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**A Simultaneous Optimization Approach  
for Heat Exchanger Network Synthesis**

by

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**A SIMULTANEOUS OPTIMIZATION APPROACH  
FOR HEAT EXCHANGER NETWORK SYNTHESIS**

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## **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 simultaneously. 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 a representation of a series of stages where, within each stage, potential exchanges between each hot and cold stream can occur. A simplifying assumption of using stage temperatures 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, e.g. no stream splits, forbidden matches, required and restricted matches, can be easily included in the model, as well as handling the case of multiple utilities. 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

Over the past two decades, extensive research efforts have made the systematic design of heat exchanger networks (HEN) the most mature field within process synthesis (Gundersen and Naess, 1988). In spite of this fact, there are important limitations that still need to be overcome. In general, current methods rely on decomposing the problem in order to progressively determine targets for synthesizing a network. 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 partitioned 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 programming approach built into the interactive program MAGNETS (Floudas et al., 1986). The design problem is decomposed into three steps. The first two steps involve the solution of the LP and MILP transshipment 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 the solution of an NLP model (Floudas et al., 1986) to determine the optimal network configuration.

The limitation behind these types of sequential decomposition schemes is that the effectiveness of each subsequent step relies heavily on the decisions of all the previous steps. In this way, restrictive assumptions and decisions taken in the initial steps may lead to topology traps. Furthermore, since trade-offs between the different types of cost are not simultaneously considered, sequential design methods may often lead to suboptimal networks. A good detailed discussion of these limitations is given in Gundersen and Grossmann (1988).

Several papers have been published to better relate the different types of costs. Amongst them, Gundersen and Grossmann (1988) introduced the Vertical MILP Transshipment Model to bring in area considerations when determining the minimum number of matches. Colberg and Morari (1989) have proposed an NLP transshipment model to more accurately predict, for a specified set of matches, the minimum area for non-vertical heat transfer and for restricted matches. Ciric and Floudas (1988) developed an MINLP model to simultaneously optimize the selection of process stream matches and the

network configuration 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. Optimization of the model identifies which of the embedded matches are needed to minimize the total investment cost of the exchangers. The use of the hyperstructure was also extended for the retrofit design case (Ciric and Floudas, 1988a).

Ideally, for the HEN design problem, it is desirable to account for all types of costs simultaneously. Dolan et al. (1987, 1989) and Yee and Grossmann (1988) proposed methods to handle such design objectives. Dolan et al. proposed the method of simulated annealing as a synthesis technique, 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 Figure 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, a simple synthesis model is proposed which will account for all the costs simultaneously yet requiring very reasonable computational times. The model is based on a stage-wise superstructure representation which does not require the specification of subnetworks nor the selection of fixed temperature approaches. Based on a simplification for stream splits, 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 number of units and on stream splitting 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, ie. 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 cooled and a set of cold process streams *CP* to be heated. 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 are also 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 least annual cost. The solution defines the network by providing the following:

1. Utilities required (HRAT)
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. Major assumptions in the proposed method include the following:

- Constant heat capacity flow rates
- Constant heat transfer coefficients
- Countercurrent heat exchangers
- Each match corresponds to one exchanger

In the proposed method, no parameters are required to be fixed; ie. 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. However, to simplify the problem, the type of stream splitting will be restricted. As will be discussed later, this restriction simplifies the proposed model significantly and allows for efficient and very reasonable solution times.

## 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. This model has also been extended by Yee et al. (1989) for determining area targets which can account for different heat transfer coefficients as well as trade-off with utility consumption. Furthermore, the model can be used for simultaneous optimization and heat integration in process flowsheets.

The proposed stage-wise superstructure in Figure 2 can be viewed as an extension of the one presented in Grossmann and Sargent (1977) where within each stage, potential exchanges between any pair of hot and cold stream can occur. The superstructure also resembles that of the spaghetti design brought forth by Linnhoff and coworkers, where the network is divided into sections or a series of stages. In the spaghetti design, the number of stages is equal to the number of energy intervals (e.g. see Figure 3). In each section of the composite curve, the corresponding cold streams are matched with the corresponding hot streams in order to obtain vertical heat transfer. As a result, spaghetti designs usually require a large number of exchangers.

In the proposed superstructure, the number of stages does not have to be equal to the number of energy intervals since the temperatures corresponding to each stage will be treated as variables to be optimized. This in fact allows for opportunities for criss-cross heat exchange when streams have different heat transfer coefficients. Furthermore, in using this representation, the determination of a pinch point and the partitioning into subnetworks is not required. In general, the number of stages needed to synthesize a network with the proposed superstructure will seldom be greater than either the number of hot streams  $N_H$  or the number of cold streams  $N_C$ . This is in view of the fact that an optimal design usually does not require a large number of exchangers, meaning that a particular stream does not exchange heat with many streams.

The superstructure for the proposed model is then derived as follows:

1. Fix the number of stages, typically at  $\max(N_H, N_C)$
2. For each stage, the corresponding stream is split and directed to an exchanger for each potential match between each hot stream and each cold stream. The outlet of the exchangers are mixed which then defines the stream for the next stage.
3. The outlet temperatures of each stage are treated as variables.

An example of a superstructure involving two hot and two cold streams is shown in Figure 2. The



two stages are represented by eight exchangers, with four possible matches in each stage. In this case, the temperatures at locations  $i=1$  and  $i=3$  are fixed, while at  $i=2$ , they would be variables ( $t_{m,i}$ ,  $t_{mv}$ ,  $t_{cl,2}$ ,  $t^{\wedge}$ ). Note that alternative parallel and series configurations are embedded as well as possible rematching of streams.

Although in principle, each utility stream can be treated as any other process stream, for simplicity in the presentation, it will be assumed that utility streams will be placed at the end of the sequence of stages. As mentioned previously, an assumption on the type of stream splitting allowed in the proposed superstructure can significantly simplify the model formulation. This restriction is illustrated in Figure 4. The assumption specifies that the outlet temperature of a particular stream at each exchanger of a stage is the same as the outlet temperature of the stage. As shown in Figure 4, for stream H1, the outlet temperature of both exchanger H1-C1 and exchanger H1-C2 at each stage are assumed to be equal. The motivation behind this assumption is that by setting these temperatures to be the same, nonlinear heat balance and heat mixing equations can be eliminated. Only an overall heat balance must be performed within each stage, and furthermore, there is no need to include the flows as variables in the model. As a result, not only is the dimensionality of the problem reduced, but the feasible space of the problem can be defined by a set of *linear* constraints as will be shown in the next section. The nonlinearities are then isolated in the objective function that involve the cost terms for the areas which are expressed in terms of stage temperatures. The model therefore becomes very robust and can be solved with relative ease.

It should be noted that the simplifying assumption on the temperatures for the stream splits 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. In order to partially overcome this limitation, the scheme shown in Figure 5 is proposed. The idea is to use the MINLP model to determine an optimal structure. If this structure involves split streams, then an NLP sub-optimization 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 sub-optimization 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 by-passes. For clarification, these structures are shown in Figure 6. In general, disregarding stream by-passes is not a significant limitation since these are usually not required and more importantly, not favorable. In very particular cases, however, the use of by-passes 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, in some instances, 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 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 such 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 stream splits and their temperatures is presented. Binary variables are introduced to designate the existence of each potential heat exchanger in the superstructure. 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. Also, for simplicity, we assume only one type of hot and one type of cold utility. These two assumptions, though, can be easily relaxed to accommodate cases of multiple utilities with various temperatures.

In order to formulate the proposed MINLP model, the following definitions are necessary:

### (i) Indices

$i$  = hot process or utility stream

$j$  = cold process or utility stream

$k m$  index for stage  $1..JVOK$  and temperature location  $1..JV0AT+1$

(ii) Sets $HP = \{i|i \text{ is a hot process stream}\}$  $HU = \text{hot utility}$  $CP = \{j|j \text{ is a cold process stream}\}$  $CU = \text{cold utility}$  $ST = \{k|k \text{ is a stage in the superstructure, } k=1,..,NOK\}$ (iii) Parameters $TIN = \text{inlet temperature of stream}$  $TOUT = \text{outlet temperature of stream}$  $F = \text{heat capacity flow rate}$  $U = \text{overall heat transfer coefficient}$  $CCU = \text{per unit cost for cold utility}$  $CHU = \text{per unit cost for hot utility}$  $CF = \text{fixed charge for exchangers}$  $C = \text{area cost coefficient}$  $B = \text{exponent for area cost}$  $NOK = \text{total number of stages}$  $\Omega = \text{an upper bound for heat exchange}$  $\Gamma = \text{an upper bound for temperature difference}$ (iv) Variables $dt_{ijk} = \text{temperature approach for match } (i,j) \text{ at temperature location } k$  $dtcu_i = \text{temperature approach for the match of hot stream } i \text{ and cold utility}$  $dthu_j = \text{temperature approach for the match of cold stream } j \text{ and hot utility}$  $q_{ijk} = \text{heat exchanged between hot process stream } i \text{ and cold process stream } j \text{ in stage } k$  $qcu_i = \text{heat exchanged between hot stream } i \text{ and cold utility}$  $qhu_j = \text{heat exchanged between hot utility and cold stream } j$  $t_{i,k} = \text{temperature of hot stream } i \text{ at inlet of stage } k$  $t_{j,k} = \text{temperature of cold stream } j \text{ at outlet of stage } k$  $z_{ijk} = \text{binary variable to denote existence of match } (i,j) \text{ in stage } k$  $zcu_i = \text{binary variable to denote that cold utility exchanges heat with hot stream } i$  $zhu_j = \text{binary variable to denote that hot utility exchanges heat with cold stream } j$ 

With the definitions above, the formulation can now be presented.

### Overall heat balance for each stream

An overall heat balance is needed to ensure sufficient heating or cooling of each process stream. The constraints stated below in (1) are for the case when inlet and target temperatures are given as exact values. The constraints specifies that the overall heat transfer requirement of each stream must equal the sum of the heat it exchanges with other process streams at each stage plus the exchanges with utility streams.

$$\begin{aligned} (T_i^* - TOUT_i) F_i &= \sum_{k \in ST} \sum_{j \in CP} q_{jk} + q_{cu}, & i \in HP \\ (TOUT_j - TIN_j) F_j &= \sum_{k \in ST} \sum_{i \in HP} q_{ik} + q_{cu}, & j \in CP \end{aligned} \quad (1)$$

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.

### Heat balance at each stage

An energy balance is also needed at each stage of the superstructure to determine the temperatures. Note that for a superstructure with  $NOK$  stages,  $NOK+1$  temperatures are involved. This takes into consideration the fact that for two adjacent stages, the outlet temperature of the first stage corresponds to the inlet temperature of the second stage. To properly define the temperature variables and stages, the index  $k$  is used. The set  $k=1..NOK$  is used to represent the  $NOK$  stages of the superstructure, while the set  $k=1..MOK+1$  is used to define the temperature location in the superstructure (see Figure 2). In both cases, stage or temperature location  $k=1$  involves the highest temperatures. With this in mind, the heat balances for each stage are as follows:

$$\begin{aligned} (T_{i,k} - T_{i,k+1}) F_i &= \sum_{j \in CP} q_{jk} - \sum_{k \in ST} q_{ik}, & i \in HP \\ (T_{j,k} - T_{j,k+1}) F_j &= \sum_{i \in HP} q_{ik} - \sum_{k \in ST} q_{jk}, & j \in CP \end{aligned} \quad (2)$$

### Assignment of superstructure Inlet temperatures

Assuming fixed inlet temperatures of the process streams  $\{TIN\}$  these are assigned as the inlet temperatures to the superstructure. For hot streams, this corresponds to temperature location  $k=1$ , and for cold streams, this corresponds to location  $k=NOK+1$ .

$$TIN_i = t_{iX} \quad i \in HP \quad (3)$$

### Feasibility of temperatures

Assuming matches involving one hot and one cold stream, constraints are also needed to specify a monotonic decrease of temperature at each successive stage  $k$ . In addition, a bound is set for the outlet temperature of each stream superstructure at the respective stream's outlet temperature. Note that the outlet temperature of each stream at its last stage does not necessarily correspond to the stream's target temperature since utility exchanges can occur at the outlet of the superstructure.

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

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

$$TOUT_j \geq t_{jX} \quad j \in CP \quad (4)$$

### Hot and cold utility load

Hot ( $q_{hu}$ ) and cold ( $q_{cu}$ ) utility requirements are determined for each process stream in terms of the outlet temperature in the last stage and the target temperature for that stream. The following constraints are for the heat load requirements:

$$\begin{aligned} (TOUT_i - t_{JA}) F_i &= q_{cu_i} & i \in HP \\ (TOUT_j - t_{JA}) F_j &= q_{hu_j} & j \in CP \end{aligned} \quad (5)$$

### Logical constraints

Logical constraints and binary variables are needed to determine the existence of process match (*ij*) in stage *k* and also any match involving utility streams. The binary variables are represented by  $z_{ijk}$  for process stream matches,  $z_{cu}^k$  for matches involving cold utilities, and  $z_{hu}^k$  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:

$$\begin{aligned}
 q_{ijk} - Q z_{ijk} &\leq 0 && ieHP, \quad jeCP, \quad keST \\
 q_{cu}^k - C_l z_{cu}^k &\leq 0 && ieHP \\
 q_{hu}^k - a z_{hu}^k &\leq 0 && jeCP \\
 z_{ijk}, z_{cu}^k, z_{hu}^k &= 0, 1
 \end{aligned} \tag{6}$$

where the corresponding upper bound  $Q$  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  $dt$  be determined. To ensure feasibility in assigning stage temperatures for existing driving forces, the binary variables are used to activate or deactivate the following constraints:

$$\begin{aligned}
 dt_{ijk} &\leq K_{ijk} (T_{ij} - T_{jk}) + T (1 - z_{ijk}) && keST, \quad ieHP, \quad jeCP \\
 dt_{ijk+1} &\leq U_{M|} (T_{i+1} - T_{j+1}) + r (1 - z_{ijk}) && k*ST > i*HF > J*C^p \\
 dt_{cu}^k &\leq t_{iNO}^k - T_{OUT}^{CU} + T (1 - z_{cu}^k) && ieHP \\
 dt_{hu}^k &\leq T_{OUT}^{HU} - t_{jA} + T (1 - z_{hu}^k) && jeCP
 \end{aligned} \tag{7}$$

Note that these constraints can be expressed as inequalities because the cost of the exchangers decreases with higher values for the temperature approaches  $dt$ . Also, the role of the binary variables in the constraints in (7) is to ensure that non-negative driving forces exist for an existing match. When a match (*ij*) occurs in stage *k*,  $z_{ijk}$  equals one and the constraint becomes active so that the approach temperature is properly calculated. However, when the match does not occur,  $z_{ijk}$  becomes zero, and the contribution of the upper bound  $r$  on the right hand side deems the equation inactive. Similar constraints are used for utility exchangers when the outlet temperature of the utility stream,  $T_{OUT}$ , is not strictly

higher (for hot utility) or lower (for cold utilities) than the target temperature of the process stream. Also, in order to avoid infinite areas, small positive lower bounds are specified for the approach temperature variables  $dt$ .

### 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.

$$\begin{aligned}
 & \text{MIN} \sum_{i \in \text{HP}} \text{CCU} \, qcu_i + \sum_{j \in \text{CP}} \text{CHU} \, qhu_j + \\
 & \sum_{i \in \text{HP}} \sum_{j \in \text{CP}} \sum_{k \in \text{ST}} \text{CF}_{ij} \, z_{ijk} + \sum_{i \in \text{HP}} \text{CF}_{i,\text{CU}} \, zcu_i + \\
 & \sum_{j \in \text{CP}} \text{CF}_{\text{HU}j} \, zhu_j + \quad (8) \\
 & \sum_{i \in \text{HP}} \sum_{j \in \text{CP}} \sum_{k \in \text{ST}} C_{ij} \left[ q_{ijk} / (U_{ij} [(dt_{ijk}) (dt_{ijk+1}) (dt_{ijk}+dt_{ijk+1}) / 2]^{1/3}) \right]^{B_{ij}} + \\
 & \sum_{i \in \text{HP}} C_{i,\text{CU}} \left[ qcu_i / (U_{i,\text{CU}} [drcu_i (TOUT_i - TIN_{\text{CU}}) (drcu_i + (TOUT_i - TIN_{\text{CU}})) / 2]^{1/3}) \right]^{B_{i,\text{CU}}} + \\
 & \sum_{j \in \text{CP}} C_{\text{HU}j} \left[ qhu_j / (U_{\text{HU}j} [dthu_j (TIN_{\text{HU}} - TOUT_j) (dthu_j + (TIN_{\text{HU}} - TOUT_j)) / 2]^{1/3}) \right]^{B_{\text{HU}j}}
 \end{aligned}$$

In the last three summation terms in the objective function, the driving force terms are calculated by the following LMTD approximation given by Chen (1987):

$$\text{LMTD} \approx \left[ (dt_1) (dt_2) \frac{dt_1 + dt_2}{2} \right]^{1/3} \quad (9)$$

Approximations to the LMTD term are primarily used to prevent numerical difficulties arising when  $dt_1 = dt_2$ . However, the Chen approximation also has an added advantage compared to other well-known approximations:

$$LMTD \sim \frac{1}{3} \overline{dt} + \frac{1}{3} \epsilon \frac{1}{2} \Delta T \quad \text{Paterson(1984)} \quad (10a)$$

$$LMTD \sim \frac{1}{2} (0.3275 \overline{dt} + dt^{0.3275}) \quad \text{Chen (1987) extending Underwood (1970) (10)}$$

In both of the above equations, the approximation to LMTD predicts a non-zero value when either  $\overline{dt}$  or  $dt$  equals zero. This inaccuracy is avoided using the Chen approximation in equation (9).

The proposed MINLP model for the HEN synthesis problem consist then of minimizing the objective function in (8) subject to the feasible space defined by equations {1) to (7)}. The continuous variables ( $r$ ,  $q_y$ ,  $dt$ ) are non-negative and the discrete variables  $z$  are 0-1. Constraints on stream matches can be easily incorporated into the MINLP formulation by fixing certain binary values or providing bounds on the heat load variables. The number of units can be controlled by adding an integer constraint so that the sum of the all binary variables are fixed or bounded at a particular value. Furthermore, stream splitting can be controlled by limiting the number of matches that can occur at each stage. To represent the case where no splitting is allowed, integer constraints are added to the formulation so that a maximum of one match can exist at each stage for each stream.

$$\sum_j z_{jk} \leq 1 \quad ieHP, \quad keST$$

$$\sum_{j,k} z_{jk} \leq S - 1 \quad jeCP, \quad keST$$

One way of accounting for the cost of splitting stream is to introduce assignment variables into the formulation so that if more than one match exist in a particular stage, the assignment variable becomes positive and a cost is added to the objective value. In this way, there is a corresponding penalty for having splits in the network configuration.

Finally, the proposed MINLP model can be easily extended to handle inlet and outlet temperatures that are specified as inequalities (see case 4 of Example 1). Also, the model can be easily modified to account for "matches between pairs of hot streams or pairs of cold streams (see Example 5).



## REMARKS

The attractive feature of the proposed model is that equations (1) to (7), which define the feasible space, are all linear. This has the effect that when applying a reduced gradient method (e.g. MINOS, Murtagh and Saunders, 1983) to the relaxed NLP (where binary variables are not restricted to integral values) and to the NLP's with fixed 0-1 variables, superlinear convergence will be guaranteed. In addition, there is no need to approximate the feasible region by any type of linearization scheme. In general, as a result of this, the MINLP problem can be solved with reasonable computational time. 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. However, unlike other heat exchanger models which generate configurations, the nonconvex terms appear only in the objective function (Floudas et al., 1986, Ciric and Floudas, 1988, Yee and Grossmann, 1988).

In view of the nature of the MINLP model, the Combined Penalty Function and Outer-Approximation Method by Viswanathan and Grossmann (1989) can be applied to solve the proposed MINLP model. The solution scheme for the method is shown in Figure 7. The initial step involves the solution of the relaxed NLP. If the relaxed NLP is non-integer, 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 terms 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 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 has been developed to ensure a good relaxed NLP solution. The proposed procedure, which relies on an LP approximation of the MINLP, is outlined in Appendix A. 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 annual cost.

## EXAMPLES

### Example 1

Example 1 is from Linnhoff et al. (1982) involving two hot and two cold streams along with steam 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 Figure 8. The corresponding MINLP formulation involves 62 equations and 50 variables of which 9 are binary. Since the cost equation does not have an explicit 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, 9 instead of 12 binary variables are needed. The model was solved by the package DICOPT++ (Viswanathan and Grossmann, 1989) via GAMS (Brooke et al., 1988) using MINOS5.2 (Murtagh and Saunders, 1983) and MPSX (IBM, 1979). Three major iterations were required using a total CPU time of 12.5 seconds on an IBM 3083. The network structure obtained did involve split streams. As a result, a sub-optimization was performed to determine the proper split ratios and temperatures. The final optimal network is shown in Figure 9. This network minimizes the utility to just \$8,000/yr 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 353-358.56K. It is interesting to note that in the proposed network, three of the exchangers (2,3,4) are placed across this pinch and the minimum approach

temperature (EMAT) is just 2.69K.

The problem was also solved with MAGNETS with a fixed HRAT-1 OK. The solution obtained, which is the same as the one reported by Linnhoff et al. (1982), has an annual cost of \$89,832 (see Figure 10), which is 11% higher than the proposed network in Figure 9. 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 (353-363K), six units were required as compared to five for the simultaneous solution. It is interesting to note that for HRAT-1 OK, 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.

#### Case 2: No stream splitting

An important difference between the proposed network of Figure 9 and the MAGNETS network of Figure 10 is that the proposed network requires stream splitting. Since in general, a network with stream splitting is more difficult to operate, it may be desirable to design a network which does not require stream splitting. As mentioned earlier in the paper, a no split network simply corresponds to selecting at most one unit for each stage 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 (11), the MINLP formulation involved 95 equations and 66 variables of which 13 are binary. The optimal solution was obtained in 4 iterations after 15.0 CPU seconds on the IBM 3083. The network is shown in Figure 11 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 appears rather insignificant in view that the two stream splits are now not necessary. Once again, only five units are required and exchangers 2 and 4 are placed across the internal pinch (353-358.56K), and EMAT for the network is just 2.65K.

#### 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 equations, 50 continuous variables and 9 binary variables. The problem was solved in 3 iterations using 16.25 CPU seconds on the IBM 3083. The network, with five units, and an annual cost of \$87,225 is shown in Figure 12. Again, the solution compares well with the one obtained from MAGNETS which requires, for HRAT=10K, 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 m<sup>2</sup> less area. However, due to a different distribution of area in the exchangers and economies of scale ( a 0.6 exponent on the area cost equation), the annual cost required 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 3.55K.

#### 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 413K to a range such that  $373K \leq TOUT_{C2} \leq 413K$ . 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 equations and 41 continuous and 9 binary variables was solved in 12.6 CPU seconds on the IBM 3083 using DICOPT++. As shown by the optimal network in Figure 13, 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 373K. 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 413K is specified. The cost of cooling water appears to be sufficiently cheap so that the cost of capital is more

significant. Hence, the network 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 \$3,000/yr as compared to the network of case 1 where the target temperature for C2 is fixed at 413K.

### **Example 2**

Example 2 is from Gundersen and Grossmann (1988) which was also analyzed by Colberg and Morari (1989). In both papers, no cost data are presented for utility streams and the level of energy recovery is fixed at  $HRAT \ll 20^{\circ}\text{C}$ . As a result, for comparison purposes, the utility usage is fixed for the proposed method at  $HRAT \ll 20^{\circ}\text{C}$ , 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, however, the cost equation for exchangers involves an explicit fixed charge for each unit. The problem data are shown in Table 2.

For the proposed method, a superstructure with two stages is constructed and the corresponding MINLP model is formulated. The formulation involves 67 equations and 53 variables with 12 being binary. The solution procedure using DICOPT++ required 3 iterations and 17.9 CPU seconds on the IBM 3083. The optimal network obtained is shown in Figure 14. 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 (1989). In both of the previous papers which presented this result, the problem was decomposed into subnetworks, and the optimal network required six units and 2960 m<sup>2</sup> of area. The optimal solution from the proposed method also requires 6 units, however, the area requirement is 3045.5 m<sup>2</sup>, which is about 85 m<sup>2</sup> more. However, the total cost actually turns out to be less. One reason is that one of the temperature approaches in exchanger 1 lies below 20 °C, and the other is the distribution of area to optimally account for economies of scale. This example then illustrates clearly that the minimization of area does not necessarily go hand-in-hand with the minimization of cost. It should also be noted that exchanger 5 is placed across the pinch at 70-90 °C. Despite this fact, the driving force is relatively high which again shows that not placing exchangers across the pinch is a heuristic that often may not hold. On the other hand, exchanger 1 exhibits the smaller driving force but this is compensated by the effect of economies of scale in the area cost. One final point to note is 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 (1989) of \$716,000.

**Example 3**

Example 3 is from the MAGNETS user manual. The main purpose for 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 Figure 15. In networks where several stream splits may be required, the restriction on the type of split allowed in the model, as illustrated by Figure 4, 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 equations and 104 continuous and 31 binary variables. The solution time was obtained in 3 iterations using DICOPT++, which required 2.78 CPU minutes on the IBM 3083. The network obtained from the MINLP optimization involves nine units and three split streams. However, the number of units was reduced to seven in the sub-optimization step and the optimal network is shown in Figure 16. The annual cost for the network is \$576,640, which is slightly higher than the MAGNETS network at \$575,332, which was solved with HRAT fixed at 5K. Comparing the two networks, the MAGNETS network requires two additional units and four additional split streams. The energy requirement is lower in the MAGNETS network but has a higher investment cost. In fact, its total area is 295.5 m<sup>2</sup>, which is almost 50% higher than the total area of 200.9 m<sup>2</sup> for the network in Figure 16.

Overall, this result is very encouraging in view of the fact that despite the simplifying assumption used in the proposed method for stream splits, the method indeed obtained a network very close to the optimum.

**Example 4**

Example 4 is from Colberg and Morari (1989), 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 (1989) requires a split stream going through exchangers in series as shown in Figure 6a, 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<20K. Also, since no cost equation was given, the exchanger cost equation from Example 2 of

$8600 + 670^{\#}(\text{Area})^{0.83}$  was assumed.

The superstructure for the problem was constructed with four stages. The formulation involved 231 equations and 151 continuous and 48 binary variables. Solution of the problem to optimality required 3 iterations and 13.8 CPU minutes on the IBM 3083. Two split streams are required in the solution, and therefore the NLP sub-optimization is performed to determine the optimal split ratios. The final network is shown in Figure 17. The cost for the network is \$150,998. This compares well with the Colberg network which, using the same cost equation, is at \$177,385, roughly 17.5% higher. However, the Colberg solution does achieve their objective of minimizing the total area. Their network requires 188.9 m<sup>2</sup> vs. 217.8 m<sup>2</sup> for the network from the proposed approach. The trade-off, though, is that the Colberg network also requires three additional units and ten 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 solution 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 required and hence 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,  $q_{cc,j1,k}$ , to represent the heat transfer from cold stream  $j$  to cold stream  $j1$ , where  $j1 \neq j$ .
2. Relax the monotonic decrease of temperatures along the stages by removing the constraint in (4):

$$t_{j,k} \geq t_{j,k+1} \quad k \in ST, \quad j \in CP$$

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

$$(TOUT_j - TIN_j) F_j = \sum_{k \in ST} \sum_{i \in HP} q_{ijk} - \sum_{k \in ST} \sum_{\substack{j1 \in CP \\ j1 \neq j}} (q_{jj1,k} - q_{j1j,k}) + q_{hu_j} \quad j \in CP$$

$$(t_{j,k} - t_{j,k+1}) F_j = \sum_{i \in HP} q_{ijk} - \sum_{\substack{j1 \in CP \\ j1 \neq j}} (q_{jj1,k} - q_{j1j,k}) \quad k \in ST, \quad j \in CP$$

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 equations and 70 continuous and 15 binary variables. Solution of the problem using DICOPT++ required 23.31 CPU seconds on the IBM 3083. The optimal solution derived is as shown in Figure 18. The solution obtained indeed requires a cold-to-cold match between stream C1 and C2, where C2 is considered the "hot" stream. The total annual cost for the network is \$13,800, which is identical to the solution from Dolan et al. (1987). Comparing the two networks, the configurations are the same and both networks achieve minimum energy requirement. The heat load distribution, however, is slightly different although 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 Figure 19. Again, the same network configuration is obtained, with one cold-to-cold match involved in the network. The heat load distribution, 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. 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.

## CONCLUSION

In this paper, a systematic procedure has been proposed for the synthesis of heat exchanger networks. Unlike previous synthesis methods, the proposed approach does not rely on any sequential decomposition of the problem, but rather 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 representation that is modeled as a mixed integer nonlinear programming 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. A simplifying assumption on the type of stream splits in the superstructure eliminates flow and heat mixing considerations in the problem formulation. This allows the feasible space for the model to be defined by a set of linear equations; the model thus can be solved efficiently. Overall, the assumption may lead to an overestimation of exchanger areas in networks with split streams. As a result, a sub-optimization is performed to determine optimal split ratios when the predicted network requires stream splits. A positive effect from the simplifying assumption is that the model will generally favor no split structures where exchanger areas are determined precisely.

The 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 a very significant one in view of the combinatorial nature of the synthesis problem, where several alternative configurations may be very close to the global optimum.

The example problems presented have also shown that pinch considerations may not be very relevant for synthesizing the network structure when all the trade-offs are accounted simultaneously; this is even for the case when heat transfer coefficients for the streams are the same. Considerations for economies of scale 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, it is often the

case that optimal networks involve exchangers that are placed across the pinch.

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## REFERENCES

1. Brooke, A., Kendrick, D., and Meeraus, A., Scientific Press, *GAMS: A User's Guide*, Palo Alto, 1988.
2. Chen, J.J.J., " Letter to the Editors: Comments on Improvement on a Replacement for the Logarithmic Mean", *Chemical Engineering Science*, Vol. 42, 1987, pp. 2488-2489.
3. Ciric, A.R. and Floudas, C.A., "Global Optimum Search in Heat Exchanger Networks - Part II: Simultaneous Optimization of Network Configurations and Process Stream Matches", *Presented at the Annual AIChE Meeting*, Washington D.C., November 1988.
4. Ciric, A.R. and Floudas, C.A., "A Mixed Integer Nonlinear Programming Model for Retrofitting Heat Exchanger Networks", *Presented at the Annual AIChE Meeting*, Washington D.C., December 1988a.
5. Colberg, R.D., and Morari, M., "Area and Capital Cost Targets for Heat Exchanger Network Synthesis with Constrained Matches and Unequal Heat Transfer Coefficients", *submitted for publication to Computer and Chemical Engineering*, March 1989.
6. Dolan, W.B., Cummings, P.T., and LeVan, M.D., "Heat Exchanger Network Design by Simulated Annealing", *Proceedings of the First International Conference on Foundations of Computer Aided Process Operations*, Park City, UT, July 5-10 1987.
7. Dolan, W.B., Cummings, P.T., and LeVan, M.D., "Process Optimization via Simulated Annealing: Application to Network Design", *AIChE J.*, Vol. 35, 1989, pp. 725-736.
8. Floudas, C.A., Ciric A.R. and Grossmann, I.E., "Automatic Synthesis of Optimum Heat Exchanger Network Configurations", *AIChE J.*, Vol. 32, 1986, pp. 276-290.
9. Grimes, L.E., Rychener, M.D. and Westerberg, A.W., "The Synthesis and Evolution of Networks of Heat Exchange that Feature the Minimum Number of Units", *Chem. Eng. Commun.*, Vol. 14, 1982, pp. 339-360.
10. Grossmann, I.E. and Sargent, R.W.H., "Optimum Design of Heat Exchanger Networks", *Computers and Chemical Engineering*, Vol. 2, 1978, pp. 1-7.
11. Grossmann, I.E., *MAGNETS User's Guide*, Carnegie Mellon University, Pittsburgh, PA, 1985.
12. Gundersen, T. and Grossmann, I.E., "Improved Optimization Strategies for Automated Heat Exchanger Network Synthesis through Physical Insights", *Presented at the Annual AIChE Meeting*, Washington D.C., December 1988.
13. Gundersen, T. and Naess, L., "The Synthesis of Cost Optimal Heat Exchanger Network Synthesis - An Industrial Review of the State of the Art", *Computers and Chemical Engineering*, Vol. 12, No. 6, 1988, pp. 503-530.
14. *IBM Mathematical Programming System Extended/370 (MPSX/3709), Basic Reference Manual*, White Plains, 1979.
15. Lee, K.F., Masso, A.H., and Rudd, D.F., "Branch and Bound Synthesis of Integrated Process Designs", *I&EC Fundamentals*, Vol. 9, No. 1, 1970, pp. 48-58.

16. Linnhoff, B. et al., *A User Guide on Process Integration for the Efficient Use of Energy*, The Institute of Chemical Engineering, UK, 1982.
17. Linnhoff, B. and Hindmarsh, E., "The Pinch Design Method for Heat Exchanger Networks", *Chemical Engineering Science*, Vol. 38, 1983, pp. 745-763.
18. Murtagh, B.A. and Saunders, M.A., "MINOS 5.0 User's Guide", Tech. report SOL 83-20, Systems Optimization Laboratory, Dept. of Operations Research, Stanford University, 1983.
19. Papoulias, S.A. and Grossmann, I.E., "A Structural Optimization Approach in Process Synthesis - II. Heat Recovery Networks", *Computers and Chemical Engineering*, Vol. 7, 1983, pp. 707-721.
20. Paterson, W.R., "A Replacement for the Logarithmic mean", *Chemical Engineering Science*, Vol. 39, 1984, pp. 1635.
21. Viswanathan, M. and Evans, L.B., "Studies in the Heat Integration of Chemical Process Plants", *AIChEJ.*, Vol. 33, 1987, pp. 1781-1790.
22. Viswanathan, J. and Grossmann, I.E., "A Combined Penalty Function and Outer-Approximation Method for MINLP Optimization", *Annual TIMS/ORSA - Canadian Operations Research Society*, Vancouver B.C., July 1989.
23. Wood, R.M., Wilcox, R.J. and Grossmann, I.E., "A Note on the Minimum Number of Units for Heat Exchanger Network Synthesis", *Chemical Engineering Communications*, Vol. 39, 1985, pp. 371-380.
24. Yee T.F. and Grossmann, I.E., "A Screening and Optimization Approach for the Retrofit of Heat Exchanger Networks", *Presented at the Annual AIChE Meeting*, Washington D.C., December 1988.
25. Yee T.F., Kravanja, Z. and Grossmann, I.E., "A New Model for Heat Exchanger Network Area Targeting and Simultaneous Optimization and Heat Integration of Processes", *Manuscript in Preparation*, 1989.

## APPENDIX A: Initialization procedure for solving the MINLP

As shown in Figure 7, 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.

An initialization procedure can be outlined as follows:

1. Estimate a value of HRAT.
2. Estimate a driving force for each match by:
  - a. Determining the  $LMTD_n$  for each enthalpy interval  $n$  (see Figure 3).
  - b. Using the following weighting equation to calculate an average driving force for each match  $(i,j)$ :

$$ALMTD_{ij} = ( \sum_n q_{ijn} LMTD_n ) / \sum_n q_{ijn}$$

where  $q_{ijn}$  is the maximum heat transfer that can occur between hot stream  $i$  and cold stream  $j$  in enthalpy interval  $n$ .

3. Set the driving forces in the objective function (8) with fixed values for the average driving forces  $ALMTD_{ij}$ , and replace the nonlinear cost term of the area by a linear approximation with a fixed charge. This reduces the MINLP in (1) to (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.

Stream	TIN (C)	TOUT (C)	Fcp (kW/C)	Cost (\$/kW-yr)
H1	443	333	30	-
H2	423	303	15	-
C1	293	408	20	-
C2	353	413	40	-
S1	450	450	-	80
W1	293	313	-	20

$U = 0.8 \text{ (kW/m}^2 \text{ C)}$  for all matches except ones involving steam

$U = 1.2 \text{ (kW/m}^2 \text{ C)}$  for matches involving steam

Annual Cost =  $1000 * (\text{Area(m}^2))^{0.6}$  for all exchangers except heaters

Annual Cost =  $1200 * (\text{Area(m}^2))^{0.6}$  for heaters

**Table 1 Problem Data for Example 1**

Stream	TIN (C)	TOUT (C)	Fcp (kW/C)
H1	150	60	20
H2	90	60	8.0
C1	20	125	25
C2	25	100	30
S1	180	180	-
W1	10	15	-

$U = 0.05 \text{ (kW/m}^2 \text{ C)}$  for all matches

Cost =  $8600 + 670 * (\text{Area(m}^2\text{)})^{0.83}$  for all exchangers

**Table 2 Problem Data for Example 2**

Stream	TIN (C)	TOUT (C)	Fcp (kW/C)	Cost (\$/kW)
H1	500	320	6	-
H2	480	380	4	-
H3	460	360	6*	-
H4	380	360	20	-
H5	380	320	12	-
C1	290	660	18	-
S1	700	700	-	140
W1	300	320	-	10

$U = 1.0 \text{ (kW/m}^2 \text{ C)}$  for all matches

Annual Cost =  $1200 * (\text{Area(m}^2\text{)})^{0.6}$  for all exchangers

Table 3 Problem Data for Example 3

Stream	TIN (C)	TOUT (C)	Fcp (kW/C)	h (kW/m <sup>2</sup> K)
H1	626	586	9.802	1.25
H2	620	519	2.931	0.05
H3	528	353	6.161	3.20
C1	497	613	7.179	0.65
C2	389	576	0.641	0.25
C3	326	386	7.627	0.33
C4	313	566	1.690	3.20
S1	650	650	-	3.50
W1	293	308	-	3.50

$$1/U = (1/h_h + 1/h_c)$$

Cost « 8600 + 670 \* (Area(m<sup>2</sup>))<sup>0.83</sup> for all exchangers

**Table 4 Problem Data for Example 4**



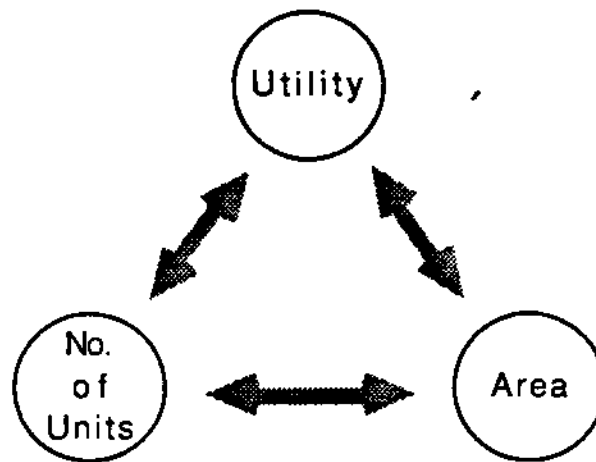
Stream	TIN (F)	TOUT (F)	Fcp (Btu/F)	Cost (\$/1000Btu-yr)
H1	320	200	16,666.8	-
H2	480	280	20,000	-
C1	140	320	14,450.1	-
C2	240	500	11,530	-
S1	540	540	-	12.76
W1	100	180	-	5.24

$U = 150$  (Btu/ft<sup>2</sup> F) for all matches except ones involving steam

$U = 200$  (Btu/ft<sup>2</sup> F) for matches involving steam

Annual Cost -  $35 * (\text{Area}(\text{m}^2))^{0.6}$  for all exchangers

Table 5 Problem Data for Example 5



**Figure 1 Trade-off Between Costs in Design**

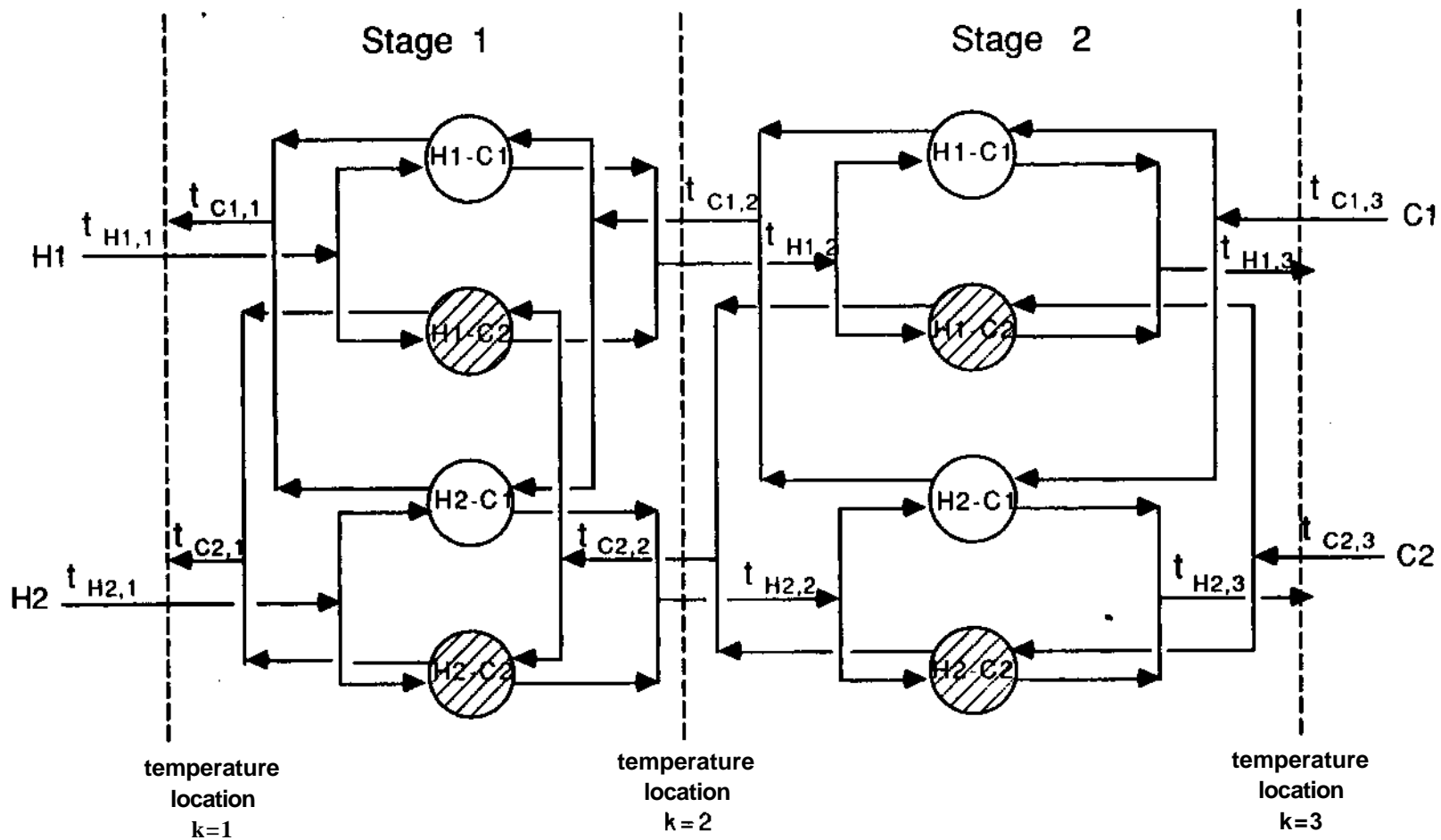
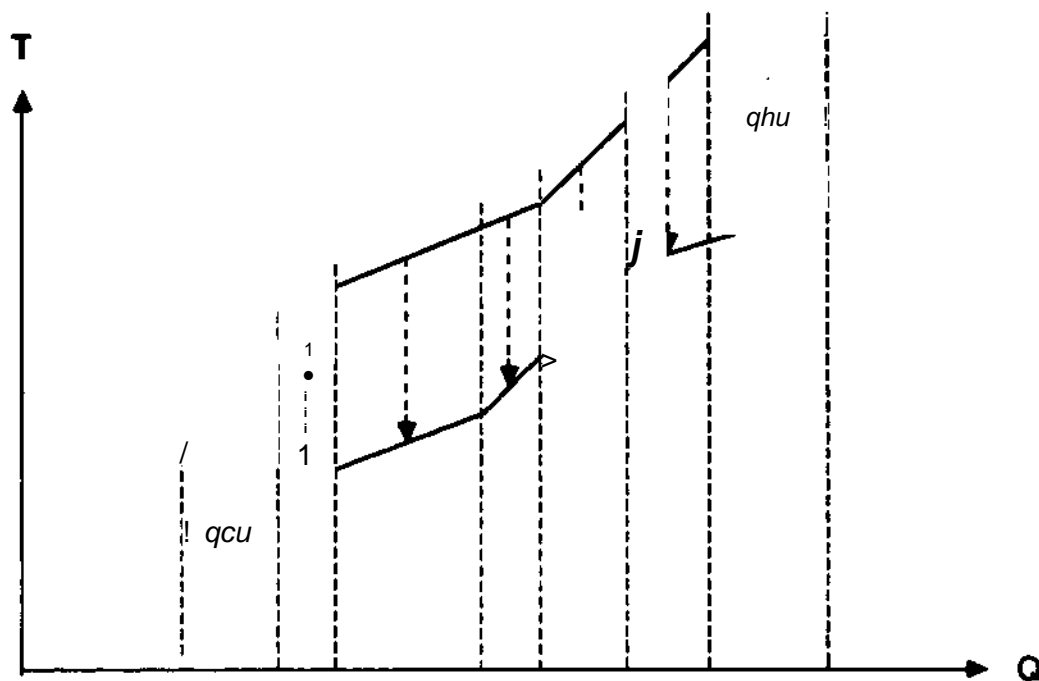


Figure 2 Two Stage Superstructure



**Figure 3 Vertical Heat Transfer Between Composite Curves  
Leading to Spaghetti Design**

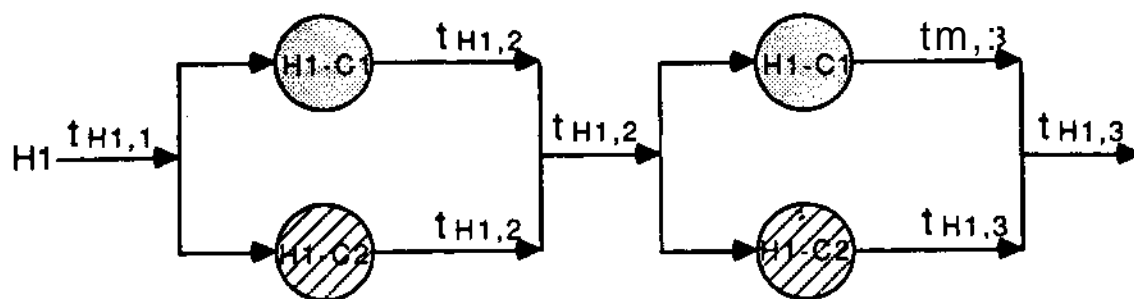


Figure 4 Restrictions on Split Temperatures

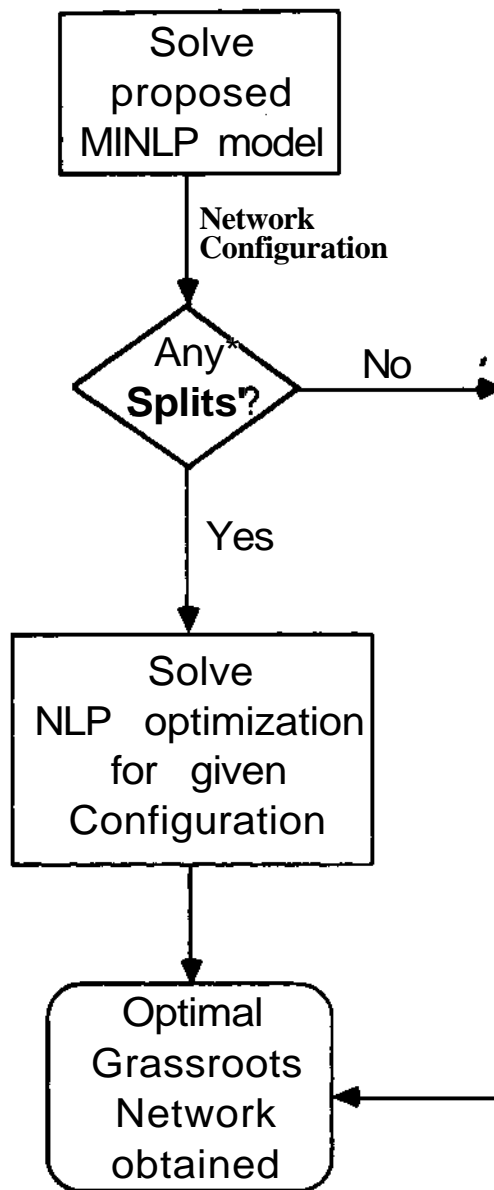
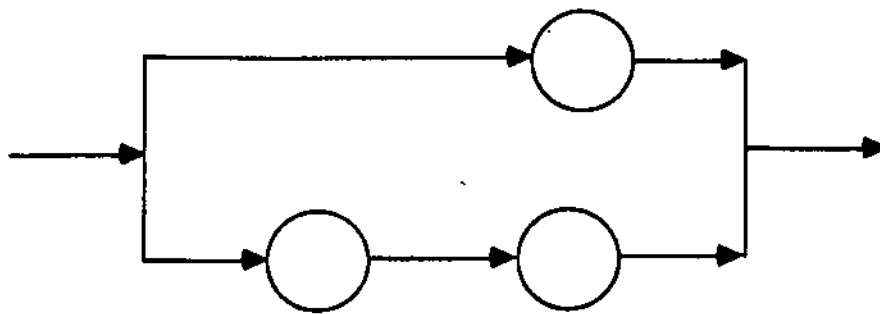
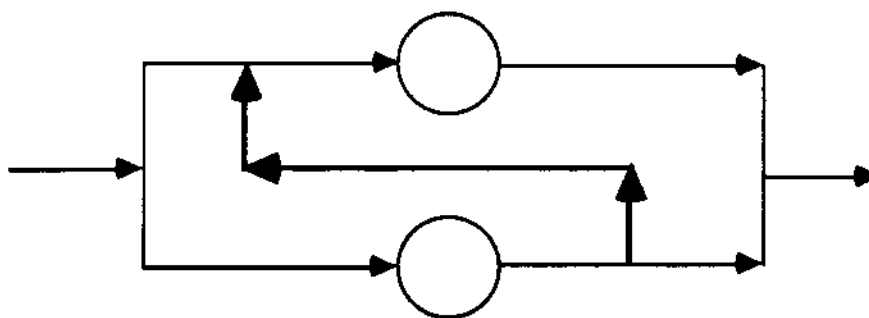


Figure 5 Proposed Synthesis Strategy



a) A split stream going through exchangers in series



b) A stream by-pass

Figure 6 Limitations of Superstructure

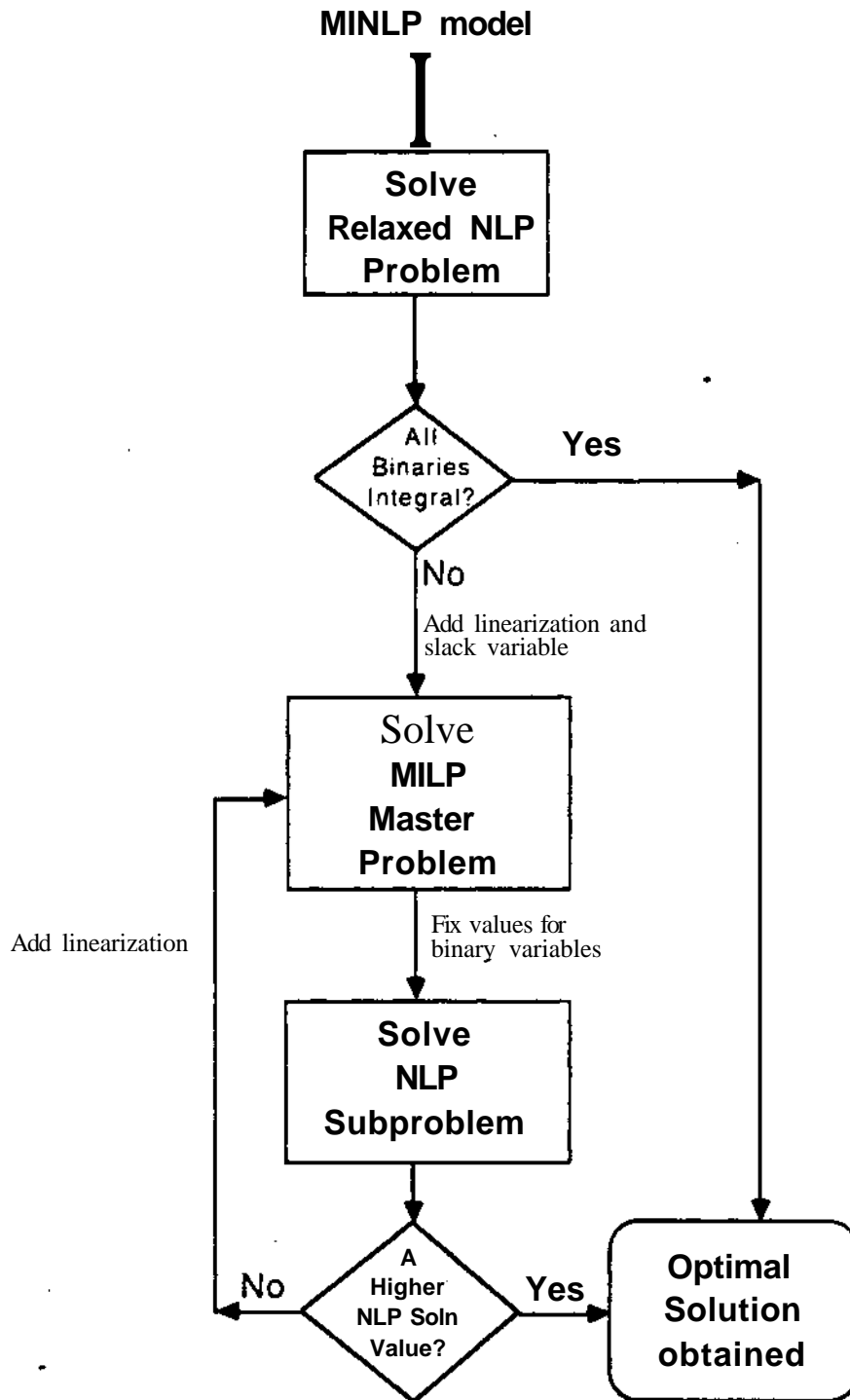


Figure 7 Combined Penalty Function & Outer Approximation Method



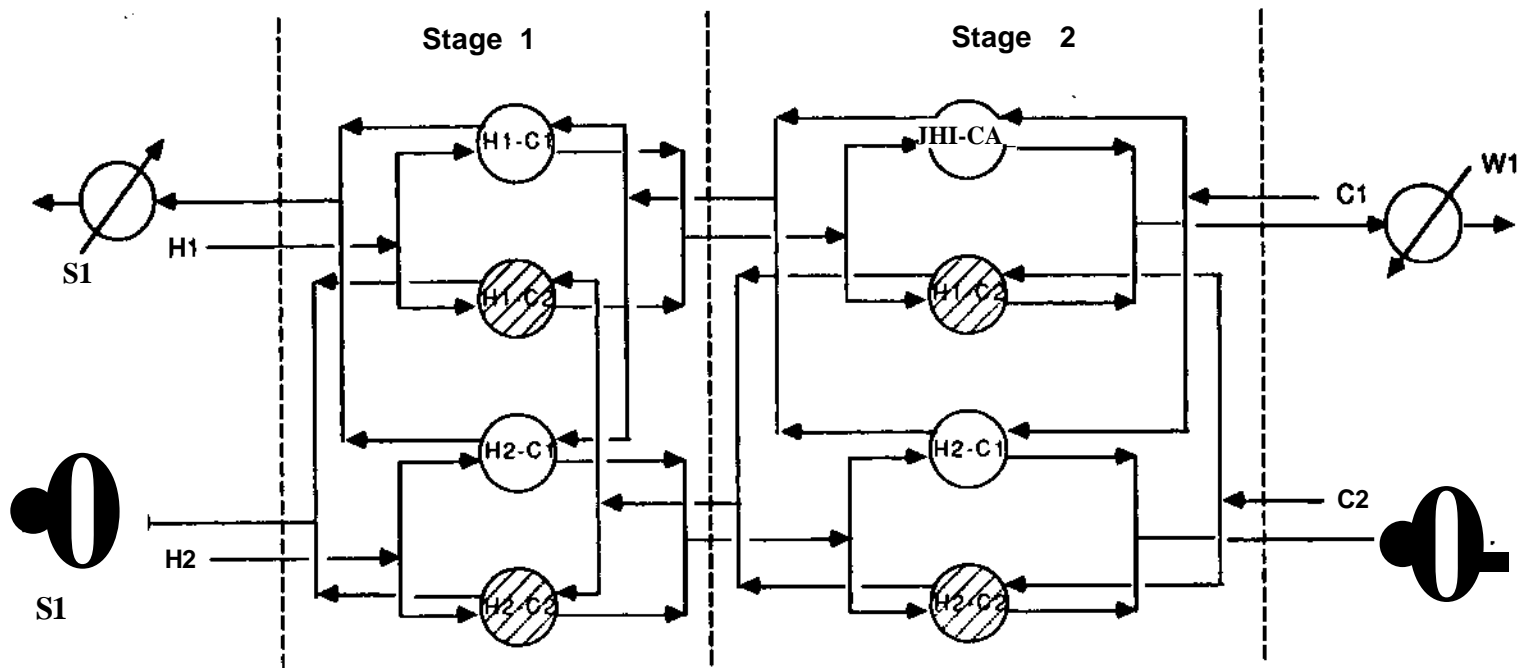
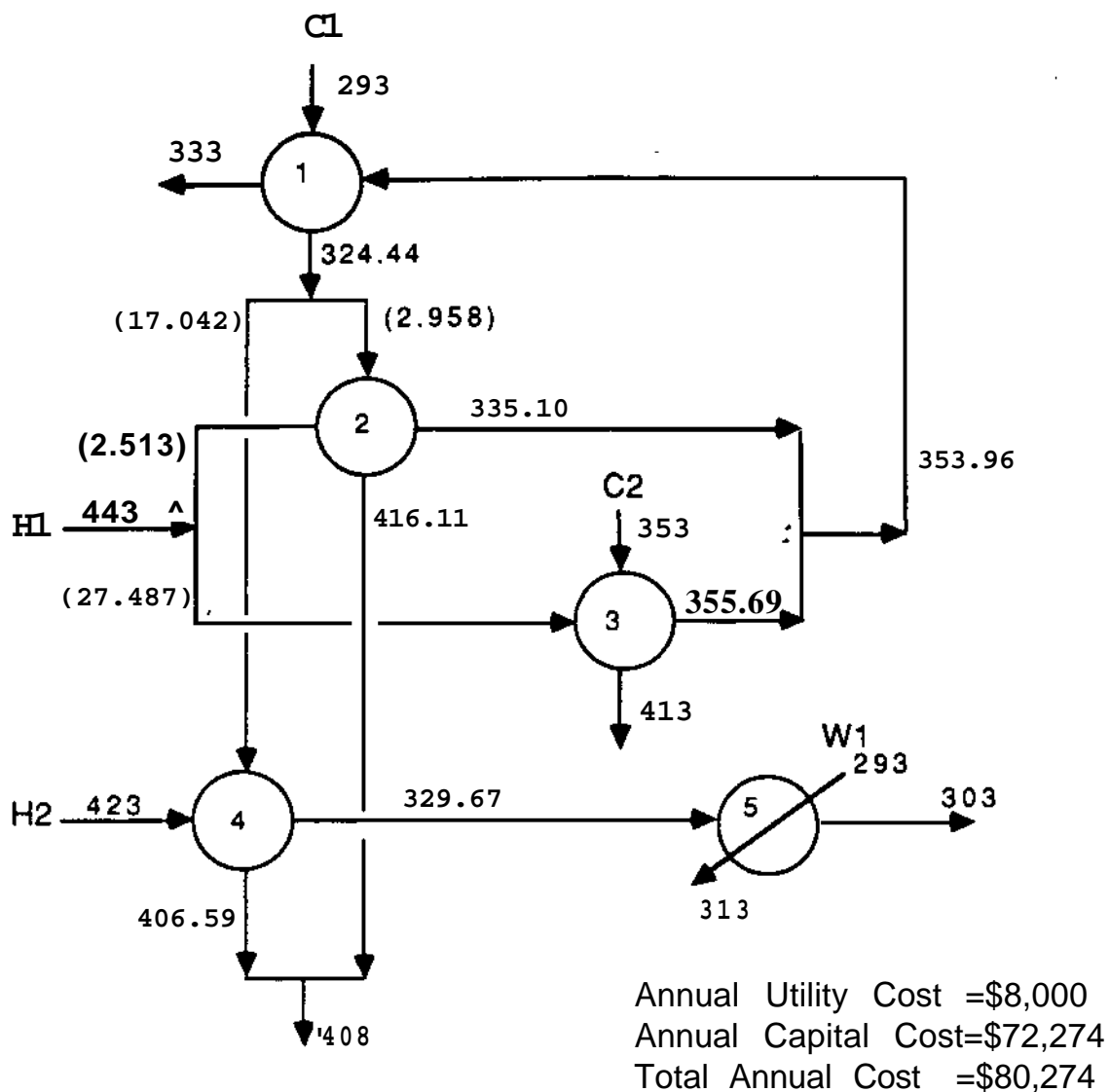
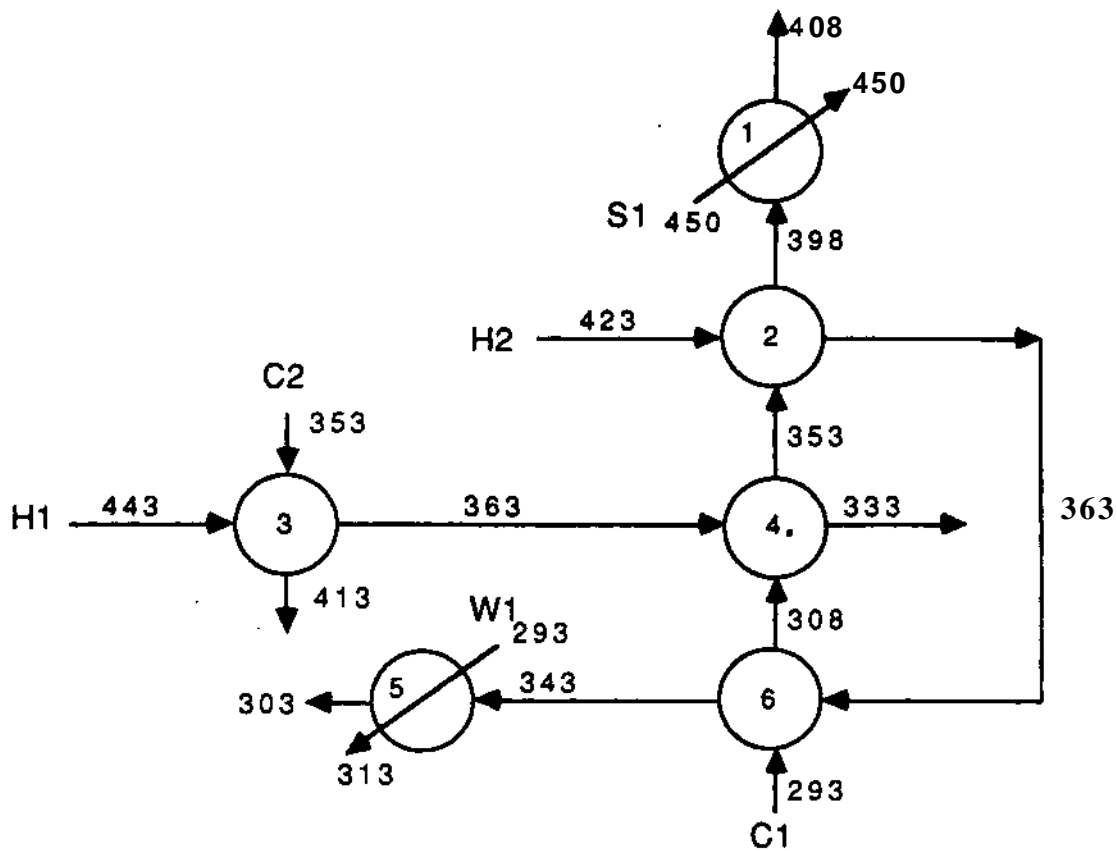


Figure 8 Superstructure for Example 1



Exch.	Heat Load (kJ)	Area(m <sup>2</sup> )
1	628.8	22.8
2	271.2	19.3
3	2400	265.1
4	1400	179.0
5	400	38.3

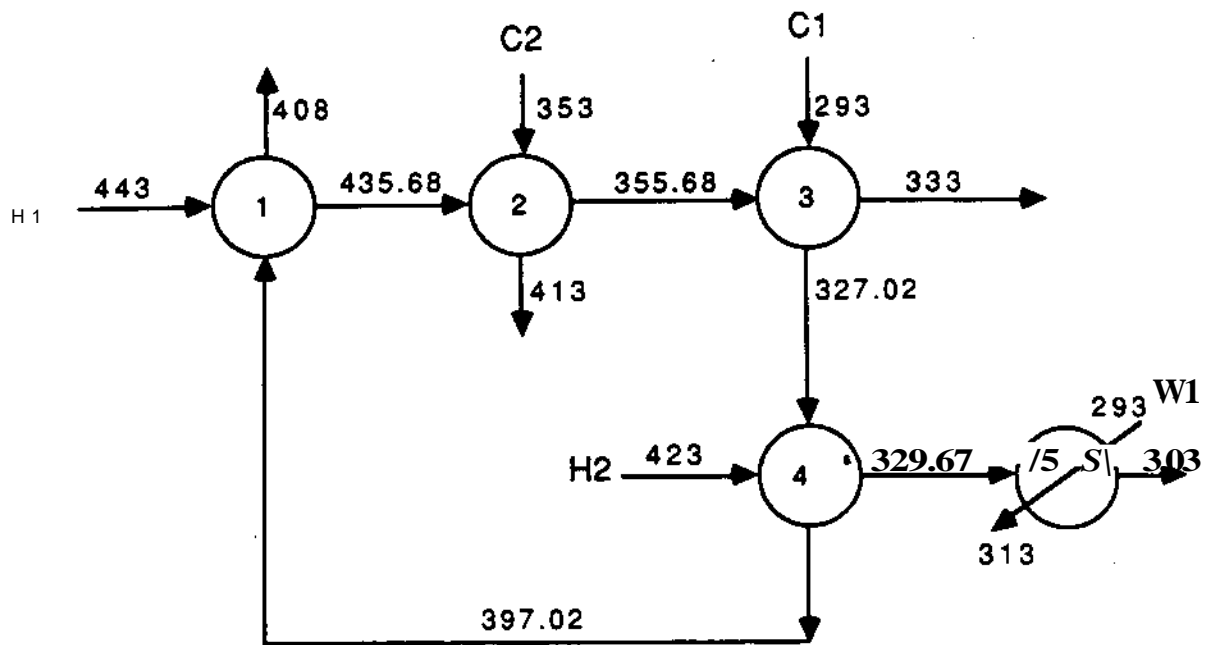
Figure 9 Example 1: Unrestricted Case



Annual Utility Cost = \$28,000  
 Annual Capital Cost = \$61,832  
 Total Annual Cost = \$89,832

Exch.	Heat Load (kW/M)	Area(m <sup>2</sup> )
1	200	3.6
2	900	68.7
3	2400	164.8
4	900	68.7
5	600	41.2
6	300	7.1

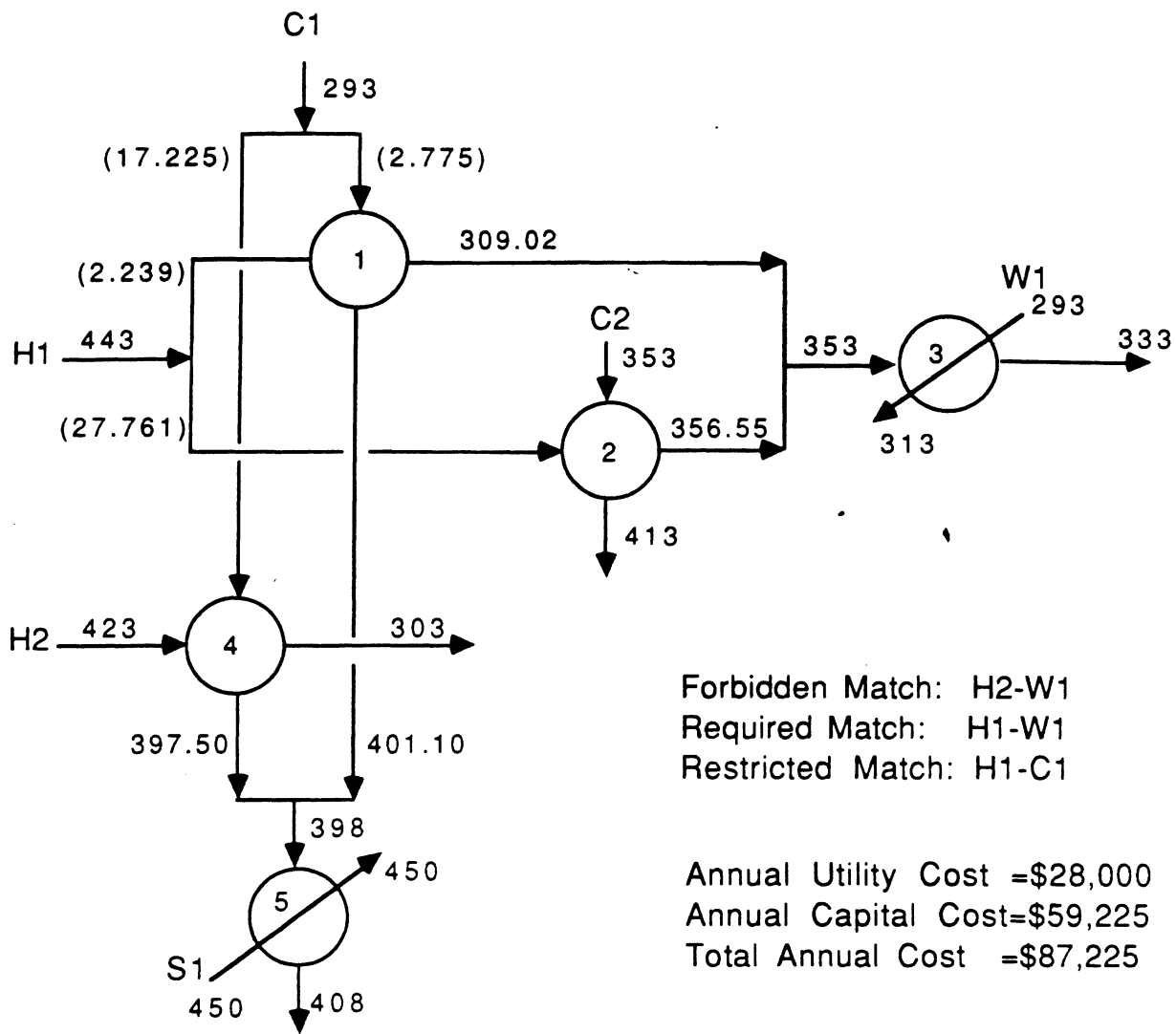
Figure 10 MAGNETS Solution for Example 1



Annual Utility Cost = \$8000  
 Annual Capital Cost = \$72,909  
 Total Annual Cost = \$80,909

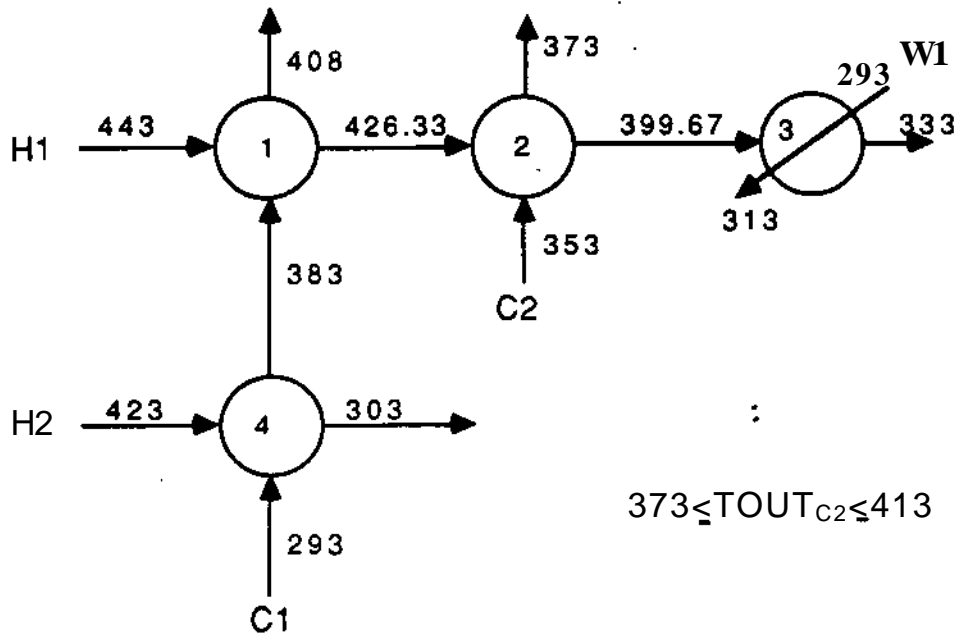
Exch.	Heat Load (kW)	Area(m <sup>2</sup> )
1	219.6	7.5
2	2400	320.3
3	<b>680.4</b>	25.0
4	<b>1400</b>	171.3
5	<b>400</b>	38.3

Figure 11 Example 1: No Split Case



Exch.	Heat Load (kW)	Area(m <sup>2</sup> )
1	300	13.9
2	2400	242.1
3	600	18.7
4	1800	135.9
5	200	3.6

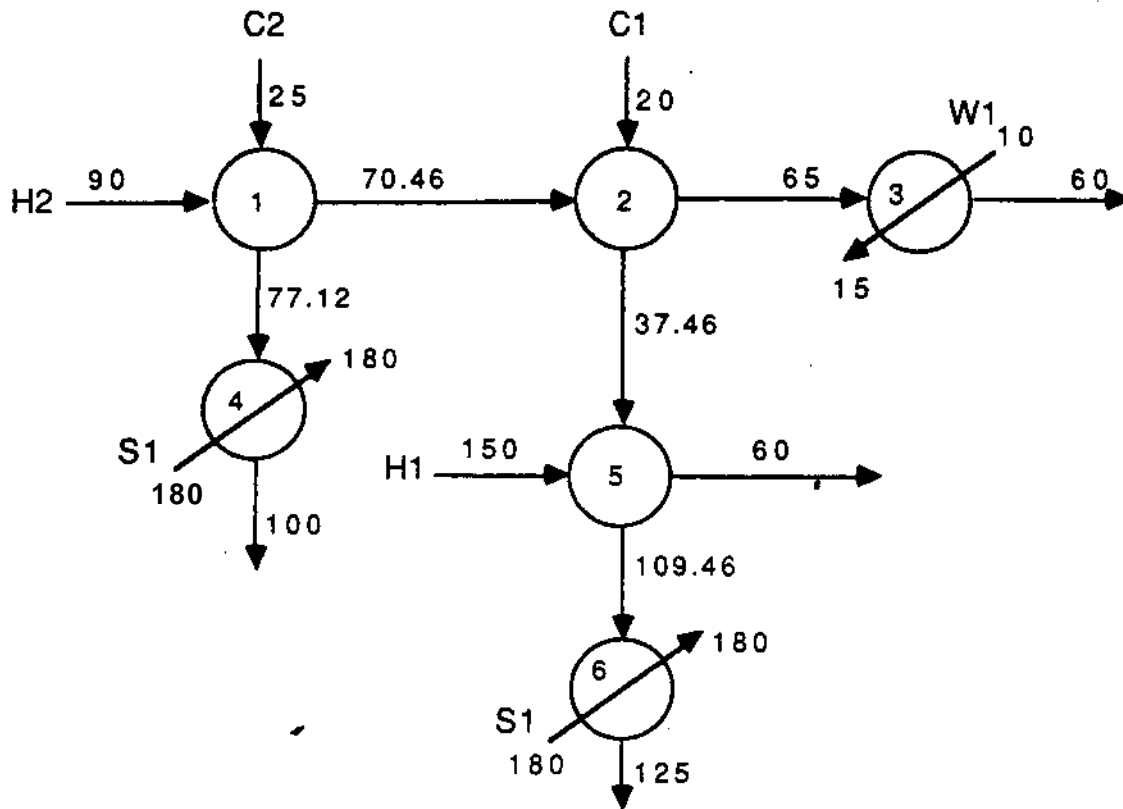
Figure 12 Example 1: Restricted Case



Annual Utility Cost = \$40,000  
 Annual Capital Cost = \$36,880  
 Total Annual Cost - \$76,880

Exch.	Heat Load (kW)	Area(m <sup>2</sup> )
1	500	16.0
2	800	20.0
3	2000	41.4
4	1800	104.0

Figure 13 Example 1: Target Temperature as Inequalities



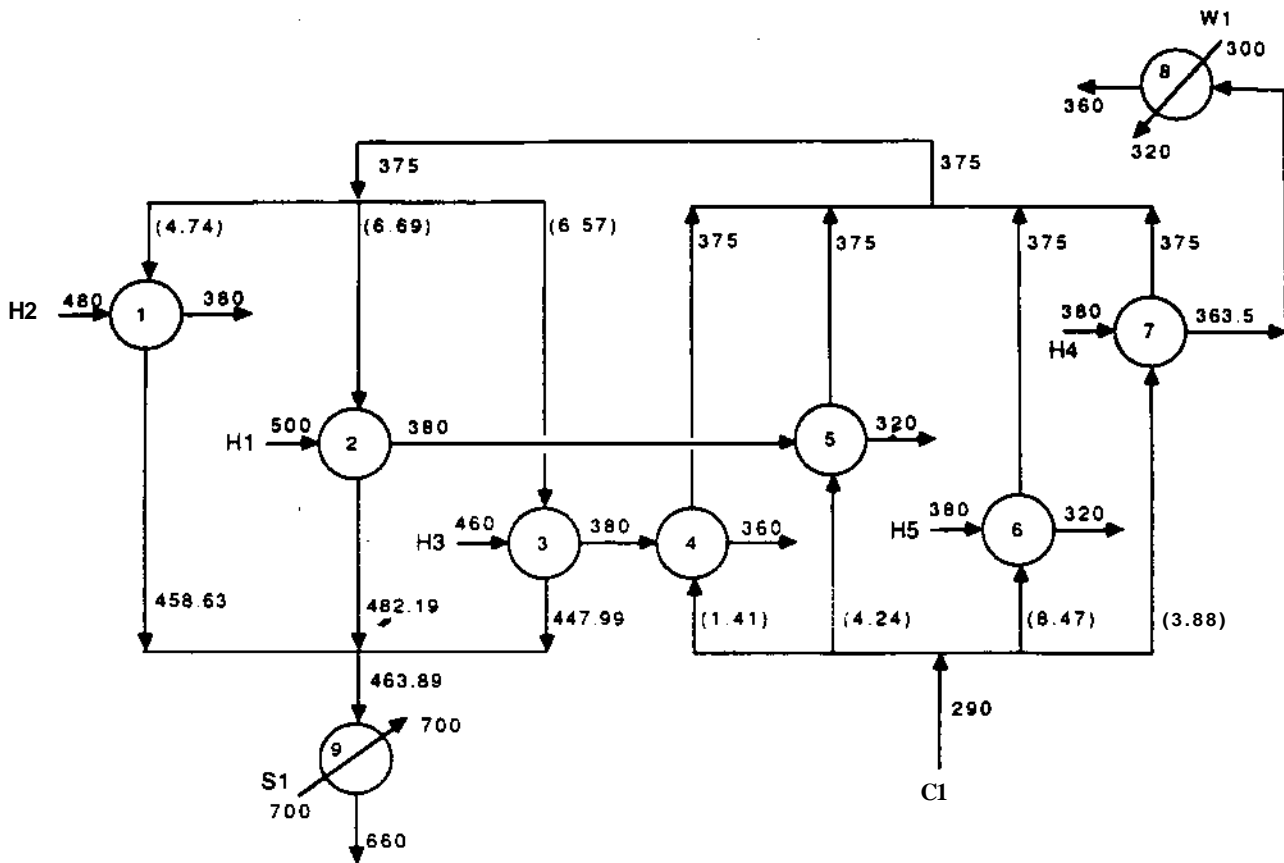
HRAT fixed at 201)

Total Capital Cost = \$715,970

Total Area = 3045.4 m<sup>2</sup>

Exch.	Heat Load (kW)	Area(m <sup>2</sup> )
1	1563.5	1210.3
2	436.5	225.7
3	400	160.0
4	686.5	150.95
5	1800	1174.1
6	388.5	124.4

Figure 14 Optimal Network for Example 2

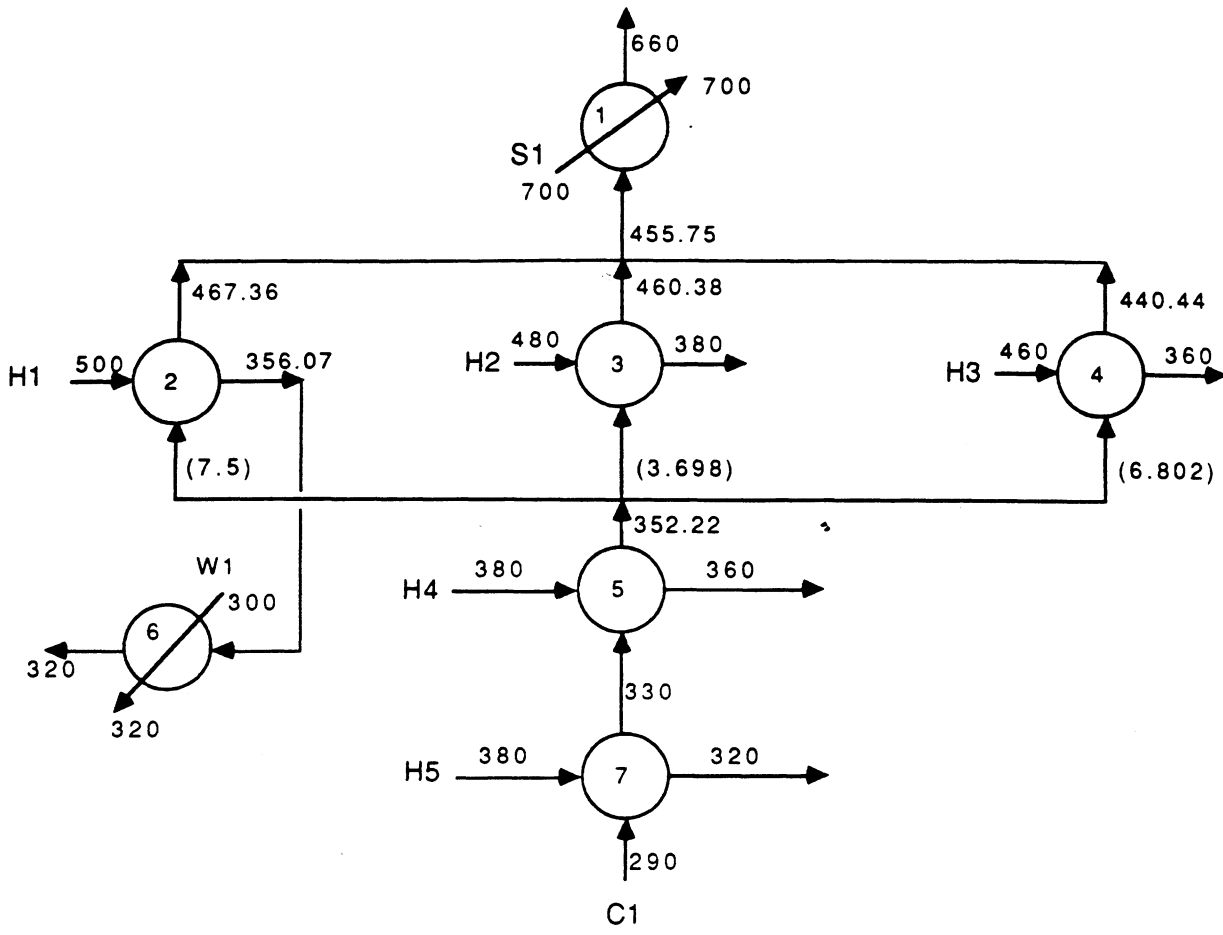


Exch	Heat Load (kAM)	Area (m <sup>2</sup> )
1	400	35.5
2	720	71.4
3	480	60.0
4	120	4.9
5	360	25.8
6	720	51.6
7	330	12.9
8	70	1.4
9	3530	32.0

Pinch location: 380-375K  
 Annual Utility Cost \* \$494,900  
 Annual Capital Cost \* \$80,695  
 Total Cost = \$575,595  
 Total Area = 295.5 m<sup>2</sup>

Figure 15 MAGNETS Solution for Example 3

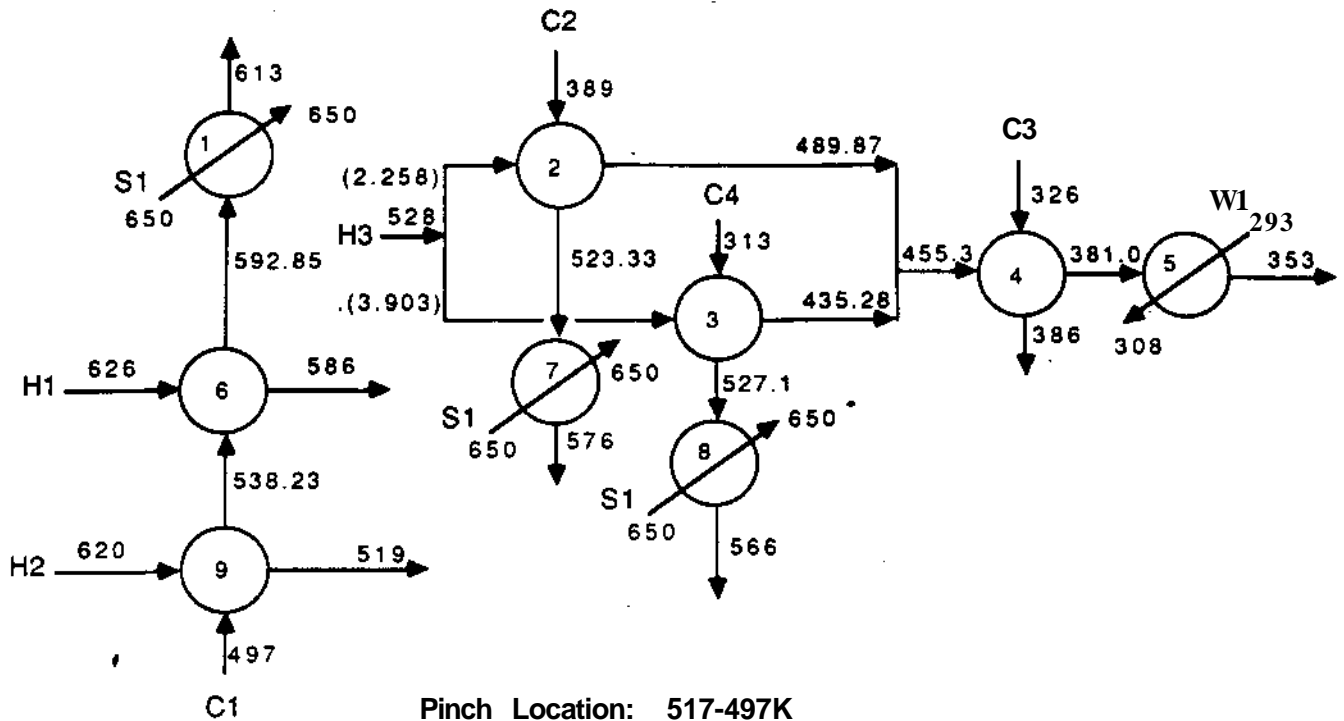




Exch.	Heat Load (kW)	Area (m <sup>2</sup> )
1	3676.4	32.6
2	863.6	64.1
3	400	17.1
4	600	47.0
5	400	13.8
6	216.4	7.9
7	720	18.4

Pinch Location: 380-366.9K  
 Annual Utility Cost = \$516,860  
 Annual Capital Cost = \$59,780  
 Total Annual Cost = \$576,640  
 Total Area = 200.9 m<sup>2</sup>

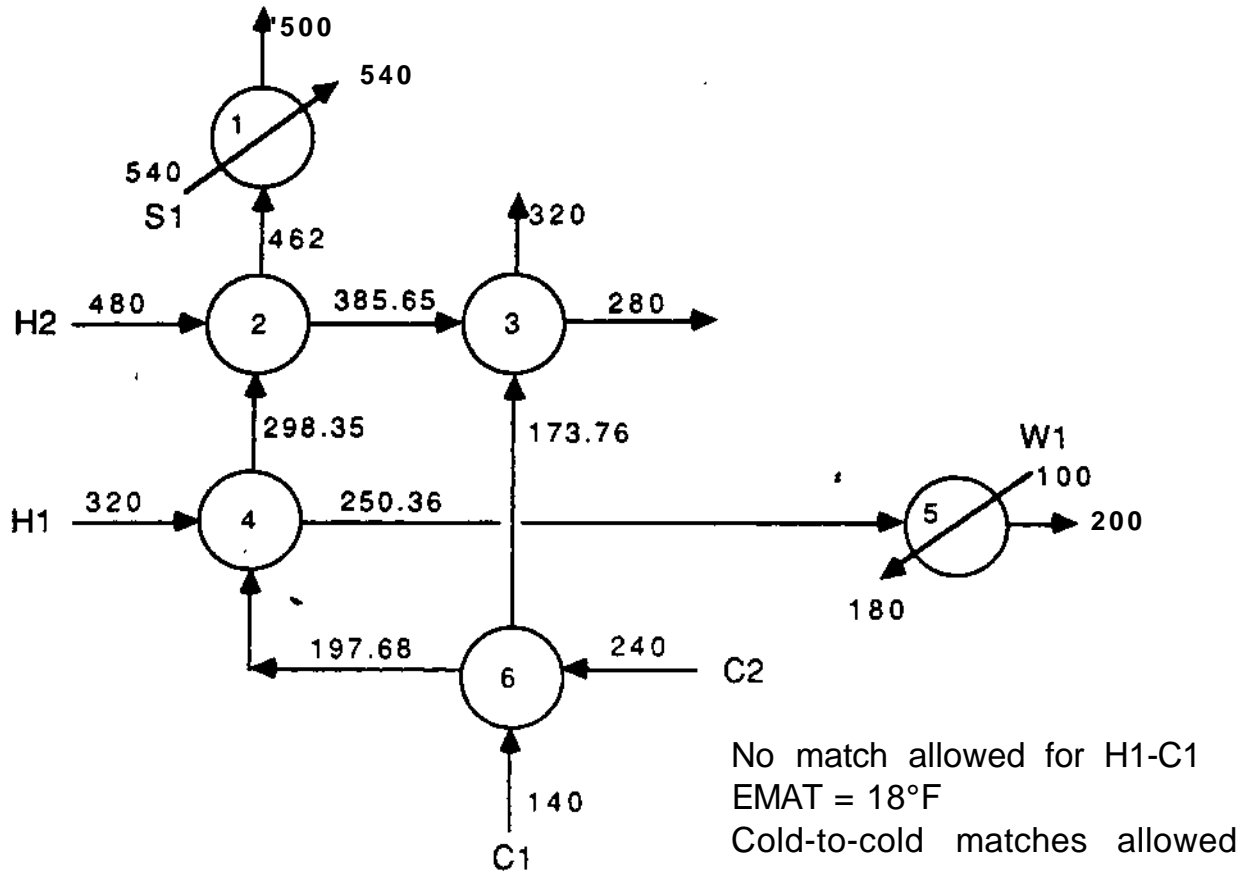
Figure 16 Optimal Network for Example 3



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

Exch.	Heat Load	Area (m <sup>2</sup> )
1	144.6	5.69
2	86.1	11.86
3	361.9	9.18
4	457.6	24.72
5	172.6	1.56
6	392.1	22.91
7	33.8	1.48
8	65.7	0.39
9	296.0	140.06

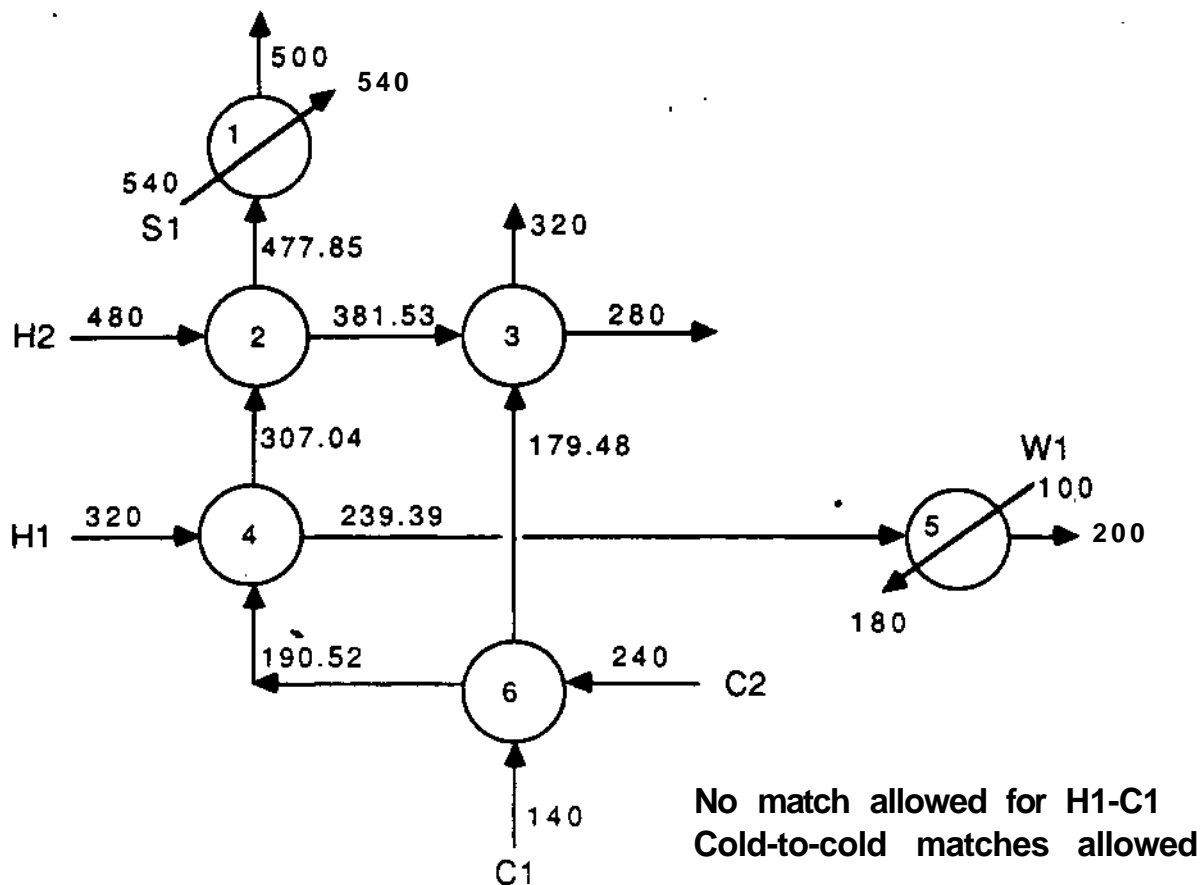
Figure 17 Optimal Network for Example 4



Annual Utility Cost = \$9988  
 Annual Capital Cost = \$3817  
 Total Annual Cost = \$13,800  
 Total Area = 832.9 ft<sup>2</sup>

Exch.	Heat Load MOO(Btu)	Area(ft <sup>2</sup> )
1	438.1	38.5
2	1886.9	286.6
3	2113.1	167.1
4	1160.7	221.7
5	839.3	66.4
6	487.9	52.6

Figure 18 Example 5: Restricted Case with EMAT = 18 °F



Annual Utility Cost = \$6,698  
 Annual Capital Cost = \$4,676  
 Total Annual Cost > \$11,374  
 Total Area = 1295.4 ft<sup>2</sup>

Exch.	Heat Load MOOQBtu	Area(ft <sup>2</sup> )
1	255.4	25.4
2	1969.4	643.7
3	2030.6	170.4
4	1343.5	331.1
5	656.6	56.2
6	570.5	68.7

Figure 19 Example 5: Restricted Case with no EMAT Specification

