Procedure for Optimization of Preliminary Process Designs," Paper 104c, AIChE ann. meet., San Francisco (Nov., 1984).

Flower, J. R. and B. Linnhoff, "A Thermodynamic-Combinatorial Approach for the Design of Optimum Heat Exchanger Networks," *AIChE J.*, **26,** 1 (1980).

Grimes, L. E., M. D. Rychener, and A. W. Westerberg, "The Synthesis and Evolution of Networks of Heat Exchange that Feature the Minimum Number of Units," *Chem. Eng. Comm.*, 14, 339 (1981).

Grossmann, I. E., and R. W. H. Sargent, "Optimum Design of Heat Exchanger Networks," *Computers and Chem. Eng.*, **2,** 1 (1978).

Hama, A., "Computer-Aided Synthesis of Heat Exchanger Networks; An Iterative Approach to Global Optimum Networks," *Proc. 1st U.K. Natl. Heat Transfer Conf.*, Leeds, 567 (July, 1984).

Hohmann, E. C., "Optimum Networks for Heat Exchange," Ph.D. Thesis, Univ. Southern California (1971).

Lee, K. F., A. H. Masso, and D. F. Rudd, "Branch and Bound Synthesis of Integrated Process Designs," *Ind. Eng. Chem. Fund.* **9,** 48 (1970).

Linnhoff, B., and J. R. Flower, "Synthesis of Heat Exchanger Networks. I: Systematic Generation of Energy Optimal Networks," *AIChE J.*, **24,** 633 (1978).

Murtagh, B. A., and M. A. Saunders, "A Projected Lagrangian Algorithm and Its Implementation for Sparse Nonlinear Constraints," Tech. Rpt. SOL 80-1R, Systems Optimization Lab., Dept. Operations Research, Stanford University, Palo Alto (1981).

Nishida, N., Y. A. Liu, and L. Lapidus, "Studies in Chemical Process Design and Synthesis. III: A Simple and Practical Approach to the Optimal Synthesis of Heat Exchanger Networks," *AIChE J.*, **23,** 77 (1977).

Nishida, N., G. Stephanopoulos, and A. W. Westerberg, "Journal Review: Process Synthesis," *AIChE J.*, **27,** 321 (1981).

Papoulias, S. A., and I. E. Grossmann, "A Structural Optimization Approach in Process Synthesis. II: Heat Recovery Networks," *Computers and Chem. Eng.*, **7,** 707 (1983).

Paterson, W. A., "A Replacement for the Logarithmic Mean," *Chem. Eng. Sci.* 39 (11), 1,635 (1984).

Pho, T. K., and L. Lapidus, "Synthesis of Optimal Heat Exchanger Networks by Tree Searching Algorithms," *AIChE J.*, **19,** 1,182 (1973).

Ponton, J. W., and R. A. Donaldson, "A Fast Method for the Synthesis of Optimal Heat Exchanger Networks," *Chem. Eng. Sci.*, **29,** 2,375 (1974).

Scharge, L., *User's Manual of LINDO*, Scientific Press, Palo Alto (1981).

Su, J. L., and R. L. Motard, "Evolutionary Synthesis of Heat Exchanger Networks," *Computers and Chem. Eng.*, **8,** 67 (1984).

Wood, R. M., R. J. Wilcox, and I. E. Grossmann, "A Note on the Minimum Number of Units for Heat Exchanger Network Synthesis, *Chem. Eng. Comm.* (1985).

Manuscript received Nov. 13, 1984, and revision received Apr. 16, 1985.