SYNTHESIS OF HEAT EXCHANGER NETWORKS 16

16.1 INTRODUCTION

In Chapter 10, a number of powerful insights were presented that can greatly simplify the problem of synthesizing heat exchanger networks. These insights can be summarized as follows:

- Given a minimum temperature approach, the exact amount for minimum utility consumption can be predicted prior to developing the network structure.
- Based on the pinch temperatures for minimum utility consumption, the synthesis of the network can be decomposed into subnetworks.
- The fewest number of units in each subnetwork is often equal to the number of process and utility streams minus one.
- It is possible to develop good a priori estimates of the minimum total area of heat exchange in a network.

While these insights narrow down the alternative designs for a network very considerably, by themselves they do not provide an explicit procedure for deriving the configuration of a heat exchanger network. In other words, the user has to examine by trial and error matches and stream interconnections that will hopefully come close to satisfying the targets for utility consumption, number of units, and total area. Quite often, this might not be a trivial task, especially when one is faced with a rather large number of process streams, and when splitting of streams is required. Furthermore, if we were to rely only on these insights, it is rather difficult to develop a computer program that can automatically synthesize heat exchanger networks of arbitrary structure (e.g., with stream splitting, bypassing of streams). Moreover, networks satisfying the targets may not necessarily correspond to designs with minimum cost.

In this chapter we will present algorithmic optimization models for the synthesis of heat exchanger networks that illustrate two major synthesis strategies: sequential optimization and simultaneous optimization. First, we consider sequential optimization models that exploit the above insights, and at the same time provide systematic procedures that allow the automation of this synthesis problem in the computer. The models (LP, MILP, NLP) will also allow us to expand the type of problems that we can consider (e.g., multiple utilities, constraints on the matches, stream splitting). Secondly, we will present an MINLP model in which the energy recovery, selection of matches, and areas are all optimized simultaneously.

Three basic heuristic rules that are motivated by the insights of Chapter 10 will be used in the development of algorithmic methods based on sequential optimization. In particular, it will be assumed that an optimal or near optimal network exhibits the following characteristics:

Rule 1. Minimum utility cost
Rule 2. Minimum number of units
Rule 3. Minimum investment cost

Clearly, it is possible in general to have conflicts among these rules. Therefore, we will assume that Rule 1 has precedence over Rule 2, and Rule 2 over Rule 3. In this way, our objective will be to consider first candidate networks that exhibit minimum utility cost, among these the ones that have the fewest number of units, and among these the one that has the minimum investment cost. We will show in this chapter how for each of these three steps we can develop appropriate optimization models to generate networks with all possible options for sequencing, stream splitting, mixing and bypassing. We can consider the optimization of the minimum heat recovery approach temperature (HRAT) either in an outer loop of this procedure or else through the approximate procedure presented in Part III. Also, the precedence order of the heuristics can be indirectly challenged through constraints on matches. In section 16.3 we will present a simultaneous MINLP model in which the above rules do not have to be applied.

16.2 SEQUENTIAL SYNTHESIS

16.2.1 Minimum Utility Cost

Let us consider the following example to motivate a useful problem representation for the prediction of the minimum utility cost.

EXAMPLE 16.1

Determine the minimum utility consumption for the two hot and two cold streams given below:

	Fcp (MW/C)	Tin (C)	Tout (C)
H1	1	400	120
H2	2	340	120
C1	1.5	160	400
C2	1.3	100	250

Steam : 500°C
Cooling water: 20–30°C
Minimum recovery approach temperature (HRAT): 20°C

The data for this problem are displayed in Table 16.1, where heat contents of the hot and cold processing streams are shown at each of the temperature intervals, which are based on the inlet and highest and lowest temperatures. The flows of the heat contents we can represent in the heat cascade diagram of Figure 16.1. Here the heat contents of the hot streams are introduced in the corresponding intervals, while the heat contents of the cold streams are extracted also from their corresponding intervals. The variables R_1, R_2, R_3, represent heat residuals, while Q_s, Q_w represent the heating and cooling loads respectively.

TABLE 16.1 Temperature Intervals and Heat Contents (MW) for Example 16.1

Temperature Intervals (K)			Heat Contents (MW)				
Hot	Interval	Cold	*C1*	*H1*	*H2*	*C1*	*C2*
420		400	↑				
	int 1					30	
H1 400		380					
	int 2			60		90	
H2 340		320	250				
	int 3		↑	160	320	240	117
180		160					
	int 4			60	120		78
120		100	C2	280	440	360	195

The usefulness of the heat cascade diagram in Figure 16.1 is that it can be regarded as a transshipment problem that we can formulate as a linear programming problem (Papoulias and Grossmann, 1983). In terms of the transshipment model, hot streams are treated as source nodes, and cold streams as destination nodes. Heat can then be regarded as a commodity that must be transferred from the sources to the destinations through some intermediate "warehouses" that correspond to the temperature intervals that guarantee feasible heat exchange. When not all of

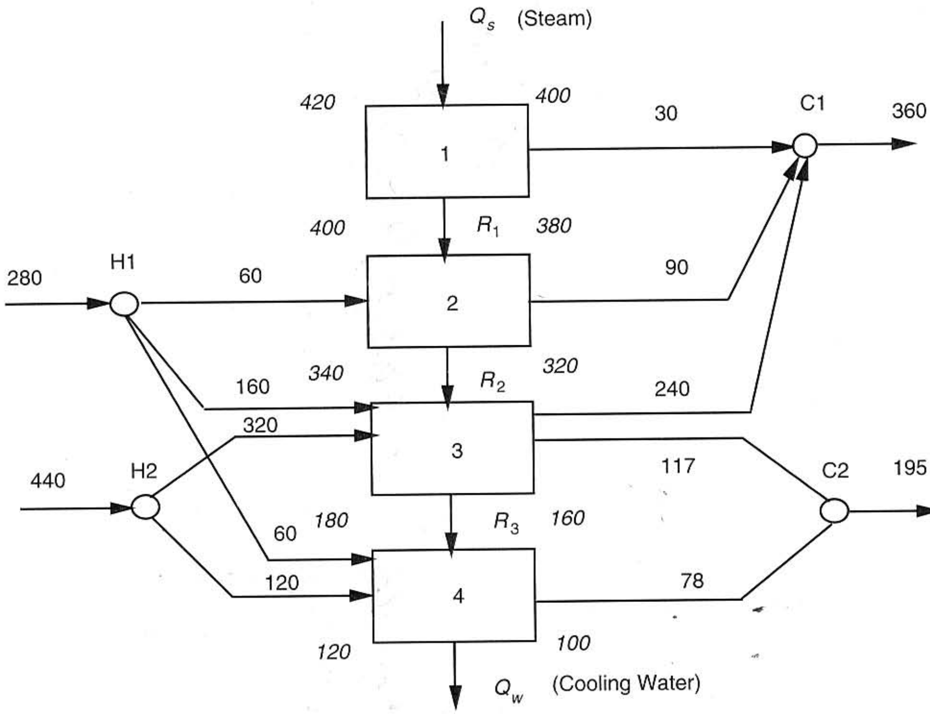


FIGURE 16.1 Heat cascade diagram.

the heat can be allocated to the destinations (cold streams) at a given temperature interval, the excess is cascaded down to lower temperature intervals through the heat residuals.

To show how we can formulate the minimum utility consumption in Table 16.1 as an LP transshipment problem, let us consider first the heat balances around each temperature level in Figure 16.1. These are given by:

$$\begin{aligned} R_1 + 30 &= Q_s \\ R_2 + 90 &= R_1 + 60 \\ R_3 + 357 &= R_2 + 480 \\ Q_w + 78 &= R_3 + 180 \end{aligned} \tag{16.1}$$

From Eq. (16.1) it is clear that we have a system of 4 equations in 5 unknowns: R_1, R_2, R_3, Q_s, Q_w. Thus, there is one degree of freedom, which in turn implies that we have an optimization problem.

By considering the objective of minimization of utility loads, rearranging Eq. (16.1) and introducing nonnegativity constraints on the variables, our problem can be formulated as the LP:

$$\begin{aligned} &\min Z = Q_s + Q_w \\ &s.t.\quad R_1 - Q_s = -30 \\ &\qquad R_2 - R_1 = -30 \\ &\qquad R_3 - R_2 = 123 \\ &\qquad Q_w - R_3 = 102 \\ &\qquad Q_s, Q_w, R_1, R_2, R_3 \geq 0 \end{aligned} \tag{16.2}$$

If we solve this problem with a standard LP package (e.g., LINDO), we obtain for the utilities $Q_s = 60$ MW, $Q_w = 225$ MW, and for the residuals $R_1 = 30$ MW, $R_2 = 0$, $R_3 = 123$ MW. Since $R_2 = 0$ this means that we have a pinch point at the temperature level 340°–320°C, which lies between intervals 2 and 3 (see Figure 16.1).

The above example then shows that we can formulate the minimum utility consumption problem as an LP. This model is actually equivalent to the calculation of the problem table that was given in Part III. This can be shown if we rearrange the constraints in Eq. (16.2) by successively substituting for the heat residuals so as to leave the right-hand sides as a function of Q_s; that is,

$$\begin{aligned} &\min Z = Q_s + Q_w \\ &s.t.\quad R_1 = Q_s - 30 \\ &\qquad R_2 = R_1 - 30 = Q_s - 60 \\ &\qquad R_3 = R_2 + 123 = Q_s + 63 \\ &\qquad Q_w = R_3 + 102 = Q_s + 165 \\ &\qquad R_1, R_2, R_3, Q_s, Q_w \geq 0 \end{aligned} \tag{16.3}$$

Suppose we now want to determine the smallest Q_s such that all the variables in the left-hand side are nonnegative. Clearly if $Q_s = 0$, the largest violation of the nonnegativity constraints will be −60 in the second equation of Eq. (16.3). Therefore, if we set $Q_s = 60$ MW, this will be the smallest value for which we can satisfy all nonnegativity constraints. By then substituting for this value in Eq. (16.3), we get $R_1 = 30$, $R_2 = 0$, $R_3 = 123$, $Q_W = 225$, which is the same result that we obtained for the *LP* in Eq. (16.2).

Thus, we have shown that the LP for minimum utility consumption leads to equivalent results as the problem table given in Chapter 10. We may then wonder what the advantages are of having such a model. As we will see, the transshipment model can be easily generalized to the case of multiple utilities, and where the objective function corresponds to minimizing the utility cost. Furthermore, we will show in the next sections how this model can be expanded so as to handle constraints on the matches, and so as to predict the matches for minimizing the number of units. In Chapters 17 and 18 we will also see how we can embed the equations of the transshipment model within an optimization model for synthesizing a process system (e.g. separation sequences, process flowsheets) where the flows of the process streams are unknown.

The transshipment model for predicting the minimum utility cost given an arbitrary number of hot and cold utilities can be formulated as follows. First, we consider that we have K temperature intervals that are based on the inlet temperatures of the process streams, highest and lowest stream temperatures, and of the intermediate utilitites whose inlet temperatures fall within the range of the temperatures of the process streams (see Chapter 10). We assume as in the above example that the intervals are numbered from the top to the bottom. We can then define the following index sets:

$$\begin{aligned} H_k &= \{\, i \mid \text{hot stream } i \text{ supplies heat to interval } k\} \\ C_k &= \{\, j \mid \text{cold stream } j \text{ demands heat from interval } k\} \\ S_k &= \{\, m \mid \text{hot utility } m \text{ supplies heat to interval } k\} \\ W_k &= \{\, n \mid \text{cold utility } n \text{ extracts heat from interval } k\} \end{aligned} \tag{16.4}$$

When we consider a given temperature interval k, we will have the following known parameters and variables (see Figure 16.2):

Known parameters:	Q^H_{ik}, Q^c_{jk}	heat content of hot stream i and cold stream j in interval k
	c_m, c_n	unit cost of hot utility m and cold utility n
Variables:	Q^S_m, Q^W_n	heat load of hot utility m and cold utility n
	R_k	heat residual exiting interval k

The minimum utility cost for a given set of hot and cold processing streams can then be formulated as the LP (Papoulias and Grossmann, 1983):

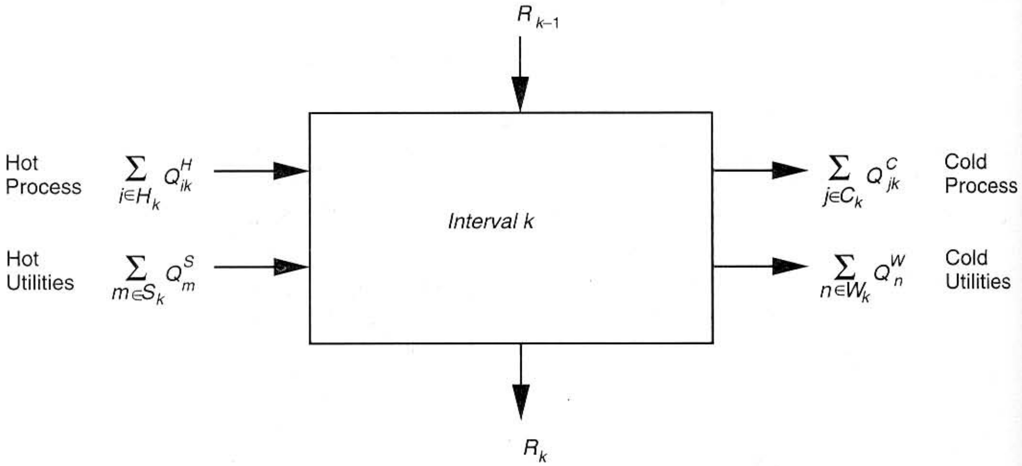


FIGURE 16.2 Heat flows in interval k.

$$\min Z = \sum_{m \in S} c_m Q_m^S + \sum_{n \in W} c_n Q_n^W$$
$$s.t.\ R_k - R_{k-1} - \sum_{m \in S_k} Q_m^S + \sum_{n \in W_k} Q_n^W = \sum_{i \in H_k} Q_{ik}^H - \sum_{j \in C_k} Q_{jk}^C \qquad k = 1, \dots K \tag{16.5}$$
$$Q_m^S \geq 0 \quad Q_n^W \geq 0 \quad R_k \geq 0 \quad k = 1, \dots K-1$$
$$R_0 = 0,\ R_K = 0$$

In the above, the objective function represents the total utility cost, while the K equations are heat balances around each temperature interval k. Note that this LP will in general be rather small as it will have K rows and $n_H + n_c + K - 1$ variables. The model in Eq. (16.5) we will denote as the condensed LP transshipment model to differentiate it from the LP that will be given in section 16.3 for constrained matches. It should also be noted that in the above formulation it would be very easy to impose upper limits on the heat loads that are available from some of the utilities (e.g., maximum heat from low pressure steam).

EXAMPLE 16.2

Given the data in Table 16.2 for two hot and two cold processing streams and two hot and one cold utility, determine the minimum utility cost with the LP transshipment model in Eq. (16.5). By considering the temperature intervals in Table 16.3, and calculating the heat contents of the process streams at each interval, the *LP* for this example is:

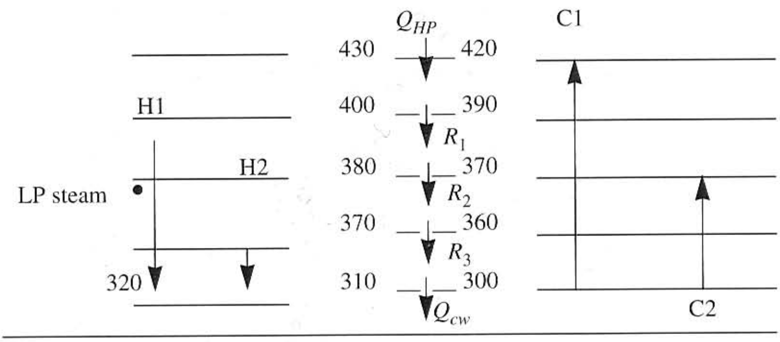
$$\begin{aligned} \min Z = \quad & 80000\, Q_{HP} + 50000\, Q_{LP} + 20000\, Q_{CW} \\ s.t. \quad & R_1 - Q_{HP} = -60 \\ & R_2 - R_1 = 10 \\ & R_3 - R_2 - Q_{LP} = -15 \\ & -R_3 + Q_{CW} = 75 \\ & R_1, R_2, R_3, Q_{HP}, Q_{LP}, Q_{CW} \geq 0 \end{aligned} \tag{16.6}$$

TABLE 16.2 Data for Example 16.2

	FCp (MW/K)	T_{in}(K)	T_{out}(K)
H1	2.5	400	320
H2	3.8	370	320
C1	2	300	420
C2	2	300	370

HP Steam: 500K $80/kWyr
LP Steam: 380K $50/kWyr
Cooling Water: 300K $20/kWyr
Minimum Recovery Approach Temperature (HRAT): 10K

TABLE 16.3 Temperature Intervals of Example 16.2



The solution to this LP yields the following results:

Utility cost: $Z = 6{,}550{,}000$ \$/yr.
Heat load high pressure steam: $Q_{HP} = 60\ MW$
Heat load low pressure steam: $Q_{LP} = 5\ MW$
Heat load cooling water: $Q_{CW} = 75\ MW$
Residuals: $R_1 = 0$, $R_2 = 10\ MW$, $R_3 = 0$.

The two above zero residuals imply that there are two pinch points for this problem: at 400–390 K, and at 370–360 K. This means that the temperature intervals in this problem can be partitioned into three subnetworks:

Subnetwork 1:	above 400–390 K
Subnetwork 2:	between 400–390 K and 370–360 K
Subnetwork 3:	below 370–360 K

16.2.2 Minimum Utility Cost with Constrained Matches

In practice it might not always be desirable or possible to exchange heat between any given pair of hot and cold streams. This could be due to the fact that the streams are too far apart or because of other operational considerations such as control, safety or startup. Therefore, it would be clearly desirable to extend our LP transshipment formulation to the case when we impose certain constraints on the matches. The most common would simply be to forbid the heat exchange between certain pairs of streams. We could also think of requiring that a minimum or maximum amount of heat be exchanged between certain pairs of streams (e.g. forcing the use of utilities on some of the streams).

The LP transshipment model in Eq. (16.5) implicitly assumes that any given pair of hot and cold streams can exchange heat since there was no information as to which pairs of streams actually exchange heat. In order to develop an LP formulation where we do have that information, we can consider the two following alternative models:

1. Transportation model where we consider directly all the feasible links for heat exchange between each pair of hot and cold streams over their corresponding temperature intervals (Cerda and Westerberg, 1983). Figure 16.3 illustrates this representation for Example 16.1.
2. Expanded transshipment model (Papoulias and Grossmann, 1983) where we consider within each temperature interval a link for the heat exchange between a given pair of hot and cold streams, where the cold stream is present at that interval and the hot stream is either also present, or else it is present in a higher temperature interval. Figure 16.4 illustrates this representation for Example 16.1.

In principle we could use either of the two representations. However, we will concentrate on the second one for continuity with the previous section, and also because it leads to LP problems of smaller size. So let us now try to explain in greater detail on how the representation in Figure 16.4 is obtained.

The basic idea in the expanded transshipment model is as follows. First, instead of assigning a single overall heat residual R_k exiting at each temperature level k, we will assign individual heat residuals R_{ik}, R_{mk} for each hot stream i and each hot utility m that are present at or above that temperature interval k. Secondly, within that interval k we will define the variable Q_{ijk} to denote the heat exchange between hot stream i and a cold stream j. Likewise, we can define similar variables for the exchange between process streams and

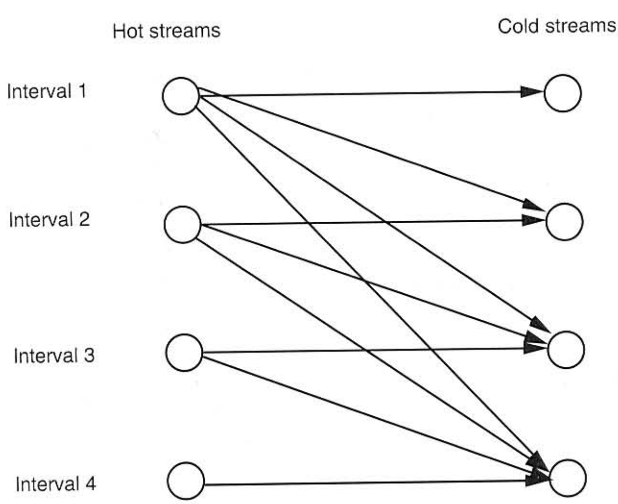


FIGURE 16.3 Representation of heat flows for transportation model.

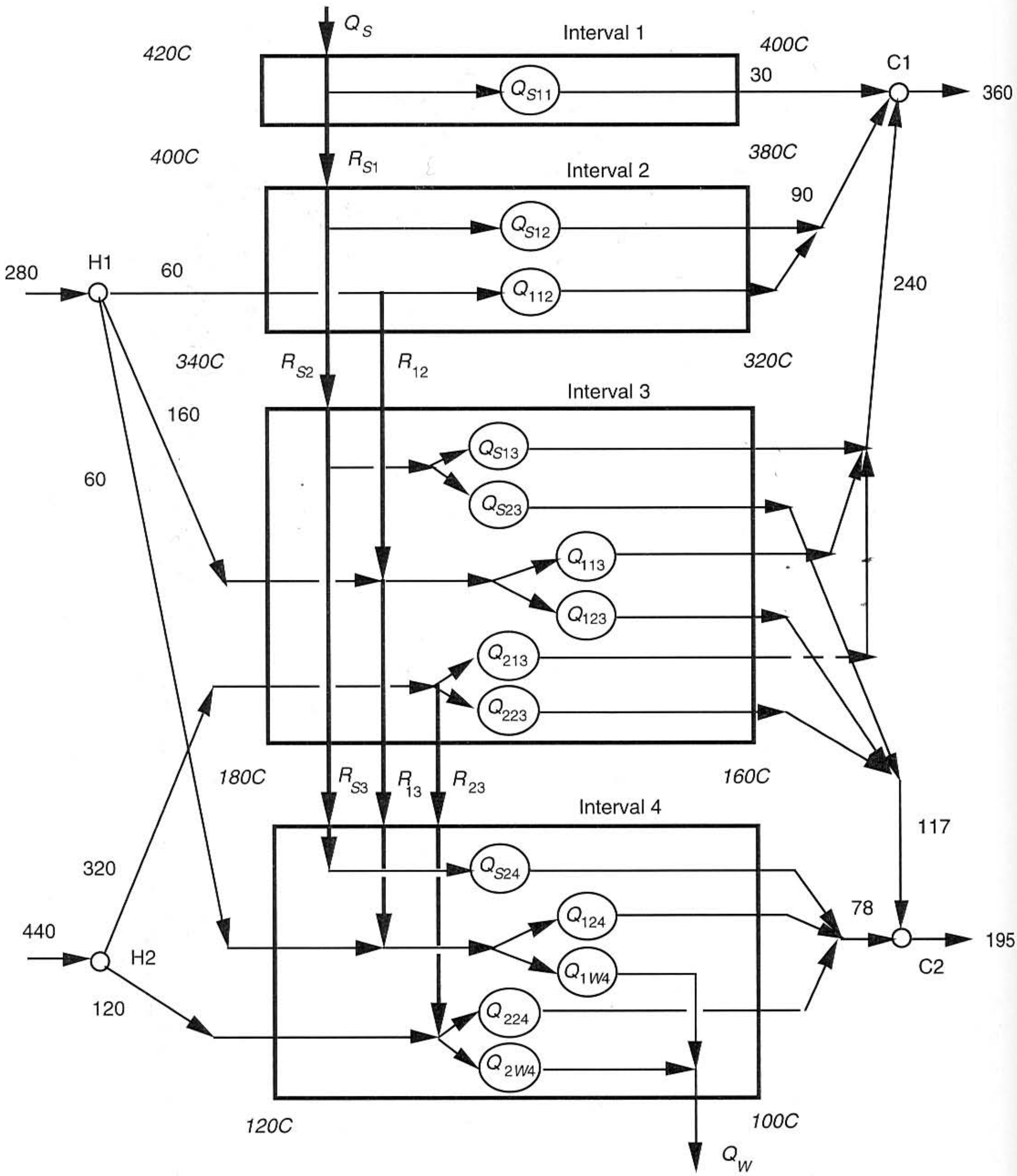


FIGURE 16.4 Representation of expanded transshipment model for Example 16.1.

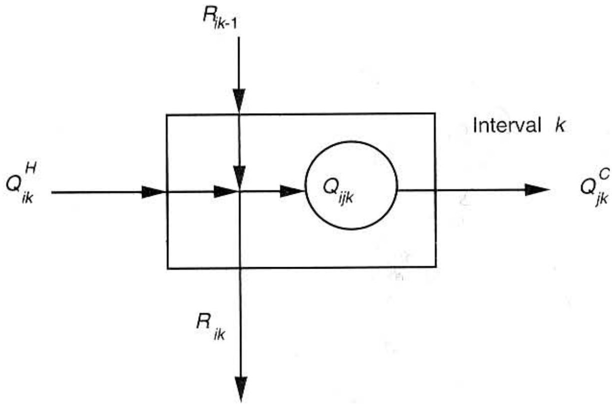


FIGURE 16.5 Interval for expanded transshipment model.

utilities. Figure 16.5 illustrates the above ideas for an interval k where we consider a hot stream i and a cold stream j.

We should note that in general a given pair of streams can exchange heat within a given temperature interval k if either of the two following conditions hold:

1. Hot stream i and cold stream j are present in interval k. This case is obvious as seen in Figure 16.5.
2. Cold stream j is present in interval k, but hot stream i is only present at a higher temperature interval. An example of this case is shown in Figure 16.6, where hot stream i can exchange heat at interval 3, although it is not present there. The reason the heat exchange can take place is simply because hot stream i is transferring heat to interval 3 through the residual R_{i2} that is coming from interval 2. Another example is shown in Figure 16.4 where steam can exchange heat with cold stream C1 at interval 2.

Based on the above observations we can then formulate an expanded LP transshipment model where we do include the information on the exchange of heat between any given pair of streams. Let us define first the following index sets:

$$H'_k = \{i \mid \text{hot stream } i \text{ is present at interval } k \text{ or at a higher interval}\} \qquad (16.7)$$
$$S'_k = \{m \mid \text{hot utility } m \text{ is present at interval } k \text{ or at a higher interval}\}$$

The index sets C_k, W_k are defined the same as in Eq. (16.4).

As for the parameters and variables, we will have the following (see Figure 16.7):

Q_{ijk}: Exchange of heat of hot stream i and cold stream j at interval k
Q_{mjk}: Exchange of heat of hot utility m and cold stream j at interval k
Q_{ink}: Exchange of heat of hot stream i and cold utility n at interval k (16.8)
R_{ik}: Heat residual of hot stream i exiting interval k
R_{mk}: Heat residual of hot utility m exiting interval k

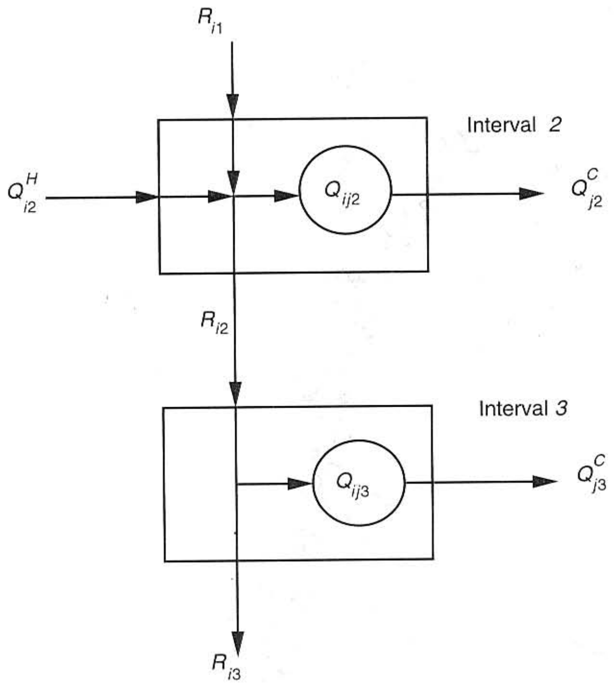


FIGURE 16.6 Example of heat flows in case a hot stream does not provide heat to all intervals.

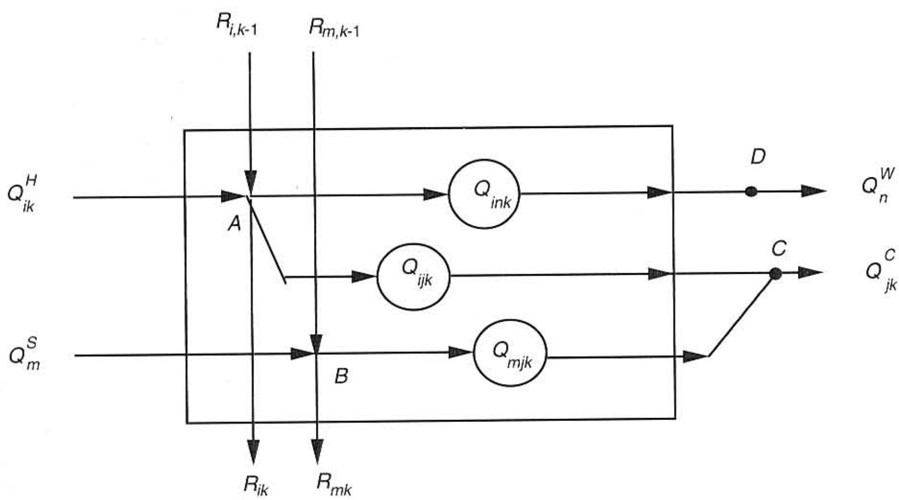


FIGURE 16.7 Heat flows in expanded transshipment model.

The variables Q^S_m, Q^W_n and the parameters Q^H_{ik}, Q^C_{jk}, c_m, c_n are identical to those of the previous section.

In contrast to the compact LP transshipment model Eq. (16.5) where we simply did an overall heat balance around each temperature level, in this case we have to perform balances at the following points within each temperature interval:

1. For the hot process and utility streams at the internal nodes that relate the heat content, residuals, and heat exchanges (i.e., nodes A and B in Figure 16.7).
2. For the cold process and utility streams at the destination nodes that relate the heat content and heat exchanges (i.e., nodes C and D in Figure 16.7).

In this way the expanded LP transshipment model by Papoulias and Grossmann (1983) can be formulated as:

$$\min\ Z = \sum_{m\in S} c_m Q^S_m + \sum_{n\in W} c_n Q^W_n$$

$$\begin{aligned}
\text{s.t.}\quad & R_{ik} - R_{i,k-1} + \sum_{j\in C_k} Q_{ijk} + \sum_{n\in W_k} Q_{ink} = Q^H_{ik} \quad i \in H'_k \\
& R_{mk} - R_{m,k-1} + \sum_{j\in C_k} Q_{mjk} - Q^S_m = 0 \quad m \in S'_k \\
& \sum_{i\in H_k} Q_{ijk} + \sum_{m\in S_k} Q_{mjk} = Q^C_{jk} \quad j \in C_k \\
& \sum_{i\in H_k} Q_{ink} - Q^W_n = 0 \qquad n \in W_k \quad k = 1,\ldots K \\
& R_{ik},\ R_{mk},\ Q_{ijk},\ Q_{mjk},\ Q_{ink},\ Q^S_m,\ Q^W_n \geq 0 \\
& R_{i0} = R_{iK} = 0
\end{aligned} \tag{16.9}$$

Note that the size of this LP is obviously larger than the one in Eq. (16.5). The importance of the formulation in Eq. (16.9) is the fact that we can very easily specify constraints on the matches. For example, if we want to forbid a match between hot i and cold j all we need to do is to set $Q_{ijk} = 0$ for all intervals k. Or, alternatively, we just simply delete these variables from our formulation. For the case when we want to impose a given match we can do this by specifying that its total heat exchange, which is the sum of Q_{ijk} over all intervals, must lie within some specified lower and upper bounds. That is,

$$Q^L_{ij} \leq \sum_{k=1}^{K} Q_{ijk} \leq Q^U_{ij} \tag{16.10}$$

Obviously we can also simply specify a fixed value for the sum in Eq. (16.10).

EXAMPLE 16.3

Let us consider the example in Table 16.1 that we examined in section 16.2. For that example we found that by not imposing any restriction on the matches, the minimum heating is 60 MW, and the minimum cooling is 225 MW. If the cost of the heating and cooling utilities is $80/kWyr and $20/kWyr, respectively, this would mean an annual cost of $9,300,000/yr. In addition, we found a pinch point at 340–320°C. Let us assume now that we were to impose as a constraint that the match for stream H1 and C1 is forbidden. Referring to Figure 16.4, the formulation in Eq. (16.9) leads to the LP problem shown in Table 16.4. The solution to this LP is as follows:

Minimum utility cost	Z	= $15,300,000/yr
Heating utility load	Q_S	= 120 MW
Cooling utility load	Q_W	= 285 MW

TABLE 16.4 Expanded LP for Restricted Match in Example 16.3

Utility Cost:	$\min Z = 80000\, Q_S + 20000 Q_W$
Interval 1:	s.t. $R_{S1} + Q_{S11} - Q_S = 0$
	$Q_{S11} = 30$
Interval 2:	$R_{12} + Q_{112} = 60$
	$R_{S2} - R_{S1} + Q_{S12} = 0$
	$Q_{S12} + Q_{112} = 90$
Interval 3:	$R_{13} - R_{12} + Q_{113} + Q_{123} = 160$
	$R_{23} + Q_{213} + Q_{223} = 320$
	$R_{S3} - R_{S2} + Q_{S13} + Q_{S23} = 0$
	$Q_{113} + Q_{213} + Q_{S13} = 240$
	$Q_{123} + Q_{223} + Q_{S23} = 117$
Interval 4:	$-R_{13} + Q_{124} + Q_{1W4} = 60$
	$-R_{23} + Q_{224} + Q_{2W4} = 120$
	$-R_{S3} + Q_{S24} = 0$
	$Q_{124} + Q_{224} + Q_{S24} = 78$
	$Q_{1W4} + Q_{2W4} - Q_W = 0$
Forbidden match:	$Q_{112} = Q_{113} = 0$ (H1–C1 do not exchange heat)

In other words, the heating utility consumption has doubled, while the utility cost has increased by $6,000,000/yr with respect to the case when no matches are forbidden. In addition, there is no longer a pinch point since the sum of heat residuals exiting each interval is greater than zero. It is interesting to note that if we specify the match H2–C2 as a forbidden match, the utility cost will be identical to the case when no constraints are imposed. This example, then, shows that by imposing constraints on the matches the minimum utility cost may or may not increase.

16.2.3 Prediction of Matches for Minimizing the Number of Units

As was shown in Chapter 10, the fewest number of units in a network is very often equal to the number of process streams and utilities minus one. This estimate applies either to each subnetwork when we partition the problem by pinch points or to the overall network when we do not perform the partitioning. In this section we will show how we can extend the expanded transshipment model Eq. (16.9) to rigorously predict the actual number of fewest units, as well as the stream matches that are involved in each unit, and the amount of heat that they must exchange.

Our first reaction might be to think that the expanded LP in Eq. (16.9) is already giving us the information on the stream matches, and that therefore we can work from there the required number of units. The reason why this is not true in general, is because the objective function in Eq. (16.9) does not have the information that we want to minimize the number of units. In fact, it is quite possible to have solutions of the expanded LP that have the same minimum cost but involve different number of matches. Therefore, it is clear that we require a formulation where we explicitly include the objective of minimizing number of matches.

Since at this point we would have performed the minimum utility cost calculation with or without match constraints, we would know the heat loads of the heating and cooling utilities. Therefore, at this point hot process streams and hot utilities can be treated simply as additional hot streams i, while cold process streams and cold utilities can be treated as cold streams j.

Assume we partition our problem into subnetworks. Each subnetwork q will then have an associated set of K_q temperature intervals. In addition, to represent the potential match of a given pair of hot and cold streams, we will define the following binary variables at the subnetwork q:

$$y_{ij}^q = \begin{cases} 1 & \text{hot stream } i\text{, cold stream } j \text{ exchange heat} \\ 0 & \text{hot stream } i\text{, cold stream } j \text{ do not exchange heat} \end{cases} \tag{16.11}$$

It should be noted that for each of the predicted matches as given by the above binary variables with a value of one, we will be able to associate it to a single exchanger unit. Therefore, the sum of units in the subnetwork will be simply given by the sum of the binary variables in Eq. (16.11). Since our objective is to minimize the number of units, it can be expressed as:

$$\min \sum_{i \in H} \sum_{j \in C} y_{ij}^q \tag{16.12}$$

As for the constraints, we will use the heat balances in Eq. (16.9) since they contain the information on the heat exchange between pairs of streams. However, we can simplify these equations for the two following reasons. One is that we know the heat contents of the utility streams, the other is that we use a common index i for hot process and utility streams, and the common index j for cold process and utility streams. In this way, the equations for the heat balances can be written for each interval k as:

$$R_{ik} - R_{i,k-1} + \sum_{j \in C_k} Q_{ijk} = Q_{ik}^H \qquad i \in H_k' \qquad k = 1, \ldots K_q$$

$$\sum_{i \in H_k} Q_{ijk} = Q_{jk}^C \qquad j \in C_k \tag{16.13}$$

$$R_{ik}, Q_{ijk} \geq 0$$

Finally, in a similar way as in the fixed cost charge model that we considered in Chapter 15, we need a logical constraint that states that if the binary variable is zero, the associated continuous variable must also be zero. In this case, we want to express the fact that if the match is not selected (i.e., $y_{ij}^q = 0$), then the heat exchanged for that match should also be zero. For any pair of hot i and cold j, this constraint can be written as:

$$\sum_{k=1}^{K_q} Q_{ijk} - U_{ij}\, y_{ij}^q \leq 0 \tag{16.14}$$

In this case, the upper bound U_{ij} will be given by the smallest of the heat contents of the two streams. For example, if hot i has 100 MW and cold j has 200 MW, then we can set U_{ij} to 100 MW as this is the maximum amount of heat that the two streams can exchange.

In this way, the problem defined by the objective function in Eq. (16.12), subject to the heat balances in Eq. (16.13), the logical constraints in Eq. (16.14), zero-one constraints in Eq. (16.11), and non-negativity constraints for the heat residuals and heat exchanges in Eq. (16.13), corresponds to an MILP transshipment problem (Papoulias and Grossmann, 1983). This problem we can solve independently for each subnetwork q (as implied by the above equations) or simultaneously over all the subnetworks. We can, of course, also develop a virtually identical formulation when we do not partition the problem into subnetworks.

The solution of the MILP transshipment problem will then indicate the following:

- Matches that take place $\left(y_{ij}^q = 1\right)$
- Heat exchanged at each match $\sum_{k=1}^{K_q} Q_{ijk}$

This information can then be used to derive a network structure, either manually or automatically, as will be shown in the next section.

An important point to be noted here is the fact that the solution of this MILP is not necessarily unique. This follows from the fact that there might be several network configurations for the same number of units and utility cost. Furthermore, a given network configuration may not necessarily have its heat loads defined in a unique way due to the presence of heat loops.

EXAMPLE 16.4

Let us consider again the problem in Table 16.1. We will assume that no constraints are imposed on the matches, so that 60 MW will be required for the heating and 225 MW for the cooling. Referring to Figure 16.8, which follows from Figure 16.4, Eqs. (16.12) to (16.14) lead to the problem shown in Table 16.5. If we solve the MILP, the solution that we obtain involves the six following matches:

Above pinch:

Match Steam–C1	60 MW	($y_{S1A} = 1$, $Q_{S11} = 30$, $Q_{S12} = 30$)
Match H1–C1	60 MW	($y_{11A} = 1$, $Q_{112} = 60$)

Below pinch:

Match H1–C1	25 MW	($y_{11B} = 1$, $Q_{113} = 25$)
Match H1–C2	195 MW	($y_{12B} = 1$, $Q_{123} = 117$, $Q_{124} = 78$)
Match H2–C1	215 MW	($y_{21B} = 1$, $Q_{123} = 215$)
Match H2–W	225 MW	($y_{2WB} = 1$, $Q_{2W4} = 225$)

TABLE 16.5 MILP Model for Example 16.4

Number of units:		$\min Z = y_{S1}{}^A + y_{11}{}^A + y_{11}{}^B + y_{12}{}^B + y_{1W}{}^B + y_{21}{}^B + y_{22}{}^B + y_{2W}{}^B$
Interval 1:	s.t.	$R_{S1} + Q_{S11} = 60$ $Q_{S11} = 30$
Interval 2:		$R_{12} + Q_{112} = 60$ $R_{S2} - R_{S1} + Q_{S12} = 0$ $Q_{S12} + Q_{112} = 90$
Interval 3:		$R_{13} - R_{12} + Q_{113} + Q_{123} = 160$ $R_{23} + Q_{213} + Q_{223} = 320$ $Q_{113} + Q_{213} + Q_{S13} = 240$ $Q_{123} + Q_{223} + Q_{S23} = 117$
Interval 4:		$-R_{13} + Q_{124} + Q_{1W4} = 60$ $-R_{23} + Q_{224} + Q_{2W4} = 120$ $Q_{124} + Q_{224} + Q_{S24} = 78$ $Q_{1W4} + Q_{2W4} = 225$
Matches above pinch:		$Q_{S11} + Q_{S12} - 60\, y_{S1}{}^A \leq 0$ $Q_{112} - 60\, y_{11}{}^A \leq 0$
Matches below pinch:		$Q_{113} - 220\, y_{11}{}^B \leq 0$ $Q_{123} + Q_{124} - 195\, y_{12}{}^B \leq 0$ $Q_{1W4} - 220\, y_{1W}{}^B \leq 0$ $Q_{213} - 240\, y_{21}{}^B \leq 0$ $Q_{223} + Q_{224} - 60\, y_{22}{}^B \leq 0$ $Q_{2W4} - 225\, y_{2W}{}^B \leq 0$

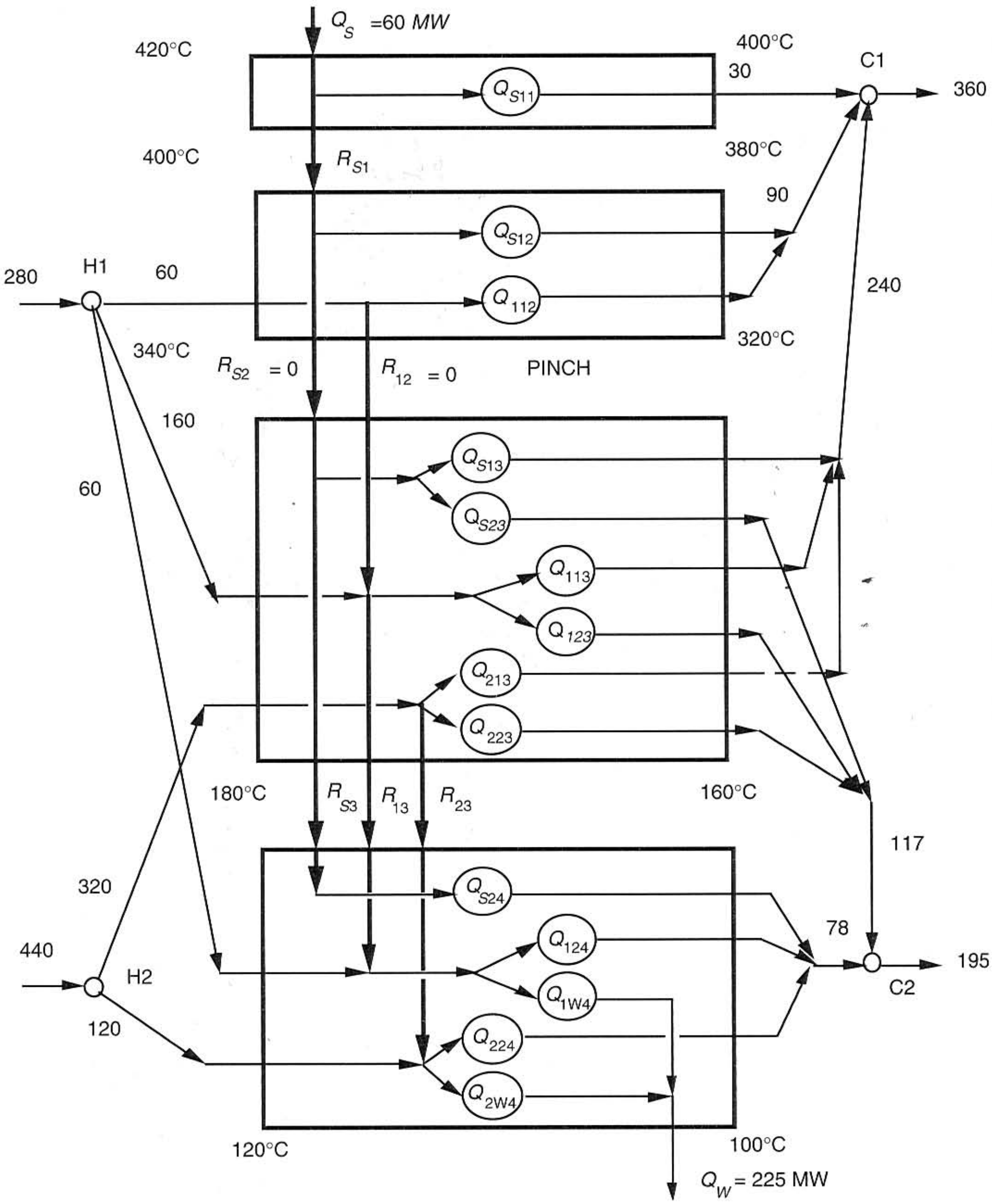


FIGURE 16.8 Representation of heat flows in MILP transshipment.

Based on the above information of matches and heat loads, we can manually derive the network configuration, shown in Figure 16.9, with six units. The solution of the MILP, however, is not unique. If we set the binary variable $y^B_{11} = 0$ for the match H1–C1 below the pinch, we obtain a different set of six matches:

Above pinch:

Match Steam–C1	60 MW	$(y_{s1A} = 1, Q_{s11} = 30, Q_{s12} = 30)$
Match H1–C1	60 MW	$(y_{11A} = 1, Q_{112} = 60)$

Below pinch:

Match H1–C2	195 MW	$(y_{12B} = 1, Q_{123} = 117, Q_{124} = 78)$
Match H2–C1	240 MW	$(y_{21B} = 1, Q_{213} = 240)$
Match H1–W	25 MW	$(y_{1WB} = 1, Q_{1WB} = 25)$
Match H2–W	200 MW	$(y_{2WB} = 1, Q_{2WB} = 200)$

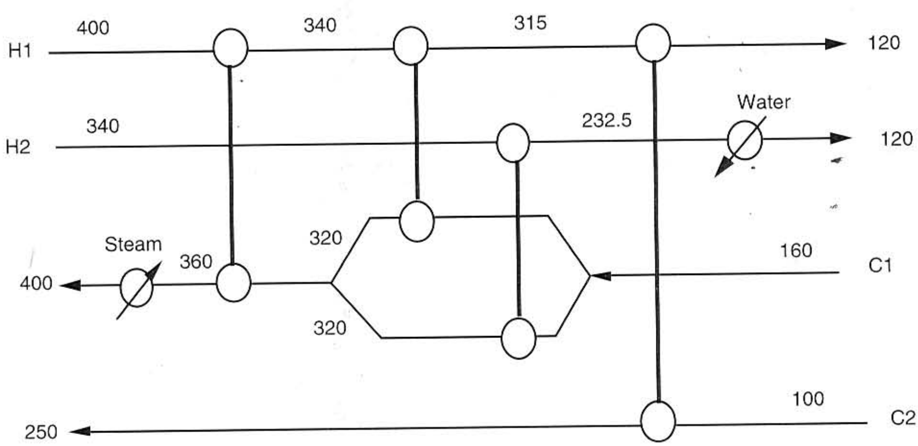


FIGURE 16.9 Network configuration for matches predicted from MILP in Example 16.4.

Thus, there are different matches and changes in the heat loads below the pinch. The above matches can be translated into the network configuration shown in Figure 16.10.

Finally, we could also solve the above MILP problem without partitioning into subnetworks. In this case, the only change required in the formulation of Table 16.5 is that for each potential match only one binary variable is defined, and the logical conditions are written also for each potential match. For example, the match H1–C1 is denoted by the binary y_{11}, and its logical condition is given by (see Figure 16.8):

$$Q_{112} + Q_{113} - 220\, y_{11} \leq 0$$

If we solve the MILP with no pinch partitioning, we obtain the following five matches:

Match Steam–C1	60 MW
Match H1–C1	85 MW
Match H1–C2	195 MW

Match H2–C1	215 MW
Match H2–W	225 MW

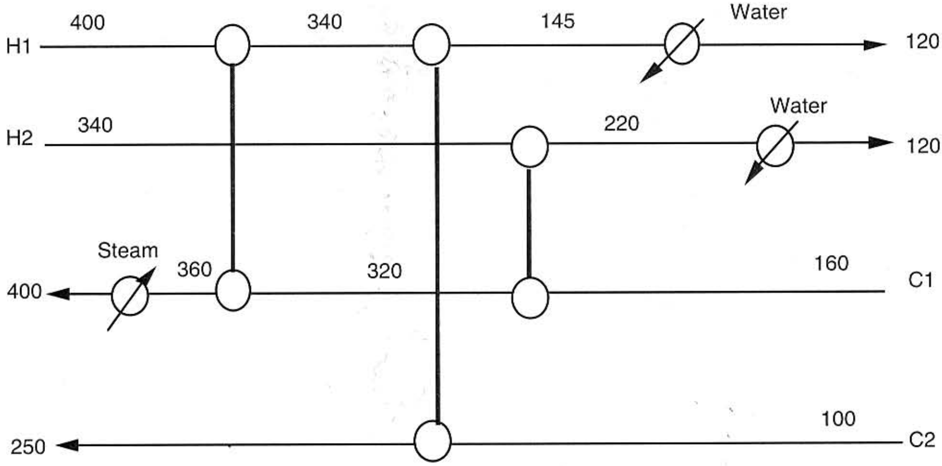


FIGURE 16.10 Alternative network configuration for Example 16.4.

These results would suggest that we should be able to derive a network with only five units. This is, in fact, possible if the match H1–C1 is placed across the pinch, has a driving force equal to the temperature approach (20°C), and if we introduce bypass streams in the network (see Wood et al., 1985). The configuration that has been derived manually for the above five matches is shown in Figure 16.11. Note that the match H1–C1 would require a large area due to its small driving force. It is of course not that trivial to derive manually a network like the one in Figure 16.11. Can we possibly automate this procedure?

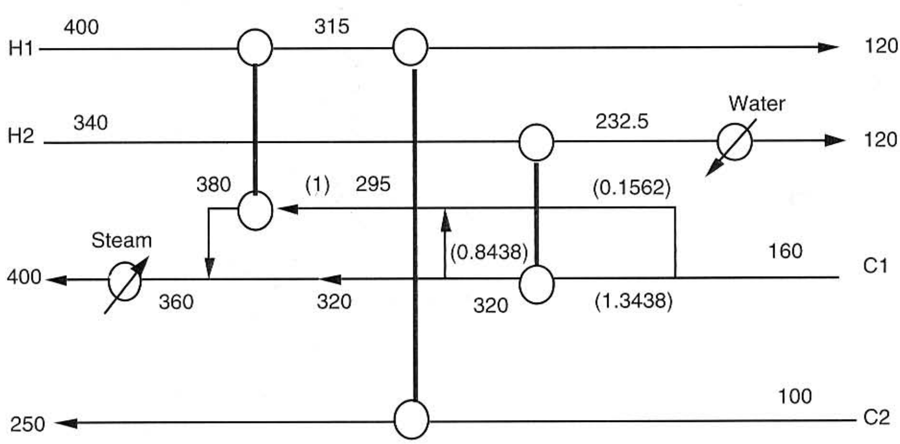


FIGURE 16.11 Five-unit network for Example 16.4.

16.2.4 Automatic Derivation of Network Structures

In this section we will show how we can make use of the information provided by the MILP transshipment model to automatically derive heat exchanger network configurations (Floudas, Ciric, and Grossmann, 1986).

The basic idea here will be to postulate a superstructure for each stream that has the following characteristics:

- Each exchanger unit in the superstructure corresponds to a match predicted by the MILP transshipment model (with or without pinch partitioning). Each exchanger will also have as heat load the one predicted by the MILP.
- The superstructure will contain those stream interconnections among the units that can potentially define all configurations with no stream splitting, with stream splitting and mixing, and with possible bypass streams. The stream interconnections will be treated as unknowns that must be determined.

An example of such a superstructure is given in Figure 16.12 for the case of one hot and two cold streams in which the two predicted matches are H1–C1 and H1–C2. Note that in this superstructure stream H1 is split initially into two streams that are directed to the two units. The outlets of these units are then also split into two streams: one that is directed to the inlet of the other unit, and one that is directed to the final mixing point.

By "deleting" some of the streams in the superstructure of Figure 16.12, we can easily verify that it has embedded all possible network configurations for the two matches. As shown in Figure 16.13, we have embedded the following alternatives:

1. Units H1–C1, H1–C2 in series
2. Units H1–C2, H1–C1 in series

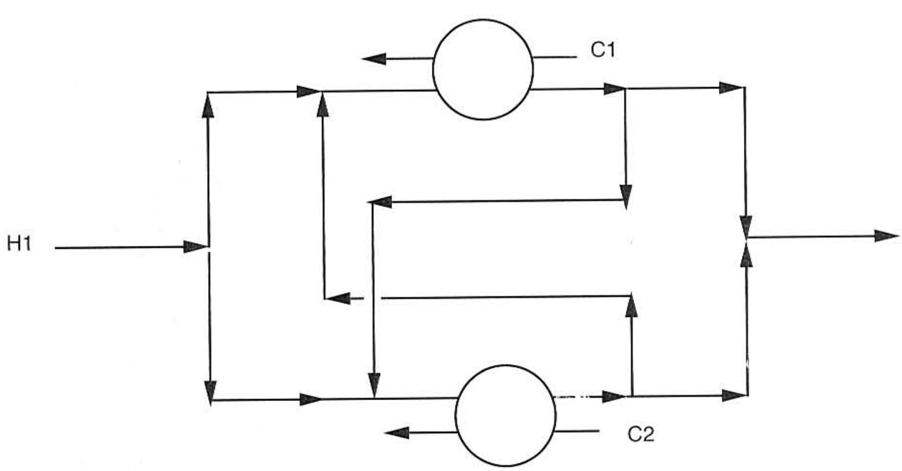


FIGURE 16.12 Superstructure for matches H1–C1, H1–C2.

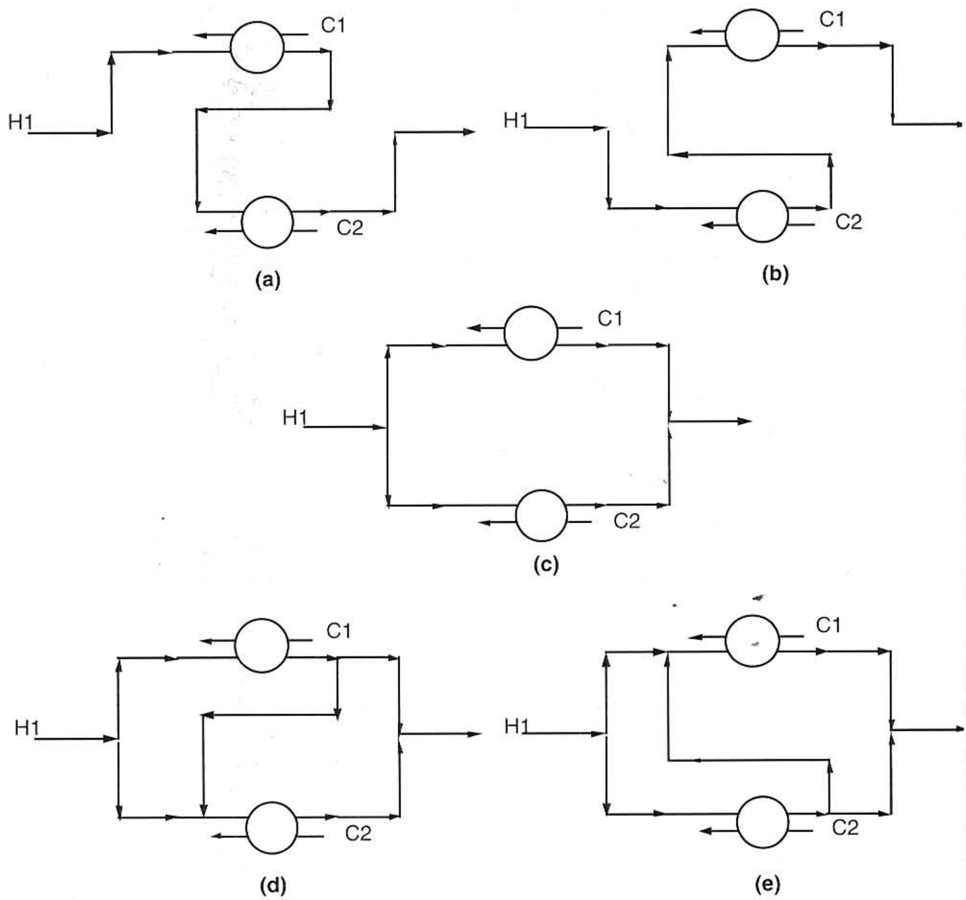


FIGURE 16.13 Alternatives embedded in the superstructure of Figure 16.12.

3. Units H1–C1, H1–C2 in parallel
4. Units H1–C1, H1–C2 in parallel with bypass to H1–C2
5. Units H1–C1, H1–C2 in parallel with bypass to H1–C1

Thus, in the network superstructure of Figure 16.12 we have embedded all possible configurations for a two-unit network.

Before we consider the extension of the superstructure to an arbitrary number of stream matches, let us see how we can model the superstructure in Figure 16.12 in order to determine the network structure with minimum investment cost. First, we assign the variables representing heat capacity flowrates (F, f), temperatures (T, t), heat loads (Q), and areas as shown in Figure 16.14. Note that the following variables are known:

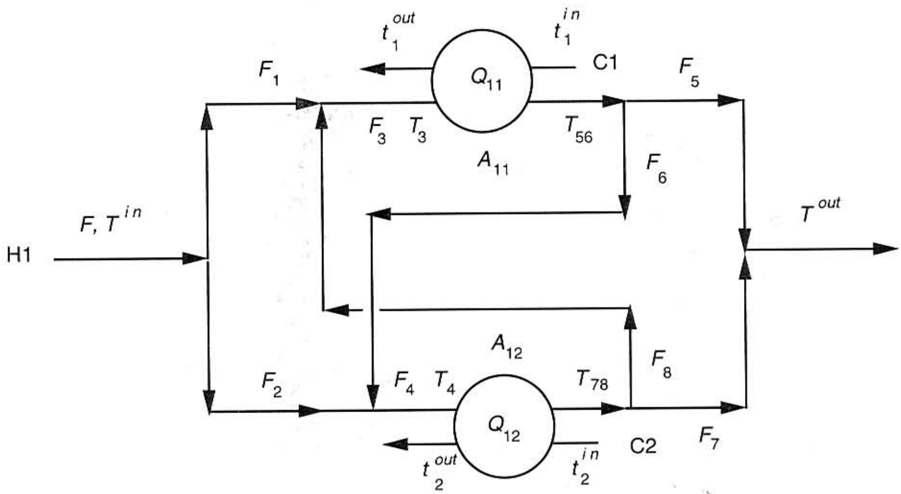


FIGURE 16.14 Variables for superstructure with two matches.

- For stream H1, the heat capacity flowrate F, and the inlet and outlet temperatures T^{in}, T^{out}.
- For stream C1, the heat capacity flowrate f_1 and the inlet and outlet temperatures t_1^{in}, t_1^{out}.
- For stream $C2$, the heat capacity flowrate f_2, and the inlet and oulet temperatures t_2^{in}, t_2^{out}.
- The heat loads Q_{11}, Q_{12} as predicted by the MILP transsphipment model.

The objective function representing the minimization of the investment cost will be given by:

$$\min \ C = c_1 A_{11}^{\beta} + c_2 A_{12}^{\beta} \tag{16.15}$$

where c_1, c_2, β are cost parameters. We can express this objective function in terms of temperatures by replacing the areas through the design equation $Q = \text{UALMTD}$ for countercurrent heat exchangers. However, the LMTD function can lead to numerical difficulties when the temperature differences θ_1, θ_2, at both ends are the same. Therefore, we replace the definition of the LMTD

$$\text{LMTD} = \frac{\theta_2 - \theta_1}{\ell n \dfrac{\theta_2}{\theta_1}} \tag{16.16}$$

by the Chen (1987) approximation $\text{LMTD} \cong [\theta_1 \, \theta_2 \, (\theta_2 + \theta_1)/2]^{1/3}$

That is,

$$\min\ C = C_1\left[\frac{Q_{11}}{U_{11}\left[\theta_1^1\theta_2^1(\theta_1^1+\theta_2^1)/2\right]^{1/3}}\right]^{\beta} + C_2\left[\frac{Q_{12}}{U_{12}\left[\theta_1^2\theta_2^2(\theta_1^2+\theta_2^2)/2\right]^{1/3}}\right]^{\beta} \tag{16.17}$$

where U_{11}, U_{12} are the overall heat transfer coefficients for the two exchangers.

Thus, the constraints that apply to the superstructure are as follows (see Figure 16.13):

1. Mass balance for initial splitter

$$F_1 + F_2 = F \tag{16.18}$$

2. Mass and heat balances for mixers at inlet of two units

$$\begin{aligned} &F_1 + F_8 - F_3 = 0\\ &F_1\,T^{\text{in}} + F_8\,T_{78} - F_3\,T_3 = 0\\ &F_2 + F_6 - F_4 = 0\\ &F_2\,T^{\text{in}} + F_6\,T_{56} - F_4\,T_4 = 0 \end{aligned} \tag{16.19}$$

3. Mass balance for splitters at outlet of exchangers

$$\begin{aligned} &F_3 - F_6 - F_5 = 0\\ &F_4 - F_7 - F_8 = 0 \end{aligned} \tag{16.20}$$

4. Heat balances in exchangers

$$\begin{aligned} &Q_{11} - F_3\,(T_3 - T_{56}) = 0\\ &Q_{12} - F_4\,(T_4 - T_{78}) = 0 \end{aligned} \tag{16.21}$$

5. Definition temperature differences

$$\begin{aligned} &\theta_1^1 = T_3 - t_1^{\text{out}}\\ &\theta_2^1 = T_{56} - t_1^{\text{in}}\\ &\theta_1^2 = T_4 - t_2^{\text{out}}\\ &\theta_2^2 = T_{78} - t_2^{\text{in}} \end{aligned} \tag{16.22}$$

6. Feasibility constraints for temperatures

$$\begin{aligned} &\theta_1^1 \geq \Delta\,T_{\min}\\ &\theta_2^1 \geq \Delta\,T_{\min}\\ &\theta_1^2 \geq \Delta\,T_{\min}\\ &\theta_2^2 \geq \Delta\,T_{\min} \end{aligned} \tag{16.23}$$

7. Nonnegativity conditions on the heat capacity flowrates

$$Fj \geq 0 \qquad j = 1, 2, \ldots 8 \tag{16.24}$$

The optimization problem defined by the objective function in Eq. (16.17) subject to the constraints in Eqs. (16.18) to (16.24) corresponds to a nonlinear programming problem that has as variables the flows F_j, j = 1,2,..8, and the temperatures T_3, T_4, T_{56}, T_{78}. Those flowrates that take a value of zero will then "delete" the streams that are not required in the superstructure.

It should be noted that the likelihood of multiple local optima in this problem is somewhat reduced because the areas of the units cannot take a value of zero due to the fixed heat loads. We may recall the example on selection of reactors in section 15.5 of Chapter 15, where local solutions were mainly due to the deletion of the reactors.

The superstructure and its nonlinear programming formulation can be readily extended to the case of an arbitrary number of stream matches with the following procedure:

1. Develop a superstructure for any stream involving two or more matches according to the following scheme:
   a. Initial split where the streams are directed to all the units in that superstructure.
   b. Outlet of units is split and mixed with the inlets of other units and with the final mixing point.

2. All stream superstructures are joined through an NLP formulation similar to Eqs. (16.17) to (16.23), having the heat loads predicted by the MILP transshipment model Eqs. (16.12) to (16.14).

3. The resulting NLP is solved to obtain the optimal network configuration. This NLP can be solved with a large-scale reduced gradient method (e.g., MINOS).

This strategy for automatic network synthesis has been implemented in the interactive computer program MAGNETS, developed by Amy Ciric, as described by Floudas, Ciric, and Grossmann (1986). The optimization of the minimum temperature approach can be performed in an outer loop, and constraints on matches can be easily handled as discussed in section 16.3. Figure 16.15 shows an example of a network configuration that was automatically synthesized with MAGNETS for the data given in Table 16.6.

16.3 SIMULTANEOUS MINLP MODEL

While the sequential targeting and optimization approach presented in the previous sections has the advantage of decomposing the synthesis problem, it has the disadvantage that the trade-offs between energy, number of units and area are not rigorously taken into account. The reason for this is that the optimization problem:

$$\min \text{Total Cost} = \text{Area Cost} + \text{Fixed Cost Units} + \text{Utility Cost} \tag{16.25}$$

is being approximated by a problem that conceptually can be stated as follows: