Heat and Work Integration
in the Synthesis of Chemical Plants

by

Hyung-Jae Alexander Yoon

M.S.C.E.P. Massachusetts Institute of Technology (1985)

Submitted to the Department of Chemical Engineering
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Signature of Author

Department of Chemical Engineering
January 16, 1990

Certified by

Lawrence B. Evans
Thesis Supervisor

Accepted by

William M. Deen
Chairman, Committee for Graduate Students
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Abstract

In many chemical process plants, a large portion of the annual operating cost is consumed by the energy network which supplies the hot and cold utility needs, and the power and electricity needs of the process. Furthermore, when building such a plant, a major portion of the capital cost can be also attributed to the energy network. Therefore, savings in the energy network can lead to large savings in the capital and the operating costs of the chemical process plant.

However, the overall design problem results in a very large combinatorial non-linear optimization problem. Therefore, previous approaches had decomposed the overall design problem into three distinct subproblems: chemical process synthesis, heat recovery network synthesis, and the utility plant synthesis. Two strategies have been used to solve different aspects of each subproblem. First is the heuristics/logic based approach where the rules of thumb developed over the years and the theory of thermodynamics and chemical engineering were used to solve the decomposed problems. The second strategy applied mathematical programming techniques to each decomposed problem.

Recently, efforts have been made to solve the subproblems simultaneously in order to obtain a better overall solution. Townsend and Linnhoff [1983] developed a set of rules to correctly place heat engines and heat pumps within the framework of the heat recovery network, thus combining an aspect of the utility plant synthesis problem with the heat recovery network synthesis problem.

In this research, a new method was developed to solve the utility plant synthesis problem and the heat exchanger network synthesis problem simultaneously.

First, heuristics were developed to account for the relationship between the utility plant and the heat recovery network. These heuristics were developed based on the thermodynamic and economic analyses. They reduce the number of alternatives that need to be examined in order to find an optimum solution to the combined utility plant and heat exchanger network synthesis problem. Placement rules for hot and cold, condensing and non-condensing utilities with match dependent $\Delta T_{\text{min}}$ with respect to the heat exchanger network have been established. Placement of heat engines, heat pumps and refrigeration cycles can be systematically established.

Second, based on the heuristics which established feasibility criteria for unit opera-
tions, numerical unit operation models were developed for heat engines, heat pumps, refrigeration cycles and other assorted units in the utility plant. Simulation and optimization with these models were performed to reduce the number of design alternatives further. The resulting data were linearized to eliminate the non-linear aspect of the overall problem.

Third, in order to find an optimum solution from the reduced number of alternatives, a mixed integer linear programming (MILP) approach is used to formulate the synthesis problem. A standard linearization procedure coupled with the linearized unit operation data from above are used to formulate the problem. The optimization is done using a standard MILP solution package LINDO utilizing Branch and Bound scheme. [Schrage, 1980]

Lastly, the optimization of the minimum approach temperature, $\Delta T_{\text{min}}$ was explored. A method was developed to properly balance the tradeoff between the heat recovery network and the utility plant. It has been applied to both the grass-root design case and the retrofit case.

This research has demonstrated a new strategy for synthesizing utility plant and the heat recovery network while properly accounting for the interaction between the two. The new method utilizes best of both heuristics approach and mathematical approach to find the design solution that neither approach could find separately. It has brought into light the fact that the heat exchanger network is not the only place where energy savings can be generated. The utility plant and the associated heat and work integration also offer large savings potential. Furthermore, it has been shown that the utility plant synthesis combined with the heat exchanger network results in a more integrated and thus lower cost design than doing either separately.

Thesis Supervisor: Dr. Lawrence B. Evans
Title: Professor of Chemical Engineering
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Chapter 1

Introduction

Over the past fifteen years the process industries have made a major effort to reduce their cost of energy. Energy conservation has been the subject of many studies. Energy conservation can be achieved through building more efficient plants or through retrofitting existing plants using more efficient process units or configurations.

Two major areas of research have been energy conservation through heat and work integration. Heat integration involves improving the energy efficiency of a plant by recovering heat from hot streams and using it to heat cold streams. Work integration is distinguished from heat integration by the fact that the former considers the use of power producing cycles such as heat engines and power consuming cycles such as heat pumps to minimize the overall manufacturing cost whereas the latter only considers interconnection of heat exchangers to minimize the utility usage. A good review of the literature of both heat and work integration can be found in the paper by Gunderson [1987] which surveys previous work on heat exchanger network design.

The problem of designing a heat and work integrated process plants can be thought of as a process synthesis problem. As such, there are two distinct types of synthesis technique: algorithmic and heuristic.

Since the goal of the process synthesis problem is to determine the optimal structure with the interconnection of various functional units, a combinatorial problem has to be solved. Additionally, process parameters for this optimal structure have
to be determined simultaneously. Algorithmic methods have been used to solve the mathematical formulation of the synthesis problem; however, this kind of approach is generally limited to simpler problems. If a mathematical formulation is not possible, it is necessary to solve the combinatorial problem approximately using heuristics even though such methods can not be guaranteed to find the optimum.

To solve the combinatorial problem, various search methods and heuristic methods have been utilized. A detailed listing of these were given in a review paper by Umeda. (1983) Most industrial research efforts have emphasized the use of a heuristic evolutionary method. In this approach the energy efficiency of the plant is improved through unit by unit optimization. This leads to optimum unit operations, but does not result in a global optimum solution for the overall process.

Since the process engineer is faced with a wide spectrum of tasks in solving the energy recovery problem, it is not surprising that there is no single all-embracing theory to effectively cope with all of them. The aim of this research is to combine the numerical techniques and the heuristics to provide a solution methodology suitable for synthesis of heat and work integrated plants.

1.1 Heat and Work Integration Problem

The problem definition for heat integration, first stated by Masso and Rudd [1969], is as follows:

Given a set of process streams: n hot streams to be cooled from supply temperature $T_{hot,supply,i}$ ($i = 1, 2, \ldots n$) to target temperature $T_{hot,target,i}$ ($i = 1, 2, \ldots n$) and m cold streams to be heated from supply temperature $T_{cold,supply,i}$ ($i = 1, 2, \ldots m$) to target temperature $T_{cold,target,i}$ ($i = 1, 2, \ldots m$) and the accompanying mass-heat capacity flow rates $mC_p i$, determine the structure of the heat exchanger network to achieve the above temperature change at minimum total cost.

The problem of work integration involves addition of the following.

In addition, given I streams whose pressures have to be changed, also given primary hot utility load (MW) and level (temperature), cold utility load and level, and primary power requirement from the chemical plant.
Synthesize an energy network subject to minimum total cost. An energy network includes all power producing and power consuming units, all hot utility and cold utility producing units, and all heat exchangers and their interconnections.

The primary hot and cold utility load and temperature levels refer to those hot and cold utilities required for uses other than heating and cooling process streams; the use of steam directly in the process would be an example.

From a purely theoretical point of view, the number of ways in which these streams can be matched through heat exchangers, heater, coolers, pumps, turbines, etc. are considerably large. Consider just the number of heat exchanger matches that are possible for a problem with \( N_h \) hot streams, \( N_c \) cold streams, \( N_{hu} \) hot utilities, and \( N_{cu} \) cold utilities. The total maximum number of heat exchanger matches possible, assuming no matches between the utilities, are

\[
N_{\text{max}} = [(N_h + N_{hu})(N_c + N_{cu})] - (N_{hu}N_{cu})
\]

The number of heat exchanger structures that would involve this maximum number of matches are given below.

\[
N_{\text{structure, max}} = [(N_h + N_{hu})(N_c + N_{cu}) - N_{hu}N_{cu}]!
\]

However, there are other possible structures involving a fewer number of matches than \( N_{\text{max}} \). The absolute minimum number of matches required is

\[
N_{\text{min}} = \max(N_h, N_c)
\]

The implicit assumption is that the smaller of \( N_h, N_c \) can be either completely cooled or heated by the opposite streams, and then only \( \max(N_h, N_c) - \min(N_h, N_c) \) streams would need to be heated or cooled using the utility.

The total number of networks possible are then the sum of all networks from \( N_{\text{min}} \) to \( N_{\text{max}} \) as shown below.

\[
N_{\text{total}} = N_{\text{max}}! + (N_{\text{max}} - 1)! + \ldots + N_{\text{min}}!
\]

Therefore, even for a simple problem of two hot streams, two cold streams, and one hot and cold utility each, total number of networks is over 24 million as shown in Table 1.1.
Table 1.1: Theoretical number of possible structures

<table>
<thead>
<tr>
<th>Hot/Cold streams and utilities¹</th>
<th>HEN alone²</th>
<th>Utility alone³</th>
<th>HEN &amp; Utility Plant ⁴</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/1, 1/1</td>
<td>153</td>
<td>401</td>
<td>61,506</td>
</tr>
<tr>
<td>2/2, 1/1</td>
<td>24,227,424</td>
<td>401</td>
<td>9.7\times10⁹</td>
</tr>
<tr>
<td>2/2, 2/1</td>
<td>24,227,424</td>
<td>160,400</td>
<td>3.9\times10¹²</td>
</tr>
<tr>
<td>5/5, 5/1</td>
<td>3.5\times10^{32}</td>
<td>1.1\times10^{13}</td>
<td>3.5\times10^{45}</td>
</tr>
</tbody>
</table>

¹First two numbers are the numbers of hot and cold streams
Second two numbers are the number of hot and cold utilities
²From equation 1.4
³From equation 1.5
⁴From product of equations 1.4 and 1.5

Consider a simple utility plant supplying a single hot and cold utility, with the cold utility at a specified temperature, Assume that we allow for the possibility that the hot utility might be supplied at any temperature between 100°C and 500°C. Considering each possible hot utility level at 1°C interval, then, there would be 401 possible combination of hot and cold utilities.

For a simplest utility plant that only produces $N_{hu}$ and $N_{cu}$ number of hot and cold utilities, with $N_{Thu}$ and $N_{Tcu}$ temperature levels of hot and cold utilities to consider, the number of possible utility plant configuration is:

$$N_{util} = \frac{N_{Thu}!}{(N_{Thu} - N_{hu})!} \frac{N_{Tcu}!}{(N_{Tcu} - N_{cu})!}$$  \hspace{1cm} (1.5)

For a simple utility plant with one possible cold temperature level and hot utility temperature level ranging from 100~500°C, there would be 401 possibilities as shown in Table 1.1.

If this simplest utility plant is combined with the heat exchanger network, the total number of possibility can be calculated by the product of equations 1.4 and 1.5. following equation. As shown in Table 1.1, the number of alternatives becomes far too large even for a small problem.
Furthermore, due to the additional possibilities arising from interconnections between pumps, compressors, turbines and other work producing and consuming units that would be included in a complete utility plant, it is not surprising that there has not been any methodology that can guarantee to find a globally optimal solution every time. Therefore, the emphasis in the recent past has been to decompose the problem into smaller subproblems and develop strategies to solve each subproblem separately.

1.2 Literature Review

The synthesis of heat and work integrated plants is a part of the overall field of process synthesis. Since the overall problem is too complex to tackle, Papoulias and Grossmann [1983c] outlined a decomposition approach breaking the problem into simpler subproblems as shown in Figure 1.1.

The chemical process consists of reactors, distillation towers, mixers etc. Its purpose is to perform all necessary chemical changes in order to make a set of products from a set of given raw materials. The problem of synthesis of the process is decoupled from the rest of the plant by assigning costs to the input variables and output variables. Input variables consist of raw material feeds to the chemical process, hot and cold utilities and the power from the utility plant. Output variables are the products and any waste streams that effect the overall economics. Therefore, this subproblem can be optimized for maximum profit with respect to the input and output variables and the associated costs.

However, using hot and cold utilities for heating and cooling all the process streams could be a very expensive option. Therefore, once the process conditions are set, process streams could be used to replace the hot utility by exchanging heat with another process stream which needs heating. Similarly, a process stream could be used to replace a cold utility. By assuming fixed process conditions and fixed utility levels and the associated costs, this heat recovery problem is also decoupled from the rest of the synthesis problem. The optimization involves tradeoff between the heat
Figure 1.1: Total Process Plant

TOTAL PROCESS SYSTEM

Chemical Process
- reactor
- separators
- mixers

Cold Streams

Heat Recovery Network
- heat exchangers

Hot Streams

Utility Plant
- boilers
- turbines
- electric generator
- etc

Raw Materials

Electricity & Power

Fuel Water

Product

Hot & Cold Utilities
exchanger costs and the utility costs to minimize the sum of two costs. In addition to the stream to stream match information, the optimized solution would yield the amount of hot and cold utility needed at the specified levels.

Finally, the utility plant can be designed to supply the hot and cold utility requirement specified from the heat recovery network and also to supply the power demand from the chemical plant. Since all the demands are specified including the temperature levels, the utility plant optimization is a matter of interconnecting cost efficient unit operations to achieve minimum cost design.

The solution to the decoupled overall synthesis problem is, then, the sum of the optimal solutions from each subproblem. Because this solution neglects interactions between subsystems, it is suboptimized. In the next few sections, we will briefly review the previous work on these three subproblems.

1.2.1 Synthesis of the Chemical Process

To synthesize the chemical process, decoupled from the heat exchanger network and plant utility system, the costs for all the input variables such as raw materials, hot and cold utilities and output variables are fixed. The capital costs for unit operations in the plant are also predetermined. Subject to these constraints, an economical chemical plant is designed. The amount of heating, cooling and power requirement for each stream in the plant can be determined at this point.

Since the synthesis procedure is somewhat a creative process, the heuristic approach has found success in solving this problem. Many different heuristics for synthesizing reaction paths, reactor network, separation sequence have been reviewed extensively by Westerberg [1980] and by Nishida, Stephanopoulos and Westerberg [1981]. Some of these heuristics have been implemented in an expert system environment such as BALTAZAR. [Motard et al., 1978] More recently, these heuristics have been organized into a systematic procedure so that they can be used directly to synthesize a variety of chemical processes. [Douglas, 1988]
Although these heuristics were used to obtain an economical design, it was unclear whether better designs existed or not without resorting to complete enumeration. This limitation led to the application of a mathematical programming approach by Santibanez and Grossmann [1980]. In this approach the units in the existing design were represented as mathematical models whose interconnections can be determined numerically. Since all the units that might be present in the process had to be represented using the model, this gave rise to a design configuration called the superstructure with all the unit models embedded in it. In order to guarantee that the solution was the best, complete enumeration was still needed. However, the mathematical representation made the computation time relatively short.

1.2.2 Synthesis of Heat Recovery Networks

The process streams in the chemical plant that were assumed to be heated and cooled strictly with the hot and cold utilities represent an opportunity for savings in the total cost through heat recovery. A number of methods have been developed to tackle this problem as discussed in the review paper by Gunderson [1987]. The complicating factor in this problem was that the number of possible heat exchanger networks to achieve this heat recovery is very large even for a small problem as shown by equation [1.4]. Although many of these networks can be eliminated from the standpoint of thermodynamic feasibility, other complications such as minimum approach temperature, \( \Delta T_{\text{min}} \), and constrained matches would add complications so as to make the problem almost intractable. Therefore, the earlier methods by Hwa [1965], Masso and Rudd [1969], Ponton and Donaldson [1974], and Rathore and Powers [1975] have relied on heuristics to find an acceptable solution rather than the best solution.

Then, Hohmann [1971] formulated the pinch point concept to determine the minimum utilities target for a given problem. This was a significant breakthrough in that it was a first systematic procedure used to reduce the combinatorial nature of the problem. This work was further extended and popularized by Linnhoff and
coworkers [Linnhoff and Flower, 1978; Linnhoff et al., 1982; Linnhoff and Hindmarsh, 1983] who presented the pinch as the bottleneck in the energy recovery. They divided the problem at the pinch and designed the heat exchanger network based on new heuristics they developed.

The pinch concept can be explained simply using the temperature enthalpy diagram such as shown in Figure 1.2. The hot composite curve shown in this diagram is composed of all hot process streams, and the cold composite curve is composed of all cold process streams. These diagrams are commonly used to quickly determine the minimum utility targets for heat exchanger networks. Since the heat content of the composite curves is a relative measure, the horizontal positions of the curves are not fixed. If they are brought together until some specified minimum approach temperature is reached between the two curves, the utility targets can be read directly from the diagram. The point or points at which the two curves are exactly offset by the minimum approach temperature are called pinch points.

The pinch divides the heat exchanger network problem into two subproblems, one below the pinch where only cooling is needed and the other above the pinch where only heating is needed. The streams above the pinch must not exchange heat with streams below the pinch, otherwise the utility requirement for the problem increases.

Although there would be a physically limiting minimum approach temperature, EMAT, for energy recovery which would limit the maximum amount of recoverable heat, the minimum approach temperature, $\Delta T_{\text{min}}$, can be varied to find the minimum cost network. This variable minimum approach temperature is called HRAT. As $\Delta T_{\text{min}}$ is varied, the cost tradeoff between the heat exchanger network cost and the utility cost would be examined. For example, as $\Delta T_{\text{min}}$ is increased, the two composite curves on Figure 1.2 are pushed apart. The heat exchanger area cost decreases because of the higher temperature driving force, but the utility cost increases because of the increase in the amount of hot and cold utility required.

Extending this concept further, Linnhoff et al. [1982] developed heuristic-evolutionary technique to synthesize the heat exchanger network. The method re-
Figure 1.2: A typical pinch diagram
sulted in heat exchanger network designs that were very close to the minimum cost
design. However, since the procedure relied exclusively on heuristics, it could not
guarantee the synthesis of the optimal network,

and it did not lend itself to computer implementation. Furthermore, additional
constraints such as forbidden matches and preferred matches couldn't be accounted for
efficiently. This led to the development of the mathematical programming approach.

Cerda and Westerberg [1983] reformulated the heat exchanger network design
problem as a network flow problem. The transportation model algorithm was then
applied to solve the problem. Papoulias and Grossmann [1983b] applied a more effi-
cient transshipment model algorithm to solve the same problem. The mathematical
nature of the two approaches made them applicable to implementation in a com-
puter program. However, these approaches still lacked ability to account for the non-
ideality such as forbidden and preferred matches. To account for these non-idealities,
Viswanathan and Evans [1987] developed a new strategy using a modification of the
transshipment model. Other issues such as flexibility and operability have been ex-
amined by Calandranis and Stephanopoulos. [1985]

The limiting factor in application of these approaches lies with the fact that
although the stream matches and utility targets could be determined, the sequence
and load at each match required for the actual network still had to be done manually.
Furthermore, the effect of heat exchanger design, such as material of construction
and flow of match (counter-current, co-current, etc.) has not been fully examined.
Finally, the arbitrary utility levels and the associated costs assumption has to be also
examined. The variation in these would imply that the procedures mentioned above
will have to be reapplied for each combination of utility level and cost.

1.2.3 Synthesis of Utility Plants

In the decoupled approach to overall process synthesis, the output of the utility
plant is specified from the synthesis of the chemical process and the heat recovery
network in the form of specific amounts of power, and hot and cold utilities at specified
levels. The synthesis of the utility plant can be accomplished by simply connecting the most efficient units into an overall network. This has been the general design procedure used by the industry. There have been numerous publications on how to select most economical, energy efficient unit operations for a variety of output conditions such as power load, heat load and level, and cooling load and level; and also for input conditions such as fuel, load variation etc.

However, it was recognized that when these units were connected together to form a utility plant, a lower cost overall design might be achieved through the combination of efficient units and less efficient units. For example, in a utility plant a gas turbine and a steam boiler might be both present because each were determined to be most efficient in their respective duty under the conditions of the problem. However, if the steam boiler is connected directly to a steam turbine, power generation and heating need may be met at lower total cost.

To account for such interaction, mathematical programming techniques were applied to the problem. One of the first to do this was Nishio and Johnson [1979] who developed a linear programming method to optimize the utility plant. It was an iterative method which optimized the fuel, steam and power flows and equipment sizes. Several iterations were required to adjust for changes in the header operating conditions and equipment efficiencies. Petroulas and Reklaitis [1984] have also developed a similar two level method. Dynamic programming is used in the first level to optimize the steam header level and minimize the energy loss. In the second level, linear programming technique is used to optimize the flows and the equipment sizes. However, these methods were designed only to minimize the energy cost (operating cost) of the existing utility plant and not for general synthesis of the utility plant. For synthesis of the energy network, these methods were inadequate because complete reprogramming is required for different problems.

To synthesize the utility plant, Papoulias and Grossmann [1983a] used mixed integer linear programming (MILP) technique to solve the problem. The basic approach is still the same as in the standard linear programming method; however, the advantage of MILP over LP is that binary variables can be used in addition to the
continuous variables to represent nonlinearities in operating conditions and equipment cost. Therefore, the MILP model of a utility plant can optimize simultaneously the utility plant structure using binary variables, and the fuel/steam/power flows using continuous variables. Nath and Holliday [1985] at Union Carbide has also developed utility system optimizer based on the MILP model.

Since the output variables such as temperature and amount of hot and cold utility were specified, there were a relatively small number of possible structures to be examined. Therefore, a minimum cost solution was always guaranteed assuming that all feasible unit operations were included in the model formulation.

1.2.4 Discussion of the Decomposition Approach

The original problem of total process synthesis has been successfully decoupled into three subproblems. In each of the three areas, many new solution strategies have been developed to solve each subproblem. Chemical process synthesis is an area that still needs to be explored further since new processes are being discovered every day. The emphases are on reaction paths, reactor network, and separation sequences. The synthesis of heat recovery networks has seen the most activity in the last decade, and the improvement in solution strategy has been dramatic especially with the discovery of the pinch. The current emphasis is on operability, flexibility, and control issues. The decoupling strategy, however, has resulted in a very rigid utility plant subproblem where all the outputs are fixed a priori by the other two subproblems. The resulting design task is a simple one and the optimization strategy developed can guarantee a minimum cost solution. In this way, an acceptable solution was obtained to the originally intractable total process synthesis problem.

However, this solution, which is the sum of the three solutions to each subproblem, may be far from the optimum design of the overall plant. As the simple utility plant synthesis case showed, combining the most efficient options to each subproblem is not guaranteed to yield the best overall solution. For example, even the simplest interaction of the utility plant and the heat recovery network by letting the utility
plant dictate the levels and load of utilities it supplies could result in a better solution than the arbitrary level selection procedure currently used. In addition, the chemical plant could be designed simultaneously with the heat recovery network, so that an energy intensive chemical plant option would not be ruled out without realizing the heat recovery potential and thus lowering the overall cost of the combined design. Furthermore, heat engines and heat pumps could be used to replace hot and cold utilities and to lower the overall cost.

Therefore, recent researches have concluded that the interaction between the chemical plant and the heat recovery network, between the utility plant and the chemical plant, between the utility plant and the heat recovery network, or among all three plants must be examined to find the best overall solution. In the next few sections, we will briefly examine the previous work that looked into subsystem interactions.

1.2.5 Chemical Plant and Heat Recovery Network Interaction

One of the first workers to recognize the interaction between the heat recovery network and the chemical plant was Wilcox [1985]. He developed heuristics to account for the effect of process stream pressure changes on the heat recovery network. For example, raising the operating temperature of a hot process stream by compression before the stream is delivered to the heat recovery network could result in the movement of the stream from below the pinch to above the pinch. This would reduce both heating and cooling requirement. However, the heuristics could not account for interactions other than pressure changes with the chemical plant.

To better account for the interaction between the chemical plant and the heat recovery network, Duran and Grossmann [1986] proposed a mathematical strategy for simultaneous optimization of the chemical plant and heat recovery network. With their scheme, the flowrates and the temperature of the process streams were treated as decision variables. Therefore, the pinch point could be calculated at each point in the

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optimization and the utility cost minimized. This method was extended further and was interfaced with a process flowsheet optimizer to be applicable to a wide variety of chemical plant problems by Lang, Biegler, and Grossmann [1988]. Viswanathan [1989] developed another strategy to account for the interaction. Similar in concept to Duran and Grossmann method, however, his method could account for forbidden match constraints. These approaches were still limited to problems with a fixed chemical process.

1.2.6 Heat Recovery Network and Utility Plant Interaction

Although each subproblem has been solved separately, there has not been any previous work that completely accounts for the interaction of these two subproblems. Even the MILP approach by Papoulias and Grossmann [1983c] that claims to perform simultaneous synthesis is in reality a sequential method where the heat recovery network is synthesized first, and then the utility plant is designed. Their important contribution was that the same MILP technique was used to solve each subproblem.

The methods developed in the previous work examined only a partial interaction of the utility plant and the heat recovery network. For example, the pinch concept can be extended further to integrate heat engines and heat pumps into the heat recovery network since the hot and cold utilities are equivalent to the heat intakes or heat rejections from heat engines and heat pumps. This extension was presented in a paper by Townsend and Linnhoff [1983a] where they discuss correct placement of heat engines and heat pumps with respect to the process pinch.

To illustrate this concept, they developed the temperature interval diagram shown in Figure 1.3. The interval temperatures are derived from the kinks on the composite curves in the pinch diagram. In each interval, an enthalpy balance of cold and hot streams is made. If there are excess enthalpy from the hot streams, then that interval is said to have heat surplus which can be either removed using cold utility or transferred to the interval below to exchange heat with streams in the lower interval.
If there are excess enthalpy need from cold streams in the interval, then the interval has heat deficit. This heat deficit has to be met with either the hot utility or the heat surplus from the interval above. The heat from the interval above can always exchange heat with interval below since, by definition, the heat from interval above has temperature that is greater by the minimum approach temperature allowed in the heat exchanger than the highest cold interval temperature.

With this temperature interval diagram, correct placement of heat engines and heat pumps can be easily determined. Since it has been already established that the only hot utility is needed above the pinch, a heat engine should be placed completely above the pinch to replace the hot utility. This is shown in Figure 1.4 (a). Heat engine (1) takes in hot utility and converts part of energy to work and rejects rest to the interval where heat is needed. Heat engine (2) takes in heat surplus from one interval and converts some to work and rejects the rest to an interval below with heat deficit. However, below the pinch only cold utility is needed. Therefore, as shown in Figure 1.4 (b), a heat engine should be placed completely below the pinch to replace the cold utility, i.e., use waste heat as heat engine intake.

If these simple rules are not followed when placing heat engines, increased utility consumption results. For example, if the heat engine exhaust is placed below the pinch as shown in Figure 1.5, then the cold utility requirement increases by the same amount as the heat engine exhaust. The rules derived here were very qualitative; however, many of these rules were indeed not considered by engineers until Townsend and Linnhoff showed them so succinctly.

As for heat pumps, the reverse is true. Heat pumps should only be placed across the pinch as shown in Figure 1.6 (a). In this case the heat pump replaces the hot utility by $Q_1 + Q_2 + W$ and reduces the cold utility by $Q_1 + Q_2$. If the heat pump is placed completely above the pinch as shown in Figure 1.6 (b), the final effect is converting the electricity into heat which can be achieved at much lower cost by a simple immersion heater. A heat pump placed completely below the pinch is even more disastrous because not only is electricity being converted to heat but also that heat has to be removed with the cold utility. With these rules, any energy network
Figure 1.3: Derivation of Temperature Interval diagram
\[ \Delta H_i = \sum \Delta H_i \text{ cold} - \sum \Delta H_i \text{ hot} \]

\[ \Delta Q_i = \Delta Q_{i-1} - \Delta H_i \]

Figure 1.4: Correct heat engine placement
Figure 1.5: Incorrect heat engine placement
can be easily checked for an inappropriate placement of these units, and if found, they can be correctly placed to increase the efficiency of the plant.

However, these rules by themselves were insufficient to synthesize an optimum network. They were very effective in the analysis of the existing designs. Even with these rules, the number of possible alternatives were staggering. To find the optimum network manually was not an easy task.

Recently, Colmenares and Seider [1986] developed a non-linear programming strategy to incorporate the placement rules developed by Townsend and Linnhoff. Their results indicated large potential savings from integrating heat engines and heat pumps. However, the effect of work integration on the utility plant or the heat recovery network was not examined.

1.2.7 Motivation for Development of a New Strategy for Utility Plant and Heat Recovery Network

With the discovery of the pinch in the heat recovery network, the analysis of the heat recovery network problem became more systematic. The extension of the pinch concept to integration of heat engines and heat pumps has been a powerful analysis tool. However, the interaction between the two subproblems can not be accounted fully with these methods.

For example, a heat pump could be placed across the pinch based on the heuristics developed by Townsend and Linnhoff; however, this may cause the utility plant to operate at a very low efficiency level. The overall cost of the operation may be higher than the design without the heat pump installed. Without proper methods to account for such interaction, the problem can only be solved by tedious trial and error method. The qualitative rules that were derived were very helpful in designing heat and work integrated plant. However, more specific rules and quantitative methods are needed to find the optimal solution.

A simple way to account for the interaction between the utility plant and the
Figure 1.6: Placement of heat pumps
heat exchanger network has been to assign costs to key variables. For example, a hot utility is assigned a cost based on the incremental fuel cost necessary to produce this high temperature hot utility and also based on the credit from the power production from this hot utility. This cost would be charged to the heat exchanger network and the chemical plant. The design of each would be done to minimize the total cost including the charges for the utility. The utility plant would be credited with producing this utility, and it would be designed to maximize the profit.

The implicit assumption is that a power production system exists and that credit will be given for producing a high temperature working fluid with work producing potential regardless of the existence of a work producing turbine. In many cases, the cost of installing a high temperature and pressure turbine far exceeds the cost of the heat exchanger network and the fuel. Therefore, only a simple boiler would be used. Yet, the design of the heat exchanger network and the process plant would not reflect this. Of course, one could go back and redesign the system based on the new cost, but then the cost of the utilities may change again. It is apparent, then, this is not a very efficient method.

Furthermore, when the utility plant and the heat exchanger network are considered simultaneously, the problem has been shown to be combinatorially intractable. Add to this, the non-linearities involved would make the finding of the global optimal solution next to impossible. The heuristic approaches have been too general to be used in finding a global optimal solution. And the mathematical programming approaches have been only applicable to the subproblems. Therefore, a new method with adequate heuristics to reduce the combinatorial nature and with a mathematical approach that is applicable to the combined problem is needed.

1.3 Thesis Overview

The objective of this research was to develop a new methodology for solving the utility plant and the heat recovery network problem simultaneously. The previous approaches have emphasized heuristics as the only method to account for the inter-
action. However, these heuristic methods could not account for all the interactions and furthermore could not be used to generate a design; they only identify attractive and unattractive possibilities. On the other hand, if a completely mathematical programming technique is used, the number of possible alternatives is astronomical due to the combinatorial nature as shown in Table 1.1. Furthermore, simply applying a mathematical formulation strategy results in a mixed integer non-linear programming (MINLP) problem. The current solution methods for solving a large MINLP are impractical in light of these complications.

Therefore, the aim of this research is to overcome these problems by developing a methodology to simultaneously synthesize the utility plant and the heat recovery network. It will be assumed that the design of the chemical process has been fixed. Although this assumption neglects the important interaction between the process and the heat exchange network/utility system, the solution methodology still represents a major advance over the present state of the art.

The new design methodology is outlined in Figure 1.7. It starts with a fixed design of the chemical process – decoupled from the heat recovery network and the utility plant. All of the process data are derived from this design, including the heating and cooling requirements for the process streams. Therefore, the hot and cold composite enthalpy vs. temperature curves (of Figure 1.2) are known for the underlying chemical process. We also assume, initially, that the minimum approach temperature, $\Delta T_{\text{min}}$, is specified.

In the traditional approach one would, at this point, determine targets for the minimum hot and cold utilities and design the heat recovery network assuming the availability of hot and cold utilities at specified temperature levels and at specified arbitrary costs. Although such a design strategy results in an optimum heat recovery network, it is optimum only with respect to the assumed utilities and their arbitrary costs. Furthermore, integration of units into the heat exchanger network from the utility plant, such as heat engines and heat pumps, can not be done effectively.

The new strategy overcomes this problem by postponing the actual design of
Begin Design

Specify chemical plant design and determine composite enthalpy curves for heating and cooling

Select ΔTmin

Determine pinch, determine feasible utility temperature levels and maximum and minimum amounts

Develop superstructure and solve MILP for optimum integrated utility plant including heat engines, heat pumps, and refrigeration units where applicable

Design and cost heat exchanger network

Compare the total cost

improvement, new ΔT

no improvement

End of Design

Figure 1.7: New Simultaneous Synthesis Strategy
the heat recovery network until the appropriate utility plant integration is determined. In Chapter 2, it is shown that there are only a comparatively small number of temperature levels (corresponding to “kinks” in the composite enthalpy curves) at which it is economically attractive to provide hot or cold utilities. Rules based on thermodynamic and economic analysis were developed to determine these levels and the maximum and minimum amount of utility at each level that can be used by the process. Although these rules, by themselves, do not allow complete design of the utility plant or the heat recovery network, they do reduce the number of utility level alternatives that need to be examined, thereby reducing the combinatorial nature of the overall problem. At the same time, these rules ensure that the minimum cost solution is included in the remaining alternatives.

If no heat pumps or heat engines were to be used and if the heating and cooling utilities were to be supplied using a traditional utilities plant providing steam at various levels and rejecting heat to an ambient sink, it would be straightforward to synthesize the utility plant using one of the mixed integer linear programming (MILP) techniques described earlier. A superstructure would be set up, including all of the allowable temperature levels for utilities described above and including models for all the traditional units in the utility plant (pumps, boilers, turbines, etc.) The solution to the MILP then selects which units and temperature levels will appear in the final optimized network. This approach is illustrated in Chapter 4.

To permit consideration of heat engines and heat pumps in the network, a set of rules were developed to identify those utilities (and their temperature levels) which could serve as a heat source or sink for a heat engine or a heat pump. Criteria based on thermodynamic and economic feasibility were developed to determine the candidate heat sources and sinks. Ones that do not meet the criteria are discarded to reduce the number of alternatives.

For each feasible combination of heat source and sink, a nonlinear model of the appropriate heat pump or heat engine was developed and optimized with respect to the local variables (operating pressures and type of working fluid) with net power production as the objective function. Input and output temperatures were not variable.
since they were already known for a given heat sink and source. Because the operating range of the units were limited, the models could be placed in a linearized form and included in the MILP superstructure for the plant utility system. The solution of the MILP then included the heat pumps and/or heat engines that lead to the economic optimum. The optimization determines the existence of units, operating conditions and the flowrates from the units. Although the problem is still combinatoric due to the discrete decision variables, the problem size has been reduced to an extent that a simple branch and bound scheme can be used to solve the problem efficiently.

In a similar way to the incorporation of heat pumps and heat engines, the elements of a refrigeration system were also included in the superstructure to provide for utilities at below ambient temperature.

To complete the synthesis, the heat exchanger network is derived with the utility plant interaction specified. The utility plant interaction consists of the temperature levels and amounts of each utility to be supplied, the presence of each heat pump and heat engine, and the configuration of the refrigeration system (if any). Since the heat exchanger network synthesis is constrained by the specified utility plant interaction, any of the previous heat exchanger network design technique can be used to synthesize the network. In this work, the heuristic evolutionary method by Linnhoff et al. [1982] was used. The method offers an advantage in that the actual heat exchanger network can be derived directly from the heuristics.

Finally, the underlying assumption that appropriate minimum approach temperature can be selected a priori is relaxed. By varying the minimum approach temperature in the outer loop as shown in Figure 1.7, the tradeoff between the utility plant and the heat recovery network was examined. As $\Delta T_{min}$ (HRAT) is decreased, the heat recovery potential increases and the interaction with utility plant decreases. On the other hand increasing $\Delta T_{min}$ decreased the heat recovery potential and increased interaction with the utility plant. The method developed properly balances the tradeoffs involved to find the optimum $\Delta T_{min}$. The method is applicable in both the grass-root design case and also the retrofit case.
The conclusion of the new strategy developed in this research is that a systematic procedure can be applied effectively to the general synthesis of utility plant and heat recovery networks while properly accounting for the interaction between the two. The new method utilizes best of both heuristics approach and mathematical approach to find the design solution that neither approach could find separately. It has brought into light the fact that the heat exchanger network design is not the only place where energy savings can be generated. The utility plant and associated heat and work integration also offer large savings potential. Furthermore, it has been shown that the utility plant synthesis combined with the heat exchanger network results in a more integrated and thus lower cost design than doing either separately.

The effectiveness of the methods developed in this thesis have been demonstrated with prototype software. For use on a large scale, they should be incorporated into a comprehensive, user-friendly software system.
Notations used in Chapter 1

- $C_{ann}$: annualized total cost
- $C_{util}$: $/ per kw-yr cost of utilities
- $C_{fuel}$: $/ per kw-yr cost of kerosine
- $C_{exchanger}$: capital cost of heat exchanger
- $F_j$: flow rate of stream $j$ in kg/sec
- $l$: total number of streams that need pressure change
- $m$: total number of cold streams
- $mCp_i$: mass-heat capacity flow rate
- $N_i$: total number of streams in each heat exchanger
- $N_c$: number of cold streams
- $N_{cu}$: number of selected cold utilities
- $N_h$: number of hot streams
- $N_{hu}$: number of selected hot utilities
- $N_{max}$: maximum number of heat exchanger matches possible
- $N_{min}$: minimum number of possible hot utility types
- $N_{Thu}$: number of possible hot utility types (usually temperature level)
- $N_{util}$: number of possible utility plant configuration
- $n$: total number of hot streams
- $\eta_{boiler}$: thermal efficiency of boiler
- $q_i$: heat content of stream $j$ usually associated with specific temperature range
- $Q_i$: utility added at $T_i$
- $Q_{min,cold}$: minimum cold utility required at lowest temperature
- $Q_{min,hot}$: minimum hot utility required at highest temperature
- $\Delta T_{min,global}$: global minimum approach temperature allowed in the heat exchanger
- $\Delta T_{min,utility}$: minimum approach temperature in a heat exchanger with utility to process stream match
- $T_{cold,supply,j}$: supply temperature of cold stream $j$
- $T_{cold,target,j}$: target temperature of cold stream $j$
- $T_{hot,supply,i}$: supply temperature of hot stream $i$
- $T_{hot,target,i}$: target temperature of hot stream $i$
Chapter 2

Hot and Cold Utilities Placement in Heat Exchanger Network

Given a set of process streams with their supply and target temperatures and a set of utilities with associated cost, a heat exchanger network can be designed to maximize the recovery of heat from the process streams and at the same time minimize the amount of hot and cold utilities used. However, in designing this network, previous methods assumed that the temperatures of hot and cold utilities were fixed, and only the demand varied depending on process parameters such as minimum approach temperature, forbidden matches, preferred matches, etc. This assumption invariably eliminated consideration of different utility temperatures and the more economical designs resulting from such consideration. Although one could repeatedly run the algorithms developed in previous methods while varying the utility temperatures to find the minimum cost network, this is at best clumsy and could result in a problem so large that it is impractical to solve with present MILP algorithms.

Furthermore, previous methods used a global minimum approach temperature in all matches whether they were between a process stream and a process stream, or between a process stream and a utility stream. However, in most heat exchanges between utility streams such as condensing steam and a process stream, the minimum approach temperature can go much lower than the minimum approach temperature in a typical process to process stream match. Even more crucial is the match between
refrigeration utility streams and the process streams. Here, the approach temperature can be less than 5°C and sometimes can be as low as 1°C or 2°C. However, except for some heuristic methods [Pho & Lapidus, 1973], methods developed previously have been able only to use a global minimum approach temperature for all the matches and could not account for these differences in the matches. And the typical $\Delta T_{\text{min}}$’s were in the 10°C ~ 20°C range. The resulting design or the cost data can not be termed reliable if these non-idealities are present in the given problem.

To overcome these non-idealities, a new method has been developed based on thermodynamics and economic analysis. The new method allows consideration of multiple temperatures for utilities. Selection of the most appropriate temperature can be made based on true cost economics rather than the levels set a priori by some existing utility plant. Furthermore, the utility stream to process stream matches can have different $\Delta T_{\text{min}}$’s from the process to process stream matches. The heuristics developed here can be considered one at a time; or as will be shown in the following chapters, they can be incorporated into a rigorous numerical algorithm so that optimization with respect to utility levels and loads can be performed.

2.1 Selection of utility temperatures

If one takes a look at all of the previous work in the area of heat exchanger network design, all assume that the hot utility is available at specific temperatures at specific cost, because the purpose of their research was to design – from the minimum utility load or minimum units stand-point – a good heat exchanger network given these utilities. The origin of these temperature levels is unclear, but they seem to propagate through hundreds of research papers in the last ten years. The classic heat exchanger network design problems, (4SP1, 4SP2, 5SP1, etc.) that have been used to test the effectiveness of the solution strategy for heat exchanger network design [Cerda and Westerberg, 1983], mostly use heating utility at two temperature levels: 235°C condensing steam for medium pressure steam and 150°C condensing steam for low pressure steam.
Table 2.1: Stream Data for 4SP2

<table>
<thead>
<tr>
<th>Stream</th>
<th>$T_s$(°C)</th>
<th>$T_i$(°C)</th>
<th>mCp(kw/°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>204</td>
<td>43</td>
<td>15.83</td>
</tr>
<tr>
<td>H2</td>
<td>260</td>
<td>43</td>
<td>10.55</td>
</tr>
<tr>
<td>H3</td>
<td>221</td>
<td>110</td>
<td>26.38</td>
</tr>
<tr>
<td>C1</td>
<td>-4</td>
<td>216</td>
<td>36.96</td>
</tr>
</tbody>
</table>

For example, consider the 4SP2 problem. The problem data are shown in Table 2.1. In this problem, condensing steam at 235°C supplies all the heating requirement of 365 kW. The total cost is $272,900 in capital cost and $39,895 in annual operating cost. The total annualized cost, based on a 10 year straight line capital recovery factor, is $67,184 per year. The cost data are derived from the previous work by Linnhoff and Hindmarsh, [1983]; Colmenares and Seider [1986] and adjusted to 1985 dollars using Chemical Process Equipment Index from Chemical Engineering [October, 1988] as shown in Appendix A-1. (The capital cost accounts for heat exchangers only, and the operating cost accounts for only the fuel needed to produce steam at 235°C. For the moment the boiler and the feed water pump costs are neglected.) The minimum cost network is shown in Figure 2.1. However, this network is the minimum cost network based on the assumption that the steam is available only at 235°C. What if the steam is available at a lower temperature or higher temperature? How would this affect the cost of the network? Will the design shown on Figure 2.1 still be the lowest cost network?

The effect of steam temperature on the total cost – annualized heat exchanger capital cost and the utility cost expressed in terms of steam cost as a function of steam temperature – of the minimum cost network for given steam temperature is shown in Figure 2.2. To obtain the total annualized cost curve, a utility temperature was selected, and then the heat exchanger networks were derived by hand. From the derived networks, the least expensive network was selected and combined with the utility cost to get the total annualized cost for heat exchanger network with the
Figure 2.1: minimum cost heat exchanger network for 4SP2
selected utility temperature.

The absolute minimum cost network occurs when the steam is supplied at 110°C. The cost increases for \( T_{\text{steam}} < 110^\circ\text{C} \) because at this temperature, two levels of steam – one at \( T_{\text{low}}(< 110^\circ) \) and one at 110°C – are required. The resulting design has one more heat exchanger than the design A. The cost also increases for \( T_{\text{steam}} > 110^\circ\text{C} \), because the area decrease due to higher temperature steam is more than offset by the increase in the cost of the higher temperature steam. Steam cost data as a function of temperature are derived from the linear interpolation of steam costs given in the paper by Colmenares and Seider. [1986] The global minimum cost network is shown in Figure 2.3.

It has been found that the general shape of the total cost vs. utility temperature for other problems is similar to that of saw-tooth curve shown in Figure 2.4. Each discontinuity represents a reduction in the number of units in the minimum cost network. This curve would apply to the case of hot utility supplied at a single temperature or if there are multiple temperature levels, for fixed values of the other levels. After each discontinuity, the cost increases with increasing temperature because of the increased cost of producing a higher temperature utility more than offsets the reduction in cost of heat exchanger area. In general, short of designing a minimum cost network for each utility temperature level and then costing each network, it is not possible to predict for every problem what the utility temperature levels are that correspond to global minimum cost network. Such a complete enumeration of all temperatures would take exorbitant time. Furthermore, previous approaches using numerical techniques, such as MILP, would be almost unsolvable since the size of the problem is almost exponentially dependent on the number of temperature levels considered.

From Figure 2.4 it is apparent that if the discontinuities can be found a priori, then the heat exchanger network can be designed for each combination of utilities at the temperature corresponding to the discontinuities. Furthermore, the global minimum cost network must be among this set of heat exchanger network and utilities combination. Using thermodynamic reasoning and insight into the problem, new
Figure 2.2: Effect of steam level
Operating Cost = $20,440/yr
Capital Cost = $247,408 total
Annualized Cost = $45,100/yr

Figure 2.3: Global minimum cost heat exchanger network
Figure 2.4: General Curve for effect of utility temperature on total cost
heuristics and algorithms have been developed that allow determination of these discontinuities without doing a complete enumeration of utility levels and heat exchanger network combinations.

2.1.1 Hot Utility Temperatures

From the example problem 4SP2, it is obvious that the selection of the utility levels plays a major role in lowering the overall cost of the network. Through simple thermodynamic and economic analyses, most temperature levels can be ruled out. A few selected levels can then be incorporated into a numerical algorithm and optimized for the load at each level.

**Single Utility Problem**

Let's first examine problems whose heating need can be satisfied using a single hot utility. Furthermore, it is assumed that the temperature range at which hot utility is required is narrow enough that multiple levels would only increase the capital cost. Although heat can be supplied using a single very high temperature utility for every problem, we are concerned with problems that allow a single hot utility where

\[ T_{\text{max,process}} > T_{\text{util}} > T_{\text{min,process}} \]

The reason that many temperature levels can be dismissed at the initial stage is due to the fact the certain levels cause the network to have more heat exchangers than other levels.

Shown in Figure 2.5 is a section of the pinch diagram above the pinch for Example Problem 2-1. There are one cold stream and one hot stream above the pinch. The hot utility can be added at any one temperature level higher than \( T_a \) as long as minimum utility requirement of 10 kw is satisfied.

The lowest utility cost design in terms of the available energy would involve adding infinitesimal hot utility at every temperature from \( T_a \) to \( T_{\text{max}} \) where the fol-
Figure 2.5: Above the pinch diagram for Example 2-1
lowing is satisfied.

\[ \int_{T_a}^{T_{\text{max}}} \delta Q \frac{\delta T}{\delta T} = Q_{\text{min, hot}} \quad (2.1) \]

For this problems, \( Q_{\text{min, hot}} = 100 \text{ kw} \). This design is represented on the composite diagram as shown in Figure 2.6 (a). There is a pinch at every temperature level, and the utility cost would be lowest if the cost of each utility reflected the availability difference. However, this design is clearly uneconomical from the overall capital cost stand-point since the number of heat exchangers needed would be infinite as shown in Figure 2.7 (a). (If the boilers, pumps, pressure reducer, and the turbine were taken into account, the picture would be worse for design A.)

There is no need, then, to consider all temperature levels. Clearly, a better design is shown in Figure 2.6 (b) with \( T_{\text{steam}} = 130^\circ C \). The corresponding network shown in Figure 2.7 (b) has three heat exchangers and one utility pinch. As a matter of fact, all designs with \( T_{\text{steam}} < 155^\circ C \) have three heat exchangers.

Under the assumption that the boiler cost is already sunk, an economic analysis can be performed on the designs with \( T_{\text{steam}} < 155^\circ C \) represented by Figure 2.7 (b) and compared to the designs with \( T_{\text{steam}} = 155^\circ C \) represented by Figure 2.7 (c). The annualized cost is as follows:

\[ C_{\text{ann}} = \frac{1}{DP_yr} \sum_{i=1}^{N} CC_{\text{exchanger, i}} + C_{\text{util}} \quad (2.2) \]

The capital cost of heat exchangers can be calculated using the following:

\[ CC_{\text{exchanger, i}} = c + bA_{\text{rea}}^a \quad (2.3) \]

Since the boiler cost is sunk, the total fuel cost is the utility cost.

\[ C_{\text{util}} = C_{\text{fuel}}\eta_{\text{boiler}} F_{\text{low, steam}} \frac{[H_{T, \text{steam}} - H_{b, f,w}]}{\Delta H_{\text{fuel}}} \quad (2.4) \]

The heat exchanger area can be estimated from the Bath Formula. [Tjoe and Linnhoff, 1984]

\[ A_{\text{rea}} = \sum_{i=1}^{M} \frac{1}{\Delta T_{\text{im}, i}} \left[ \sum_{j} \frac{q_j}{h_j} \right]_i \quad (2.5) \]
Figure 2.6: Hot utility level alternatives
Figure 2.7: minimum cost heat exchanger network for various utility levels
Table 2.2: Result of economic costing for Example 2-1

<table>
<thead>
<tr>
<th>Design</th>
<th>first term$^1$</th>
<th>second term$^1$</th>
<th>third term$^2$</th>
<th>Total$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design A (140°C)</td>
<td>$42,000</td>
<td>$34,765</td>
<td>$13,116</td>
<td>$26,583</td>
</tr>
<tr>
<td>Design B (155°C)</td>
<td>$28,000</td>
<td>$29,756</td>
<td>$13,487</td>
<td>$23,619</td>
</tr>
<tr>
<td>Design C (170°C)</td>
<td>$28,000</td>
<td>$26,739</td>
<td>$13,896</td>
<td>$23,499</td>
</tr>
</tbody>
</table>

$^1$Cost before annualization factor
$^2$Total annualized cost with $DP_yr = 5.7$

For designs (designated Design A) with $T_{steam} < 155°C$.

$$C_{ann} = \frac{1}{DP_yr} \left[ 3c + \frac{b(A_{ex1}^a + A_{ex2}^a + A_{ex3}^a)}{C_{util,1}} \right] + \frac{C_{util,1}}{C_{util,2}}$$  \hspace{1cm} (2.6)

For $T_{steam} = 155°C$ designs (designated Design B),

$$C_{ann} = \frac{1}{DP_yr} \left[ 2c + \frac{b(A_{ex4}^a + A_{ex5}^a)}{C_{util,2}} \right] + \frac{C_{util,1}}{C_{util,2}}$$  \hspace{1cm} (2.7)

The ratios of the first term to the second term to the third term vary depending on different $DP_yr$'s and also on the problem. But in this example problem the first and second terms account for about 80% of the $C_{ann}$ if $DP_yr = 1$. An analysis shows that the difference in the first terms is at least 33%. If that isn’t enough to favor the Design B, the second terms also differ by 10 to 15% in Design B’s favor. Only the third terms favor Design A, but the effect is negligible since it is only 1 to 2%. This result is shown in Table 2.2. Based on this consideration Design B is far superior. Figure 2.8 shows the effect of selection of hot utility temperatures on the total annualized cost. In fact given two utility temperature levels, the level that results in a design with fewer number of exchangers is always a better design based on the total annualized cost.

For designs with $T_{steam} > 155°C$, as shown in Figure 2.6 (d) with $T_{steam} = 170°C$, there is no utility pinch, and only two heat exchangers are needed as shown in Figure 2.7 (d). Thus, design C and design B have heat exchanger networks of identical
Figure 2.8: Effect of utility temperature on two stream problem
structure. The only differences arise from the increased area in Design B and increased utility cost in Design C. The difference in the total annualized cost is only $119 between 155°C and 170°C steam levels. This analysis is done assuming that the boiler cost is sunk, and the boiler and the accompanying piping can handle any temperature steam.

However, in the grass-root design case, the boiler cost would have to considered at the least. In that case, the cost difference between 155°C and 170°C boilers are much higher than $119 per year. The relevant calculations are shown in Appendix A-1. Since this research is concerned with the grass-root design, the cost advantage favors the 155°C steam system. Any design with $T_{steam} > 155$ °C is more costly than the 155°C steam system.

It is obvious then, that Design B with $T_{steam} = 155$ °C is the minimum cost network. The question is should we have known, before we examined all the temperature levels, that $T_{steam} = 155$ °C is the utility level for the global minimum cost network. The answer is we should have, because 155°C is the only candidate utility temperature for this problem. The candidate hot utility temperatures consist of the kinks in the hot composite curves above the pinch and also the $T_{cold,max} + AT_{min}$. This is the first set of heuristics developed, and a detailed explanation is provided in the following paragraphs.

In this example problem, there is a kink at 170 °C (where-ever a hot stream enters the hot composite curve is considered a kink), but this is eliminated because it is greater than $T_{cold,max} + AT_{min}$. Therefore, there is only $T_{steam} = T_{cold,max} + AT_{min} = 155$ °C to consider. Thus, without having to enumerate all the temperature levels, a minimum cost design should have been made based on the 155°C steam. Therefore, for any problem with two streams above the pinch, subject to single utility, only the few candidate points picked by above rules need to be considered rather than every temperature level extending from $T_{hot,min}$ to $T_{cold,max}$.

Figure 2.9 shows the only other alternative for a problem with two streams above the pinch based on the heuristics, the minimum cost network should be at one of the
candidate points. The only candidate point occurs at $T_{steam} = T_{cold,max} + \Delta T_{min}$, and indeed the global minimum cost network has utility at the candidate point.

The reasons that only these candidate points need to be considered are many. First, any utility added below $T_{kink}$ results in an extra exchanger compared to the design with utility added at $T_{kink}$. This is shown in Figure 2.10. This problem has two hot streams and one cold stream above the pinch. Design (1) has three heat exchangers and one heater for a total of four exchangers whereas the Design (2) has five exchangers. Clearly, the Design (1) is better than Design (2) without going into the details of analysis using equations [2.1 - 2.4].

As a matter of fact, designs using $T_{steam,1}$ is always better than designs with $T_{steam,2}$ no matter how many kinks are present above the $T_{steam,1}$. The portion of the network above $T_1$ will be identical, but for the design of the network between $T$ and $T_{hot,pinch}$, the advantage goes to $T_{steam,1}$ system.

However, there are always a few exceptions. If the temperature difference at point (a) on the composite diagram shown in Figure 2.10 is wide enough, loop breaking techniques can be used to combine EX1 and EX3 in Design (2) to form Design (2'). In this case we can not conclude that $T_1$ is better than $T_2$ based solely on equation [2.1]. In fact, Design (2') has lower total cost compared to Design (1).

However, this special case arises because $Q_{1,max} \geq Q_{hot,min}$ where $Q_{1,max}$ is the maximum amount of hot utility that can be added at $T_1$ till that utility causes a pinch as shown in Figure 2.11. Of course, the actual hot utility load $Q_1$ would never be greater than $Q_{hot,min}$ from the composite diagram. In this case, the heuristic needs to be updated to include $T_1'$ where $Q_{1',max} = Q_{hot,min}$ and eliminate the old $T_1$ from the candidate utility levels. Since Design (1') is structurally identical to Design (1), it is not shown separately. Furthermore, Design (2') is not possible for $T_2 < T_1'$, and only Design (2) is possible which was already determined to be more costly than Design (1). Therefore, only $T_1'$ found with above heuristic needs to be considered to account for this special case.

Second, hot utility added above $T_{kink}$ offers no advantage. There are three
Figure 2.9: Utility level alternative for two stream problem
Figure 2.10: Minimum cost heat exchanger network for three stream problem
Figure 2.11: Special utility level for single utility problem
possible designs for problem shown in Figure 2.12 (a). As before, all heat must be supplied at one temperature. In case (b), steam is supplied at $T_{kink}$ where $Q_{kink,\text{max}} = Q_{\text{hot, min}}$, and four exchangers are needed. (Although only three exchangers are shown in the composite diagram, heat exchanger EX1 actually consists of two separate exchangers. Thus, the total number of exchangers is four.) In case (c), steam is supplied at $T_{steam,3} > T_{kink}$ and, six exchangers are needed. There is no question, then, that case (b) is a less expensive design.

However, if $T_{steam,3}$ is selected such that $T_{steam,3} - T_{cold,\text{max}} \geq \Delta T_{\min}$, the design shown in Figure 2.12 (d) can be found. This design has three heat exchangers and is less expensive than the design shown in (b). Of all possible utility temperatures $T_{steam,3}$ where $T_{steam,3} - T_{cold,\text{max}} \geq \Delta T_{\min}$, the lowest cost design occurs at $T_{steam,3} = T_{cold,\text{max}} + \Delta T_{\min}$.

However, this is not a contradiction of the utility temperature heuristics since $T_{steam,3} = T_{cold,\text{max}} + \Delta T_{\min}$ was already established as one of the possible candidates for the minimum total cost utility level. Therefore, the minimum total cost design would have been found from examining the only two possible candidate points selected from the heuristics. The temperatures lying in between the candidate points need not be considered.

The heuristics developed here will limit the number of levels that need to be considered so that an optimization can be performed with respect to temperature levels, and the minimum cost utility can be found for a single utility problems.

**Multiple Level Utility Problem**

The problems considered thus far needed only one utility level to meet all of its heating demand. Furthermore, it was assumed that supplying utility at multiple levels only increases the capital cost without decreasing the fuel consumption. In such problems, the hot utility must be added at the temperatures specified by the single utility heuristics, namely the kinks.
Figure 2.12: Alternate designs for $T_{hot}$ above $T_{kink}$
However, there will be problems where if the utility is supplied at multiple levels, a lower cost design may result as shown in Figure 2.13. This type of problem arises if the adjacent kink temperatures cover a large range. Although the network shown in Figure 2.13 (a) has fewer heat exchangers than the network shown in Figure 2.13 (b), the total annualized cost is slightly higher because all its utility need is supplied at the very expensive level. By replacing a portion of the expensive hot utility with lower temperature utility at $T_{util} = 190^\circ C$, the total annualized cost is lowered even though an additional heat exchanger is required.

In this section, the heuristics from the single utility case are extended so that selection of candidate utility temperatures for multiple level utilities can be made without complete enumeration of all possible levels and combinations.

Let's begin by considering a two level utility design. Extending the heuristics from the single level utility section, the number of alternatives can be reduced to a more reasonable size without eliminating the minimum cost combination. The new heuristic for two utility case is simply that the candidate temperature levels are the kink points and the $T_{cold, max} + \Delta T_{min}$.

The reason for choosing these temperature levels is simple. If two utility temperature levels are not at the kink points, the resulting design would cost more than the similar two utility temperature levels at the kinks. For example, shown in Figure 2.14 (a) is a composite diagram where hot composite curve is shifted to the right at the points of hot utility injection. If the hot utilities are added at the kink temperatures, the heat exchanger network would have 5 units. On the other hand, if the hot utilities are added at the non-kink points, the resulting design would have 7 units as shown in Figure 2.14 (b). Clearly, the injection of both hot utilities at the kink points will yield a lower total cost design than a design using injection of both hot utilities at the non-kink temperatures.

However, there is another possibility for the two utility problem. A third design would have one utility at the kink temperature and the other at a non-kink temperature. This is shown in Figure 2.15 as utility combination (1) & (2), and
Figure 2.13: Minimum cost network for multiple level utilities

(a) Total Cost = $90,000/yr

(b) Total Cost = $88,000/yr
Figure 2.14: Effect of non-kink temperature utilities
levels (1) and (3) are kink points, the utility combination of (1) & (3) should be better than combinations involving non-kink level (2) according to the heuristics.

In comparing combination (1) & (2) with kink combination, the former invariably causes triple levels of utility, i.e. utility level (3) is needed because $Q_1 + Q_2 < Q_{min,hot}$. Therefore, it can be eliminated first. Please note that if level (2) could have satisfied all heating demand, i.e. $Q_{2, max} = Q_{min}$, then level (3) would have been lowered already such that $Q_{2, min} < Q_{min}$. This belongs to one of those special cases mentioned in the previous section where the kink temperature needs to be updated.

The other alternative is utility combination (2) & (3). Comparison of this combination with combination (1) & (3) shows that the latter utility combination always results in a lower cost design as long as two utility levels are to be used. This is numerically proven for any type of hot and cold composite curves in the appendix A-2. Simply extending this analysis further for multiple level utilities, it is apparent that only the temperatures selected by above heuristics need to be examined to get the minimum cost design.

Since the number of utility level combinations have been reduced drastically, the global minimum cost design can be found among the utility levels selected either manually or by numerical algorithms. For example if there are 5 hot streams above the pinch, at the most there will be six candidate points. The total number of alternatives is only 31 which, as shown in Chapter 4, can easily be handled by the algorithm for utility plant optimization.

One final note is regarding the question “when is a single level utility system better than multiple level system?” The heuristics developed do not answer that question. They only pick the correct utility temperature levels that must be in the minimum cost design. The numerical algorithms in Chapter 4 deals with the optimization of utility loads and the number of levels.
Figure 2.15: Inter-kink utility level combination
2.1.2 Cold Utility Temperatures

From the pinch diagram, the minimum amount of cold utility, $Q_{\text{min,cold}}$, needed for a given problem is known. But in order to determine the temperature levels at which this load should be distributed to achieve a minimum cost network design, the number of alternatives that have to be examined is very large. In this section, we develop the similar rules as in the previous section to reduce the number of levels that need to be considered to find the minimum cost network, i.e. for cold utilities the candidate levels corresponds to the kinks on the cold composite curve and the $T_{\text{hot,min}} - \Delta T_{\text{min}}$. Of course, the cold kink temperatures below $T_{\text{hot,min}} - \Delta T_{\text{min}}$ need not be considered.

Only the condensing cold utility (supplied by a refrigeration system) will be considered in this section. Non-condensing cold utility such as cooling water will be dealt with in a subsequent section.

**Single Utility Problem**

Shown in Figure 2.16 (a) is a section of a typical pinch diagram below the pinch. The cold utility can be supplied at $T_1$ which corresponds to $T_{\text{hot,min}} - \Delta T_{\text{min}}$, or at $T_2$ where $T_2 < T_1$, or at $T_3$ where $T_3 > T_1$. For now, only single level utility designs will be considered. The design based on $T_1$, shown in Figure 2.16 (b), will have same number of exchangers as the design based on $T_2$, but latter’s area will be smaller. However this cost savings in area is minor compared to the increased power consumption which can be calculated easily using the following equation.

$$\Delta C_{\text{cost}} = C_{\text{power}} \eta_{\text{compressor}} Q_{\text{cold util}} T_{\text{cooling water}} \left[ \frac{1}{T_1} - \frac{1}{T_2} \right]$$  \hspace{1cm} (2.8)

In this cost equation, we assumed that the capital cost of the compressor in the refrigeration cycle is already sunk. Therefore, the cold utility cost can be estimated from the extra power input for using cold utility at $T_2$ instead of at $T_1$. Comparison of cost savings due to heat exchanger area decrease by using $T_2$ cold utility versus the extra cost of pumping has been made for various temperature levels and loads. From
this analysis, we can conclude that $T_1$ is always better than $T_2$.

The analysis of $T_1$ vs. $T_3$ is not as clear cut. Although the design [b] using cold utility at $T_3$ shown in Figure 2.16 (c) does have one more exchanger than the design [a], $\Delta C_{\text{ost}}$ from equation 2.8 for this case could overwhelm the effect of the extra exchanger. This is especially true with large $DP_{yr}$ and for high power cost.

But for cases where $T_1 \geq T_{\text{cooling water}} - 25^\circ C$, the total cost for design [a] is always lower. Therefore, the cold utility should always be added at the kink temperatures or at $T_{\text{hot,min}} - \Delta T_{\text{min}}$. This is true for multi-stream cases also.

For low temperature refrigeration, i.e. $T_1 \leq T_{\text{cooling water}} - 25^\circ C$, temperature levels that need to be looked at are still the cold kink temperatures and $T_{\text{hot,min}} - \Delta T_{\text{min}}$. But if the difference between the kink temperatures are large, it is sufficient to consider mid-kink temperatures, i.e. $\frac{T_{\text{kink},i} + T_{\text{kink},i+1}}{2}$. However, the utility at mid-kink temperature must still meet the condition that $Q_{\text{mid-kink}} = Q_{\text{min,cold}}$. Even with the inclusion of the mid-kink temperatures, the number of levels are considerably less. Furthermore, unless a mid-kink temperature is proved to be needed in the final design, other non-kinks need not be considered to find the minimum cost design.

**Multiple Utility Problem**

For multiple level cold utilities, the same kink temperature cold utility rule applies as in the single level cold utility case. As shown in Figure 2.17, the cold utilities must be added at the kinks on the cold composite curve corresponding to $T_1$ & $T_2$ in order to avoid having extra heat exchangers. Utility level combination of (1) & (2) will always be lower cost than combination of (1) & (3). This is further reinforced by the fact that if the latter combination could not satisfy the cooling demand, then the level (2) must be included causing it to have three levels instead of two.

As before, the kink temperature must be checked to make sure that the following
Figure 2.16: Pinch diagram for single level cold utility placement below the pinch and the resulting network.
If this condition does not hold, then the kink temperature is raised until the condition becomes true. The corresponding temperature is selected as a candidate point instead of the original kink temperature.

Additional levels need to be considered if the first $T_{kink}$ or the difference between $T_{kink,i}$'s are large. Mid-kink temperatures can be used to determine the viability of the additional levels. In most cases, the load on the mid-kink levels turns out to be very small and can be economically replaced with utilities at the kink points.

2.2 Non-point Temperature Utilities

Even today, some industrial sites still use non-condensing hot utilities such as hot oil because of safety and controllability issues. Furthermore, cooling water is used for process cooling at most plants. These hot and cold utilities are called non-point temperature utilities since the target temperature of the utility can be varied. With the exception of the work by Viswanathan and Evans [1987], none of the previous work could account for this type of utility in terms of calculating the utility load or the target temperature of such utility. In this section, a simple set of heuristics are developed that would allow an engineer to quickly determine the target temperatures and the maximum load on these non-point temperature utilities.

2.2.1 Non-condensing Cold Utility

In most plant situations, there is normally only one type of non-condensing cold utility, i.e. cooling water; therefore, this problem reduces to the single utility case. (Some plants do have chilled water system. But this can be thought of as a cooling water system with different supply and target temperatures. Thus, this analysis is equally applicable.) The supply temperature of the cooling water is specified by the utility plant. This temperature is based on the cost of cooling, water evaporation...
Figure 2.17: multiple level cold utilities
rate, ambient temperature, and other cooling tower process parameters. In addition, the maximum allowable return temperature ($T_{cw,\text{target}}$) for cooling water is also set by the cooling tower process. Although the heat exchanger network can not set the supply temperature, the target temperature could be set such that both the cooling tower process and the heat exchanger network can have minimum cost.

Here again, thermodynamic reasoning and simple economic analysis can reduce the number of alternatives that have to be looked at in order to find the minimum cost target temperature and the load.

Let's begin by examining the below pinch section of the two stream pinch diagram as shown in Figure 2.18. First, the load on the cooling water is not really a variable. In the minimum cost network, each utility supplies as much load as it can without violating the pinch. Therefore, in this example problem, the load for any target temperature is $Q_{\text{cold,min}}$.

According to the heuristics from condensing cold utilities, the only candidate point for condensing cold utility is $T_2$ which corresponds to $T_{\text{hot,min}} - \Delta T_{\text{min}}$. However, for non-condensing utilities there are other candidate points because the utility pinch does not occur on the left side of the utility curve as in the condensing utilities case.

There are three other typical temperature levels. First is any $T_1$ where $T_1 < T_2$. Second is $T_3$ where it causes the utilities pinch with the hot composite curve. The third alternative is $T_4$ where the cold utility with $T_{\text{target}} = T_4$ is shifted to the right, and a lower portion of cold stream is shifted to the left. $T_4$ is calculated based on the assumption that it causes utility pinch when shifted to the right and that $Q_{cw,T4} = Q_{\text{cold,min}}$.

The design resulting from selecting $T_{cw,\text{target}} = T_4$ has three exchangers. This is one more than the design for $T_3$ utility. Since $T_3$ causes a utility pinch, any $T_{cw,\text{target}} > T_3$ utility necessarily has one more exchangers resulting in a higher cost design. For various combinations of hot and cold stream target and supply temperatures and loads, $T_{cw,\text{target}} = T_3$ always yields lower cost design than $T_4$ utility. Therefore,
temperatures above $T_3$ need not be examined.

The network with $T_1$, $T_2$, $T_3$ all have same number of exchangers. Therefore, the comparison is made using the capital cost savings due to area decrease for lower temperature and using the power savings due to decreased cooling water flow for higher target temperature. The result of comparison for different hot stream data was that $T_3$ always gives the lower cost design.

Therefore, in most problems, it is sufficient to calculate the target temperature $T_3$ causing a utility pinch and use it as the optimum non-condensing utility target temperature. However, it must be noted that the maximum cooling water return temperature is set by the cooling tower operation at around 50°C [Crozier, 1980]. Thus, in cases where $T_3 > T_{cw, max, return}$, the latter temperature must be used instead of $T_3$. In light of this fact, it is apparent that some of the previous research showing cooling water temperature rising beyond 80°C is only of theoretical interest and does not reflect actual design consideration.

For multiple stream problems as shown in Figure 2.19, the same heuristics can be used. Therefore, only candidate points are the utility pinch causing $T_4$ and $T_5$. Unlike the previous one hot and one cold stream problem, $T_5$, which looks identical to $T_4$ from Figure 2.18, must be included because the number of exchangers for a multi-stream case is an unknown term that must determined after the utility is selected.

The temperatures causing a utility pinch such as $T_4$ and $T_5$ in Figure 2.19 or $T_3$ in Figure 2.18 can be calculated simply by using the following equation.

$$ T_i = \frac{\sum_{j} T_{kink,j} \text{ Enthalpy}_{cold streams}}{\sum_{j} T_{kink,j \, hot} \text{ mC}_{hot streams}} - \Delta T_{min} \quad (2.10) $$

With these target temperatures, the network can be designed and costed to find the lowest cost combination of heat exchanger network and utility. Design of the heat exchanger network is simplified in that when cold utility at $T_5$ is placed, a portion of cold composite curve is shifted to the left from $T_{kink2}$.

In addition, $T_4$ and $T_5$ should be compared to the $T_{cw, max, return}$. If either is greater than $T_{cw, max, return}$, then the list is altered to include $T_{cw, max, return}$ and $T_i$ which
Figure 2.18: Non-point cooling utility
Figure 2.19: Alternate cooling water design for multi-stream case
satisfy $T_i \leq T_{cw,max,return}$ condition. Using these heuristics, most of temperatures can be eliminated, and the result is that minimum cost design can be found among the remaining alternatives. This analysis is equally applicable for high heat capacity cooling fluid other than the cooling water.

2.2.2 Non-condensing Hot Utility

Non-condensing hot utility is handled in the same manner as non-condensing cold utility. The purpose here is again to reduce the range of target temperature to a few that can be examined by complete enumeration.

With the condensing utility, the utility temperatures correspond to the kink temperatures. However, for non-condensing utility although the shift in the hot composite curve occurs at the kinks, the target temperature of the utility is lowered to $T^*$ as shown in Figure 2.20 to minimize the flow of the utility. Therefore, for each kink $T^*$ is calculated, and the maximum load is calculated. Maximum load is determined by shifting the portion of the hot composite curve that is above the kink until the shifted portion causes a new pinch as shown on the right half of Figure 2.20.

It is important to note that until now $T_{target}$ or $Q_{load}$ couldn't be calculated because the relationship between the kink temperature, where the part of the composite curve is shifted, and the utility target temperature was ignored. But from the heuristics regarding the condensing utility temperature, it was apparent that the shift of either composite curve should be at the kink points.

Therefore, for every non-condensing type of hot utility, there will be a few possible target temperatures, $T^*$'s, corresponding to the kink temperatures on the hot composite curve. With these temperatures, minimum cost utility and heat exchanger network can be found manually for small problems or using numerical algorithm for more complex problems.
Figure 2.20: Non-point temperature hot utility
2.3 Variable $\Delta T_{\text{min}}$'s

Heretofore, it was assumed that the global minimum approach temperature was sufficient to account for all types of heat exchanger matches, be it stream to stream or stream to utility, for the purpose of determining minimum utility load. However, it is important that different $\Delta T_{\text{min}}$ be used for process stream to utility match as opposed to process stream to process stream match in order to accurately determine the utility cost.

This is especially important for low temperature refrigeration. Here, the $\Delta T_{\text{min}}$ can be as small as 1°C as opposed to 10°C typically used for process to process stream match. In previous research [Shelton and Grossmann, 1985], this problem was handled by using a small global $\Delta T_{\text{min}}$ when refrigeration is involved. However, this was unsatisfactory since a small global $\Delta T_{\text{min}}$ caused infeasibilities in the process to process stream matches when the actual design was attempted.

However, with the approach developed in this chapter for determining hot and cold utility temperatures and loads, multiple $\Delta T_{\text{min}}$'s can be used to account for utility to process stream matches that require $\Delta T_{\text{min}}$ that is very different from $\Delta T_{\text{min,global}}$.

Each utility, such as condensing hot utility, non-condensing hot utility, condensing cold utility would have with it associated $\Delta T_{\text{min}}$. The shifting of the hot composite curve for hot utility and cold composite curve for cold utility placement still occurs at the kink points.

However, the utility can be placed at the lower temperature where the utility pinch occurs due to its $\Delta T_{\text{min,utility}}$ rather than due to $\Delta T_{\text{min,global}}$ as shown in Figure 2.21. The hot composite curve is still shifted at the kink but the hot utility is added at the temperature which gives a pinch on one end of the match. $Q_{\text{max,utility}}$ is calculated by pushing the shifted portion of the hot composite to the right until a pinch based on $\Delta T_{\text{min,global}}$ is formed with the cold composite curve. The corresponding $T_{\text{utility}}$ is calculated based on $Q_{\text{max}}$. The relationship between the variables is algebraic. These temperatures and loads would be used to determine the minimum
cost design.

Additional hot utilities beyond $Q_{\text{max}}$ should not be added because a violation of the minimum approach temperature would occur in the process to process stream match as shown in Figure 2.22. Although the hot utility to cold curve match does not violate the pinch, the shifted hot composite curve matched with the cold composite curve violates the minimum approach temperature for the process to process stream match.

2.4 Pinch Point and Minimum Utility

Although Hohmann developed the concept of pinch and the graphical minimum utility requirement calculation procedure, other workers in the area of heat exchanger network design have developed their own procedure for pinch and minimum utilities calculation. Namely, Linnhoff and Flower [1978] developed the problem table method, and Cerda and Westerberg [1981] developed the transportation model method. Since their methods could not be incorporated into the new heat and work design approach developed for this research, a new algorithm was developed to determine the pinch point(s) and the minimum utilities.

Some of the advantages of the new algorithm over the previous methods are the direct result of the heuristics developed earlier. This algorithm can handle utilities that go through temperature changes such as cooling water and hot oil. It can also calculate utility requirements for utilities that have different $\Delta T_{\text{min}}$ than from process $\Delta T_{\text{min}}$. In addition, the method can handle heating and cooling curves that have discontinuities in temperature. Most important of all, the temperature levels for hot and cold utilities and the maximum allowable heat injection or rejection at those levels are automatically calculated.

The algorithm first identifies the candidate pinch points and checks them for $\Delta T_{\text{min}}$ violation. The candidate pinch points are entering and exiting temperatures of hot and cold process streams and their projections, i.e. $T_i \pm \Delta T_{\text{min}}$. To reduce
Figure 2.21: Utility dependent $\Delta T_{\text{min}}$
Figure 2.22: Incorrect utility placement
the number of candidate pinch points further, the minimum approach temperature violation is examined for each candidate point set. For example, for \( T_{hp,1} \) and \( T_{cp,1} \) shown in Figure 2.23 to be pinch points, the following must hold:

\[
T_j - T_{cp,j} \geq \Delta T_{min} \quad \forall \ j
\]  

(2.11)

\( T_j \)'s are calculated using modified successive linearization algorithm to solve the discontinuous algebraic equations arising from the enthalpy balances on the cold composite curve and the hot composite curve. If equation [2.11] holds for \( T_{hp,1} \) and \( T_{cp,1} \), then they are still possible candidate pinch point set. Other \( T_{hp,i} \) and \( T_{cp,i} \) are examined with equation [2.11] for violation of the \( \Delta T_{min} \) assuming that \( T_{hp,i} - T_{cp,i} = \Delta T_{min} \).

For the remaining candidate pinch point sets, hot and cold utility requirements are calculated using the following equations.

\[
Q_{hot,i} = \sum_{T_{hot,j,i} > T_{hp,i}} \Delta H_{stream} - \sum_{T_{cold,j,i} > T_{cp,i}} \Delta H_{stream}
\]  

(2.12)

\[
Q_{cold,i} = \sum_{T_{hot,j,i} < T_{hp,i}} \Delta H_{stream} - \sum_{T_{cold,j,i} < T_{cp,i}} \Delta H_{stream}
\]  

(2.13)

The pinch point set for a given problem is the set with the smallest absolute utility requirement as shown in the next equation.

\[
\text{minimum : } |Q_{hot,i}| + |Q_{cold,i}| \quad \forall \ i
\]  

(2.14)

To test the effectiveness of the algorithm, problems presented in the previous research papers were solved. Solutions from the new algorithm agreed with the reported values. The result is tabulated in the appendix C.

**Discontinuous temperature problem**

As shown in Figure 2.24, the pinch diagrams may have discontinuities which cause determination of the pinch point(s) to be impossible using the numerical methods such as transhipment or transportation model and at best awkward for the graphical or table problem methods. The algorithm developed allows inclusion of these discontinuities since this method is not tied to the continuous temperature interval.
Figure 2.23: Pinch Diagram

\[ T_{cp,i} + \Delta T_{min} = T_{hp,i} \]
Figure 2.24: Discontinuous Composite Curves
scheme used in other methods. Multiple discontinuities are also accounted for in the same manner.

**Multiple level minimum utility**

Heretofore, the minimum utility calculation showed the absolute enthalpy value of the hot and cold utilities. However, to optimize the utility temperature level, the maximum amount of utility that can be used at each level should be known. The temperature levels are picked based on the heuristics. $Q_{u,i,max}$ is calculated graphically as shown in Figure 2.25. This procedure is also implemented in the algorithm. $Q_{u,i,max}$ obtained are used in the formulation of the MILP overall optimization problem described in Chapter 4.

### 2.5 Summary

In this chapter, new heuristics have been developed that would allow a designer to correctly pick utility temperatures be it hot or cold, condensing or non-condensing utility and determine the maximum load which can be used at each level. The heuristics can be used to design an optimum heat exchanger network with minimum cost utilities for small problems. In addition, these heuristics can be used as a framework for solving larger problems using numerical algorithms as discussed in Chapter 4.
Figure 2.25: Maximum utility load diagram
Notations used in Chapter 2

- $a$: area exponentiation factor for heat exchanger cost
- $A_{rea,ex,i}$: area for heat exchanger $i$
- $b$: variable charge for heat exchanger $$/m^2$
- $c$: fixed charge for heat exchanger
- $C_{ann}$: annualized total cost
- $C_{util}$: $$/per kw-yr cost of utilities
- $C_{fuel}$: $$/per kw-yr cost of kerosine
- $CC_{exchanger}$: capital cost of heat exchanger
- $DP_{yr}$: depreciation years represented in annualization factor
- $F_j$: flowrate of stream $j$ in kg/sec
- $H_bf_{w}$: enthalpy of boiler feed water
- $h_j$: heat transfer coefficient for stream $j$
- $H_{T,steam}$: enthalpy of condensing steam at $T$
- $\Delta H_{fuel}$: heat content of fuel
- $M$: total number of heat exchangers
- $N_i$: total number of streams in each heat exchanger
- $\eta_{boiler}$: thermal efficiency of boiler
- $q_j$: heat content of stream $j$ usually associated with specific temperature range
- $Q_{cw,T_i}$: cooling water load with target temperature $T_i$
- $Q_i$: utility added at $T_i$
- $Q_{i,max}$: maximum utility that can be added at $T_i$
- $Q_{min,cold}$: minimum cold utility required at lowest temperature
- $Q_{min,hot}$: minimum hot utility required at highest temperature
- $\Delta T_{lm,i}$: log-mean temperature difference for heat exchanger $i$
- $\Delta T_{min,global}$: global minimum approach temperature allowed in the heat exchanger
- $\Delta T_{min,utility}$: minimum approach temperature in a heat exchanger with utility to process stream match
- $T_{cw,\text{max,return}}$: maximum allowable return temperature for cooling water
- $T_{hot,min}$: lowest hot stream temperature
- $T_{cold,\text{max}}$: highest cold stream temperature
- $T_{util}$: temperature (condensing) of utility
Chapter 3

Unit Operation Simulation

With the heuristics from chapter 2, the combinatorial nature of the hot and cold utilities represented in equation (1.5) is reduced to a manageable level. However, in order to integrate heat engines and heat pumps with the heat recovery network, the number of possible structures that would have to be examined again poses a combinatorial explosion. Furthermore, the optimization of these units is further complicated by the presence of discrete decision variables such as type of working fluid and continuous decision variables such as operating temperatures and pressure levels which would result in not only a non-linear but also a non-differentiable optimization problem. Inclusion of the auxiliary units in order to completely synthesize the utility plant aggravates the situation even more.

To overcome this problem, we have developed a new strategy to perform preliminary examination of feasible options before they are considered simultaneously with other units in the overall optimization of the utility plant. Ones that are deemed uneconomical are discarded. The underlying assumption is that an uneconomical heat engine taking heat at one temperature level and rejecting at another temperature level will not suddenly become economical when it is included in the overall utility plant.

In addition, the utility levels selected from the Chapter 2 heuristics can also be used as heat engine and heat pump heat rejection and heat intake levels. The maximum loads calculated at each level, then, correspond to the maximum loads for
these unit operations. Therefore, for each combination of utility levels, a non-linear model of the unit operation is developed for different combination of working fluid.

Simple optimization with respect to maximum efficiency is performed with these non-linear models in order to determine the optimum working fluid and the corresponding operating parameters for each combination.

These non-linear models could be used directly within a superstructure to determine the interconnections of the units they represent within the integrated utility plant. However, this would result in a mixed integer non-linear programming (MINLP) problem. With the problem at hand, an efficient linearization strategy is possible because the operating range over which the model has to be linearized has been reduced with the heuristics. This makes the substitution of linear models developed from non-linear optimization possible without loss of accuracy or unacceptable increase in size of the binary variables which are used in the standard linearization technique. The resulting mixed integer linear programming (MILP) problem is much easier to solve than the corresponding MINLP.

The number of non-linear optimization for decoupled unit operations would still be very large; however, targets or feasibility criteria have been established for various cases to quickly rule out options without having to do the non-linear optimization. For example, if a heat engine were to be used between a process heat source and a process heat sink, as a minimum the following condition must hold for the scheme to be thermodynamically feasible.

\[ T_{\text{source}} - 2 \times \Delta T_{\text{min}} > T_{\text{sink}} \]  

Furthermore, economic necessity may dictate that \( W_{\text{produced}} \) be greater than \( W_{\text{min}} \) specified by an engineer to prevent the design from having too many small heat engines.

In the following sections, the specifics of the non-linear optimization strategy and linear approximation will be explained.
3.1 Power Unit Operation Modelling

Once the minimum utility load for the problem and the maximum utility load that could be supplied at each utility temperature have been determined, utilization of these heat sources and heat sinks for heat engine, heat pump, or refrigeration can be examined. For each possible work integration combination, a simple Rankine cycle model is used to determine the economic feasibility. However, the simulation and optimization of all possible combinations are still a daunting task.

As explained before, heuristics can eliminate many possible combinations without going through the detailed simulation and optimization calculation. The algorithms developed in the following sections have resulted in good rules of thumb that can be used to reduce the problem size immediately. Once this is done, the remaining alternatives can be incorporated into the overall heat and work integration optimization problem. The formulation and handling of the non-linear constraints are explained in Chapter 4.

3.1.1 Heat engine modelling

The purpose of a heat engine model is to get an accurate idea of the size of the turbine, the compressor, the flowrate, and other process parameters such as pressures so that a heat engine for each combination of heat sources and heat sinks can be studied individually. A typical heat engine is modelled with a process flow diagram as shown in Figure 3.1. For each combination of heat sources and heat sinks, inlet and outlet temperatures are defined, i.e. $T_{in}$ and $T_{out}$ for heat source, and $T_{cool,in}$ and $T_{cool,out}$ for heat sink.

In addition, the maximum amount of heat intake and/or heat rejection is also known. For example, for a topping cycle integrated with a process, the maximum amount of heat the cycle can reject is $Q_{out,topping-cycle}$ as shown in Figure 3.2 (a). On the other hand, maximum amount of heat intake is bounded for a bottoming cycle by $Q_{in,bottoming-cycle}$. In a special case where the hot and cold composite curves
Figure 3.1: Power Plant Cycle
are wide apart as shown in Figure 3.2(b), it is possible to install an inter-process heat engine. In this case, the maximum amount of heat rejection is bounded by $Q_{out,inter-process-cycle}$.

**Power plant cycle modelling**

A general model of a heat engine cycle is developed so that an optimized operating condition can be determined for each combination of heat sources and heat sinks and a specific working fluid. The objective is to produce maximum net power from the cycle by varying the flowrate of the working fluid, the boiler outlet pressure and the temperature of the working fluid.

The steps of the power plant cycle will be examined in the order in which they appear in the optimization program. There are four steps as shown in Figure 3.1. In the first step, the working fluid is pumped up to a specified pressure. For simplicity, constant volume pressurization is assumed with mechanical efficiency term to account for the non-ideality. The pump outlet temperature, $T_2$, is dependent on the $P_3$ which has to be optimized. An enthalpy balance and entropy balance are made with departure functions and ideal gas heat capacities. (A detailed procedure is shown in Appendix D.) Peng-Robinson equation of state, shown below, is used in modelling the working fluid. [Modell and Reid]

$$P = \frac{RT}{V - b} - \frac{a(\omega, T_R)}{V(V + b) + b(V - b)}$$  \hspace{1cm} (3.2)

$$a(\omega, T_R) = \frac{0.45724R^2T_R^2}{P_c} \alpha(\omega, T_R)$$  \hspace{1cm} (3.3)

$$\alpha(\omega, T_R) = [1 + (0.3746 + 1.542\omega - 0.26992\omega^2)(1 - \sqrt{T_R})]$$  \hspace{1cm} (3.4)

$$b = \frac{0.0778RT_c}{P_c}$$  \hspace{1cm} (3.5)

Appropriate enthalpy and entropy equations are derived from the above equation of state. Parameters for different working fluids are listed in Table T3-4 in Appendix D.

In the second step of the cycle, boiler flowrate($m_{wf}$) of the working fluid, boiler outlet temperature($T_3$) of the working fluid, and boiler pressure($P_3$) are optimized to meet the minimum approach temperature specification inside the boiler. For example,
Figure 3.2: Heat Engine Integration
if $T_{out}$ is set, $P_3$ and $m_{wf}$ can be varied to find a combination that gives maximum net power production. The effect of varying $P_3$ is shown in Figure 3.3 (a). For a given working fluid flowrate, $P_3$ can be increased for additional power production until a pinch occurs inside the boiler or until the net power production declines because of the increased pumping requirement. The effect of varying flowrate, $m_{wf}$, is shown in Figure 3.3 (b). For a given $P_3$, the flowrate of the working fluid can be increased or decreased (until a pinch occurs in the boiler) to increase the net power production.

On the other hand, if $T_3$ but not $T_{out}$ is set, then $m_{wf}, P_3, T_{out}$ are varied to yield a closely matching heat intake curve. If the boiler is a direct-fired kind as in most steam generators, $T_3$ and $P_3$ are set at the maximum allowable temperature and pressure for the material of construction assumed to be 500 °C and 100 bars.

In the third step, the turbine, an iso-entropic efficiency of 85% is assumed. An enthalpy balance and an entropy balance are made on each stage and converged using the Newton-Raphson method. From these balance equations, $T_4$ is estimated. $P_4$ is the vapor pressure corresponding to condenser temperature, $T_1$. $P_4$ is estimated from $T_1$ using an empirical correlation shown below [Milora & Tester] or from Reidlich vapor pressure equation.[Reid,Prausnitz,Sherwood]

$$\ln P_{r}^{sat} = A - B_r/T_r - C \ln T_r - D_r T_r + E_r T_r^2$$

(3.6)

Normally, the outlet vapor would be superheated to avoid the condensate formation on the turbine or two phase expansion may occur resulting in a lower efficiency. However, in this simulation even if condensation does occur, the isentropic efficiency of 85% is still assumed for enthalpy calculation purposes.

In the final step, working fluid is condensed at constant pressure using a process heat sink or cooling water and returned to the pump. A more detailed calculation procedure with the appropriate balance equation for the whole cycle is shown in Appendix D.

This model can handle a variety of working fluids. For each combination of heat source and heat sink, the optimization is performed. Based on this enumeration,
Figure 3.3: The effect of pressure and flowrate on the heat intake curve
a working fluid with the highest cycle efficiency is selected for a given temperature range. In addition, for a given heat source and heat sink combination, the model can be linearized with the following equations:

\[ W_{\text{topping-cycle}} = \eta_{\text{topping}} Q_{\text{out}} \]  
\[ W_{\text{bottoming-cycle}} = \eta_{\text{bottoming}} Q_{\text{in}} \]  

The \( \eta \)'s are calculated from the optimization of the model for a given heat source and heat sink combination.

With variable target temperature of the heat source, \( T_t \), the selection of working fluid becomes harder. Constant \( \eta \) is used for range of \( Q_{\text{in}} \) even though as \( Q_{\text{in}} \) is varied the \( T_t \) changes and thus performance, \( \eta \), changes. The error tolerance in \( \eta \) is set at 5% in this simulation. In other words, \( \eta \) is used only in the region of \( Q_{\text{in}} \) where \( \eta_{Q_{\text{in}}, \text{max}} \) and \( \eta_{Q_{\text{in}}, \text{min}} \) do not change more than 5%. if \( \eta \) does vary by more than 5%, then \( Q_{\text{in}} \) region is divided into sub-regions where \( \eta \) variation is less than 5%.

**Supercritical Rankine Cycle**

In cases where the temperature difference in the boiler is large, it is necessary to increase the pressure in the system to extract more work from the system by decreasing the temperature difference in the boiler. This would necessitate that the model handle supercritical rankine cycle as well as a simple rankine cycle. To handle supercritical fluids, a better equation of state, such as Martin-Hou equation of state, would normally be used for more accurate result. However, for the purpose of this research such accuracy is not required, and the Peng-Robinson equation of state is sufficient.

Consider, R-22 used in a work integration scheme as shown in Figure 3.4, the cycle efficiency for this example is 3.8% at \( P=16.9 \) bars. But the efficiency can be increased by operating the cycle in the supercritical region as shown in Figure 3.4 (b) with \( P=50 \) bars. This increase in the pressure results in the movement of point B on the Figure 3.4 (a) closer to the vapor equilibrium line as shown in Figure 3.4 (b). The flowrate increases, and less heat is released to the heat sink from the superheated
vapor at point C. This results in greater work production for given heat intake in the boiler.

As the pressure is increased further to 70 bars as shown in Figure 3.4 (c), the heat transfer in the boiler approaches an ideal condition in that the temperature difference between the working fluid and the process fluid is nearly uniform throughout the boiler. However, at this higher pressure, the amount of work required in the pump has increased from 4015 J/Kg to 6280 J/kg while the work output has only increased from 33415 J/kg to 33525 J/kg. The extra power production is insufficient to cover the increased power requirement of the pump resulting in a lower efficiency. Furthermore, the expansion from point B results in a two phase system further reducing the efficiency in a real system. (However, in this simulation the effect of two phase expansion is not taken into account.) Any further increase in pressure would only worsen the overall cycle efficiency.

**Result and discussion**

Depending on the cycle temperatures, \((T_{Q,m}, T_{Q,out})\) different working fluid will yield different cycle efficiencies. The purpose of the model is to determine which working fluid should be used for given a heat source and heat sink temperature regime. Once the selection is made, the optimized model is transformed into a set of linear constraints. These constraints are included in the overall problem and optimized along with other unit operations.

The selection of optimal working fluid for low temperature heat source has been studied by others. For example, Milora and Tester studied the utilization efficiency, as defined below with equation (3.9), of geothermal heat source for various working fluids, and the result is shown in Figure 3.5.

\[
\eta_u = \frac{P_{\text{power,produced}}}{m_{sf} * [C_p(T_{in} - T_o) - C_p T_o \ln(T_{in}/T_o)]} \tag{3.9}
\]

The condenser temperature, \(T_o\), is set at 26.67°C. Their result indicated that at temperatures near 100°C, all working fluids operate in the subcritical pressure region.
Figure 3.4: Supercritical Rankine Cycle (R-22)
Figure 3.5: Performance of organic rankine cycle fluids using low temperature heat source
resulting in a uniformly low utilization efficiency which translates into uneconomical systems. As the temperature of the heat source is increased, the working fluids with lowest critical temperatures are the first to improve, indicating transition to supercritical operation. At temperatures in $160 \sim 230^\circ C$ range, R-22 appears to be best suited. Below $150^\circ C$, R-115 appears to give best result. R-32 has relatively high efficiency over the broadest range of temperature.

In the work integration simulation for this work, the condenser temperature is another variable that needs to be considered when determining the optimum fluid. In Figure 3.6 (a) through (d), cycle efficiencies are plotted for working fluids at various $T_{source}$ and $T_{sink}$. These figures appear to extend the conclusions of Milora and Tester that certain fluids perform better under different heat source temperatures. Examining figure (a), all fluids perform their worst around $100^\circ C$, and the relative differences are minor. However, as $T_{source}$ increases, the performance of R-115 peaks above others up to about $170^\circ C$, and then R-22 performs better up to the $T_{source, max} = 300^\circ C$. Comparing this figure to Figure 3.5, it seems apparent that relative ranking in terms of performance did not change with increasing $T_{sink}$.

However, as $T_{sink}$ is raised further as shown in figures (b), (c), and (d), most fluids become unsuitable because of their low critical temperatures. For $T_{sink}$ above $110^\circ C$, only three fluids were examined. R-113 appears to be best suited for high $T_{source}$ and $T_{sink}$ power production. Steam didn't turn out to be a good working fluid in this temperature range; however, with the likelihood of higher temperature steam turbine cycle being present in most process plant sites, incorporation of the low temperature cycle with the high temperature cycle may give it an advantage over other working fluids. Indeed, this is the case in many current process plant operations. The waste heat is invariably used for steam reheating to increase the performance of steam turbine cycle rather than for use with an organic fluid rankine cycle. Since vacuum condenser is not included in the simulation, $\eta_{70^\circ C}$ and $\eta_{40^\circ C}$ are same. The performance of R-717 is very low because the operating pressure is very high and results in very high pump power requirement.

With the optimum working fluid selected, the economics of the cycle can be
Figure 3.6: Performance of Bottoming Cycle with various working fluid and conditions
studied in more detail for given heat source and heat sink. For example, consider a
heat source at 200°C and a heat sink at 60°C. Since R-22 has the highest cycle efficiency
in this temperature range, it will be used in the detailed study. Five different pressures
were examined to study the effect on the economics of the cycle. These are shown
in Table 3.1. In the second column, $W_{\text{net}}$ represents difference between the amount
of work produced in the turbine and the amount consumed in the pump per kg of
working fluid. The columns three through five show the profit for the work integration
scheme at different sizes based on the following equation with 10 year capital cost
depreciation.

$$P_{\text{profit}} = C_{\text{power}} W_{\text{net}} m_w - C C_{\text{turbine,ann}} - C C_{\text{pump,ann}}$$ (3.10)

The capital costs of evaporator and condenser are neglected because if the cycle
isn’t profitable without taking into account these costs, then it won’t be profitable
with these costs included. However, in the overall MILP optimization later, the
capital costs of evaporator and condenser are included. The above equation is used
to quickly rule out unpromising alternatives. The capital costs of turbines and pumps
are estimated from equations (3.24) and (3.25) shown in section 3.2.3. If the heat is
rejected to the cooling water instead of process heat sink, the cost of cooling water
would also have to be subtracted from equation (3.10).

From Table 3.1, one can see that the cycle pressure corresponding to the maxi-
mum $W_{\text{net}}$ always results in the least cost regardless of the amount of $Q_{\text{in}}$. Therefore,
for a given heat source and heat sink, simulation is run to find a maximum $W_{\text{net}}$ cycle.
From then on, $\eta$ and other process parameters such as T’s and P’s corresponding to
$W_{\text{net, max}}$ are used in linearizing the work integration option.

From this analysis another important criterion can be established for viable
power production cycles regarding the size of the heat sink and heat source. As seen
from Table 3.1, there is a minimum size necessary for a power production cycle to
be economical according to equation (3.10). Profits for various combination of heat
sources and heat sinks are plotted against $Q_{\text{in}}$ in Figure 3.7 (a). As $Q_{\text{in}}$ is varied for
given combination at maximum $W_{\text{net}}$, the profit only turns positive beyond a specific
Table 3.1: Minimum cost comparison data for heat engine

<table>
<thead>
<tr>
<th>Pres (bar)</th>
<th>( W_{\text{net}} )</th>
<th>Profit</th>
<th>$1000/yr | ( Q_{\text{in}} = 4\text{MW} )</th>
<th>( Q_{\text{in}} = 10\text{MW} )</th>
<th>( Q_{\text{in}} = 20\text{MW} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>34</td>
<td>10,408</td>
<td>-93</td>
<td>-66</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>49</td>
<td>21,764</td>
<td>-88</td>
<td>6.9</td>
<td>227</td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>23,981</td>
<td>-77</td>
<td>75</td>
<td>403</td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>23,051</td>
<td>-79</td>
<td>72</td>
<td>405</td>
<td></td>
</tr>
</tbody>
</table>

size. This point is the minimum \( Q_{\text{in}} \) for that temperature combination. Going back to the original problem with heat sources and heat sinks, the minimum heat available for work integration has to be greater than \( Q_{\text{in,\text{min}}} \) for that heat source and heat sink. Furthermore, similar analysis can be performed on \( Q_{\text{out}} \), and \( Q_{\text{out,\text{min}}} \) are calculated for various heat source and heat sink combinations as shown in Figure 3.7 (b). Since these \( Q \)'s are based on equation (3.10), they represent absolutely minimum \( Q_{\text{out}} \) and \( Q_{\text{in}} \). Therefore, any process combination of heat sources and heat sinks that does not meet this requirement can be quickly ruled out.

As the temperature of the heat source decreases, the amount of available energy for power production also decreases. Below \( T_{\text{source}} = 92^\circ\text{C} \), available energy is too low for an economical system. The cycle efficiency for this \( 92^\circ\text{C} \) temperature heat source coupled with \( 30^\circ\text{C} \) heat sink is only about 3% at best. Therefore, any work integration combination involving \( T_{\text{source}} < 92^\circ\text{C} \) can be purged from the list of alternatives.

If a work integration combination passes the above criterion or does not fit them, a quick simulation/optimization is run to check the feasibility. From this simulation cycle efficiency is backed out and compared to the minimum \( \eta \). From the analysis of various heat engine combinations, minimum cycle efficiency for economically feasible power production was determined to be around 8%. This in no way requires that the final solution have all the work integration combination with \( \eta > 8\% \), but only that they be included in the final formulation. Once formulated this way, the problem is optimized to solve for the minimum cost design.

It has been also found that for a inter-process stream heat engine to be feasible,
Figure 3.7: Minimum heat engine intake and exhaust data
the temperature difference between the condenser and the boiler has to be at least 120°C. Since minimum work production is 300 kW based on a general rule of thumb, minimum $Q_{in}$ would be around 2 MW based on the observed $\eta_{max}$. This is another criteria that is used to eliminate any combination of heat source and heat sink from further consideration.

Up to this point, there was no mention of variable $T_i$; however, target temperature of the heat source would change as $Q_{in}$ changes. In this simulation $\eta$ is assumed to be constant for a range of $T_i$ where $\eta$ does not change by more than 5%. Thus, multiple values of $\eta$ would be used for same $T_s$ but for varying $T_i$. On the average for $\eta$ to change 5%, the value of $T_i$ would have to change about 10°C. Therefore, for $T_i$ varying 20°C only two $\eta$'s need to be included in the final formulation.

Steam turbine cycle is modelled using the same algorithm with minor changes. For example, the working fluid is set to water and the corresponding data are entered in the model. The performance data are shown in Figure 3.8 for various heat sink temperatures. Since efficiencies are relatively high, any high temperature heat source will exclusively use steam as working fluid.

Since needed data for overall optimization formulation can be accurately obtained from fluids examined so far, other more exotic fluids will not be tested using the algorithm. Another power production scheme, gas turbines, will be dealt with in section 3.2.4 later in this chapter.

**Conclusions**

A versatile model has been developed for simulating and optimizing bottoming cycle, topping cycle, and inter-process cycle. This simulation can account for a supercritical rankine cycle to improve the efficiency. From examining various working fluids, a small database has been developed to determine type of working fluids to be used for different range of $T_{sink}$ and $T_{source}$. Various elimination criteria have been established to quickly purge unpromising alternatives from the list of possible work integration schemes.
Figure 3.8: Cycle efficiency of steam turbine
Note that this simulation and optimization module only tests the viability of the stand-alone option. If the option is not viable, it is excluded from further consideration. On the other hand, a viable stand-alone option is included in the final MILP formulation and optimized with other options to find the overall minimum cost design. For example, the low temperature heat source may be used more economically in steam reheating if a steam turbine system is already present instead of using the heat source for its own power production. But this fact would not be known until the overall formulation is optimized.

3.1.2 Heat pump modelling

The heat pump is modelled with a simple Reverse Rankine cycle shown in Figure 3.9. Heat is supplied in the evaporator from the process heat source. Temperatures \( (T_{in}, T_{out}) \) of the heat source are known, and \( Q_{in} \) is bounded by the heuristics from Chapter 2. Evaporator temperature is set at \( T_{out} - \Delta T_{min} \). In the condenser, \( T_{enter} \) and \( T_{exit} \) are known. \( Q_{out} \) is a function of \( Q_{in} \). Flowrate of the working fluid can be varied along with \( T_4 \) as shown in Figure 3.10 to satisfy the condition that point of the closest approach in the condenser is just equal to \( \Delta T_{min} \). Once \( T_4 \) has been optimized this way, \( P_4 \) can be backed out from equation (3.6).

The Peng-robinson equation of state is used as in the power plant cycle. Isoenthalpic expansion is assumed in the valve, and the compressor’s iso-entropic efficiency is set at 85%.

Although a turbo-expander could be used in place of a simple expander, the cost of a such system would be very high due to the two phase expansion of the working fluid. However, it is used in a large scale operations such as cryogenic refrigeration plants. This subject can be a research topic all on its own and will not be discussed further here.

Result and discussion

Among the variables that determine the performance of a heat pump system is
Figure 3.9: Typical Heat Pump Cycle
Figure 3.10: Heat pump condenser temperature profile
the $\Delta T_{\text{raise}}$ as shown in Figure 3.11 and defined below.

$$\Delta T_{\text{raise}} = T_4 - T_2$$

(3.11)

The subscripts above refer to the location on Figure 3.9. In other words, $\Delta T_{\text{raise}}$ represents, in terms of the working fluid temperatures, the rise in the temperature of the heat source necessary in order to reject heat to the higher temperature heat sink without violating the $\Delta T_{\text{min}}$ in counter current heat exchangers. In Figure 3.11 the heat available at $(T_s, T_i)$ is raised in temperature by means of a working fluid so that it can supply its heat to the heat sink at $(T_{\text{cool,in}}, T_{\text{cool,out}})$.

In other publications, different definitions of $\Delta T_{\text{raise}}$ were given; however, as long as consistency prevails, the comparison of performance for various working fluids would be correct, regardless. [TEnSA, 1988] Furthermore, the definition given by equation (3.11) above would give more accurate account of temperature rise even for a large difference between $T_s$ and $T_i$.

A standard definition of coefficient of performance, $COP$, as defined in equation (3.12) below are used to examine the performance of various working fluids under different conditions.

$$COP = \frac{H_2 - H_1}{H_3 - H_2}$$

(3.12)

Figure 3.12 shows the performance of various working fluids at $\Delta T_{\text{raise}} = 30, 40, 50^\circ \text{C}$, respectively. On the abscissa is the temperature of the heat source, assumed to be constant.

An appropriate selection of working fluid can be made from these figures for a given heat source temperature and heat sink temperatures. For example, if heat source is available at $T = 20^\circ \text{C}$ and heat sink is available at $T = 30^\circ \text{C}$, from Figure 3.12 (a) the best working fluid is R-22 with $COP = 6.25$. (Note: $\Delta T_{\text{raise}} = 30^\circ \text{C}$ because it is assumed that $\Delta T_{\text{min,condenser}} = \Delta T_{\text{min,evaporator}} = 10^\circ \text{C}$.)

As $\Delta T_{\text{raise}}$ is increased the performance of the heat pump cycle drops as shown in Figure 3.12 (b) and (c). However, the optimum working fluid for the given heat source temperature is still the same. Therefore, once the optimum working fluid
Figure 3.11: Definition of $\Delta T_{raise}$.
Figure 3.12: Heat pump COP of fluids at various conditions
is chosen for a specific heat source temperature, selection of the working fluid is no longer a variable that needs to be included in the overall optimization problem. Table T3-4 in appendix D shows complete data for all working fluids examined.

Examining the $COP$'s in specific range, it appears that the selection of the working fluid will not play an important role since the difference in $COP$ between two working fluids rarely exceeds 10%. For a moderately sized heat pump system requiring 100kW of work, the difference in annualized cost would be only about $4000 per year, a minor sum in comparison to other factors. More important is the feasibility of the working fluid ($T_4 < T_{critical}$) at the given heat sink temperature. Theoretically, $T_{critical} > T_{cool, out} + \Delta T_{min}$; however, in reality $T_{critical}$ must be much greater than $T_{cool, out}$ in order to avoid high working fluid flow rate and thus inefficient operation. Other factors such as safety, ease of availability etc. would play a more important role.

For $\Delta T_{raise} > 60^\circ C$, the $COP$ values are below 3 for most working fluid. The heat pump systems with $COP < 3$ are not economically viable and can thus be excluded from any further consideration. The reason can be found in the following simple economic analysis.

There are four factors that determine the economic viability of the heat pump system as shown in the following equation.

$$\text{Profit} = Q_{cold}C_{cu} + Q_{hot}C_{hu} - W_{power}C_{power} - \Delta C_{ann,exchanger} - C_{ann,comp}$$  \hspace{1cm} (3.13)

$Q_{cold}$ and $Q_{hot}$ are the amount of cold and hot utility replaced by the heat pump, and $C_{cu}$ and $C_{hu}$ are the cost coefficients. These two terms represent the savings resulting from the placement of a heat pump. The power requirement is $W_{power}$ and is multiplied by its cost coefficient. The fourth term represents incremental cost associated with having larger area heat exchangers because the temperature driving forces are reduced in the condenser and the evaporator of the heat pump system in comparison to hot and cold utility heat exchangers. The last term is the annualized capital cost of the compressor.

Simply, a heat pump is economically viable if profit is positive and not viable if
profit is negative. Above equation can be simplified further to determine approximate values of COP for a viable heat pump system. A typical value of cost coefficients are given below.

\[ C_{cu} = 6.02/\text{kW-yr} \]
\[ C_{power} = 420.00/\text{kW-yr} \]
\[ C_{hu} = 89.88 \text{ to } 103.7/\text{kW-yr} \]

The cost of the hot utility varies according to the temperature of the utility. The effect of the fourth term is minor and is neglected especially since it is an annualized cost. The last term can vary with the size of the compressor. But since the purpose of this analysis is to develop a good rule of thumb in order to rule out majority of heat pump systems quickly, any system that doesn’t meet the produce some profit without the last term would surely not satisfy equation (3.13).

Substituting the coefficients and solving for minimum \( COP \) results in the following equation.

\[ 6 + \left(1 + \frac{1}{COP}\right)C_{hu} - \frac{420}{COP} = 0 \]

Solving this equation, \( COP_{min} = 3.02 \). Therefore, any heat pump system with \( COP < 3.0 \) can be ruled out immediately. Furthermore, for a given heat sink temperature, a minimum hot utility temperature can be estimated. Using this temperature, \( C_{hu} \) can be derived and equation (3.14) can be solved for minimum \( COP \). These minimum \( COP \) values are shown in Figure 3.13.

Since the values from Figure 3.13 are worst case scenario minima, they can be used to purge all unpromising alternatives from a list of heat pump placement possibilities. For example, if there are two heat sources and two heat sinks as shown in Figure 3.14, there are four possible heat pump systems. Instead of including all four combinations in the overall optimization formulation, Figure 3.13 can be used to eliminate unpromising combinations immediately. At worst, there would still be four combinations that need to be formulated in the overall optimization problem. At best, there may be none.
Figure 3.13: Minimum COP economics criteria for heat pump
Figure 3.14: Heat Pump Integration Alternatives
Once a heat pump system passes this test it is formulated in terms of linear variables and integer variables and then optimized with other options in the overall MILP problem. The formulation procedure is explained in Chapter 4.

**Direct Vapor Recompression (DVR) Cycle**

Recently, DVR cycle has been touted by the industry as a highly viable option to drastically decrease the energy consumption in the distillation sequences. However, without proper placement decisions based on the pinch concept, it could end up driving the overall cost higher. The fundamental rule is that the DVR should be used only if $T_{\text{condenser}}$ is below the pinch and $T_{\text{reboiler}}$ is above the pinch.

The simulation algorithm developed here can also be used to model DVR cycle by setting $\Delta T_{\text{evaporator}} = 0$ and by replacing the working fluid properties with the distillate properties. The end effect is that for a given heat sink temperature $\Delta T_{\text{raise}}$ is lower for DVR than for a heat pump, and thus higher efficiency results.

However, it must be noted that obtaining the distillate data is not very easy for a mixture, and the non-idealities may cause the simulation to yield inaccurate results.

**Multiple Stage Heat Pump**

To increase the performance of the heat pump over a large $\Delta T_{\text{raise}}$, multiple stage heat pumps as shown in Figure 3.15 can be used. Again, the program can handle multiple stages with only slight modifications. A variety of working fluid combinations for binary cycles have been tested. However, the improvement in the performance is minor compared to the extra cost of a heat exchanger and a compressor.

This should have been apparent without going into the details of optimization by simple COP analysis. The COP of the binary cycle is defined as below:

$$
COP_{1+2} = \frac{Q_{\text{in}}}{COP_1} + \frac{Q_{\text{in}} + \frac{Q_{\text{in}}}{COP_2}}{COP_2}
$$

For a binary cycle with $COP_1 = 6$ and $COP_2 = 6$, the combined cycle COP is only 2.76, still lower than the minimum required.
Figure 3.15: Binary Heat Pump Cycle
Furthermore, the added cost of the heat exchanger and the compressor may not be recovered in the energy saved. In an example with R-22 as a working fluid, COP increases from 3 to 3.34 with double stage for a case where \( T_{\text{source}} = -25^\circ\text{C} \) and \( T_{\text{sink}} = 35^\circ\text{C} \). For a moderately sized heat pump with work load of 100 kW, this would result in a reduction of 10 kW translating into $4200 per year in savings. However, this would not offset the annualized cost of extra heat exchanger and a compressor.

**Conclusions**

An accurate simulation and optimization program has been written that can handle multitude of working fluids for simple heat pumps, DVR and multiple stage heat pumps. This program is incorporated with other programs to form a general synthesis technique for heat and work integration problems as will be shown in later chapters.

The important conclusion from this analysis is that there is very little latitude for placement of heat pumps. An important COP vs viability relation has been established that can quickly limit the scope of the problem by eliminating unpromising alternatives without time-consuming simulation. In addition, multiple stages have been found to be uneconomical and need not be considered. This translates into less complex overall problem than previously thought when heat pump integration is included. Previously mentioned combinatorial explosion with respect to the number of possible heat pump combinations in the overall optimization problem is not expected. This makes the problem of heat pump integration tractable.

### 3.1.3 Refrigeration

Refrigeration cycle is modelled the same way as the heat pump using the reverse Rankine cycle. Only difference is that the heat has to be removed regardless of the cost. Objective is, then, to minimize the compression cost. Heat must be rejected to the cooling water eventually.

A typical single stage refrigeration cycle is identical to the heat pump and is
shown in Figure 3.16 (a). In today’s typical cryogenic refrigeration cycles, the valve would be replaced with a turbine to recover some work. However, in this modelling, turbine is not considered. Optimization is done with $m_{wf}$, $T_3$, $T_{exit}$, and the cooling water flow rate. (Note that not all these variables are independent.)

With very low temperature and large quantity of refrigeration need, it may be necessary to install multistage refrigeration cycle as shown in Figure 3.16 (b). Since the calculation procedure for the second stage is identical to the first stage, the algorithm is easily modified to handle the multi-stage refrigeration cycle.

**Result and discussion**

A number of working fluid are examined under different cooling situations to determine the performance. Two condenser configurations are studied in detail. The first rejects heat to cooling water whose temperature rises from 10°C to 20°C. The second rejects heat to cooling fluid (possibly process heat sink) whose temperature rises from -30°C to -20°C.

In the first configuration, working fluids examined were ammonia, R-22, propylene, iso-butane, R-114, and R-115. Temperature of the working fluid in the evaporator was varied from -75°C to 5°C in ten degree increments. A plot of COP's and $T_{evap, wf}$ is shown in Figure 3.17. As expected, COP’s decrease for every fluid as $\Delta T_{raise}$ is increased. Ammonia was found to give the highest COP in each case except at -75°C, where R-22 performed better. The spread of COP results for each $\Delta T_{raise}$ varied from 0.3 at -75°C to almost 1.0 at 5°C. The only working fluid that gave below average performance throughout was R-115. Performance of other working fluids were very similar.

The second configuration transferred heat into a condenser cooling fluid (possibly process heat sink) whose temperature rose from -30°C to -20°C. Temperature of the working fluid in the evaporator was varied from -115°C to -35°C in ten degree increments. These temperatures were used to test R-13 and ethylene as working fluid. The critical temperatures of these two compounds are less than the temperature of the cooling water in the first configuration, so the saturated liquids in the condenser
Figure 3.16: Typical Refrigeration Cycles
Figure 3.17: Performance of working fluids for single stage refrigeration cycle
were not obtainable in the first cycle and thus not tested. Ammonia and R-22 were also included in the second configuration simulation since they performed best in the first configuration. The COP results are plotted in Figure 3.18. Although one would expect the COP's of working fluids with lower critical temperatures to be larger, the result of the simulation proved otherwise. R-22 turned out to be the best performer over others with lower critical temperatures. As in the first configuration, the spread in COP increased with decreasing $\Delta T_{rise}$. Only ethylene performed below average over the whole range of temperature.

From these optimized simulations, one can conclude that R-22 is best suited for refrigeration around -115 to -35°C and R-717 is best suited for refrigeration around -35 to 5°C. However, the difference in performance is not large enough to favor R-22 over R-717 or vice versa, rather the availability at the locale would play more important role.

For problems where there are large temperature differences between the condenser and the evaporator, single stage refrigeration may not be the best alternative. By combining number of high efficiency cycles, the overall performance can be increased. Several working fluid combinations in a two stage refrigeration system are examined to get good simulation data. As will be shown later, even two stage cycles are hard to justify compared to the single stage cycles in temperature range considered; therefore, any more complex cycles will not be dealt with here. A good technique for designing the multiple refrigeration system alone can be found in a paper by Shelton and Grossmann. [1987]

Since there would be more room for improvements in the worst performing cycle, $T_{evap} = -115^\circ$C was examined to determine the benefits resulting from the binary cycle. COP's for this temperature were around 1.0 for single cycle. Two cycles each with COP of 3.0 or more were combined to form the binary cycle. The upper loop working fluid was condensed using cooling water whose temperature rose from 10°C to 20°C same as in the first configuration of single cycle simulation. The combinations of working fluid examined are shown in Table 3.2.
Figure 3.18: Performance of various fluids in single stage low temperature refrigeration cycle
Table 3.2: Binary Cycle Working Fluid

<table>
<thead>
<tr>
<th>Upper loop</th>
<th>R-22</th>
<th>R-13</th>
<th>R-717</th>
<th>R-13</th>
<th>R-115</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lower loop</td>
<td>R-22</td>
<td>R-22</td>
<td>R-717</td>
<td>R-717</td>
<td>R-115</td>
</tr>
</tbody>
</table>

Table 3.3: Binary COP result

<table>
<thead>
<tr>
<th>upperfluid</th>
<th>COP\text{single}</th>
<th>lowerfluid</th>
<th>COP\text{binary}</th>
</tr>
</thead>
<tbody>
<tr>
<td>R-22</td>
<td>.82</td>
<td>R-22</td>
<td>.96</td>
</tr>
<tr>
<td>R-22</td>
<td></td>
<td>R-13</td>
<td>.94</td>
</tr>
<tr>
<td>R-717</td>
<td>.80</td>
<td>R-717</td>
<td>.92</td>
</tr>
<tr>
<td>R-717</td>
<td></td>
<td>R-13</td>
<td>.95</td>
</tr>
<tr>
<td>R-115</td>
<td>.55</td>
<td>R-115</td>
<td>.87</td>
</tr>
</tbody>
</table>

Each cycle is optimized the same way as in single cycle case; however, the $T_{\text{evap, upperloop}}$ is also an optimization variable for the binary cycle case. $T_{\text{evap, upperloop}}$ was varied in ten degree increments to find the temperature that gave the largest COP for a given combination of fluids. The COP is defined in this case as the ratio of refrigeration in the lower loop evaporator to total power consumed in the two compressors.

The results of this simulation are shown in Figure 3.19. It is apparent that the peaks which represent the optimum COP for the given combination of working fluids occur at different temperatures and thus $T_{\text{evap, upperloop}}$ is indeed an important optimization parameter. Overall, R-22 combination performed best with COP of 0.96; R-13 and R-717 combination performed second best. Other combinations fared worse and need not be considered further. Although R-13 and R-717 combination performed only slightly worse than R-22 combination, the narrow range of $T_{\text{evap, upperloop}}$ over which this performance was achieved indicate that R-22 combination is superior.

Table 3.3 compares the COP for binary cycle with single cycle COP. The improvement in terms of absolute COP is not drastic. However, in terms of percentage increase in COP, they range from 15% for R-717 combination to over 55% for R-115 combination. In the grass root design problems that this research is concerned with,
1. Evaporator temperature of upper loop

* R-115 by R-115
* R-22 by R-22
* R-717 by R-717
* R-13 top R-717 bottom
* R-13 top by R-22 bottom

Figure 3.19: Performance of various binary refrigeration cycle
the improvement factor is not as important as the absolute value of COP. Therefore, R-22 combination would still be chosen for binary cycle over R-115 combination. However, this simulation result would be useful in the case of retrofitting existing refrigeration system. The secondary fluid for either upper or lower cycle would be chosen based on the COP improvement.

A quick economical analysis of two stage cycle for R-22 shows that for moderate cooling load of 100kW, the power cost decreases from $51,219 to $43,750. This $7,469/year savings would not offset the cost of the extra compressor and the extra heat exchanger. However, as the cooling load is increased, the binary cycle would become more economical. But over the range which we are interested in (up to 1MW of refrigeration) the single stage cycle simulation is sufficient to give accurate data to be used in the overall optimization.

**Conclusion**

Since refrigeration is not an option rather a necessity, it would be always included in the final formulation. Therefore, elaborate criteria for inclusion need not be established. A good simulation model to generate operating parameter as described above is all that is needed. Most likely, this option would be compared to the heat pumping to determine the most economical route to removing the excess heat.

Due to the versatility of R-22 in both single cycle and binary cycle refrigeration simulation, it is used exclusively in modelling the refrigeration in this research.

### 3.2 Modeling of Miscellaneous Units

There are many other units that are present in the utility plant than described above. However, these do not represent opportunity for heat and work integration. They only need to be included in the overall optimization to determine the effect on the cost of the heat and work integration options. For this purpose simple linear simulation models developed in the following sections are sufficient.
3.2.1 Boiler

A simple capital cost equation are all that is needed for a boiler. This is shown in equation 3.16. The correlation was derived from Ulrich[1984]. This correlation is for a steam boiler. The boilers in the heat engine cycle, especially the organic rankine fluid cycle, are assumed to be simple heat exchangers whose cost are given by equation (3.29).

\[ C_{\text{capital, cost}} = 349,600 f_t f_p m_{\text{steam}}^{0.82} \] (3.16)

where

\[ f_t = 1 - 6.1 \times 10^{-4} \Delta T_{\text{superheat}} + 1.3 \times 10^{-5} \Delta T_{\text{superheat}}^2 \] (3.17)

\[ f_p = 1.0187 - 2.724 \times 10^{-3} P_{\text{boiler}} + 9.865 \times 10^{-5} P_{\text{boiler}}^2 \] (3.18)

Operating cost is calculated based on 95% efficiency assumption and $98/kw-yr fuel cost. Therefore, equation 3.19 is used for operating cost calculation.

\[ O_{\text{operating, cost}} = \frac{98.00}{0.95} [m_{\text{w,f}} \Delta H_{\text{w,f,boiler}}] \] (3.19)

If the capital cost of the boiler is assumed to be sunk, then the operating cost becomes the cost of the hot utility charged to the plant. The utility costs thus calculated are quite different from the costs used in previous research work as shown in Table 3.4 The discrepancy is due to the fact that in all previous research the presence of steam turbine system was assumed. However, the goal of this research is to design the utility plant with the process and the heat exchanger network, taking into account the work integration potential. Therefore, presence of steam turbine system could not be assumed a priori. The result is that the heat exchange network designed assuming existence of steam turbine system is vastly different from the heat exchanger network designed with optimum work integration. This is further explained in Chapter 5.

3.2.2 Cooling Water System

To be a complete synthesis tool, a model of cooling water system would have to be included. However, the cooling water system doesn't play an important role in
Table 3.4: Hot Utility Cost Data

<table>
<thead>
<tr>
<th>Type</th>
<th>T(K)</th>
<th>P(bar)</th>
<th>cost¹($/kw-yr)</th>
<th>cost²($/kw-yr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>High</td>
<td>672.4</td>
<td>68.95</td>
<td>103.7</td>
<td>103.7</td>
</tr>
<tr>
<td>Medium</td>
<td>605.4</td>
<td>17.24</td>
<td>73.319</td>
<td>99.7</td>
</tr>
<tr>
<td>Low</td>
<td>411.0</td>
<td>3.45</td>
<td>56.286</td>
<td>89.88</td>
</tr>
</tbody>
</table>

¹cost data used in the work by Colmenares and Seider
²cost data from equation 3.19

work integration but only in heat integration. The model doesn’t need to be complex as long as it provides accurate cost data for analysis. In light of this, cost correlations are developed based on the work by Burger [1979,1983] and Crozier [1980].

The major variables in the cooling tower are the inlet temperature \( T_{cw,in} \) and the outlet temperature \( T_{cw,out} \) shown in Figure 3.20. \( T_{cw,in} \) can be optimized for different conditions. The tradeoff would be between the lower pumping cost for high \( T_{cw,in} \), and the higher water make-up cost and treating cost. (As the \( T_{cw,in} \) is increased the cost of water treating increases.) For typical plants, the optimal \( T_{cw,in} \) is 50°C, and that is used throughout this work.

\( T_{cw,out} \) is bounded by the wet-bulb temperature on the lower side and by the minimum process outlet temperature on the upper side. A good rule of thumb has been to set \( T_{cw,out} = T_{wet-bulb} + 5°C \). In this work, \( T_{cw,out} \) is set at 30°C for typical operation in the SouthWest. [Crozier, 1980]

The capital cost of cooling water system for different load is estimated from the correlation shown in equation 3.20 through 3.22.

\[
Capital\text{Cost,cooling tower system} = 225.87[m_{cw}] + 195,229 \quad (3.20)
\]

valid for \( 100gpm < m_{cw} < 999gpm \) (equivalent to 500kw and 4Mw)

\[
Capital\text{Cost,cooling tower system} = 90.88[m_{cw}] + 332,220 \quad (3.21)
\]
Figure 3.20: Simplified Cooling Tower System
valid for 1000gpm < \( m_{cw} < 4999gpm \) (equivalent to 5Mw and 24Mw)

\[
Capital \text{Cost,cooling tower system} = 57.746[m_{cw}] + 498,450 \quad (3.22)
\]

valid for 5,000gpm < \( m_{cw} < 15,000gpm \) (equivalent to 25Mw and 80Mw) For cooling need below 1 Mw, it is better to use the plain air cooler to reduce the capital cost expenditure.

Instead of calculating the operating cost for each unit in the cooling tower system, they are lumped into one correlation. This correlation takes into account the operating cost factor of pumps, fan, water treating and make-up water. This correlation is shown in equation 3.23.

\[
Operating \text{Cost,cooling water system} = 31.12[m_{cw}] \quad (3.23)
\]

The derived correlations are used to determine the economic feasibility of cooling water system compared to other types of cooling such as direct air cooling or heat pumping.

### 3.2.3 Pump, Compressor, Turbine

The models developed for heat engines, heat pumps, and refrigeration cycles gave accurate performance data. However, the overall objective is the determination of the minimum cost design. In order to cost the work integration design, the cost data for each unit in the work integration design have to be derived.

Following non-linear correlations are derived for capital costs of various units from the graphical data in Urlich[1984].

\[
Capital \text{Cost,turbine} = 173,495 \ W_{turbine}^{0.424} \quad (3.24)
\]

valid for 300kw < \( W_{turbine} < 16Mw \)

\[
Capital \text{Cost,pump} = 3,120 \ [2 + 0.96 \ D_{in}^{0.383}] \ W_{in}^{0.368} \quad (3.25)
\]
valid for $50kw < W_{in} < 3Mw \quad P_{in} < 22bars$

$$C_{apitalCost,compressor} = \$1,925 \ W_{in}^{0.963} \quad (3.26)$$

valid for $600kw < W_{in} < 15Mw$

Since these correlations are non-linear, the resulting formulation of the objective function would be also non-linear. However, this non-linearity is solved by using standard linearization technique described in detail in Chapter 4.

### 3.2.4 Gas Turbines

Power production platforms discussed in the previous sections did not include a model of a gas turbine system because it is used mainly for the sole purpose of generating power and not necessarily integrating with the rest of the process. In addition, ever present steam requirement of the chemical plant favors steam turbine system over gas turbine. However, in plants where power demand exceeds steam demand such as paper mills, integration of gas turbine for power production and utilization of exhaust gas as a heat source has proved to be economically viable. [Otto 1980]

A simple performance model is developed based on the design shown in Figure 3.21. Simplification is made by setting the bulk of the cycle parameters constant based on optimal design consideration outlined in the Gas Turbine Handbook. [1966] For example, $T_3$ is set to $1,100^\circ C$, mass flow rate of fuel to air is set at 0.0137, and the fuel type is set to methane. Other cycle parameters are listed in the Appendix F. $T_{exhaust}$ and $m_{fuel}$ are only independent variables in the model.

Simulation runs are made by varying the $T_{exhaust}$, and the cycle efficiencies are calculated. The result is shown in Figure 3.22. As expected, the performance increases as $T_{exhaust}$ is lowered. $T_{exhaust}$ actually corresponds to the hot utility supply temperature alluded to in Chapter 2. Therefore, once the candidate hot utility temperatures are selected based the heuristics in Chapter 2, cycle efficiency for work integration using gas turbine is backed out using Figure 3.22. The fuel flowrate is
Figure 3.21: Simplified Gas Turbine System
Figure 3.22: Cycle Efficiency of Gas Turbine System
calculated, and the sizing is done. The capital cost and operating costs are estimated using the following equations [3.27,3.28].

\[ C_{\text{Cost, gas turbine cycle}} = 173,495(W_{out})^{0.424} + 176(W_{out})^{0.83} + 1,925(W_{in})^{0.963} + 14,000 \]  

(3.27)

\[ O_{\text{perating Cost, gas turbine cycle}} = \$0.181m_{fuel,methane} \]  

(3.28)

Since the purpose of this research is not to optimize the stand-alone gas turbine cycle, rather to determine economic viability of gas turbine cycle in comparison with other work integration options, above simulation model and the resulting data are sufficient.

### 3.2.5 Heat Exchangers

The capital cost of heat exchangers is estimated using equation 3.29. [Linnhoff and Hindmarsh, 1983] This equation has been used in many other research work and has been found to give good estimation. Furthermore, using this already accepted correlation would allow easy comparison of economic result. It assumes a simple counter-current shell and tube exchanger with plain steel.

\[ C_{\text{Capital Cost, heat exchanger}} = \$1,090[A_{rea}]^{0.83} + 14,000 \]  

(3.29)

Since area is an unknown term until the heat exchanger network is designed, the Bath formula for area estimation is used to estimate an approximate area for the heat exchanger network and determine the impact on the heat exchanger cost. [Tjoe and Linnhoff, 1985]

### 3.3 Summary

Models developed in this chapter for both the performance and the cost data are more accurate than previously used data. Furthermore, these models are used to
simulate various designs to determine economic feasibility of the entire plant. Next task is to incorporate the heuristics and models into a rigorous numerical optimization method.
Notations used in Chapter 3

\[ \Delta H_{wf,boiler} \] enthalpy change of working fluid in the boiler.

\[ m_{cw} \] flow rate of cooling water in gallons per minute.

\[ m_{fuel,methane} \] flow rate of methane fuel in kg/sec.

\[ m_{gf} \] mass flow rate of geothermal fluid.

\[ T_{evap,wf} \] temperature of working fluid in unit evaporator.

\[ T_{cond,wf} \] temperature of working fluid in unit condenser.

\[ T_{enter} \] temperature of cooling fluid (cooling water or process stream) entering condenser.

\[ T_{exit} \] temperature of cooling fluid leaving condenser.

\[ \Delta T_{raise} \] temperature difference between \( T_{evap,wf} \) and \( T_{cond,wf} \).

\[ T_{cw,in} \] temperature of cooling water returning from the process.

\[ T_{cw,out} \] temperature of cooling water from the bottom of the tower.
Chapter 4

Mathematical Formulation of Utility Plant Synthesis with Heat & Work Integration

The strategy for simultaneous synthesis of the plant utilities system and heat recovery network was first to identify the types of utilities and the temperature levels needed for the heat recovery network. In Chapter 2 a method and algorithm were developed to identify a small set of temperature levels that would be present in an optimized heat recovery network and the maximum amount of utility that could be used at each level.

In Chapter 3, we identified all of the units that could be present in the utility system, including heat engines, heat pumps, and refrigeration units. Heuristics were developed to drastically reduce the number of possibilities to those that are economically and thermodynamically viable.

In this chapter, our goal is to develop a superstructure containing all possible utility levels and interconnecting units. Then, the problem of selecting the optimum combination of temperature levels and units and the operating parameters (such as flowrates of streams and capacities of units) of heat and work integrated plant can be formulated as a mixed integer linear programming (MILP) problem and solved. Although the problem is still combinatoric, the heuristics and linearization schemes have reduced the size to the extent that the simple branch and bound method can
solve the resulting optimization problem.

4.1 Mathematical Programming Approach

In the general synthesis of processing system, the goal is to determine the configuration and the operating parameters of a flowsheet that optimizes a specific objective function subject to design specifications. The objective function is most likely to be a cost or a profit function that includes annualized capital cost and annual operating cost for the former and also includes revenue term for the latter. To optimize the objective function, a mathematical programming strategy is applied to the synthesis problem.

In order to solve this problem, a superstructure that encompasses every possible structural alternative has to be derived. Since the size of such formulation is extremely large, general rules of thumb based on prior experience are used to limit the number of alternatives. Santibanez and Grossmann, 1980] This superstructure is mathematically represented and optimized to determine the optimal structure of process units with their corresponding interconnections.

The performance and constraints on the units in the superstructure can be described by a system of linear and nonlinear equations as shown below.

\[ Ax = b \]  \hspace{1cm} (4.1)

\[ f_i(x) = 0 \quad i = \ldots, n \]  \hspace{1cm} (4.2)

where \( A \) is a matrix of constant coefficients for the continuous process variable vector \( x \) with vector \( b \) as the right-hand side, and \( f \) is a vector of non-linear equations. For example, a mass balance on a pump would be one of the linear equations whereas a mass balance on a reactor with non-linear rate law would be one of the non-linear equations. These equations will be indeterminate thus allowing number of degrees of freedom.

If \( y_i \)'s are binary variables representing existence of units, the degrees of freedom
can be bounded by design specifications and physical constraints as shown below.

\[
\begin{align*}
    b_L & \leq C_1 x + C_2 y \leq b_U \\
    d_L & \leq g(x, y) \leq d_U
\end{align*}
\]  

(4.3) (4.4)

Here C's are matrices of constants, \( b_L \) and \( b_U \) are lower and upper bounds on the linear constraints. The function \( g \) is a vector of nonlinear constraints with \( d \)'s as its bounds.

A typical problem would involve maximization of a profit function or minimization of a cost function as shown here.

\[
\begin{align*}
    \text{max : } & \quad P_{\text{profit}} = P(x, y) \\
    \text{min : } & \quad C_{\text{cost}} = C(x, y)
\end{align*}
\]  

(4.5)

The design problem, then, would require solving either function for optimal values of vectors \( x \) and \( y \) subject to linear and nonlinear, equality and inequality constraints shown in equations (4.1) through (4.4). Because of the nonlinear constraints and the discrete integer variables, the problem would be solved using mixed-integer nonlinear programming (MINLP) technique.

However, due to the difficulty associated with a large scale MINLP, this problem is reformulated as a mixed-integer linear program (MILP) by converting the nonlinear function vectors \( f \) and \( g \) to linear approximations. For example, temperatures and pressures need not be continuous if heuristics developed in Chapter 2 are used to select discrete levels of these operating conditions. A steam boiler generating steam at a known set of conditions is represented by a set of linear constraints instead of a non-linear function of temperature and pressure. A binary variable vector \( z_j \) would represent the existence or non-existence of discrete set of operating conditions, in this case, of a steam boiler.

Since each unit can operate at only one condition, the following constraint ensures that only one operating condition is active for each unit.

\[
\sum_{j=1}^{t} z_{ij} = y_i \quad i = 1, \ldots, m
\]  

(4.6)
where $l$ is number of discrete set of operating conditions for unit $i$. If unit $i$ exists ($y_i = 1$), then one of the $z_{ij}$'s must be 1. Furthermore equations (4.1) through (4.4) are transformed into the following linear equality and inequality constraints.

\[
\begin{align*}
A_1z + A_2x &= b \\ 
d_L &\leq C_1x + C_2y + C_3z \leq d_U
\end{align*}
\]  

(4.7)  
(4.8)

The matrices $A_1$ and $C_3$ are constants arising from discretizing the operating parameters. The profit function, $P$, is also linearized to the following form.

\[
\max : \quad P_{\text{profit}} = a^Ty + b^Tz + c^Tx
\]  

(4.9)

where $a, b, c$ are cost coefficient vectors. The resulting MILP is shown in Table 4.1. When applied to an actual problem, the number of binary variables is smaller than the product, $lxm$, that Table 4.1 would indicate because not all $m$ units would have $l$ number of $z$'s.

**Linearization of Process Data**

The non-linear equations are approximated using a standard linearization technique as shown in Figure 4.1. For example in Figure 4.1 (a), the non-linear $mC_p$ is approximated using a straight line $mC_p_{\text{constant}}$. The error tolerance as measured in terms of end temperatures is set at 5% for convex functions. For concave functions, the error tolerance as measured in terms of largest temperature difference between $mC_p_{\text{constant}}$ line and the $mC_p$ curve is less than 5%. In addition, the $mC_p_{\text{constant}}$ line...
is always below the actual \( mC_p \) curve for hot streams and always above the actual \( mC_p \) curve for cold streams so that the minimum approach temperature requirement is always met.

For non-linear equations that span a wider range such as shown in Figure 4.1 (b), multiple sectioning is done to keep the error tolerance in the ordinate variable under 5%. The function is then represented as shown in equation (4.10).

\[
C_{\text{capital, turbine}} = m_i W_i + b_i z_i
\]

\[
z_i W_i^L \leq W_i \leq z_i W_i^U \quad z_i = 0, 1
\]

In this piece-wise linear function, \( z_i \) is activated \((z_i = 1)\) if \( W \) is in the range specified by \( W_i^L \) and \( W_i^U \). If the unit doesn't exist at all \((\sum z_i = 0)\), the capacity bounds deactivate the whole equation by setting everything to zero. Lower and upper bounds could be varied to reduce the error of approximation. But this results in an increased number of variables and constraints. A proper balance has been reached by limiting the linearization error tolerance to 5%.

## 4.2 MILP formulation of Utility Plant

To develop an MILP formulation of the utility plant synthesis problem, the superstructure mentioned in the previous section is developed. It is also important that this configuration not be limited to just the utility plant. It must also be amenable to inclusion of possible heat and work integration with the process. First, however, we will illustrate the synthesis of a simple utility system with no heat or work integration devices and hot and cold utility requirements specified arbitrarily. (Presumably, this information would come from the design of the chemical process.)

The utility plant is subdivided into three sections, 1) power production, 2) heating and cooling, and 3) miscellaneous support units.

Power production is accomplished in two ways. First, an open air gas turbine shown in Figure 3.22 can be used. The performance and cost data were derived in
Figure 4.1: Linear Approximation
Chapter 3. Second, a steam turbine system can be used to generate power. Since steam is also used for process heating, a back pressure turbine with extraction is employed. For problems with large power demand, a condensing steam turbine with a vacuum condenser is included as an option. For simplicity, it is assumed that these turbines are connected to an electricity generator so that the electricity can be distributed to the process, instead of motive power. The electricity can also be purchased from the local utility, but this is unlikely given the large demand. Normally, only the start-up electricity demand is purchased. However, if excess electricity is generated from the utility plant, it is sold to the utility grid. The revenue generated may or may not be credited depending on the problem specification.

Hot utility is generated from a direct-fired boiler or waste heat boiler. The working fluid is normally steam. The operating pressure and temperature of the steam is determined by heuristics from Chapter 2. Back pressure extraction turbines would be coordinated with these operating parameters. The cooling requirement is met with cooling water. Cooling water return temperature is a continuous variable, but the optimized maximum temperature of 50°C is used from Chapter 3. Refrigeration and heat pumping are considered in the later sections.

Other support units include the feedwater pump to the boiler and de-aerator to provide water to the process and the boiler. A water treater is needed for make-up water that goes into the de-aerator. A superstructure which includes all these units are shown in Figure 4.2

**Derivation of MILP Model**

With the configuration shown in Figure 4.2, the utility plant synthesis problem is formulated as a mixed-integer linear program. The continuous variable vector $\mathbf{x}$ represents the flowrates of streams and the size of units. The vector $\mathbf{y}$ is a binary vector representing existence or non-existence of units. Furthermore, vector $\mathbf{z}$, represents a discrete set of operating parameters, discrete size, and other linearized constraints.

For example, the flowrate for each unit has to be defined. Into each unit $i$, the mass flowrate is $F_{Ij}$ from unit $j$. Out of each unit $i$, the mass flowrate is defined as
The mass balance equation is written below.

\[ \sum_j F_I^j - \sum_k F_O^k = 0 \quad i = 1, \ldots, m \]  
(4.11)

If \( h_i^j \) is the enthalpy of stream from unit \( j \) entering unit \( i \), the energy balance can be also written assuming that \( Q_i \) is heat added and \( W_i \) is power generated by the unit \( i \).

\[ \sum_j F_I^j h_i^j - \sum_k F_O^k h_k^i + Q_i - W_i = 0 \]  
(4.12)

If the unit exists at discrete conditions, third script is used to account for this. For example, if unit \( i \) exists at \( l \) conditions, flowrate from unit \( j \) at condition \( l \) into unit \( i \) is defined as \( F^l_{i}^j \). An extra summation over \( l \) would be required.

In order to set the flow to zero if the unit doesn’t exist, the following constraint is used.

\[ F_O^k - U_i y_i \leq 0 \quad i = 1, \ldots, m \]  
(4.13)

Here \( U_i \) is the maximum output flowrate from each unit \( i \). If \( y_i = 0 \), \( F_O^k \) has to be zero to satisfy the above equation. \( F_O^k \) can not be a negative number. Flowrate into unit \( i \), \( F_{i}^j \) is then forced to zero based on equation (4.11).

To determine the interconnections between units, the following set of constraints are developed. First, if unit \( i \) exists, unit \( j \) must exist or vice versa. For example, if steam boiler exists, feedwater pump must exist; or if feedwater pump exists, steam boiler must exist.

\[ y_{\text{boiler}} = y_{\text{feedwater pump}} \]  
i.e. \[ y_i = y_j \]  
(4.14)

If on the other hand, existence of unit \( i \) implies existence of unit \( j \) but not vice versa, a different constraint is used. For example, if a high pressure steam turbine exists, an electric generator exists. But the existence of the generator does not imply existence of a high pressure steam turbine. The generator may be connected to a medium pressure turbine or even a gas turbine. This is shown by the following constraint.

\[ y_i - \sum_j y_j = 0 \]  
(4.15)
Here, $y_i$ is the generator, and $y_j$'s are high and medium pressure turbines and the gas turbines.

Since a unit can operate at multiple conditions, constraints are needed that will ensure that only one operating condition exists for a given unit, and this is connected to an appropriate unit. This is accomplished by the following equations.

$$\sum_{k} y_i^k - y_j \leq 0$$ \hspace{1cm} (4.16)

$$\sum_{k} y_i^k \leq 1$$ \hspace{1cm} (4.17)

For example, if a high pressure boiler $y_i$ can operate at $k$ conditions, equation (4.17) ensures that only one operating condition is valid. Furthermore, equation (4.16) ensures that the boiler at this one operating condition is connected to a high pressure turbine $y_j$.

Other design considerations are also included as constraints. The power demand is met by power produced and/or purchased. The slack variable $W_x$ is the excess power produced which may or may not be sold depending on the problem specification. In order to prevent the utility plant from becoming just another power plant, $W_x$ can be forced to zero. To account for seasonal variation on $W_{demand}$, the worst case value is used.

$$W_{demand} = \sum_{i} W_i$$ \hspace{1cm} (4.18)

Heating demand is differentiated into multiple categories. For example, high temperature heating demand can be met only by a high temperature heat producing unit. However, the medium temperature heating demand can be met with both the high and medium temperature heat producing units, etc. The cooling demand is also expressed as a constraint.

$$Q_{hot,high} = - \sum_{i}^{high\text{ temp only}} Q_i$$ \hspace{1cm} (4.19)

$$Q_{hot,med} = - \sum_{i}^{high\text{ mid}} Q_i$$ \hspace{1cm} (4.20)

$$Q_{hot,low} = - \sum_{i}^{M} Q_i$$ \hspace{1cm} (4.21)
Furthermore, flowrates and capacities are bounded by following set of constraints. As explained before, these constraints ensure that the bounded variables are set to zero if the unit does not exist, i.e. \( y_i = 0 \).

\[
y_i L_B \leq F_i, Q_i, W_i \text{ etc.} \leq y_i U_B
\]  

The objective function is derived as shown below.

\[
\min: C_{\text{cost,ann}} = \sum_i a_i y_i + \sum_i CC_i(Q, W, F) + \sum_i OC_i(Q, W, F)
\]  

The constant fixed charge coefficient is shown as \( a_i \) and is activated only if unit \( i \) is present. The capital cost coefficients and operating cost coefficients are derived in appropriate units to account for the heat load, work load or the flowrate. The coefficients derived in Chapter 3 are used here. The last term accounts for the fuel cost, power cost and the cost of other feeds to the utility plant.

This general MILP was solved using the commercially available MILP solver "LINDO." [Scientific Press, 1980] To make sure that the formulation is consistent; and this is very necessary since the number of variables and constraints involved are large as will be shown in the next section, binary variables are set to 1 or 0 individually and in conjunction with the flow variables. If infeasibility exists, then the formulation is re-examined. Although there were very few cases of inconsistent formulation, here an expert system type of environment to automatically generate the LINDO input files from the MILP formulation would be valuable in the ultimate implementation of this methodology for use by engineers in a production environment.

**Result and Discussion**

The problem solving technique described above has been applied to an example problem. The data for this problem is shown in Table 4.2. The hot utility demands were specified by the designer of the chemical process along with the power requirement. The minimum pressure of the steam and therefore the minimum condensing
temperatures of the steam have also been specified. The heating demand is given in terms of mass flowrate instead of enthalpy. There is no external cooling water requirement. The purpose here is to demonstrate the effectiveness, yet the simplicity of the method.

The solution involves determining which of the units shown in Figure 4.2 are presents and how they are interconnected and at what conditions they operate. Table 4.2 also lists optimum operating conditions of the units determined from the Chapter 3 models. Some important cost data are also listed. The capital cost estimates are made from the equations derived in Chapter 3. These data are formulated as a MILP problem. The resulting formulation has 45 binary variables, 97 continuous variables, and 155 constraints. The coefficients used such as H's, CC's, CO's, efficiencies, and capacities are also derived from the Chapter 3 simulation and optimization models.

The problem was solved using the LINDO optimizer on a DEC MicroVAX in less than two, real time, minutes. The optimized utility plant is shown in Figure 4.3. The design has three different turbine systems, and two boilers. There is no need for a vacuum condenser since the power demand is completely met with the three turbines chosen. The total annualized cost is $29,072,972. It is interesting to note that of the total cost $18,003,671 is due to the fuel cost. In terms of percentages, it appears that the reduction in fuel cost plays a more important role than the capital cost. But this must be weighed against the annualization factor. In some previous work, 10yr straight line depreciation was used. However, it is quite inadequate for it would include the units that would be very capital intensive. The 5 year straight line or 10 year discounted rate is better. [Ulrich, 1984] In this work, the latter rate was used.

The design has a gas turbine, high pressure steam turbine, and medium pressure steam turbine. This is an unexpected result, since Townsend and Linnhoff [1983b] had concluded in their paper that it is rarely economical to have the combined system using both gas turbine and steam turbine system. However, in this example problem if gas turbine is eliminated from consideration, the total annualized cost is $36,503,552.
Table 4.2: Problem Data for Example 4-1

<table>
<thead>
<tr>
<th>Utility Demand</th>
<th>MP steam</th>
<th>LP steam</th>
<th>Total Power (kW) demand from chemical process</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utility Plant Units &amp; Operating Conditions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP steam</td>
<td>500°C</td>
<td>100. bar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>482°C</td>
<td>70.7 bar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>482°C</td>
<td>50. bar</td>
<td></td>
</tr>
<tr>
<td>MP steam</td>
<td>454°C</td>
<td>34.5 bar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>426°C</td>
<td>24. bar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>426°C</td>
<td>17. bar</td>
<td></td>
</tr>
<tr>
<td>LP steam</td>
<td>204°C</td>
<td>5.17 bar</td>
<td></td>
</tr>
<tr>
<td>Boiler</td>
<td></td>
<td></td>
<td>operates at 6 conditions specified above</td>
</tr>
<tr>
<td>Vacuum Condenser</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cooling water</td>
<td></td>
<td></td>
<td>57°C</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>30°C to 50°C</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.34bar</td>
</tr>
<tr>
<td>Gas Turbine</td>
<td>T_{combustion}</td>
<td>1,100°C</td>
<td>Pressure Ratio= 11</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>T_{exhaust}=450, 410, 385°C</td>
</tr>
<tr>
<td>Cost Data</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Annualization factor</td>
<td>0.175</td>
<td>10yr, 15% discount rate</td>
<td></td>
</tr>
<tr>
<td>Gas Turbine Fuel (methane)</td>
<td>$0.172/kg</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Boiler Fuel (kerosine)</td>
<td>$0.143/kg</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1 These represent the condensing temperature of steam.
2 These represent temperature of superheated steam.
Air 100bar, 500°C

Air Preheater

H Ps sam head

EA '0

7

8.8MW Turbine

Compressor 32MW

MP steam head

LP steam head

34.5bar, 45.1°C

34.7kg/sec

34.7kg/sec

MP Economiser

To Process

BFWpump

MP boiler

Deaerator

From Process

5bar, 204°C

To process

10 kg/sec

Total Ann Cost: $29,072,000
The resulting design is shown in Figure 4.4. This design is over 25% more costly than the optimum configuration shown in Figure 4.3.

However, their conclusion is not completely inapplicable. As the power demand is reduced and the heating demand is increased, the utility plant with a steam turbine system alone becomes more economical. But as the power demand is increased and the heating demand reduced, a utility plant with gas turbine system alone becomes more economical. The power demand and the steam demand, where the change-overs occur, vary depending on the problem. The problem Townsend and Linnhoff examined falls into a grey region where the change-over occurs. The method outlined here can cover a wider range of problems than an approach based on over-simplified heuristics.

Using this formulation method, the combinatorial nature of the problem is eased through the use of computing power. It is important to note that the superstructure must include all possible options. If other options or more operating conditions need to be examined, the formulation can easily handle this. Increasing the number of high pressure steam levels by one increases the formulation size of the original example problem 4-1 by 2 binary, 8 continuous variables, and 3 additional constraints. Although the size of the binary variable vector would increase the computation time, judicious selection of operating conditions using heuristics from Chapters 2 and 3 allows optimization of industrial size problems.

4.3 MILP for Heat Engine Integration

It was shown in the previous section that a properly optimized plant can save millions of dollars in the total annualized cost compared to a base case. However, even more savings can be realized if process heat sources and heat sinks are used to integrate heat engines from the utility plant. The MILP formulation developed in the previous section allows natural inclusion of these possibilities.

In Chapter 2 heuristics were developed that showed appropriate temperature
Figure 4.4: Optimized Utility Plant without gas turbine

HP boiler

MP boiler

BFW pump

Deaerator

MP Economiser

Waste boiler

LP Economiser

Condensate Return

Make-up water

Cooling Tower

Vacuum Cond
levels for hot utility and also cold utility. These levels can now be incorporated into the MILP model described in the previous section. The units and the possible operating parameters that were in the original superstructure would still be there. However, the superstructure is extended to include other operating parameters from Chapter 2.

The hot utility injection levels can be combined with heat engine heat exhaust. The cold utility injection levels can be combined with heat engine heat intake. We realize from Chapter 2 heuristics that these are the levels that might be in the global optimum solution. Therefore, it is sufficient to look only at these levels to find the global optimum solution. But first, these various heat engine integration options – either to inject heat into the process or to reject heat from process to heat engines – are examined using the models from Chapter 3. Only the ones that pass the conditions outlined in section 3.2 are considered. The MILP formulation is then developed to optimize and find a solution that gives the lowest cost (operating/capital) integrated plant configuration.

The MILP model need not be developed anew. The MILP formulation from the previous section is just extended to include the new feasible options and operating conditions. The extension of the model involves setting up binary variables and associated continuous variables for integrated heat engines. Furthermore, appropriate flow and connection constraints must be set. For topping cycles, i.e. with the heat engine placed above the pinch, steam is used as a working fluid. For bottoming cycles, an appropriate fluid is chosen from Figure 3-7 based on the temperature levels selected from the Chapter 2 heuristics. For example, if the heat source is available at 200°C, R-114 from Figure 3-7 would be used for the power cycle. The cost, enthalpy, efficiency coefficients are again derived from the models in Chapter 3. These coefficients would be used in equations (4.11) through (4.21).

The main constraint that would take into account the presence of a heat engine is shown below. For each hot utility level $T_{u,j}$, heat can be added from the boiler
where \( T_{\text{boiler},i} \geq T_{u,j} \) and also from the heat engine where \( T_{\text{heat engine outlet}} \geq T_{u,j} \).

\[
Q_{u,j} = Q_{\text{boiler},i} + Q_{\text{heat engine},i}
\]

(4.25)

At each temperature level the amount of heat injected or removed up to that level is limited by \( Q_{u,i,\text{max}} \) as shown below.

\[
\sum_{i} Q_{i} \leq Q_{j,\text{max}} \quad j = 1, \ldots, M
\]

(4.26)

For example, if \( Q_{u,1} \) is the heat added at level \( T_{u,1} \), \( Q_{u,2} \) can be at most equal to \( Q_{u,2,\text{max}} - Q_{u,1} \). (Please refer to Figure 2.25) If additional \( Q_{u,2} \) is added that would violate the pinch at \( T_{u,2} \) The values for \( Q_{u,i,\text{max}} \) are calculated using the method described in section 2.4 earlier.

**Result and Discussion**

Example 4.2 is an extension of Example 4.1 so that it also has the heat exchanger network problem, i.e. hot and cold stream data and minimum approach temperature allowed in the heat exchanger network. The data for this problem is shown in Table 4.3. First, the pinch points and possible hot utility levels are determined. A minimum approach temperature of 10°C is used. (The utility demand data for Example problem 4.1 were actually derived from the stream data above the pinch.) The minimum hot and cold utility demands were calculated to be 106 MW and 13 MW, respectively. For each utility level selected, the maximum amount of utility that can be added are calculated and are shown in Table 4.3. Using the models and heuristics from section 3.2, hot utility levels are examined for possible topping cycle.

Given multiple heat source temperatures and multiple heat sink temperatures, the simulation model can optimize the operation of heat engines and other units in the utility plant to yield coefficients such as operating cost, annualized capital cost, heat exchanger load and power output for promising integration options.

Since the stream data from which the original utility demands were obtained are available, the fixed utility demand can be relaxed. For example, medium pressure
Table 4.3: Example 4-2 Stream and utility data

<table>
<thead>
<tr>
<th>Stream No.</th>
<th>T$_{supply}$ (°C)</th>
<th>T$_{target}$ (°C)</th>
<th>Enthalpy (MW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>400.</td>
<td>175.</td>
<td>19</td>
</tr>
<tr>
<td>2</td>
<td>180.</td>
<td>130.</td>
<td>7.5</td>
</tr>
<tr>
<td>3</td>
<td>130.</td>
<td>120.</td>
<td>4.12</td>
</tr>
<tr>
<td>4</td>
<td>130.</td>
<td>50.</td>
<td>9.14</td>
</tr>
<tr>
<td>5</td>
<td>120.</td>
<td>150.</td>
<td>30</td>
</tr>
<tr>
<td>6</td>
<td>120.</td>
<td>170.</td>
<td>12.5</td>
</tr>
<tr>
<td>7</td>
<td>140.</td>
<td>170.</td>
<td>90</td>
</tr>
<tr>
<td>Pinch</td>
<td>Hot 130°C</td>
<td>Cold 120°C</td>
<td></td>
</tr>
</tbody>
</table>

Utility Data
- Hot utility 1: 180°C, 106 MW
- Hot utility 2: 175°C, 102 MW
- Hot utility 3: 150°C, 22 MW
- Cold utility 1: 30°C, 13 MW

Steam can be used to meet the low pressure steam demand. Therefore, $Q_{med} \leq 44.7kg/sec$ is used as a constraint instead of $Q_{med} = 34.7kg/sec$ used in the stand-alone utility plant formulation. The possibility of adding a bottoming cycle for at T=130°C was examined using the model from Chapter 3. However, the size of the heat source did not meet the criterion established in Figure 3.8 and thus was eliminated from consideration.

The addition of an extra hot utility level and the accompanying topping cycle increased the formulation size by 3 binary, 8 continuous variables, and 6 constraints. These are in addition to 45 binary, 97 continuous variables and 155 constraints for the utility plant design from the previous section. Optimization of this new MILP resulted in a optimum network costing only $24,693,000 per year shown in Figure 4.5. The optimized design has only one steam turbine operating from pressure of 70 bar to 10 bar. There is no LP steam head, and all heating demand is met with 10 bar steam.

The cost savings resulted mainly from the elimination of a boiler and a MP turbine. This is counter-intuitive and against the normal design rule of thumb where
Figure 4.5: Utility plant integrated with HEN

- HP boiler
- Air Preheater
- Fuel
- Compressor
- Gas Turbine
- BFW pump
- Deaerator
- From Process

- 70.7 bar, 482°C
- 19.5 MW
- 47.4 kg/sec
- 10 bar 195°C
- MP steam head
- MP Economiser
- To Process

Total Annualized COST: $24,693,000
HP turbine and MP turbine are always present together. However, when the trade-off between the cost of extracting the last bit of energy and the benefit is closely examined, the former overwhelms the latter in the case of this example. If the steam and power demand were to change, the formulation can be easily modified and optimized again.

One other counter-intuitive result is that multiple utility levels that would complicate the heat exchanger network design did not take place. To maximize the efficiency of the utility plant, one would have expected to see MP steam at both 175°C and at 180°C. However, when optimized from the cost stand-point, this is not the case and only one MP steam level is selected in the final solution.

This example problem illustrates the benefit of designing the utility plant with complete heat exchanger network data instead of just utility demands specified a priori by the designer. (This is not quite the simultaneous synthesis since the actual design of heat exchanger network is not done.) The normal design procedure would have been to design the HEN based on the assumption of available hot utility level. Then, the utility plant would be designed to meet the hot utility demand of the HEN. However, by integrating the utility plant design with the HEN and using both heuristic simplification and mathematical programming techniques, the global optimum solution can be found within the superstructure.

Another advantage of this method is the ease with which problem specifications can be changed. For example, the design shown in Figure 4.5 would change if the LP steam demand is increased. This would happen if process conditions changed. At about 70kg/sec of LP steam demand, it is no longer cheaper to use the MP steam for all the heating need. A new optimum design with high pressure steam header at 70 bar and medium pressure steam at 17 bar and LP steam at 5 bar with steam turbines between each level is found. This design is structurally identical to Figure 4.3 but with different operating conditions. This new design was found simply by changing the constraint \( Q_{LP} \leq 10kg/sec \) to \( Q_{LP} \leq 70kg/sec \).

If the initially rejected bottoming cycle is included, the resulting MILP formu-
lation has additional 3 binary, 6 continuous variables, and 11 constraints. (These are in addition to the variables and constraints for extra hot utility level case.) However, the optimized result is still the same one without the bottoming cycle in the final structure. If the option is forced, and this can be easily accommodated by setting associated binary variables to 1, the total annualized cost is $29,553,000 over 20% larger than the optimum case. This example indicates that the pruning heuristics method is an effective way of reducing the problem size without eliminating the optimum solution. However, care should be taken so as to ensure that marginally economical stand-alone systems are included since their effect when connected to other units are unknown. The models and heuristics from Chapter 3 ensure this.

The heat engine integration problems examined so far followed the basic rules of Townsend and Linnhoff. There was always a heat sink available above the pinch for a heat engine to reject heat to and a heat source below the pinch for a heat engine to take heat. This allowed placement of heat engines either completely below the pinch or above the pinch, shown in Figure 4.6.

However, there are some cases where these rules would not hold. These cases arise from the unpinched or unconventional temperature enthalpy diagram as shown in Figure 4.7. Unlike a conventional pinch diagram, the process plotted in Figure 4.7 (a) has a pinch but no heating is required above the pinch. Normally, this would preclude any possibility of heat engine integration. However, using the low temperature utility shown in bold line to heat the cold streams and incorporating the hot stream above the pinch with heat intake from a heat engine could produce an economically viable co-generation scheme.

Furthermore, heat engines could be placed across the pinch to produce more work as shown in Figure 4.7 (b). Both of these cases violate the heuristics proposed by Townsend and Linnhoff, but they can result in a more economical solution. The new algorithm developed in Chapter 3 for pinch point location and utility demand calculation can easily handle theses situations.

The example problem shown in Figure 4.7 (a) and whose stream data are listed
Figure 4.6: Typical Heat engine integration
Figure 4.7: Alternate Heat Engine Integration
Table 4.4: Example 4-3 Stream Data

<table>
<thead>
<tr>
<th>Stream No.</th>
<th>( T_{supply} ) (°C)</th>
<th>( T_{target} ) (°C)</th>
<th>Enthalpy (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>500.</td>
<td>220.</td>
<td>16,500</td>
</tr>
<tr>
<td>2</td>
<td>250.</td>
<td>80.</td>
<td>1,500</td>
</tr>
<tr>
<td>3</td>
<td>90.</td>
<td>40.</td>
<td>7,000</td>
</tr>
<tr>
<td>4</td>
<td>40.</td>
<td>130.</td>
<td>2,250</td>
</tr>
<tr>
<td>5</td>
<td>110.</td>
<td>130.</td>
<td>14,500</td>
</tr>
<tr>
<td>Pinch</td>
<td>Hot</td>
<td>90°C</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Cold</td>
<td>80°C</td>
<td></td>
</tr>
</tbody>
</table>

Utility Data

| Cold utility 1 | 30 | 50 | 8,250 |
| Power          |    |    | 4,050 |

in Table 4.4, is not an unusual configuration. A typical Ethylene-Oxide plant design has a process composite diagram very similar to this. In order to show the advantage of simultaneous method, this problem is first solved without the utility plant. Then, the problem is solved with the utility plant simultaneously.

There are a few assumptions that need to be made before the problem can be solved. Since the utility plant is not considered in the first case, the power demand is met by purchase ($420/kWyr), by process stream integration or some combination, which-ever is cheaper. If hot utility is needed because of internal power production using hot process streams, hot utility is assumed to be available at any temperature based on the fuel cost and pumping cost only. (The capital cost of boiler and pump is already sunk.)

There are two power production options. First is a steam turbine system which operates at 480°C, 17 bar inlet turbine conditions and at 155°C, 5 bar condenser outlet. The second is an organic fluid rankine cycle with R-113 operating at 45bar, 480°C and 155°C, 12.2 bar. Power production using hot streams through condensing turbine is ruled out because that would be identical or worse than purchasing power from outside.

Since the operating conditions specified in Figure 3.8 are significantly different
from this example, the figures can not be used for basis of selecting suitable working fluids. For example, if Figure 3.8 (c) were used for comparison, a steam system with 17% efficiency would be chosen over the R-113 system with 10% cycle efficiency. However, it must be realized that in that example problem the heat source was at constant temperature. In this example the heat source temperature goes from 500 to 150 °C. New efficiency and enthalpy coefficients were derived from the models in Chapter 3. Since this problem falls into a category where the cycle efficiency would change by more than 5% as $Q_m$ is changed, multiple coefficients are used.

The MILP formulation has 6 binary variables, 21 continuous variables and, 33 constraints. When the problem is optimized for size and type of operation, R-113 cycle is chosen with the total annualized cost of $1,320,000 per year. Power production is 1.6MW, and the rest is purchased. No hot utility is needed, but 6.6MW of cooling water is needed.

However, in many cases the power can not be purchased from outside, or the utility plant already exists. Then, the problem must be reformulated with the utility plant and optimized simultaneously. The result is quite surprising in that no direct power production is done from the heat sources in the process. With the MILP formulation of the utility plant superstructure from Example 4-1, the heat engine integration is formulated simultaneously. The optimum configuration found from this MILP problem has only a gas turbine for power production and cooling water for cold utility. This is probably due to the fact that there is no need for MP or LP steam demand in this example. The total annualized cost is $3,236,000.

This problem can not be generalized, since depending on the shape of the composite curves or depending on the power demand the economics would change. However, the method is applicable to a wide variety of problems. Especially, it is very suitable for studying the power generation potential of process streams not only for new plants, but also existing plants.

Finally, the example shown in Figure 4.7 (b) is another case where violation of Townsend and Linnhoff's rules occur. If the heat exchanger network and the
work integration system are designed with the Townsend and Linnhoff heuristics, the resulting design has a MP steam turbine rejecting heat to the cold streams above the pinch. However, when this problem is formulated as an MILP problem with integrated utility plant and optimized, the resulting solution has a steam turbine rejecting heat below the pinch which is a violation of the Townsend and Linnhoff's heuristics. The total cost is indeed lower than strictly following their rules.

Again, whether these violation are economical depends not only on the heat sources and sinks in the problem but also on the utility plant design. The method developed here allows simultaneous consideration of both so that a global optimum solution can be found instead of a local optimum. Furthermore, better designs that violate the Townsend and Linnhoff heuristics can be easily found using this approach.

4.4 MILP heat pump placement

The same strategy for heat engine integration is used to solve the problem of heat pump integration. First, heuristics are used to reduce the size of the problem, and then the problem is mathematically formulated and optimized to find the minimum cost solution. Since the hot and cold utilities can be replaced with the condenser and the evaporator of the heat pump, the heuristics developed in Chapter 2 for hot and cold utility levels can be used to determine the appropriate temperature levels for the heat pump placement. The heat pumps operating under a combination of these temperature levels are optimized using the model developed in Chapter 3. Heat sink and heat source combination that meet the minimum criteria are transformed into a linear set of equations. These are then formulated as a mixed integer linear programming problem, with the integer variable representing the discrete combination of the heat sinks and heat sources.

In order to account for the interaction of the heat pump with the utility plant and the integrated heat engines, this formulation is combined with the MILP formulation developed for the latter two in the previous sections. This summation involves connecting flows of various heat pump operations to that of heat engine integrated
utility plant. Capital cost and operating cost contributions are added to the objective function.

The main difference between this formulation and the previous formulation for a heat engine integrated utility plant is the fact that the hot and cold utilities could be replaced by a heat pump simultaneously. In addition, the amount of hot and cold utilities displaced is set by the coefficient of performance (COP) of the heat pump. Therefore, following additional constraints for hot and cold utilities are included in the formulation.

\[
Q_i = Q_{boiler,i} + Q_{heat\ engine,i} + Q_{heat\ pump,i}
\]
\[
Q_j = Q_{cooling\ water,j} + Q_{heat\ engine,j} + Q_{heat\ pump,j}
\]

where \(Q_i\) is the amount of heat injection at temperature \(T_i\), \(Q_j\) is the amount of heat removal at temperature \(T_j\), and \(Q_{unit,i}\) is the amount of heat injection from the unit to \(T_i\), and \(Q_{unit,j}\) is the amount of heat removal by the unit from \(T_j\). The maximum amount of heat injection or removal constraint given by equation (4.26) would still hold. However, unlike the heat engine case, heat injection and rejection from the heat pump would be further constrained by the following equation to account for the thermodynamic coefficient of performance.

\[
Q_{heat\ pump,j} = Q_{heat\ pump,i} + W_{heat\ pump}
\]

The optimization of this MILP then should tell us whether the integration with the heat pump is necessary for an optimum (minimum cost) operation of the total plant.

**Result and Discussion**

Example 4-2 is further explored for possible heat pump integration. Applying the heuristics for heat pump placement from Chapter 2, the possible levels where heat pump can be added are shown in Figure 4.8 in the next page. Since no cold streams are present below the pinch, the heat intake equivalent to cold utility can be added at any point. However, the heat pump heuristic dictates that the preferred levels are temperatures where the kinks occur in the hot composite curve in the absence of the
cold kinks. Therefore, 120°C and 50°C are possible levels. The actual heat pump working fluid evaporator temperature would be lower by $\Delta T_{\text{min}}$, i.e. 110°C and 40°C.

On the heat exhaust side, the heat pump should be placed at the hot composite kinks. At this point, the models and heuristics from section 3.2.2 are used to determine which of the options need to be included in the MILP formulation.

All combinations involving heat exhaust at 180°C do not meet the heat pump placement criteria and are eliminated from the list of integration options. Of the combinations with $T_{\text{exhaust}} = 150^\circ\text{C}$, only $T_{\text{intake}} > 100^\circ\text{C}$ meet the capacity, efficiency, and economic criteria. Differential economic study is done to determine which levels between 100 $\sim$ 120°C are most efficient. In this case $T_{\text{intake}} = 110^\circ\text{C}$ has the highest economic potential.

The heat pump integration is formulated directly as an extension of the previous MILP instead of developing a separate formulation and later combining the two. The resulting MILP has 4 binary, 8 continuous, 12 constraints for a total of 52 binary, 113 continuous variables and 173 constraints when combined with the heat engine integrated utility plant MILP formulation. The optimized design for a heat engine and heat pump integrated utility plant does have the heat pump installed. The total annualized cost for the optimized design is $24,438,700 slightly lower than for the case without the heat pump as shown in Figure 4.5.

In using the strategy developed here to solve the heat engine and heat pump integration with the utility plant, other situations may be encountered where the Townsend and Linnhoff heuristics are not applicable. For example, in a problem such as shown in Figure 4.9, strict adherence to the heat pump placement rules of Townsend and Linnhoff could result in a design where the condenser 1 heat is pumped and rejected to the reboiler 2. However, since other process streams can not meet the demand of reboiler 3, low temperature hot utility is needed below the pinch. The end effect is to replace the hot utility 1 with hot utility 2. But the amount of work and the capital cost is not offset by the savings generated. In the current methodology, equation 4.26 would force utility demands to balance so that such designs do not
Figure 4.8: Heat pump integration
result.

In another case as shown in Figure 4.10, the addition of heat engine exhaust below the pinch can yield an economical design. In this design a heat pump is added to pump heat from $T_4$ to $T_1$. When the problem is optimized without the heat pump, the design has a steam turbine exhausting heat to $T_1$. However, when a heat pump and a gas turbine exhausting to $T_3$ are included, a lower cost design results which utilizes the gas turbine and the heat pump. This is another violation of Townsend and Linnhoff’s rule. This is especially applicable when $T_{\text{pinch}}$ is high and a suitable working fluid for the heat pump can be found in the specified temperature range.

These are special cases to the general rules developed by Townsend and Linnhoff. But they can be easily recognized, and the MILP formulation can be extended to account for such possibilities.

### 4.5 MILP of refrigeration

In many processes, there are process streams that need to be cooled below the minimum cooling water temperature. If cold process streams are available to cool these hot streams, then they would be used in lieu of refrigeration. However, if the cooling needs are larger than the available cold streams, some form of refrigeration will be required.

A strategy is developed to consider the refrigeration cycle that would allow mathematical formulation of the problem with a subsequent conversion to MILP formulation which can be integrated with the other MILP formulations developed earlier. Given a problem with associated pinch diagram as shown in Figure 4.11, the problem must be decoupled into two sections, one that needs only the cooling water and the other section requiring refrigeration. The division occurs at $T_{CW,\text{min}} + \Delta T_{\text{min}}$ on the hot side and at $T_{CW,\text{min}}$ on the cold composite side. The design for the regular pinch section has been discussed already. The design procedure for the refrigeration section will now be discussed.
Figure 4.9: Uneconomical heat pump usage
Figure 4.10: Special heat engine and heat pump application
Figure 4.11: Division of Pinch Diagram
The refrigeration section from Figure 4.11 is redrawn in Figure 4.12. As discussed in section 2.3.2, there are only a few places where cold utility can be added economically. These are shown as $T_i$'s. At each level, the maximum load that utility can remove without violating the $\Delta T_{\text{min}}$ constraint is shown as $Q_{i, \text{max}}$. The solution to the problem involves determining which of the levels are present and what load they carry in the optimum design.

To solve the problem, the MILP formulation technique is again applied. Here, each level of refrigeration can be thought of as a separate unit operation represented by a binary variable. This is shown in Figure 4.13. Each level can remove $Q_i$ amount of heat from the process. However, $Q_i$ is bounded by $Q_{i, \text{max}}$ by following constraints.

\[
\sum_{i} Q_i \leq Q_{j, \text{max}} \tag{4.30}
\]
\[
\sum_{i=1}^{L} Q_i = Q_{\text{cold, min}} \tag{4.31}
\]

The first constraint assures that the minimum approach temperature is not violated. For example, if $Q_{j, \text{max}}$ is the maximum amount of heat that can be removed at $T_j$ without violating the minimum approach temperature, the actual $Q_j$ has to be less than this value minus the $\sum_{i<j} Q_i$. The second constraint assures that the total amount of heat removed from the process is minimum calculated from the pinch diagram. In addition, each level can also take heat from the levels below it and reject heat to levels above it. This is shown by the following constraint.

\[
Q_i + \sum_{j=1}^{i-1} Q_{j,i} - \sum_{k=1}^{0} Q_{i,k} + \sum_{k=1}^{0} W_{i,k} = 0 \tag{4.32}
\]

Other constraints such as flow activation, connectivity, mass balance, energy balances are also developed to complete the formulation. The coefficients such as cycle efficiency, capacity bounds are found from the models in section 3.3. The optimization of the resulting MILP formulation is accomplished using LINDO. The solution will be the minimum cost design with refrigeration level and load information for the given problem.

**Result and Discussion**
Figure 4.12: Pinch diagram of refrigeration section
Q3 + W3,2 + W3,1 + W3,0 - Q3,2 - Q3,1 - Q3,0 = 0
Q2 + W2,1 + W2,0 + Q3,2 - Q2,1 - Q2,0 = 0

Q1 <= Q1\text{max}
Q1 + Q2 <= Q2\text{max}
Q1 + Q2 + Q3 <= Q3\text{max}
The problem shown in Figure 4.12 was solved using this procedure. There are 10 binary, 26 continuous variables, and 18 constraints in the MILP formulation. The optimized solution has levels $T_1$ and $T_3$. $Q_1$ and $Q_3$ are 50kw each, but level $T_3$ rejects heat to $T_1$ as shown in Figure 4.14.

Since the possibility of using a low temperature Rankine cycle within the refrigeration segment is very low, this refrigeration MILP formulation does not need to be solved simultaneously with the integrated utility plant formulation. (Of course, a cryogenic plant would be an exception, but this can be a topic all on its own and is not explored here.) This optimization can be completed first, and the optimized result can be expressed as constraints in the MILP formulation of the integrated utility plant. The power demand from the refrigeration section would be an additional demand that needs to be satisfied by the utility plant. Cooling water demand would also be included. In this way, even the problems requiring refrigeration can be solved effectively using the MILP strategy.

4.6 Summary

In this chapter, a new strategy for designing an optimum integrated utility plant has been developed. The method uses heuristics developed in previous chapters to reduce the problem size. Combined with the simulation and optimization models developed in chapter 3, a mixed integer linear programming formulation is generated which can calculate the optimum solution. The MILP formulation approach is used to optimize utility plant alone, with heat engines, with heat pumps, and/or with refrigeration schemes for complete integration. The resulting solutions were the lowest cost designs that were obviously better than the designs found using the previous approaches which did not account for the interactions.

The accuracy of the linearization scheme can be checked at the end by comparing the capacity to the bounds set by linearization. If the capacity is outside the region, then additional binary variables are used to include the outside region. The problem is re-optimized to find a new optimum solution. In all cases examined, the structure
$Q_0 = 136 \text{kW}$

Secondary condenser

$Q_1 = 50 \text{kW}$

Secondary evaporator or primary condenser

$Q_3 = 50 \text{kW}$

-30°C

Primary evaporator

10°C

Figure 4.14: Optimum Refrigeration Schematic Diagram
of the system stayed the same, but the operating conditions and the total annualized cost changed somewhat. This does not preclude the fact that the structure could change; however, because the error tolerance in the linearization step was low enough that this problem has not been encountered in this research.
### Notation used in Chapter 4

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CC</td>
<td>Capital cost coefficient</td>
</tr>
<tr>
<td>OC</td>
<td>Operating cost coefficient</td>
</tr>
<tr>
<td>$H_{j,i}^{k}$</td>
<td>Enthalpy of stream entering $j$ from $i$ at condition $k$</td>
</tr>
<tr>
<td>$F_{j,i}^{k}$</td>
<td>Flowrate of stream entering $j$ from $i$ at condition $k$</td>
</tr>
<tr>
<td>$l$</td>
<td>Number of operating conditions</td>
</tr>
<tr>
<td>$m$</td>
<td>Number of units</td>
</tr>
<tr>
<td>$L$</td>
<td>Total number of cold utility levels.</td>
</tr>
<tr>
<td>$M$</td>
<td>Total number of hot utility levels.</td>
</tr>
<tr>
<td>$Q_{u,i}$</td>
<td>Utility at level $T_i$</td>
</tr>
<tr>
<td>$W_{\text{demand}}$</td>
<td>Primary power demand from the process</td>
</tr>
<tr>
<td>$W_i$</td>
<td>Work produced or used by unit $i$</td>
</tr>
</tbody>
</table>
Chapter 5
Optimization of $\Delta T_{\text{min}}$

One of the important design variables in the heat exchanger network synthesis problem is the global minimum approach temperature, $\Delta T_{\text{min,global}}$. In the result presented so far, this value was assumed to be fixed by the designer. However, by varying the minimum approach temperature, utility demand and thus the structure of the integrated utility plant can be changed. The MILP solution strategy developed in the previous chapter can be applied further to this variable $\Delta T_{\text{min}}$ problem. Variable $\Delta T_{\text{min}}$ has implications in both the grass-root design case and the retrofit case. In this chapter the MILP solution strategy is applied to both.

5.1 Selection of $\Delta T_{\text{min,global}}$ in Grass-root Design

Up to this point, it was assumed that the minimum approach temperature based on prior experience was sufficient to give an optimal design of both heat exchanger network and the utility plant. However, this may not necessarily be the case since the present design problem may have no relation to the prior design from which the minimum approach temperature was obtained. In such a case, there must be an outer loop in the design procedure to vary $\Delta T_{\text{min}}$ as shown in Figure 5.1.

In the previous research that was limited to the synthesis of heat exchanger network, the design of the integrated utility plant block in Figure 5.1 was replaced with a simple costing routine that assigned costs to a few selected utilities. To determine
Begin Design

Specify chemical plant design and determine composite enthalpy curves for heating and cooling

Select ΔTmin

Develop superstructure and solve MILP for optimum integrated utility plant including heat engines, heat pumps, and refrigeration units where applicable

Design and cost heat exchanger network

Compare the total cost

improvement, new ΔT

no improvement

End of Design

Figure 5.1: synthesis procedure for utility plant and heat exchanger network
the optimum $\Delta T_{\text{min}}$ and the corresponding heat exchanger network, a plot of total cost curve versus various $\Delta T_{\text{min}}$ was constructed as shown in Figure 5.2.

First, $\Delta T_{\text{min}}$ was picked. Then, using the pinch technique, the minimum utility loads and the pinch were determined. The two components of the total cost are annualized capital cost of heat exchangers and the operating cost due to utilities cost. The capital cost of the heat exchangers were calculated after the design for the network was completed for a given $\Delta T_{\text{min}}$ and pre-selected utilities. The utility cost is determined from the minimum load that is distributed over a number of pre-selected utilities and multiplied by an arbitrary cost for each utility. (The utility cost is termed arbitrary because there are wide variety of methods for costing the utility. Therefore, depending on the choice of costing method, one would expect different cost for the same utility.) This procedure is repeated for various $\Delta T_{\text{min}}$ until the minimum on the total cost curve shown in Figure 5.2 is determined.

On the left side of the curve shown in Figure 5.2 where the minimum approach temperature is very small, the capital cost of the heat exchangers overwhelms the utility cost, and the resulting total cost is very high. As $\Delta T_{\text{min}}$ is increased for a given problem, the minimum hot and cold utility loads increases which in turn causes the utility cost to rise. However, the amount of total area required in the heat exchanger network decreases because of the larger driving force resulting in a lower capital cost for heat exchangers. At the other extreme, utility cost could overwhelm the heat exchanger cost for a large $\Delta T_{\text{min}}$ and results in large total cost. Therefore, to determine the optimum $\Delta T_{\text{min,global}}$ for a heat exchanger network, tradeoff between the extra operating cost due to increased utility loads and the savings in the capital cost of the heat exchangers due to decreased area need to be examined.

This is a very tedious task especially since the heat exchanger network costing can be performed only after the actual network is designed. However, good heat exchanger area estimation techniques have been developed recently so that the cost of the heat exchangers can be accurately estimated without actually designing the network. [Ahmad 1985, Viswanathan 1989] This would allow faster determination of the minimum cost heat exchanger network since time-consuming network derivation
Figure 5.2: Total Cost Curve for Heat Exchanger Network Designed with Arbitrary Utility Costs
at each $\Delta T_{\text{min}}$ does not need to be performed.

**$\Delta T_{\text{min}}$ Selection for Simultaneous Synthesis of Utility Plant and HEN**

However, when the utility plant synthesis is considered together with the heat exchanger network synthesis, the simple utility costing relationship will not give an accurate result. This is especially true if the change in $\Delta T_{\text{min}}$ causes a structural change in the utility plant. Therefore, the assumption that the utilities are available at constant cost needs to be relaxed for determining the optimum minimum approach temperature for simultaneous synthesis case.

To apply the new procedure to the determination of an optimum $\Delta T_{\text{min}}$, first an arbitrary $\Delta T_{\text{min}}$ is selected. Second, the minimum utilities and the pinch are determined. Third, and this is what differentiates the new procedure from the old, the utility plant is designed and costed using the MILP procedure described in the previous chapter. This procedure, then, replaces the arbitrary costing of utilities with costs of fuel, water, and the capital costs of units. The heat exchanger network is designed last to find the capital cost contribution.

This procedure is repeated for different $\Delta T_{\text{min}}$'s to find the optimum approach temperature and the corresponding utility plant and the heat exchanger network. To facilitate a faster search of the optimum $\Delta T_{\text{min}}$, the area estimation technique can be used instead of designing the complete heat exchanger network.

**Result and Discussion**

The methodology is demonstrated using the example problem 4SP1 and compared to the result from previous research using constant utility cost assumption. The stream data for example problem 4SP1 are given in Table 5.1.

Since the original problem assumed that the power requirement was zero, the utility plant formulation degenerates to a simple problem of selecting an efficient unit to supply the hot utility at the lowest cost. Steam heater, oil heater, and direct-fired heater were included in the MILP formulation. Obviously, the optimization selected direct-fired heater operating at 411°C as the best utility design. The total cost for this
heater is $52 per kW-year of heating supplied in 100 ~ 350 kw capacity. (Therefore, total annualized cost for the utility plant including the fuel cost would be the product of the heating demand and the cost coefficient, $52.)

At this point $\Delta T_{\text{min}}$ of 10°C was selected for heat exchanger network design. (In more complex problems utility plant optimization would be done after selecting $\Delta T_{\text{min}}$. However, in this example the degenerative nature led to a priori optimization.) The minimum cost heat exchanger network for $\Delta T_{\text{min}} = 10^\circ\text{C}$ is shown in Figure 5.3 with total annualized cost of $19,475. Summing up the cost of the heat exchanger network and the utility plant yields $27,631.

For various values of $\Delta T_{\text{min}}$, the resulting heat exchanger cost and the utility plant cost were calculated. For other values of $\Delta T_{\text{min}}$, the structure of the minimum cost heat exchanger network were identical to network shown in Figure 5.3; however, temperatures and areas of heat exchangers varied. This result is plotted as the sum of the two costs in Figure 5.4 (a). The optimal value of $\Delta T_{\text{min}}$ corresponding to global minimum cost heat exchanger network and the utility plant occurs at 8.2°C.

If the assumption of fixed utility plant is not relaxed, then the previous method with arbitrary utility costing is used to find the optimum $\Delta T_{\text{min}}$. The utility cost data from the paper by Colmenares and Seider [1986] are used for this purpose. The resulting heat exchanger network cost and the utility cost is summed and plotted as the total annualized cost shown in Figure 5.4 (b). The breakdown of the cost is shown in the Appendix F-1.

The optimal value of $\Delta T_{\text{min}}$ corresponding to the global minimum cost heat exchanger network and the utility cost occurs at 4.2°C. Please note that this method

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kw/°C)</th>
<th>$T_s$ (°C)</th>
<th>$T_l$ (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.79</td>
<td>160.</td>
<td>93.</td>
</tr>
<tr>
<td>2</td>
<td>10.55</td>
<td>249.</td>
<td>138.</td>
</tr>
<tr>
<td>3</td>
<td>7.62</td>
<td>60.</td>
<td>160.</td>
</tr>
<tr>
<td>4</td>
<td>6.08</td>
<td>116.</td>
<td>260.</td>
</tr>
</tbody>
</table>
Figure 5.3: Minimum cost of heat exchanger network for 4SP1 with $\Delta T_{min} = 10^\circ C$
(a) Optimum $\Delta T_{min}$ with heat exchanger network and utility plant

(b) Optimum $\Delta T_{min}$ with fixed utility

Figure 5.4: Cost Curves
is valid if the utility pricing structure holds regardless of the load. However, as will be shown in the retrofit case, this assumption can not hold for large utility load fluctuation.

It is apparent that the two methods yield quite different answers, and that is expected since previous methods did not consider utility plant synthesis along with heat exchanger network synthesis. Since this new method does not involve any arbitrary decision on the designers part with regard to the utilities, it gives a more accurate account of the tradeoffs involved.

Furthermore, for more complex problems the structure of the minimum cost heat exchanger network may change with varying $\Delta T_{\text{min}}$. This structural change inevitably affects the utility plant because, for example, previous utility levels may not be sufficiently high in temperature to supply all the heating requirement to the new heat exchanger network. However, the previous utility costing method would not reflect this change. Therefore, it is doubly important to do the utility plant synthesis simultaneously in order to account for the tradeoffs between the heat exchanger network and the utility plant.

For example, the problem whose pinch diagram is shown in Figure 5.5 could amplify the effect of incorrect costing further. The problem stream data are given in Table 5.2. The pinch occurs at 160\degree C, and the minimum utility loads are 4.97 MW of hot utility and 2.28 MW of cold utility. Again, this problem is solved for optimum $\Delta T_{\text{min}}$ using the simultaneous method and the previous sequential method with constant utility costs.

For the sequential method, the same data from Colmenares and Seider [1986] are used. Hot utilities are available at 280\degree C, 234\degree C, and 150\degree C in the form of condensing steam. The costs are distributed at $109, $76, and $56 per kw-yr, respectively. (It is assumed that steam at other temperatures can be obtained but since these would be just depressurized steam from one of the three, the cost would be same, i.e. steam at 200\degree costs same as steam at 234\degree.) Cold utility is cooling water available at $6 per kw-yr.
Figure 5.5: Example problem 5-2
Table 5.2: Example Problem 5-2 Stream Data

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kw/C)</th>
<th>$T_s$(°C)</th>
<th>$T_t$(°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>80.</td>
<td>130.</td>
<td>224.</td>
</tr>
<tr>
<td>2</td>
<td>48.</td>
<td>160.</td>
<td>270.</td>
</tr>
<tr>
<td>3</td>
<td>6.2</td>
<td>224.</td>
<td>270.</td>
</tr>
<tr>
<td>4</td>
<td>20.</td>
<td>260.</td>
<td>234.</td>
</tr>
<tr>
<td>5</td>
<td>89.</td>
<td>260.</td>
<td>140.</td>
</tr>
<tr>
<td>6</td>
<td>42.</td>
<td>160.</td>
<td>110.</td>
</tr>
</tbody>
</table>

With the heat exchanger network synthesis alone, using the arbitrary utility levels, the optimum $\Delta T_{min}$ occurs at 5°C. The utilities are supplied at 280°C and at 234°C in the amount of 2.77 MW and 1.8 MW respectively. The resulting utility plant has steam being produced at 280°C from a boiler and at 234°C through a pressure reducer from 280°C steam. The power need of 500 kW is produced from a gas turbine. The reason power is not produced from the 280°C steam expanding through turbine to 234°C steam is that insufficient power is produced by this route. Simply using the gas turbine is more efficient and more economical than having a combined cycle system of steam and gas turbines. The total annualized cost for this heat exchanger network and the utility plant is $2,990,000.

However, for the simultaneous synthesis problem using the new approach, the optimum $\Delta T_{min}$ turns out to be 10°C. The utilities are supplied at 280°C and at 234°C in the amount of 2.53 MW and 2.44 MW respectively. The resulting utility plant has a steam system to supply both the heating and the power demand. This is possible because the $\Delta T_{min}$ selected allowed the steam turbine to be more economical than the gas turbine. In the previous method, the steam turbine system alone could not supply sufficient power, thus resulted in a steam boiler for heating and a gas turbine for power. However by increasing the utility load using larger $\Delta T_{min}$, the steam turbine could replace gas turbine completely. The total annualized cost for this heat exchanger network and the utility plant is $2,510,000.

It is apparent that the selection of correct $\Delta T_{min}$ is very important in finding the lowest cost design. The previous method was prone to err due to arbitrary utility
costing decisions. However, the new method addresses the problem of utility costing correctly by going back one step to incorporate the utility plant synthesis. Therefore, the error due to arbitrary utility costing decision is eliminated which results in a more accurate design and costs which reflect the changes in overall plant.

The only time the previous approach would offer an advantage in terms of the time involved in finding the optimum $\Delta T_{\text{min}}$ would be in the simple heat exchanger retrofit case. The simple retrofit case occurs when the retrofit of heat exchanger network does not affect the utility plant cost structure at all. However, there would be very limited number of cases that involve heat exchanger network retrofit with no structural change to the utility plant. [Gunderson, 1989] Therefore, as shown in the next section the simultaneous synthesis procedure is better in general even for the retrofit case. (The accuracy using the previous approach is not improved for heat exchanger retrofit case since the MILP utility plant synthesis procedure can be formulated to exactly mirror the utility plant costing method that would be used.)

5.2 Retrofit

We will now discuss the application of the new MILP formulation approach to the retrofit of an existing utility plant. Since the cost of building a new plant is very high, retrofitting has become an important problem. Strategies for retrofitting the heat exchanger network by itself has been explored already. [Tjoe and Linnhoff, 1984,1986] [Witherell, 1986] In the present work, a strategy for interfacing the utility plant formulation to a retrofit problem is developed. The MILP formulation strategy developed in the previous chapter can be easily modified to accommodate the retrofit problems.

Furthermore, retrofitting the heat exchanger network without simultaneously retrofitting the utility plant can be a futile exercise in designing. For example, steam usage could be reduced through retrofitting of a heat exchanger network; however, this may reduce power production and require installation of expensive condensing steam turbine or gas turbine resulting in a higher overall cost. In such a case the heat
exchanger network retrofit would have been pointless. [Gunderson, 1989] Therefore, it is quite important that the utility plant be considered together with the heat exchanger network even in the retrofit case. The stream data for the retrofit case would be derived from the existing heat exchanger network minus the utility streams.

Modification of the MILP formulation developed to handle the retrofit case in the previous chapter is fairly simple. First, the existing units in the utility plant are identified. Their binary existence variables are set to 1. However, the binary variables are not included in the total cost objective function since their capital costs are already sunk, i.e. \( CC_i \cdot y_i = 0 \). Furthermore, the capital costs associated with the flowrates are set to zero, i.e. \( CC_i \cdot F_j = 0 \). These variables, \( y_i \)’s and \( F_j \)’s, associated with the existing units would only appear in the constraint equations.

Second, using the method from Chapter 4, heat engine, heat pump, and refrigeration cycle integration is examined along with the utility plant. Basically, new operating conditions and possible new configurations are identified. These are formulated as a MILP problem and then optimized. If the optimized solution is the same as the existing configuration, the utility plant retrofit alone is not necessary. However, retrofit by varying \( \Delta T_{\text{min}} \) needs to be looked at.

Third, by varying the \( \Delta T_{\text{min}} \) for the heat exchanger network, the hot and cold utility demand would be changed. These changes would in turn, affect the utility plant. The utility plant MILP is reformulated with this new information in the same way as the second step. The resulting formulation is optimized. Again, if the optimized solution of the utility plant is the same as the existing configuration, a new \( \Delta T_{\text{min}} \) is used and the process repeated. However, if the optimization with varying \( \Delta T_{\text{min}} \) and utility demand gives a lower cost utility plant design, then the heat exchanger network is retrofitted with the new utility information. If the total cost of the retrofitted utility plant and the heat exchanger network is lower than the existing design, then the new design is implemented. To insure that this new design is the global minimum cost solution, \( \Delta T_{\text{min}} \) is varied further to construct the tradeoff diagram similar to Figure 5.2.
Although the method is brute force trial and error with respect to $\Delta T_{\text{min}}$, this approach offers an advantage in that the design of the heat exchanger network need not be done until it can be determined that the utility plant can utilize the possible savings resulting from the HEN retrofit. The HEN retrofit data are obtained from a simple pinch diagram. (In our work this graphical procedure was implemented in a program) By ensuring the inclusion of the utility plant before the HEN retrofit, the time consuming heat exchanger network design problem need not be done at every $\Delta T_{\text{min}}$ step.

**Result and Discussion**

To test the effectiveness of the method, the same problem as shown in Figure 5.5 is solved again, except this time as a retrofit case. The existing heat exchanger network has a minimum approach temperature of 10°C and minimum heating and cooling load of 4.97 Mw and 2.28 Mw, respectively. The existing utility plant has one high pressure steam boiler operating at 310°C and 77 bar. In addition, there is a steam turbine ejecting at 234°C and 34 bar producing 500 kW of power needed by the process. The total operating cost is $760,000 which is derived from the total annualized cost of $2,510,000 calculated in the previous section minus the capital costs which are assumed to be sunk since this is a retrofit case.

Since it has been already determined in the previous section that there is no better solution at $\Delta T_{\text{min}} = 10^\circ \text{C}$, the only other option is to vary $\Delta T_{\text{min}}$ to get a different utility structure. As $\Delta T_{\text{min}}$ is lowered from 10°C, the minimum utility demand changes and is calculated from the pinch diagram. The MILP formulation of the utility plant is changed to reflect the new utility demand data. In order to ensure adequate power production, gas turbine option is included. In addition, the option of producing excess steam from the steam turbine cycle to meet the power demand is included. This excess steam would be just vented and returned to the boiler.

The resulting total cost data are shown in Figure 5.6. The reason for increase in the total cost as $\Delta T_{\text{min}}$ is decreased is due to the heat exchanger area increase. (In the actual implementation of this procedure, the heat exchanger network area would not
need to be calculated unless the utility plant cost turned out to be lower.) Normally, there would be a corresponding decrease in the utility cost. However, because of the power need, the steam turbine operated at the same condition as before. The utility savings from the heat exchanger network did not show up as savings in the overall cost because of this. The excess steam was simply vented and returned to the boiler.

Other possibilities such as installing a gas turbine or installing a new steam turbine all gave higher total cost. Although this may appear to be counter-intuitive at first, the result is correct if one realizes that the capital cost of the existing units is assumed to be sunk already. Therefore, any option using the existing units will have much lower total cost.

For $\Delta T_{min} > 10^\circ C$, the total cost also increases as shown in Figure 5.6. Although the area of the heat exchanger network would decrease, there is no savings resulting from this since the old heat exchangers could not be sold. Again, the decrease in the heat exchanger areas would not be calculated unless the utility plant gives lower cost design from new $\Delta T_{min}$. The utility cost goes up because the demand increases for higher $\Delta T_{min}$. Therefore, the total cost increases. (Although there is excess power production from the steam turbine, no credit was given toward the total cost since it was assumed that there was no market for the excess power.) Although the cost curve in Figure 5.6 is continuous, this would not be the case always. For example, if the existing boiler could not supply the needed steam, due to the capacity limitation or pressure and temperature limitation, a new boiler would have to brought on-line. The result of this addition would be a discontinuity in the cost curve at a point where the new boiler is activated.

Previous methodology would have redesigned the heat exchanger network for each $\Delta T_{min}$ first, and then expected the utility plant to be redesigned to utilize the savings. However, this procedure often leads to cases where utility plant becomes uneconomical and results in the total cost being higher. Therefore, the heat exchanger design step would have been in vain.

However, with the new strategy of utility plant formulation with rudimentary
Figure 5.6: Retrofit Total Cost Curve
heat exchanger network information the retrofit can be done faster. In addition, the new retrofit procedure has brought into light often neglected design rule of thumb mentioned by Gunderson [1989] that unless the power demand from the process can be reduced at the same time as the hot and cold utility savings generated in the retrofit of the heat exchanger network, the combined retrofit will not result in a lower cost solution. Furthermore, the new strategy offers more thorough retrofit of heat exchanger network since utility levels are also considered as variables unlike the previous retrofit approaches where utility levels were assumed to be fixed.

5.3 Heat Exchanger Network Design

Since the heat exchanger network design problem has been studied extensively, existing methods were used to do this part. For simple heat exchanger network design problems, the heuristic procedure by Linnhoff and Flower [1978]; Linnhoff et al. [1981] were adequate. These procedures were automated into a program and was used to derive the heat exchanger networks used in the example problems.

Since the utility load and levels would have been determined at this point, these utilities can be treated as simple hot streams and cold streams with supply and target temperatures. The hot and cold streams from the process are included in the analysis. These streams are divided into two sections one below the pinch and one above the pinch. (For problems with refrigeration need, a third section is needed according to the rules provided in section 4.4.) To equalize the number of hot and cold streams in each section, deficient streams are split. For example, if there are three cold streams above the pinch and only one hot stream above the pinch, then the hot stream would be split into three streams with heat capacity flow closely matching the cold streams. Heuristics regarding split ratios have been developed by Linnhoff et al. [1982]

Hot and cold streams are then connected until all the streams are used up in the heat exchange. If the pinches or utility load is required, then this implies that initial matches were incorrect. Therefore, other matches are tried until the constraints are met. For small problems up to 10SP1, exhaustive search of all possible combination
are examined to find a minimum unit heat exchanger network. In most cases this was sufficient to find the minimum cost heat exchanger network. However, in some cases heat exchanger may exhibit loops from the stream splits. Since loop-breaking technique could not be programmed, this step was done manually at the end.

However, for more complex problems the mathematical strategy developed by Papoulias and Grossmann [1983b] would be more efficient. Although this method has not been implemented with the procedure developed here, it would be an relatively easy task to do so since both methods are based on the mixed integer linear programming strategy. But the above method does not actually give the heat exchanger network as does the Linnhoff et al. approach. To overcome this problem, Floudas and Grossmann [1986] proposed a superstructure approach to designing of the heat exchanger network. Their method relies on developing heat exchanger network superstructure that encompasses all possible alternatives for a given problem. Since the superstructure is represented mathematically, optimization can be done more efficiently to find the minimum cost heat exchanger network design. Interfacing the method developed here with their method has not been explored.
Notations used in Chapter 5

- $C_{\text{ann}}$: annualized total cost
- $C_{\text{util}}$: $\text{per kw-yr}$ cost of utilities
- $C_{\text{fuel}}$: $\text{per kw-yr}$ cost of kerosine
- $CC_{\text{exchanger}}$: capital cost of heat exchanger
- $CC_i$: capital cost coefficient of unit $i$
- $DP_{\text{yr}}$: depreciation years represented in annualization factor
- $F_i$: flowrate of stream from unit $i$ into unit $j$
- $y_i$: binary existence variable for unit $i$
Chapter 6

Future Work

There are three most likely avenues of future research. First is with the more friendly user interface to allow the design procedure to become an every day design tool. Second is an extension toward incorporating the chemical process plant. Third is flexibility and operability problem.

It is often the criticism of the industrial users about the mathematical approach that the concept is simple enough to understand quickly more so than the heuristics approach; however, the actual implementation of the strategy is much too hard for a typical engineer to be a useful tool in the design. The strategy developed in this research would also run into this implementation barrier. The methodology is very much straight-forward. However, the actual time involved in solving a real problem is much greater than the 2-3 minutes of optimization time mentioned previously. Setting up the problem so that the pinch can be determined is time consuming. Furthermore, identifying the possible utility levels and loads would also take some time. These data have to be then fed to the unit operation optimizer to get the correct operating parameters. Finally, the objective function and the constraint equations have to be written for the problem. This last task is actually very time consuming and often times takes two to three days to complete.

Therefore, to be a useful synthesis tool in an engineering production environment, this methodology needs to be incorporated into a comprehensive computer-aided engineering system, so many of the tasks can be automated. The interconnec-
tion shown in Figure 5.1 which are done manually needs to be done automatically. This would save a lot of time in converting the data from one part of the procedure to be used in another part. In addition, an expert-system-like user interface to implement the level selection procedure, maximum load calculation, appropriate unit selection, and appropriate operating parameter selection would also help in this. Automatic formulation of the MILP problem to be fed into a commercial MILP optimization package would also be needed.

It has been shown in numerous previous research that the simultaneous optimization of the heat exchanger network with the chemical process can result in a large savings to the overall cost. [Gunderson, 1987] Therefore, it seems likely that further savings can be extracted with simultaneous optimization of chemical plant, heat exchanger network, and the utility plant. Future research in this area is needed.

Finally, we have not addressed the important problem regarding the operability of the process. Especially, important is the start-up question. Since the plants designed with the procedures developed here assumed steady state operation, the units in the design are the ones that are needed for steady state operation. However, in the start-up more units that these minimum would be required. There is a tradeoff between the amount of time the plant would be off-spec versus the extra capital cost of having these units to reduce the off-spec time. Furthermore, integrating heat engines and heat pumps with the process might introduce additional operability problems.

In addition, in the problems examined up to now, flexibility has been completely neglected. This omission was possible because the design was always done with the worst case scenario. But the tradeoff between the flexibility and the total cost must be examined in order to ensure that waste of capital doesn’t result from the overemphasis on the flexibility.
REFERENCES


Crozier, R., “Designing near optimum cooling-water system,” Chemical Engineering, pp. 118-127, April 21, 1980


APPENDIX A

Problem 4sp1 cost data are derived as follows.

The \( CPI = \frac{760.8}{788.6} \) is used from the equipment index for 1985 and 1983. [Chemical Engineering, Oct. 1988]

Linnhoff and Hindmarsh [1983] gave a correlation on the cost of the heat exchanger network. This is adjusted with CPI values.

\[
C_{\text{heat exchanger}} = 14,000 + 1,090 (Area)^{0.83}
\]  

(1)

for \( 0 < Area < 300 \text{m}^2 \). Area is calculated from the following equation,

\[
Area = \frac{Q}{\Delta T_{\text{lm}}} \sum \frac{1}{h_i}
\]  

(2)

based on the assumptions: \( h_{\text{stream}} = 1 \text{m}^2\text{oC/kw} \) and \( h_{\text{utility}} = 3 \text{m}^2\text{oC/kw} \)

For utility cost without the utility plant, Colmenares and Seider [1985] data are used. The highest temperature utility cost is same as fuel cost $109.3/kw-yr. The rest are shown below.

- 110°C: $56/kw-yr
- 204°C: $73/kw-yr
- 235°C: $109/kw-yr

To get the cost of steam at temperatures in between the data points, linear approximation with the closest data are used.

Calculation procedure for cost of heat exchanger network using 170°C steam versus 155°C steam is as follows. Heat exchanger costs are estimated from equation (1). The utility cost are estimated from the fuel cost necessary to produce the hot utility at the specified temperature as shown below. We assume that the boiler feed water is provided at 35°C amount of fuel needed is

\[
U_{\text{utility, cost}} = F_{\text{fuel, cost}} \frac{\Delta Q_{\text{hot, min}}}{\Delta H_{\text{condensation}, T}} \times (H_{P, \text{vap}} - H_{\text{water, 35°C}})
\]  

(3)
The following data are used for utility cost for comparison with the Colmenares and Seider derived data.

\[ \text{Fuel cost} = \$109/\text{kw-yr} \]
\[ H_{\text{condensation}, 155^\circ C} = 902 \text{ Btu/lbm} \]
\[ H_{155^\circ C, \text{vap}} = 1183 \text{ Btu/lbm} \]
\[ H_{\text{water}, 35^\circ C} = 70 \text{ Btu/lbm} \]

From these equations, utility at different cost can be estimated. Note that this is only for comparison with other work or for quick and dirty example calculation. For the actual costing, the MILP model of the utility plant has to be optimized.
APPENDIX B

This appendix is divided into two sections, grass-root design case and retrofit case. Heuristics provided here are used with the ones provided in Chapter 2. Although these heuristics are sufficient for small design problems, they only provide a framework on which to build the MILP model for the overall optimization of the problem.

Grass-root Design Case

First determine the power need and the hot and cold utility needs from the pinch diagram.

If the ratio of the amount of hot utility need versus the amount of inter-process heat exchange exceeds 1.7, then the utility plant is built first with only the hot utility needing section, i.e. cold streams that can not be heated with the process hot streams. The reason for this comes from examination of various heat exchanger problems where the heating requirement for cold streams were increased while holding the amount of process to process stream heat exchange constant. It has been found that it costs more to place hot utilities within the process to process stream matches by breaking the hot streams, even if these breaks are at the kinks.

Furthermore, this rule can be applied to a simple power production scheme. The analysis was done assuming maximum efficiency of 37% for a power cycle. The result was that if the power demand expressed as hot utility need (by conversion factor of \( \frac{1}{0.37} \)) and the hot utility need from the pinch analysis is greater than 1.7 times the inter-process heat exchange, a sequential optimization of utility plant and the HRN is adequate.

The hot utility levels are chosen such that the power production is met and at the same time minimum utility temperature is met. The hot utility levels are selected from the kinks on the cold composite curve since there are no hot streams present in the new section. For each kink, maximum allowable heat load is calculated. Higher utility levels are selected from the turbine pressure ratio rule, i.e. \( \frac{P_i}{P_{i+1}} = 0.7 \) Generally accepted correlation for minimum superheating as shown below is used to calculate
the corresponding temperature.

\[ T_{\text{boiler}} = 10 + 0.1545(T_{\text{cond}} - 120) \]  (4)

The corresponding \( T_{\text{condensation}} \) can be calculated from a vapor pressure correlation for a given working fluid. Since \( T_{\text{cond}} \) is the pinch causing temperature and not the \( T_{\text{boiler}} \), it is used in the analysis here. However, \( T_{\text{boiler}} \) would be used in the MILP optimization or the unit operation modelling for enthalpy and entropy calculation purposes.

Although not recommended, it is possible to lower the hot utility temperature by shifting process hot streams. But for this to be even considered, this shifted process hot stream must not divide the utility to process matches. Furthermore, this hot process stream must be used completely in a single match. (This only occurs in very odd shaped pinch diagram problems where a lone hot stream skews the hot composite curve.)

If the ratio is less than 1.7, then the hot utility levels and the process to process stream heat exchange must be examined together. In effect, the hot utility is interspersed within the hot composite curve.

Hot utility levels are chosen from the kinks on the hot composite curve.

Above the pinch, the candidate hot utility temperatures are kinks in the hot composite curve caused by streams entering or leaving the curve and \( T_{\text{cold, max}} + \Delta T_{\text{min}} \).

From this list of candidate temperatures, if \( T_{kink} \geq T_{\text{cold, pinch}} + \Delta T_{\text{min}} \), then \( T_{kink} \) is deleted. In addition, if \( T_{kink} \geq T_{\text{cold, max}} + \Delta T_{\text{min}} \), then \( T_{kink} \) is deleted from the list of candidate temperatures.

In order to reduce the utility temperature further, the next rule is used. If \( Q_{\text{max}, i} < Q_{\text{min}, \text{hot}} \) then the \( T_{\text{util}} \) is lowered until \( Q_{\text{max}} = Q_{\text{min}} \). If kink temperature difference is large, then cold kinks plus \( \Delta T_{\text{min}} \) is used. If that is still large 10 degree heuristic is used. However, if these still represent large temperature differences, the utility level using the 0.7 pressure rule is used.
If $Q$ optimized is less than $Q_{max}$, then $T_i$ is lowered till $Q_i = Q_{max,i}$. If $Q_i = Q_{max}$, then $T_i$ is increased and optimized until $Q_i$ is just less than $Q_{max,i}$.

Although the hot utility should not be placed below the pinch, this is not an absolute rule. Especially, in the case of excess cooling capacity below the pinch, it is ideal to place the hot utility below the pinch rather than above the pinch. Furthermore, if heat pump and heat engine configuration are simultaneously used, it is necessary to include the possibility of hot utilities below the pinch. An example of this was shown in Chapter 4. The temperature levels below the pinch are still same as above the pinch.

However, cold utilities should never be placed above the pinch.

Below the pinch, candidate cold utility temperature are kinks in the cold composite curves plus $T_{hot,min} - \Delta T_{min}$. Same method of candidate elimination and temperature updating is used as in the above the pinch hot utility level selection.

If there are no cold kinks for the cold utilities, the kinks on the hot utilities are used. In such a case the preferred kinks are the ones caused by the streams entering the hot composite curve rather than the kinks caused by exiting streams.

**Retrofit**

First rule with the retrofit design is that the power production must be met. Unless the plant is operating at extremely low efficiency the capital cost of installing a whole new power production and hot utility is rarely justified. (This is the conclusion from the cases that we looked in this research; however, there were a few cases reported in the literature of theoretical studies where such replacement was more economical. But the annualization factor plays an important role in this case, and the 5 year straight line or 10 year discount rate used in this research gives more realistic cost than 10 year straight line method used previously.) Therefore, if power need can not be reduced in the process, there is no point in reducing the low temperature utility load. Although the temperature of the low temperature utility can be lowered to increase power production, the savings is minimal. The cost is paid with the loss of
flexibility and sometimes higher heat exchanger area.

Only time the retrofiting can be economical is if the power demand increases to an extent that the existing system cannot handle the load. In such a case instead of just installing a new unit to meet the incremental demand, retrofit of the whole utility plant to better optimize the operation should be done. The utility levels can now be selected in the same manner as in the grass-root design case.

Furthermore, if power need can be reduced, the first objective should be to shift power production to fewer units. Also, the heating load should be shifted to fewer units. (These are the units in the utility plant and not the heat exchangers.) The new operating conditions should be selected based on the heuristics from grass-root design case.

This result runs counter to many of the previous research which have shown that the hot utility load reduction can save a lot of operating cost. However, these cases were studied without considering the power demand.
APPENDIX C

In this appendix, typical heat exchanger network design problems that have been published in the literature are tabulated. These problems are solved with the new algorithm, and the results are compared to the published ones. The units on the utility load are kW. The hot utility is 235°C steam and 25-50°C cooling water except where noted otherwise.

Table 1: Hot and cold utility result for 4SP1

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>T_s</th>
<th>T_t</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>8.79</td>
<td>160</td>
<td>93</td>
</tr>
<tr>
<td>H2</td>
<td>10.55</td>
<td>249</td>
<td>138</td>
</tr>
<tr>
<td>C1</td>
<td>7.62</td>
<td>60</td>
<td>160</td>
</tr>
<tr>
<td>C2</td>
<td>6.08</td>
<td>116</td>
<td>260</td>
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</table>

<table>
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<th>(\Delta T_{\text{min}})</th>
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<td>249-239</td>
</tr>
<tr>
<td>11^4</td>
<td>133.8</td>
<td>256.2</td>
<td>249-238</td>
</tr>
</tbody>
</table>

1Duran and Grossmann, 1986.
2Papoulias and Grossmann, 1983.
3Grimes et al., 1982.
4Our result.
### Table 2: Hot and cold utility result for 4SP2

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_s$</th>
<th>$T_t$</th>
</tr>
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<tbody>
<tr>
<td>H1</td>
<td>15.83</td>
<td>204</td>
<td>43</td>
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<td>H2</td>
<td>10.55</td>
<td>260</td>
<td>43</td>
</tr>
<tr>
<td>H3</td>
<td>26.38</td>
<td>221</td>
<td>110</td>
</tr>
<tr>
<td>C1</td>
<td>36.96</td>
<td>-4</td>
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</tbody>
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<table>
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<tr>
<th>$\Delta T_{\text{min}}$</th>
<th>$Q_{\text{hot, min}}$</th>
<th>$Q_{\text{cold, min}}$</th>
<th>Pinch (°C)</th>
</tr>
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<tbody>
<tr>
<td>11.11$^1$</td>
<td>336.95</td>
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<td>11.11$^2$</td>
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</tr>
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</table>

$^1$Ponton and Donaldson, 1974.  
$^2$Our result.

### Table 3: Hot and cold utility result for 5SP1

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_s$</th>
<th>$T_t$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>16.61</td>
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<td>121</td>
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<tr>
<td>H2</td>
<td>13.29</td>
<td>204</td>
<td>66</td>
</tr>
<tr>
<td>C1</td>
<td>11.39</td>
<td>38</td>
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<tr>
<td>C2</td>
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<td>13.03</td>
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<th>$Q_{\text{hot, min}}$</th>
<th>$Q_{\text{cold, min}}$</th>
<th>Pinch (°C)</th>
</tr>
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<tbody>
<tr>
<td>11.11$^1$</td>
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<tr>
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<td>875.7</td>
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</table>

$^1$Linnhoff and Flower, 1978.  
$^2$Our result.
Table 4: Hot and cold utility result for 6SP1

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_s$</th>
<th>$T_t$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>14.77</td>
<td>226.7</td>
<td>65.6</td>
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<tr>
<td>H2</td>
<td>12.56</td>
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<td>H3</td>
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<td>198.9</td>
<td>65.6</td>
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<tr>
<td>C1</td>
<td>8.44</td>
<td>221.1</td>
<td>37.8</td>
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<tr>
<td>C2</td>
<td>17.2</td>
<td>176.7</td>
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<td>C3</td>
<td>13.9</td>
<td>204.4</td>
<td>93.3</td>
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<th>$Q_{\text{cold, min}}$</th>
<th>Pinch (°C)</th>
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</table>

$^1$Linnhoff and Flower, 1978.
$^2$Our result.

Table 5: Hot and cold utility result for 6SP2

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_s$</th>
<th>$T_t$</th>
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</thead>
<tbody>
<tr>
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<td>H2</td>
<td>5860.0</td>
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<td>203.9</td>
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<tr>
<td>H3</td>
<td>29.3</td>
<td>177</td>
<td>121</td>
</tr>
<tr>
<td>C1</td>
<td>5860.0</td>
<td>93.3</td>
<td>93.8</td>
</tr>
<tr>
<td>C2</td>
<td>43.95</td>
<td>66</td>
<td>149</td>
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<tr>
<td>C3</td>
<td>58.6</td>
<td>82</td>
<td>121</td>
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</tbody>
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<table>
<thead>
<tr>
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<th>$Q_{\text{hot, min}}$</th>
<th>$Q_{\text{cold, min}}$</th>
<th>Pinch (°C)</th>
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<tbody>
<tr>
<td>11.11$^1$</td>
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<td>11.11$^2$</td>
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<td>none</td>
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</tbody>
</table>

$^1$Grimes et al., 1982.
$^2$Our result.
Table 6: Hot and cold utility result for 7SP1

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>T, °C</th>
<th>Tt, °C</th>
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</thead>
<tbody>
<tr>
<td>H1</td>
<td>14.77</td>
<td>227</td>
<td>66</td>
</tr>
<tr>
<td>H2</td>
<td>12.55</td>
<td>271</td>
<td>149</td>
</tr>
<tr>
<td>H3</td>
<td>17.72</td>
<td>199</td>
<td>66</td>
</tr>
<tr>
<td>C1</td>
<td>8.44</td>
<td>38</td>
<td>221</td>
</tr>
<tr>
<td>C2</td>
<td>17.3</td>
<td>82</td>
<td>177</td>
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<tr>
<td>C3</td>
<td>13.9</td>
<td>93</td>
<td>204</td>
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<td>C4</td>
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<table>
<thead>
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<th>Qc, kW</th>
<th>Pinch, °C</th>
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<tr>
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<td>11.112</td>
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1 Pehler and Liu, 1984.
2 Our result.

Table 7: Hot and cold utility result for 7SP2

<table>
<thead>
<tr>
<th>Stream</th>
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<th>T, °C</th>
<th>Tt, °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>12.53</td>
<td>310</td>
<td>204</td>
</tr>
<tr>
<td>H2</td>
<td>8.32</td>
<td>244</td>
<td>93</td>
</tr>
<tr>
<td>H3</td>
<td>6.96</td>
<td>278</td>
<td>66</td>
</tr>
<tr>
<td>C1</td>
<td>8.44</td>
<td>93</td>
<td>204</td>
</tr>
<tr>
<td>C2</td>
<td>8.44</td>
<td>38</td>
<td>221</td>
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<tr>
<td>C3</td>
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<th>ΔTmin, °C</th>
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<th>Qc, kW</th>
<th>Pinch, °C</th>
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<tr>
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</table>

1 Masso and Rudd, 1969.
2 Our result.
Table 8: Hot and cold utility result for 7SP4

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_s$</th>
<th>$T_t$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>675</td>
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<td>H2</td>
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<td>590</td>
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<td>H3</td>
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<td>C1</td>
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<td>345</td>
</tr>
<tr>
<td>C2</td>
<td>12.0</td>
<td>400</td>
<td>100</td>
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<tr>
<td>C3</td>
<td>125.0</td>
<td>300</td>
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<table>
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<th>$Q_{hot,min}$</th>
<th>$Q_{cold,min}$</th>
<th>Pinch (°C)</th>
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</thead>
<tbody>
<tr>
<td>20$^1$</td>
<td>8390</td>
<td>6617</td>
<td>430-410</td>
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<tr>
<td>20$^2$</td>
<td>8390</td>
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<td>430-410</td>
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</table>

$^1$Papoulias and Grossmann, 1983.
$^2$Our result.

Table 9: Hot and cold utility result for 10SP1

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_s$</th>
<th>$T_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>8.79</td>
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<td>H2</td>
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<td>138</td>
</tr>
<tr>
<td>H3</td>
<td>14.8</td>
<td>227</td>
<td>66</td>
</tr>
<tr>
<td>H4</td>
<td>12.6</td>
<td>271</td>
<td>149</td>
</tr>
<tr>
<td>H5</td>
<td>17.7</td>
<td>199</td>
<td>66</td>
</tr>
<tr>
<td>C1</td>
<td>7.6</td>
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</tr>
<tr>
<td>C2</td>
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<td>116</td>
<td>222</td>
</tr>
<tr>
<td>C3</td>
<td>8.44</td>
<td>38</td>
<td>221</td>
</tr>
<tr>
<td>C4</td>
<td>17.3</td>
<td>82</td>
<td>177</td>
</tr>
<tr>
<td>C5</td>
<td>13.9</td>
<td>93</td>
<td>204</td>
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</tbody>
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<table>
<thead>
<tr>
<th>$\Delta T_{min}$</th>
<th>$Q_{hot,min}$</th>
<th>$Q_{cold,min}$</th>
<th>Pinch (°C)</th>
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<tbody>
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<td>10.00$^2$</td>
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<td>10.00$^3$</td>
<td>0.0</td>
<td>1902</td>
<td>none</td>
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</tbody>
</table>

$^1$Grimes et al. 1982.
$^3$Our result.
Table 10: Hot and cold utility result for Duran and Grossmann (1986) problem

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_s$</th>
<th>$T_t$</th>
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<tbody>
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<td>29.75</td>
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<td>9.24</td>
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<td>176.8</td>
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<tr>
<td>C3</td>
<td>107.7</td>
<td>46.85</td>
<td>129.6</td>
</tr>
</tbody>
</table>

$\Delta T_{\text{min}}$ | $Q_{\text{hot, min}}$ | $Q_{\text{cold, min}}$ | Pinch (°C)
15° | 1684 | 10632 | 110.6-95.5 |
15° | 1685 | 10631 | 110.6-95.5 |

1Duran and Grossmann, 1986.
2Our result.

Table 11: Hot and cold utility result for Floudas et al. (1985) problem

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_s$</th>
<th>$T_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>7.9</td>
<td>357.4</td>
<td>65.7</td>
</tr>
<tr>
<td>H2</td>
<td>5.8</td>
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<td>232.3</td>
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<tr>
<td>H3</td>
<td>2.4</td>
<td>282.3</td>
<td>46.3</td>
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<tr>
<td>H4</td>
<td>31.7</td>
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<td>H5</td>
<td>6.3</td>
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<td>149.5</td>
<td>110.</td>
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<td>C1</td>
<td>24.8</td>
<td>15.7</td>
<td>377.</td>
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</table>

$\Delta T_{\text{min}}$ | $Q_{\text{hot, min}}$ | $Q_{\text{cold, min}}$ | Pinch (°C)
6.38° | 2341 | 1822 | 221.3-214.9 |
6.4°  | 2341 | 1822 | 221.3-214.9 |

1Floudas et al., 1985.
2Our result.

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Table 12: Hot and cold utility result for Tjoe and Linnhoff (1986) problem

<table>
<thead>
<tr>
<th>Stream</th>
<th>CP (kW/°C)</th>
<th>$T_a$</th>
<th>$T_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>0.2</td>
<td>160</td>
<td>30</td>
</tr>
<tr>
<td>H2</td>
<td>1.6</td>
<td>100</td>
<td>90</td>
</tr>
<tr>
<td>H3</td>
<td>1.0</td>
<td>65</td>
<td>40</td>
</tr>
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<td>C1</td>
<td>0.05</td>
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<td>150</td>
</tr>
<tr>
<td>C2</td>
<td>0.8</td>
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<td>75</td>
</tr>
<tr>
<td>C3</td>
<td>0.2</td>
<td>90</td>
<td>150</td>
</tr>
</tbody>
</table>

$\Delta T_{\text{min}}$ | $Q_{\text{hot,min}}$ | $Q_{\text{cold,min}}$ | Pinch (°C) |
<table>
<thead>
<tr>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>10$^1$</td>
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<td>30$^1$</td>
<td>14.5</td>
<td>24</td>
<td>65-35</td>
</tr>
<tr>
<td>10$^2$</td>
<td>3.0</td>
<td>12.5</td>
<td>100-90</td>
</tr>
<tr>
<td>30$^2$</td>
<td>14.5</td>
<td>24</td>
<td>65-35</td>
</tr>
</tbody>
</table>

$^1$Tjoe and Linnhoff, 1986.

$^2$Our result.
The working fluids data from Milora and Tester were used in the simulation and optimization.

Pump Calculation

Assuming constant volume pressurization,
\[ W_{ideal} = \int V \delta P. \]

Real work is calculated by applying mechanical efficiency term.
\[ W_{real} = \frac{W_{ideal}}{\eta} \]

The pump outlet temperature is calculated by an enthalpy balance.
\[ W_{real} = \Delta H = [H(T_{out}, P_{out}) - H(T_{in}, P_{in})] \]

The only unknown term is \( T_{out} \). Since this is a complex function in terms of \( T_{out} \), the Newton-Raphson convergence technique is used.

Turbine Calculation

Pressure ratio on the turbine is 0.7, i.e. \( \frac{P_{out}}{P_{in}} = r^n \) where \( P_{out} \) is the final exhaust pressure, \( P_{in} \) is the turbine inlet pressure, and \( n \) is the number of stages in the turbine.

The following procedure is used to calculate the temperatures around the turbine. (The entropy and enthalpy equations from Appendix E should be used.)

1. determine whether \( P_{in, stage} > P_c \) if so go to step 4
2. Calculate \( T^{sat}, H^V, H^L, S^V, S^L \)
3. Given \( T_{in} \) and \( P_{in} \), calculate \( S(T_{in}, P_{in}) \) and determine liquid fraction.
4. Calculate enthalpy change for constant entropy expansion.
5. determine \( T_{out} \) from \( \Delta H_{real} = \eta_{real} \Delta H_{isentropic} \)
6. repeat steps 3 through 5 until calculation for each stage is complete.
7. Total work output is the sum of each stage \( \Delta H_{real} \)
APPENDIX E

Heat Pump Calculation

The Peng-Robinson equation of state and parameters are used here and also in the previous appendix. The equations were shown in Chapter 3.

The enthalpy and entropy balance equations are derived here. The change in enthalpy from one real state to another real state is represented as a three step process. First, the fluid goes from real to ideal state under constant temperature. Second, the fluid is heated in the ideal state. Third, the fluid goes from a new ideal state to the second real state. This is shown in the following equation.

\[
H(T_2, V_2) - H(T_1, V_1) = [H(T_2, V_2) - H^o(T_2, V_2^o)]
- [H(T_1, V_1) - H^o(T_1, V_1^o)]
+ [H^o(T_2, V_2^o) - H^o(T_1, V_1^o)]
\]

where \(^\circ\) represents an ideal gas state.

The first and the third steps are calculated using the departure function shown below.

Enthalpy Departure Function (from ideal to real):

\[
[H(T, V) - H^o(T, V^o)] =
\left\{ \frac{a}{2\sqrt{b}} \ln \left[ \frac{V + b(1 - \sqrt{2})}{V + b(1 + \sqrt{2})} \right] \right\} \left[ 1 + \frac{aT}{\sqrt{(\alpha TT)}} \right] + (PV - RT)
\]

The second step is calculated using the following equation.

Ideal Enthalpy:

\[
[H^o(T_2, V_2^o) - H^o(T_1, V_1^o)] =
T_c R [C_o(T_{2R} - T_{1R}) + \frac{C_1}{2}(T_{2R}^2 - T_{1R}^2)]
+ \frac{C_2}{3}(T_{2R}^3 - T_{1R}^3) + \frac{C_4}{4}(T_{2R}^4 - T_{1R}^4)]
\]

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where $T_{IR} = \frac{T_2}{T_R}$.

The entropy balance equations are derived in the same manner. The three step division is shown with the following equation.

\begin{equation}
S(T_2, V_2) - S(T_1, V_1) = \left( S(T_2, V_2) - S^o(T_2, V_2^o) \right) \\
- \left( S(T_1, V_1) - S^o(T_1, V_1^o) \right) \\
+ \left( S^o(T_2, V_2^o) - S^o(T_1, V_1^o) \right)
\end{equation}

where $^o$ represents an ideal gas state.

The first and the third terms on the right-hand side are calculated using the entropy departure function shown below.

Entropy Departure Function (from ideal to real):

\begin{equation}
[S(T, V) - S^o(T, V^o)] = -R \ln \left( \frac{V^o}{V-b} \right) + \frac{a}{\sqrt{TTR}} \ln \left( \frac{V+b(1+\sqrt{2})}{V+b(1+\sqrt{2})} \right)
\end{equation}

The ideal entropy change (second step) is calculated with the next equation.

Ideal Entropy:

\begin{equation}
[S^o(T_2, V_2^o) - S^o(T_1, V_1^o)] = S^o(T_2, P_2) - S^o(T_1, P_1) = \\
R[C_\infty \ln \frac{T_2}{T_1} + C_1(T_2 - T_1) + \frac{C_2}{2}(T_2^2 - T_1^2)] \\
+ \frac{C_4}{3}(T_2^3 - T_1^3) - \ln \frac{P_2}{P_1}
\end{equation}

where $T_{IR} = \frac{T_2}{T_R}$. 

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APPENDIX F

Gas Turbine Calculation

Refer to Figure 3.21 for gas turbine configuration.

Following assumptions were made in modelling the gas turbine.

\[ T_3 = 1,100^\circ C \]
\[ T_1 = 25^\circ C \]
\[ P_1 = 1\text{ atm} \]

Compressor isentropic efficiency = 0.85

Turbine isentropic efficiency = 0.85

Combustion Chamber pressure loss = 5%

Heat exchanger pressure loss air-side = 3%

Heat exchanger pressure loss exhaust-side = 4kPa

Heat Exchanger \( \Delta T_{min} = 40^\circ C \)

Exhaust to Air ratio = 1.0137

The cost data are derived with the following procedure and equations. The operating cost is simply the fuel cost; therefore, the total operating cost is the product of fuel flow and fuel cost of \$0.181 per kg of fuel. The capital cost has three components - 1) capital cost of turbine, 2) capital cost of compressor, 3) capital cost of heat exchanger. This is given by the following equation.

\[ C_{cost} = 173,495(W_{out})^{0.424} + 1,925(W_{in})^{0.963} + 1,090(A_{rea})^{0.83} + 14,000 \quad (11) \]

Since the area is proportional to \( W_{out} \) by the following relationships, \( \Delta H_{fuel} = W/\eta \) and \( \Delta H_{fuel} - W = \Delta H_{turbine - T_{exhaust}} \), the area term is given by the following equation.

\[ A_{rea} = \frac{\Delta H_{t-T}}{(U\Delta T_{im})} \quad (12) \]

\[ = W_{out} \ast (1/\eta - 1)/(U\Delta T_{im}) \quad (13) \]
Therefore, the capital cost of gas turbine system is give by the equation below.

\[ C_{st} = 173,495(W_{out})^{0.424} + 274(W_{out})^{0.83} + 1,925(W_{in})^{0.963} + 14,000 \quad (14) \]