Studies in the Heat Integration of Chemical Process Plants

A method for solving the problem of heat exchanger network synthesis in chemical process plants is presented based on the use of the out-of-kilter algorithm. The method represents an extension of previous approaches based on network flow problem formulations. A new approach to overcome the constraints in forbidden-match problems, termed the dual stream approach, has been developed based on the use of a stream as both a hot and a cold stream. This approach results in considerable savings in utility costs in certain forbidden-match problems. An algorithm to deal with heating or cooling utilities that undergo temperature changes, termed non-point-temperature utilities, is presented using the transshipment model. The new algorithm determines the utility mass flow rates and pinch points accurately.

Murali Viswanathan, L. B. Evans
Department of Chemical Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139

Introduction

The problem of heat exchanger network synthesis (HENS) has been the subject of many studies over the past decade. Excellent reviews of this subject have been presented by Westerberg (1980), Nishida et al. (1981), and Umeda (1983).

This paper presents improvements in existing HENS solution methods to permit solution of a broader range of problems, including those with multiple forbidden matches and non-point-temperature utilities. The improvements are based on the use of the out-of-kilter algorithm to solve the transportation or transshipment network flow problems that occur.

The HENS problem was first stated formally by Masso and Rudd (1969). A typical chemical process involves streams that have to be heated (cold streams) or cooled (hot streams). The costs involved include the cost of heating and cooling utilities and the cost of the heat exchangers. The objective is to heat and cool the process streams from specified supply temperatures to specified target temperatures at a minimum total cost. The problem can be defined as follows:

> A set of H hot streams with flow rates m_{hi} ($i = 1, 2, \ldots, H$) have to be cooled from temperatures T_{hsi} ($i = 1, 2, \ldots, H$) to target temperatures T_{hti} ($i = 1, 2, \ldots, H$). A set of C cold streams with flow rates m_{cj} ($j = 1, 2, \ldots, C$) have to be heated from supply temperatures T_{csj} ($j = 1, 2, \ldots, C$) to target temperatures T_{ctj} ($j = 1, 2, \ldots, C$). It is required to determine the structure of the heat exchanger network to achieve this objective at minimum total cost.

Correspondence concerning this paper should be addressed to L. B. Evans.

Masso and Rudd (1969) proposed a systematic method for arriving at the minimum cost heat exchanger network while meeting process specifications. They suggested a set of heuristics that could be used to match the streams, but their heuristics did not always result in minimum-cost networks. Kesler and Parker (1969), Kobayashi et al. (1971), and Cena et al. (1977) formulated the problem in a more rigorous mathematical manner as an assignment problem in linear programming. However, the cost objective function based on the heat exchange surface area was both nonlinear and nonconvex and had to be approximated. The method hence generated networks with large numbers of heat exchangers.

Hohmann (1971), and Linnhoff and Flower (1978) suggested that the difficulties associated with optimizing the nonconvex cost function could be avoided by breaking up the objective function into two specific performance targets:

1. First determine the minimum utility requirement, that is, maximum energy recovery
2. Then determine the heat exchange matches that result in the minimum number of heat exchangers subject to maximum energy recovery

This led to the definition of the pinch point and to the development of the so-called pinch design method (Linnhoff, 1982), and demonstrated that one could predict the minimum utility and minimum heat exchanger unit requirements prior to actually developing the network and then synthesize the network in order to meet these targets.

In the pinch design method, hot and cold stream composite enthalpy curves are constructed, as in Figure 1, by adding the

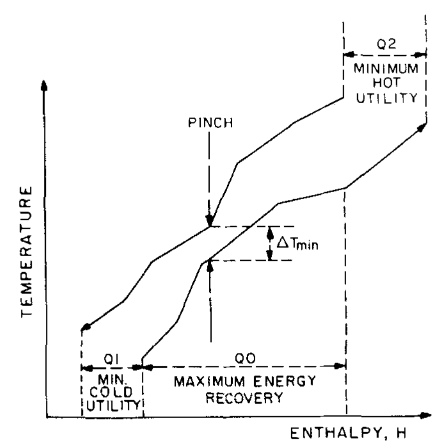


Figure 1. Composite enthalpy curves and the pinch.

heat contents of the hot and cold streams, respectively, over the temperature ranges involved. These temperature ranges are obtained by considering the supply and target temperatures of the hot and cold streams. The two composite curves are then moved parallel to the enthalpy axis until the point of closest approach reaches ΔT_{min}, the minimum temperature difference allowed between the streams exchanging heat. The point of closest approach of the curves is called the pinch point. The pinch divides the system into two separate subsystems, each of which is in enthalpy balance with its relevant utility. At maximum energy recovery, Figure 1,

1. Only heating, $Q2$, is required above the pinch
2. Only cooling, $Q1$, is required below the pinch
3. No heat is transferred across the pinch

The overlap, $Q0$, between the curves represents the maximum heat recovery possible. Once the minimum utility requirement is determined, the network is derived by dividing the problem at the pinch and designing each part separately.

Cerda et al. (1983) and Cerda and Westerberg (1983) formulated the pinch design problem as a network flow problem and used the transportation model and standard optimization algorithms to determine the minimum utilities and minimum number of heat exchangers. They developed a linear programming transportation model for the minimum utilities problem and solved it using the northwest corner algorithm. To determine the minimum number of heat exchangers subject to maximum energy recovery, they developed a mixed integer linear programming (MILP) approach based on the transportation model and then used several relaxations to reduce it to a transportation problem. This approach requires an initial feasible solution. Cerda et al. (1983) describe a row-and-column reordering algorithm to determine an initial feasible solution.

In the transportation model, heat flows from the hot streams/utilities that act as sources directly to the cold streams/utilities that act as destinations. Papoulias and Grossman (1983) approached the problem using the transshipment model. In this model, heat flows from the hot streams/utilities to the cold streams/utilities via intermediate nodes or "warehouses." The temperature intervals obtained by applying the rules of Cerda et al. serve as the intermediate nodes. Papoulias and Grossmann solved the resulting MILP for the minimum units and did not apply the relaxations of Cerda and Westerberg (1983). The minimum utilities transshipment model involves fewer variables than the corresponding transportation problem.

Floudas et al. (1985) and Wilcox (1985) proposed a split-mix bypass technique using a superstructure in order to automatically generate heat exchanger network configurations that feature minimum investment cost subject to minimum utility cost and minimum number of units. The heat exchanger area is minimized using a nonlinear program. Many of the stream connections in the superstructure are reduced to zero flow, resulting in realistic and practical designs.

The generally accepted approach today for implementing the pinch design methodology involves first formulating the minimum utilities problem as a transportation or transshipment problem and solving the resulting linear program using the Simplex algorithm. The minimum number of heat exchanger units for maximum energy recovery is determined either by formulating the problem as an MILP and reducing it to the transportation problem (Cerda and Westerberg, 1983) or solving the resulting MILP using branch-and-bound methods (Papoulias and Grossman, 1983).

In this paper, a method for solving the minimum utilities and heat exchanger units network problems using the out-of-kilter algorithm (Ford and Fulkerson, 1961) will be presented. The out-of-kilter algorithm can effectively replace both the Simplex and MILP algorithms used earlier. The transshipment model has been used for determination of the minimum utilities and the transportation model for determination of the minimum number of units. Both these models were modified to facilitate solution by the out-of-kilter algorithm. Forbidden and restricted matches can be handled.

Using the above modeling approach as a tool, a new method termed the dual stream approach is presented to overcome the heat-recovery limitations imposed by the forbidden matches. The dual stream approach is based on choosing a process stream or a set of process streams to behave both as hot and as cold streams. Using this method, it is possible to reduce the utility requirement for forbidden-match problems, at times even back to the utility requirement for the corresponding unrestricted problem.

The transshipment and transportation models treat the hot and cold utilities as point-temperature sources or sinks; that is, the utilities are assumed to be at a single temperature. If a utility (such as cooling water) undergoes a temperature change and thereby flows through more than one temperature interval in the transshipment model (non-point-temperature utility), the utility flow has to be redistributed after solving the model. This may affect the choice of utilities if multiple utilities are involved and also the location of the pinch point. For such problems, an algorithm has been presented to redistribute the non-point-temperature utilities if necessary and determine the final temperature to which the utility has to be heated or cooled.

Out-of-Kilter Algorithm

The out-of-kilter algorithm (OKA) is a general algorithm for solving capacitated, deterministic network flow problems. It has been developed (Ford and Fulkerson, 1961) based on the concepts of linear programming duality theory and complementary slackness conditions. An important feature of the OKA is that it is completely symmetric with respect to the primary and dual optimization problems and can be initiated with any starting vector (not necessarily feasible) that satisfies the conservation-of-flow equations at all nodes. The null vector will always satisfy the algorithm. This makes the determination of an initial feasible solution unnecessary. Using the OKA for the transportation and transshipment problems allows bounds to be included on flows, a feature that normally adds a complication to the conventional transportation problem. Moreover, the broad applicability of the OKA adds to the flexibility of the synthesis process. An excellent description of the algorithm can be found in Phillips and Garcia Diaz (1981).

Determination of Minimum Utilities and Units Using the OKA for Unconstrained Problems

The transshipment model was used for the minimum utility determination and the transportation model for determination of the minimum number of heat exchanger units. Both models were solved using the OKA. The theory behind the transshipment model is given in Papoulias and Grossmann (1983) and the transportation model is described in Cerda et al. (1983). These will not be repeated here.

The basis behind the OKA formulation is the establishment of a capacity cost triplet $(U_{i,j}, L_{i,j}, C_{i,j})$ for each arc (i, j) directed from node i to node j, Figure 2, where

$U_{i,j}$ = maximum possible flow along the arc

$L_{i,j}$ = minimum required flow along the arc

$C_{i,j}$ = cost per unit flow along the arc

The value of each capacity-cost triplet is set based on the problem data and the optimization objective. The algorithms to formulate the minimum utilities transshipment and minimum units transportation models and establish the capacity-cost triplets before solving using the OKA are given in the appendix.

Forbidden-Match Problems

An algorithm was developed using the OKA to solve the minimum utilities problem with any number of forbidden matches.

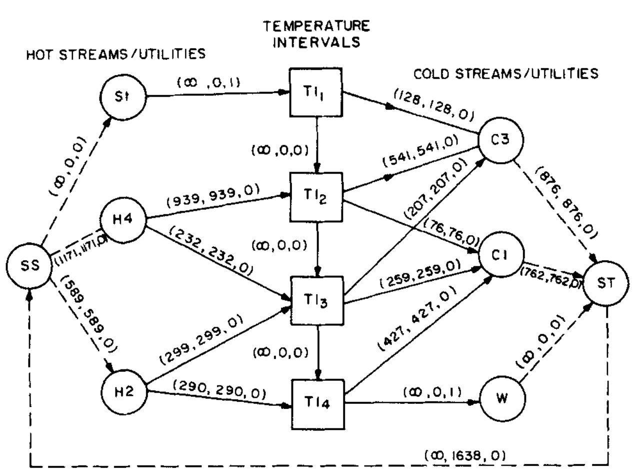


Figure 2. Minimum utilities transshipment model, 4SP1 problem.

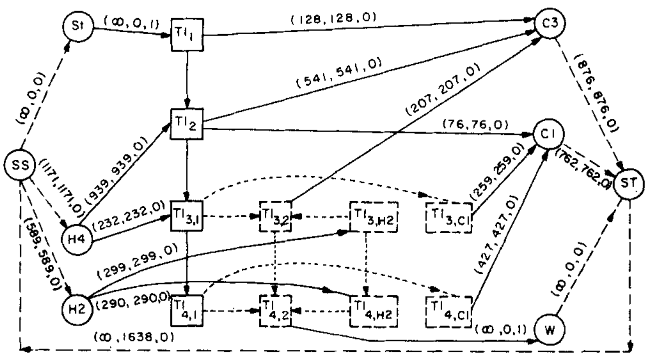


Figure 3. Minimum utilities transshipment model, 4SP1 with *H2-C1* match forbidden.

The algorithm constructs a modified version of the transshipment network that does not allow the flow of heat across any forbidden match. The sequence of steps to develop this model is given below. Here, the temperature intervals are split into subsidiary temperature intervals (the subsidiary temperature interval nodes are shown as dashed lines in Figure 3) and the connecting arcs formed, based on the matches that are forbidden. The constraints to forbid a match (or matches) are incorporated directly into the transshipment model such that heat cannot flow in the forward direction along any forbidden match and at the same time, the other matches are not affected. The model is formulated as follows:

1. Form the source, destination, and temperature interval (TI) nodes as for the unrestricted case. Set up the dummy arcs as mentioned in the appendix and connect each TI to the next lower TI.

Let:

$p \rightarrow q$ denote the formation of an arc from node p to node q

p —$II\rightarrow$ $p1, p2$ denote splitting node p into nodes $p1$ and $p2$ and forming an arc from $p1$ to $p2$

TI_k = temperature interval k ($k = 1, 2, \ldots, K$)

2. Let

P = set of forbidden matches (p, q)

HP, CP = sets of hot and cold streams, respectively, in P

H_k, C_k = sets of hot and cold streams/utilities passing through TI_k

Consider the coldest temperature interval TI_{k0} that the cold stream q of the forbidden match (p, q) passes through.

For $k \geq k0$ and $(p, q) \in P$, if $(p \in HP, p \in H_k)$ or $(q \in CP, q \in C_k)$ then:

(a) Split all the TI_k's that the hot stream of the forbidden match passes through, for which $k \geq k0$, Figure 3. Once this is done, attention need be focused only on the split TI's during the model formulation.

$$TI_k \text{ —}II\rightarrow TI_{k,1}, TI_{k,2}$$

If a node has already been split, do not split it again.

(b) $TI_{k-1,2} \rightarrow TI_{k,2}$ (if both $TI_{k-1,2}$ and $TI_{k,2}$ exist)

$TI_{k-1,2} \rightarrow TI_k$ (if $TI_{k-1,2}$ and TI_k exist but not $TI_{k,2}$)

3. For $k = 1, 2, \ldots, K$

(a) For all nonsplit TI's

$$i \rightarrow TI_k \quad i \in H_k, j \in C_k, TI_k \notin TI_{sp}$$
$$TI_k \rightarrow j \quad TI_{sp} = \text{set of all nodes split in 2(a) above}$$

(b) For all split TI's, for streams not involved in the forbidden matches

$$i \rightarrow TI_{k,1} \quad i \in H_k, j \in C_k, i \notin HP, j \notin CP$$
$$TI_{k,2} \rightarrow j \quad TI_k \in TI_{sp}$$

(c) For all split TI's, for streams involved in the forbidden matches

$$\left.\begin{array}{l} TI_{k,2} \text{ —II→ } TI_{k,i}, TI_{k,2} \\ i \rightarrow TI_{k,i} \\ TI_{k,1} \text{ —II→ } TI_{k,1}, TI_{k,j} \\ TI_{k,j} \rightarrow j \\ TI_{k-1,i} \rightarrow TI_{k,i} \text{ if both exist} \\ TI_{k,i} \rightarrow TI_{k,j} \quad (i,j) \notin P \end{array}\right| \begin{array}{l} i \in H_k, j \in C_k \\ i \in HP, j \in CP \\ TI_k \in TI_{sp} \end{array}$$

4. Thus, in each TI, the forbidden-match streams are handled with a separate set of nodes. Amongst the nodes in this set, connections are made between streams that can exchange heat. For example, if the $H4$-$C3$ and $H2$-$C1$ matches are forbidden, the matches $H4$-$C1$ and $H2$-$C3$ should be allowed. This set is then connected to the corresponding main TI so that heat can flow from or to all other streams in that interval.

5. Set up capacity-cost triplets for all TI-TI arcs as (a high number, 0, 0) and for all other arcs as in the unrestricted case transshipment model outlined earlier.

The model is now ready for solution by the OKA for any number of forbidden matches. After solving the model using the OKA, it is necessary to sum the flows from each TI and all its subsidiary TI's to the next TI and all its subsidiary TI's to determine the pinch points. The number of variables involved in this method depends on the nature of the problem. For a problem involving two hot streams, two cold streams, one hot utility, one cold utility, four temperature intervals, and two hot streams and two cold streams involved in forbidden matches, the formulation given above set up the transshipment model with 39 variables (the flow rates of the utilities and the flow from one TI to another TI). Moreover, a feasible starting point is not needed. For the determination of the minimum number of matches for maximum energy recovery, once again the transportation model can be used, with the appropriate stream connections left out, and the model can be solved using the OKA.

Consider the 4SP1 problem (Lee et al., 1970) for the data given in Table 1, with the $H2$-$C1$ match forbidden. The above method was used to formulate the minimum utilities model and the OKA used to solve it. The transshipment model for this is shown in Figure 3. The utility requirement was calculated to be 260 kW of steam and 382 kW of cooling water. The unconstrained problem needed 128 kW of steam and 250 kW of cooling water. So, the $H2$-$C1$ forbidden-match problem involves transferring 132 kW heat across the pinch (249–239°C), and the hot and cold utility requirements each increase by 132 kW. The transportation model was used to determine the minimum units. This gave five matches and the results agreed with those reported by Papoulias and Grossmann (1983).

Table 1. 4SP1 Problem Data

Stream	FC_p kW/°C	T^s °C	T^t °C
Steam	—	270	270
$H4$	10.55	249	138
$H2$	8.79	160	93
$C3$	6.08	116	260
$C1$	7.62	60	160
Cooling water	—	38	82

$\Delta T_{min} = 10°C$

Forbidden-Match Problems—The Dual Stream Approach

In problems involving forbidden matches, the constraints—which forbid the transfer of heat between the hot and cold streams involved in the forbidden matches—often result in a considerable increase in the utility requirement.

In such problems, that is, those in which the utility requirements increase on forbidding a match, our studies show that if it were possible to make one of the streams (hot/cold) of the forbidden match release/absorb heat into/from another like stream (hot/cold) and then utilize the heat content of the second stream, the utility requirement could be reduced considerably. This second stream thus behaves in a dual fashion, that is, as a hot stream in a few temperature intervals and as a cold stream in a few temperature intervals. For example, consider the minimum utility transshipment model in Figure 2. On forbidding the match between $H2$ and $C1$, the utility requirement may go up considerably, because $H2$ is not hot enough to supply most of the heating requirements of $C3$. If, on the other hand, $C1$ is used to cool $C3$, Figure 4, $C3$ can be brought to such a temperature level that it can exchange much more heat with $H2$. So when $C1$ cools $C3$, $C3$ behaves as a hot stream, $\overline{C3}$. This brings $C3$ up to TI_4 and it then behaves as a cold stream. Using the conventional approach, if the match between $H2$ and $C1$ were forbidden, cold utility W would have to supply the cooling requirements of $H2$ both in $TI4$ (fully) and $TI3$ (partially). Using the dual stream approach, $C3$ can meet part or all of the heating requirements of $H2$ in TI_4. The amount of savings in utility depends on two factors:

- Choice of the dual stream
- Nature of the problem

As regards choice of the dual stream, the following heuristics would help in choosing the best possible stream to behave in this fashion.

1. Assume that the match between hot stream i and cold stream j is forbidden.

$i \in H, j \in C$ (H, C set of hot and cold streams, respectively)

$h_{i,k}$ = amount of heat that hot stream i can dump into hot stream k, $k \in H$, $k \neq i$

$c_{j,l}$ = amount of heat that cold stream j can absorb from cold stream l, $l \in C$, $j \neq l$

$$h_{i,k} = \max_{\substack{k \in H \\ k \neq i}} h_{ik}$$

$$c_{j,L} = \max_{\substack{l \in C \\ l \neq j}} c_{jl}$$

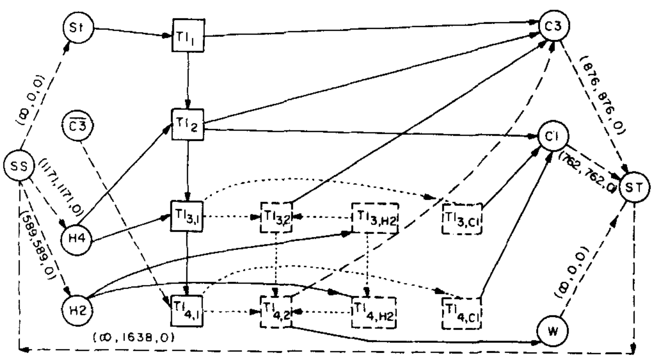


Figure 4. Minimum utilities transshipment model, 4SP1 problem.

$H2$-$C1$ match forbidden; dual stream approach with $C3$ as dual stream

2. If $h_{iK} > c_{jL}$, stream K is the dual stream and is heated by stream i

If $h_{iK} < c_{jL}$, stream L is the dual stream and is cooled by stream j

If $h_{iK} = c_{jL}$, either stream can be chosen as the dual stream

So, for a forbidden-match problem, the forbidden-match transshipment model has to be formulated first. Once the choice of dual stream is made, the forbidden-match transshipment model has to be modified to incorporate the dual stream behavior; then the pinch points can be determined. This will be illustrated later using an example. The amount of energy savings by this approach, over the conventional approach for forbidden matches, depends on the nature of the problem. Studies show that the energy requirements using this approach fall into three categories;

- Best case—same minimum utilities as for the unrestricted case
- Worst case—same minimum utilities as the conventional approach for forbidden-match problems
- Likely case—utility requirements between the best and worst cases

The price one has to pay on using the dual stream approach is a possible increase in heat exchanger area, for the dual stream is first heated/cooled and then cooled/heated, whereas in the conventional approach the increased energy requirement is supplied directly using utilities. The dual stream approach is worthwhile if the savings in energy more than offsets the cost of increased heat exchanger area.

The dual stream approach avoids the pumping and piping costs involved in using an external carrier stream and hence results in considerable savings in transportation costs over the external carrier-stream approach. The savings in transportation costs will be significant if the dual stream approach eliminates the extra need for a utility entirely, that is, if it results in the same minimum utility requirement as for the unconstrained case.

Based on the nature of the problem, the decisions to be taken are:

1. Whether to use the dual stream approach; if so, the stream or streams that behave in this dual manner must be chosen
2. The temperature interval(s) in which the stream(s) will behave in this dual manner

The decision on whether to use a dual stream involves a trade-off between capital cost (increased heat exchanger area and decreased piping) and operating cost (reduced pumping cost and reduced utility requirement).

Now consider the 4SP1 problem once again. The utility requirement for the unconstrained problem is 128 kW of steam and 250 kW of cooling water. This was determined by solving the minimum utilities transshipment model, Figure 2, using the OKA. If the $H2$-$C1$ match is forbidden, the utility requirements go up from 128 to 260 kW of steam, and from 250 to 382 kW of cooling water. The OKA formulation of the minimum utilities transshipment model for this is given in Figure 3. On using the dual stream approach described above, $C3$ was chosen as the dual stream; upon resolving the problem, the utility requirements turned out to be 128 kW of steam and 250 kW of cooling water. A pinch point occurred at 249–239°C. This is the same as in the unrestricted case problem. The dual stream transshipment model is shown in Figure 4. Thus, from the point of utility consumption, the dual stream approach negated the effect of the forbidden match. These results, along with the results of prohibiting the $H4$-$C3$ match are summarized in Table 2. For the latter case, the utility requirement went down considerably on using the dual stream approach, but did not go back to that of the unrestricted problem. These two cases fall into the best-case and likely case categories described earlier in connection with the performance categories of the dual stream approach.

The concept of the dual stream approach is not restricted to the OKA formulation. It can be used with the transshipment or transportation models and any algorithm used to solve the models in order to determine the minimum utility and heat exchanger unit targets for the network. The resulting energy target will be in the region between the constrained and the unconstrained targets, depending on the stream data.

Non-Point-Temperature Utilities

Previously, all the work using the transshipment model has been limited to point-temperature utilities, that is, utilities that are assumed to be at a single temperature. Non-point-temperature utilities have been approximated as point-temperature utilities in each temperature interval. If a utility goes through a temperature change and thereby flows through more than one temperature interval in the transshipment model (non-point-temperature utility) it is necessary to redistribute the utility after solving the model. This is because a utility mass flow rate in one temperature interval may result in the availability of

Table 2. 4SP1 Problem: Minimum Utility Requirement

Restrictions	Hot Utility (Steam) kW	Cold Utility (Cooling water) kW
None	128	250
$H4$-$C3$ match forbidden (conventional approach)	669	791
$H2$-$C1$ match forbidden (conventional approach)	260	382
$H4$-$C3$ match forbidden (dual stream approach with $H2$ as dual stream)	189	311
$H2$-$C1$ match forbidden (dual stream approach with C3 as the dual stream)	128	250

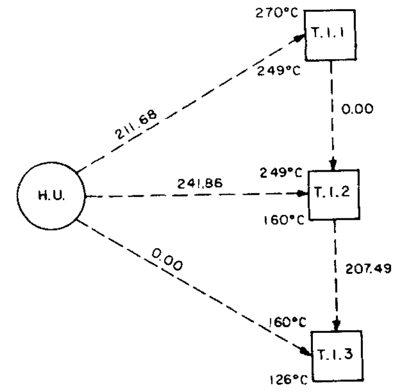
Table 3. **Modified 4SP1 Problem**

Stream	FC_p kW/°C	T^s °C	T^t °C
$H4$	10.55	249	138
$H2$	8.79	160	93
$C1$	7.62	60	160
$C3$	10.08	116	260
Hot utility	—	270	140
Cooling water	—	38	82

$\Delta T_{min} = 10°C$

excess heat or may not be sufficient to satisfy the heat demand at some other temperature interval. Our studies show that redistributing the utility may affect the choice of utilities and also the location of the pinch point, and the final temperature to which the utility is heated or cooled has to be determined.

For example, consider the problem shown in Table 3. Here, hot utility HU is available at 270°C and can be cooled to 140°C. The solved minimum utility transshipment model is shown in Figure 5. Here, the non-point-temperature hot utility has been approximated as three different hot utilities, each flowing into a different temperature interval. The problem appears to be pinched both at 249–239°C and at 160–150°C. From this, it is clear that a heat flow of 211.68 kW along the arc HU-TI_1 necessitates a flow rate of 10.08 kW/°C of utility HU. When the utility goes through the temperature range corresponding to TI_2 (89°C), it will produce 897.12 kW of heat. Of this, only 34.37 kW is needed at TI_2. Even if the excess flows down from TI_2 to TI_3, it will result in a surplus, for only 207.49 kW of heat is needed at TI_3. So, utility HU need not go through TI_2 fully, but need only be cooled such that the heat demands at all the TI's are met. If the flow rate of 10.08 kW/°C obtained by considering arc HU-TI_1 is just enough to meet the heat demand at TI_2 but not enough to meet that at TI_3, the mass flow rate of the utility has to be increased so as to just satisfy the demand. When this is done, the increase in mass flow rate will result in an increase in heat flow along the arcs HU-TI_1 and HU-TI_2 and the excess will cascade down. Hence, the mass flow rate has to be increased such that the sum of the excess flow that cascades down from all the upper TI's and the flow along the arc HU-TI_3 is just enough to satisfy the demand at TI_3. This has to be repeated once again if HU flows through TI_4 also and the mass flow rate is not enough to meet the demand at TI_4. A generalized algorithm to redistribute the utilities, if necessary, is presented in this section.



THE FINAL TEMPERATURE OF THE HOT UTILITY = 225°C

Figure 6. Modified 4SP1 problem.
Flow of hot utility HU after redistribution

Figure 6 shows the section of Figure 5 corresponding to the heat flow for utility HU after redistribution was performed. This shows that whereas earlier the problem was pinched at both 249–239°C and 160–150°C, on redistributing the utilities it is actually pinched only at 249–239°C. The flow along arc HU-TI_3 is now zero and the utility need be cooled only to 225°C. In Figure 5 HU was treated as a set of point-temperature utilities, that is, as three separate utilities that respectively supply heat to TI_1, TI_2, and TI_3. In Figure 6, HU was treated as the non-point-temperature utility that it really is. This changes not only the final temperature of the utility but also the location of the pinch point and hence may affect the capital cost of the network.

The composite enthalpy curves for the problem are shown in Figure 7. The dotted line segment AB represents that portion of the hot stream composite curve with the utility HU redistributed. Here, the utility streams have been incorporated into the composite enthalpy curves. The solid line segment AB represents the case without utility redistribution (here, the utility

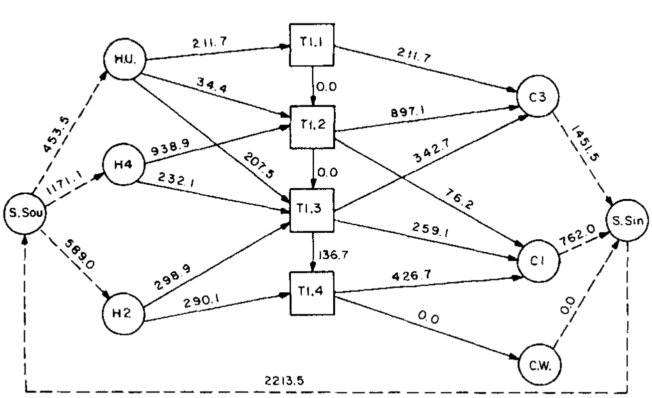


Figure 5. Modified 4SP1 problem.
Solved minimum utilities transshipment model bfore utility redistribution

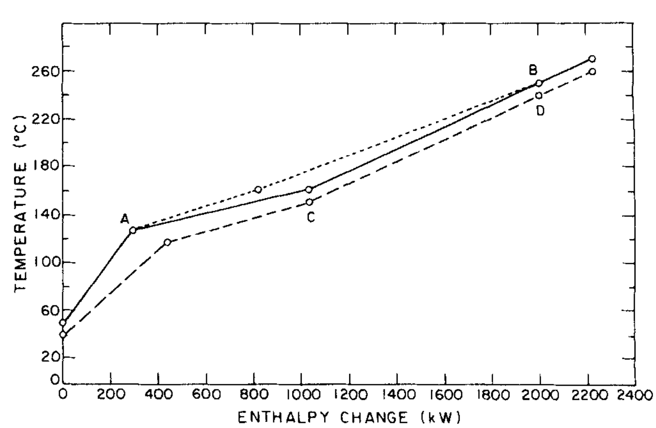


Figure 7. Modified 4SP1 problem.
Composite enthalpy curves to illustrate effect of utility redistribution

streams have not been incorporated into the composite enthalpy curves). It can be seen that the latter case falsely indicates that the two composite curves are parallel from C to D, that is, the problem is pinched at 249–239°C and at 160–150°C. When the utility was redistributed, the curves did not turn out to be parallel in this section. Redistribution helps determine the actual mass flow rate of the utility based on the heat demand at each TI and thereby plays an important role when multiple utilities are involved and the cheaper utilities are to be chosen. The above example was for a hot utility, but utility redistribution has to be considered even for a cold utility that flows through more than one TI. A general algorithm for redistributing non-point-temperature hot and cold utilities if necessary, and thereby getting a more accurate estimate of the pinch-points, is presented below.

For each utility j that flows through more than one TI, consider the arcs and nodes associated with that utility, as in Figure 6.

Let:

U_H = set of all such hot utilities

U_c = set of all such cold utilities

TI_U = set of all TI's that utility j passes through

TI_1, TI_N = hottest and coldest TI's that utility j flows through

$F2_i$ = total residual heat flow from TI_{i-1} to TI_i if $j \in U_H$, and from TI_i to TI_{i+1} if $j \in U_C$, $i = 1, 2, \ldots, N$

N = number of TI's that utility j flows through

d_i = heat demand at TI_i; corresponds to the heat flow from the utility to TI_i if $j \in U_H$, and the heat flow from TI_i to the utility if $j \in U_C$. Before redistribution, the flows along the utility arcs will be equal to d_i

SM = mass flow rate of the utility

$F3_i$ = flow along the utility arcs after redistribution, $i = 1, 2, \ldots, N$; this corresponds to the flows in the arcs from the utility to TI_i if $j \in U_H$, and the arcs from TI_i to the utility if $j \in U_C$

R_i = residual flow of the utility from TI_{i-1} to TI_i if $j \in U_H$, and from TI_i to TI_{i+1} if $j \in U_C$, $i = 1, 2, \ldots, N$

t_i = part of TI_i that the utility flows through; for example, if TI_i is from 80 to 40°C and the utility has a supply temperature of 160°C and can be cooled to 70°c, t_i = 10°C

For each such utility j:

1. Set $F3_i, R_i = 0, i = 1, 2, \ldots, N$
2. Set $i = 1$ if $j \in U_H$
   $i = N$ if $j \in U_C$

The utility is originally at its supply temperature. Calculate the mass flow rate assuming that the arc flowing into or out of TI_i (depending on whether it is a hot or cold utility) determines the critical flow rate.

$F3_i = d_i$

3. $SM = F3_i/t_i$
4. If the heat demand at TI_i is greater than the supply at that node, assume that the utility goes through the entire temperature range of TI_i and increment the flow along $F3_i$ accordingly (the final temperature of the utility will be determined later).

Demand at $TI_i = d_i$

Supply at $TI_i = F3_i + R_i$

If $(F3_i + R_i) < d_i$, set $F3_i = F3_i + (SM \cdot t_i)$

If ($j \in U_H, i = N$) or ($j \in U_C, i = 1$) go to step 6

5. If $d_i = 0$, check if any heat flow is required in any of the arcs flowing from utility j into the TI's below TI_i (if $j \in U_H$) or from the TI's above TI_i to utility j (if $j \in U_C$). If so,

$F3_i = F3_i + (SM \cdot t_i)$

6. If $(F3_i + R_i) = d_i$, that is, if the demand at any TI is just satisfied, examine the next arc.

If $j \in U_H$, set $i = i + 1$, go to step 4 if $i \leq N$
go to step 9 if $i > N$

If $j \in U_C$, set $i = i - 1$, go to step 4 if $i \geq 1$
go to step 9 if $i < 1$

7. If $(F3_i + R_i) > d_i$, then:

If $j \in U_H$, set $R_{i+1} = F3_i + R_i - d_i, i = i + 1$
go to step 4 if $i \leq N$
go to step 9 if $i > N$

If $j \in U_C$, set $R_{i-1} = F3_i + R_i - d_i, i = i - 1$
go to step 4 if $i \geq 1$
go to step 9 if $i < 1$

8. Once again, check if $(F3_i + R_i) < d_i$. If so, there is an unsatisfied demand at node TI_i.

UD_i = unsatisfied demand at node TI_i

$UD_i = d_i - (F3_i + R_i)$

This has to be met by an increase in the flows for all the utility arcs flowing into TI_k (all $k \leq i$ if $j \in U_H$, all $k \geq i$ if $j \in U_C$), that is, by an increase in the mass flow rate.

Add all the T_i's that the utility goes through up to this stage:

sumtemp $= \Sigma\, t_k$
$k \leq i$ if $j \in U_H$
$k \geq i$ if $j \in U_C$

$F3_k = F3_k + (UD_k \cdot t_k/\text{sumtemp})$, for all $k \leq i$ if $j \in U_H$
for all $k \geq i$ if $j \in U_C$

If $j \in U_H$, set $i = 1$ and go to step 3

If $j \in U_C$, set $i = N$ and go to step 3

9. Now the final temperature to which the utility has to be cooled or heated has to be determined.

If there is an excess flow at TI_l ($l = \max i$ if $j \in U_H$, $l = \min i$ if $j \in U_C$), or

If for any $TI_i \in TI_U$, $F3_i = 0$,

excess flow $= EX = F3_l + R_l - d_l$

$m = \max i$ such that $F3_i \neq 0$, if $j \in U_H$

$n = \min i$ such that $F3_i \neq 0$, if $j \in U_C$

reduce the flow along the utility arc flowing through TI_m or TI_n by EX.

$F3_i = F3_i - EX$

($i = m$ if $j \in U_H$)

($i = n$ if $j \in U_C$)

Now set the target temperature of the utility by considering the fraction of $TI_{m \text{ or } n}$ that the utility flows through, and subtract EX from all R_i($i > m$ if $j \in U_H$, $i < n$ if $j \in U_C$).

10. Add R_i to $F2_i$ for all i involved. Now $F3_i$ and $F2_i$ represent the redistributed arc flows for the concerned section of the network.

This has to be repeated for each utility $j \in U_H$ or $j \in U_C$. The transshipment model has to be examined with the redistributed flows in order to determine if any TI-TI flow is zero, that is, in order to determine if there are any pinch points. Due to the driving force requirements, a particular utility's target temperature may be different from the temperature to which it may be heated or cooled. Hence, a utility may not be used in its full temperature range. In such cases it may be worthwhile to investigate the cost effectiveness of using a less expensive utility with a narrower supply-target temperature range.

If a utility flows through more than one TI and is part of a forbidden match at some TI, subsidiary TI's will be created on using the forbidden match algorithm described earlier. In such cases, on redistributing the utility the flows in all the TI-TI arcs involved would have to be adjusted before the model is examined for the presence of pinch points. To our knowledge, this is the first analysis of the minimum utilities transshipment model for the redistribution of non-point-temperature utilities wherein both the mass flow rate of the utilities and the location of the pinch points may be affected.

Conclusions

The out-of-kilter algorithm can be used to calculate the minimum utilities and the minimum number of units for maximum energy recovery. The algorithm does not need a feasible starting point.

For forbidden-match and high transportation cost problems, the dual stream approach can be used to reduce the utility requirement but may result in an increased capital cost; therefore, the trade-off determines whether or not it is to be used. Unlike the external carrier stream approach, the dual stream approach does not involve extra pumping and piping costs; but if used, the dual stream must be incorporated as both a hot stream and a cold stream in the minimum utilities transshipment model and also in the determination of the minimum number of heat exchanger units for maximum energy recovery. The dual stream approach will be valuable when the process has to be optimized simultaneously along with the heat integration and forbidden matches are involved, for it can provide the process optimizer with a better estimate of the maximum energy recovery possible.

Finally, an algorithm to deal with non-point-temperature utilities in the transshipment model has been presented. The algorithm redistributes the utilities that flow through a temperature range and also flow through more than one temperature interval in the transshipment model. Using example problems, it has been shown that this sort of redistribution can affect the mass flow rate and final temperature of the utility and also the location of the pinch points. The final temperature and mass flow rate of the utility help choose the appropriate utility if multiple utilities are involved.

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Notation

A = set of all arcs in network
arc(i, j) = arc directed from node i to node j
$c_{j,l}$ = amount of heat that cold stream j can absorb from cold stream l
$C_{i,j}$ = cost per unit flow along arc(i, j)
C = set of all cold stream nodes
d_i = heat flow from utility j to TI_i if $j \in U_H$, and from TI_i to utility if $j \in U_C$
$D1$ = $(C \cup W)$
$f_{i,j}$ = actual flow along arc(i, j)
$F2_i$ = total residual flow of heat from TI_{i-1} to TI_i if utility $j \in U_H$, and from TI_i to TI_{i+1} if $j \in U_C$
$F3_i$ = flow along utility arcs after redistribution
$h_{i,k}$ = amount of heat that hot stream i can dump into hot stream k
H_k, C_k = sets of hot, cold streams/utilities passing through TI_k
H_n, C_n = set of all hot, cold stream/utility nodes in subnetwork n
m_{hi} = mass flow rate of hot stream i
HP, CP = sets of hot, cold streams/utilities in P
H = set of all hot stream nodes
$L_{i,j}$ = minimum required flow along arc(i, j)
m_{cj} = mass flow rate of cold stream j
P = set of forbidden matches
$Q0$ = overlap between composite enthalpy curves = maximum energy recovery possible
$Q1$ = minimum cold utilities required
$Q2$ = minimum hot utilities required
R_i = residual flow of utility j from TI_{i-1} to TI_i if $j \in U_H$, and from TI_{i+1} to TI_i if $j \in U_C$
S = set of hot utility nodes
$S1$ = $(H \cup S)$
SM = utility mass flow rate
t_i = part of TI_i that utility flows through
T_{csj} = supply temperature of cold stream j
T_{ctj} = target temperature of cold stream j
T_{hsi} = supply temperature of hot stream i
T_{hti} = target temperature of hot stream i
TI = set of temperature interval nodes TI_k
TI_k = temperature interval k
TI_{sp} = set of split temperature intervals
TI_U = set of TI's that utility j to be redistributed passes through
ΔT_{min} = minimum approach temperature
U_H, U_C = set of hot, cold utilities that pass through more than one temperature interval in minimum utilities transshipment model
$U_{i,j}$ = maximum possible flow along arc(i, j)
W = set of cold utility nodes

Appendix: Determination of Minimum Utilities and Heat Exchanger Units Using OKA

The transshipment model was used for the minimum utility determination and the transportation model for the determination of the minimum number of heat exchanger units. Both these models were solved using the OKA.

Minimum utilities transshipment model—out-of-kilter formulation

The formulation of the minimum utilities transshipment model is illustrated in Figure 2 for a problem involving hot streams $H4$ and $H2$, cold streams $C3$ and $C1$, hot utility St, and cold utility W. The temperature intervals TI_1 to TI_4 are determined using the rules outlined by Cerda et al. (1983). The heat flow pattern for each temperature interval is as follows (Papoulias and Grossmann, 1983):

1. Heat flows into a temperature interval TI_k from all hot streams and heating utilities i whose temperature range includes TI
2. Heat flows out of a temperature interval TI_k to all cold streams and cooling utilities j whose temperature range includes TI
3. The residual heat R_k flows from one temperature interval TI_k to the next lower temperature interval TI_{k+1}

The flow of heat from the hot streams to the temperature intervals and from the temperature intervals to the cold streams is usually fixed. Only the flow rates of the utilities and the residual heat flows are variables. A capacity cost triplet $(U_{i,j}, L_{i,j}, C_{i,j})$ is associated with each arc (i, j) directed from node i to node j, where

$U_{i,j}$ = maximum possible flow along the arc
$L_{i,j}$ = minimum required flow along the arc
$C_{i,j}$ = cost per unit flow along the arc

The objective is to determine the flow along each utility arc and the residual flow R_k from TI_k to TI_{k+1} ($k = 1, 2, \ldots, K - 1$) such that the cost of flow is a minimum and at the same time, the flow along each arc (i, j) is between the maximum and minimum values $(U_{i,j}, L_{i,j})$ that are set. The problem hence is:

$$\text{Minimize} \sum_{(i,j)\in A} C_{i,j} f_{i,j}$$

subject to $L_{i,j} \leq f_{i,j} \leq U_{i,j}$
and conservation of flow is satisfied at all the nodes
A = set of all arcs in the network
$f_{i,j}$ = flow in arc connected node i to node j

The arcs and their corresponding capacity cost triplets are set as follows:

1. For all the process streams, based on the rules for the heat flow pattern given above,

$$\left.\begin{array}{l} U_{i,k} = L_{i,k} \\ U_{k,j} = L_{k,j} \\ C_{i,k} = 0 \\ C_{k,j} = 0 \end{array}\right] \begin{array}{l} \text{calculated from supply and target temperatures and flow rates} \\ i \in H, j \in C, k \in TI \\ H = \text{set of all hot stream nodes} \\ C = \text{set of all cold stream nodes} \\ TI = \text{set of temperature interval nodes} \end{array}$$

2. Between two temperature intervals:

$U_{TIk-1,TIk}$ = a very high number (to correspond to infinity)
$L_{TIk-1,TIk} = 0$, $C_{TIk-1,TIk} = 0$, $TI_{k-1} \in TI$, $TI_k \in TI$

3. For all the utilities, based on the rules for the heat flow pattern:

$U_{i,k}, U_{k,j}$ = a very high number if there is no limit on the amount of utility available; otherwise set as the maximum amount available
$L_{i,k}, L_{k,j}$ = 0 (a utility may or may not be used)
$C_{i,k} = CS_i$, $i \in S$, $k \in TI$, CS_i = cost per unit flow of hot utility i
$C_{k,j} = CW_j$, $j \in W$, $k \in TI$, CW_j = cost per unit flow of cold utility j

4. Let $p \rightarrow q$ denote the formation of an arc from node p to node q.

In order to satisfy conservation of flow at each node (a feature required for the OKA), the following procedure is adopted.
(a) A super source node SS and a super sink node ST are created.

(b) $SS \rightarrow i$

$$\left.\begin{array}{l} U_{SS,i} = \sum_{k\in TI} U_{i,k} \\ L_{SS,i} = \sum_{k\in TI} L_{i,k} \\ C_{SS,i} = 0 \end{array}\right| \begin{array}{l} \text{for } \forall\, i \in S1, S1 = (H \cup S) \\ S = \text{set of hot utility nodes} \end{array}$$

(c) $j \rightarrow ST$

$$\left.\begin{array}{l} U_{j,ST} = \sum_{k\in TI} U_{k,j} \\ L_{j,ST} = \sum_{k\in TI} L_{k,j} \\ C_{j,ST} = 0 \end{array}\right| \begin{array}{l} j \in D1, D1 = (C \cup W) \\ W = \text{set of cold utility nodes} \end{array}$$

(d) $ST \rightarrow SS$

$$U_{ST,SS} = \sum_{j\in D1} U_{j,ST}$$

$$L_{ST,SS} = \sum_{j\in D1} L_{j,ST}$$

$$C_{ST,SS} = 0$$

All arcs created using steps (a) through (d) above are termed dummy arcs.

Because of this sort of "cost biasing," the OKA will automatically utilize the heat of the process streams as much as possible (since their cost is set to zero) and only if necessary will go to the utilities. The "from" and "to" nodes of each arc and the corresponding capacity-cost triplet values are fed to the OKA, and after the model has been solved the flows in the arcs from the hot utilities or to the cold utilities give the minimum utility requirements. A zero residual flow R_k indicates the presence of a pinch point.

Example

The formulation of the above model and its solution using the OKA will be illustrated using the 4SP1 (Lee et al., 1970) problem as an example. The problem data are shown in Table 1. The ΔT_{min} value is taken to be 10°C. The rules of Cerda and Westerberg (1983) were used to determine the pinch point candidates from among the supply temperatures of the streams and the temperature intervals were set up using a ΔT_{min} of 10°C. The "from" and "to" node of each arc and its corresponding capacity-cost triplet were fed to the OKA, which was called as a FORTRAN subroutine from LISP. No starting solution was provided. The minimum utility requirement was 128 kW of steam and 250 kW of cooling water. A pinch point occurred at 249–239°C (hot and cold stream temperatures). This agrees with the results reported by Papoulias and Grossmann (1983). The method was also tested for a number of standard heat exchanger network synthesis problems from the literature and the results were found to agree with reported values.

Minimum units transportation model—out-of-kilter formulation

After determining the minimum utility requirement using the method specified above, the problem is divided at the pinch and the transportation model is used to determine the minimum number of heat exchanger units needed in each subnetwork for maximum energy recovery. For a subnetwork n, let:

H_n = set of all hot stream/utility nodes
C_n = set of all cold stream/utility nodes

For each arc directed from source i to destination j:

$U_{i,j}$ = maximum possible heat flow from i to j
$L_{i,j}$ = 0 (two streams may or may not exchange heat)
$C_{i,j}$ = $1/U_{i,j}$ (to use the higher capacity matches as much as possible)

For the dummy arcs,

$$U_{SS,i} = L_{SS,i} = \sum_{j\in C_n} U_{i,j},\ C_{SS,i} = 0,\ \forall i \in H_n$$

$$U_{j,ST} = L_{j,ST} = \sum_{i\in H_n} U_{i,j},\ C_{j,ST} = 0,\ \forall j \in C_n$$

$$U_{ST,SS} = L_{ST,SS} = \sum_{j\in C_n} U_{j,ST},\ C_{ST,SS} = 0$$

The problem hence is,

$$\text{Minimize} \sum_{(i,j)\in A} f_{i,j}(1/U_{i,j})$$

$$\text{subject to } L_{i,j} \le f_{i,j} \le U_{i,j}$$

and conservation of flow is satisfied at all nodes

The model is now ready for solution by the OKA. The modeling has been done such that the algorithm always tends to minimize the number of units.

Once again, considering the 4SP1 problem as an example, the network is first divided at the pinch (249–239°C). Above the pinch, the only match turned out to be between St and $C3$ (128 kW). Below the pinch, the minimum units transportation model was formulated as described above. Once again, the OKA was used to solve the problem. The number of units needed for maximum energy was five and agreed with the results reported by Papoulias and Grossmann (1983).

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