

**SIMULTANEOUS OPTIMIZATION OF A CHEMICAL PROCESS,  
ITS HEAT EXCHANGER NETWORK, AND THE UTILITY SYSTEM  
USING A PROCESS SIMULATOR**

by

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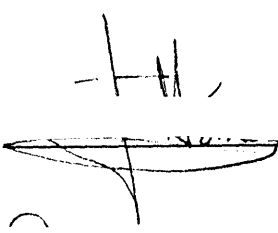
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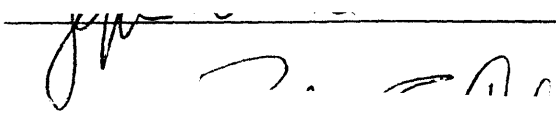
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**Abstract**

The main contribution of this thesis is the development of a strategy for the simultaneous optimization of a chemical process, its heat exchanger network, and the utility system. The simultaneous optimization is accomplished by incorporating the subsystems' heat and work interactions in the optimization. The simultaneous optimization method is developed by analyzing and providing new insights into the heat and work interactions between the subsystems, proposing and developing mathematical models that account for the subsystem's heat and work interactions, and using the developed mathematical models to formulate an optimization problem.

The analysis and the development of new insights into the heat and work interactions between the subsystems leads to the development of mathematical programs that account for the subsystems' heat and work interactions. The expansion of Duran and Grossmann's (1986) pinch location method to not only account for heat integration but also to target for the capital cost of the heat exchanger network (as done in pinch analysis) is identified as a method that accounts for the heat and work interactions between a chemical process and its heat exchanger network. A superstructure for the design and optimization of integrated utility systems is also developed. Although this superstructure accounts for the heat and work interactions between heat exchanger networks and utility systems, it requires solving a large and difficult mixed integer nonlinear program. Therefore, the superstructure is not solved in the thesis. However, the superstructure is used as a guideline to develop a new method that predicts the capital and operating costs of integrated utility systems without their rigorous design.

The simultaneous optimization strategy is obtained by expanding Duran and Grossmann's method (to account for all the heat and work interactions between a chemical process and its heat exchanger network) and combining it with the new method to target for the capital and operating costs of utility systems (to account for the heat and work interactions with the utility system). In this thesis, the simultaneous optimization method is solved with an optimizer contained in a rigorous sequential process simulator. This combines the advantages of current industrial-scale rigorous process simulators, flowsheet optimizers, pinch analysis,

and the new method to target for the capital and operating costs of the utility system without its rigorous design.

Today, process simulators allow rigorous and efficient simulations of even the most complicated chemical processes. Flowsheet optimization strategies presently available in process simulators are typically equivalent to only 3-10 flowsheet simulations (Lang, Biegler and Grossmann, 1988). Since pinch analysis can be used to quickly target for the approximate energy consumption and capital cost of a heat exchanger network without actual design (Linnhoff and Ahmad, 1990), significant savings in computational time can be achieved if this targeting technique is used to expand Duran and Grossmann's method and embedded in the optimization step of a process simulator. Similarly, the new method that targets for the capital and operating costs of the utility system can be embedded in the optimization step of a process simulator. Again, this significantly reduces computation time. The key result is the first tractable method that can simultaneously optimize the decision variables of a complicated real-life chemical process, its heat exchanger network, and the utility system together with parameters for heat and work integration (minimum approach temperatures for the process heat or utility system integration).

The simultaneous optimization method, the sequential approach, and Lang, Biegler, and Grossmann's (1988) method (Duran and Grossmann's method in a process simulator) are used to solve two complete process optimization problems. Since the sequential approach and Lang, Biegler and Grossmann's method fix some of the heat and work interactions between subsystems, they can't simultaneously optimize all decision variables. Some decision variable are either fixed permanently (the supply and target temperatures of the utilities) while other require post-optimization (the parameters for process heat and utility system integration). On the other hand, the simultaneous method requires no iterations in the optimization of all three subsystems' decision variables (because all subsystems' heat and work interactions are included in the optimization). This significantly reduces the total time required to optimize the complete system.

In the atmospheric petroleum crude tower optimization problem process heat integration is very important to obtain low total cost solutions. The sequential approach initially ignores process heat integration. Therefore, it is not surprising that it obtained the solution with the highest total system cost. Lang, Biegler, and Grossmann's method accounts for heat integration and, it obtained a low total cost solution. In this example, both of these methods had multiple solutions. This is attributed to their inability to account for all the subsystems' heat and work interactions.

In the cold end of an ethylene plant optimization problem heat and work integration with the refrigeration system is crucial to obtain solutions with a low total cost. The sequential approach and Lang, Biegler, and Grossmann's method fix the heat and work interactions with the utility system. Their solutions have a much higher total system cost than the solution obtained with the simultaneous method. As in the previous example, the sequential approach has multiple solutions. Again, this is probably due because many subsystems' heat and work interactions are ignored.

In both problems Lang, Biegler, and Grossmann's method had difficulty converging. This occurred because, as a result of ignoring the capital cost of the heat exchanger network in the optimization, their solutions have essentially two pinches. Two near pinches can cause the pinch to change from one iteration to the next and create problems calculating derivatives for the optimization.

The simultaneous optimization method always obtained the lowest total system cost. It had a unique optimum and it required no iterations in the optimization of all the operating conditions. All these advantages are attributed to its ability to account for all the heat and work interactions between a chemical process, its heat exchanger network and the utility system.

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## CHAPTER 1 : INTRODUCTION AND OBJECTIVES

The main objective of this thesis is to develop a method for the total cost optimization of a complete chemical process. A complete chemical process consists of the chemical processing equipment, the heat exchanger network, and the utility system to supply work, steam, cooling water, refrigeration, etc. (Figure 1.1). Unlike process synthesis, process optimization does not involve optimization over the structure of the chemical process, and the utility system is dedicated to the specific process. The goal in total process optimization is to obtain the values of the decision variables of a conceptual complete chemical process that produces required products from given raw materials at minimum total cost while satisfying process constraints and design specifications.

In the past, because the overall problem is so complex, a decomposition approach described by Linnhoff and Townsend (1982) and Douglas (1988) was used to make the optimization tractable. These approaches are sequential and the problem was decomposed into three subproblems and each one was optimized separately. The chemical process steps involving chemical reaction and separation are usually optimized first, followed by the optimization of the heat exchanger network and then the utility system. In order to optimize the chemical process separately from the heat exchanger network and the utility system, the heat and work interactions between the chemical process and the other two subsystems are usually fixed. The heat and work interactions with the utility system are fixed by assuming the number and temperature levels of the utilities present, their unit costs for thermal energy, and the unit cost for supplying work. The heat and work interactions with the heat exchanger network are initially eliminated by assuming all heating and cooling will be done with utilities.

Once the optimization of the nonintegrated chemical process is done, its interactions with the heat exchanger network are now allowed, but fixed, by working with the previously optimized process stream data. In order to optimize the heat exchanger network its heat and

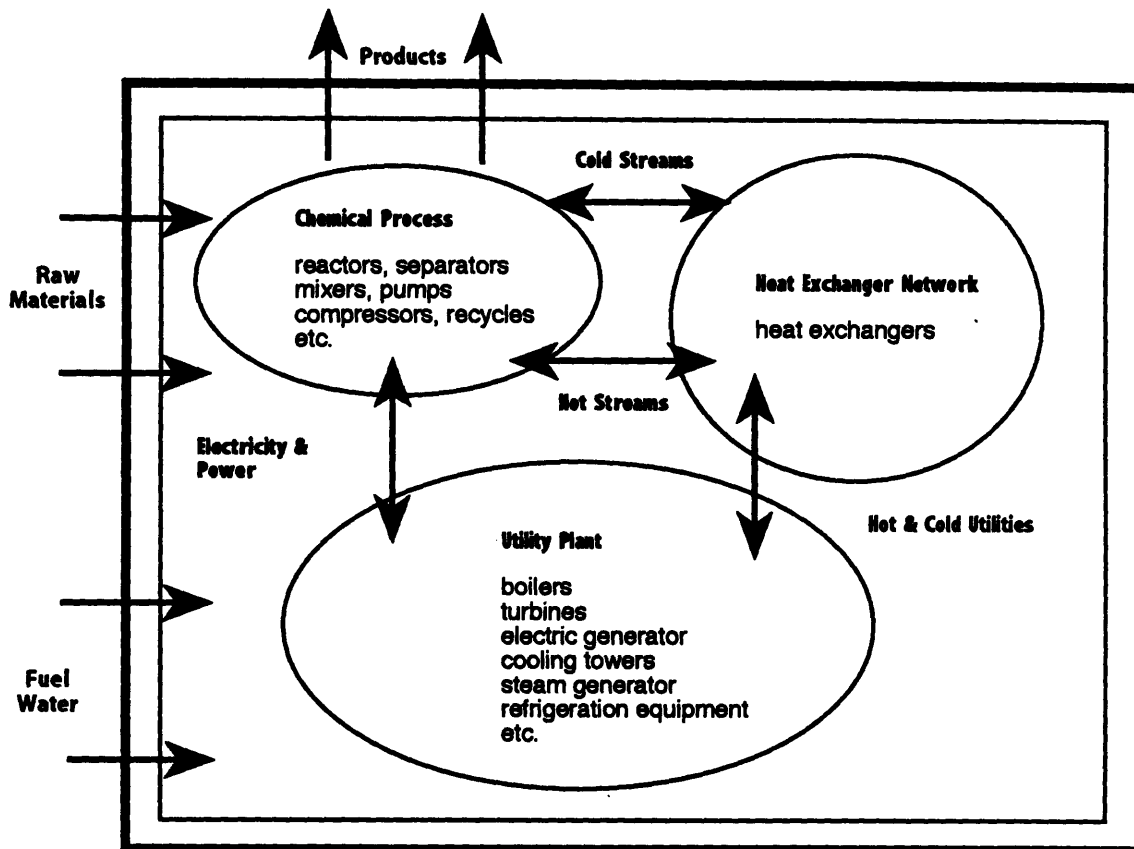


FIGURE 1.1 The heat and work interactions between the chemical process, its heat exchange network, and the utility system. (Yoon, 1990)

work interactions with the utility system must also be specified. This is usually done by using the same utility mix and unit costs for thermal energy. With these assumptions, recent developments in pinch analysis allow the rapid targeting (prediction) and design of a near cost-optimal heat exchanger networks. Linnhoff and Ahmad (1990) showed how heat exchanger networks can be developed that are typically within 5% of their cost target. They also showed that this cost target is a true minimum if all heat transfer coefficients of the process streams are the same, and very close to a true minimum if they differ by less than one order of magnitude. The optimization of the total system is now completed by designing a utility system that provides the work needed by the chemical process as well as the assumed utilities needed by the heat exchanger network.

The main problem with the sequential approach to complete process optimization is that it cannot systematically deal with the significant heat and work interactions that often exist between the three subsystems. Figure 1.1 depicts the heat and work interactions that occur between a chemical process, its heat exchanger network and the utility system. Changes in process operating conditions can lead to stream flow rates and temperatures that can significantly affect the chemistry and the cost of the chemical process, the amount of heat and work integration possible, and the utility requirements for the total system. In general, the sequential approach to complete process optimization cannot properly account for the tradeoffs between capital and operating costs of a chemical process, its heat exchanger network, and the utility system, since it neglects their heat and work interactions.

Iteration is used often between the steps of the sequential approach in order to accommodate these interactions, but there is no suggestion of which order can give the best solution. Pinch targeting methods certainly improve the designers capability to explore heat interactions between chemical processes and heat exchanger networks (Linnhoff et al., 1982).



They can quickly iterate between proposed process changes and the resulting minimum heat exchanger network cost. Linnhoff and Dhole (1989) developed a work targeting method that can sometimes help in quickly discovering some of the heat and work interactions with the utility system. However, the success of this trial-and-error approach depends mostly on the skill of the designer and the experience with the process involved. The results are nearly always suboptimal, or at least there is doubt about optimality.

This thesis presents a strategy for the simultaneous optimization of a chemical process, its heat exchanger network, and the utility system. The simultaneous method incorporates the heat and work interactions between the subsystems in the optimization. The method also exploits the advantages of current industrial-scale rigorous process simulators, flowsheet optimizers, pinch analysis, and a new method to target for the capital and operating costs of the utility system that does not require a rigorous simulation or design of the entire utility system.

Today, process simulators allow rigorous and efficient simulations of even the most complicated chemical processes. Although flowsheet optimization strategies presently available in process simulators cannot guarantee finding the global optimum for nonconvex problems, their computational requirements are typically equivalent to only 3-10 flowsheet simulations (Lang, Biegler and Grossmann, 1988). Since pinch analysis can be used to quickly target for the minimum energy consumption and approximate minimum capital cost of a heat exchanger network without actual design (Linnhoff and Ahmad, 1990), significant savings in computational time can be achieved if this targeting technique is embedded in the optimization step of a process simulator. Similarly, the new method that targets for capital and operating costs of utility systems can be embedded in the optimization step of a process simulator. Again, this significantly reduces computation time. The result is the first method

that can simultaneously optimize the operating conditions of all three subsystems (by including their heat and work interactions) with reasonable computational expense. The specific tasks accomplished to develop the simultaneous optimization method are listed below.

(1) Improved understanding of the heat and work interactions between subsystems. In order to develop the tools necessary for simultaneous flowsheet optimization, the subsystems' heat and work interactions must be well understood. With this, engineers can gain physical insight, offer explanations, and evolve the flowsheets beyond the mathematical optimization techniques proposed.

(2) Develop mathematical programs to account for subsystems' heat and work interactions. Even if the interactions are well understood it would be an arduous task, if not an impossible one, to optimize a flowsheet without mathematical programs.

(3) Implement the developed mathematical programs in a rigorous sequential modular process simulator. If the operating conditions of the chemical process, its heat exchanger network and the utility system are going to be simultaneously optimized by taking into account their heat and work interactions, it can be done so rigorously. Today's sequential modular process simulators can rigorously and efficiently simulate even the most complicated chemical processes. They also usually contain a number of flowsheet optimization strategies that allow them to tackle a variety of flowsheet optimization problems (Lang, Biegler and Grossmann, 1988).

The thesis concludes by presenting the advantages of the simultaneous method over previously used methods (sequential approach and Lang, Biegler, and Grossmann's method) with flowsheet optimization examples. An atmospheric petroleum crude tower and the cold end of an ethylene plant are the complete process optimization example problems presented.

## **CHAPTER 2 : LITERATURE REVIEW**

The steps where the chemical engineer chooses the unit operations and their interconnections to create a process flowsheet is usually referred to as process synthesis. The goal of process synthesis is to choose the structure and operating conditions of a complete chemical process that produces the required products from given raw materials at minimum cost while satisfying process constraints and design specifications. The specific tasks in process synthesis include selecting the chemical reactions pathways, designing the reactor network, separation sequence, heat exchanger network, and utility system. Since the overall problem is typically very complex, a decomposition approach described by Linnhoff and Townsend (1982) and Douglas (1988) has been used. In these sequential approaches, the overall problem is broken into subproblems and each subproblem is solved separately.

Optimization usually refers to the step in process synthesis where the total system cost is reduced by manipulation of operating conditions once the structure of the complete chemical process is selected. The optimization method presented in this thesis targets for the capital and operating costs of the heat exchanger network and the utility system without actually designing them. Therefore, optimization is performed without the selection of a rigorous structure for the complete system. In this context, synthesis and optimization have become harder to distinguish. Ideally synthesis and optimization of complete chemical processes would be done simultaneously. The literature review that follows is of both synthesis and optimization of complete chemical processes.

### **2.1 Synthesis and Optimization of Chemical Processes**

Historically, process synthesis has been done using heuristics. The heuristic approach has found success in reducing the vast number of structures that a chemical process could have to produce a given set of products. Heuristics for the synthesis of reaction pathways, reactor

networks, and separation sequences have been reviewed by Westerberg (1980) and by Nishida, Stephanopoulos and Westerberg (1981). Artificial intelligence techniques have been used in programs such as AIDES (Sirola et al., 1971) and BALTAZAR (Motard et al., 1978) to implement some of these heuristics. Recently, Douglas (1988) has organized these heuristics into a somewhat more systematic procedure for process synthesis. A major problem in utilizing heuristics is that, since they represent general observations, the optimal solution cannot be guaranteed.

In order to synthesize and optimize the chemical process independently from the heat exchanger network and the utility system, the heat and work interactions between the chemical process and the other two subsystems are fixed. This is usually done by assuming the number and temperature level of the utilities present and assigning them unit costs for thermal energy. The cost of providing work is usually also needed. These costs can vary widely depending on the heat and work interaction between the chemical process, the heat exchanger network, and the utility system. Assigning the same cost to utilities and work for all structures and types of chemical processes is clearly incorrect. Nevertheless, with these assumptions and the correlations for the capital costs of unit operations, the optimization of a chemical process can be attempted while still incorporating the gross effects of heat and work interactions between subsystems. Once the optimization procedure is understood at this level, these assumptions can be removed to fine-tune the results.

The limitations of heuristics in process synthesis and optimization has led to an alternative mathematical programming approach by Santibanez and Grossmann (1980) and Papoulias and Grossmann (1983c). In their methods, a nonlinear nonconvex optimization problem is linearized by assuming operating conditions, with the interconnections between units determined numerically. All units that might be present in the process must be included in the model which takes on the framework of a superstructure (Santibanez and Grossmann, 1980). A key problem with the mixed integer linear program (MILP) superstructure approach for chemical processes is the large number of structural alternatives required. In addition, to

perform the linearization of nonlinear processes, operating conditions must be assumed; this effectively reduces the method to one of comparing many, many alternatives rather than generating new structures in the synthesis.

Once different structures have been evaluated, either by the heuristic methods or by mathematical techniques, the most promising alternatives are optimized further. For example, if enough is known about the process, this optimization could be carried out in a process simulator. An advantage of rigorous sequential modular process simulators over nonlinear equation solvers is that a number of optimization methods are usually readily available to tackle a variety of optimization problems. The successive quadratic programming (SQP) algorithm (Biegler and Cuthrell, 1985), the simultaneous modular approach (Chen and Stadtherr, 1985), and the inside-out strategy (Jiraphongpan et al., 1980) are some of the flowsheet optimization strategies that could be used. The lowest total cost option is selected as the optimized process.

## 2.2 Synthesis and Optimization of Heat Exchanger Networks

The heat integration problem was stated by Masso and Rudd (1969) as :

*"Given a set of process streams:  $N_H$  hot streams to be cooled from supply temperature  $T_i^{\text{in}}$  ( $i = 1, 2, \dots, N_H$ ) to target temperature  $T_i^{\text{out}}$  ( $i = 1, 2, \dots, N_H$ ) and  $N_C$  cold streams to be heated from supply temperature  $t_j^{\text{in}}$  ( $j = 1, 2, \dots, N_C$ ) to target temperature  $t_j^{\text{out}}$  ( $j = 1, 2, \dots, N_C$ ) and the accompanying mass-heat capacity flow rate  $F_i C_i$  for hot streams and  $f_j c_j$  for cold streams, determine the structure of the heat exchanger network to achieve the above temperature change at minimum total cost. "*

The heat exchanger network provides opportunities for savings in total cost by matching process streams to partially recover heat instead of using utilities to provide all the heating and cooling demands of the process streams. Initially, the problem was transformed into a mathematical model and solved numerically. Hwa (1965), Kesler and Parker (1969), and Kobayashi, Umeda, and Ichikawa (1971) are some of the researchers who transformed the problem into an assignment linear program (LP). The tree search method was first tried by

Lee et al. (1970) and later by other researchers including Menzies and Johnson (1972), and Rathore and Powers (1975). At the same time, some methods that include heuristics and mathematics were presented by Masso and Rudd (1969) and Ponton and Donaldson (1974). The simplifications needed for the above models coupled with the combinatorial nature of the problem led to only moderate success in solving the heat integration problem (Gundersen and Naess, 1987).

Hohmann (1971) formulated a thermodynamic approach where minimum utilities targets were determined ahead of design. He also discussed the tradeoffs among network area, energy consumption, and the number of heat exchangers. Hohmann's work contributed little to the mathematical approach but his understanding of the problem led not only to a better solution to the heat integration problem but also to a better understanding of the complete process synthesis and optimization problem.

Hohmann's work was popularized and substantially extended by Linnhoff and coworkers (Linnhoff and Flower, 1978; Linnhoff et al., 1982; Linnhoff and Hindmarsh, 1983). In their work, they identify the pinch as the bottleneck in energy recovery and they divide the heat exchanger network design at the pinch. The design of the network is based on thermodynamic targets and design rules to achieve these targets. This method is now known as the pinch design method.

The pinch concept can be explained with the composite curves, first used by Huang and Elshout (1976). The hot streams are merged into a composite heat source curve (the overall heat rejection profile for the process) and the cold streams into a composite heat sink curve (the overall heat demand profile for the process), Figure 2.1. The enthalpy position of the composite curves is a relative measure, so in a temperature-enthalpy diagram their horizontal position is not fixed. The curves can then be brought together until some specified minimum

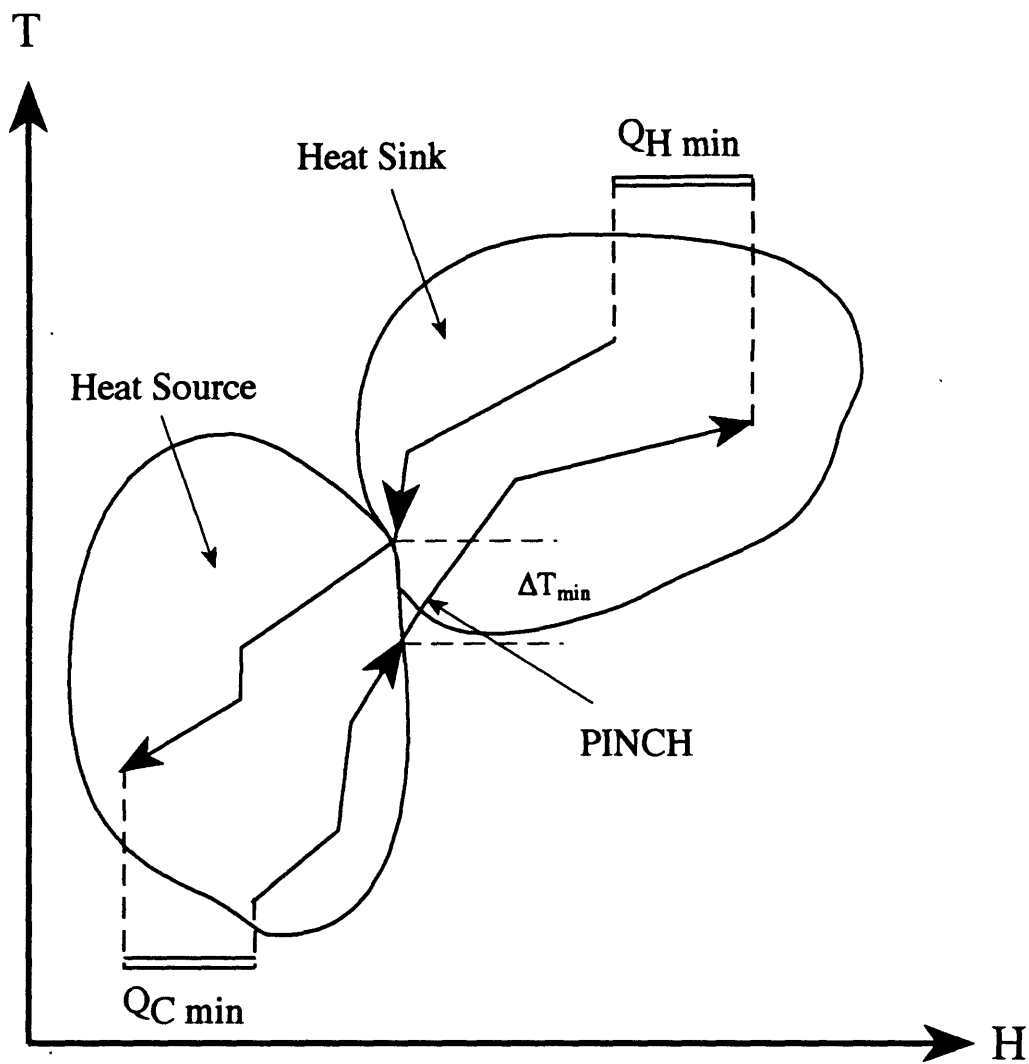


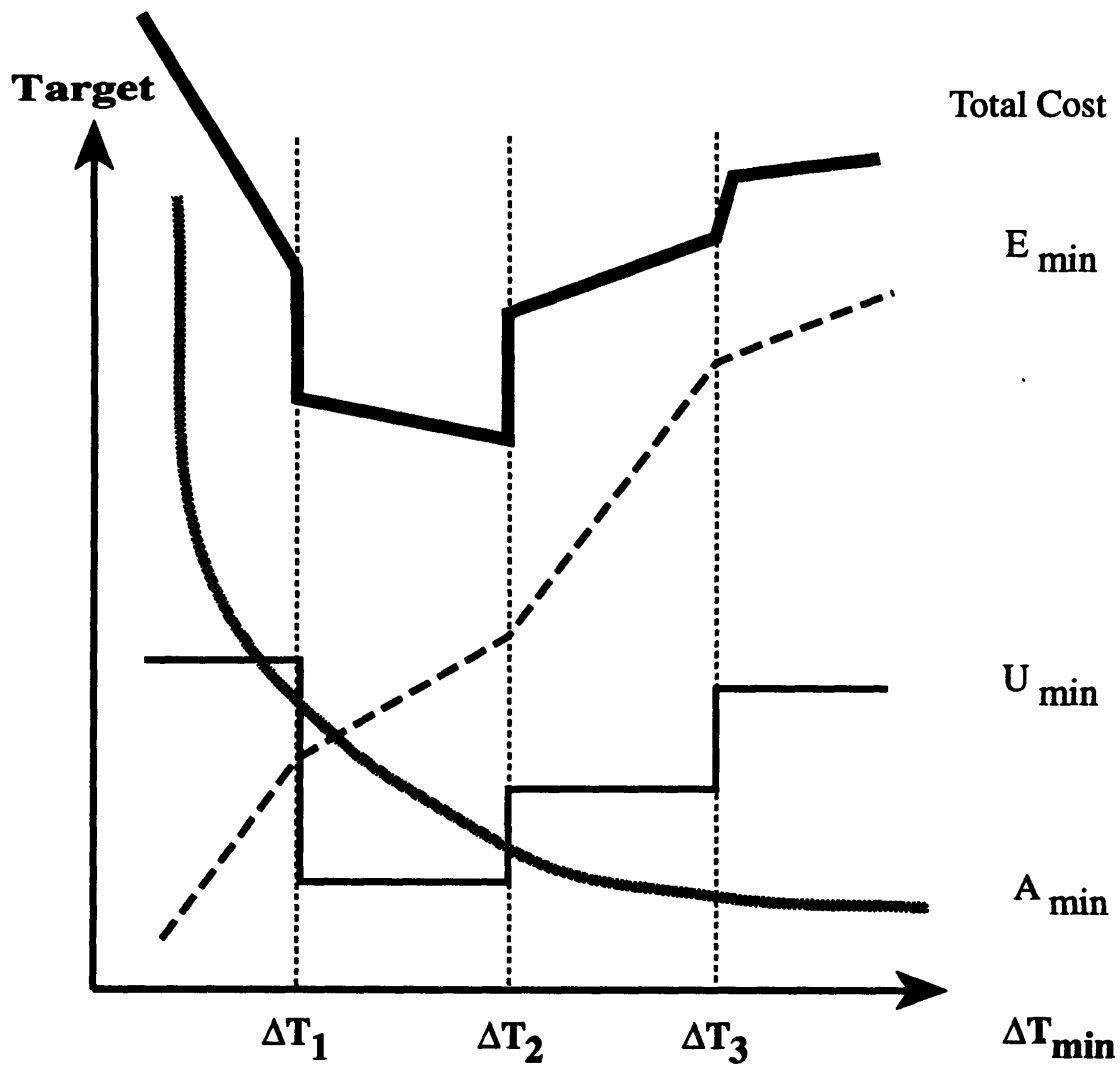
FIGURE 2.1 Illustration of the hot and cold composite curves. (Linnhoff et. al., 1982)



approach temperature is reached and the utility targets can be read directly from the diagram. The points where the two curves are offset by the minimum approach temperature is called the pinch.

The pinch design method has evolved further. Townsend and Linnhoff (1984) developed a simple but approximate method to target for the network's minimum heat transfer area ( $A_{\min}$ ). Ahmad and Linnhoff (1984) combined targets for maximum energy recovery, minimum network heat transfer area ( $A_{\min}$ ), and minimum number of heat exchanger units for maximum energy recovery ( $U_{\min-MER}$ ) to predict the heat exchanger network total cost ahead of design. Their cost targeting method predicts the optimal minimum approach temperature for process heat exchange ( $\Delta T_{\min}$ ) before design. Provided the associated costs of the available utilities are known, the  $\Delta T_{\min}$  obtained in this fashion provides the appropriate tradeoff between the capital cost of the network and its energy consumption. The cost targeting technique is depicted in Figure 2.2. A key finding here is that for a given problem, the discontinuities in the energy, area, and units targets occur at the same values of  $\Delta T_{\min}$ . This is because the discontinuities are caused by the kinks (changes in slope) on the composite curves.

Gundersen and Grossmann (1990) showed that a  $\Delta T_{\min}$  pre-optimization constrains the design of the heat exchanger network. Yee and Grossmann (1990) proposed a mixed integer nonlinear programming (MINLP) superstructure approach for the design of heat exchanger network. In general, this method obtains lower total cost than the pinch design method. Unfortunately, since an MINLP is computationally very expensive, only small problems can be solved. Since, in the pinch design method the  $\Delta T_{\min}$  optimization is done at the targeting stage (not at the design stage) and the  $\Delta T_{\min}$  is allowed to evolve, the optimization results are usually close to the global optimum. In fact, Linnhoff and Ahmad (1990) showed how networks can be developed which are typically within 5% of their cost target.



$E_{min}$  = annualized cost target for minimum energy consumption

$U_{min}$  = annualized cost target for minimum number of units for maximum energy recovery

$A_{min}$  = annualized cost target for minimum heat transfer area

FIGURE 2.2 The components in the cost targeting method for the heat exchange network versus  $\Delta T_{min}$ . (Ahmad and Linnhoff, 1984)

For the design of near-minimum area networks Linnhoff and Vredeveld (1984) introduced the driving force plot. Thereafter, Ahmad (1985) suggested the remaining problem analysis to make sure each exchanger placed in the network is consistent with the total cost target. Figure 2.3 from Ahmad (1985) shows schematically how to apply the pinch design method with such enhancements.

Other factors like forbidden matches and preferred matches have been considered by Cerda and Westerberg (1983) and Papoulias and Grossmann (1983b) and other non-idealities by Viswanathan and Evans (1987). Flexibility and operability have been examined by Calandranis and Stephanopoulos (1985) and by Kotjabasakis and Linnhoff (1987). Sama (1992) explored a second law approach for the design of heat exchanger networks. A good review for design of cost optimal heat exchanger networks is given by Gundersen and Naess (1987).

### **2.3 Synthesis and Optimization of Utility Systems**

The purpose of the utility system is to provide the work and heating and cooling requirements of the chemical process and its associated heat exchanger network. The utility system consists of fired and/or waste heat boilers, different types of turbines, electric motors and generators, compressors and refrigeration equipment, cooling towers, and other auxiliary equipment. The utility system synthesis problem consists of choosing the structure and operating conditions of the utility system such that the demands of the chemical process and the heat exchanger network are met at a minimum total cost (capital and operating).

The synthesis of a utility system could be accomplished by connecting the most efficient units into a network. However, it was recognized (Nishio and Johnson, 1979) that a lower cost design could be achieved through the combination of some less efficient units. For example, a gas turbine might be the most efficient way to produce work and a steam boiler the most efficient way to produce steam; but if a steam boiler is connected to a steam turbine, work and heating demands could be met at a lower cost.

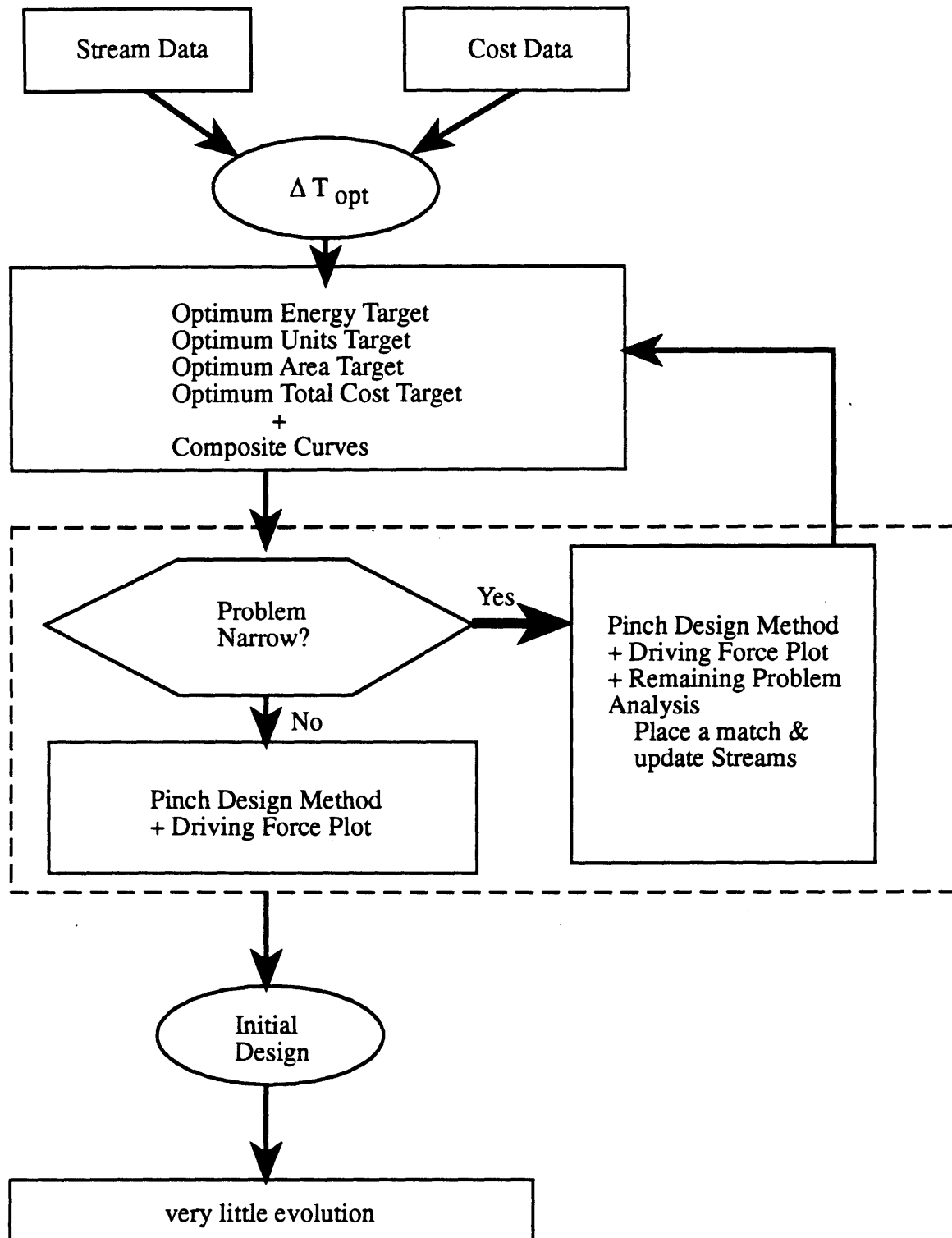


FIGURE 2.3 The pinch design method with the driving force plot and the remaining problem analysis. (Ahmad, 1985)

To account for the heat and work interaction, Nishio and Johnson (1979) and Petroulas and Reklaitis (1984) applied mathematical programming techniques. Their methods were designed only to minimize energy costs, treated as operating costs, and not to optimize the general synthesis of the utility network. Their reasoning was that in utility systems the operating costs are usually dominant. Papoulias and Grossmann (1983a) developed an MILP method to synthesize utility systems. In MILP binary variables can be used to represent the existence or absence of units and/or operating conditions, thereby permitting the development of a superstructure. Provided the superstructure contains all feasible combinations, the MILP method can be used to simultaneously synthesize and optimize utility systems. Since the number of possible units in a utility system is not as great as in a chemical process, the MILP approach can be a powerful tool when combined with insight to select the operating conditions needed for linearization. Nath and Holiday (1985) at Union Carbide also developed a strategy to optimize utility systems based on an MILP model but their model only minimized operating cost. None of the above methods considers the refrigeration section of the utility system. Up to now, the above and below ambient sections of utility systems have been treated as separate systems.

Procedures for optimizing refrigeration systems have been reported in academic and industrial literature. Barnes and King (1974) developed a two-stage approach for the optimization of cascade refrigeration systems. The first stage uses heuristics and graph decomposition principles to identify promising configurations and design parameters. Dynamic programming is then used to obtain the minimum cost alternative. This method relies heavily on heuristics. Industrial literature tends to be problem specific. Mehra (1979,1982) developed charts for evaluating work requirements for propylene and ethylene refrigeration systems. Piccotti (1979) has an optimization procedure for the ethylene plant refrigeration system.

## **2.4 Subsystem Heat and Work Interactions**

The sequential approach to process optimization decouples the complete problem, and formulates strategies to solve each subproblem. Consequently, the overall solution, which is the sum of three solutions, may be far from the global optimum. Combining the most efficient options of each subproblem, in general, does not lead to the overall best solution. In order to improve the overall solution, researchers have developed methods that incorporate some of the heat and work interactions between the subsystems.

### **2.4.1 Chemical Process and Heat Recovery Network Heat and Work Interactions**

The chemical process and the heat exchanger network interact through the hot and cold streams that require heat exchange to reach their target temperatures. In the chemical process optimization step of the sequential approach it is assumed that all cold streams will require hot utilities and all the hot streams will require cold utilities to reach their target temperatures. Therefore, increasing the load or temperature level of a hot stream or increasing the load or decreasing the temperature level of a cold stream can only lead to higher utility requirements or the use of more expensive utilities. When the chemical process and the heat exchanger network are considered simultaneously, the process changes that increase utility demand are different than when they are considered sequentially.

Linnhoff and Vredeveld (1984) noticed that by changing pressures of process streams a hot stream could be moved from below the pinch to above the pinch. This will reduce both the overall heating and cooling duties required. Wilcox (1985) developed heuristics to account for this observation. His heuristics only deal with pressure changes. Linnhoff and Vredeveld (1984) also developed the plus/minus rules which demonstrate qualitatively that incremental costs of heating or cooling process streams are not always positive and constant; in fact, for

some process streams, it's negative. The plus/minus rules suggest process changes that decrease utility consumption. These rules incorporate pressure changes and will be discussed later.

The main problem with the process changes proposed by the plus/minus rules is that they are guided only in terms of reducing total utility consumption. The effects on the capital cost of the heat exchanger network, the chemical process's chemistry and costs, and the utility system's performance and costs are considered only after the process changes are made. Indeed, Linnhoff, Smith, and Williams (1990) have shown examples where the plus/minus rules lead to process changes that increase the total system cost.

In order to better account for the heat interaction between the chemical process and the heat exchanger network, Duran and Grossmann (1986) developed a mathematical strategy for the simultaneous optimization of the chemical process with heat integration. In their approach the flowrates as well as the supply and target temperatures of the process streams are treated as decision variables. Their pinch location method calculates the pinch and minimum utilities required at each step in the optimization. Unfortunately, since the capital cost of the heat exchanger network is not included in the optimization, the heat integration is constrained to satisfy a specified minimum approach temperature for process heat integration ( $\Delta T_{\min}$ ). Lang, Biegler and Grossmann (1988) implemented this procedure, but using a process simulator. Current process simulators are able to efficiently and rigorously model complicated chemical processes.

Yee, Grossmann and Kravanja (1990) proposed an MINLP superstructure approach for the design of heat exchanger networks that could be solved together with the chemical process equations. Since their model is not based on pinch analysis, it does not require a fixed  $\Delta T_{\min}$ . The capital cost of the heat exchanger network is obtained from the network design solution obtained for the MINLP. Unfortunately, since an MINLP is computationally expensive, only small problems with simplifications (in material and/or energy balances and in calculation of

physical properties) can be solved. The largest problem Yee, Grossmann and Kravanja solved had only fifty-five binary variables. Yee, Grossmann and Kravanja's (1990) method, Duran and Grossmann's (1986) method, and Lang, Biegler and Grossmann's (1988) method all fix the heat and work interactions with the utility system, by assuming the number and temperature levels of the utilities present and their unit costs for thermal energy. The cost of providing work is also assumed.

#### **2.4.2 Heat Recovery Network and Utility System Heat and Work Interactions**

The heat recovery network and the utility system interact through the hot and cold utilities produced by the utility system to satisfy the heat exchanger network thermal demands. These demands can be satisfied by any number of utilities at many different temperature levels. The utility system's production or consumption of work depends on the number of utilities and their temperature levels it provides. In the sequential approach to process synthesis and optimization, the demands of the heat exchanger network are lumped into an arbitrary number of temperature levels (eg. high, medium, and low temperature steam or refrigeration levels) and the utility system is designed to satisfy these demands. This fixes some of the heat and work interactions between the heat exchanger network and the utility system. When solving the problem simultaneously, the number of utilities and their temperature levels should be treated as variables to be optimized.

Papoulias and Grossmann (1983c) used an MILP for both the heat exchanger network and the utility system and claimed that it solved the problem simultaneously. In their approach they still lumped utility demands into arbitrary groups, therefore ignoring important heat and work interactions between both subsystems. They only discussed the above ambient section of the utility system (no refrigeration). Townsend and Linnhoff (1983a,b) developed the appropriate placement rules for heat engines and heat pumps and showed graphically how heat and work interplay. They also used the grand composite curve to better understand this heat and work interaction in any given chemical process.



Townsend and Linnhoff's appropriate placement rules can be explained with the composite curves. The composite curves divide the process into a heat sink in need of hot utilities above the pinch and a heat source in need of cold utilities below the pinch (Figure 2.1). A heat engine, shown in Figure 2.4, takes  $Q_1$  units of heat from a heat source, produces work ( $W=Q_1-Q_2$ ), and rejects  $Q_2$  units of heat to a heat sink at a lower temperature. For a heat engine to be appropriately placed it must be placed completely above the pinch or completely below the pinch. To see this, Figure 2.5 shows what happens if a heat engine is placed across the pinch. The engine takes  $Q_1$  units of heat, produces  $W$  units of work, and rejects  $Q_1-W$  units of heat to the process sink below the pinch where it will have to be removed, in addition to the process cooling requirements (B), by cooling water. This is a waste of capital and energy. Capital, because additional equipment is required to transfer the rejected heat, and energy, because better efficiencies could be obtained in the transformation of heat into work by rejecting heat at a lower temperature (ambient temperature).

Figure 2.6 shows the correctly placed heat engines. Above the pinch the engine rejects  $Q_1-W$  units of heat to the process heat sink so the amount of hot utility needed is reduced by  $Q_1-W$ . Overall it takes an extra  $W$  units of heat to produce  $W$  units of work. Effectively, complete conversion of heat into work is achieved by the system as a whole. Below the pinch complete conversion of heat into work can also be achieved by extracting  $Q_2$  units heat from the process heat source. Although complete conversion of heat into work can be achieved by a system containing an appropriately placed heat engine, the heat extracted from the heat source still undergoes a loss in availability (work producing potential). In summary, heat engines should be placed such that they either reject heat into the process heat sink (above the pinch) or extract heat from the process heat source (below the pinch).

The appropriate placement of heat pumps can also be explained with the process heat source and heat sink concept. A heat pump, shown in Figure 2.7, takes  $Q_1$  units of heat from a heat source, uses  $W$  units of work, and rejects  $Q_1+W$  units of heat into a heat sink at a higher temperature. The appropriate placement of a heat pump is across the pinch. Figure 2.8

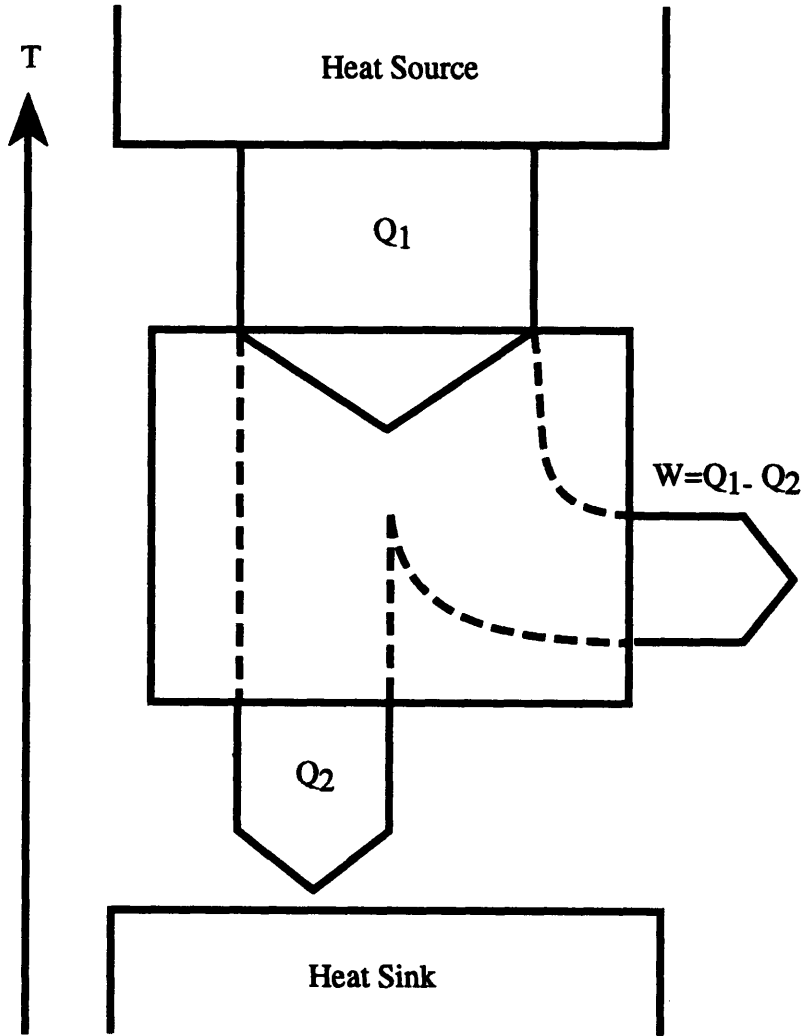


FIGURE 2.4 Illustration of a heat engine model. (Townsend and Linnhoff, 1983a)

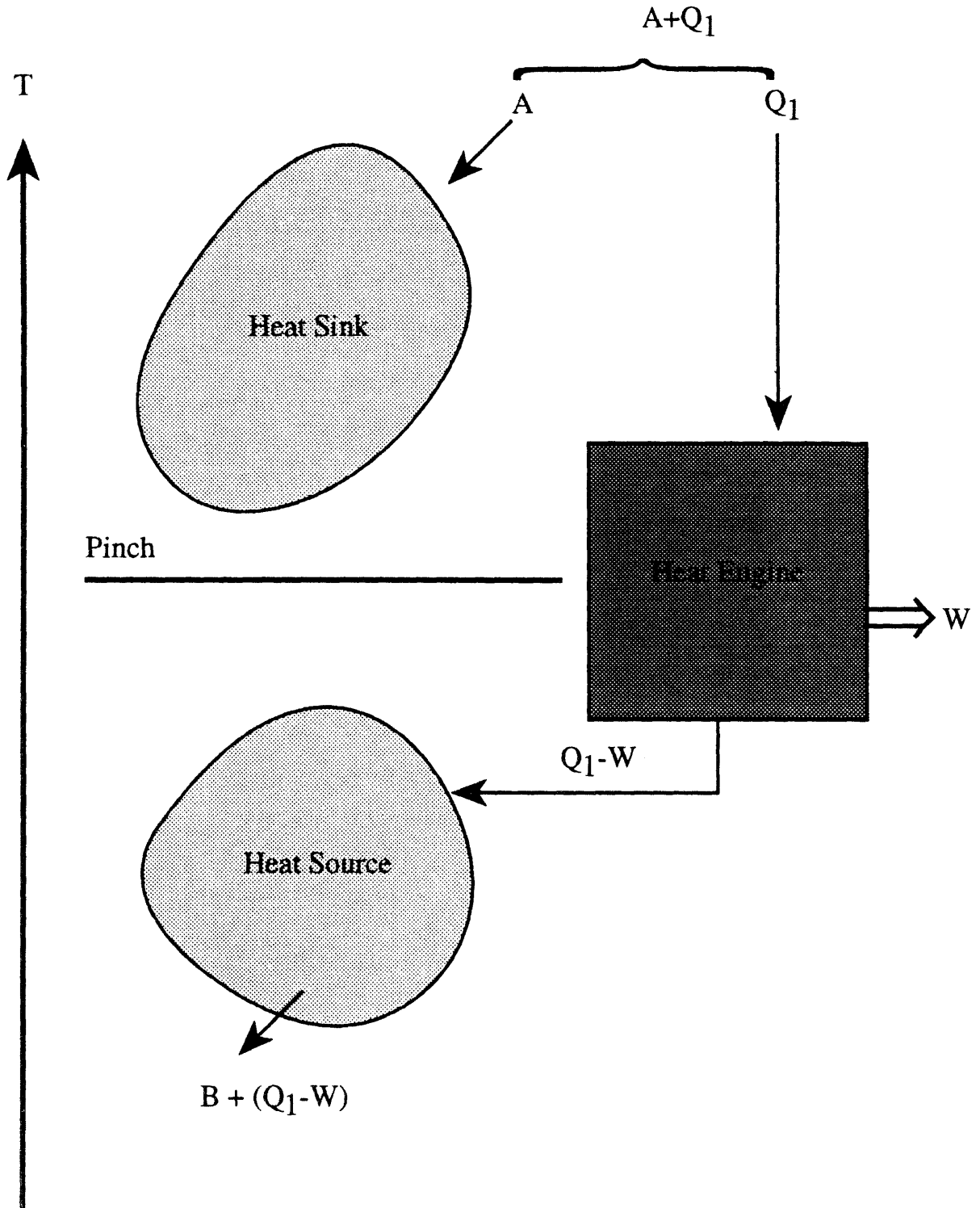


FIGURE 2.5 Diagram of an incorrectly placed heat engine. (Townsend and Linnhoff, 1983a)

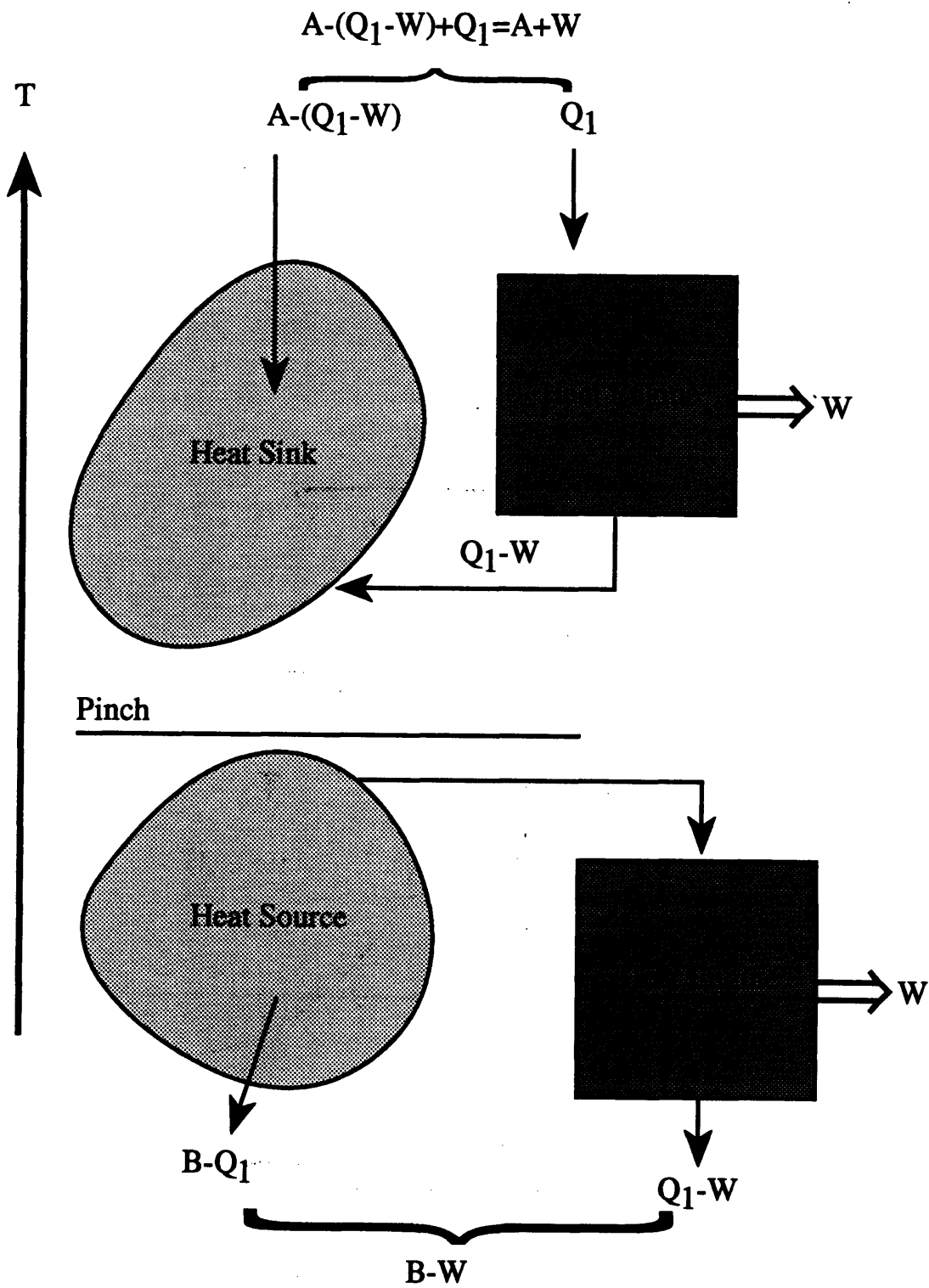


FIGURE 2.6 Diagram of correctly placed heat engines. (Townsend and Linnhoff, 1983a)

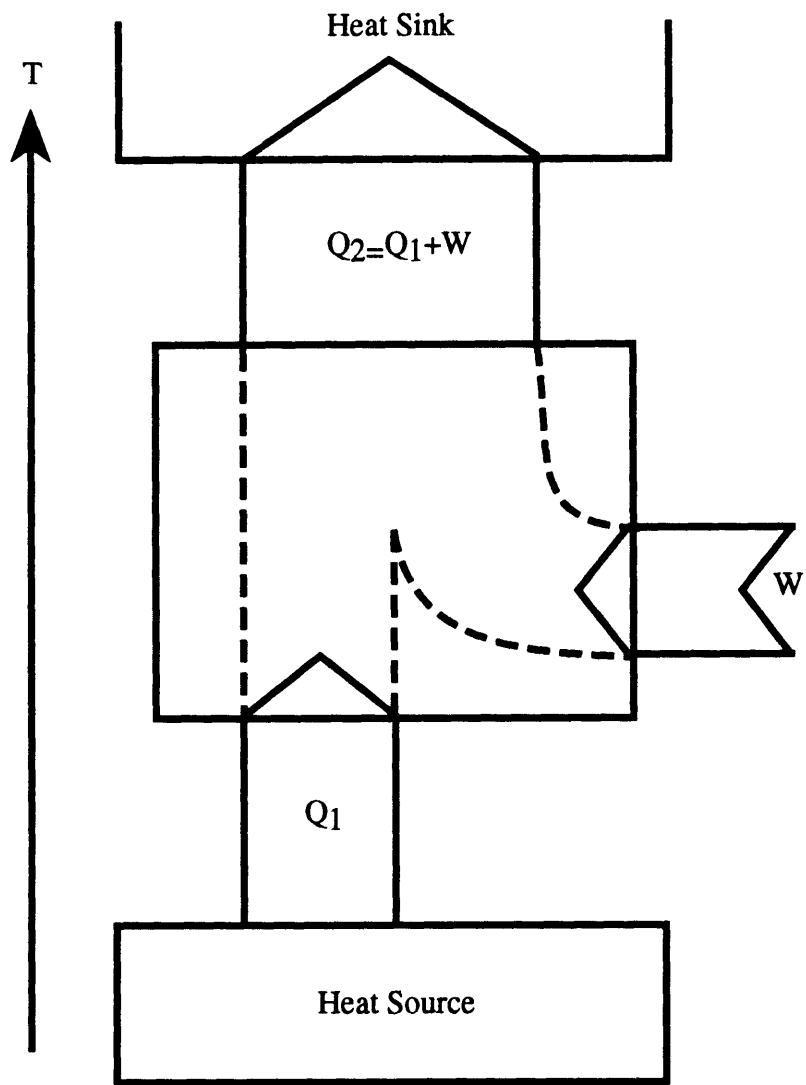


FIGURE 2.7 Illustration of a heat pump model. (Townsend and Linnhoff, 1983a)

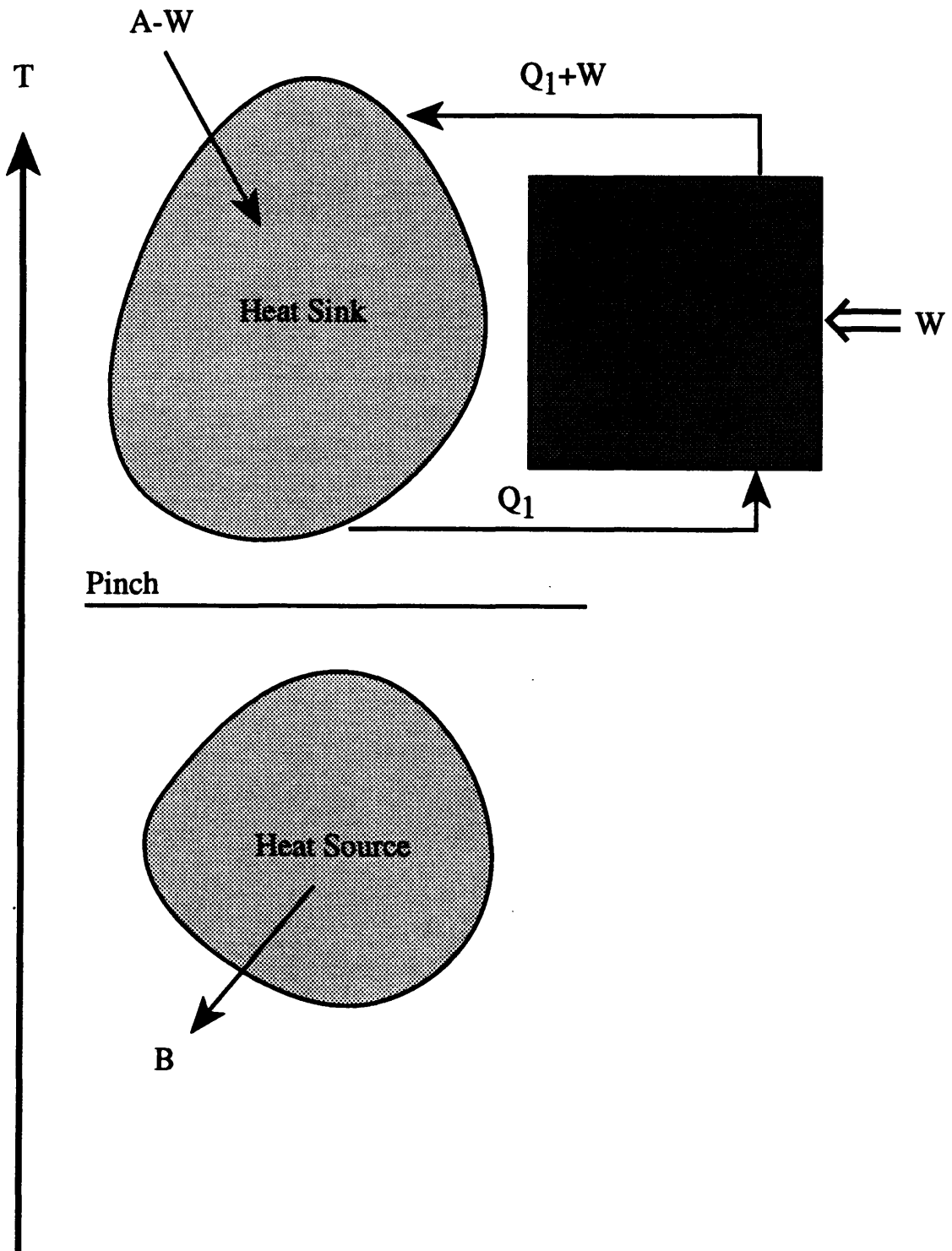


FIGURE 2.8 Diagram of an incorrectly placed heat pump. (Townsend and Linnhoff, 1983a)

shows what happens if a heat pump is placed above the pinch. It removes  $Q_1$  units of heat from the process above the pinch (making the process heat sink bigger) and rejects  $Q_1+W$  units of heat back into the process above the pinch (now making process heat sink smaller). The hot utility demand is reduced by  $W$ , but  $W$  units of work are needed to operate the pump. No net energy is saved and work is converted to heat. If the heat pump is placed entirely below the pinch,  $W$  units of work are again converted to heat. This heat is ultimately rejected into the process heat source, making the heat source larger and increasing the cold utility demand by amount  $W$ ; essentially, work is transformed into cooling water.

Figure 2.9 shows a correctly placed heat pump across the pinch.  $Q_1$  units of heat are removed from the process heat source (below the pinch) and  $Q_1+W$  units of heat are rejected into the process heat sink (above the pinch). This reduces the cold utility demand by  $Q_1$  and the hot utility demand by  $Q_1+W$ . In summary, one should place the heat pump such that it extracts heat from the process source (below the pinch) and rejects heat to the process sink (above the pinch).

Colmenares and Seider (1986) used nonlinear programming to quantify Townsend and Linnhoff's appropriate placement rules. Unfortunately, they only discussed placing simple heat engines and heat pumps. Utility system usually consist of complex heat engines (co-generation steam cycles) and heat pumps (complex and cascade refrigeration systems). Yoon (1990) combined heuristics and an MILP approach to design and optimize the heat exchanger network and utility system simultaneously. His approach reduces the number of possible temperature levels for heat exchange by various heuristics and then optimized the number of levels and loads in each level through an MILP approach. Unfortunately, the heuristics used to reduce the size of the problem are questionable. Shelton and Grossmann (1986a,b) also used the MILP superstructure approach to design integrated refrigeration systems. Their method is limited to small problems and also fixes the minimum approach temperature for the integration of refrigeration systems ( $\Delta T_{\min}$ ).

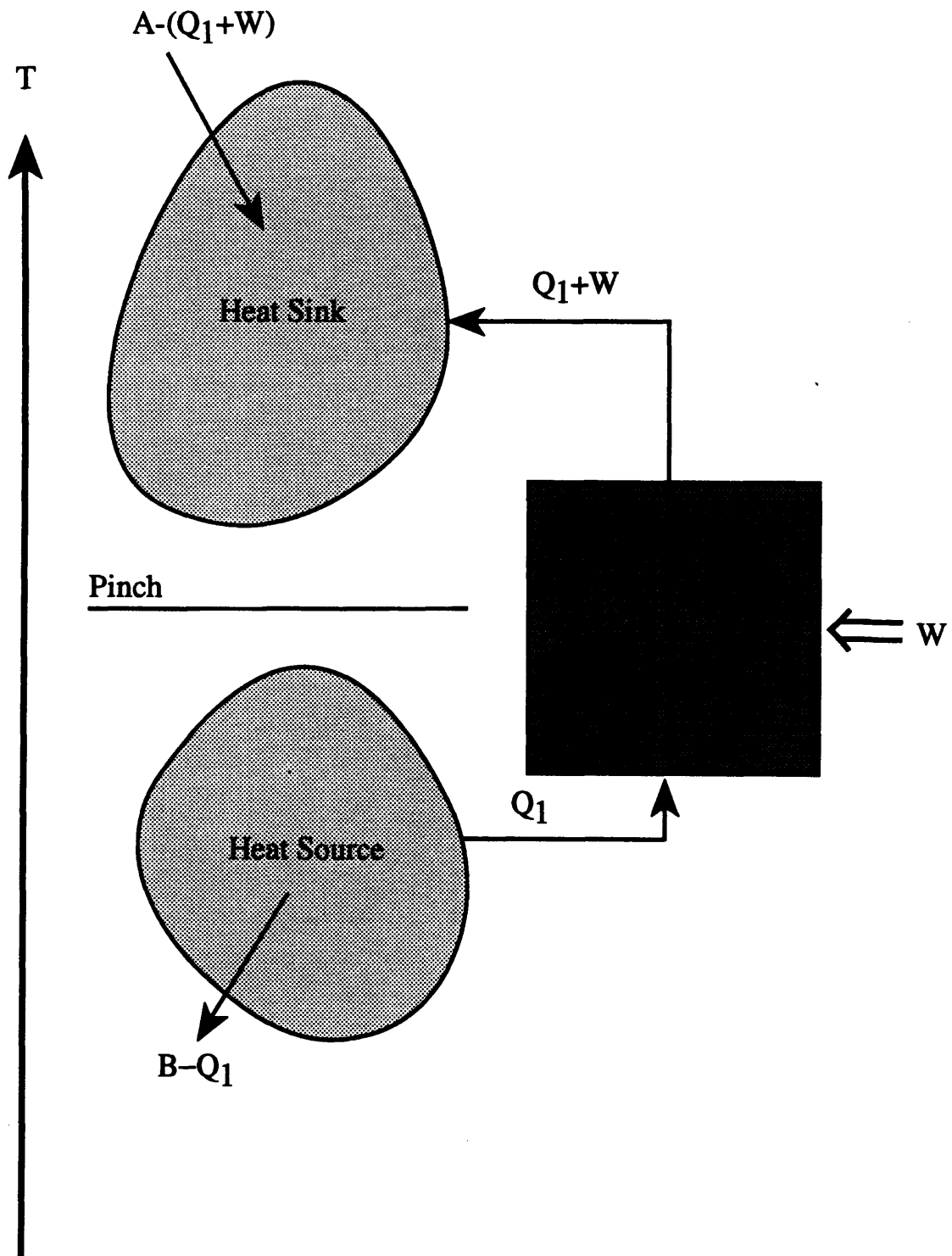


FIGURE 2.9 Diagram of a correctly placed heat pump. (Townsend and Linnhoff, 1983a)



Linnhoff and Dhole (1989) used the exergy composite curves and the exergy grand composite curve to capture some of the heat and work interactions between the heat exchanger network and refrigeration systems. From a simulation of a specific refrigeration system or from an existing refrigeration system an exergetic efficiency for that particular system is defined. The effects of different operating conditions on the total work requirement for the refrigeration system can then be calculated by assuming the exergetic efficiency stays constant.

Problems with Linnhoff and Dhole's method include the assumption of a constant exergetic efficiency and that a different exergetic efficiency must be calculated for every different refrigeration system and chemical process combination. The method predicts the work demand of the entire refrigeration system (predicts operating costs only) and not the work demand of each compressor in the refrigeration system. The work demanded by each compressor in the refrigeration system could be used to predict the refrigeration system's capital and operating costs.

#### **2.4.3 Chemical Process and Utility System Heat and Work Interactions**

The chemical process and the utility system interact directly through the work demanded by the chemical process and indirectly through the heat exchanger network. Changing the chemical process operating conditions could lead to different work and/or utility demands on the utility system. Different utility requirements could lead to different utility system structures and operating conditions. In the sequential approach it is assumed that the incremental costs of work and utilities are positive and constant. For utilities the overall incremental cost is not constant and could even be negative (plus/minus rules). It is easy to imagine that a similar relationship holds true for work demands.

Dhole (1991) extended Linnhoff and Dhole's (1989) exergy analysis to incorporate the effects of process changes on refrigeration system's work demand. Dhole's method suffers

the same drawback as Linnhoff and Dhole's method. A constant exergetic efficiency is still used and a different exergetic efficiency must be calculated for each different refrigeration system and chemical process combination. The method predicts the work demand of the entire refrigeration system (predicts operating costs only) and not the work demand of each compressor in the refrigeration system (could be used to predict the capital and operating costs of the refrigeration system).

## **2.5 Total Process Synthesis and Optimization**

Although many researchers recognize that the process synthesis and optimization problem should be solved simultaneously, no method proposed so far does so. Gundersen (1991) has a review on the achievements and future challenges on the industrial process synthesis and optimization problem. Papoulias and Grossmann (1983c) proposed an MILP that claimed to solve the complete process synthesis and optimization problem simultaneously. In their approach the thermal demands are lumped into arbitrary temperature levels, and these demands are satisfied by a pre-specified number of utilities that could have a few possible temperature values. This fixes some of the heat and work interactions with the utility system. Their MILP method reduces the search space by making binary variables turn on or off operating conditions. This significantly reduces the size of the problem since not all the operating conditions are possible. Since the choice of operating conditions is arbitrary, the method reduces to one of comparing many alternatives.

Approaches utilizing pinch analysis try to optimize the subsystems by using thermodynamic guidelines to account for the subsystem heat and work interactions. Linnhoff and Vredeveld's plus/minus rules (1984) and Linnhoff and Dhole's exergy analysis (1989) can be used to propose process changes that achieve better heat and work integration. This is really iteration in the sequential approach, but much faster, because thermodynamic targets predict the amount of heat and work integration expected without the redesign of a heat exchanger network or the utility system. The main problem with this approach is that the proposed

process changes are guided only in terms of heat and work integration. The effects on the capital cost of the heat exchanger network, the chemical process's chemistry and costs, and the utility system's capital costs are considered only after the process changes are made. The success of this trial-and-error approach depends mostly on the skill of the designer and the experience with the process involved. The results are nearly always suboptimal, or at least there is doubt about optimality.

## 2.6 Thesis Overview

The main objective of this thesis is to present a strategy for the simultaneous optimization of a chemical process, its heat exchanger network, and the utility system using a process simulator. This is accomplished by incorporating the heat and work interactions between the subsystems in the optimization.

In order to develop the simultaneous optimization method for complete chemical processes the heat and work interactions between subsystems must be well understood. Chapter 3 presents previous insights and develops new ones into the heat and work interactions between subsystems. The chapter also proposes mathematical models that could be used to account for the subsystems heat and work interactions.

An expansion on Duran and Grossmann's [1986] pinch location method is identified as a method that accounts for all major heat and work interactions between a chemical process and its heat exchanger network. This strategy not only accounts for heat integration but also targets for the capital cost of the heat exchanger network. A superstructure that could account for the heat and work interactions between heat exchanger networks and utility systems by solving a hard and difficult MINLP is also presented. This superstructure is not solved in this thesis. It is used as a guideline to develop a new method that targets for capital and operating costs of utility systems. This new method accounts for the utility systems' heat and work interactions without rigorous simulations of entire utility systems.

Chapter 4 develops the mathematical programs that incorporate subsystem's heat and work interactions proposed in Chapter 3. Even if the heat and work interactions between subsystems were very well understood it would be an arduous task, if not an impossible one, to optimize a complete chemical process without mathematical programs. A simple procedure to expand Duran and Grossmann's (1986) pinch location method is illustrated. The expanded pinch location method can account for heat integration and target for the capital costs of heat exchanger networks. A new method is introduced, that targets for capital and operating costs of utility systems (by accounting for their heat and work interactions) without rigorous simulations of entire utility systems and is based on the superstructure for integrated utility systems presented in Chapter 3. Chapter 4 illustrates the application of this new method to the two complete chemical process optimization example problems presented in this thesis.

Chapter 5 introduces the simultaneous method to complete chemical process optimization and its implementation in a rigorous sequential process simulator. The simultaneous method is a combination of the extended pinch location method and the new method to target for the utility system's capital and operating costs. The simultaneous method exploits the advantages of current process simulators, flowsheet optimizers, pinch analysis, and the new method to target for the capital and operating costs of the utility system that accounts for its heat and work interactions, but does not require a rigorous simulation of the entire utility system.

Today, process simulators allow rigorous and efficient simulations of even the most complicated chemical processes. Although flowsheet optimization strategies presently available in process simulators cannot guarantee finding the global optimum for nonconvex problems, their computational requirements are typically equivalent to only 3-10 flowsheet simulations (Lang, Biegler and Grossmann, 1988). Since pinch analysis can be used to quickly target for the approximate energy consumption and capital cost of a heat exchanger network without actual design, significant savings in computational time can be achieved if this targeting technique is embedded in the optimization step of a process simulator.

Similarly, the new method to target for the capital and operating costs of the utility system can be embedded in the optimization step of a process simulator. Again, this significantly reduces computation time. The result is the first tractable method that can simultaneously optimize all three subsystem operating conditions and account for their heat and work interactions with reasonable computational expense.

This thesis concludes by presenting the advantages of the simultaneous method over the sequential approach and Lang, Biegler, and Grossmann's method (Duran and Grossmann's method in a process simulator) by comparing and analyzing their solutions to two process optimization examples. Chapter 6 presents the atmospheric petroleum crude tower optimization problem and Chapter 7 the cold end of an ethylene plant optimization problem.

## Notations used in Chapter 2

$A_{\min}$	target for minimum heat transfer area for the heat exchanger network
$C$	index for cold process streams
$E_{\min}$	annualized minimum energy cost target
$f_i C_i$	heat capacity-flowrate product for cold process stream $i$
$F_i C_i$	heat capacity-flowrate product for hot process stream $i$
$H$	index set of hot process streams
$N_C$	number of cold stream
$N_H$	number of hot stream
$Q_1$	amount of heat extracted from a heat source by a heat engine or pump
$Q_2$	amount of heat rejected to a heat sink by a heat engine or pump
$Q_C$	minimum cold utility demand
$Q_H$	minimum hot utility demand
$t_i^{\text{in}}$	supply temperature for cold process streams
$t_i^{\text{out}}$	target temperature for cold process streams
$T_i^{\text{in}}$	supply temperature for hot process streams
$T_i^{\text{out}}$	target temperature for hot process streams
$U_{\min\text{-MER}}$	minimum number of heat exchangers for maximum energy recovery
$W$	amount of work produced by a heat engine or consumed by a heat pump
$\Delta T_{\min}$	minimum approach temperature for process heat integration
$\Delta T_{\min}$	minimum approach temperature refrigeration system integration

**CHAPTER 3 : CRITICAL ANALYSIS OF THE CHEMICAL PROCESS,  
HEAT EXCHANGER NETWORK, AND UTILITY SYSTEM  
HEAT AND WORK INTERACTIONS**

**3.1 Chemical Process and Heat Exchanger Network Heat and Work Interactions**

The sequential approach to process optimization can be summarized with the following equations taken from Lang, Biegler, and Grossmann (1988) where a set of  $N_H$  hot process streams  $i \in H$ , are to be cooled, and a set of  $N_C$  cold process streams  $j \in C$ , are to be heated.

$$\begin{aligned}
 \min \phi &= F(\underline{\mathbf{x}}, \underline{\mathbf{y}}) + \sum_i c_h^i Q_h^i + \sum_j c_c^j Q_c^j \\
 \text{s.t. } \underline{\mathbf{h}}(\underline{\mathbf{x}}, \underline{\mathbf{y}}) &= 0, \\
 \underline{\mathbf{g}}(\underline{\mathbf{x}}, \underline{\mathbf{y}}) &\leq 0, \\
 Q_h^i &= r_h^i(\underline{\mathbf{y}}), \quad i \in HU && \text{(NLP P0)} \\
 Q_c^j &= r_c^j(\underline{\mathbf{y}}), \quad j \in CU \\
 Q_h^i, Q_c^j &\in \mathbf{R}^1 : i \in HU, j \in CU \\
 \underline{\mathbf{x}} \in \mathbf{XC} &\mathbf{R}^n, \quad \underline{\mathbf{y}} \in \mathbf{YC} \mathbf{R}^m
 \end{aligned}$$

*"The vector of variables  $\underline{\mathbf{x}}$  represents process parameters such as pressures, temperatures, flowrates, or equipment sizes; the vector of variables  $\underline{\mathbf{y}} = [F_i, T_i^{\text{in}}, T_i^{\text{out}}; \text{ all } i \in H; f_j, t_p^{\text{in}}, t_p^{\text{out}}; \text{ all } j \in C]$ , represent the flowrates and temperatures of the process streams that undergo either cooling or heating. The variables  $\underline{\mathbf{x}}$  and  $\underline{\mathbf{y}}$  belong to the respective sets  $\mathbf{X}$  and  $\mathbf{Y}$ , which are typically given by known lower and upper bounds (e.g. physical constraints, specifications). The vector of constraints  $\underline{\mathbf{h}}, \underline{\mathbf{g}}$ , represents material and energy balances, or design specifications. In a nonintegrated process flowsheet, all of the heating and cooling is supplied with utilities that have been pre- assigned to process streams so as to ensure feasible heat exchange. The equations in (NLP P0) involving the expressions  $r_h^i(\underline{\mathbf{y}}): i \in HU$  and  $r_c^j(\underline{\mathbf{y}}): j \in CU$ , represent the heat balances for calculating the heating and cooling requirements,  $Q_h^i: i \in HU$  and  $Q_c^j: j \in CU$ , for the nonintegrated flowsheet.*

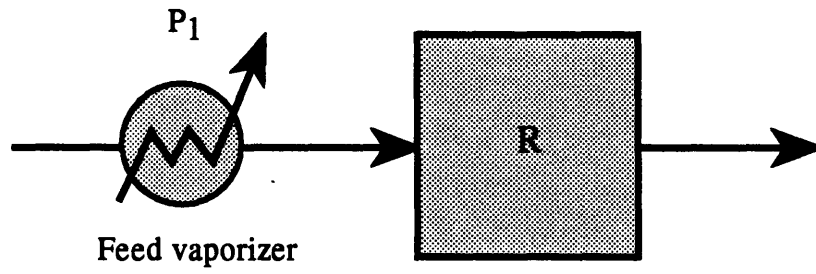
*The objective function  $\phi$  is generally economic in nature involving both investment and operating costs in the term  $F(\underline{\mathbf{x}}, \underline{\mathbf{y}})$ ; the other terms correspond to utility cost with  $c_h^i: i \in HU$  and  $c_c^j: j \in CU$ , representing unit cost for the respective heating and cooling utilities."*

The sequential approach fixes some of the heat and work interactions with the utility system by assuming the number and temperature levels of the utilities present ( $i \in \text{HU}$ ,  $j \in \text{CU}$ ) and their costs ( $c_h^i$ :  $i \in \text{HU}$  and  $c_c^j$ :  $j \in \text{CU}$ ). It fixes the heat and work interactions with the heat exchanger network by assuming that all cold streams are going to need hot utilities and all the hot streams are going to need cold utilities to reach their target temperatures. Therefore, increasing the load or temperature level of a hot stream or increasing the load or decreasing the temperature level of a cold stream can only lead to higher utility consumption or the use of more expensive utilities. When the chemical process and the heat exchanger network are considered simultaneously this is not always the case.

Consider the following examples taken from a Linnhoff-March (1990) course in pinch technology. The example on the effects of reducing the pressure of a feed vaporizer is illustrated in Figures 3.1 and 3.2. The feed vaporizer is shown in Figure 3.1a and the composite curves of the total process are given in Figure 3.1b. The feed vaporizer is a cold streams and forms part of the cold composite curves. If the vaporization pressure is decreased the temperature will also decrease and part of the cold composite curve will move downward as shown in Figure 3.2a. If the heat of vaporization is not a strong function of temperature, the energy targets will remain constant and the driving forces will be increased leading to a heat recovery network with less heat exchange area required. If we could decrease the pressure even further so the vaporization temperature is now below the pinch, both the hot and cold utility targets will be reduced; as shown in Figure 3.2b. So we see that reducing the level of a cold stream (*keep the cold streams cold*) can reduce the area requirements of the heat exchanger network or even lead to savings in utility consumption, a fact not clear in the sequential approach. Similar arguments can be made for hot streams, that is *keep the hot streams hot*.



(a)



(b)

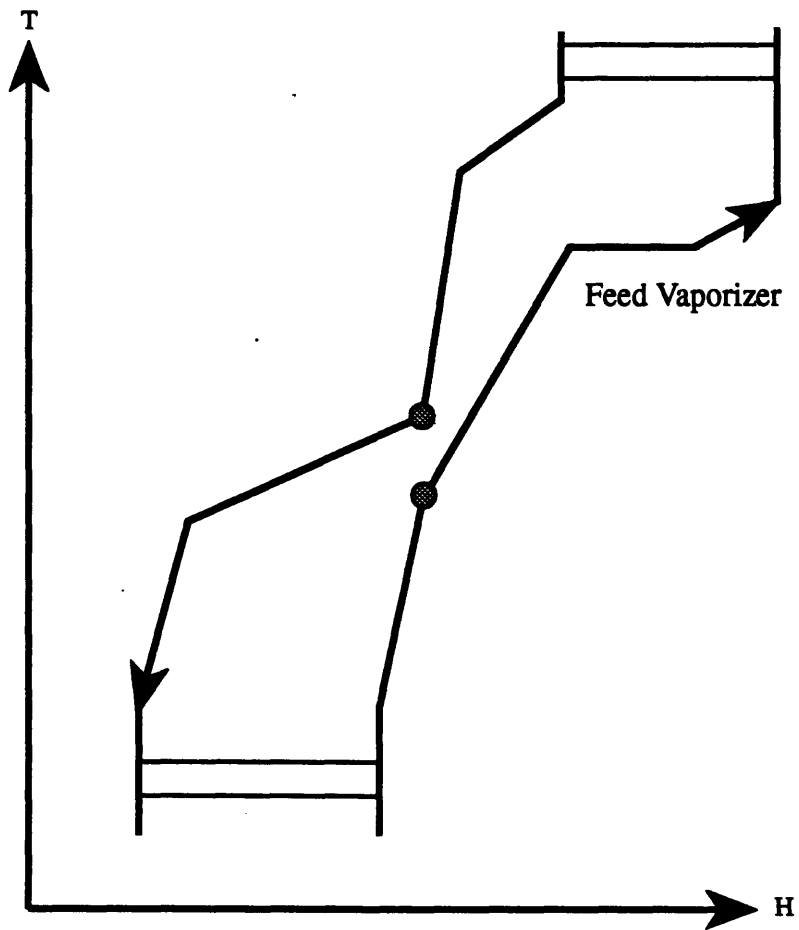


FIGURE 3.1 The example on the effects of reducing the pressure of a feed vaporizer; (a) the feed vaporizer; (b) the composite curves of the complete process. (Linnhoff-March, 1990)

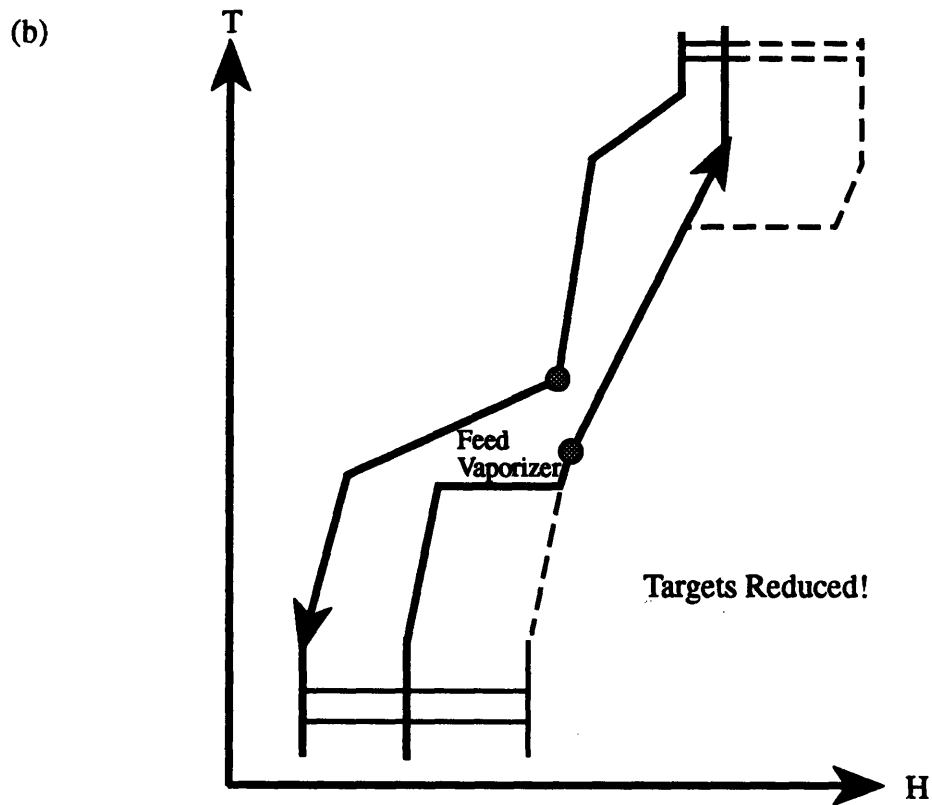
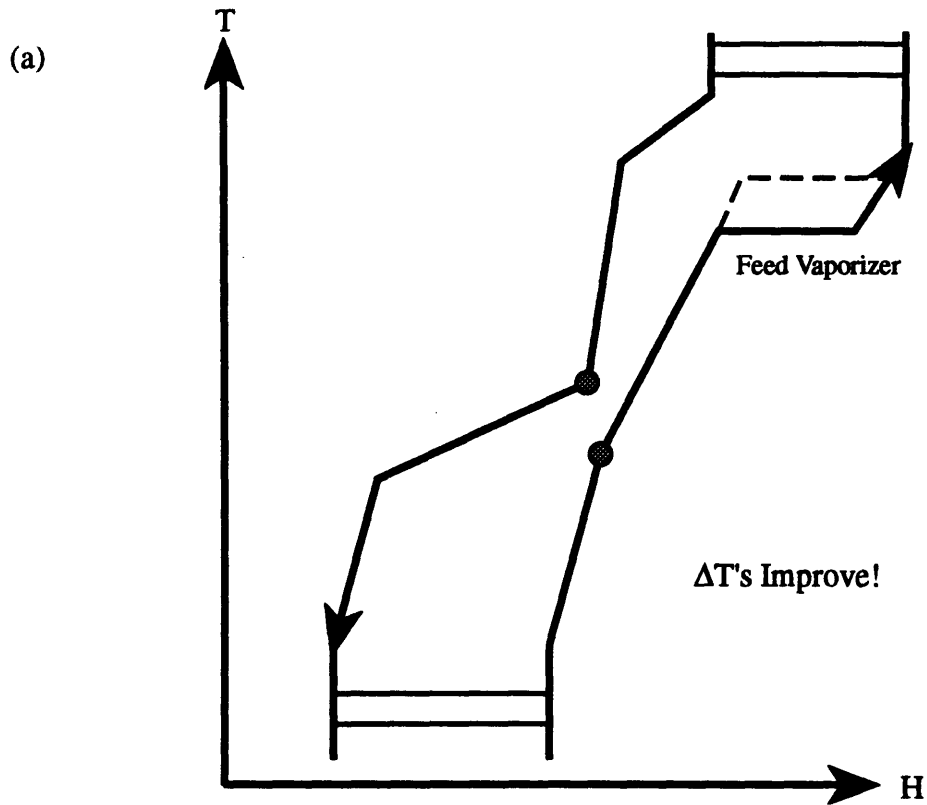
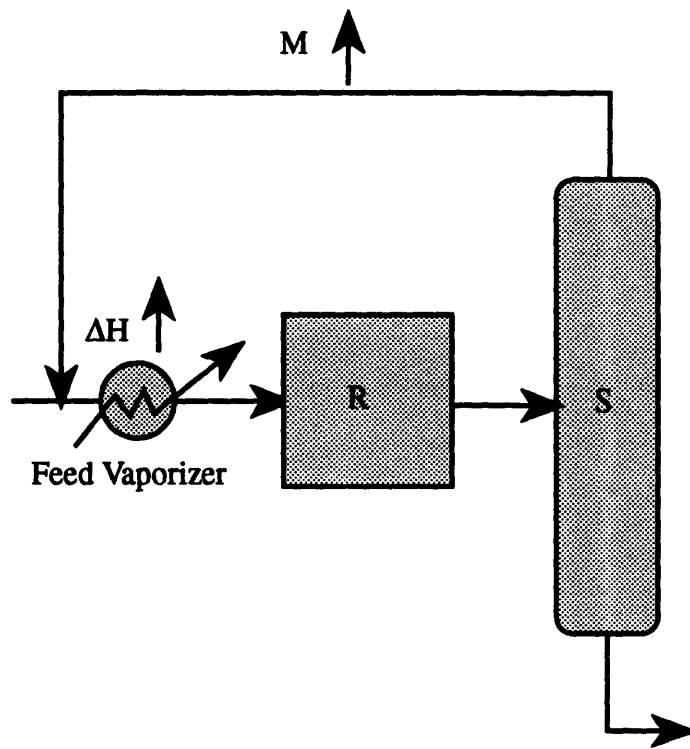


FIGURE 3.2 The effects of reducing the pressure of a feed vaporizer; (a) the composite curves of the complete process after the pressure was decreased; (b) the composite curves of the complete process after the pressure was decreased further. (Linnhoff-March, 1990)

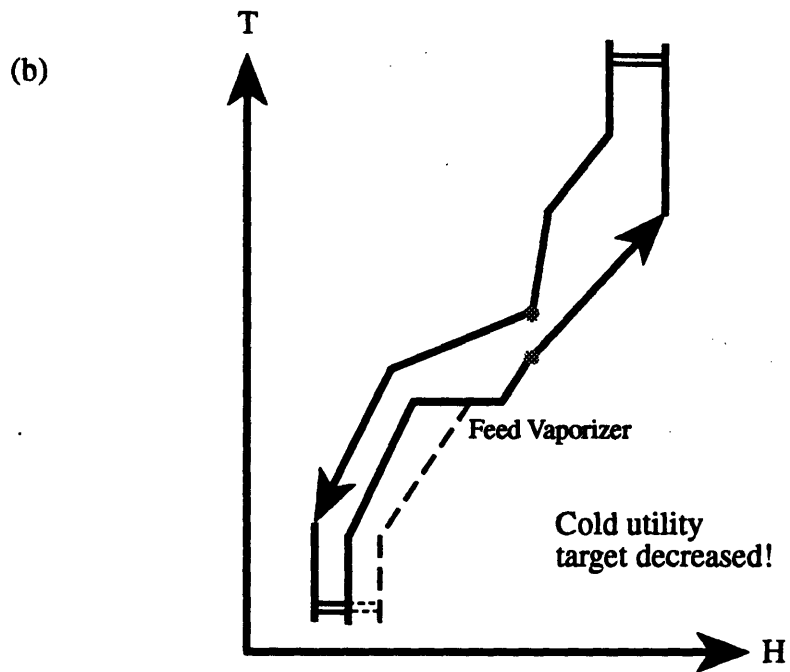
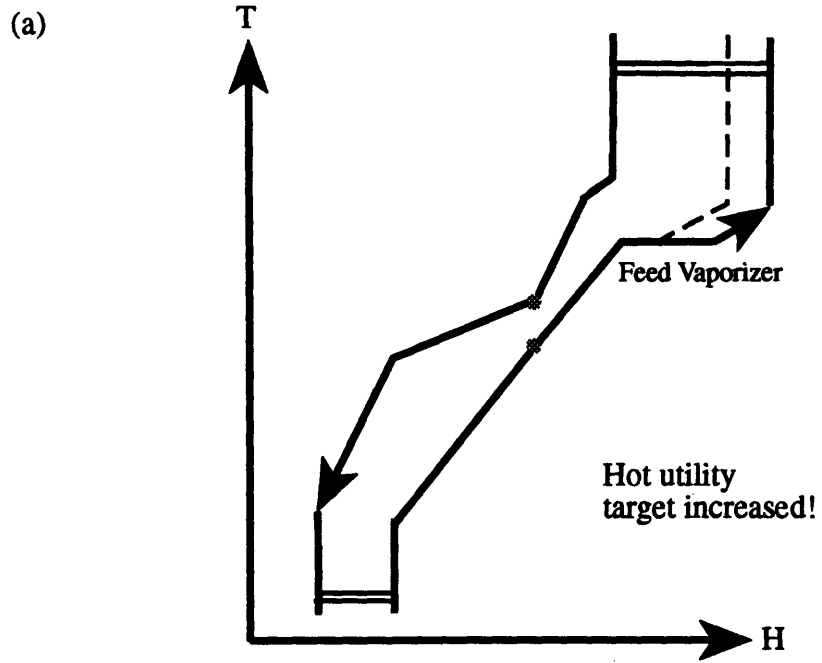
The sequential approach initially assumes that all heating and cooling will be done with utilities and not with heat integration using the heat exchanger network. Therefore, increasing the thermal load of hot streams and/or cold streams will always lead to higher utility consumption. However, the pinch concept shows that different tradeoffs arise if the subsystems are considered simultaneously instead of sequentially. The example on the effects of increasing the flowrate of a feed vaporizer which is part of the process recycle (Figure 3.3) illustrates that fact. Increasing the recycle flowrate increases the heat load on the feed vaporizer, but the overall energy consumption can increase or decrease. Figure 3.4a shows that the overall hot utility required will increase if the feed vaporizer is above the pinch, but if it is below the pinch, the overall hot utility required will stay the same and the total cold utility required will decrease (Figure 3.4b).

The general case can be explained by the plus/minus principle, as shown in Figure 3.5. Process changes that reduce utility consumption are those that decrease the size of the net heat sink above the pinch or the net heat source below the pinch. Above the pinch, the total duty of the hot composite should be increased and that of the cold composite decreased. Conversely below the pinch, the duty of the hot composite should be decreased and that of the cold composite increased. In the sequential approach the process changes that save utilities are those that decrease the load of the hot and cold process streams regardless of their locations with respect to the pinch.

By treating the heat exchanger network and the chemical process simultaneously, instead of sequentially, different tradeoffs arise. These tradeoffs are understood qualitatively, but mathematical techniques are needed to make them quantitative.



**FIGURE 3.3** The example on the effects of increasing the flowrate of a feed vaporizer which is part of the process recycle. (Linnhoff-March, 1990)



**FIGURE 3.4** The effects of increasing the flowrate of a feed vaporizer which is part of the process recycle; (a) if feed vaporizer is above the pinch; (b) if the feed vaporizer is below the pinch. (Linnhoff-March, 1990)

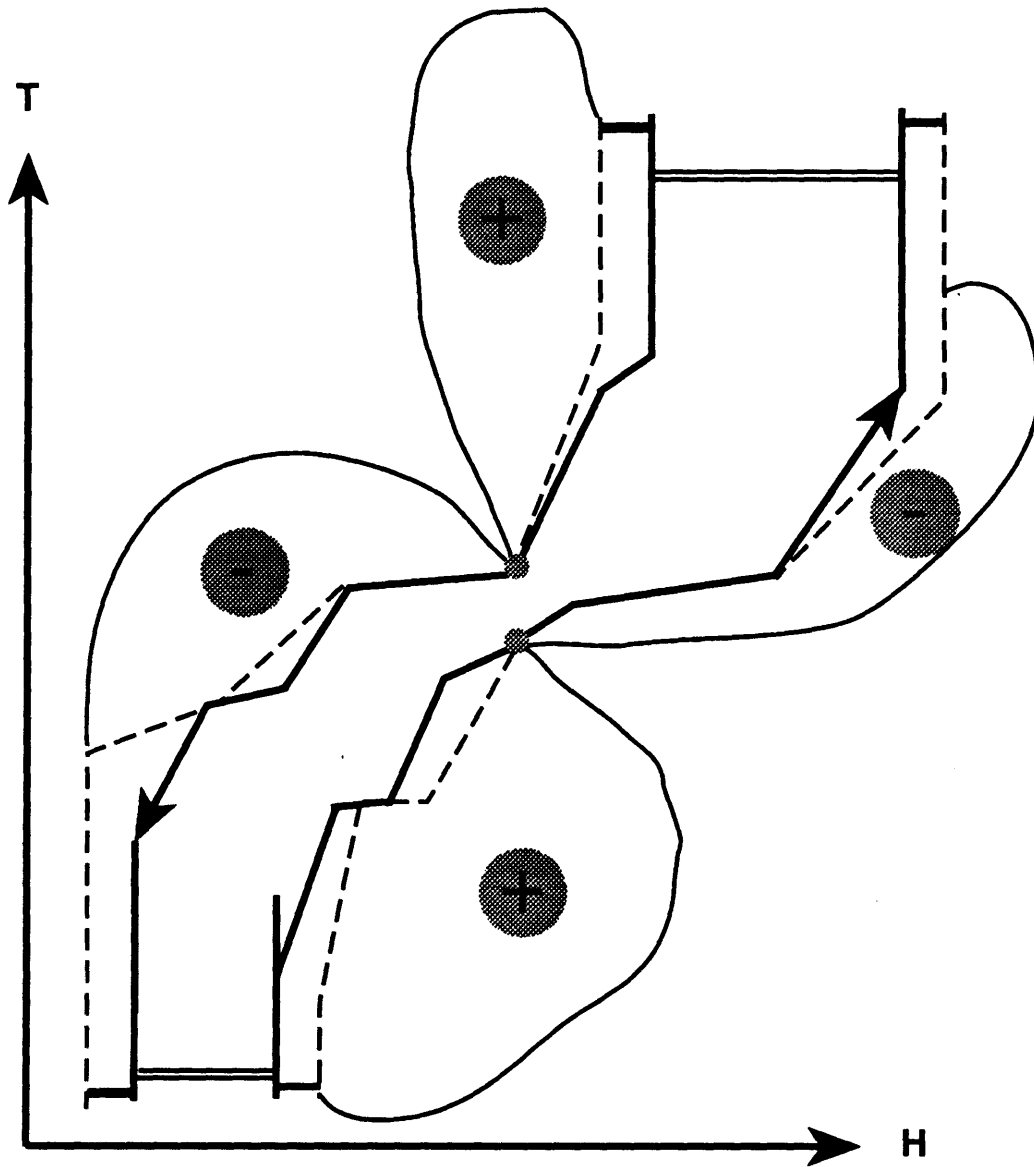


FIGURE 3.5 Illustration of the plus/minus principle of Linnhoff and Vedrevel (1984).

### 3.1.1 The Pinch Location Method : Quantifying the Plus/Minus Rules

In the sequential approach to process optimization the targets for minimum hot and cold utility consumption are usually obtained from the composite curves. The composite curves relative position is not fixed (depends on the minimum approach temperature) but their shape is, since in the sequential approach the flowrates and supply and target temperatures of the process streams undergoing heat exchange are determined from the solution to equations in NLP P0. In a simultaneous optimization approach for the heat exchanger network and the chemical process, the flowrates and the supply and target temperatures ( $\underline{y}$  variables) of the process streams undergoing heat exchange should be optimization variables. A mathematical method is needed to determine targets for the minimum hot and cold utility requirements without fixing these variables.

The pinch location method, as shown by Duran and Grossmann (1986), accomplishes this by modifying the nonlinear flowsheet optimization problem given by NLP P0 to include heat integration. This is done by replacing the heat balance equations of the nonintegrated flowsheet by a set of constraints that assure maximum heat recovery at a given minimum approach temperature. Their NLP is based on the observation that the pinch can only occur at a supply temperature of a process stream (or stream segment). They showed that if all the supply temperatures are chosen as pinch candidates,  $T^p$ , and heat balances are performed above each candidate, the candidate yielding the largest net heat sink (for the heat balance above the candidate pinch) corresponds to the process stream causing the pinch. The size of this largest net heat sink gives the minimum hot utility required,  $Q_H$ . The minimum cold utility required,  $Q_C$ , is then calculated by overall heat balance. The pinch location method has been implemented in sequential process simulators by Lang, Biegler, and Grossmann (1988).

For the case of a single hot and cold utility, NLP P0 for the nonintegrated flowsheet can be modified to include heat integration (Lang, Biegler, Grossmann, 1988).

$$\begin{aligned}
 \min \phi &= F(\underline{x}, \underline{y}) + c_h Q_H + c_c Q_C \\
 \text{s.t. } h(\underline{x}, \underline{y}) &= 0 \\
 g(\underline{x}, \underline{y}) &\leq 0 \\
 Q_H &= \max_p(z^p_H(\underline{y})) \\
 Q_C &= \Omega(\underline{y}) + Q_H \\
 Q_H &\geq 0, \quad Q_C \geq 0 \\
 \underline{x} &\in X, \quad \underline{y} \in Y
 \end{aligned}
 \tag{NLP P1}$$

where the heating deficit functions,  $z^p_H(\underline{y})$ , calculates the size of the heat sink at a given pinch candidate temperature,  $T^p$ ; and  $\Omega(\underline{y})$  represent an overall energy balance.  $z^p_H(\underline{y})$  and  $\Omega(\underline{y})$  are given by:

$$z^p_H(\underline{y}) = \text{QSIA}(\underline{y})^p - \text{QSOA}(\underline{y})^p \tag{3.1}$$

$$\text{QSIA}(\underline{y})^p = \sum_j f_j c_j [\max(0, (t_j^{\text{out}} - (T^p - \Delta T_m)) - \max(0, (t_j^{\text{in}} - (T^p - \Delta T_m)))] \tag{3.2}$$

$$\text{QSOA}(\underline{y})^p = \sum_i F_i C_i [\max(0, (T_i^{\text{in}} - T^p) - \max(0, (T_i^{\text{out}} - T^p))] \tag{3.3}$$

$$\Omega(\underline{y}) = \sum_i F_i C_i (T_i^{\text{in}} - T_i^{\text{out}}) - \sum_j f_j c_j (t_j^{\text{out}} - t_j^{\text{in}}) \tag{3.4}$$

The multiple hot and cold utility case can be treated by repeatedly redefining the stream data and reevaluating the heating deficit functions (Lang, Biegler and Grossmann, 1988).

Since the interaction of the heat exchanger network and the chemical process is understood qualitatively (plus/minus principle), let's analyze Duran and Grossmann's example problem with this insight in order to evaluate the pinch location method. Figure 3.6 shows the flowsheet of the process optimization problem used by Duran and Grossmann to illustrate



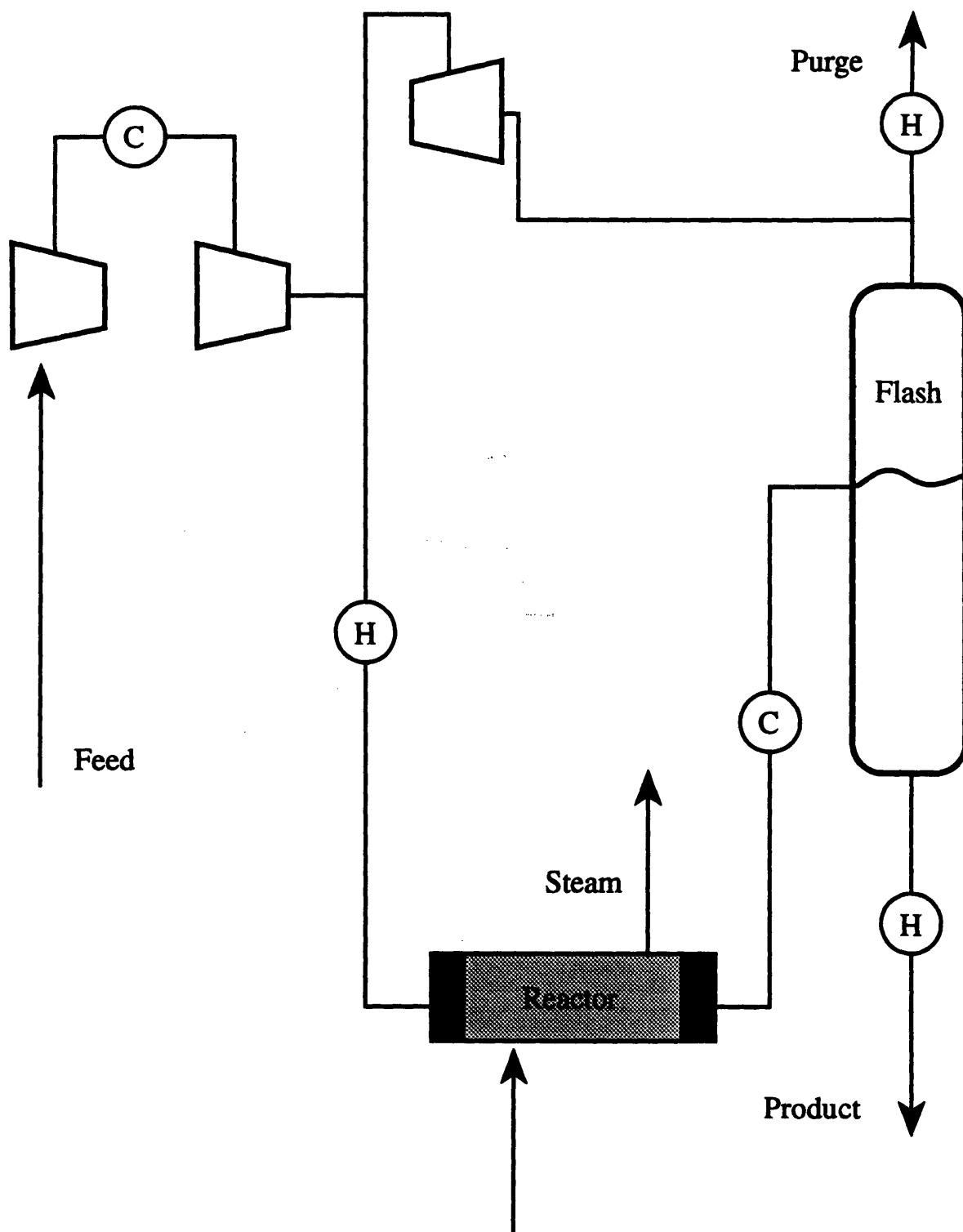


FIGURE 3.6 the flowsheet of the process optimization problem used by Duran & Grossmann (1986) to illustrate their method.

their method. A feed consisting of three components A, B and C, where C is an inert component, is compressed with a two-stage centrifugal compressor with intermediate cooling. The pressurized feed is mixed with recycle, and the resulting stream is pre-heated to reaction temperature. In the reactor components A and B react to produce D. The reaction is exothermic, so depending on how much the reactor is cooled it could be operated anywhere in the range from adiabatic to isothermal. The effluent is cooled and sent to a flash unit where most of the product is recovered in the liquid stream. The product stream is heated to deliver the required product as saturated vapor. A portion of the vapor stream is recompressed and recycled and the rest is purged to avoid accumulation of the inert C. The purge stream is heated to deliver it at a fixed temperature.

Table 3.1 shows the results of Duran and Grossmann's process optimization problem obtained using the sequential approach and their method. Their pinch location method gives annual profits 90.7% higher than the sequential approach. The main reasons for the difference are that the simultaneous approach gives a solution with higher conversion of raw materials (81.7% vs 75.1%) and much lower hot utility consumption (1,684kW vs 8,622 kW).

When one looks at the composite curves of both solutions (Figures 3.7a and 3.7b) it is clear how the simultaneous approach reached its solution. The reactor effluent is a hot stream above the pinch. According to the plus/minus principle increasing its load will decrease the size of the heat sink above the pinch. The potential for decreasing the heat sink is so high that new tradeoffs arise. Increasing the recycle rate will not only lead to higher conversion of raw materials but also to less hot utility consumption (size of the heat sink decreases because reactor effluent flowrate increases). Since in the sequential approach increasing the load of any hot or cold process stream increases utility consumption, this tradeoff is not found. The composite curves also show that the load of the cold streams below the pinch has been increased to reduce the size of the heat source.

TABLE 3.1 The results of Duran & Grossmann's (1986) process optimization problem obtained using the sequential approach and Duran & Grossmann's method.

	Duran & Grossmann's Method	Sequential Approach
<b>ECONOMIC</b>		
<i>Expenses</i>	<i>Million \$ /yr</i>	<i>Million \$ /yr</i>
Feedstock	22.6717	26.4165
Capital Investment	3.7596	3.9108
Electricity compress	2.3774	2.4871
<b>Heating Utility</b>	<b>2.8244</b>	<b>14.4586</b>
Cooling Utility	0.7900	0.7247
<i>Earnings</i>		
Product	41.530	41.5300
Purge	4.5169	6.8242
Generated Steam	5.6407	9.7441
<b>Annual Profits</b>	<b>19.2645</b>	<b>10.1003</b>
<b>TECHNICAL DESIGN AND OPERATING CONDITIONS</b>		
	<i>Million \$ /yr</i>	<i>Million \$ /yr</i>
<b>Overall conversion A</b>	<b>81.68 %</b>	<b>75.13 %</b>
Pressure Reactor	12.10 atm	13.87 atm
Conversion per pass	30.43 %	37.53 %
Inlet reactor Temperature	450.00 °K	450.00 °K
<b>Outlet reactor Temperature</b>	<b>502.65 °K</b>	<b>450.00 °K</b>
Steam generated	10,119.12 kW	17,479.60 kW
Flash Pressure	9.10 atm	10.87 atm
<b>Flash Temperature</b>	<b>320.00 °K</b>	<b>339.88 °K</b>
Purge rate	9.66 %	19.55 %
Power compressors	11,353.60 kW	11,353.60 kW
Heating utility	1,684.27 kW	8,622.04 kW
Cooling utility	10,632.04 kW	9,752.77 kW
<b>Total heat exchanged</b>	<b>31,962.20 kW</b>	<b>28,720.51 kW</b>

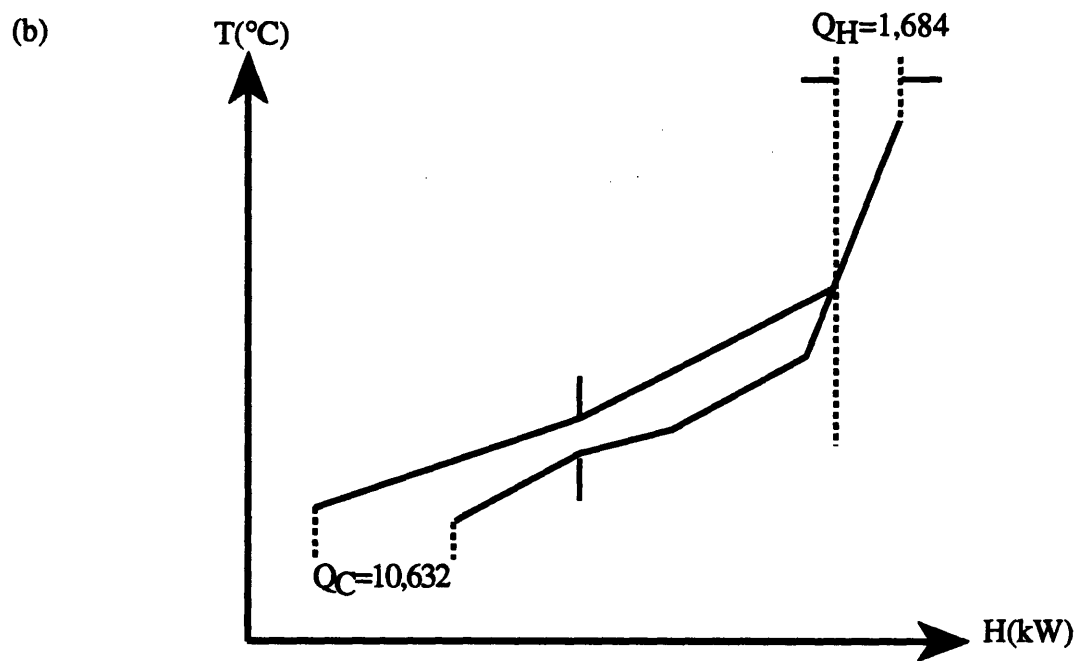
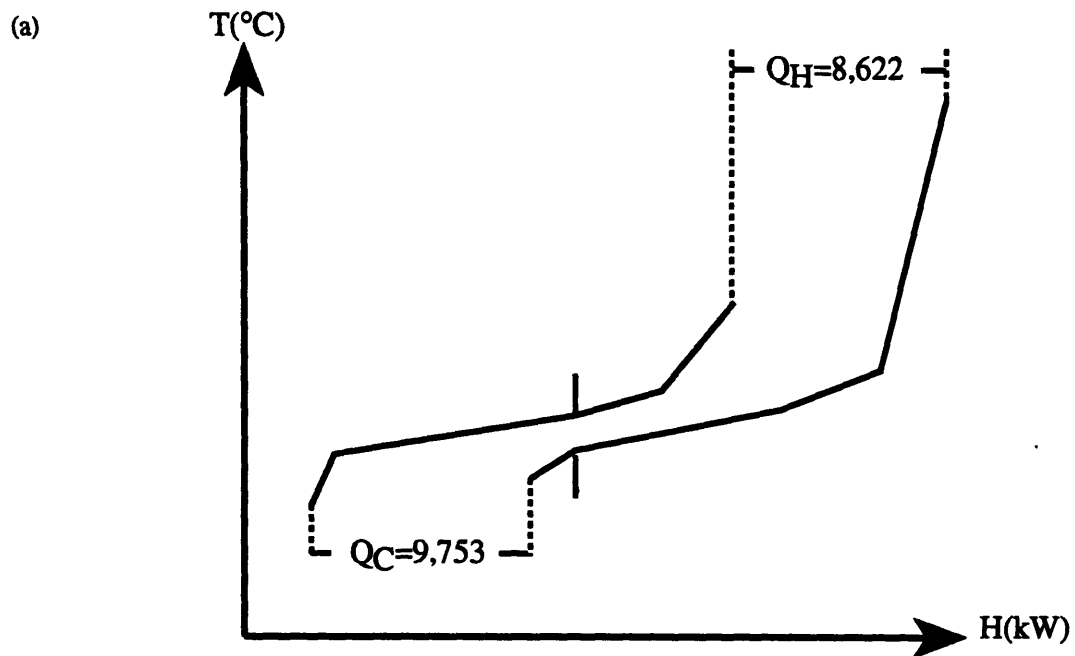


FIGURE 3.7 The composite curves of the solutions to Duran & Grossmann's (1986) process optimization problem; (a) composite curves of the solution using the sequential approach; (b) composite curves of the solution using Duran & Grossmann's method.

The fact that the quantitative pinch location method agrees with the qualitative plus/minus rules is encouraging. This agreement encourages the use of the pinch location method as a quantitative tool to find complicated tradeoffs in the heat and work interactions between the chemical processes and its heat exchanger network. Although the pinch location method can account for some of the heat and work interaction between these two subsystems, it neglects some potentially important interactions.

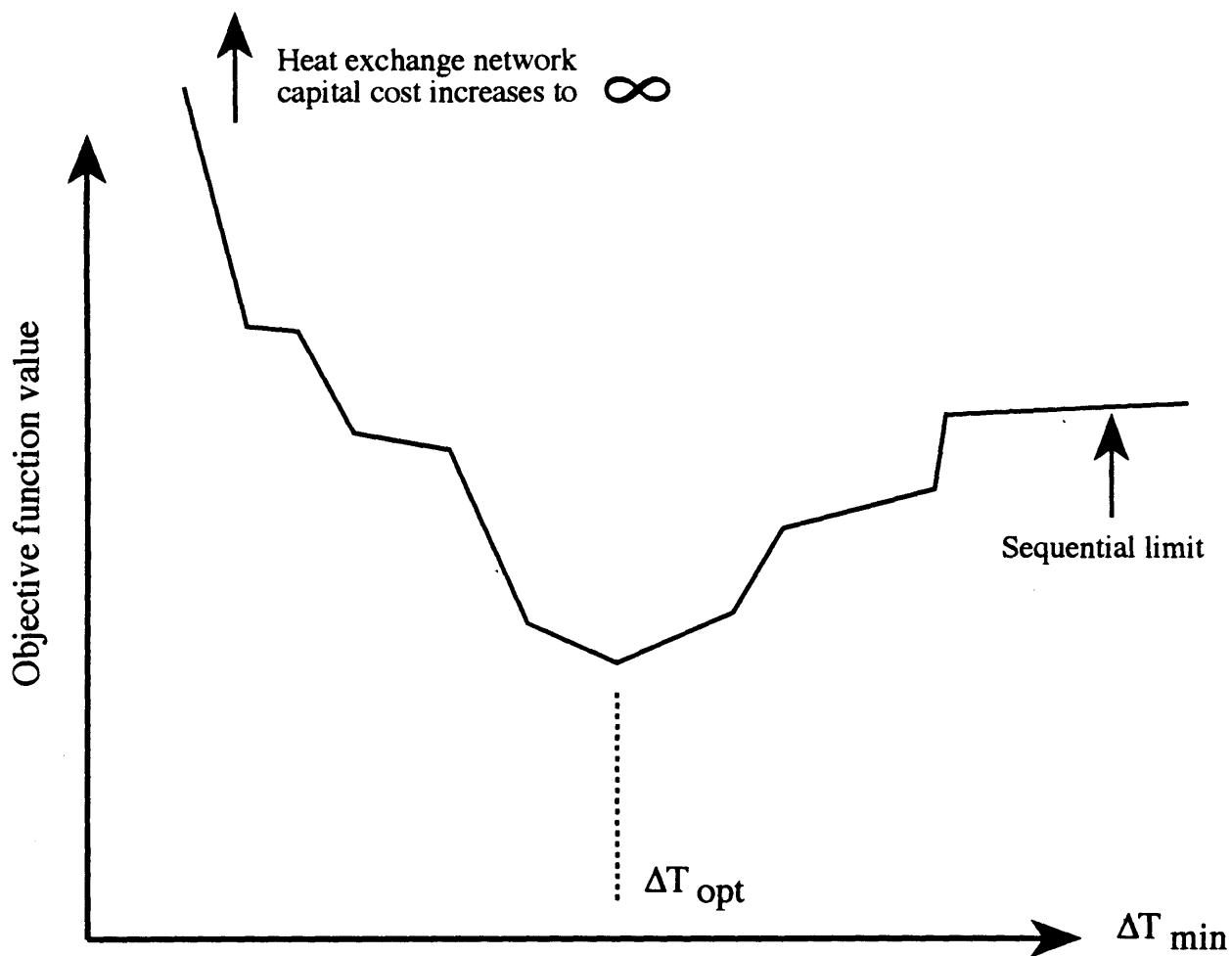
The pinch location method ignores some of the heat and work interactions between the chemical process and the heat exchanger network because the capital cost of the heat exchanger network is not included in its objective function. Therefore, the minimum approach temperature for heat exchange must be fixed and the capital cost of the network is added after the optimization. As we saw in the heat exchanger network synthesis and optimization problem (Figure 2.2), the minimum approach temperature for heat exchange is a key variable for the tradeoff between capital cost (network area and number of units) and operating cost (amount of energy recovered) of the network. As the minimum approach temperature for heat exchange is decreased more energy is recovered so the operating costs go down but the driving forces are decreased so the area cost and capital cost go up. As the minimum approach temperature for heat exchange is increased less energy is recovered so the operating costs go up but the driving forces are increased so the area cost and capital cost go down. The cost targeting method of Ahmad and Linnhoff (1984) was specifically developed to account for this tradeoff.

The composite curves of Duran and Grossmann's solution (Figure 3.7a) reflect the problems with the pinch location method. Since the capital cost of the heat exchanger network is not included in the objective function of NLP P1, heat integration is performed as long as the minimum approach temperature for heat exchange is not violated (plus/minus rules are applied

as much as possible). This leads to composite curves with two pinches. As will be seen in the petroleum crude unit and the cold end of an ethylene plant example problems presented in Chapters 6 and 7, double pinches appear to be typical of their method.

In order to optimize simultaneously the heat exchanger network and chemical process, the capital cost of the heat exchanger network should be included in the optimization and the minimum approach temperature for heat exchange ( $\Delta T_{\min}$ ) should be allowed to vary. Figure 3.8 illustrates the objective function value of the a truly simultaneous optimization method as  $\Delta T_{\min}$  varies. As  $\Delta T_{\min}$  goes to zero the area of the network will go to infinity and so will the total cost of the system. As the minimum approach temperature increases the total system cost will go through a minimum before starting to increase again. This occurs because the limit of a very high minimum approach temperature is the sequential approach. At very large values of  $\Delta T_{\min}$  no process heat integration occurs, utilities are used to perform all the heating and cooling of process streams.

The discontinuities in the curve at different minimum approach temperatures, result from different structures of the heat exchanger network. In other words, they are caused by heat exchanger networks that require different number of heat exchangers. Since the chemical process stream variables are not fixed, these discontinuities are probably impossible to predict like in Ahmad and Linnhoff's (1984) cost targeting method. It so happens, that in many real chemical processes, the cost of heat exchangers is very low when compared to the total cost of complete chemical process. Therefore, if the target for the minimum number of heat exchangers changes during the optimization the discontinuity in the objective function is masked. This will become clear in the atmospheric petroleum crude tower optimization problem of Chapter 6. The optimum minimum approach temperature for heat exchange obtained in this manner will reflect the proper tradeoff between the capital and operating costs of the chemical process and its heat exchanger network.



Objective function value =  $f(\text{Capital and operating costs of the chemical process and its heat exchanger network})$

FIGURE 3.8 Objective function value versus  $\Delta T_{min}$  in a method that accounts for all heat and work interactions between a chemical process and its heat exchanger network.

Figure 3.9 shows the prediction of the objective function value of Duran and Grossmann's method if  $\Delta T_{\min}$  is allowed to vary. Because the capital cost of the heat exchanger network is not included in the objective function, the total system cost does not go to infinity as  $\Delta T_{\min}$  goes to zero.

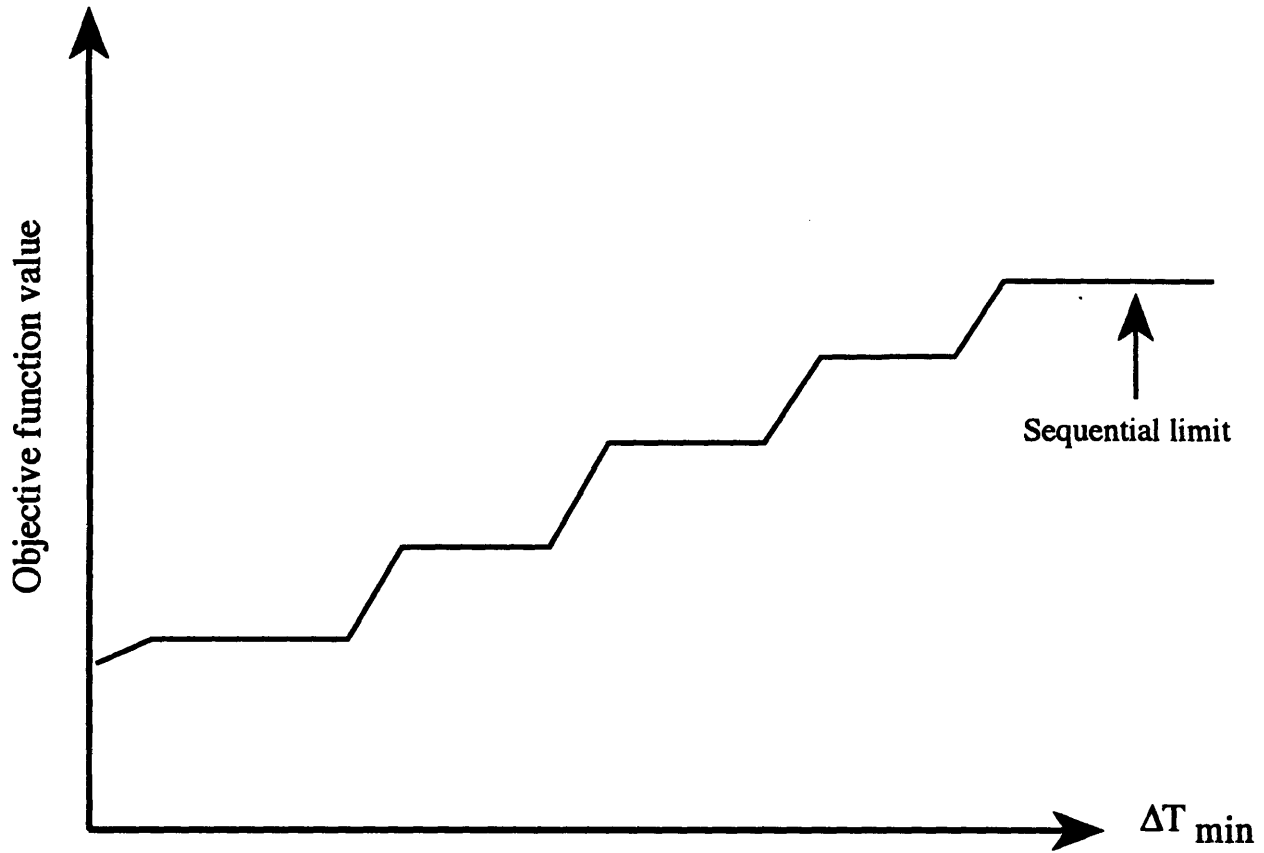
The expansion of the pinch location method to account for all heat and work interactions between the chemical process and the heat exchanger network will be discussed in Chapter 4.

### 3.2 Utility System and Heat Exchanger Network Heat and Work Interactions

In section 3.1 the heat and work interactions between the chemical process and the heat exchanger network were discussed. Some of the heat and work interactions with the utility system were assumed to be fixed. This was done because the number and temperature levels of the utilities present ( $i \in \text{HU}$ ,  $j \in \text{CU}$ ), their usage costs ( $c_h^i$ :  $i \in \text{HU}$  and  $c_c^j$ :  $j \in \text{CU}$ ), and the cost of work must be assumed in order to optimize these models. The real costs of work and utilities are the capital and operating costs of the utility system used to produce them. Since the demand for utilities and work is dependent on the chemical products produced (chemical process chosen) and the way these products are produced (chemistry chosen), it is expected that the real costs of utilities and work would vary from flowsheet to flowsheet.

In this section the heat and work interactions between the utility system and the heat exchanger network are discussed. The heat and work interactions with the chemical process are assumed to be fixed. This is done by fixing the operating conditions of the chemical process ( $\underline{x}$  and  $\underline{y}$  variables). The shape of the composite curves is fixed, since it depends only on the  $\underline{y}$  variable.





Objective function value  $\neq$  f(Capital cost of heat exchanger network)

FIGURE 3.9 Objective function value versus  $\Delta T_{\min}$  in Duran and Grossmann's (1988) method.

The pinch divides the process into a net process heat sink above the pinch and a net process heat source below the pinch (Figure 2.1). If the composite curves are partially or completely below ambient temperature, refrigeration might be needed. The design of integrated utility systems should be divided at the pinch and at the ambient temperature. This is because the ambient temperature acts as a natural pinch. Heat should not be transferred below ambient temperature because it would have to be removed by refrigeration. Figure 3.10 shows the composite curves divided at the pinch and ambient temperatures. Design of integrated utility systems based on the appropriate placement rules for each partition will be discussed.

In order to design integrated utility systems based on the appropriate placement rules the process heat sink and source must be quantified. The appropriate placement of heat engines and heat pumps has been discussed qualitatively. A quantitative method for calculating the maximum amount of heat that can be added or removed from the process heat sink or source at a given temperature without violating the pinch is needed. The tool used for this purpose is the grand composite curve (Linnhoff et al., 1982). Figure 3.11 shows how to construct the grand composite curve from the composite curves. Basically, the grand composite curve is a graph of temperature versus enthalpy difference (horizontal distance) between the hot and cold composite curves.

The grand composite curve quantitatively characterizes the process heat sink above the pinch and the process heat source below the pinch. The curve above the pinch represents the net process cold stream against which hot utilities (or heat engine or heat pump exhaust) must be matched. The curve below the pinch represents a net process hot stream against which cold utilities (or heat engine or heat pump extractions or heat recovered for preheat) must be matched. In Figure 3.12 a temperature interval with heat surplus can be easily distinguished from one with heat deficit. Portions of the graph with negative slope indicate intervals with heat surplus and portions with positive slope indicate intervals with heat deficit.

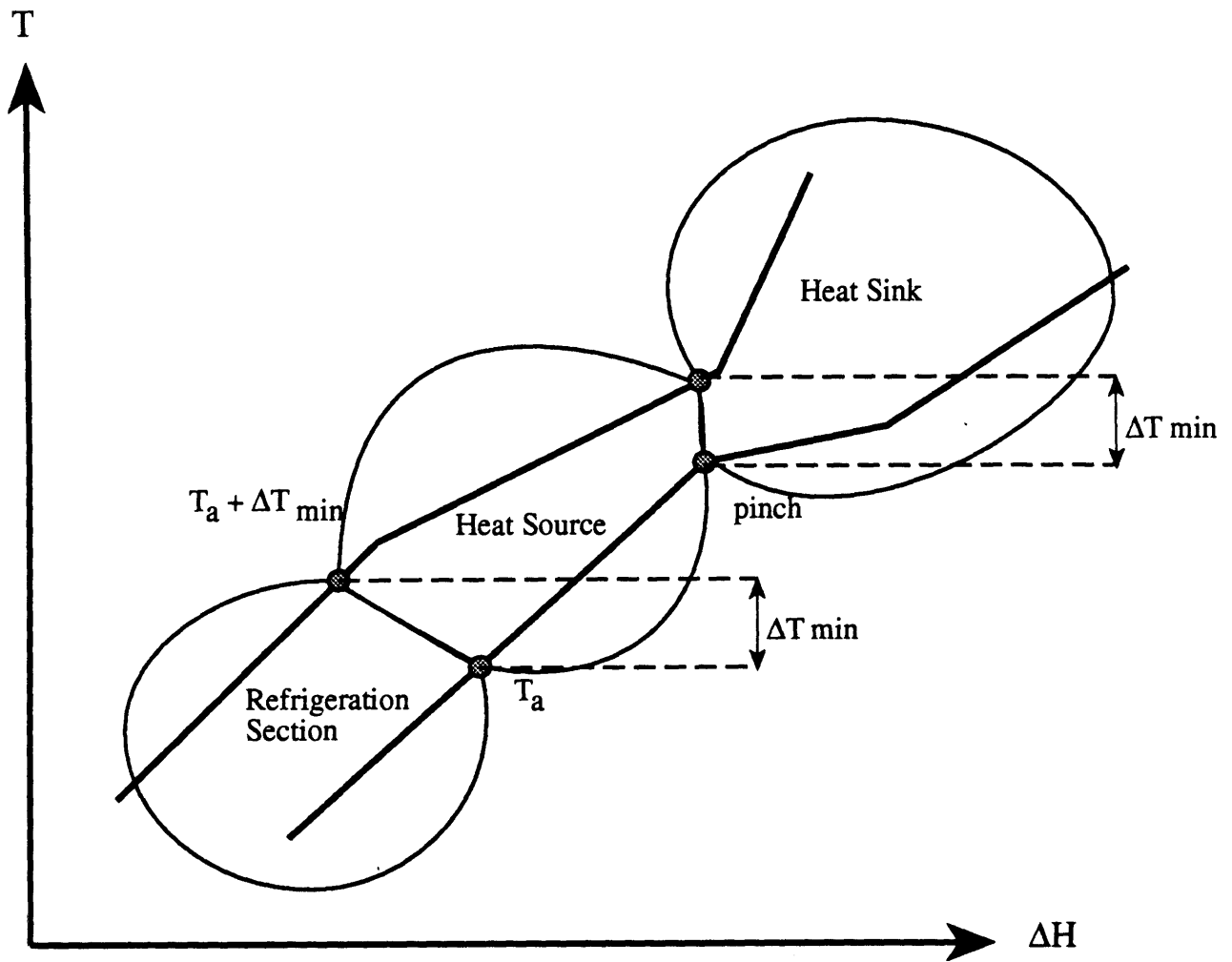


FIGURE 3.10 The composite curves divided at ambient temperature and at the pinch. (Yoon, 1990)

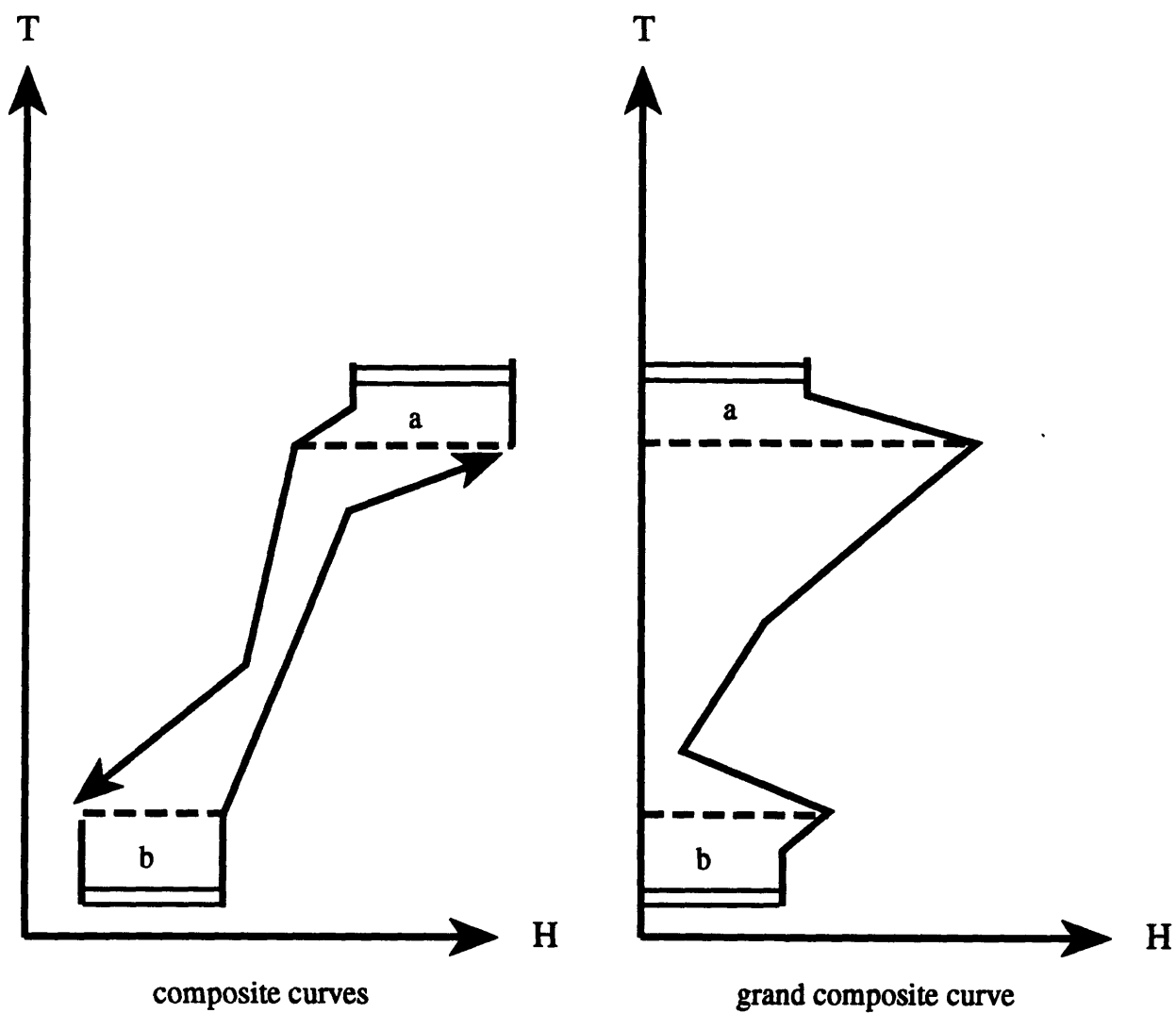


FIGURE 3.11 The relationship between the composite curves and grand composite curve. (Townsend and Linnhoff, 1983b)

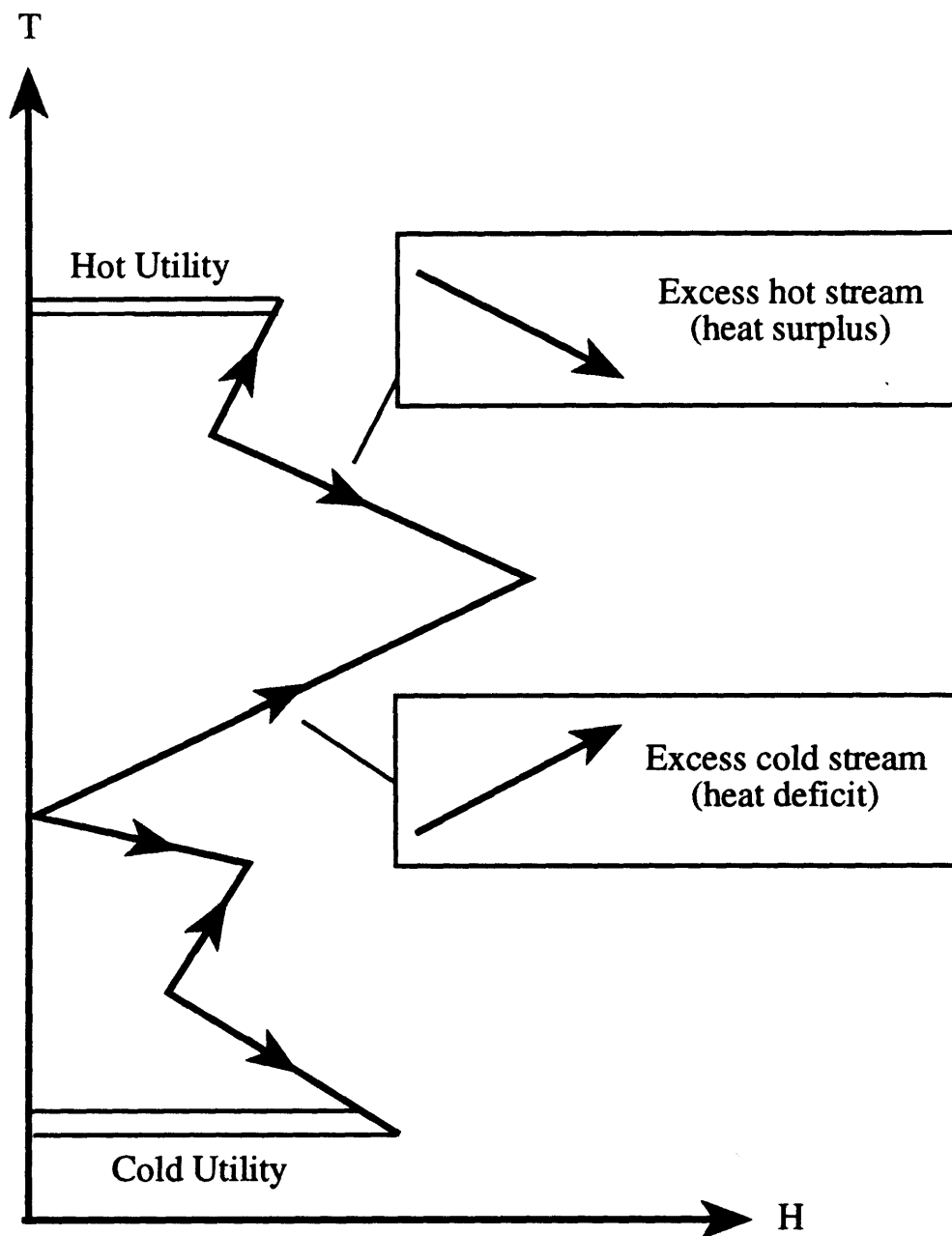


FIGURE 3.12 Identifying regions with heat surpluses or deficits in the grand composite curve. (Townsend and Linnhoff, 1983b)

Consider the shaded regions, called "pockets", in the grand composite curve shown in Figure 3.13. The part with the excess hot streams (negative slope) represents a local heat source. By the heat cascading principle, the heat of the local heat source is hot enough to be transferred into the lower temperature parts of the process. Normally, transferring this heat into the part of the process right underneath allows for the best possible use of different utility levels. The process takes care of itself (it is in energy balance) in the shaded regions. For minimum energy consumption only the parts of the graph outside the pockets need to be matched with external utilities.

### **3.2.1 Superstructure for Integrated Utility Systems : Quantifying the Appropriate Placement Rules**

As said before, the grand composite curve quantifies the process heat sink and the process heat source. The minimum hot and cold utility requirements are easy to read, and the amount of intermediate utility that could be used at any temperature without transferring heat across the pinch (condition for minimum energy consumption) is given by the horizontal distance to the grand composite curve once the shaded regions (or pockets) have been added. The rest of this section uses the grand composite curve and the appropriate placement rules to develop a superstructure that could be used for the design and optimization of utility systems and heat exchanger networks (by solving an MINLP). In this thesis, MINLP will not be used to solve the proposed superstructure. The superstructure only provides a theoretical framework that includes the heat and work interactions between the utility system and the heat exchanger network. In Chapter 4, the superstructure is used as a guideline to develop a method that targets for the capital and operating costs of the utility system and takes into accounts its heat and work interactions with the chemical process and the heat exchanger network.

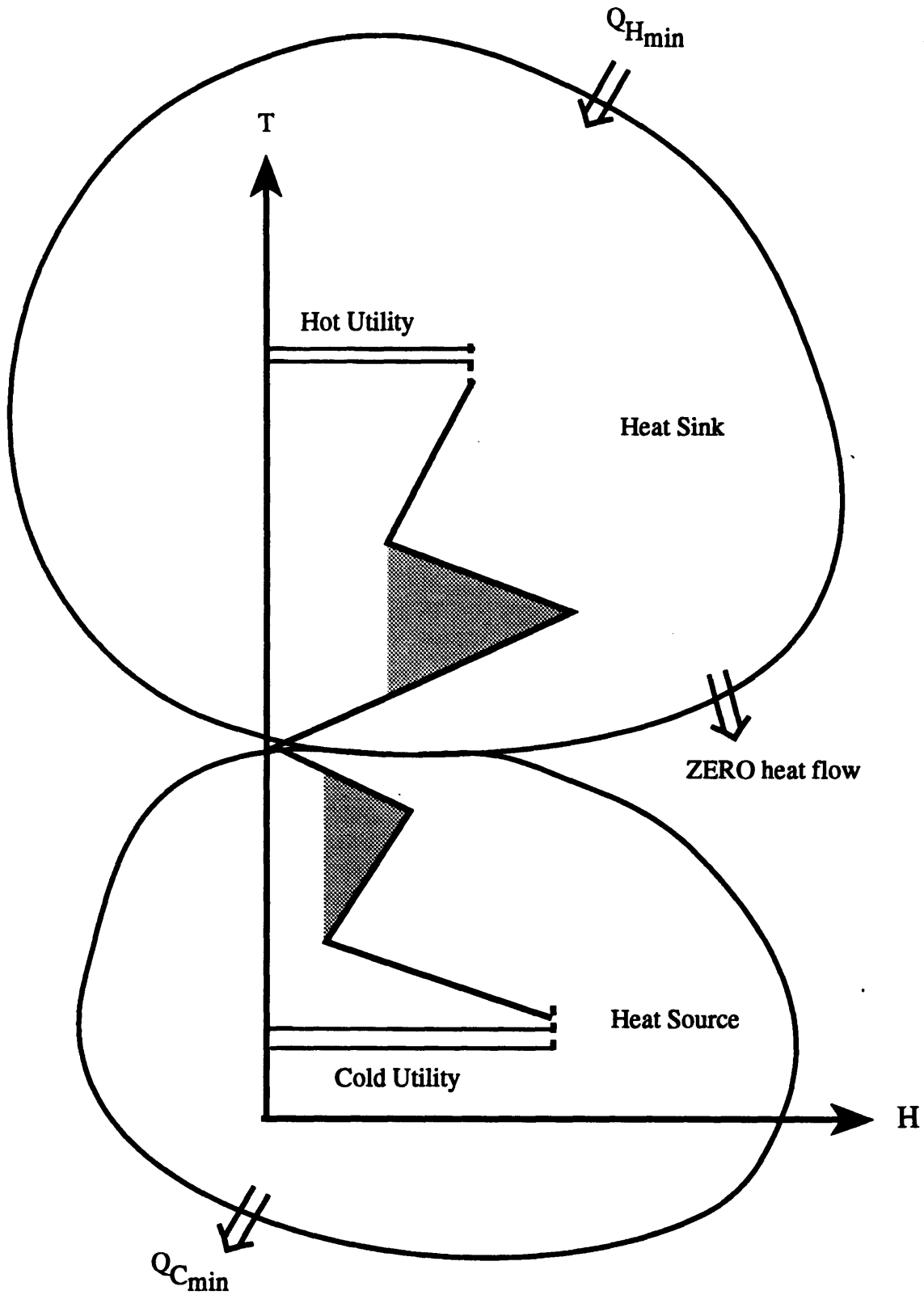


FIGURE 3.13 Illustrations of the shaded regions (or "pockets") in the grand composite curve. (Townsend and Linnhoff, 1983b)

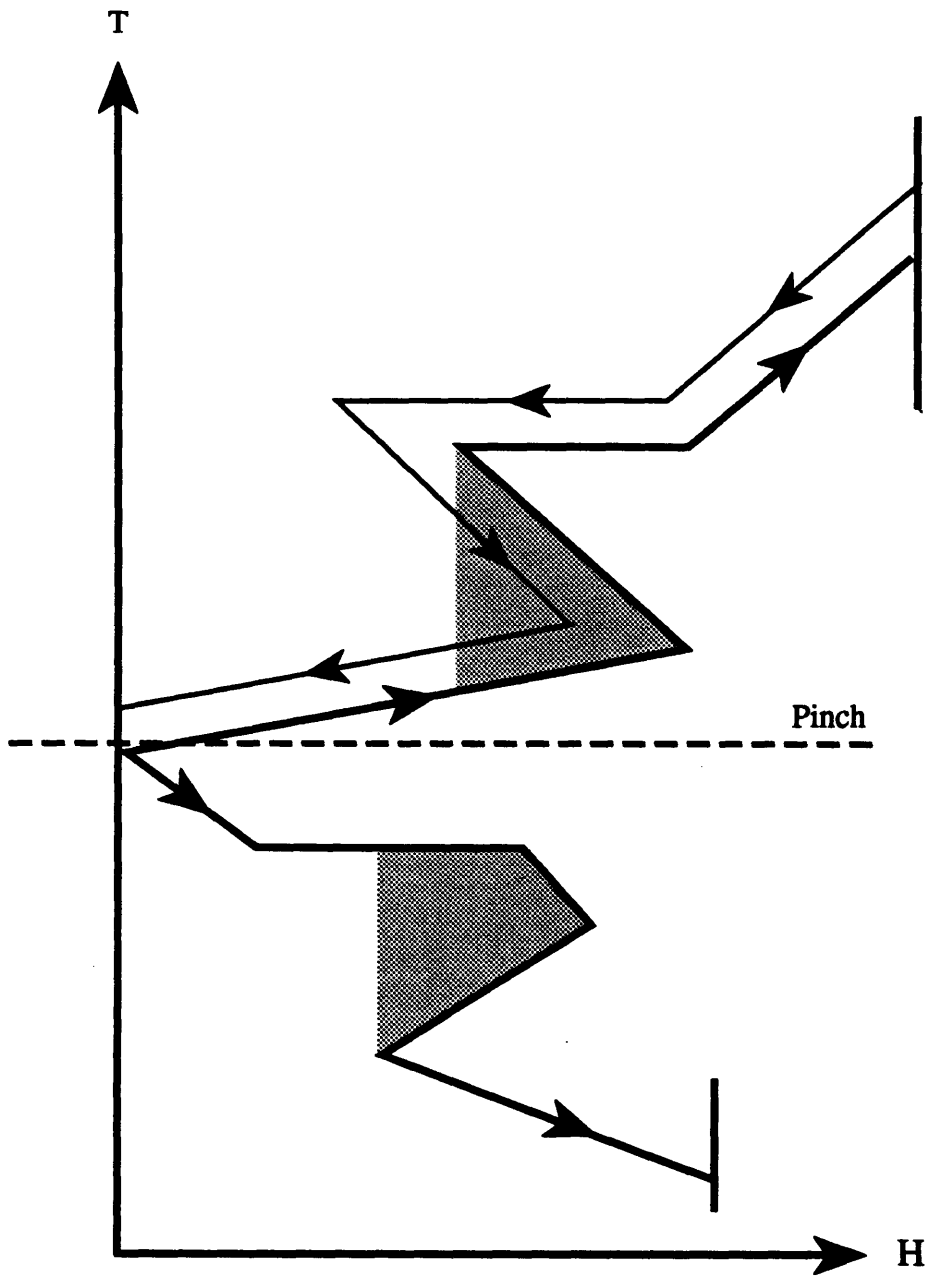
### **3.2.2 Work and Hot Utility Production Section (satisfying the process heat sink)**

Townsend and Linnhoff (1983a) showed graphically that if the process heat sink is satisfied by the exhaust of a heat engine, better overall efficiencies could be obtained for the production of hot utilities and work than stand alone use of heat engines (appropriate placement rules). A heat engine above the pinch could be thought of as the part of a utility system that produces work needed by the process and rejects heat above the pinch in the form of hot utilities. This can be done at various levels, if the economics are favorable. Figure 3.14 shows the exhaust of a theoretical heat engine that produces the maximum amount of work while delivering the minimum hot utility required. In terms of available energy, this is the best engine possible. In terms of total cost, the high capital cost involved to produce such an engine will make other designs more attractive.

For now, in order to start building the superstructure, it is assumed that steam obtained at different extraction levels from a steam turbine is the only hot utility being produced. Hot oil, exhaust from a gas turbine, hot gas from direct process heaters or other hot utilities will be considered later. The grand composite curve gives the hot and cold utility requirements of the process both in enthalpy and temperature, but it is unclear at what temperature level or how many steam levels should be produced by the utility system (Figure 3.15). An infinite number of steam levels can approximate the exhaust of the maximum (thermodynamically best) work producing engine.

Yoon (1990) reduced the size of the problem by claiming that, for a given number of steam levels, the most economical design is usually obtained if these levels provide the steam at the kinks in the grand composite curve, where a process stream either enters or leaves. Thus, when the heat exchanger network is designed, one less exchanger is needed than the case where steam is not added at a kink. This is a very questionable heuristic. The heuristic does not specify the number of steam levels but it fixes their temperature. He then uses simulations





**FIGURE 3.14** The heat absorption-rejection profile of a theoretical heat engine that produces the maximum amount of work without rejecting heat below the pinch. (Townsend and Linnhoff, 1983b)

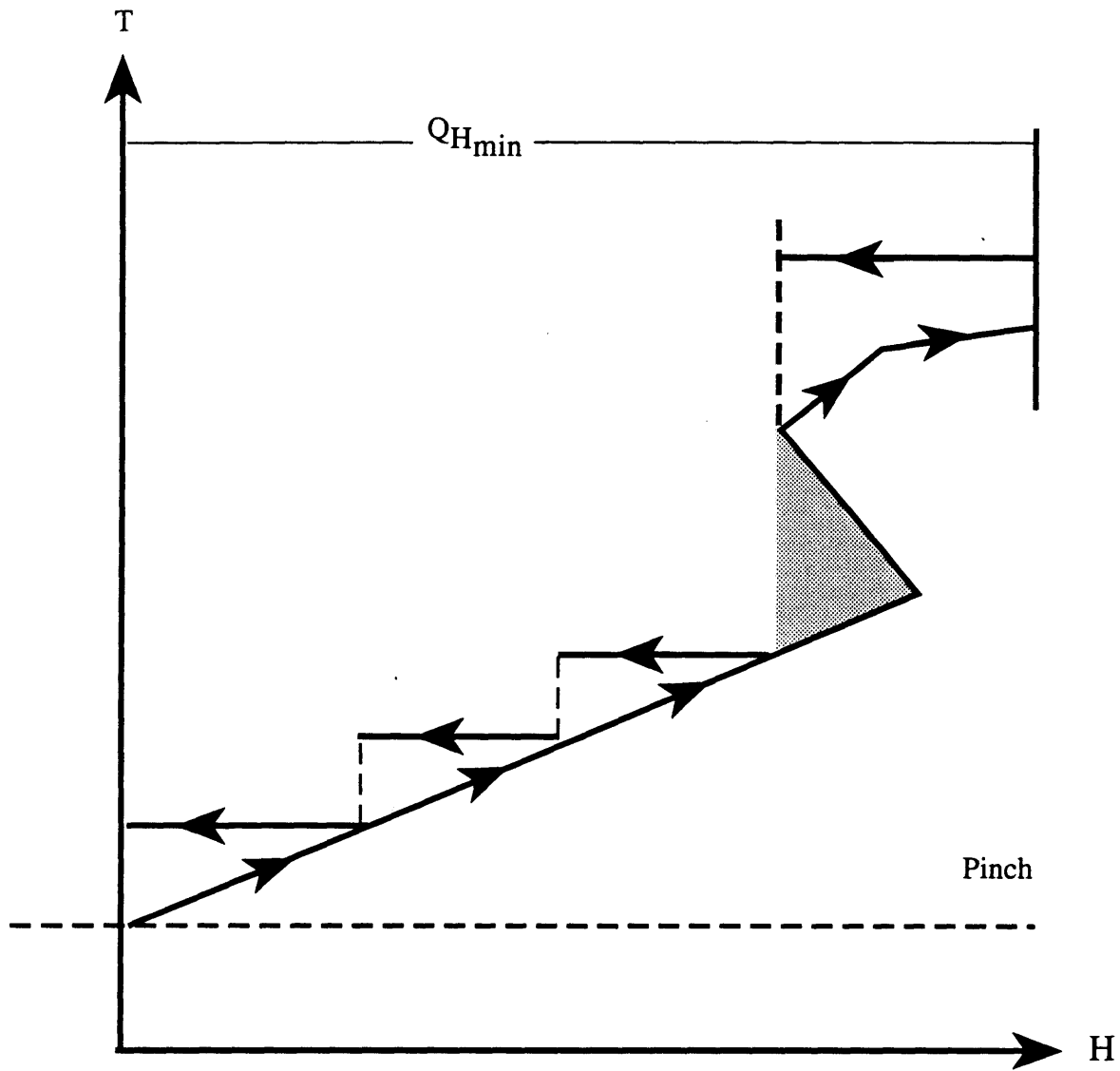
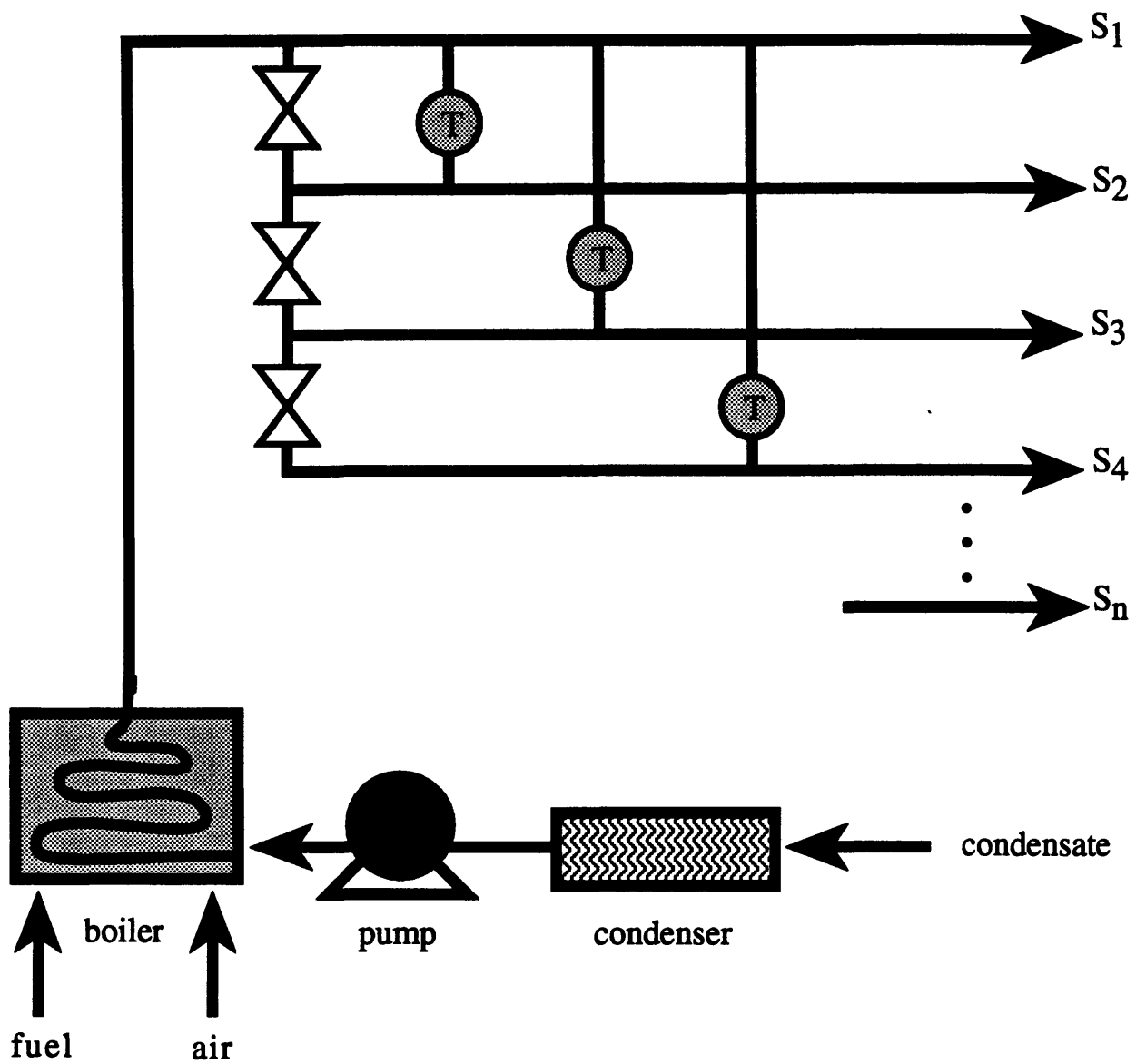


FIGURE 3.15 The possibility of using many steam levels to satisfy the process heat sink.

to capture the performance of steam turbines at the given kink temperatures. Finally, the simulation results are used to linearize the remaining problem and a superstructure that could be solved with MILP is proposed for the design and optimization of an integrated utility system above the pinch. His heuristic is questionable, but the method captures some of the heat and work interactions between the utility system and the heat exchanger network.

If Yoon's (1990) requirement that steam be produced at temperatures that match the kinks in the grand composite curve is not followed, linearization of the problem is not performed, and information on the effects of steam temperature and heat duty on the capital cost of the heat exchanger network is included in the objective function, the structure and operating conditions of the utility system and its heat exchanger network above the pinch could be optimized by solving an MINLP. The superstructure shown in Figure 3.16 does not make Yoon's (1990) simplifications and follows the appropriate placement rules. A large number of steam levels should be included in the superstructure to insure the global optimum is contained in the superstructure. This theoretical method, although able to account for most of the utility system and heat exchanger network heat and work interactions above the pinch, would be computationally very expensive.

The utility system must not only satisfy the complete process' hot utility demand but also its work demand. In order to satisfy both demands at minimum cost, the appropriate placement rules might have to be violated. Figure 3.17 shows the extension of the superstructure to allow for violations of the appropriate placement rules. The steam turbine is allowed to reject heat at ambient temperature to extract more work from the steam, and a gas turbine is added to the superstructure to produce work at a higher efficiency with the possibility of co-generation.



Pinch temperature -----

FIGURE 3.16 The superstructure of a utility system that satisfies the process heat sink without rejecting heat below the pinch.

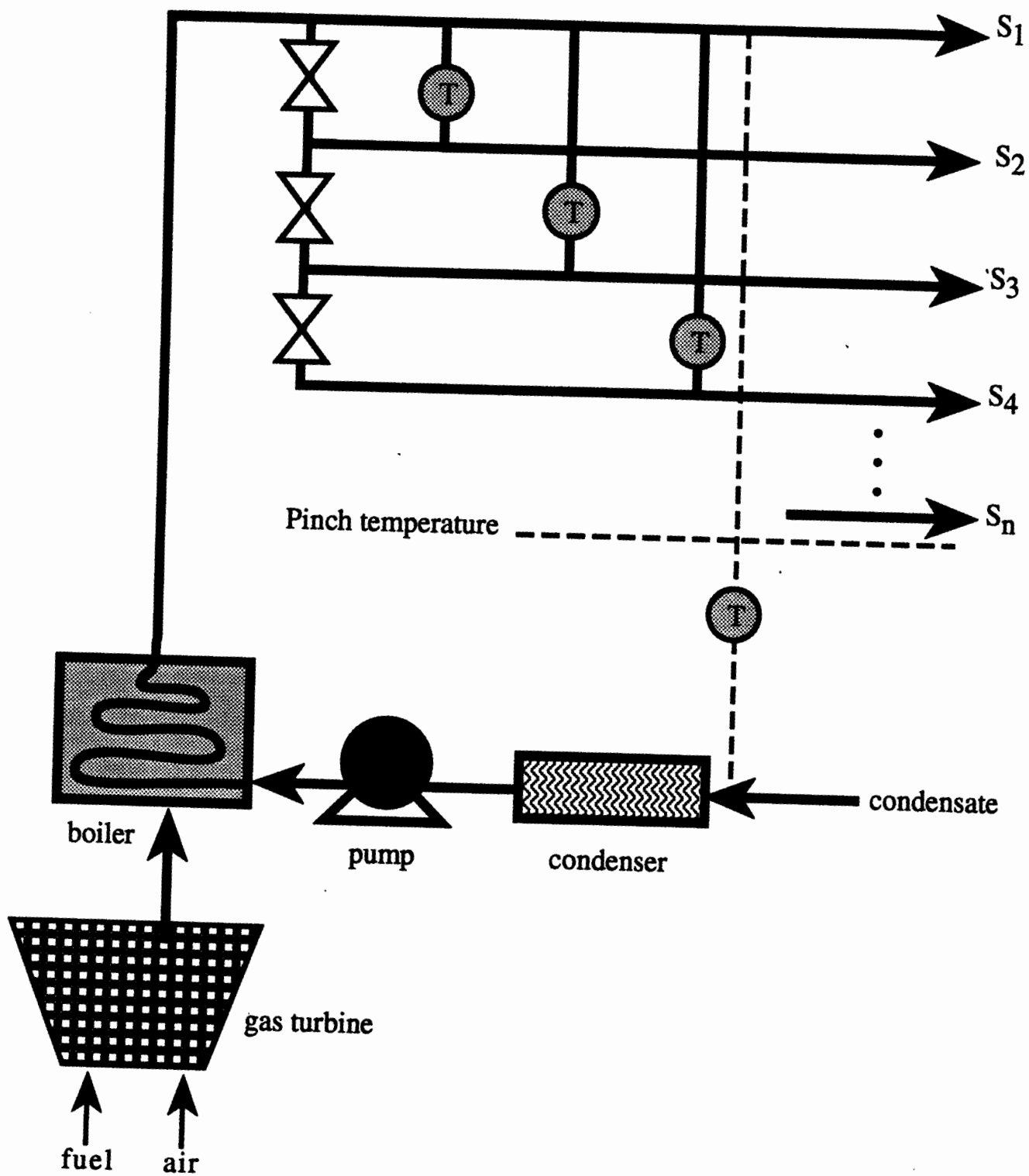


FIGURE 3.17 The superstructure of a utility system that satisfies the process heat sink but allows a condensing turbine and a gas turbine to reject heat below the pinch.

According to the appropriate placement rules, a heat engine can also be placed below the pinch. The possibility of work production below the pinch should also be explored as an alternate source of work. Figure 3.18 shows the absorption profile of a theoretical heat engine that produces the maximum amount of work from a given process source. Again, this is the best engine in terms of available energy, but not in terms of total cost. The process heat source is limited in size ( $Q_c$ ) and in temperature (pinch temperature). The principles involved in fitting organic rankine cycles to heat sources have been explored by Sega (1974) and Milora and Tester (1976).

When dealing with a process heat source, the principles remain the same. Figure 3.19 shows the advantages of choosing a working fluid that operates above critical conditions. Profile 1 is far from critical, and although the exchanger requires less area than profile 2, Milora and Tester (1976) have shown that the loss of availability in profile 1 makes profile 2 a much better alternative for work production. Figure 3.20 shows the load versus level tradeoff. Profile 1 absorbs more energy than profile 2, but at a lower level.

When incorporating work production below the pinch to the superstructure for integrated utility system, it could be assumed that the thermodynamically best engine is used. This engine cost could be determined with Milora and Tester's (1976) organic rankine cycles' cost correlations. The result is an engine that produces the maximum amount of work possible at a cheaper cost. This could be justified because, in general, according to Yoon's (1990) studies, organic rankine cycle work production below the pinch will not be economically competitive with work production above the pinch. If the MINLP solution to the superstructure where to contain the organic rankine cycle, further inspection would be required. Subsection 3.2.4 will show how the heat engine below the pinch can be incorporated into the heat engine above the pinch by using the process heat source to preheat air or boiler feed water. In general, this is a better alternative than having a separate organic rankine cycle.

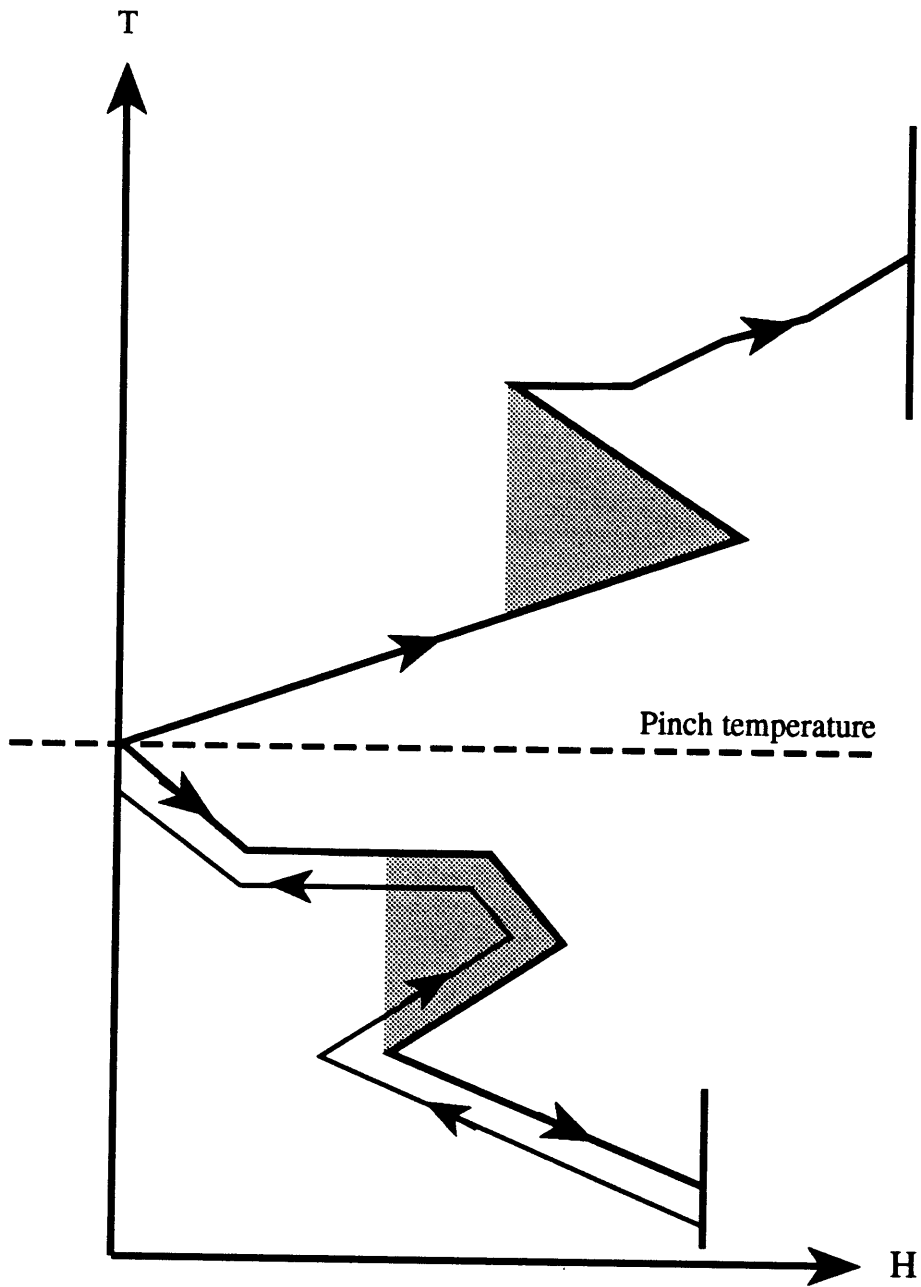


FIGURE 3.18 The heat absorption-rejection profile of a theoretical heat engine that produces the maximum amount of work and uses only the process heat source as its source of heat. (Townsend and Linnhoff, 1983b)

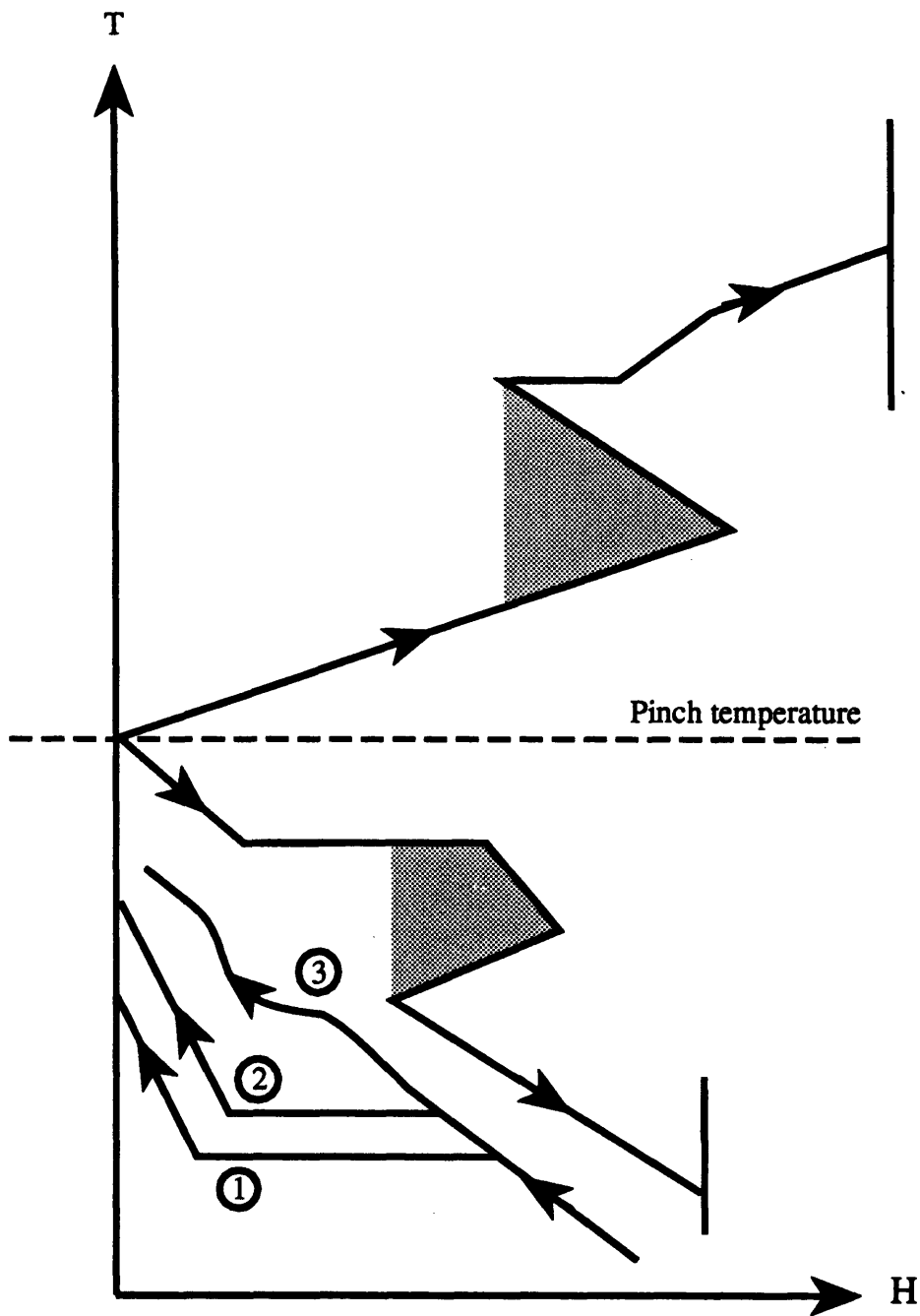


FIGURE 3.19 The advantages in work production of using a supercritical working fluid when using an organic rankine cycle to mine heat from the process heat source. (Townsend and Linnhoff, 1983b)



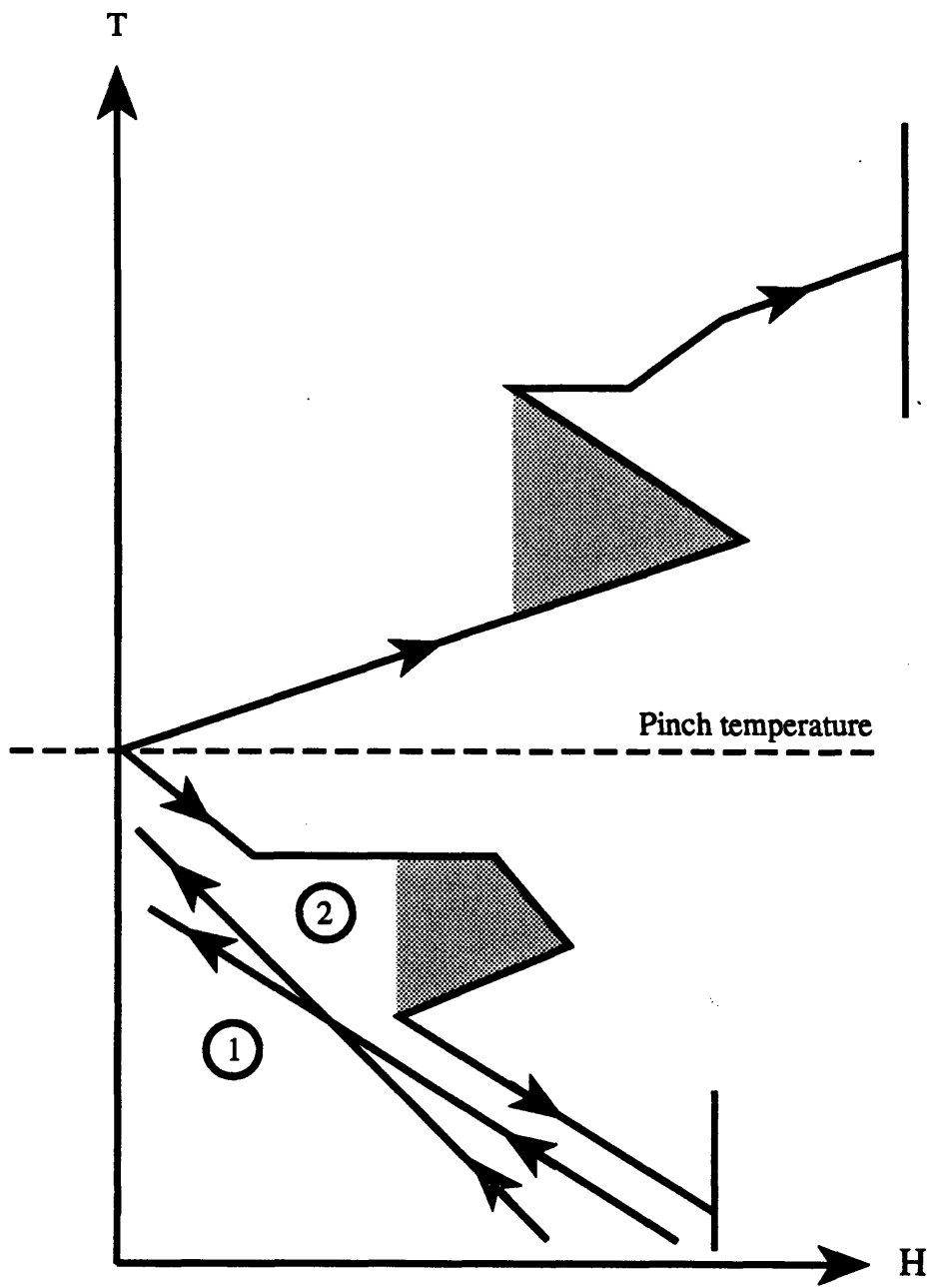


FIGURE 3.20 The heat load versus temperature level tradeoff when using an organic rankine cycle to mine heat from the process heat source. (Townsend and Linnhoff, 1983b)

Townsend and Linnhoff (1983a,b) and Colmenares and Seider (1986) recognized that a local heat source (or pocket in the grand composite curve) above the pinch could also be used for work production. If a heat engine is run by a local heat source above the pinch, the heat engine is called an interprocess heat engine. This engine could follow the appropriate placement rules by rejecting heat above the pinch or break the appropriate placement rules to produce more work by rejecting heat at ambient temperature. The principles involved in fitting an interprocess heat engine are the same as for fitting an organic rankine cycle to a heat source.

Like the process heat source, the local heat source above the pinch is limited in size and in level. Unless the local heat source above the pinch is at a high level or has a very large duty, it is unlikely that a cost efficient heat engine could utilize it for work production. Nevertheless, the engineer should be alert in case an unusually large local heat source above the pinch is present. The local heat source above the pinch is also likely to be composed of various process streams, further complicating its potential use for the production of work. The use of local heat sources above the pinch to run interprocess heat engines is left out of the proposed superstructure for integrated utility systems. Subsection 3.2.4 will show how the interprocess heat engines can be incorporated into the heat engine above the pinch by using the heat of local heat sources in the heat engine above the pinch. This concludes the analysis of the work production section of the utility system.

The process heat sink can also be satisfied with other hot utilities such as hot oil, hot gas from process heaters, or hot gas from gas turbine exhaust. Hot gas from process heaters or gas turbine exhaust as hot utilities can be dangerous and hard to control. For safety and control, it is preferred if these utilities are used to produce steam. Nevertheless, if they were to be used, they could be treated in the same manner as the hot oil utility (non-condensing hot

utility). Non-condensing hot utilities have the property that their temperatures changes significantly during heat exchange. The superstructure for integrated utility systems above the pinch should be extended to account for these types of utilities.

Although the appropriate placement rules have shown that heat pumps across the pinch reduce the hot and cold utility demand, it is not clear if they are cost effective. More capital intensive work consuming equipment is used to replace less expensive utilities, and depending on the ratio of hot utility demand decrease over work used, that is the effective coefficient of performance, it may not make economic sense. Yoon (1990) has shown that, even for moderate pinch temperatures, heat pumps are usually not a good economic alternative. For this reason, heat pumps across the pinch are not proposed in the superstructure for integrated utility systems above ambient temperature.

### **3.2.3 Work Consumption and Cold Utility Production Section**

**(satisfying the process heat source)**

As said before, the cold utility production section of the utility system should be divided at the ambient temperature. Below ambient temperature the process heat source must be satisfied by a refrigeration system. Above the ambient temperature, the process heat source can be satisfied with a cooling water system and/or used to preheat air and/or boiler feed water (if process heat source is hot and large enough it could raise steam.)

The simplest way to satisfy the process heat source above ambient temperature is a cooling water system. The cooling water system can be added to the superstructure for integrated utility system as shown by Yoon (1990). The use of the process heat source to preheat air or boiler feed water should also be explored. Using the source in this manner will reduce the size of the process heat source and therefore the load on the cooling water system. Linnhoff (1988) has shown that overall furnace efficiencies could be improved by using the process

heat source to preheat air. He also showed that the use of excess air need not be an expensive alternative and could lead to reduced emissions in the utility system. A well designed integrated utility system should examine all alternative uses for the process heat source above ambient temperature.

If refrigeration is needed by the chemical process then it must be provided by a refrigeration system. A refrigeration system can be thought of as a multi-extraction heat pump (Figure 3.21). Industrial refrigeration designers know well that pumping low level heat all the way up to ambient temperature is an expensive alternative. More economic designs could be obtained if heat is pumped into local process heat sinks at intermediate temperature levels ("economizers"). Local process heat sinks are easily identified in the grand composite curve. An important heat and work interaction with the chemical process occurs by changing process operating conditions, if the economics are favorable, to alter the size of these local process heat sinks.

Therefore, the refrigeration system should be designed as a multi-extraction, multi-rejection heat pump. In order to take into account all the heat and work interactions with the heat exchanger network, the effects of the refrigeration utilities temperature and their heat duties on the capital cost of the heat exchanger network must be included in the objective function. Figure 3.22 shows the superstructure for a refrigeration system that can, theoretically, simultaneously optimize a refrigeration system and its heat exchanger network (by solving an MINLP). A large number of extraction and rejection levels should be included in the superstructure to ensure the global optimum is contained in the superstructure.

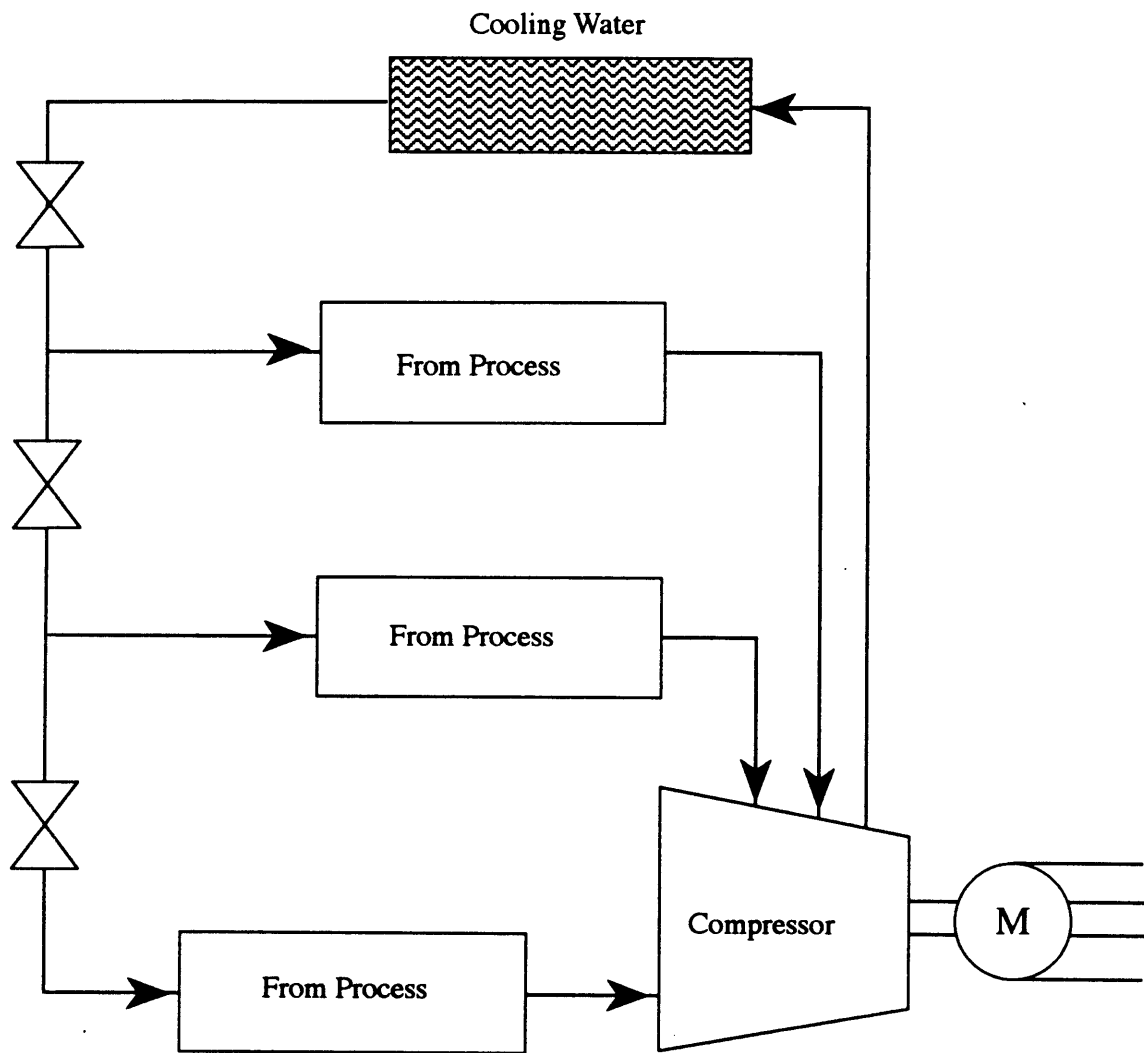
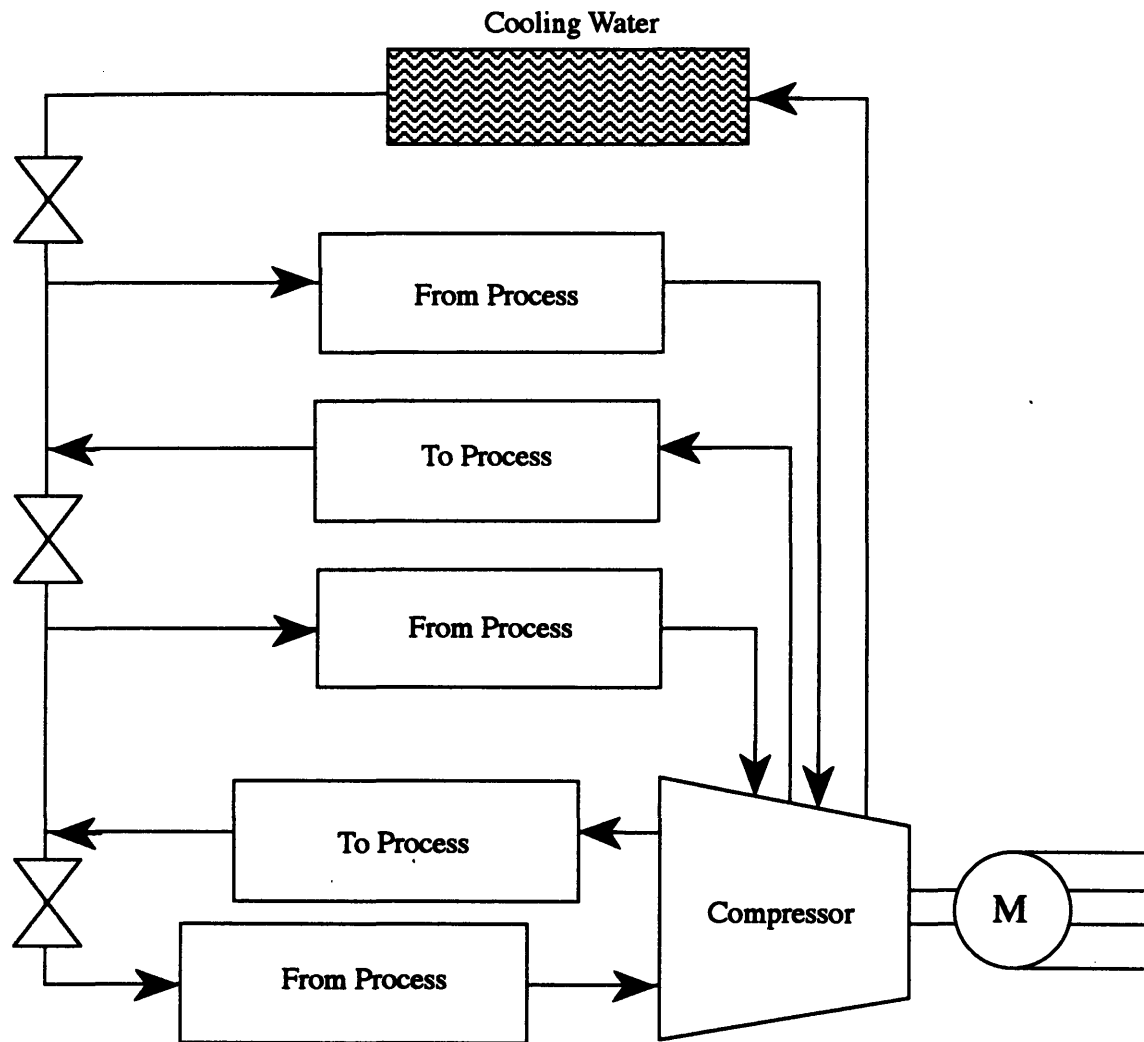


FIGURE 3.21 The below ambient temperature superstructure of the utility system that treats the refrigeration systems as a multi-extraction heat pump.



**FIGURE 3.22** The below ambient temperature superstructure of the utility system that treats the refrigeration system as a multi-extraction multi-rejection heat pump.

### **3.2.4 The Superstructure for Integrated Utility Systems**

The components for integrated utility systems discussed in sub-sections 3.2.2 and 3.2.3 are summarized in Figure 3.23. In order to reduce the size of the problem, the proposed superstructure for integrated utility systems will eliminate or merge components that, typically, were shown to be unimportant when considered alone. The engineer should be aware in case special circumstances arise where eliminating or merging these components is not a good idea.

The utility system is as a work producer above ambient temperature and a work consumer below ambient temperature. The possible sources of work above ambient temperature are the heat engine above the pinch, the heat engine below the pinch, and the interprocess heat engines (Figure 3.23). The heat engine below the pinch and the interprocess heat engines use process streams as heat sources. Therefore, their heat sources are limited in size and in temperature level. These engines are usually organic rankine cycles used for low temperature heat recovery and work production.

The heat engine above the pinch uses fuel as its heat source. Therefore, its heat source is not limited in size and the fuel's theoretical flame temperature limits its temperature level. The superstructure of the heat engine above the pinch was already shown in Figure 3.17. The heat engine above the pinch can adopt various forms. If a small amount of work is required by the process or imported work is available and inexpensive, the heat engine above the pinch will take on the form of a steam boiler. If large amounts of work are required by the process and imported power is expensive, the heat engine above the pinch will take on the form of a gas turbine co-generation cycle. If the process demand for work and the price of imported work are not at an extreme, the heat engine above the pinch could take on the form of a steam

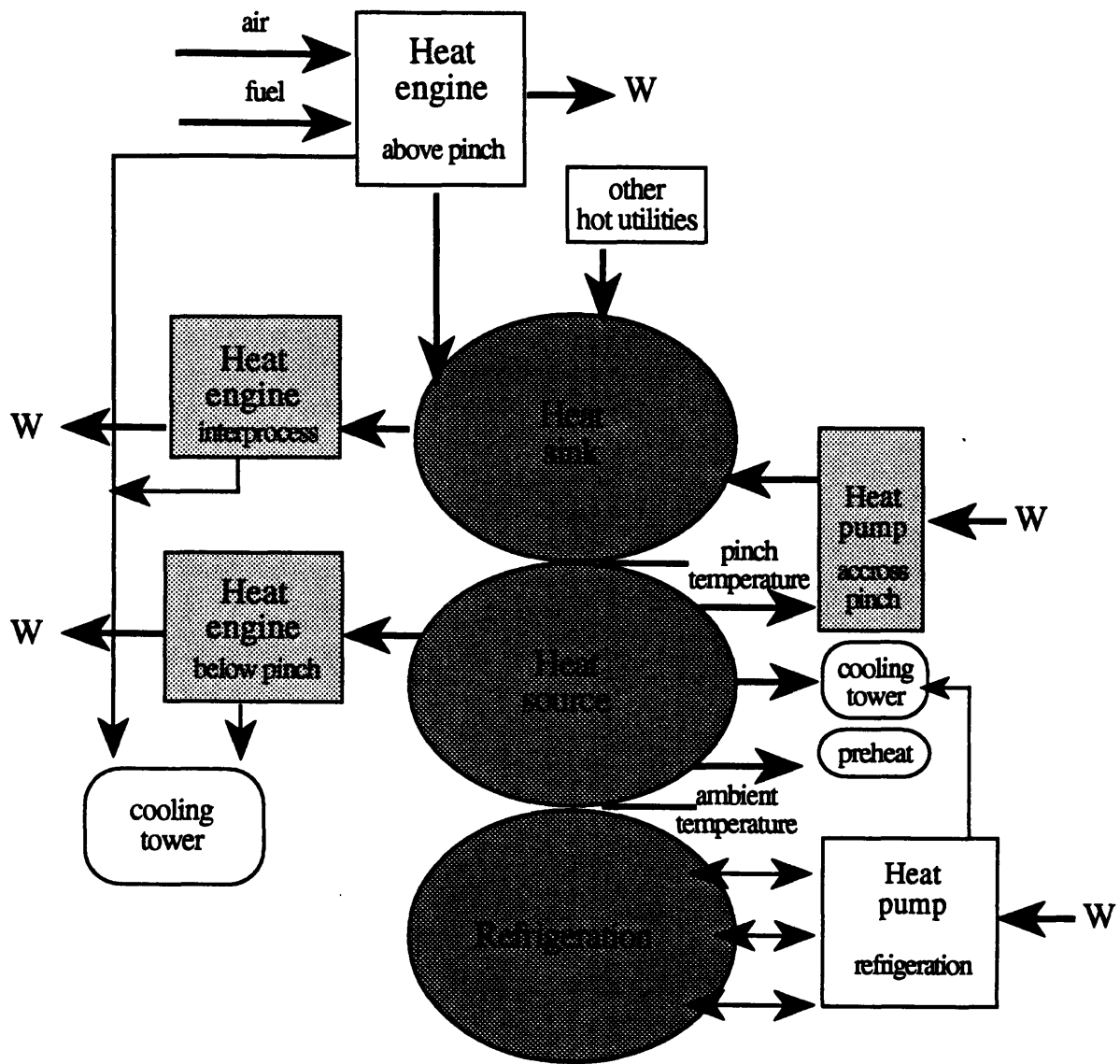


FIGURE 3.23 Summary of the previously discussed components in the superstructure for integrated utility systems.



turbine co-generation cycle. Yoon's (1990) preliminary studies suggest, that in the chemical industry, organic rankine cycles utilizing process heat sources are not economically competitive with steam cycles or co-generation steam cycles.

Linnhoff (1988) has shown that if a furnace is used to produce hot air as a hot utility, the overall furnace efficiency could be improved by using the process heat source to preheat air. The overall efficiency of the utility system should also improve if the process heat source is used to preheat air or boiler feed water.

Figure 3.24 shows the complete proposed superstructure for integrated utility systems. Since the heat engine below the pinch and the interprocess heat engines are usually not competitive with the heat engine above the pinch for the production of work and hot utilities (steam), the proposed superstructure for integrated utility system above ambient temperature could be thought of as a single heat engine (a steam cycle or co-generation steam cycle). The proposed heat engine produces the work demanded by the chemical process and the refrigeration section of the utility system, rejects heat at various levels to the process heat sink in the form of steam (hot utility), and uses the process heat source to preheat air or boiler feed water to improve the overall efficiency of the utility system. In a sense, the process heat source is incorporated into the steam or co-generation steam cycle by using it to preheat. Local heat sources above the pinch could also be incorporated into the steam or co-generation steam cycle by using them to preheat air or boiler feed water or to produce steam.

The proposed superstructure for integrated utility systems above ambient temperature is completed by allowing other hot utilities to satisfy the process heat sink and also by allowing the process heat source to reject heat into cooling water (Figure 3.24). The superstructure for integrated utility systems below ambient temperature can be envision as a multi-extraction, multi-rejection heat pump and was given in Figure 3.22. So, the proposed superstructure for integrated utility systems is basically a heat engine above ambient temperature and a heat

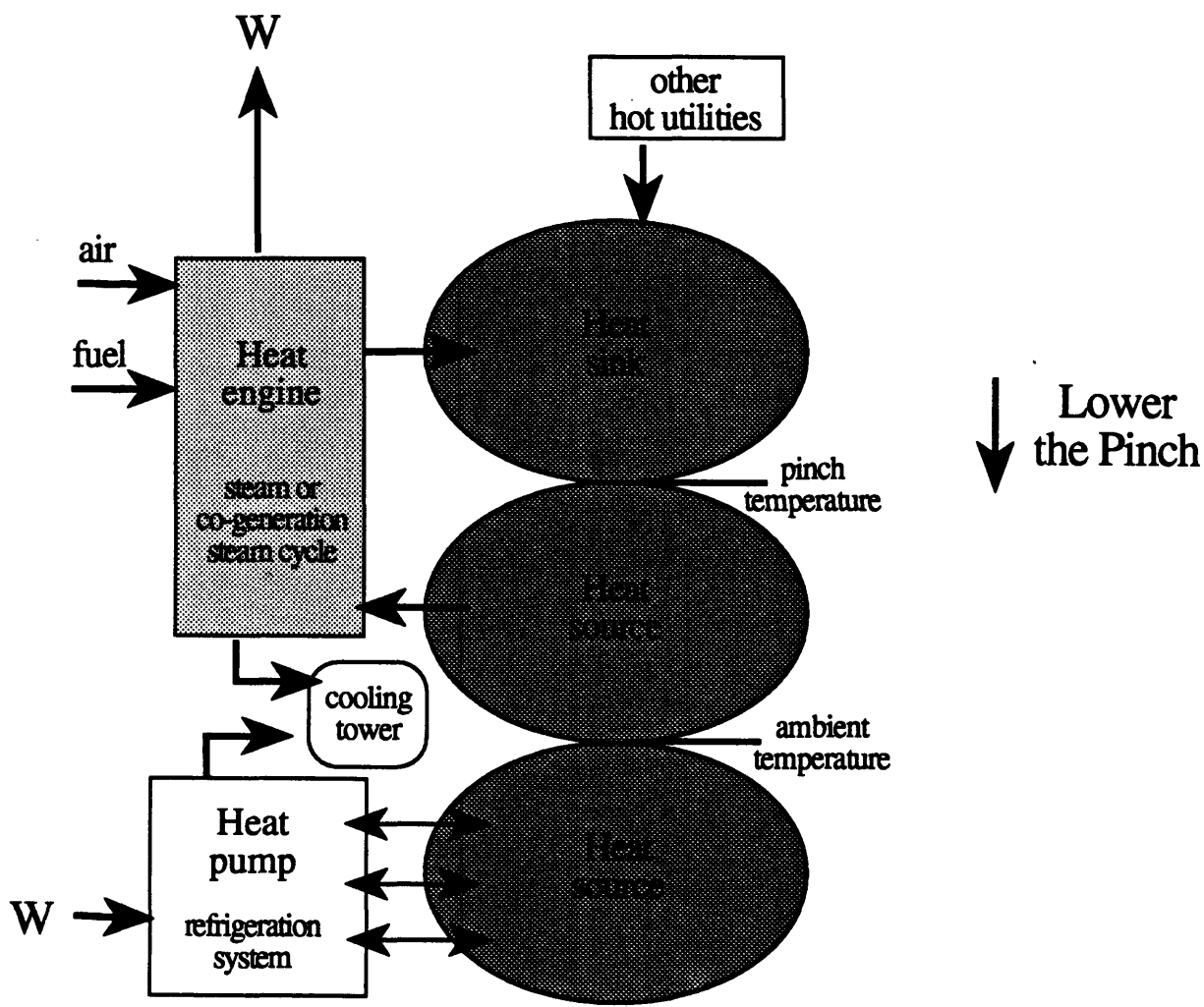


FIGURE 3.24 The proposed superstructure for the design and optimization of integrated utility systems.

pump below ambient temperature. The superstructure has the desired property that, theoretically, it can custom fit most chemical processes. Processes with high refrigeration requirement will have different superstructures solutions than processes with large process heat sources or large process heat sinks above ambient temperature.

The superstructure of Figure 3.24 is a large and difficult MINLP problem to solve. Many steam levels for the heat engine above ambient temperature and many extraction and rejection levels for the heat pump below ambient temperature need to be included in the superstructure to insure the global optimum is contained in the superstructure. In addition the effects of the utility temperatures and heat duties on the capital cost of the heat exchanger network must be included in the objective function to account for the heat and work interactions with the heat exchanger network. As said before, this superstructure will not be solved in this thesis. The purpose of this superstructure was to conceptually develop a method that can simultaneously design and optimize utility system and heat exchanger networks. In Chapter 4 this superstructure serves as guideline to develop a method that targets for the capital and operating costs of the utility system and takes into accounts its heat and work interactions with the chemical process and the heat exchanger network.

### **3.3 Chemical Process, Heat Exchanger Network and Utility System**

#### **Heat and Work Interactions**

If the utility system above ambient temperature is seen as a steam or co-generation steam cycle (Figure 3.24), an observation of a heat and work interaction between integrated utility systems and chemical processes can be formulated. The overall efficiency of the utility system above ambient temperature could be improved by changing process conditions such that the pinch is lowered to ambient temperature. Lowering the pinch below ambient temperature will improve the efficiency of the refrigeration section by lowering the rejection temperature of the multi-extraction, multi-rejection heat pump. Therefore, lowering the pinch improves the

efficiency of the integrated utility system (Figure 3.24). Linnhoff and Parker (1984) showed that if the utility system is a furnace, the overall efficiency of the furnace could be improved by lowering the pinch. The key point here is an extension of Linnhoff and Parker's (1984) observation that does not restrict the utility system to be a furnace.

The observation of improved utility efficiencies with lower pinch temperatures, like the plus/minus principle and the appropriate placement rules, is based only on improving heat or work integration. Changing process conditions to follow any of these principles can cause inefficient use of capital and raw materials and a higher total system cost.

In Section 3.1 an extended pinch location method was proposed to quantify the plus/minus principle and optimize chemical process and heat exchanger networks (fixed utility system). In Section 3.2 a theoretical superstructure was presented to quantify the appropriate placement rules. This superstructure could be used to design and optimize heat exchanger networks and utility systems (fixed chemical process) by solving an MINLP. The extended pinch location method combined with the MINLP superstructure approach for integrated utility system could be used to quantify this new observation and solve simultaneously the chemical process, its heat exchanger network, and the utility system and take into account their heat and work interactions.

The problem with combining these two methods is that the superstructure problem by itself is a hard and computationally expensive problem to solve. A new method to target for the utility system capital and operating costs without the computation expense of the superstructure approach is needed. This new method is based on the superstructure of Section 3.2 and is developed in Chapter 4. The simultaneous optimization method presented in this thesis is a combination of this new method with the extended pinch location method

proposed in Section 3.1. The result is the first tractable method that can simultaneously optimize a chemical processes, its heat exchanger network, and utility systems and take into account their heat and work interactions.

### Notations used in Chapter 3

$c_c^i$	unit thermal cost of cold utility i
$c_h^i$	unit thermal cost of hot utility i
C	index for cold process streams
CU	number of cooling utilities
$f_i$	flowrate of cold process stream i
$f_i c_i$	heat capacity-flowrate product for cold process stream i
$F_i$	flowrate of hot process stream i
$F_i C_i$	heat capacity-flowrate product for hot process stream i
$F(\underline{x}, \underline{y})$	function to evaluate the chemical process' capital and operating costs
$g(\underline{x}, \underline{y})$	vector of inequality constrains
$h(\underline{x}, \underline{y})$	vector of equality constrains
H	index set of hot process streams
HU	number of hot utilities
$N_c$	number of cold stream
$N_h$	number of hot stream
p	index set for candidate pinch
$Q_c$	minimum cold utility demand
$Q_h$	minimum hot utility demand
$Q_c^i$	thermal duty of cooling utility i
$Q_h^i$	thermal duty of heating utility i
$QSIA(\underline{y})^p$	heat sink above pinch candidate p
$QSOA(\underline{y})^p$	heat source above pinch candidate p
$t_i^{in}$	supply tempearture for cold process streams
$t_i^{out}$	target temperature for cold process streams
$T_i^{in}$	supply temperature for hot process streams
$T_i^{out}$	target temperature for hot process streams
$T^p$	pinch candidate temperature
$\underline{x}$	vector of process parameters
$\underline{y}$	vector of flowrates and temperatures of process streams
$z_h^p(\underline{y})$	heating deficit above pinch candidate p
$\Delta T_{min}$	minimum approach temperature for process heat integration
$\phi$	objective function
$\Omega(\underline{y})$	difference in heat content between hot and cold process streams

## **CHAPTER 4 : DEVELOPMENT OF MATHEMATICAL PROGRAMS TO ACCOUNT FOR THE SUBSYSTEMS' HEAT AND WORK INTERACTIONS**

### **4.1 Extending the Pinch Location Method to Target for the Capital Cost of the Heat Exchanger Network**

Section 3.1 suggested that extending Duran and Grossmann's (1986) pinch location method to target for the capital cost of the heat exchanger network would lead to a method that can simultaneously optimize a chemical process and its heat exchanger network. Since all major heat and work interactions between the chemical process and the heat exchanger network are included in such a method, the chemical process operating conditions can be simultaneously optimized along with the flowrates and supply and target temperatures of the process streams undergoing heat exchange (heat exchanger network operating conditions) as well as the minimum approach temperature for process heat exchange.

Linnhoff and Ahmad (1990) used simple models to target for the capital costs of heat exchanger networks prior to design. They showed that typically, networks can be developed that are within 5% of the total cost target. In their method, a selected utility mix is first matched against the grand composite curve. Then, the balanced composite curves are used to target for the capital cost of the heat exchanger network. The balanced composite curves are the composite curves with the fitted utilities treated as if they were process streams.

This section incorporates Linnhoff and Ahmad's (1990) method to target for the capital cost of the heat exchanger network in the pinch location method. Therefore, the rest of the section is dedicated to show how information in the heating deficit functions ( $z_H^p(\mathbf{y})$  in NLP P1) can be used to obtain the grand composite curve, the balanced composite curves, and target for the capital cost of the heat exchanger network.

#### 4.1.1 Using the Heating Deficit Functions to Obtain the Grand Composite Curve

The pinch location method is based on the observation that if all process streams or stream segments have constant heat capacity-flowrate products, the pinch can only occur at the inlet temperature of a process stream or stream segment (Linnhoff et al., 1982). Duran and Grossmann (1986) showed that if all the supply temperatures of process streams or stream segments are chosen as pinch candidates,  $T^p$ , and heat balances are performed above each pinch candidate, the pinch candidate yielding the largest net heat sink (for a heat balance above its temperature) corresponds to the process stream or stream segment causing the pinch. The pinch candidates for cold process streams or stream segments must have their value increased by the minimum approach temperature.

Consider the 4SP1 problem (Table 4.1) used by Duran and Grossmann (1986) to illustrate this fact. Figure 4.1 shows the heat sinks corresponding to each pinch candidate. The candidate with the largest heat sink corresponds with the process stream or stream segment that causes the pinch. The size of this largest net heat sink gives the minimum hot utility required,  $Q_H$ . The minimum cold utility required,  $Q_C$ , is then calculated by overall heat balance. The pinch location method has been implemented in a rigorous sequential process simulator by Lang, Biegler, and Grossmann (1988).

For easier reference, NLP P1 (Duran and Grossmann's pinch location method, 1986) is now restated. For the case of a single hot and cold utility, NLP P0 for the nonintegrated flowsheet can be modified to include heat integration (Lang, Biegler, Grossmann, 1988).

$$\begin{aligned}
 \min \phi &= F(\underline{x}, \underline{y}) + c_h Q_H + c_c Q_C \\
 \text{s.t. } h(\underline{x}, \underline{y}) &= 0 \\
 g(\underline{x}, \underline{y}) &\leq 0 \\
 Q_H &= \max_p(z_H^p(\underline{y})) && \text{(NLP P1)} \\
 Q_C &= \Omega(\underline{y}) + Q_H \\
 Q_H &\geq 0, \quad Q_C \geq 0 \\
 \underline{x} &\in X, \quad \underline{y} \in Y
 \end{aligned}$$



TABLE 4.1 The 4SP1 problem. (Lee et.al., 1970)

	FC (kW/°C)	T <sup>in</sup> (°C)	T <sup>out</sup> (°C)
H1	8.79	160	93
H2	10.55	249	138
C1	7.62	60	160
C2	6.08	116	260

$\Delta T_{\min} 10^{\circ}\text{C}$

FC = heat capacity - flowrate product

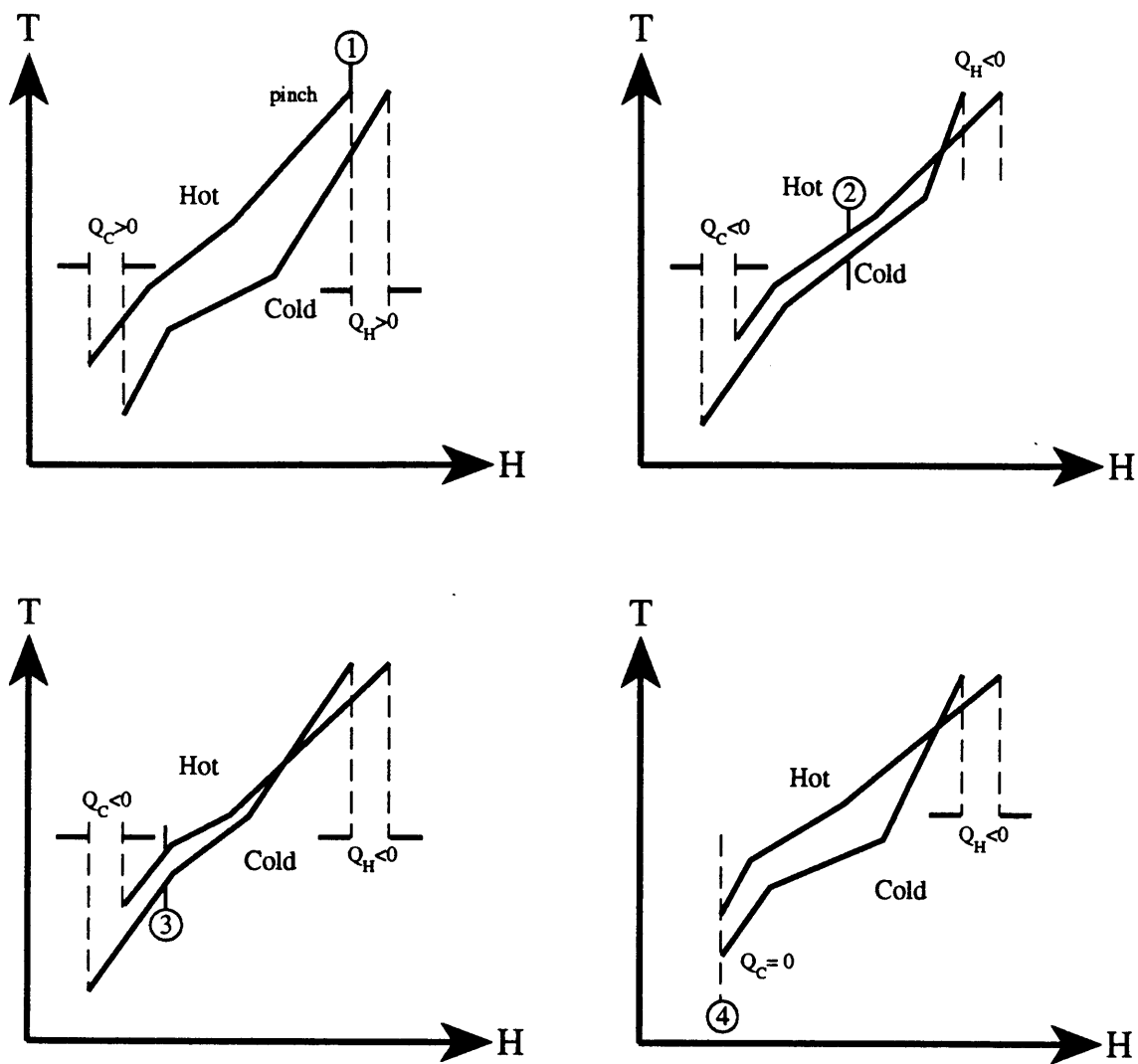


FIGURE 4.1 Heat sinks corresponding to each pinch candidate in the 4SP1 problem. (Duran and Grossmann, 1986)

where the heating deficit functions,  $z_H^p(\mathbf{y})$ , calculates the size of the heat sink at a given pinch candidate temperature,  $T^p$ ; and  $\Omega(\mathbf{y})$  represent an overall energy balance.  $z_H^p(\mathbf{y})$  and  $\Omega(\mathbf{y})$  are given by:

$$z_H^p(\mathbf{y}) = \text{QSIA}(\mathbf{y})^p - \text{QSOA}(\mathbf{y})^p \quad (4.1)$$

$$\text{QSIA}(\mathbf{y})^p = \sum_j f_j c_j [\max(0, (t_j^{\text{out}} - (T^p - \Delta T_m)) - \max(0, (t_j^{\text{in}} - (T^p - \Delta T_m)))] \quad (4.2)$$

$$\text{QSOA}(\mathbf{y})^p = \sum_i F_i C_i [\max(0, (T_i^{\text{in}} - T^p) - \max(0, (T_i^{\text{out}} - T^p))] \quad (4.3)$$

$$\Omega(\mathbf{y}) = \sum_i F_i C_i (T_i^{\text{in}} - T_i^{\text{out}}) - \sum_j f_j c_j (t_j^{\text{out}} - t_j^{\text{in}}) \quad (4.4)$$

The multiple hot and cold utility case can be solved by repeated redefinitions of the stream data and reevaluations of the heating deficit functions (Lang, Biegler and Grossmann, 1988) or, even easier, by simply fitting a selected utility mix in the grand composite curve. This subsection shows how to obtain the grand composite curve from the information in the heating deficit functions,  $z_H^p(\mathbf{y})$ .

The grand composite curve is obtained by noticing that the heating deficit functions,  $z_H^p(\mathbf{y})$ , are the differences in heat content between the cold and hot process streams above the corresponding pinch candidate temperatures,  $T^p$ . Therefore, the difference between the largest heating deficit function ( $\max_p(z_H^p(\mathbf{y}))$ ) and any other heating deficit function ( $z_H^p(\mathbf{y})$ ) is the horizontal distance between the composite curves at the latter pinch candidate temperature. The horizontal distances between the composite curves are given by  $U^p$  in equation (4.5) (the pinch candidates have been extended to include both the inlet and outlet temperatures of the process streams and arranged in descending values of temperature). The pinch candidate temperatures for cold process streams or stream segments must have their value increased by the minimum approach temperature.

$$U^p = \max_p(z_H^p(\mathbf{y})) - z_H^p(\mathbf{y}); \quad p = 1, \dots, 2^*(N_H + N_C) \quad (4.5)$$

As said before, the grand composite curve is a graph of temperature ( $T^P$ ) versus enthalpy difference between the hot and cold composite curves ( $U^P$ ). The following example illustrates how to obtain the grand composite curve from the heating deficit functions ( $z^P_H(\mathbf{y})$ ).

### Example

Consider Lang, Biegler and Grossmann's (1988) example problem in their appendix to illustrate the application of the pinch location method to a multiple utility problem. The problem's data is given in Table 4.2. In order to obtain the grand composite curve, the pinch candidates must be extended to include both the inlet and outlet temperatures of the process streams. The pinch candidate temperatures for cold process streams or stream segments must have their value increased by the minimum approach temperature. To better illustrate the method, the pinch candidates are also arranged in descending values of temperature.

Table 4.3 shows the values of the extended pinch candidates ( $T^P$ ), their corresponding heating deficit functions ( $z^P_H(\mathbf{y})$ ), and enthalpy difference between the hot and cold composite curves ( $U^P$ ) at the pinch candidate temperatures. Figure 4.2 is a graph of the extended pinch candidate temperature ( $T^P$ ) versus the enthalpy difference between the hot and cold composite curves ( $U^P$ ). Figure 4.2 is also the grand composite curve for the stream data in Table 4.2.

#### 4.1.2 Using the Heating Deficit Functions to Obtain the Balanced Composite Curves

To obtain the balanced composite curves, a selected utility mix must first be matched against the grand composite curve. This can be easily done, since the amount of intermediate utility that could be used at any temperature without violating the pinch, is given by the horizontal distance to the grand composite curve once the shaded regions have been added.

TABLE 4.2 Lang, Biegler and Grossmann's (1988) example problem to illustrate the application of the pinch location method to a multiple utility problem.

	FC (kW/K)	T <sup>in</sup> (K)	T <sup>out</sup> (K)
H1	1	450	350
H2	2	400	280
C1	2	320	480

**With the following utilities:**

HU1 = HP steam at 500 K  
HU2 = LP steam at 430 K  
CU1 = Cooling at 300 K  
CU2 = Refrigerant at 270 K  
 $\Delta T_{\min} = 10 \text{ K}$

TABLE 4.3 The temperature values of the expanded pinch candidates, their corresponding heating deficit functions, and enthalpy difference between the hot and cold composite curves.

	$T^P$ (K)	$Z_H^P(y)$ (kW)	$U^P$ (kW)	$QSIA(y)^P$ (kW)	$QSOA(y)^P$ (kW)
C	490.0	0.0	130.0	0.0	0.0
H	450.0	80.0	50.0	80.0	0.0
H	400.0	130.0	0.0	180.0	50.0
H	350.0	80.0	50.0	280.0	200.0
C	330.0	80.0	50.0	320.0	240.0
H	280.0	-20.0	150.0	320.0	340.0

$T^P$  = extended pinch candidates

$Z_H^P(y)$  = heating deficit functions for the extended pinch candidates

$U^P$  = enthalpy difference between the hot and cold composite curves at the pinch candidate's temperature.

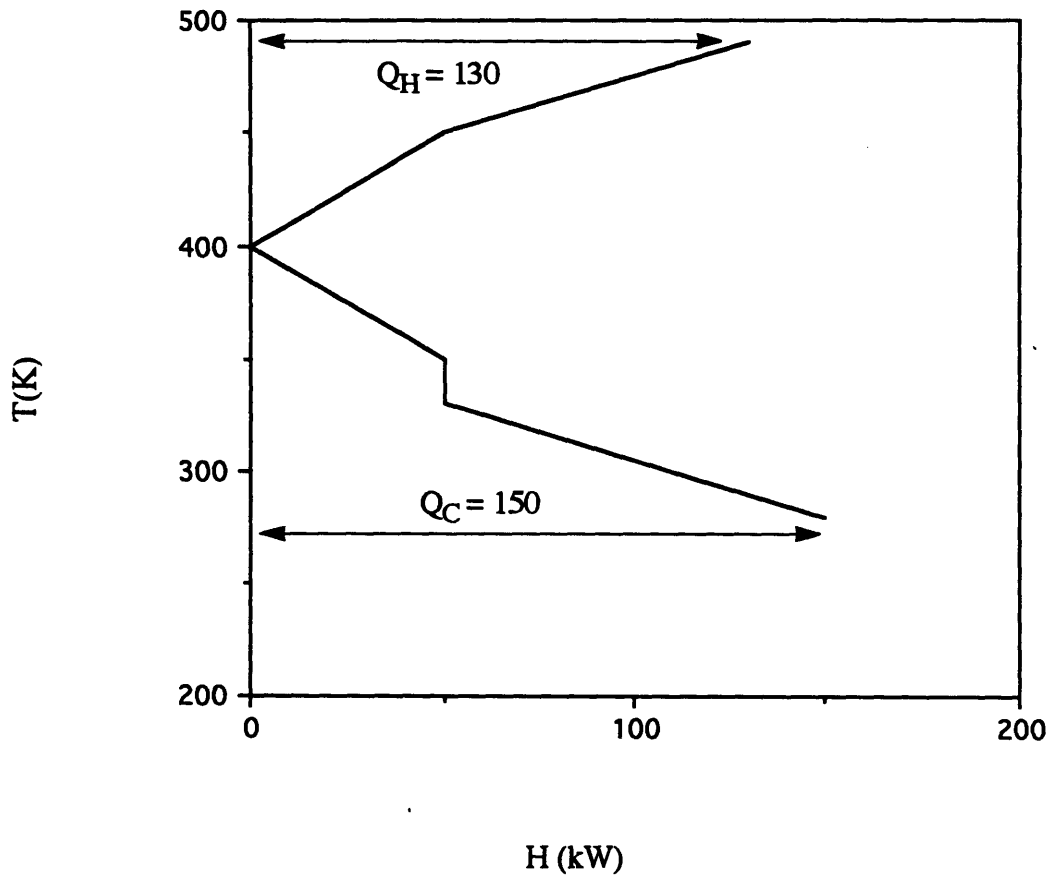


FIGURE 4.2 The grand composite curves for the stream data in Lang, Biegler, and Grossmann's (1988) example problem.

The hot utilities are fitted in ascending values of temperature and the cold utilities in descending values of temperature. For condensing utilities, their heat duty is determined by the horizontal distance to the grand composite curve once the shaded regions have been added minus the sum of the heat duties of the previously fitted utilities. This is done because, in general, the cost of hot (cold) utilities increases (decreases) steadily with increasing temperature. For condensing utilities, their heat duties are given by  $Q_h^i$ , for the hot utilities, and  $Q_c^j$ , for the cold utilities, in equations (4.6) and (4.7).  $i=1,\dots,HU$ ;  $k=1,\dots,i-1$ ;

$$Q_h^i = U^p_i - \sum_k Q_c^k; \quad i=1,\dots,HU; \quad k=1,\dots,i-1; \quad Q_h^0=0 \quad (4.6)$$

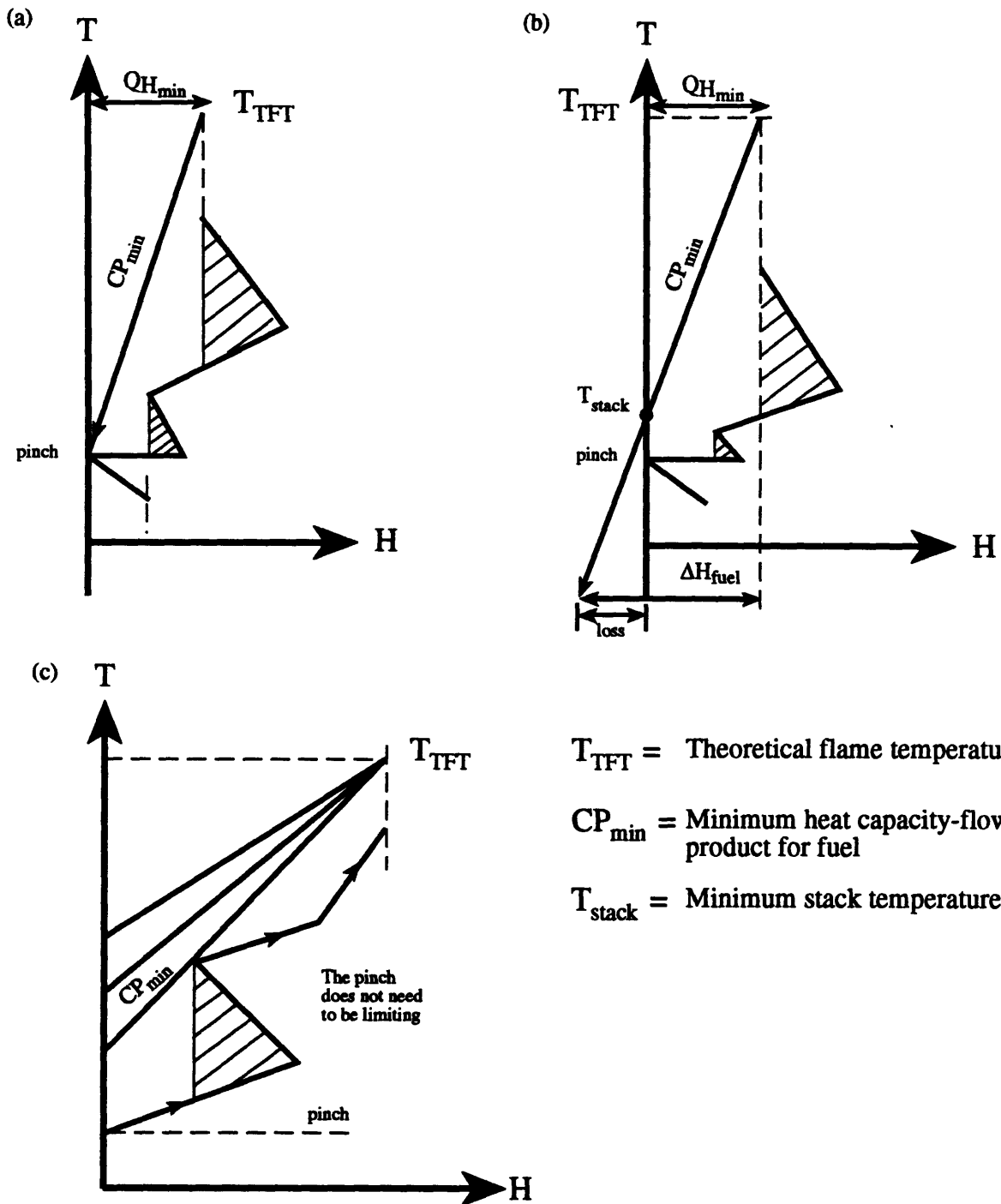
$$Q_c^j = U^p_j - \sum_k Q_h^k; \quad j=1,\dots,CU; \quad k=1,\dots,j-1; \quad Q_c^0=0 \quad (4.7)$$

Where  $U^p_i$  and  $U^p_j$  represents the distance to the grand composite curve once the shaded regions have been added at a given utility temperature.

The previous discussion was for fitting condensing utilities to the grand composite curve. Non-condensing utilities might also need to be fitted. Non-condensing utilities have the property that their temperature changes significantly during heat exchange. The duty of a non-condensing utility is determined by the most restrictive distance to the grand composite curve once the shaded regions have been added. Figure 4.3 illustrates the most restrictive region in a grand composite curve when fitting flue gas as a hot utility. The most restrictive region in the grand composite is easily seen graphically or determined mathematically. Although a mathematical program was written to fit flue gas as a hot utility in the grand composite curve of the atmospheric petroleum crude tower optimization problem (Chapter 6), this thesis will not present the detailed mathematical procedure.

Once the utilities are fit to the grand composite curve, the balanced composite curves can be obtained by treating the utilities as process streams and updating their heating deficit functions. The pinch candidates should be arranged in descending values of temperature and





$T_{TFT}$  = Theoretical flame temperature  
 $CP_{min}$  = Minimum heat capacity-flowrate product for fuel  
 $T_{stack}$  = Minimum stack temperature

FIGURE 4.3 The most restrictive region in the grand composite curve when fitting flue gas as a hot utility; (a) the pinch limits integration; (b) the minimum stack temperature limits integration; (c) a part of the grand composite curve limits integration. (Linnhoff-March, 1990)

expanded further to include the utilities inlet and outlet temperatures. The pinch candidate temperatures for the cold utilities must have their value increased by the minimum approach temperature.

The first term in the heating deficit functions ( $QSIA(\underline{y})^p$ ) is the enthalpy content of the cold process streams above the pinch candidate temperature,  $T^p$ . Therefore, the  $QSIA(\underline{y})^p$  should be updated by adding to them the total amount of cold utility used above the pinch candidate temperature,  $T^p$ . The second term in the heating deficit functions ( $QSOA(\underline{y})^p$ ) is the enthalpy content of the hot process streams above the pinch candidate temperature,  $T^p$ . Therefore, the  $QSOA(\underline{y})^p$  should be updated by adding to them the total amount of hot utility used above the pinch candidate temperature,  $T^p$ . The  $QSIA(\underline{y})^p$  and  $QSOA(\underline{y})^p$  for the utilities inlet and outlet temperatures can be obtained by linear interpolation between the original values of the process streams and then performing the updating as previously described.

The balanced composite curves are obtained by noticing that the difference between the largest first term in the heating deficit functions ( $\max_p(QSIA(\underline{y})^p)$ ) and any other first term in the heating deficit function corresponding to a cold stream (or cold stream segment or cold utility) pinch candidate temperature ( $QSIA(\underline{y})^k$ ) gives the horizontal component of the balanced cold composite curve at the cold stream (or cold stream segment or cold utility) real temperature (not pinch candidate temperature),  $T^k$ . Therefore, a graph of cold streams (or cold stream segments or cold utilities) real temperatures ( $T^k$ ) versus the difference described above, yields the balanced cold composite curve. A similar treatment to the last term in the heating deficit functions corresponding to hot streams (or hot stream segments or hot utilities) pinch candidate temperatures ( $QSOA(\underline{y})^m$ ) yields the balanced hot composite curve. The horizontal distances to the balanced cold and hot composite curves are given by  $CC^k$  and  $HC^m$  in equations (4.8) and (4.9).

$$CC^k = \max_p(QSIA(\mathbf{y})^p) - QSIA(\mathbf{y})^k \quad k=1, \dots, 2*(N_C+CU) \quad (4.8)$$

$$HC^m = \max_p(QSOA(\mathbf{y})^p) - QSOA(\mathbf{y})^m \quad m=1, \dots, 2*(N_H+HU) \quad (4.9)$$

The following example illustrates how to obtain the balanced composite curves from the updated first and second terms ( $QSIA(\mathbf{y})^p$  and  $QSOA(\mathbf{y})^p$ ) of the heating deficit functions ( $z_H^p(\mathbf{y})$ ).

### **Example**

Consider Lang, Biegler and Grossmann's (1988) example problem in their appendix to illustrate the application of the pinch location method to a multiple utility problem. The problem's data was given in Table 4.2. In order to obtain the balanced composite curves, the utility mix in Table 4.2 must first be fit to the grand composite curve (Figure 4.2). When fitting the utilities to the grand composite curve, the temperature of the cold utilities must be increased by the minimum approach temperature. Table 4.4 shows the resulting duties for the given utility mix using equations (4.6) and (4.7). The results are the same as those obtained by Lang, Biegler and Grossmann without the repeated redefinitions of the stream data and reevaluations of the heating deficit functions their method requires.

Once the utilities are fitted to the grand composite curve, the pinch candidates are expanded further to include the utilities inlet and outlet temperatures and all the heating deficit functions are updated. The pinch candidate temperatures for the cold utilities have their values increased by the minimum approach temperature and all pinch candidates are arranged in descending values of temperature. Table 4.5 shows the expanded pinch candidates and their updated heating deficit functions. Table 4.6 demonstrates the updating of the first and second terms in the heating deficit functions.

TABLE 4.4 Calculation of the thermal duties for the utilities in Lang, Biegler and Grossmann's (1988) example problem using the grand composite curve.

		$U_i^p$ (kW)	$U_i^f$ (kW)	$U_i^h$ (kW)	$U_i^c$ (kW)
HU1	= 500 K	130.0	—	100	—
HU2	= 430 K	30.0	—	30	—
CU1+ $\Delta T_{min}$	= 310 K	—	90	—	90
CU2+ $\Delta T_{min}$	= 280 K	—	50	—	60

$Q^h$  = thermal duties for the hot utilities

$Q^c$  = thermal duties for the cold utilities

$U_i^p$  - horizontal distance to the grand composite curve once the shaded regions have been added at the hot utility temperatures.

$U_i^c$  - horizontal distance to the grand composite curve once the shaded regions have been added at the cold utility temperatures plus  $\Delta T_{min}$ .

TABLE 4.5 The expanded pinch candidates and their updated deficit functions.

	$T^P(K)$	$Z_H^P(y)(kW)$	$QSIA(y)^P(kW)$	$QSOA(y)^P(kW)$
H	5010	0.0	<del>0.0</del>	0.0
H	500.0	-100.0	<del>0.0</del>	100.0
C	490.0	-100.0	0.0	<del>100.0</del>
H	450.0	-20.0	<del>80.0</del>	100.0
H	431.0	-1.0	<del>118.0</del>	119.0
H	430.0	-30.0	<del>120.0</del>	150.0
H	400.0	0.0	<del>180.0</del>	180.0
H	350.0	-50.0	<del>280.0</del>	330.0
C	330.0	-50.0	320.0	<del>370.0</del>
C	310.0	-90.0	320.0	<del>410.0</del>
C	309.0	-2.0	410.0	<del>412.0</del>
H	280.0	-60.0	<del>410.0</del>	470.0
C	280.0	-60.0	410.0	<del>470.0</del>
C	279.0	0.0	470.0	<del>470.0</del>

TABLE 4.6 Examples of updating the first and second terms in the heating deficit functions.

(a) *First term for pinch candidate 330 K*

original value	=	320 kW
cold utility used above 330 K	=	0 kW
updated value	=	320 kW

(b) *First term for pinch candidate 280 K*

original value	=	320 kW
cold utility used above 280 K	=	90 kW
updated value	=	410 kW

(c) *Second term for pinch candidate 490K*

original value	=	0 kW
hot utility used above 490 K	=	100 kW
updated value	=	100 kW

(d) *Second term for pinch candidate 430K*

original value	=	20 kW *
hot utility used above 430 K	=	130 kW
updated value	=	150 kW

\* value obtained by interpolation

Figure 4.4 is a graph of two curves. One is the real temperatures corresponding with cold process stream or cold utilities,  $T^k$ , versus the values of equation (4.8) and the other is the real temperatures corresponding with hot process streams or hot utilities,  $T^m$ , versus the values of equation (4.9). Figure 4.4 is also the balanced composite curve for the stream data and the given utility mix in Table 4.2.

#### **4.1.3 Using the Balanced Composite Curves to Target for the Capital Costs of the Heat Exchanger Network**

Linnhoff and Ahmad (1990) used the balanced composite curves and simple models for the capital costs of heat exchanger networks to target for the networks's annualized cost prior to design. They showed that typically, networks can be developed that are within 5% of the total cost target.

They argued that, if the heat transfer coefficients for all streams undergoing heat exchange ( $h_i$ ) are the same, network minimum area is achieved through overall countercurrent heat exchange. Overall countercurrent heat exchange appears as vertical heat transfer on the balanced composite curves (Figure 4.5).

Figure 4.6 (from Linnhoff and Ahmad, 1990) introduces a general way to ensure vertical heat transfer. The balanced composite curves are first divided into "enthalpy intervals" (Figure 4.6a). The intervals are determined by a change in slope in either balanced composite curve. Next, a hypothetical network design is performed in each interval that achieves the desired vertical heat transfer. Figure 4.6b demonstrates the procedure for an interval containing two hot streams and three cold streams. Each hot stream is split into the same number of branches as the number of cold streams in that interval. Similarly, each cold stream is split into the same number of branches as the number of hot streams in that same interval.

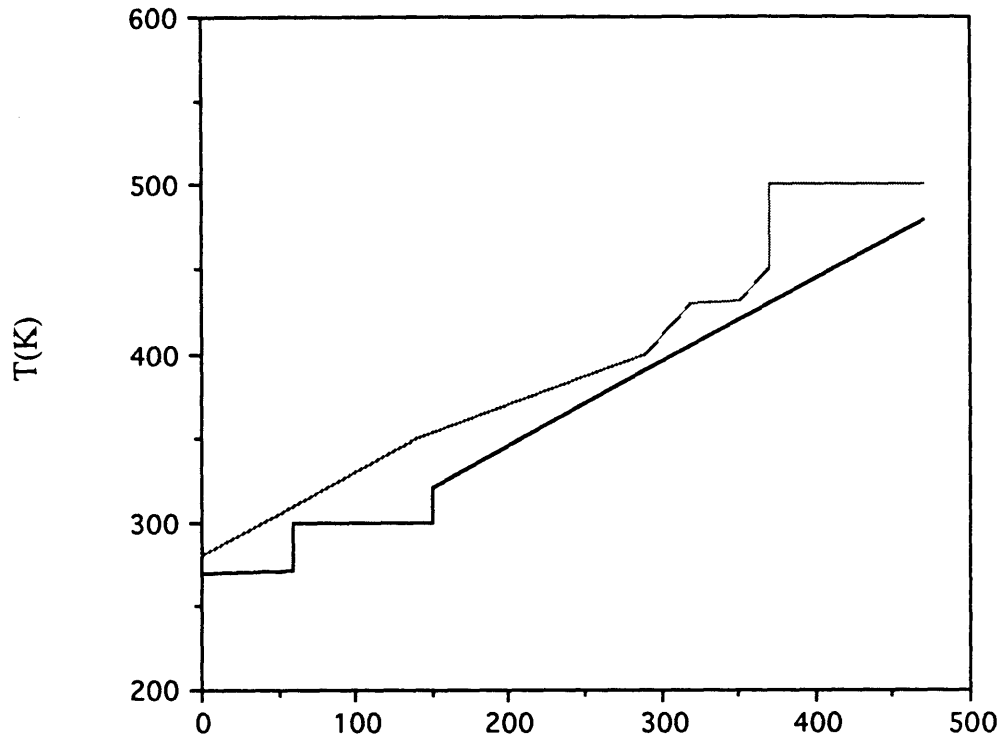
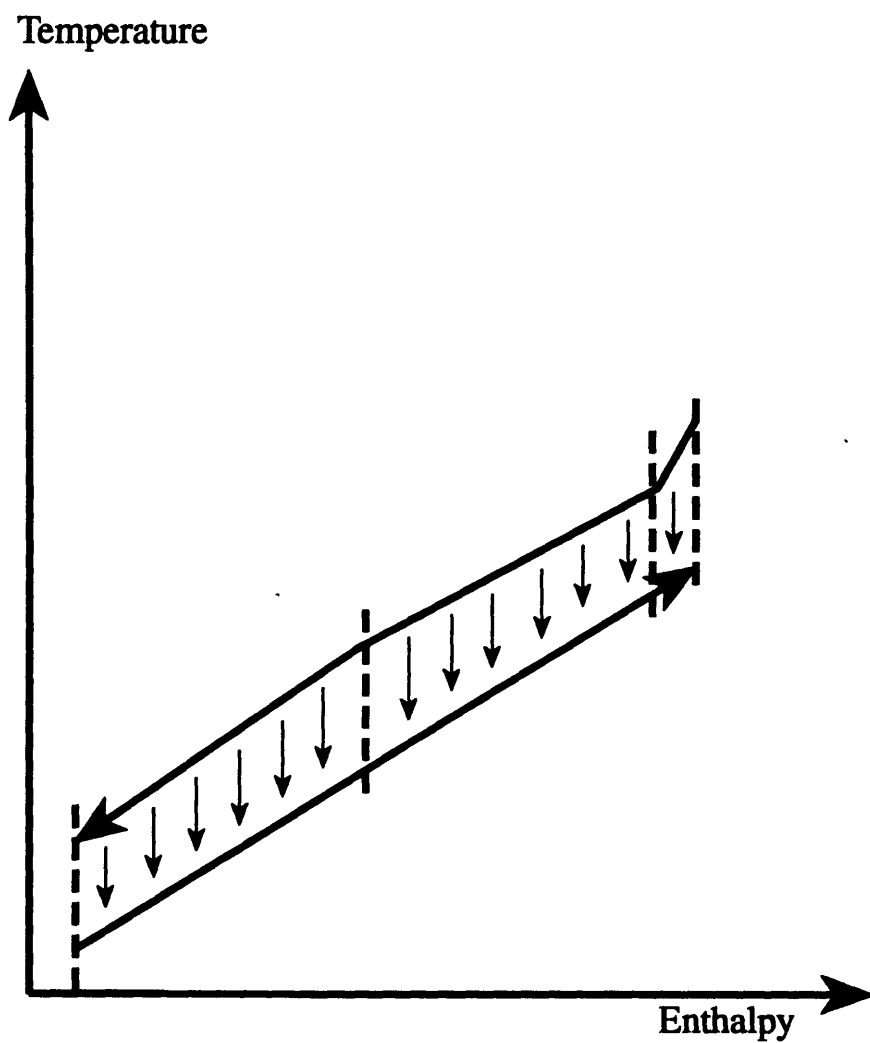


FIGURE 4.4 The balanced composite curves for Lang, Biegler, and Grossmann's (1988) example problem.





**FIGURE 4.5 Overall countercurrent process heat exchange appears as vertical heat transfer on the balanced composite curves. (Linnhoff and Ahmad, 1990)**

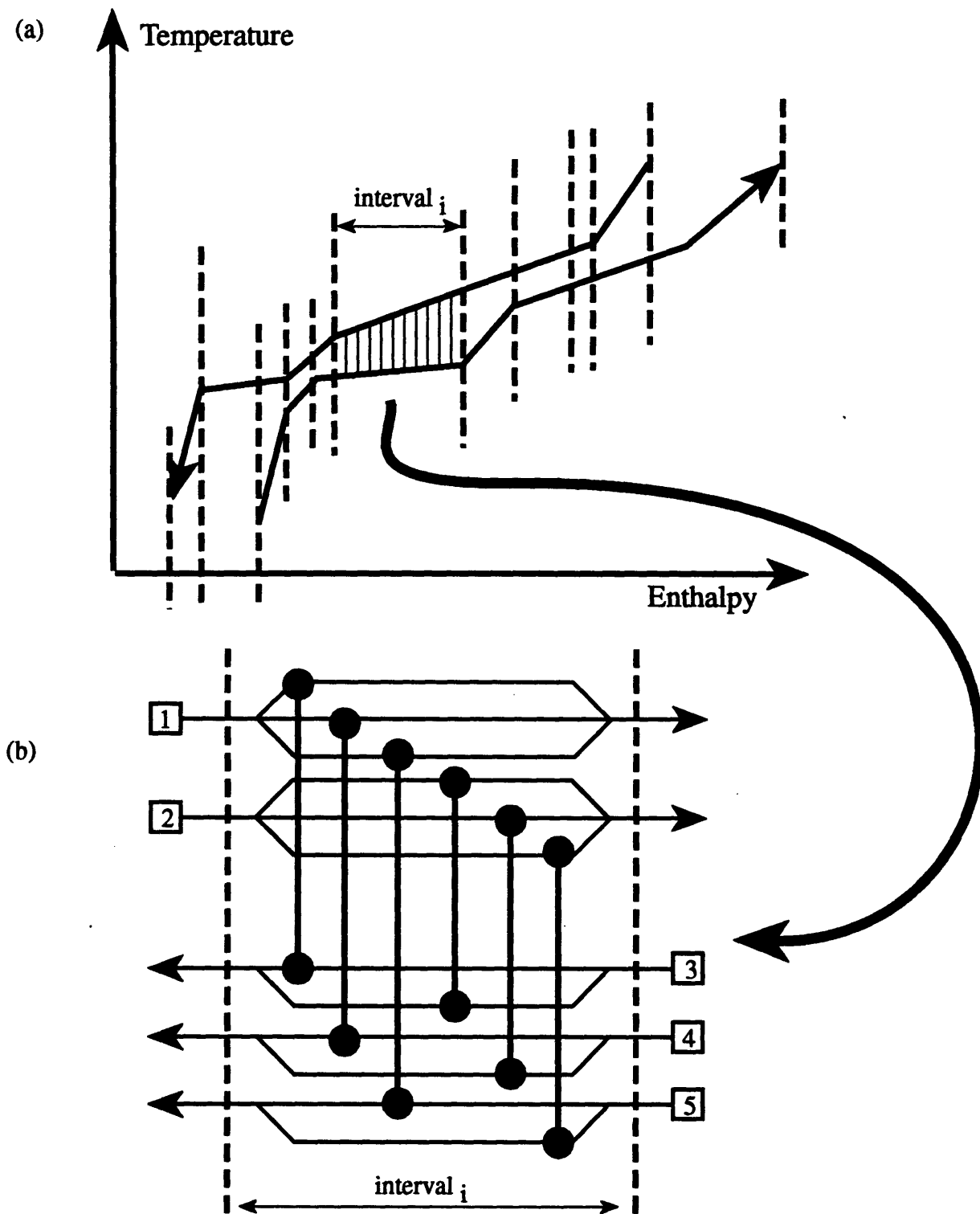


FIGURE 4.6 Example of a general stream-splitting and matching scheme to ensure vertical heat transfer in an enthalpy interval of the composite curves. (Linnhoff and Ahmad, 1990)

Each hot stream is then matched with each cold stream such that every match occurs between the corner temperatures of the enthalpy interval. The heat exchange in those matches appears as vertical heat transfer on the balanced composite curves.

Linnhoff and Ahmad (1990) showed that, if all heat transfer coefficients ( $h_i$ ) for all streams undergoing heat exchange are the same, the network minimum area is given by:

$$A_{\min} = (1/U) \sum_i (\Delta H_i / \Delta T_{LMI}) \quad i=1, \dots, 2*(N_H + N_C + HU + CU) - 3 \quad (4.10)$$

where  $U$  is the overall heat transfer coefficient,  $\Delta H_i$  is the enthalpy width of interval  $i$ , and  $\Delta T_{LMI}$  is the logarithmic mean temperature difference of interval  $i$ .

They also derived an approximate target for minimum area of the heat exchanger network when the heat transfer coefficients ( $h_i$ ) for all streams undergoing heat exchange are not the same. This formula is given in equation (4.11).

$$A_{\min} = \sum_i (1/\Delta T_{LMI}) \sum_{j=1, \dots, N_H + N_C + HU + CU} (q_j / h_j) \quad i=1, \dots, 2*(N_H + N_C + HU + CU) - 3 \quad (4.11)$$

where  $(q_j)_i$  is the enthalpy change of stream  $j$  in interval  $i$ .

Equation (4.11) allows the use of the balanced composite curves to target for the minimum area required by the heat exchanger network without the actual design of the network. Linnhoff and Ahmad (1990) and other researchers (Townsend and Linnhoff, 1984; Ahmad, 1985) have shown that the discrepancy between the minimum area target and the actual network area in the final design is usually less than 10%.

The network capital cost is predicted by assuming a cost correlation for the installed capital cost of heat exchangers, and assuming the overall area target ( $A_{\min}$ ) is achieved in the minimum number of units for maximum energy recovery ( $U_{\min-MER}$ ). Linnhoff and Ahmad (1990) demonstrated how networks can be designed that are within 5% of this total cost target.  $U_{\min-MER}$  is obtained by dividing the heat exchanger network design at the pinch and the ambient temperature and predicting the minimum number of units need in each section to achieve maximum energy recovery. The minimum number of exchangers need in each section to achieve maximum energy recovery is the total number of streams present in each section (includes hot and cold process streams and stream segments as well as hot and cold utilities) minus one. The correlation for the installed capital cost of heat exchangers is given in equation (4.12) and the prediction of the heat exchanger network capital cost in equation (4.13).

$$\text{exchanger installed capital cost} = a + b \cdot A^e \quad (4.12)$$

where  $A$  is the exchanger area and  $a$ ,  $b$ , and  $e$  are constants.

$$\text{network capital cost} = a \cdot U_{\min-MER} + b \cdot A_{\min}^e \quad (4.13)$$

A mathematical model of the method described in this sub-section to predict the capital cost of the heat exchanger network from the balanced composite curves was used in this thesis. Although this model was implemented in the atmospheric petroleum crude tower optimization problem (Chapter 6) and the cold end of the ethylene plant optimization problem (Chapter 7), this thesis will not present the detailed mathematical procedure. The network capital cost predicted from this model is the same as that reported in literature by various authors.

#### 4.1.4 Conclusions

This section showed how the information in the heating deficit functions can be used to obtain the grand composite curve (sub-section 4.1.1), the balanced composite curves (sub-section 4.1.2), and target for the capital cost of the heat exchanger network (sub-section 4.1.3). The grand composite curve and the balanced composite curves are obtained by simple manipulation of the heating deficit functions. Linnhoff and Ahmad's (1990) cost targeting method is used to target for the capital cost of the heat exchanger network from the balanced composite curves.

By incorporating the mathematical programs developed in this section, the pinch location method (NLP P1) can be expanded to not only take into account heat integration but also target for the capital cost of the heat exchanger network. As discussed in section 3.1, this expanded pinch location method considers all major heat and work interactions between a chemical process and its heat exchanger network. Therefore, it can simultaneously optimize the operating conditions of the chemical process, its heat exchanger network, and the minimum approach temperature for heat exchange. The expanded pinch location method is given by NLP P2.

$$\begin{aligned}
 \min \phi &= F(\underline{x}, \underline{y}) + \sum_i c_h^i Q_h^i + \sum_j c_c^j Q_c^j + c_a A(\underline{y}, \Delta T_{\min})^e + c_u NU(\underline{y}, \Delta T_{\min}) \\
 \text{s.t. } h(\underline{x}, \underline{y}) &= 0, \\
 g(\underline{x}, \underline{y}) &\leq 0, \\
 GCC &= r_1(\underline{y}, \Delta T_{\min}) \\
 BCC &= r_2(\underline{y}, \Delta T_{\min}) \\
 Q_h^i &= r_3(GCC), i \in HU \\
 Q_c^j &= r_4(GCC), j \in CU \\
 A &= r_5(BCC) \\
 NU &= r_6(BCC) \\
 Q_h^i, Q_c^j &\in R^1 : i \in HU, j \in CU \\
 \underline{x} &\in XCR^n, \underline{y} \in YCR^m
 \end{aligned}
 \tag{NLP P2}$$

where  $r_1$  and  $r_2$  represent functions to calculate the grand composite curve (GCC) and the balanced composite curves (BCC).  $A$  and  $NU$  are the targets for minimum area of the heat exchanger network ( $A_{\min}$  in equation (4.11)) and the minimum number of heat exchangers for maximum energy recovery ( $U_{\min-MER}$ ). They are both functions of the balanced composite curves. The annualized per unit costs of heat exchanger network area and heat exchangers are given by  $c_a$  and  $c_u$ .  $Q_h^i$  and  $Q_c^j$  represent the heating and cooling duties for the selected utility mix. They are functions of the grand composite curve (equations (4.6) and (4.7)).  $c_h^i$  and  $c_c^j$  represent the unit costs for thermal energy for the respective hot and cold utilities

The expanded pinch location method (NLP P2) of this section will not be solved in this thesis. A new NLP will be introduced that not only accounts for the heat and work interactions between the chemical process and its heat exchanger network but also the heat and work interactions with the utility system. This NLP is solved by implementing it in a rigorous sequential process simulator (Chapter 5).

#### **4.2 The New Method to Target for the Capital and Operating Costs of Utility Systems**

Section 3.2 presented a superstructure that could be used for the synthesis and optimization of integrated utility system by solving a large and difficult MINLP. The purpose of this thesis was to develop a method for the simultaneous optimization (not synthesis) of a chemical process, its heat exchanger network, and the utility system by taking into account their heat and work interactions. Therefore, the superstructure is used as a guideline to develop a new method that targets for utility systems capital and operating costs by including its heat and work interactions with the other subsystems. The method does not require a rigorous simulation of the entire utility system and therefore, significantly reduces computation time. In other words, the large and difficult MINLP of Section 3.2 becomes tractable. The steps in this method are summarized as follows :

1) Use the superstructure of Section 3.2 to select a structure for the utility system. Selecting the structure for the utility system is the same as selecting the number of hot and cold utilities but not their temperature levels. As will be seen in the following subsections, this can be a difficult or an easy task. As suggested by the utility system superstructure of Section 3.2, the structure of the utility system depends greatly on the shape and size of the process heat sink and the process heat source (grand composite curve). Therefore, the selection of the utility system must be done on an individual problem basis.

2) Take into account the utility system heat interactions with the chemical process and its heat exchanger network by fitting utilities in the grand composite curve to determine their duties. Fitting utilities in the grand composite curve to determine their duties was discussed in subsection 4.1.2.

3) Take into account the utility system work interactions with the chemical process and its heat exchanger network with the performance equations. The performance equations allow the quick prediction of work consumption or production by individual pieces of equipment in the utility system without a rigorous design of the entire utility system. The performance equations will be introduced in subsection 4.2.2.

4) Target for the capital cost and operating costs of the utility system from cost correlations and the results of steps 2 and 3.

The rest of this Section shows how to apply the above method to the atmospheric petroleum crude tower and the cold end of an ethylene plant optimization problems presented in Chapters 6 and 7.

#### **4.2.1 Targeting for the Capital and Operating Costs of the Utility System Used in the Atmospheric Petroleum Crude Tower Optimization Problem**

The first step in the new method to target for the utility system capital and operating costs is to select its structure. Figure 4.7 shows typical composite curves and grand composite curve for the atmospheric crude tower optimization problem of Chapter 6. In this problem this step is relatively easy. The utility system structure selected for this problem consists of a process heater or furnace and a cooling tower. It is unlikely that any other alternative structure available in the superstructure of Section 3.2 will yield a lower total cost.

The second step of the method accounts for the utility system heat interactions by fitting the utilities in the grand composite curve to determine their duties. The utilities in this example are furnace flue gas (hot utility) and cooling water (cold utility). Fitting non-condensing utilities in the grand composite curve was discussed in subsection 4.1.2. The duty of a non-condensing utility is determined by their most restrictive distance to the grand composite curve once the shaded regions have been added.

Figure 4.8 shows that the flue gas outlet temperature is allowed to change, and therefore, change the degree of integration of the hot end of the utility system. A new optimization variable, the minimum approach temperature for the integration of the hot end of utility system ( $\Delta T_{\text{ummin}}$ ), can be defined.  $\Delta T_{\text{ummin}}$  can be very different than the minimum approach temperature for heat exchange ( $\Delta T_{\text{min}}$ ) defined earlier.  $\Delta T_{\text{ummin}}$  determines the degree of integration of the hot end of the utility system and also the furnace heat duty.

The cooling water supply and target temperature are fixed, and a per unit cost of cooling is specified in the cost data of Table 6.1. This fixes some of the heat interactions with the cold end of the utility system. A more detailed model where the degree of integration of the cold end of the utility system can change could be defined, but this is not necessary, since the cooling costs are very low in comparison to other costs.



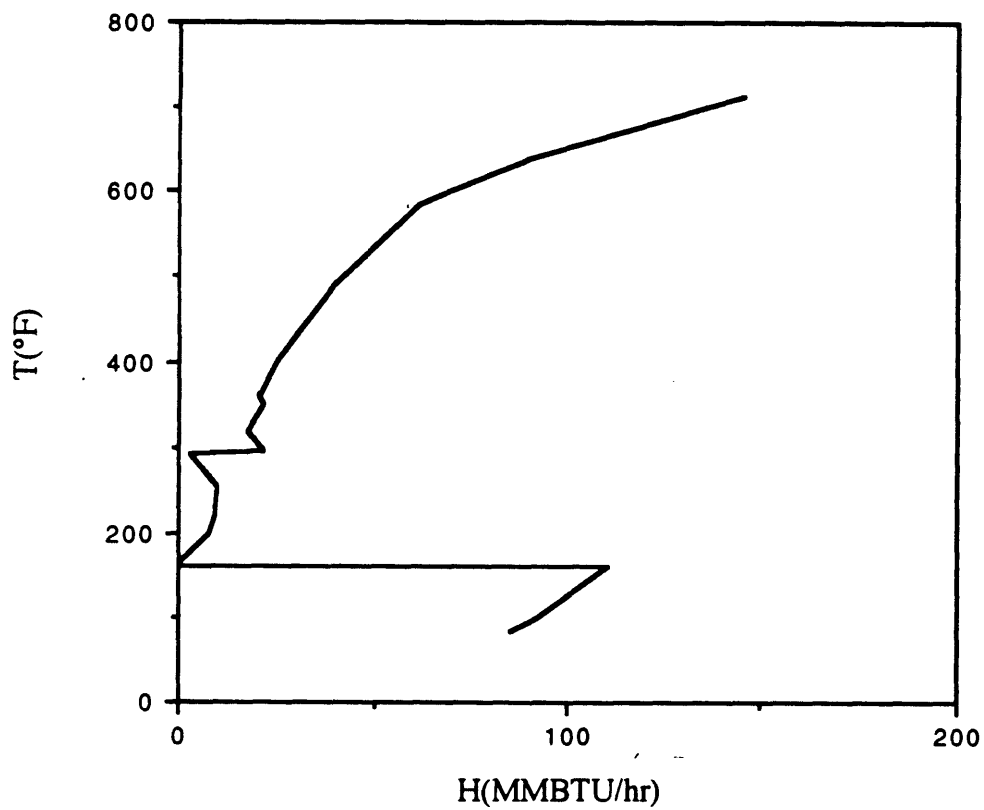
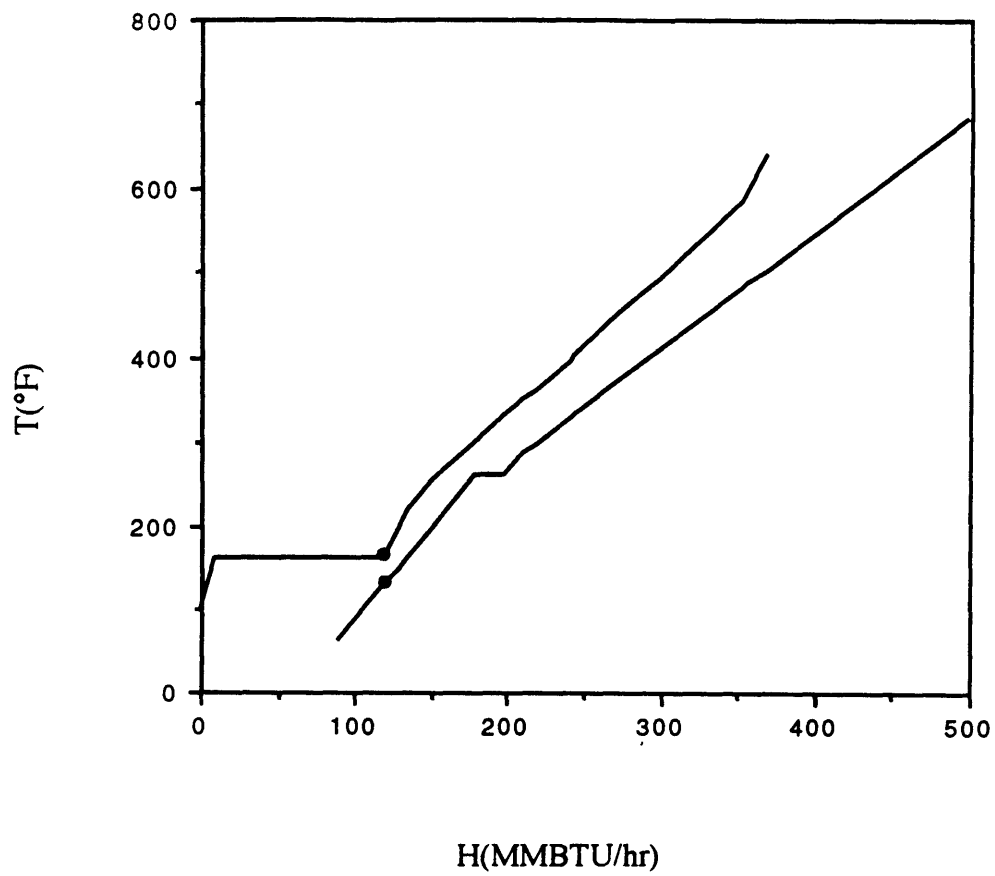
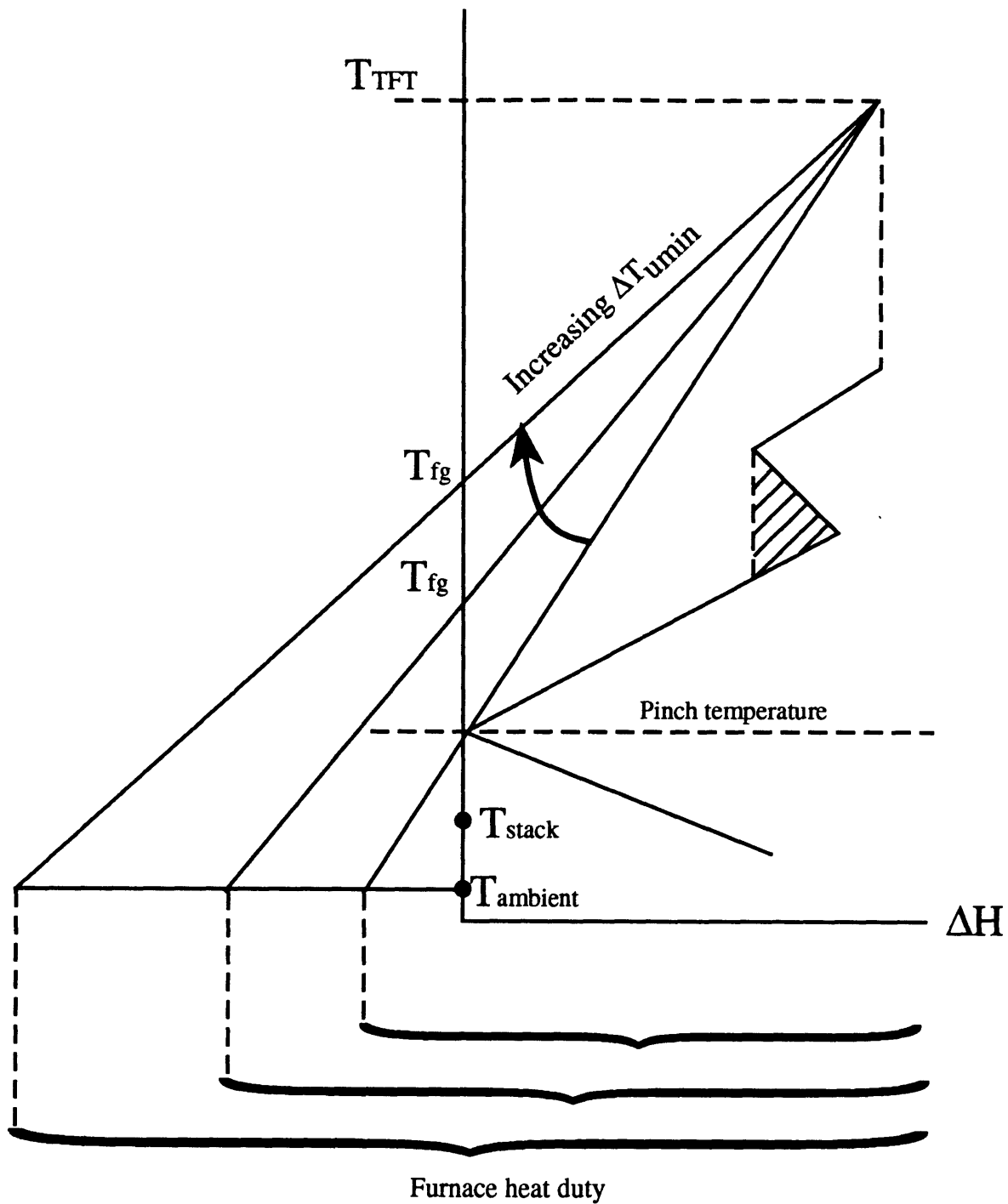


FIGURE 4.7 Typical composite curves and grand composite curve for the atmospheric petroleum crude tower optimization problem.



- $T_{TFT}$  = Theoretical flame temperature
- $T_{fg}$  = Flue gas exit temperature
- $T_{stack}$  = Minimum stack temperature
- $T_{ambient}$  = Ambient temperature

FIGURE 4.8 The effects of  $\Delta T_{umin}$  on the furnace heat duty and the flue gas exit temperature. (Linnhoff-March, 1990)

In this example, there is no work demand or production by the chemical process or the utility system. The utility system has no work interactions (only heat interactions) with the chemical process or the heat exchanger network. Therefore, the third step in the new method to target for the capital and operating costs of the utility system is not necessary. The duties of the utilities and the cost correlations of Table 6.1 are enough to target for the capital and operating costs of the utility system.

### Example

Figure 4.9 illustrates the grand composite curve of the solution obtained with Lang, Biegler, and Grossmann's (1988) method in the atmospheric petroleum crude tower optimization problem. At a  $\Delta T_{\min}$  of 45 °F the pinch temperature occurs at 304.3 °F, the minimum hot utility requirement is 149.0 MMBTU/Hr, and the minimum cold utility requirement is 93.0 MMBTU/Hr.

In order to target for the capital and operating costs of the utility system the utilities thermal duties must first be determined by fitting them in the grand composite curve. Figure 4.10 illustrates the fitting of cooling water and furnace flue gas in the grand composite curve.

Since the shape of the grand composite curve does not restrict the fitting of cooling water, the cooling water duty is given by the minimum cold utility requirement (93.0 MMBTU/Hr).

The shape of the grand composite curve and a  $\Delta T_{\min}$  of 110 °F determines the heat duty of the furnace flue gas. In this example, the pinch restricts the integration of the furnace flue gas. In order to satisfy a  $\Delta T_{\min}$  of 110 °F, the flue gas exit temperature is determined to be 369.3 °F. This is because  $\Delta T_{\min}$  is the sum of  $\Delta T_{\min}$  (45 °F) and the temperature difference between the furnace flue gas exit temperature and the pinch temperature (369.3 °F - 304.3 °F = 65 °F). The furnace flue gas exit temperature determines the furnace flue gas heat duty to be 175.0 MMBTU/Hr.

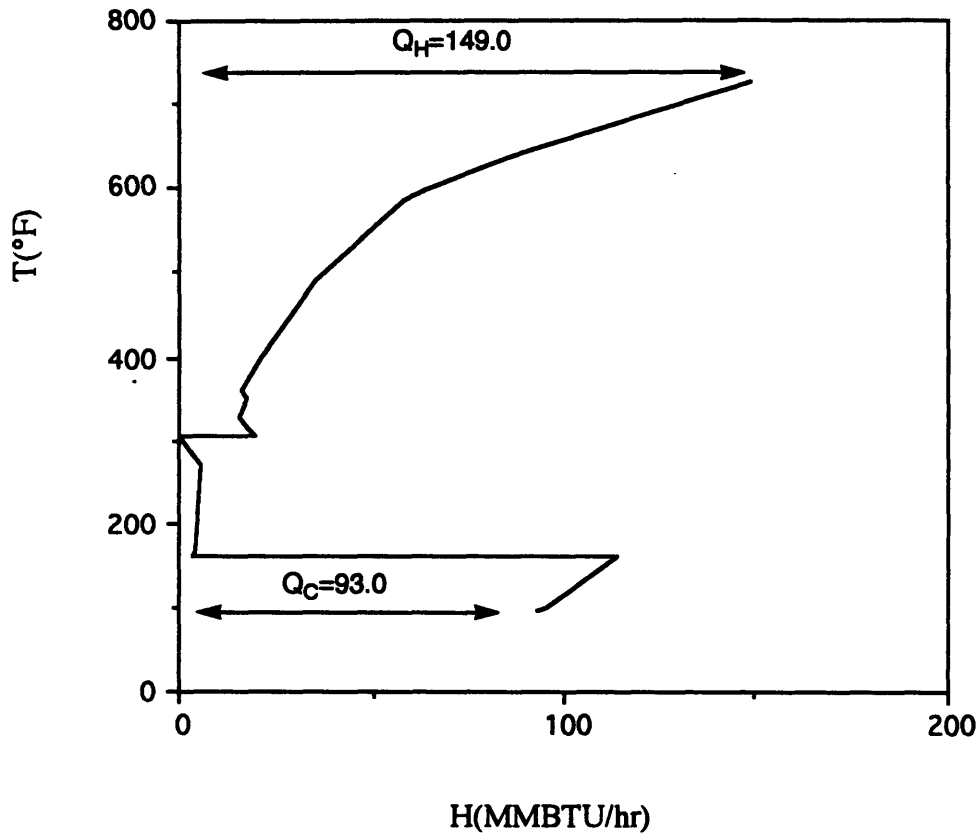


FIGURE 4.9 Grand composite curve of the solution to the atmospheric petroleum crude tower optimization problem obtained with Lang, Biegler, and Grossmann's (1988) method.

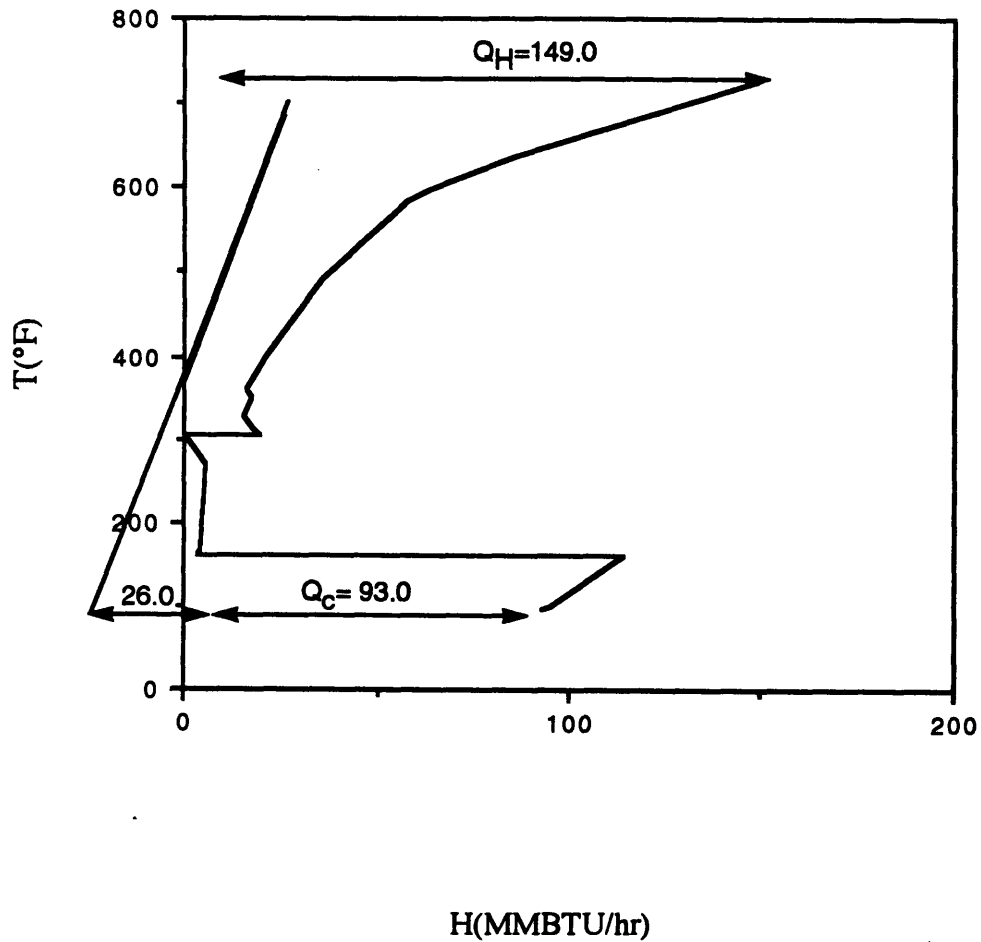


FIGURE 4.10 Fitting furnace flue gas and cooling water in the grand composite curve of the solution to the atmospheric petroleum crude tower optimization problem obtained with Lang, Biegler, and Grossmann's (1988) method.

Since the utility system in this example has no work interactions, its capital and operating costs can be predicted with the utilities thermal duties and the cost correlations of Table 6.1. Table 4.7 demonstrates the prediction of the annualized capital and operating costs for this utility system.

#### **4.2.2 Targeting for the Capital and Operating Costs of the Utility System Used in the Cold End of an Ethylene Plant Optimization Problem**

The first step in the new method to target for the utility system capital and operating costs is to select its structure. Figure 4.11 shows typical composite curves and grand composite curve for the cold end of an ethylene plant optimization problem of Chapter 7. From the large amount (and wide temperature range) of subambient cooling duty required, it is clear that the overall cost of the total process will strongly depend on the capital and operating (work consumption) costs of the refrigeration system. In this problem, heat as well as work integration of the refrigeration section of the utility system is important to obtain the minimum total cost solution.

In this problem, the selection of the structure of the utility system is not an easy step. It is unclear how many refrigeration levels should be provided or how to design the refrigeration system. The superstructure of Section 3.2 suggested that refrigeration systems should be designed as multi-extraction, multi-rejection heat pumps, but more specific information is required. A brief review of typical industrial refrigeration equipment and previous research to design integrated refrigeration systems follows.

The basic refrigeration unit is the mechanical vapor recompression cycle. A mechanical vapor recompression cycle is illustrated in Figure 4.12. It contains four principal component: an evaporator, a compressor, a condenser, and an expansion valve. The evaporator is the heat exchanger where the liquid refrigerant is evaporated and the process stream cooled. The extraction of heat from the process in the evaporator is the purpose of the entire refrigeration

TABLE 4.7 Calculating the capital and operating costs of the utility system in Lang, Biegler and Grossmann's (1988) solution to the atmospheric petroleum crude tower optimization problem.

**furnace flue gas heat duty** = 175.0 MMBTU / hr

**cooling water duty** = 93.0 MMBTU / hr

*CAPITAL COSTS*

**Installed furnace cost** =  $.682 (175.0 \times 10^6)^{.8}$   
 = 2.680 million \$

**Annualized capital cost** = 1.072 million \$ / yr

*OPERATING COSTS*

**fuel use** =  $(2.916 \frac{\$}{\text{MMBTU}}) (175 \frac{\text{MMBTU}}{\text{hr}}) (8540 \frac{\text{hr}}{\text{yr}})$   
 4.358 million \$ / yr

**cooling water cost** =  $(.343 \frac{\$}{\text{MMBTU}}) (93.0 \frac{\text{MMBTU}}{\text{hr}}) (8540 \frac{\text{hr}}{\text{yr}})$   
 = .272 million \$ / yr

**Total operating costs** = 4.630 million \$ / yr

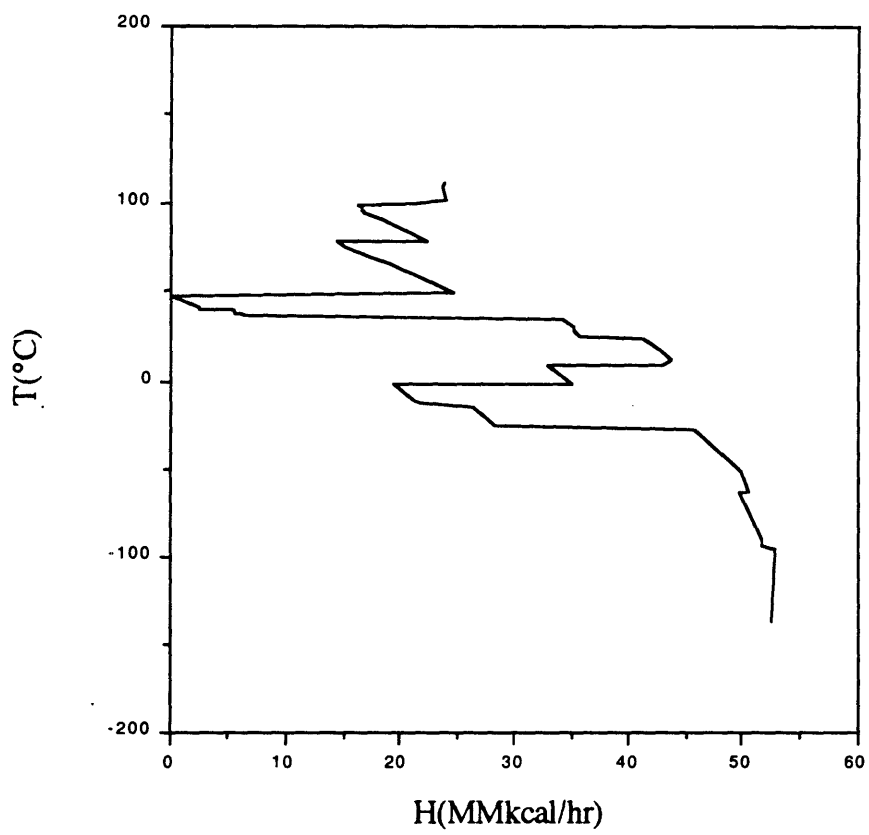
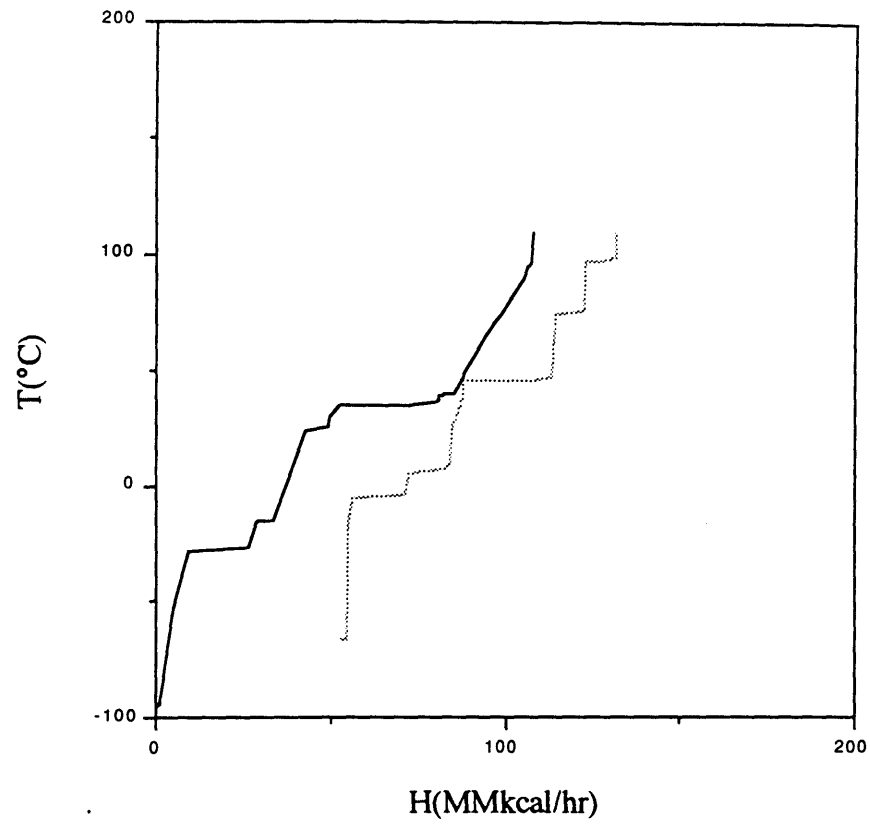


FIGURE 4.11 The composite and grand composite curves for the cold end of a typical ethylene plant.



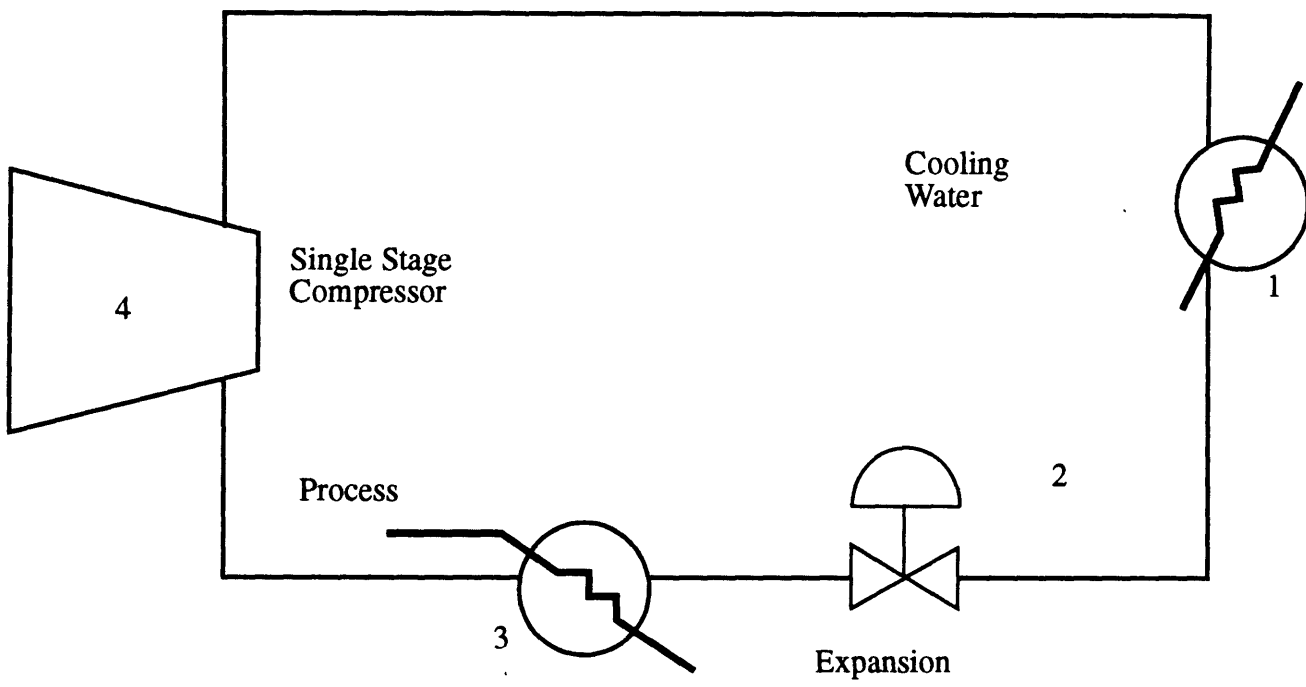
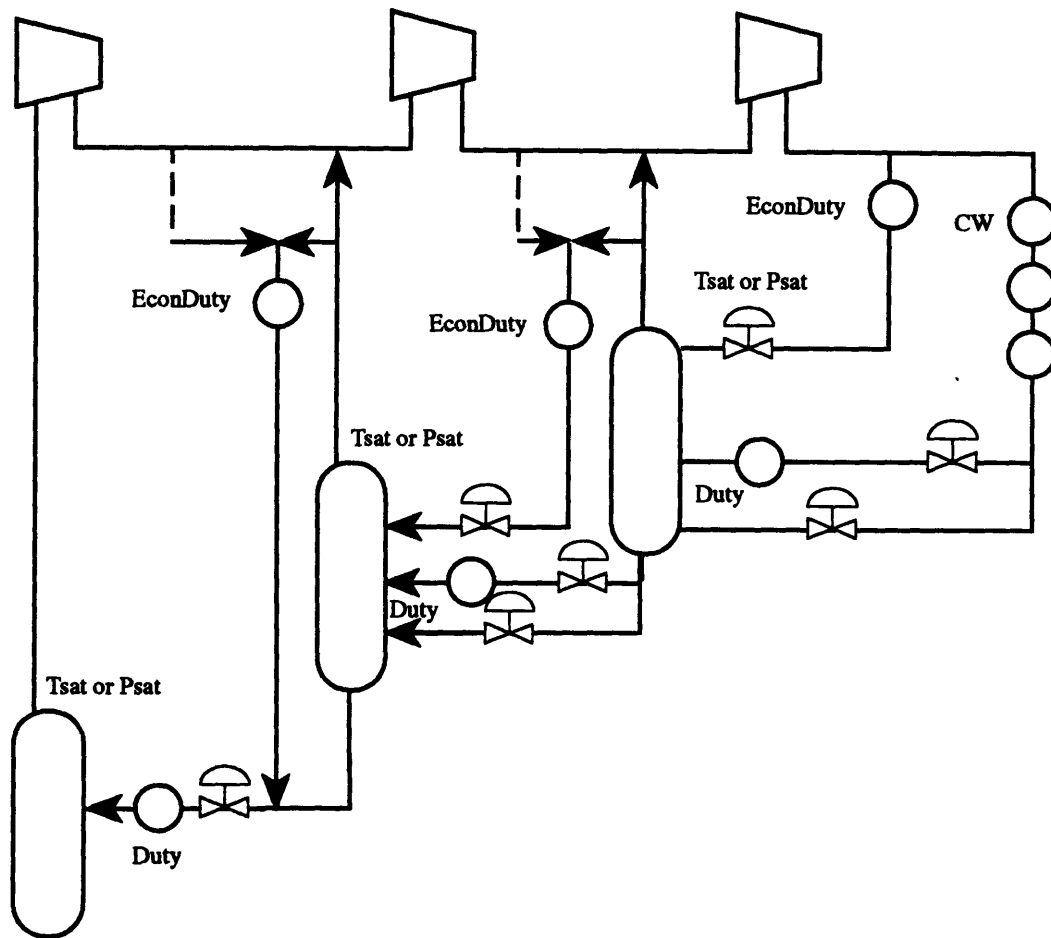


FIGURE 4.12 Illustration of a mechanical vapor recompression refrigeration cycle.

system. The compressor is the expensive part of the refrigeration system. It increases the pressure and temperature of refrigerant vapor from the evaporator and discharges it to the condenser. The condenser is the heat exchanger that liquifies the refrigerant. It removes the heat absorbed in the evaporation and compression stages. To complete the cycle, the condensed refrigerant flows through an expansion valve where the pressure and temperature levels are reduced to those in the evaporator.

Colmenares and Seider (1986) designed integrated refrigeration systems by fitting various simple mechanical vapor recompression cycles in the grand composite curve. Unfortunately, single stage mechanical vapor recompression cycles have process application limitations. As the temperature difference between the condenser and evaporator increases excessive compression ratios are encountered, excessive temperature in the discharge gas are developed, and alternative schemes can achieve energy savings that offset extra equipment cost. The alternative schemes are the complex or compound refrigeration system and the cascade refrigeration system.

A complex refrigeration system is the combination of two or more single stage mechanical vapor recompression cycles. Figure 4.13 shows a three stage complex refrigeration system. These systems contain a multi-stage compressor or two or more single-stage compressors connected in series. They also use the same refrigerant at all pressure levels of the system. The complex refrigeration system is the multi-extraction, multi-rejection heat pump suggested in the superstructure for refrigeration systems of Section 3.2. The advantage of a complex refrigeration system over single stage mechanical vapor recompression cycles is that better compression efficiencies are achieved (less horsepower). Yoon (1990) in addition to his questionable heuristics, claimed that a complex refrigeration cycle with R-22 as a working fluid is the lowest cost design for all refrigeration systems. Unfortunately, R-22 is banned due to its role in destroying ozone in the atmosphere.



**CW** = cooling water  
**Duty** = refrigeration cooling duty  
**EconDuty** = economizer heat duty

FIGURE 4.13 Illustration of a complex refrigeration cycle. (Advent User Guide, 1991)

When the range of refrigeration temperatures needed is large (as in the cold end of the ethylene plant), complex refrigeration can have operation limitations. Sub-atmospheric operation of the evaporator is undesirable (limits refrigeration temperature) and condenser temperature must be below the working fluid's critical temperature (limits rejection temperature). The alternative is a cascade refrigeration system.

Cascade systems are usually needed when evaporators must operate at low temperatures (below -60 C). Cascade systems consist of two completely independent refrigeration systems (Figure 4.14). One system is referred as the low temperature system and the other as the high temperature system. The low temperature system compresses the refrigeration load to a temperature that can be condensed by the high temperature system. The two independent systems are connected only by the cascade condenser which acts as the condenser for the low temperature system and the evaporator for the high temperature system. Refrigerants for each individual system are picked according to the temperature/pressure level in which the system operates. The cascade refrigeration system is not exactly the multi-extraction, multi-rejection heat pump suggested in the superstructure for refrigeration systems of Section 3.2. It is actually two multi-extraction, multi-rejection heat pumps. This difference was not introduced in Section 3.2 to make its reading easier.

The cold end of the ethylene plant requires refrigeration temperatures as low as -105 C, so a cascade refrigeration system is required. Since ethylene and propylene are available as products, they are usually also used as refrigerants. Ethylene provides the low temperature refrigeration and propylene the high temperature refrigeration.

Linnhoff and Dhole (1989) presented the only method to date that captures most of the heat and work interactions of industrial refrigeration systems. The exergy composite curves and the exergy grand composite curve are introduced and used to estimate the amount of exergy lost in the heat exchanger network and in the chemical process. The exergetic efficiency of the refrigeration system is then defined as the ratio of the exergy lost in the heat exchanger

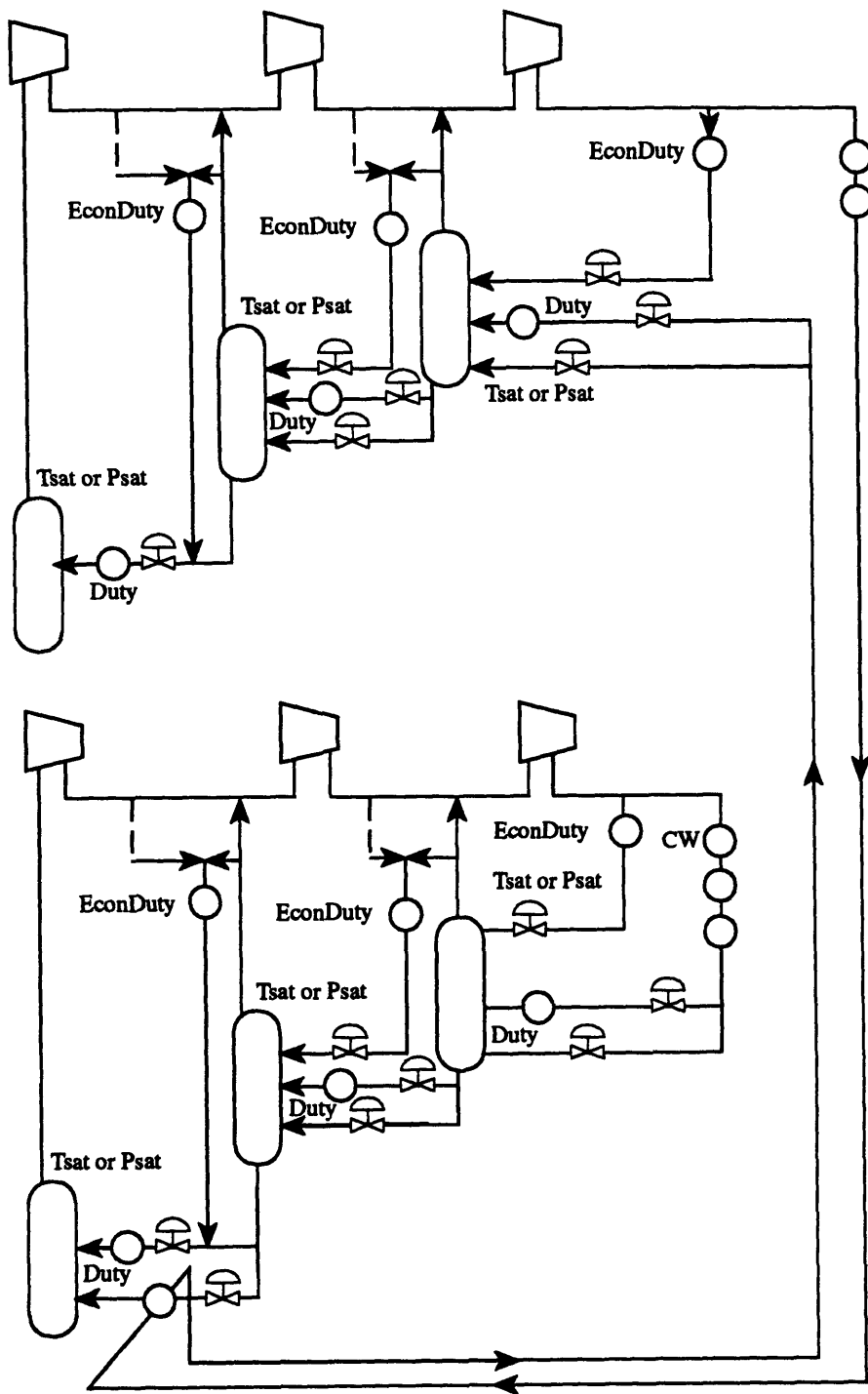


FIGURE 4.14 Illustration of a cascade refrigeration cycle. (Advent User Guide, 1991)

network and the chemical process over the actual work required to run the refrigeration compressors. The actual work can be obtained by a rigorous simulation of the entire refrigeration system or from an existing refrigeration system.

The exergetic efficiency is then assumed constant with respect to changes in refrigeration system operating conditions and process changes. The effects of any proposed change can then be evaluated in terms of its potential for heat and work integration. In Linnhoff and Dhole's (1989) method, like the plus/minus rule and the appropriate placement rules, the effects of proposed changes on the capital cost of the heat exchanger network and the chemistry and costs of the chemical process are considered only after a process change is made.

The reason the Linnhoff and Dhole (1989) method is not used in this thesis is that it only targets for operating costs of refrigeration systems and not their capital costs. Their method targets for the total work requirement (operating cost) of a particular refrigeration system (the one whose exergetic efficiency has been calculated). But, in order to target for the capital costs of refrigeration systems, the work required by each individual piece of equipment (each compressor) in the refrigeration system is needed.

Another problem with Linnhoff and Dhole's (1989) method is the assumption of constant exergetic efficiency. With changing operating conditions of the refrigeration system and the chemical process (changing shape of the grand composite curve), it is unlikely that the exergetic efficiency will remain constant. Even if the overall exergetic efficiency remains relatively unchanged, the individual efficiency of each compressor can vary widely. The individual efficiencies of each compressor determines their work demand and therefore, the capital costs of refrigeration systems. Finally, the targeting method only works for a particular chemical process and refrigeration system combination. For a different

combination, a new exergetic efficiency must be calculated. This concludes the review of typical industrial refrigeration equipment and previous research to design integrated refrigeration systems.

Now, the structure of the utility system in the cold end of an ethylene plant optimization problem is selected. In this example, the utility system must provide a significant amount of refrigeration and some cooling water and low temperature steam. The selected structure of the refrigeration system is a cascade refrigeration cycle with three levels of ethylene refrigeration in the low temperature cycle and four levels of propylene refrigeration in the high temperature cycle. A multi-stage compressor is used in both the low and the high temperature cycles. The structure was selected from previous industrial refrigeration system designs for similar ethylene plants (Zdonik, Green, and Hallee, 1970; EPRI, 1989). The low temperature steam is assumed to come from an extraction level of a steam turbine and the cooling water from a cooling tower. The optimum, minimum cost structure could only be guaranteed by solving the superstructure of Section 3.2 (a very large and difficult MINLP).

The second step of the method accounts for the utility system heat interactions by fitting the utilities in the grand composite curve to determine their duties. The utilities in this example are low temperature steam, cooling water, and seven refrigeration levels. Fitting utilities in the grand composite curve to determine their duties was discussed in subsection 4.1.2.

The degree of integration of the refrigeration system should be allowed to change. Therefore, a new optimization variable, the minimum approach temperature for the integration of the refrigeration section of the utility system ( $\Delta T_{\min}$ ), can be defined.  $\Delta T_{\min}$  can be very different than the minimum approach temperature for heat exchange ( $\Delta T_{\min}$ ) defined earlier.  $\Delta T_{\min}$  determines the degree of integration of the refrigeration section of the utility system and also the refrigeration utilities cooling duties.

Since refrigeration costs dominate the utility system costs, cooling water and low temperature steam supply and target temperatures are fixed and unit costs for thermal energy for both utilities are specified in the cost data of Table 7.1. This fixes some of the heat interactions with the above ambient temperature section of the utility system. A more detailed model where the degree of integration of the above ambient temperature section of the utility system can change could also be defined, but this is not necessary, since the refrigeration costs dominate.

Fitting utilities in the grand composite curve and calculating their duties does not account for the work interactions of refrigeration systems with chemical processes and their heat exchanger networks. As their operating conditions change, the performance of their refrigeration compressors vary. This can significantly affect the capital and operating costs of the entire refrigeration system. Information on the performance of refrigeration systems with changing operating conditions is needed in order to capture their work interactions.

Step three in the method to target for utility systems capital and operating costs takes into account the utility system work interactions with the chemical process and its heat exchanger network with the performance equations. The performance equations allow the quick prediction of work consumption or production by individual pieces of equipment in utility systems without a rigorous design of the entire utility system. In this subsection, the performance equations for refrigeration systems are presented.

The performance equations for refrigeration systems are obtained by capturing, in simple equations, the performance of simple mechanical vapor recompression refrigeration cycles (simple heat pumps). The performance of simple mechanical vapor recompression refrigeration cycles is then used to predict the performance of complex or cascade refrigeration cycles (multi-extraction multi-rejection heat pumps) and obtain the work demanded by each individual compressor. But first, the refrigeration performance equations must be developed.



Figure 4.15 and Figure 4.16 illustrates results obtained from Aspen Plus simulations of simple refrigeration cycles with ethylene and propylene as working fluids. When the utilization efficiency,  $N_u$ , is plotted against the evaporator temperature (at a given condenser temperature) a nearly linear relationship is observed. As far as I know, this has not been reported in the literature.  $N_u$  is defined as the thermodynamic ideal work necessary to transfer a given amount of heat from evaporator temperature to condenser temperature divided by the actual work obtained to transfer the same amount of heat in the simulation. For refrigeration applications,  $N_u < 1.0$ . For work producing cycles,  $N_u$  is normally define as the inverse of the refrigeration utilization efficiency. Therefore, for refrigeration systems

$$N_u = W_{ideal} / W_{actual} = W_{id} / W_{sim} \quad (4.14)$$

where  $W_{sim}$  is the calculated actual work from a simulation.

Usually the coefficient of performance, COP, is plotted against the evaporator temperature (at a given condenser temperature) to illustrate the performance of simple refrigeration cycle. The coefficient of performance is the ratio of the evaporator duty to the compression work in the simulation. When COP is plotted against evaporator temperature curves are obtained. Figure 4.17 and 4.18 are plots of COP versus evaporator temperature (at a given condenser temperature) of data obtained from the same simulations that gave Figures 4.15 and 4.16.

From the nearly linear relationship of  $N_u$  to evaporator temperature, simple and accurate performance equations for both simple refrigeration cycles at all feasible operating conditions are obtained. They are :

for ethylene,

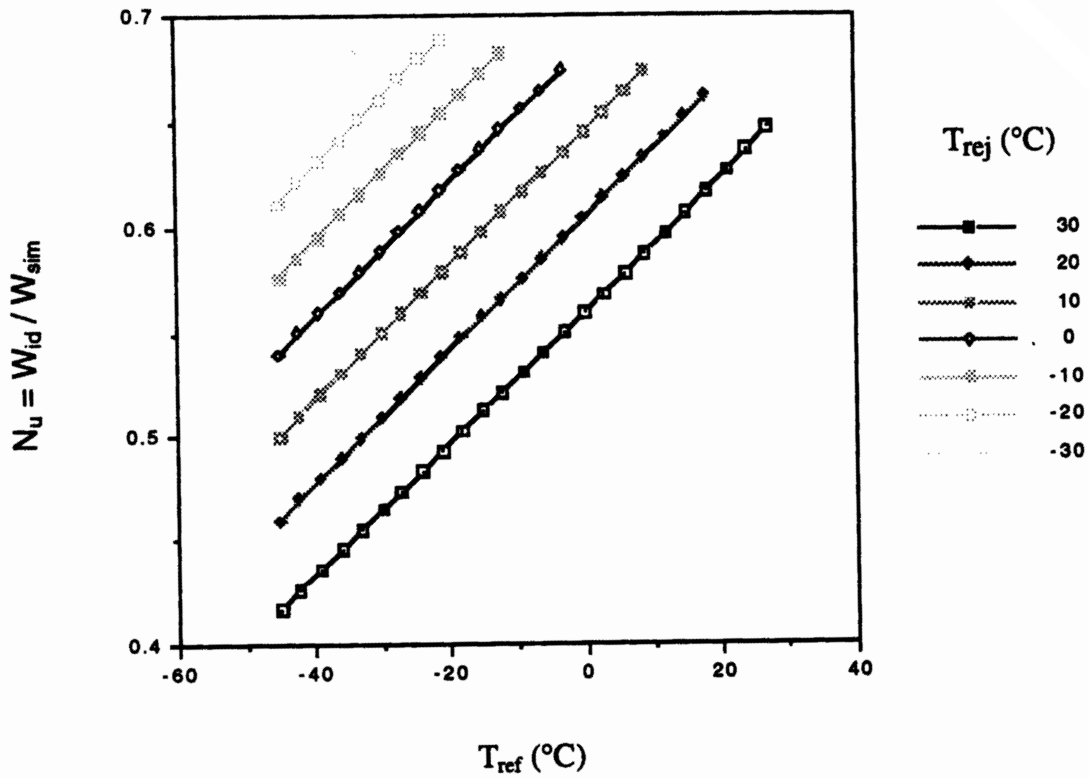


FIGURE 4.15 Graph of the utilization efficiency,  $N_u$ , versus the evaporator temperature (at various condenser temperatures) for a mechanical vapor recompression cycle with propylene as the working fluid.

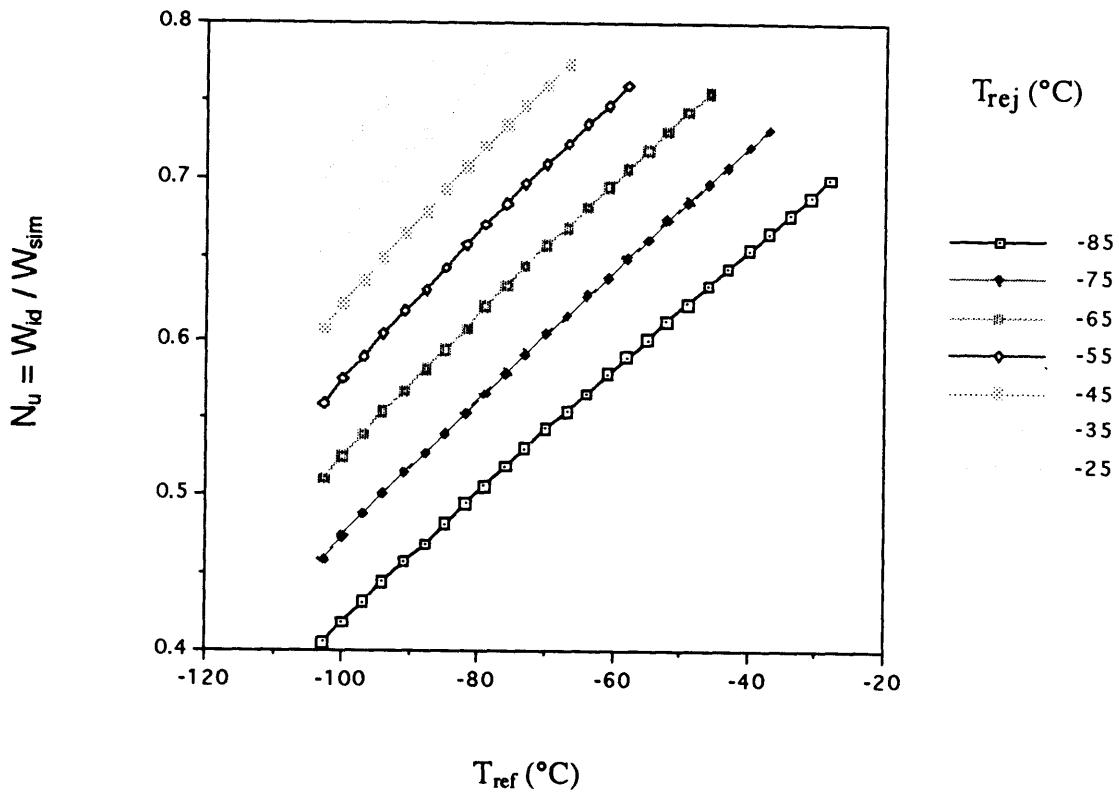


FIGURE 4.16 Graph of the utilization efficiency,  $N_u$ , versus the evaporator temperature (at various condenser temperatures) for a mechanical vapor recompression cycle with ethylene as the working fluid.

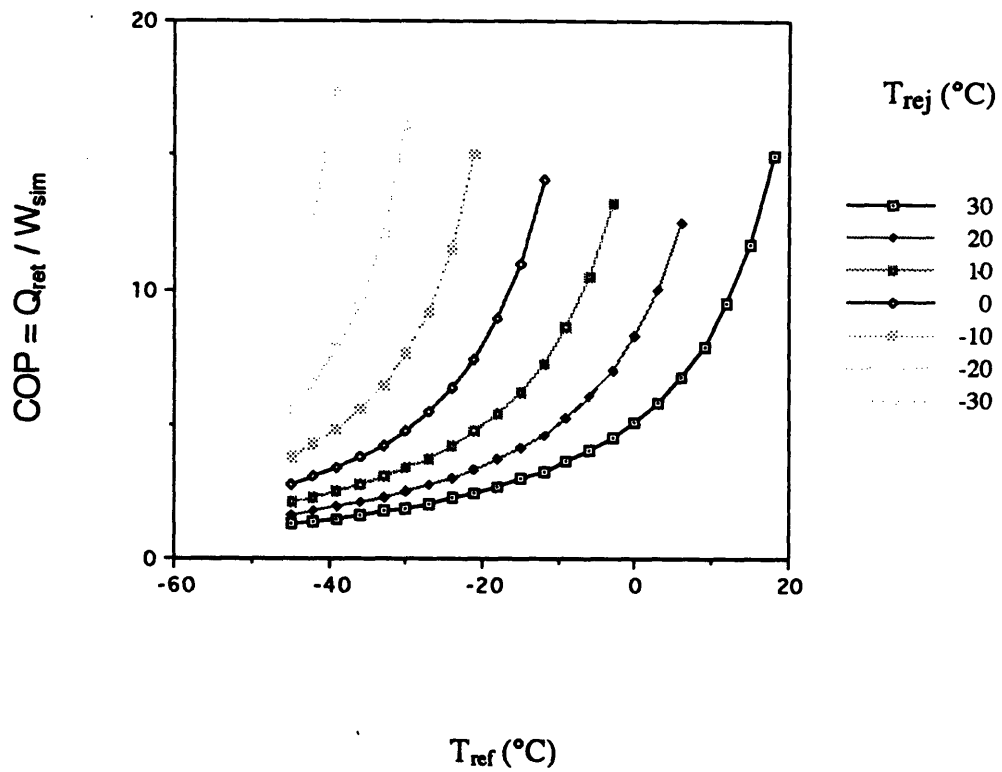


FIGURE 4.17 Graph of the coefficient of performance, COP, versus the evaporator temperature (at various condenser temperatures) for a mechanical vapor recompression cycle with propylene as the working fluid.

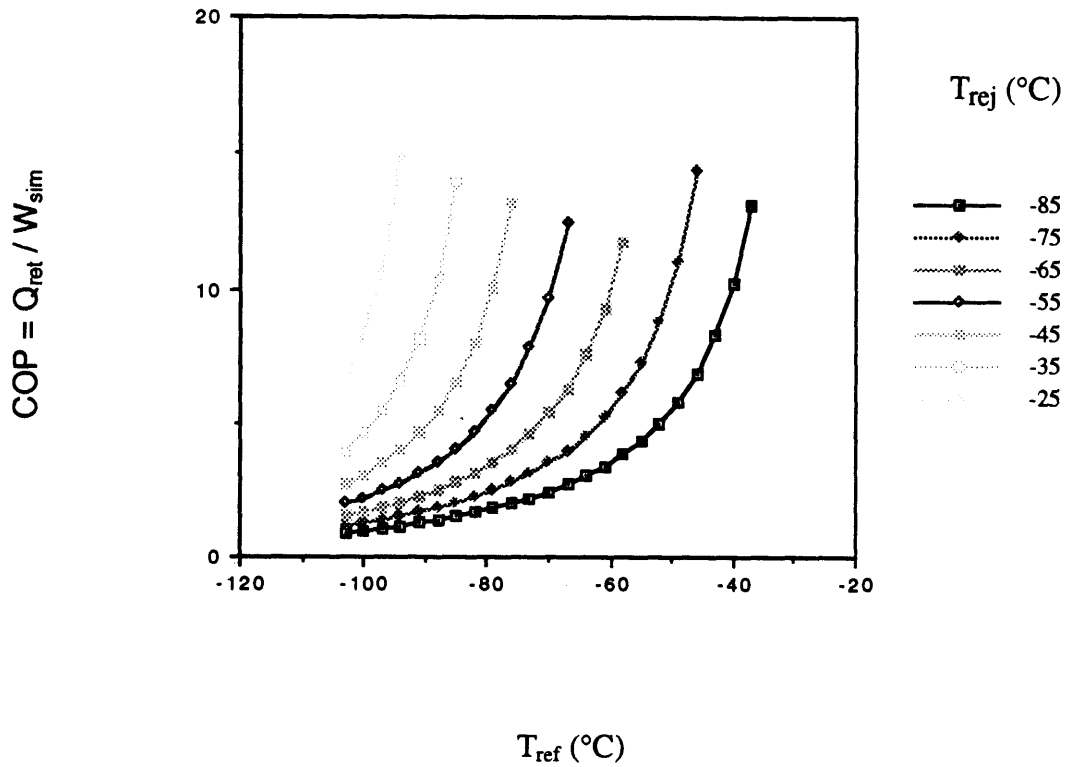


FIGURE 4.18 Graph of the coefficient of performance, COP, versus the evaporator temperature (at various condenser temperatures) for a mechanical vapor recompression cycle with ethylene as the working fluid.

$$N_u = M_e * T_{ref} + B_e \quad (4.15)$$

$$M_e = (3.1699E-3) - (3.9874E-5 * T_{rej}) - (4.5455E-7 * (T_{rej})^2) - (2.8486E-9 * (T_{rej})^3) \quad (4.16)$$

$$B_e = 0.65148 - 6.6937E-3 * T_{rej} \quad (4.17)$$

for propylene,

$$N_u = M_p * T_{ref} + B_p \quad (4.18)$$

$$M_p = (3.2052E-3) - (4.7541E-7 * T_{rej}) + (6.6733E-9 * (T_{rej})^2) - (8.5203E-10 * (T_{rej})^3) \quad (4.19)$$

$$B_p = 0.68037 - 3.8542E-3 * T_{rej} \quad (4.20)$$

where  $T_{ref}$  is the evaporator temperature and  $T_{rej}$  the condenser temperature.

These performance equations allow the quick prediction of the compression work requirement of simple refrigeration cycles (with ethylene or propylene as working fluids) for any feasible combination of evaporator and condenser temperatures and refrigeration cooling duty. The performance equations define  $N_u$  from the evaporator and condenser temperatures.  $N_u$  and the evaporator cooling duty predict the compression work. These performance equations are also used to quickly predict the compression work for each individual compressor in complex and cascade refrigeration systems with ethylene and propylene as refrigerants. Therefore, the rigorous simulations of complex or cascade refrigeration systems is not necessary.

Different performance equations must be developed for different working fluids or different refrigeration technologies. If they are linear, then the prediction of the compression work for each individual compressor is easy. It would be interesting to explore if linear performance equations can be obtained for the work producing cycles above ambient temperature. There, the reference cycle could be a Rankine cycle with water as a working fluid.

Now, the performance equations are used to calculate the individual work requirements at each compression stage (or individual compressor's work requirement if different compressors are used) for complex refrigeration systems. First, individual  $N_u$ s for each compression stage must be calculated. Since complex refrigeration cycles are a combination of two or more simple refrigeration cycles, each intermediate stage can be considered to be a condenser for the bottom cycle and an evaporator for the top cycle. In other words, the intermediate stage acts as a direct contact heat exchanger between the bottom cycle and the top cycle. Therefore, the  $N_u$  for each compression stage is defined by the performance equations and the evaporator and condenser temperature in each cycle of the complex refrigeration system. The prediction of individual work requirement at each compression stage is obtained from the individual  $N_u$ s and the cooling duties at each stage of the complex refrigeration cycle.

The use of the performance equations to predict the compression work requirement for each individual compressor in cascade refrigeration cycles is straightforward. Simply treat the low temperature cycle and the high temperature cycle as individual complex refrigeration cycles. The heat load transferred from the low temperature cycle to the high temperature cycle can be obtained by summing the refrigeration duty of the low temperature cycle and its total work requirement. Economizers in complex or cascade refrigeration systems are treated as heat duty that leaves the refrigeration system at a particular stage and does not require further compression.

The final step in the method is to target for the capital and operating costs of the utility system. This is done with the heating or cooling duties of the utilities (results of step two), the individual work requirement of each compressor (results of step three), and the cost correlations given in Table 7.1

### **Example**

Figure 4.19 illustrates the grand composite curve with its fitted utility mix for the minimum total cost solution obtained in the cold end of an ethylene plant optimization problem. Table 4.8 gives the temperatures of the utility mix and the utilities thermal duties obtained from the grand composite curve.

In order to target for the utility system's capital and operating costs its work interactions in the refrigeration section must be accounted for. This can be done with the refrigeration performance equations. The refrigeration performance equations allow the quick prediction of the work demand by each compressor in the refrigeration system without a rigorous design of the entire system.

Table 4.9 illustrates the calculation of the individual utilization efficiencies for each compression stage in the cascade refrigeration system and the prediction of the work requirement at each compression stage. The individual utilization efficiencies are obtained from the refrigeration performance equations. The work demand in each compression stage (and by each compressor) is obtained from the individual utilization efficiencies and the cooling duties at each stage of the cascade refrigeration cycle.

Table 4.10 demonstrates the prediction of the annualized capital and operating costs of the utility system. These costs are predicted with the thermal duties of the utilities, the individual work requirement of each compressor in the refrigeration system, and the cost correlations in Table 7.1.



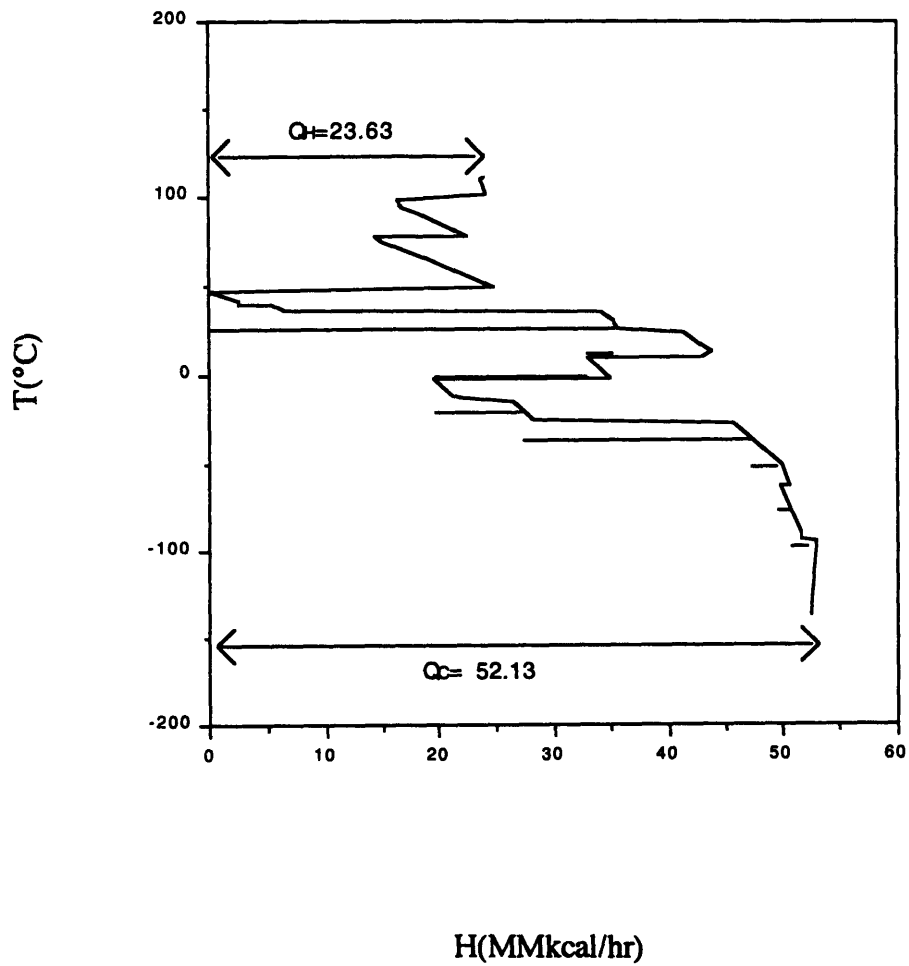


FIGURE 4.19 Grand composite curves with its fitted utility mix for the minimum total cost solution obtained in the cold end of an ethylene plant optimization problem.

**TABLE 4.8** The utility temperatures and their duties for the utility mix in the minimum total cost solution for the cold end of an ethylene plant optimization problem.

<b>Utility mix</b>	<b>Temperature (°C)</b>	<b>Duty (MMkcal / hr)</b>
<b>steam</b>	130	23.63
<b>cooling water</b>	25	35.66
<b>propylene refrigerant level 1</b>	13.7	1.95
<b>propylene refrigerant level 2</b>	0.0	14.30
<b>propylene refrigerant level 3</b>	-21.3	7.73
<b>propylene refrigerant level 4</b>	-39.3	20.01
<b>ethylene refrigerant level 1</b>	-53.4	2.27
<b>ethylene refrigerant level 2</b>	-79.5	1.01
<b>ethylene refrigerant level 3</b>	-97.0	1.69

**TABLE 4.9** The calculation of the individual utilization efficiencies and the production of the work requirement in each compression stage in the cascade refrigeration system.

	Temperature (°C)	individual $N_u$	Compression work in each stage (kW)
<b>final rejection</b>	45	.5498	6,576
<b>propylene 1</b>	13.7	.6274	2,630
<b>propylene 2</b>	0.0	.6121	6,002
<b>propylene 3</b>	-21.3	.6355	3,733
<b>propylene 4</b>	-39.3	.6812	705
<b>ethylene 1</b>	-53.4	.6564	701
<b>ethylene 2</b>	-79.5	.7084	276
<b>ethylene 3</b>	-97.0		
<b>heat rejected to cooling water =</b>			34.21 MMkcal / hr
<b>work of propylene compressor =</b>			18,941 (kW)
<b>work of ethylene compressor =</b>			1,682 (kW)

TABLE 4.10 Calculating the capital and operating costs of the utility system in the minimum total cost solution to the cold end of an ethylene plant optimization problem. (see Table 7.1 for additional information)

***CAPITAL COSTS***

<b>propylene compressor</b>	=	8215 (18,941) .73
	=	10.89 million \$
<b>ethylene compressor</b>	=	8215 (1,682) .73 x 6 units
	=	11.16 million \$
<b>Annualized capital cost</b>	=	<b>4.41 million \$ / yr</b>

***OPERATING COSTS***

<b>steam cost</b>	=	1.50 \$ / MMBTU ( 3.969 $\frac{\text{MMBTU}}{\text{MMkcal}}$ ) (23.63 $\frac{\text{MMkcal}}{\text{hr}}$ ) (8300 $\frac{\text{hr}}{\text{yr}}$ )
	=	1.17 million \$ / yr
<b>cooling water cost</b>	=	.10 \$ / MMBTU ( 3.969 $\frac{\text{MMBTU}}{\text{MMkcal}}$ ) (69.37 $\frac{\text{MMkcal}}{\text{hr}}$ ) (8300 $\frac{\text{hr}}{\text{yr}}$ )
	=	.23 million \$ / yr
<b>electric power</b>	=	20.00 \$ / MMBTU (0.03415 $\frac{\text{MMBTU}}{\text{kW hr}}$ ) (20,623 kW) (8300 $\frac{\text{hr}}{\text{yr}}$ )
	=	11.69 million \$ / yr
<b>Total operating costs</b>	=	<b>13.09 million \$ / yr</b>

### Notations used in Chapter 4

A	target for minimum heat transfer area for the heat exchanger network
$A_{\min}$	target for minimum heat transfer area for the heat exchanger network
$B_e$	y-intercept for ethylene performance equation
$B_p$	y-intercept for propylene performance equation
BCC	balanced composite curve
$c_a$	annualized cost of heat transfer area
$c_u$	annualized cost of heat exchangers
$c_c^i$	unit thermal cost of cold utility i
$c_h^i$	unit thermal cost of hot utility i
C	index for cold process streams
$CC^k$	horizontal distance to the cold composite curve
COP	coefficient of performance
CU	number of cooling utilities
$f_i$	flowrate of cold process stream i
$f_i c_i$	heat capacity-flowrate product for cold process stream i
$F_i$	flowrate of hot process stream i
$F_i C_i$	heat capacity-flowrate product for hot process stream i
$F(\underline{x}, \underline{y})$	function to evaluate the chemical process' capital and operating costs
$g(\underline{x}, \underline{y})$	vector of inequality constrains
GCC	grand composite curve
$h(\underline{x}, \underline{y})$	vector of equality constrains
$h_i$	heat transfer coefficient for stream i
H	index set of hot process streams
$HC^m$	horizontal distance to the hot composite curve
HU	number of hot utilities
$M_e$	slope of ethylene performance equation
$M_p$	slope of propylene performance equation
$N_u$	utilization efficiency
$N_c$	number of cold stream
$N_h$	number of hot stream
NU	minimum number of units for maximum energy recovery
p	index set for candidate pinch
$(q_j)_i$	enthalpy change of stream j in interval i
$Q_c$	minimum cold utility demand
$Q_h$	minimum hot utility demand
$Q_c^i$	thermal duty of cooling utility i
$Q_h^i$	thermal duty of heating utility i
$QSIA(\underline{y})^p$	heat sink above pinch candidate p
$QSOA(\underline{y})^p$	heat source above pinch candidate p
$t_i^{\min}$	supply temperature for cold process streams

$t_i^{\text{out}}$	target temperature for cold process streams
$T_{\text{ref}}$	evaporator temperature in a mechanical vapor recompression cycle
$T_{\text{rej}}$	condenser temperature in a mechanical vapor recompression cycle
$T_i^{\text{in}}$	supply temperature for hot process streams
$T^k$	temperature values at kinks in cold composite curve
$T^m$	temperature values at kinks in hot composite curve
$T_i^{\text{out}}$	target temperature for hot process streams
$T^p$	pinch candidate temperature
$U$	overall heat transfer coefficient
$U_{\text{min-MER}}$	minimum number of heat exchangers for maximum energy recovery
$U^p$	horizontal distance to grand composite curve at pinch candidate $p$
$U_i^p$	horizontal distance to grand composite curve at hot utility temperature
$U_j^p$	horizontal distance to grand composite curve at cold utility temperature
$\underline{x}$	vector of process parameters
$\underline{y}$	vector of flowrates and temperatures of process streams
$z_h^p(\underline{y})$	heating deficit above pinch candidate $p$
$\Delta H_i$	enthalpy change in interval $i$
$\Delta T_{\text{lni}}$	log mean temperature difference in enthalpy interval $i$
$\Delta T_{\text{min}}$	minimum approach temperature for process heat integration
$\Delta T_{\text{min}}$	minimum approach temperature refrigeration system integration
$\Delta T_{\text{umin}}$	minimum approach temperature flue gas integration
$\phi$	objective function
$\Omega(\underline{y})$	difference in heat content between hot and cold process streams

## CHAPTER 5 : THE SIMULTANEOUS OPTIMIZATION METHOD AND ITS IMPLEMENTATION IN A RIGOROUS SEQUENTIAL PROCESS SIMULATOR

### 5.1 The Simultaneous Optimization Method

Section 4.1 extended Duran and Grossmann's (1986) pinch location method to not only account for heat integration but also to target for the capital costs of heat exchanger networks. This expanded pinch location method (NLP P2) can simultaneously optimize a chemical process and its heat exchanger network by including all their heat and work interactions.

Unfortunately, NLP P2 fixes some important heat and work interactions with the utility system. This occurs because the number and temperature levels of the utilities present ( $i \in \text{HU}$ ,  $j \in \text{CU}$ ), their unit costs for thermal energy ( $c_h^i$ :  $i \in \text{HU}$  and  $c_c^j$ :  $j \in \text{CU}$ ), and the cost of providing work must be specified in order to solve NLP P2. The real costs of providing work and thermal utilities are the capital and operating costs of the utility system used to produce them. Since the demand for utilities and work is dependent on the chemical products produced (chemical process chosen) and the way these products are produced (chemistry chosen), it's expected that the real costs of utilities and work would vary from flowsheet to flowsheet.

Section 4.2 introduced a new method that targets for utility systems capital and operating costs by including its heat and work interactions with the chemical process and heat exchanger network. The method uses only the grand composite curve (to fit a utility mix) and simple performance equations to target for the utility system's capital and operating costs. Since a rigorous simulation of the entire utility system is not necessary, computation time is drastically reduced.

The expanded pinch location method (NLP P2) of Section 4.1 can be combined with the new method to target for the utility system capital and operating costs of Section 4.2. The result is the simultaneous optimization method presented as the main objective of this thesis. The simultaneous optimization method is the first strategy that can simultaneously optimize the operating conditions of all three subsystem along with parameters for process heat and utility system integration (e.g.  $\Delta T_{\min}$ ,  $\Delta T_{\text{ummin}}$ ,  $\Delta T_{\text{min}}$  etc.) with reasonable computational expense. This is accomplished by including the subsystem's heat and work interactions in the optimization step. The simultaneous optimization method is given by NLP P3.

$$\begin{aligned}
 \min \phi &= F(\underline{x}, \underline{y}) + c_a A(\underline{y}, \underline{z}) + c_u \text{NU}(\underline{y}, \underline{z}) + c_f F(\underline{y}, \underline{z}) + c_{cw} \text{CW}(\underline{y}, \underline{z}) + c_w W(\underline{y}, \underline{z}) + \text{CCUS}(\underline{y}, \underline{z}) \\
 \text{s.t. } &h(\underline{x}, \underline{y}) = 0, \\
 &g(\underline{x}, \underline{y}) \leq 0, \\
 \text{BCC} &= r_1(\underline{y}, \underline{z}) \\
 \text{GCC} &= r_2(\underline{y}, \underline{z}) \\
 A &= r_3(\text{BCC}) \\
 \text{NU} &= r_4(\text{BCC}) \\
 F &= r_5(\text{GCC}, \text{PE}) \\
 \text{CW} &= r_6(\text{GCC}, \text{PE}) \\
 W &= r_7(\text{GCC}, \text{PE}) \\
 \text{CCUS} &= r_8(\text{GCC}, \text{PE}) \\
 \underline{x} \in X, \underline{y} \in Y, \underline{z} \in Z
 \end{aligned}
 \tag{NLP P3}$$

The vector variables  $\underline{x}$  and  $\underline{y}$  are the same as defined in the previous NLPs. The vector variables  $\underline{z}$  represent utility system operating conditions and parameters for process heat integration and utility system heat integration (ex. utility temperature levels,  $\Delta T_{\min}$ ,  $\Delta T_{\text{ummin}}$ ,  $\Delta T_{\text{min}}$ , etc.).

The functions  $r_1$  and  $r_2$  calculate the grand composite curve (GCC) and the balanced composite curves (BCC).  $A$  and  $\text{NU}$  are used to calculate the capital costs of the heat exchanger network.  $A$  is the target for minimum heat transfer area for the heat exchanger network ( $A_{\min}$  in equation 4.11) and  $\text{NU}$  is the target for the minimum number of heat



exchangers for maximum energy recovery ( $U_{\min-MER}$ ). They are both determined from the balanced composite curves. The annualized unit costs of heat transfer area and heat exchangers are given by  $c_a$  and  $c_u$ .

$F$ ,  $CW$ , and  $W$  are used to predict the operating costs of the utility system.  $F$ ,  $CW$ , and  $W$  represent the annual consumption of fuel ( $F$ ), cooling water ( $CW$ ), and work ( $W$ ) and their local market costs are given by  $c_f$ ,  $c_{cw}$ , and  $c_w$  respectively. The prediction of the annualized capital cost of the utility system is given by  $CCUS$ .  $F$ ,  $CW$ ,  $W$ , and  $CCUS$  are functions of the grand composite curve and the performance equations (PE). The utility temperature levels are now optimization variables in the vector  $\underline{z}$  and, no unit cost for thermal energy is associated with them.

## **5.2 Implementing the Simultaneous Optimization Method in a Rigorous Sequential Process Simulator.**

In this thesis the simultaneous optimization method (NLP P3) is solved with an optimizer contained in a rigorous sequential modular process simulator. Figure 5.1 illustrates some of the earlier uses of rigorous process simulators to optimized complete chemical processes. Process simulators were first used as an interactive process optimization tool (Figure 5.1a). The simulators would converge a flowsheet and predict the capital and operating costs of a chemical process. The user would interact by changing the decision variables with the purpose of finding lower costs alternatives.

From its earlier use, the application of process simulators in complete process optimization developed in two directions. One was an early mathematical approach illustrated in Figure 5.1b and the other the pinch analysis approach depicted in Figure 5.1c.

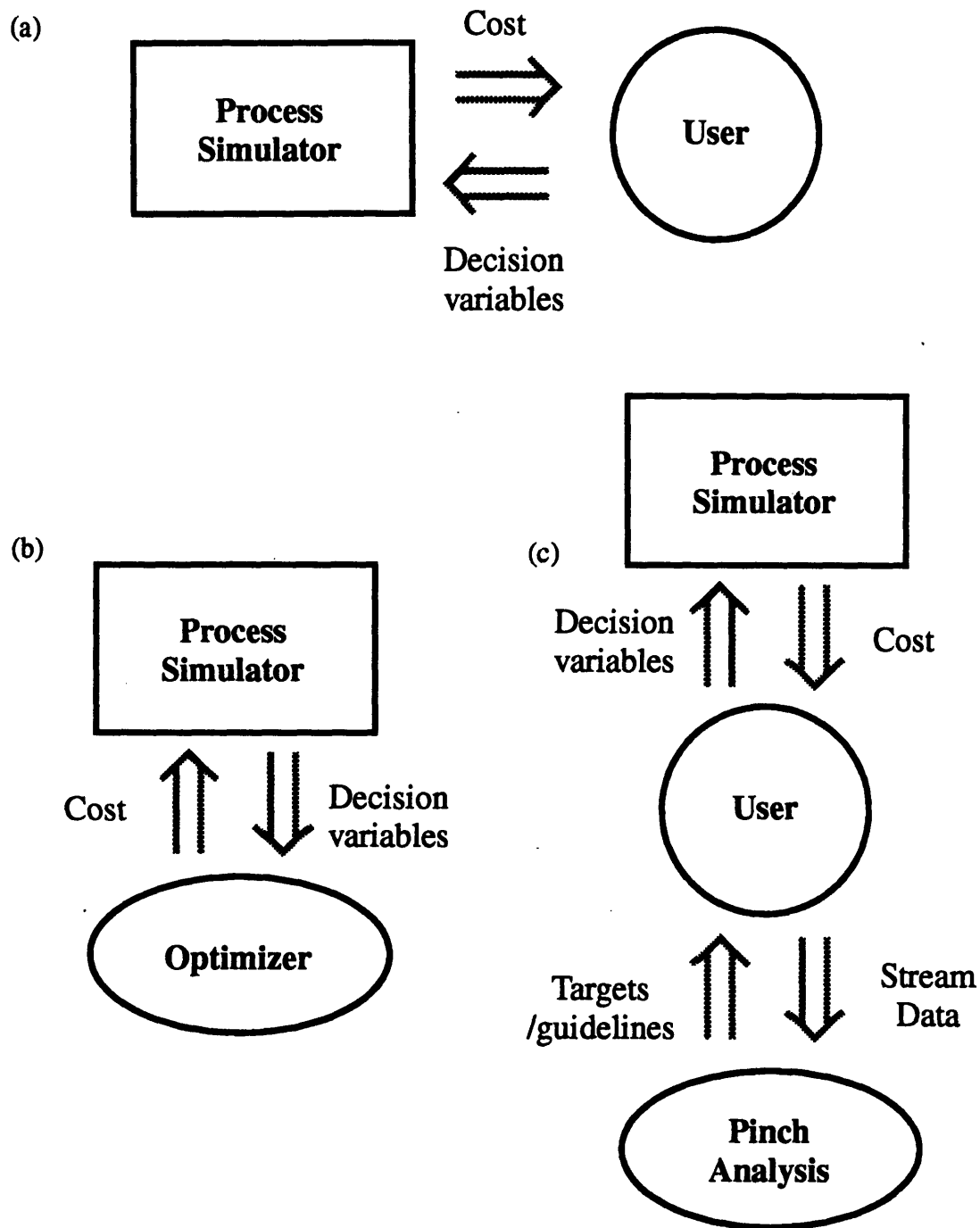


FIGURE 5.1 The early uses of process simulators in complete process optimization; (a) used as an interactive process optimization tool; (b) the early mathematical approach; (c) the pinch analysis approach.

In the early mathematical approach a flowsheet optimizer replaced the user in the optimization of the decision variables (Figure 5.1b). An objective function was formulated and the optimizer was used to simultaneously converge and optimize the flowsheet. Flowsheet optimization strategies developed were typically equivalent to only 3-10 flowsheet simulations (Lang, Biegler and Grossmann, 1988). Furthermore, they could usually guarantee finding at least a local optimum.

The disadvantage of this early mathematical approach was that the heat and work interactions with the heat exchanger network and the utility system were fixed in the formulation of the objective function. The heat and work interactions with the utility system were fixed by assuming the number and temperature levels of the utilities present ( $i \in \text{HU}$ ,  $j \in \text{CU}$ ), their unit costs for thermal energy ( $c_h^i$ :  $i \in \text{HU}$  and  $c_c^j$ :  $j \in \text{CU}$ ), and the cost of providing work. Initially, the heat and work interactions with the heat exchanger network were fixed by assuming all heating and cooling will be done with utilities.

In the pinch analysis approach, the user is still an important component of the optimization (Figure 5.1c). The flowsheet simulator converges a flowsheet, predicts the capital and operating costs of a chemical process and provides stream data. The user utilizes the stream data and pinch analysis to quickly develop targets and guidelines for better heat and work integration. The target and guidelines provide the basis for selecting the new values of the decision variables.

The advantage of pinch analysis is that it can discover some important heat and work interactions between the subsystems. However, the success of this trial-and-error approach depends mostly on the skill of the users and their experience with the process involved. The results are nearly always suboptimal, or at least there is doubt about optimality.

Lang, Biegler, and Grossmann (1988) implemented Duran and Grossmann's method (1986) in a process simulator. Their method combined some of the advantages of the early mathematical approach and pinch analysis. Figure 5.2a shows a diagram of their method. The decision variables are optimized with an optimizer and process heat integration is anticipated in a "superblock". At each iteration in the optimization the process simulator provides the current stream data to the superblock. The superblock determines targets for minimum energy consumption which are passed to the optimizer in the form of costs.

Unfortunately, Lang, Biegler, and Grossmann's method neglected some important heat and work interactions between the subsystems. The capital costs of the heat exchanger network were not included in the objective function. Therefore, process heat integration was constrained to satisfy a pre-specified  $\Delta T_{\min}$ . Of course, the optimization could be run repeatedly for a range of  $\Delta T_{\min}$ s. Their method also fixed the heat and work interactions with the utility system by selecting and costing a pre-determined utility mix. As a result, Lang, Biegler and Grossmann's method could not optimize the utility system's operating conditions or parameters for process heat or utility system integration (the variables in vector  $\underline{z}$  of NLP P3).

A diagram of the implementation of the simultaneous optimization method in a process simulator is given in Figure 5.2b. Similarly to Lang, Biegler and Grossmann's (1988) method, the simultaneous optimization strategy uses a superblock and an optimizer. However, the superblock not only anticipates process heat integration but is also able to target for the capital and operating costs of the heat exchanger network and the utility system. This is accomplished by combining Lang, Biegler, and Grossmann's method with Linnhoff and Ahmad's (1990) method to predict the capital cost of heat exchanger networks and the new method to target for the capital and operating cost of the utility system in the optimization step of a process simulator (Figure 5.3).

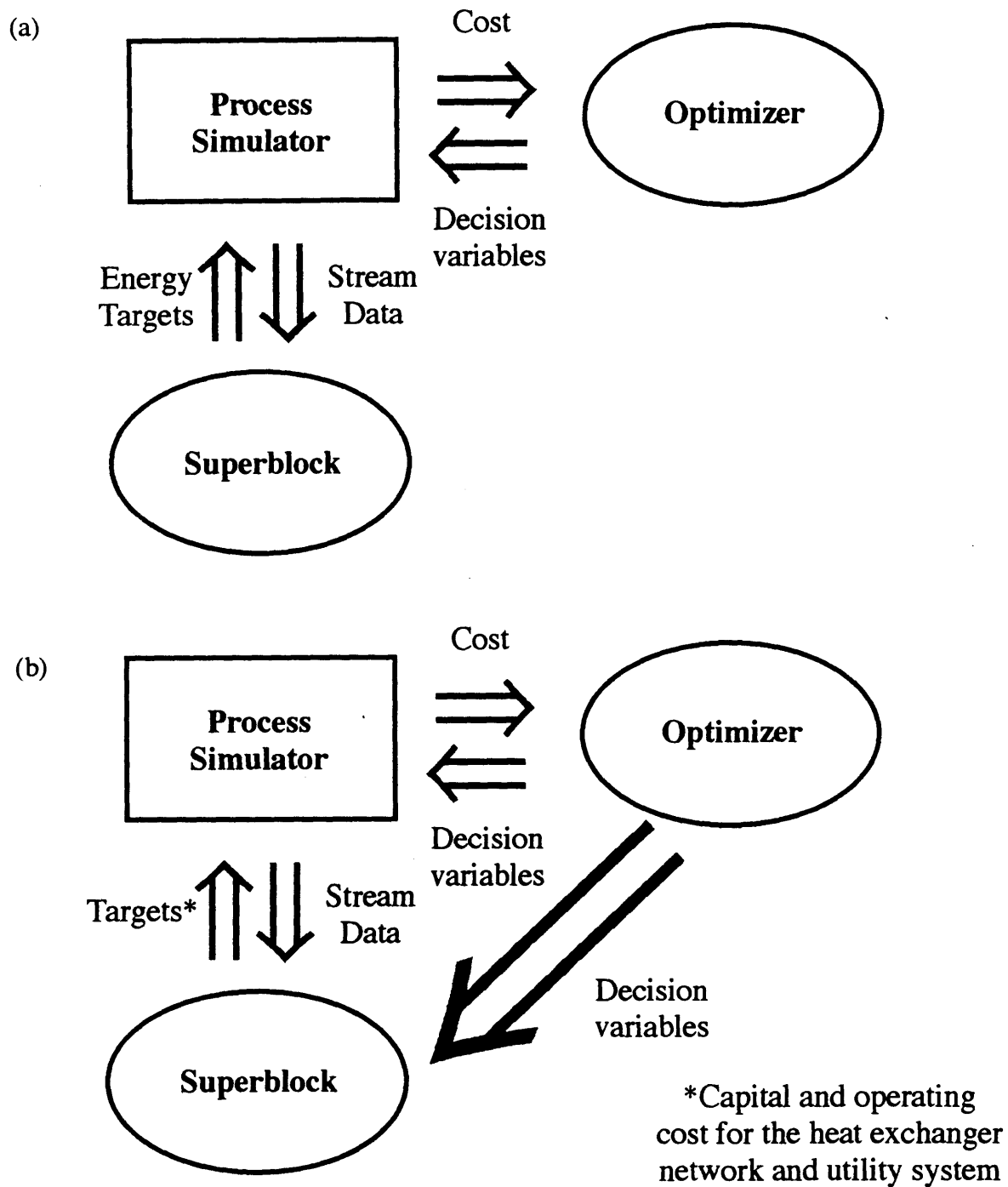


FIGURE 5.2 Recent uses for process simulators in complete process optimization; (a) Lang, Biegler, and Grossmann's (1988) method; (b) the simultaneous optimization method

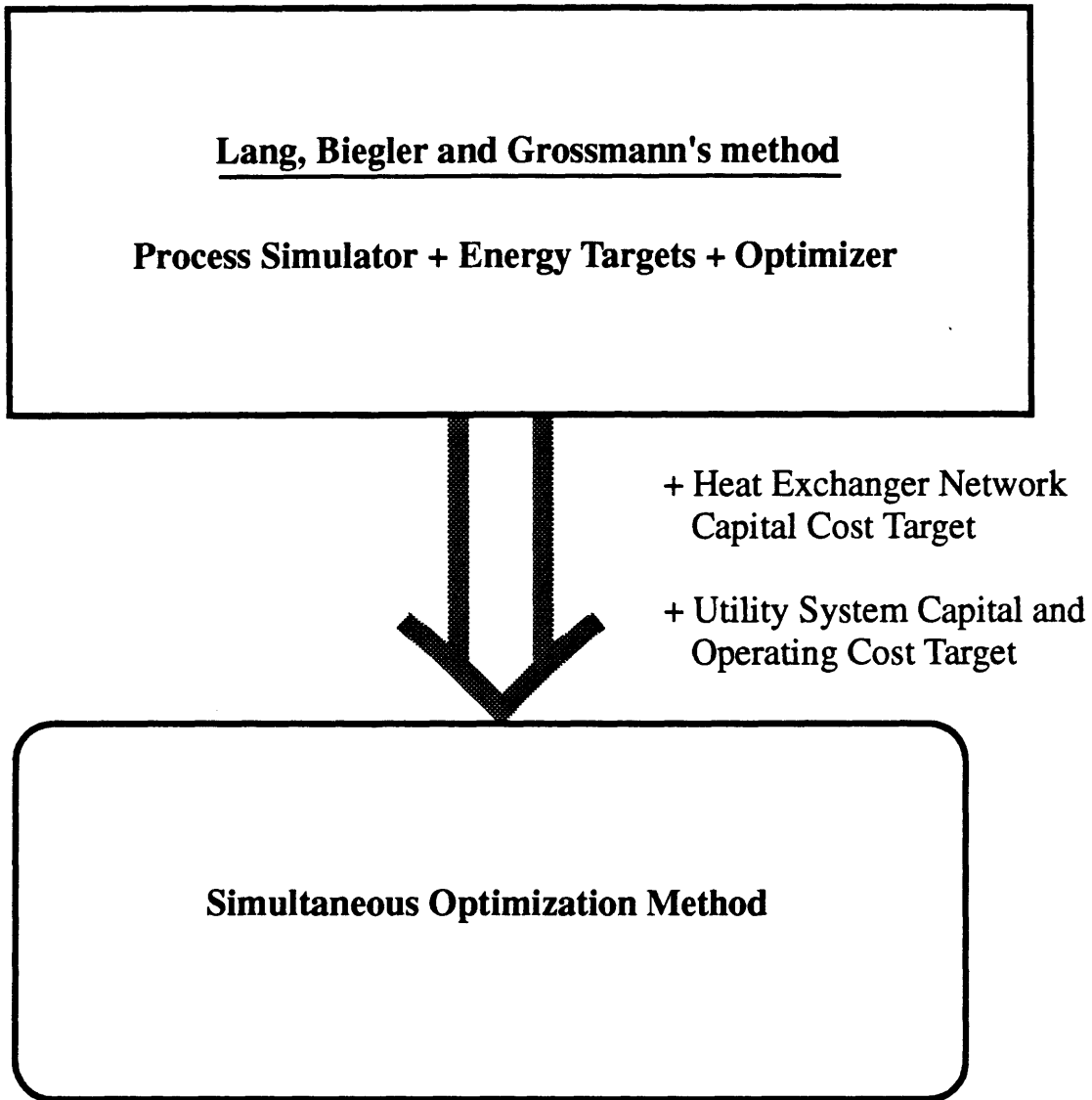


FIGURE 5.3 Diagram of the simultaneous optimization method.

Since all heat and work interactions between the subsystems are included in the optimization step, the optimizer can simultaneously converge and optimize a complicated real-life chemical process, its heat exchanger network and the utility system together with parameters for process heat and utility system integration (ex.  $\Delta T_{\min}$ ,  $\Delta T_{\text{umin}}$ ,  $\Delta T_{\text{rmin}}$ ). A flowchart for the simultaneous optimization method is given in Figure 5.4 and Table 5.1 lists the steps involved in its implementation in the optimization step of a process simulator.

The next two Chapters demonstrate the advantages of the simultaneous optimization method over the sequential approach and Lang, Biegler and Grossmann's (1988) method through flowsheet optimization examples. The sequential approach solutions were obtained by first solving NLP P0 in a rigorous process simulator (Figure 5.1b). The process stream data of these solutions and Linnhoff and Ahmad's (1990) cost targeting method were used to optimize  $\Delta T_{\min}$  and target for the capital costs of the heat exchanger network and the utilities thermal duties. Finally, the utility systems were designed to satisfy the demands for the assumed utilities and work at minimum cost. Lang Biegler and Grossmann's (1988) solutions were obtained by solving NLP P1 at various  $\Delta T_{\text{mins}}$  in a rigorous process simulator (Figure 5.2a) followed by the addition of the capital and operating costs of the heat exchanger networks and the utility systems. The simultaneous solutions were obtained by solving NLP P3 in a rigorous process simulator (Figure 5.2b). Chapter 6 presents the atmospheric petroleum crude tower optimization problem and Chapter 7 the cold end of an ethylene plant optimization problem.

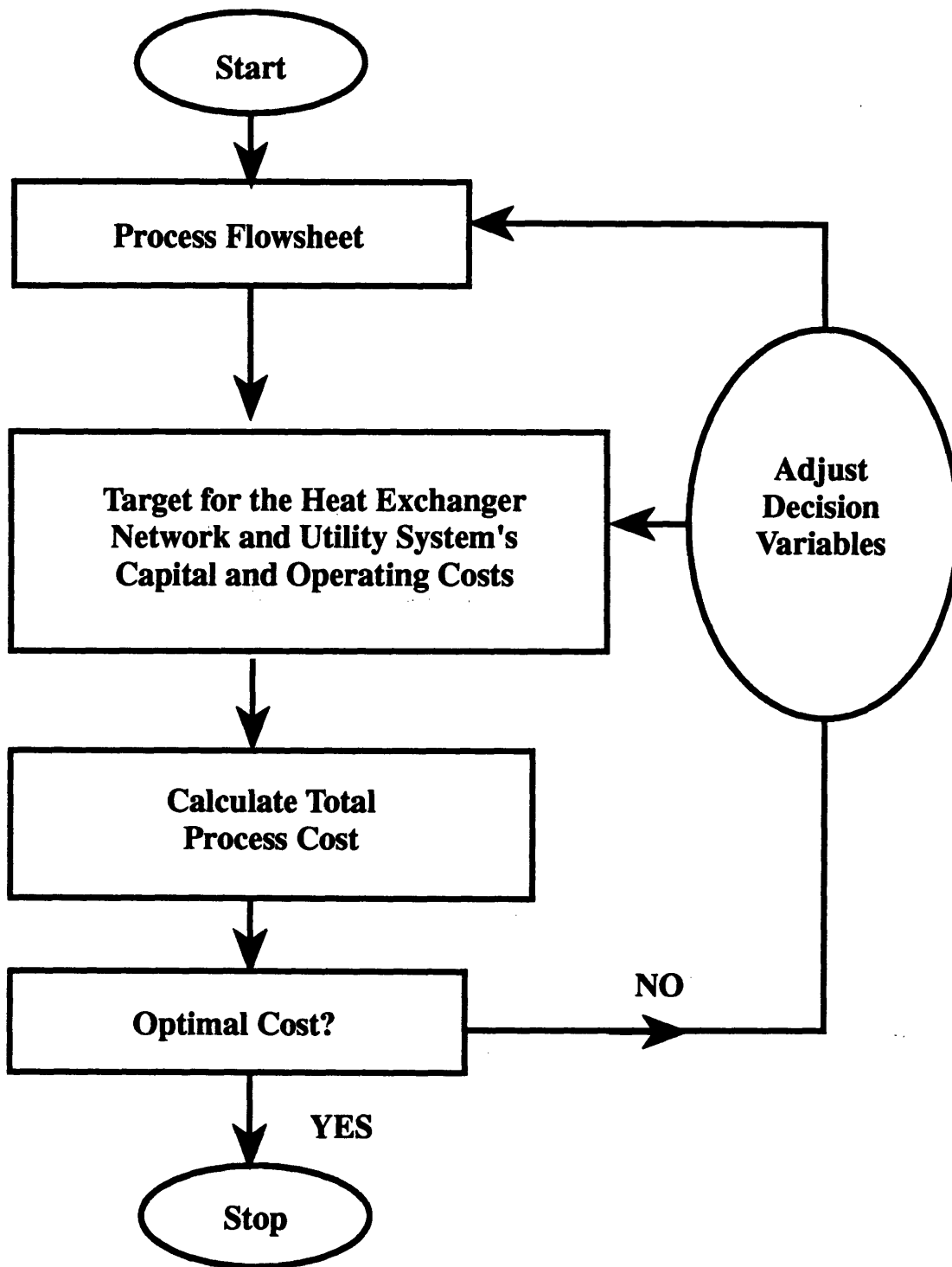


FIGURE 5.4 A flowchart for the simultaneous optimization method.



**TABLE 5.1** The steps involved in implementing the simultaneous optimization method in a rigorous sequential process simulator.

1) At a given SQP iteration, the flowrates and temperatures of all process streams undergoing heating or cooling are fixed. Therefore, the heat capacity-flowrate products of the process streams can be obtained from the process simulator by:

$$F_i C_i = [H(T^{\text{out}}_i) - H(T^{\text{in}}_i)] / (T^{\text{out}}_i - T^{\text{in}}_i); i = 1, \dots, N_h \quad (5.1)$$

$$f_j c_j = [h(t^{\text{out}}_j) - h(t^{\text{in}}_j)] / (t^{\text{out}}_j - t^{\text{in}}_j); j = 1, \dots, N_c \quad (5.2)$$

2) Arrange the pinch candidates in descending values of temperature and use equations (4.1), (4.2) and (4.3) to calculate the heating deficit functions ( $z^P_h(\mathbf{y})$ ) for each pinch candidate. The following temperatures are selected as pinch candidates.

- i) Supply temperatures of hot process streams
- ii) Target temperatures of hot process streams
- iii) Supply temperatures of cold process streams plus  $\Delta T_{\text{min}}$
- iv) Target temperatures of cold process streams plus  $\Delta T_{\text{min}}$

At a given SQP iteration, the  $\Delta T_{\text{min}}$  is fixed.

3) Obtain the grand composite curve from equation (4.5)

4) At a given SQP iteration, the temperatures of the utilities are fixed. Therefore, equations (4.6) and (4.7) can be used to fit the utilities in the grand composite curve and obtain their thermal duties.

5) Extend and arrange the pinch candidates in descending values of temperature. The new pinch candidates are the supply and target temperatures of the utilities.  $\Delta T_{\text{min}}$  must be added to the new pinch candidates corresponding with cold utilities.

6) Update the first and second terms in the heating deficit functions of all pinch candidates as described in sub-section (4.12)

7) Use equations (4.8) and (4.9) to obtain the balanced composite curves.

8) Target for the capital and operating costs of the chemical process from its current operating conditions and cost correlations.

9) Target for the capital cost of the heat exchanger network by applying Linnhoff and Ahmad's (1990) method to the balanced composite curves.

10) Target for the capital cost and operating costs of the utility system with the utilities thermal duties, the performance equations, and the cost correlations.

### Notations used in Chapter 5

<b>A</b>	target for minimum heat transfer area for the heat exchanger network
<b><math>A_{\min}</math></b>	target for minimum heat transfer area for the heat exchanger network
<b>BCC</b>	balanced composite curve
<b><math>c_a</math></b>	annualized cost of heat transfer area
<b><math>c_{cw}</math></b>	local market cost for purchasing cooling water
<b><math>c_f</math></b>	local market cost for purchasing fuel
<b><math>c_u</math></b>	annualized cost of heat exchangers
<b><math>c_w</math></b>	local market cost for purchasing work
<b><math>c_c^i</math></b>	unit thermal cost of cold utility i
<b><math>c_h^i</math></b>	unit thermal cost of hot utility i
<b>CCUS</b>	annualized capital cost of the utility system
<b>CU</b>	number of cooling utilities
<b>F</b>	annual fuel consumption
<b><math>F(\underline{x}, \underline{y})</math></b>	function to evaluate the chemical process' capital and operating costs
<b><math>g(\underline{x}, \underline{y})</math></b>	vector of inequality constrains
<b>GCC</b>	grand composite curve
<b><math>h(\underline{x}, \underline{y})</math></b>	vector of equality constrains
<b>HU</b>	number of hot utilities
<b>NU</b>	minimum number of units for maximum energy recovery
<b>PE</b>	performance equations
<b><math>U_{\min-MER}</math></b>	minimum number of heat exchangers for maximum energy recovery
<b>W</b>	annual work consumption
<b><math>\underline{x}</math></b>	vector of process parameters
<b><math>\underline{y}</math></b>	vector of flowrates and temperatures of process streams
<b><math>\underline{z}</math></b>	vector of utility system operating condition and parameters for process
<b><math>\Delta T_{\min}</math></b>	minimum approach temperature for process heat integration
<b><math>\Delta T_{\min}</math></b>	minimum approach temperature for refrigeration system integration
<b><math>\Delta T_{\min}</math></b>	minimum approach temperature for flue gas integration
<b><math>\phi</math></b>	objective function

## **CHAPTER 6 : THE ATMOSPHERIC PETROLEUM CRUDE TOWER OPTIMIZATION PROBLEM**

The sequential approach, Lang, Biegler and Grossmann's (1988) method, and the simultaneous method were implemented in a process simulator and used to solve the atmospheric petroleum crude tower optimization problem. This chapter compares and analyses their results.

The atmospheric petroleum crude tower optimization problem is based on a simulation given in the ASPEN PLUS User Guide (1988). Figure 6.1 illustrates the flowsheet for the atmospheric petroleum crude tower optimization problem. The crude tower has two pumparounds and three side-strippers. Crude oil is vaporized by a process heater and separated into four petroleum products and a residue (to be further processed in a downstream vacuum unit). Purity specifications for naphtha and gasoil are given. Steam is injected at the bottom of the tower and in each sidestripper to enhance separations. Crude oil is modeled as an assay composed of twenty-eight pseudocomponents and the physical properties are calculated by performing three-phase flash calculations using the Grayson-Streed corresponding states correlations. These correlations are applicable (in the operating temperature/pressure range of the atmospheric petroleum crude tower) to systems containing hydrocarbons and the gases typically present in hydrocarbon mixtures (ASPEN PLUS User Guide, 1988). As discussed in subsection 4.2.1 the utility system in this example consists of a process heater or furnace and a cooling tower.

This optimization problem was chosen because the decisions that lead to lower total cost solutions revolve around the optimization of the heat exchanger network. A total of nine hot streams (condenser, two pumparounds, and six outlet streams) can be used to recover heat by preheating the petroleum crude feed or raising feed steam. The lower total cost solution should balance heat recovery with capital cost in the preheat train. Since the throughput and the number of stages in the columns are fixed, the capital and operating costs of the chemical

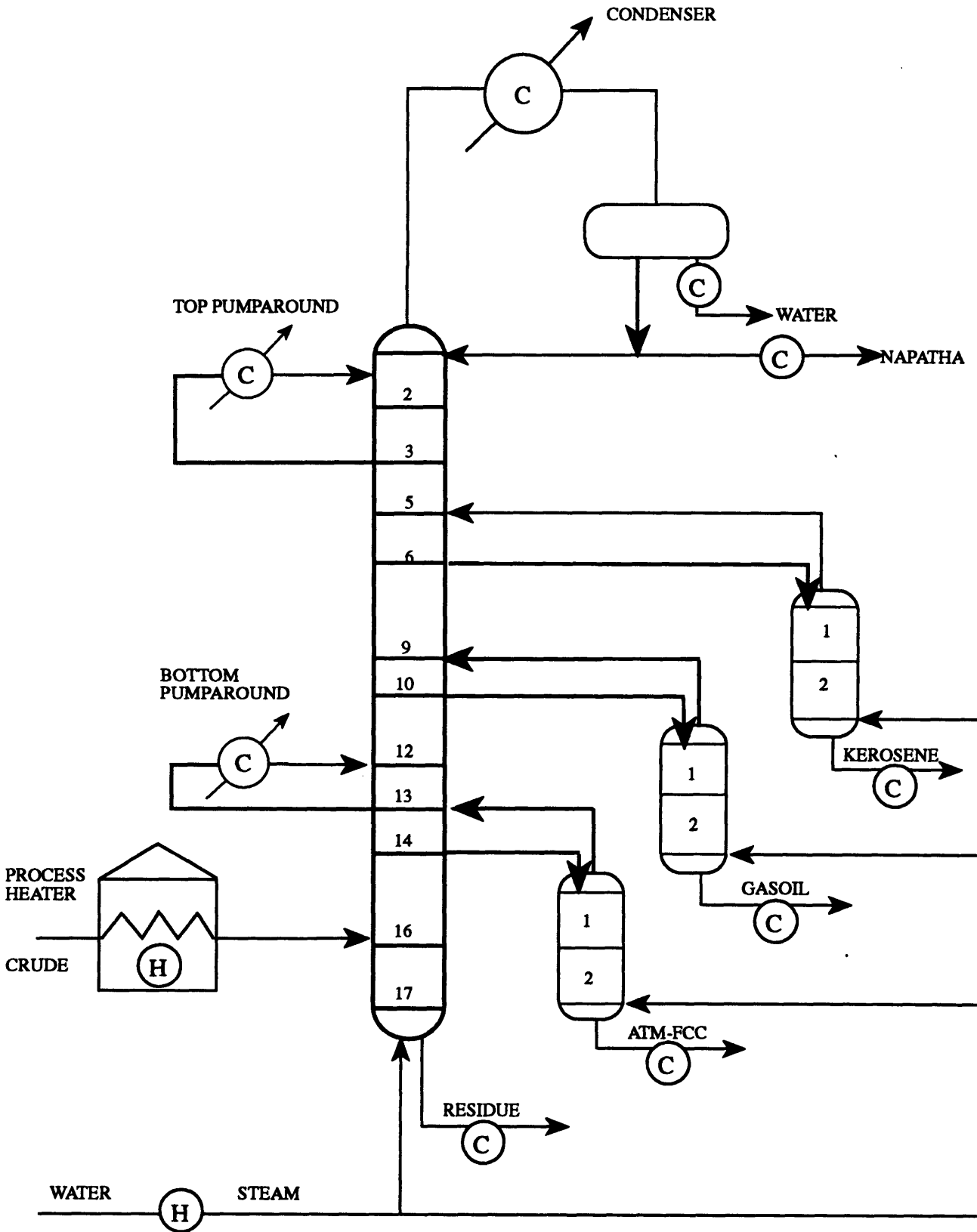


FIGURE 6.1 The flowsheet for the atmospheric petroleum crude tower optimization problem. (Aspen Plus User Guide, 1988)

process can be assumed fixed. Although utility costs are significant, their consumption depends on the amount of heat recovered in the crude preheat train. An optimization problem where heat recovery is important was desirable to explore the effects of adding the target for capital costs of the heat exchanger network to Lang, Biegler and Grossmann's (1988) method.

Table 6.1 contains a summary of the cost data for the atmospheric petroleum crude tower optimization problem. In the sequential approach and Lang, Biegler and Grossmann's method some of the heat and work interactions with the utility system are fixed by assuming the temperature levels of the utilities present and their unit costs for thermal energy. The cooling water supply and target temperatures are fixed and a per unit cost of cooling is given. The flue gas unit cost for thermal energy is obtained from the fuel cost and by an assumed efficiency for the process heater of 89% (same as choosing flue gas exit temperature of 280 °F).

Since the simultaneous method accounts for the heat and work interactions of all subsystems, the utility temperature levels can be optimization variables. Utilities unit costs for thermal energy are not necessary. Instead, the simultaneous method can target for the capital and operation cost of the utility system.

In this example, as discussed in subsection 4.2.1, the utility system has no work interactions (there is no work demand or production by the chemical process or the utility system). Therefore, the utility system's capital and operating costs can be predicted by accounting only for its heat interactions. Simply fit both utilities (furnace flue gas and cooling water) in the grand composite curve to obtain their duties. Fitting non-condensing utilities in the grand composite curve was discussed in subsection 4.1.2. The duty of a non-condensing utility is determined by their most restrictive distance to the grand composite curve once the shaded regions have been added. The utilities thermal duties and the cost correlations in Table 6.1 are enough to predict the capital and operating costs of the utility system.

**TABLE 6.1 Cost data for the atmospheric petroleum crude tower optimization problem.**

<b>A) Flue Gas</b>	
Theoretical Flame temperature	2200°F
Minimum Stack temperature	280°F
Ambient temperature	50°F
Fuel Cost	85 \$/kW yr (2.916 \$/MMBTU)
Cost	95.5 \$/kW yr (3.276 \$/MMBTU)*
<b>B) Cooling Water</b>	
Supply temperature	50°F
Target temperature	60°F
Cost	.343 \$/kW yr (3.85 \$/MMBTU)
<b>C) Installed Exchanger Capital Cost (\$)</b>	$20,000 + 500 A \text{ (m}^2\text{)}$
<b>D) Installed Furnace Capital Cost (\$)</b>	$0.682 (Q_H \text{ (BTU/hr)})^{0.8}$
<b>E) Capital Annualization Factor</b>	0.40
<b>F) Plant Operates</b>	8,540 hr/yr

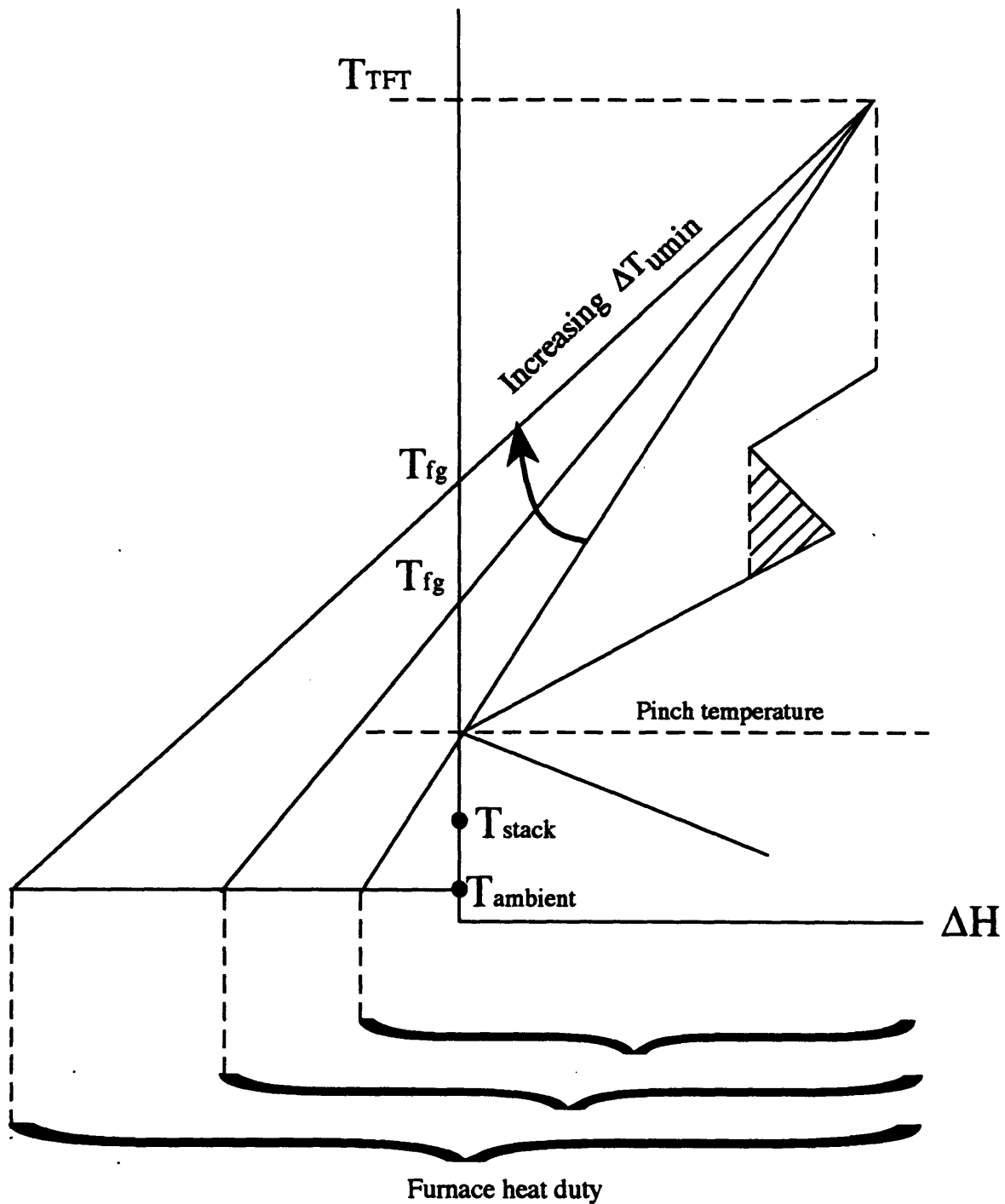
\*Not needed in the simultaneous method.

In Table 6.1 the cooling water supply and target temperatures are fixed and a per unit cost of cooling is given. This model for the cooling tower is used in all three methods. The simultaneous method could define a more detailed model where the degree of integration of the cold end of the utility system can change, but this is not necessary since the cooling costs are very low when compared to other costs.

In the simultaneous method, the degree of integration of the hot end of the utility system is not fixed. Therefore, a new optimization variable is defined, the minimum approach temperature for the integration of the hot end of the utility system ( $\Delta T_{\text{ummin}}$ ). A given  $\Delta T_{\text{ummin}}$  and the shape of the grand composite curve determines the heat duty and exit temperature of the furnace flue gas. Figure 6.2 illustrates the effects of  $\Delta T_{\text{ummin}}$  on the furnace heat duty and the flue gas exit temperature.  $\Delta T_{\text{ummin}}$  can be very different than the minimum approach temperature for process heat exchange ( $\Delta T_{\text{min}}$ ) defined earlier.

The decision variables in the atmospheric petroleum crude tower optimization problem are given in Table 6.2. The results and solution vectors obtained using the sequential approach, Lang Biegler and Grossmann's method, and the simultaneous method are given in Table 6.3. The sequential approach solution is obtained by first solving the nonintegrated flowsheet problem, NLP P0. The stream data of the solution to NLP P0 and Linnhoff and Ahmad's (1990) cost targeting method are used to optimize  $\Delta T_{\text{min}}$  and target for the capital costs of the heat exchanger network and the utilities thermal duties. Finally, the furnace heat duty and the cooling water duty are used to target for the capital and operating costs of the utility system. Lang Biegler and Grossmann's (1988) solution is obtained by solving NLP P1 at various  $\Delta T_{\text{min}}$ s followed by the addition of the capital and operating costs of the heat exchanger network and utility system. The simultaneous solution was obtained by solving NLP P3.

The sequential approach and Lang, Biegler and Grossmann's method optimized  $\Delta T_{\text{min}}$  in a one dimensional search. Since their heat interaction with the utility system are fixed, their  $\Delta T_{\text{ummin}}$  is fixed at 110 °F, which is a typical value used in practice. The simultaneous method



- $T_{TFT}$  = Theoretical flame temperature
- $T_{fg}$  = Flue gas exit temperature
- $T_{stack}$  = Minimum stack temperature
- $T_{ambient}$  = Ambient temperature

FIGURE 6.2 The effects of  $\Delta T_{min}$  on the furnace heat duty and the flue gas exit temperature. (Linnhoff-March, 1990)



**TABLE 6.2** The decision variables in the atmospheric petroleum crude tower optimization problem.

<b>Crude inlet temperature</b>	680-710°F
<b>Steam inlet temperature</b>	270-350°F
<b>Steam flowrate</b>	20,700-21,500 lbmol/hr
<b>Napatha outlet temperature</b>	100-70°F
<b>Water outlet temperature</b>	100-70°F
<b>Kerosene outlet temperature</b>	200-70°F
<b>Gasoil outlet temperature</b>	250-150°F
<b>ATM-FCC outlet temperature</b>	200-70°F
<b>Residue outlet temperature</b>	350-180°F
<b>Top pumparound outlet temperature</b>	300-130°F
<b>Top pumparound flowrate</b>	3,400-3,600 lbmol/hr
<b>Bottom pumparound outlet temperature</b>	550-350°F
<b>Bottom pumparound flowrate</b>	1,500-1,600 lbmol/hr
$\Delta T_{\min}$	5-80°F
$\Delta T_{\min}$	40-300°F

TABLE 6.3 The results and solution vectors to the atmospheric petroleum crude tower optimization problem obtained with the sequential approach, Lang, Biegler and Grossmann's (1988) method, and the simultaneous method.

<b>Decision Variables</b>	<b>Sequential Solution</b>	<b>LBG's Solution</b>	<b>Simultaneous Solution</b>
Crude inlet temperature	680	680	680*
Steam inlet temperature	270*	270*	327.5
Steam flowrate	20,700*	20,700*	20,700*
Napatha outlet temperature	100*	100*	100*
Water outlet temperature	100*	100*	100*
Kerosene outlet temperature	200*	166.3	200*
Gasoil outlet temperature	250*	161.7	217.3
ATM-FCC outlet temperature	200*	168.3	200*
Residue outlet temperature	350*	270	252.5
Top pumparound outlet temperature	200	160.6	162.6
Top pumparound flowrate	3,500	3,600*	3,600*
Bottom pumparound outlet temperature	425	350	350*
Bottom pumparound flowrate	1,525	1,600*	1,600*
$\Delta T_{\min}$	31**	45**	34.7
$\Delta T_{\min}$	110***	110***	222.2
<b>COSTS (million \$)</b>			
Energy cost	5.35	4.63	4.69
Heat exchanger network's capital cost	2.82	2.99	2.75
Utility system's capital cost	1.21	1.07	1.09
Total cost	9.38	8.69	8.53

\* Value at end of range

\*\* Optimized in one dimensional search

\*\*\* Not optimized

optimized  $\Delta T_{\min}$  and  $\Delta T_{\text{ummin}}$  with the rest of the optimization variables for the three subsystems.

The solution obtained with the sequential approach has an objective function value of 9.38 million \$/yr. It requires 181.3 MMBTU/hr of furnace duty, utilizes 12,146 m<sup>2</sup> of heat transfer area, has a process heater efficiency of 89%, and a  $\Delta T_{\min}=20$  °F. The composite curves and the grand composite curve corresponding to this solution are given in Figure 6.3. Further pinch analysis with the plus/minus rule could be applied to try an improve the solution. This will require many sequential iterations and its success depends on the designers experience. There is no guarantee the minimum total cost solution will be obtained.

The main reason the sequential approach obtained a suboptimal solution using is that it does not anticipate process heat integration. Therefore, all outlet hot process streams (petroleum crude tower products) are kept as hot as possible and not fully utilized to preheat petroleum crude feed or to raise steam. This occurs because the sequential approach assumes all cooling of hot process streams is done with cooling water and not by process heat integration. Therefore, cooling an outlet hot process stream beyond its upper temperature limit always increases the objective function value of NLP P0 by increasing the total cooling load.

Another problem with the sequential approach in this example is that of multiple solutions. The sum of the condenser and the two pumparounds cooling duties is nearly constant. Therefore, the same amount of cold utility is needed to cool these three hot streams irregardless of their cooling load distribution. This causes NLP P0 to have multiple solutions. Multiple solutions can cause a process optimizer to slow down or even fail. In this example, the cooling load distribution between the condenser and the two pumparounds was usually determined by the initial guess.

The solution obtained with Lang, Biegler and Grossmann's method has an objective function value of 8.69 million \$/yr. It requires 149.0 MMBTU/hr of furnace duty, utilizes 12,768 m<sup>2</sup>

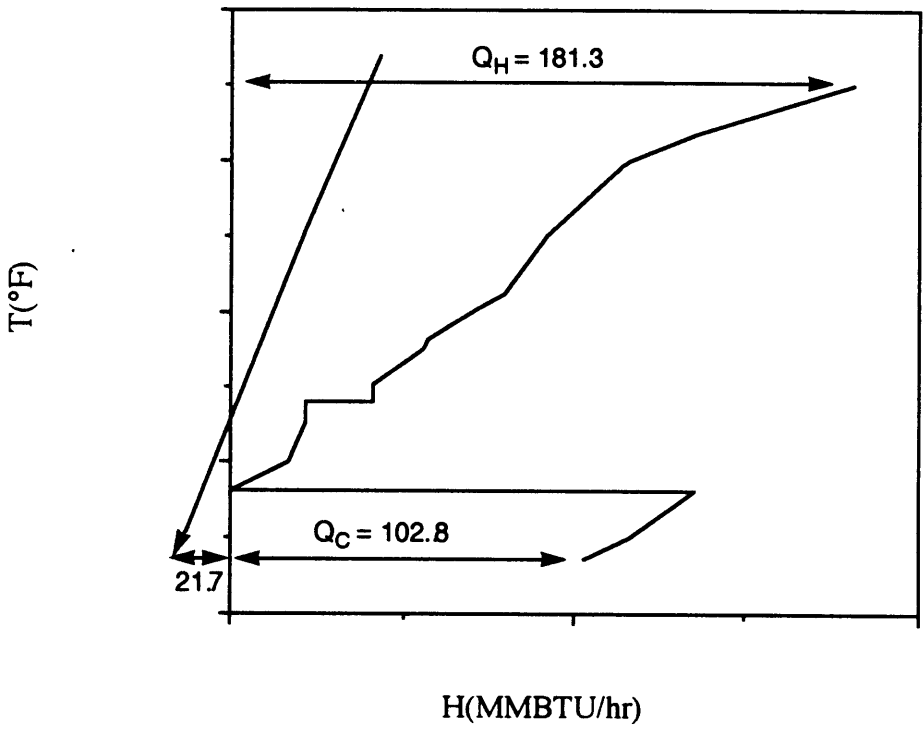
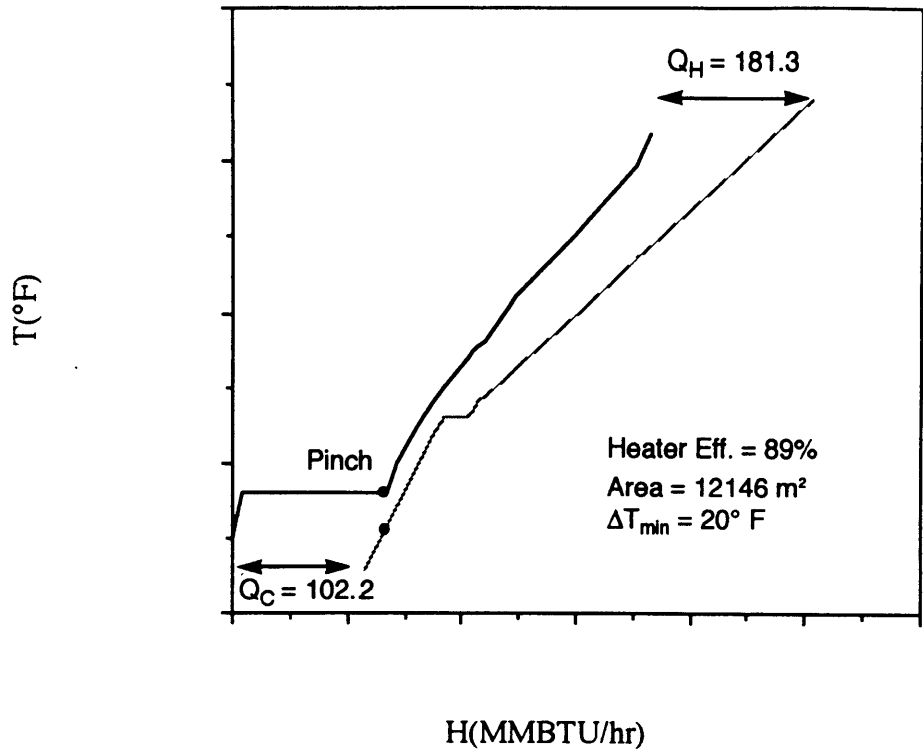


FIGURE 6.3 The composite and grand composite curves of the solution to the atmospheric petroleum crude tower optimization problem obtained with the sequential approach.

of heat transfer area, has a process heater efficiency of 85%, and a  $\Delta T_{\min}=45$  °F. The composite curves and grand composite curve corresponding to this solution are given in Figure 6.4.

The reason Lang, Biegler and Grossmann's method obtained a suboptimal solution is that NLP P1 does not consider the effects of process heat integration on the capital cost of the heat exchanger network and the performance of the utility system (furnace). Therefore, process heat integration of outlet hot process streams is performed as long as the  $\Delta T_{\min}$  is not violated (plus/minus rules are applied as much as possible). Here, Lang, Biegler and Grossmann's method performs too much process heat integration.

Other problems with Lang, Biegler and Grossmann's method in this example include double pinches and multiple solutions. The solution obtained with their method has two pinches and a highly constrained region in between (Figure 6.4). Double pinches can cause the pinch temperature to change from one iteration to another. Shifting pinch temperatures can cause convergence problem in optimizers (Lang, Biegler and Grossmann, 1988). The constrained region occurs because, in that region, many hot process stream are available to transfer heat but not all are allowed to do so because  $\Delta T_{\min}$  would be violated. NLP P1's objective function is indifferent as to which hot process streams transfer heat in that region. Therefore, NLP P1 has multiple solutions. Because of shifting pinch temperatures and multiple solutions in this example, the process optimizer was slow and had trouble converging.

The solution obtained with the simultaneous method has an objective function value of 8.53 million \$/yr. It requires 145.1 MMBTU/hr of furnace duty, utilizes 11,934 m<sup>2</sup> of heat transfer area, has a process heater efficiency of 81%, and a  $\Delta T_{\min}=34.7$  °F. The composite curves and grand composite curve corresponding to this solution are given in Figure 6.5. The optimized  $\Delta T_{\min}$  was found to be 222.2 °F.

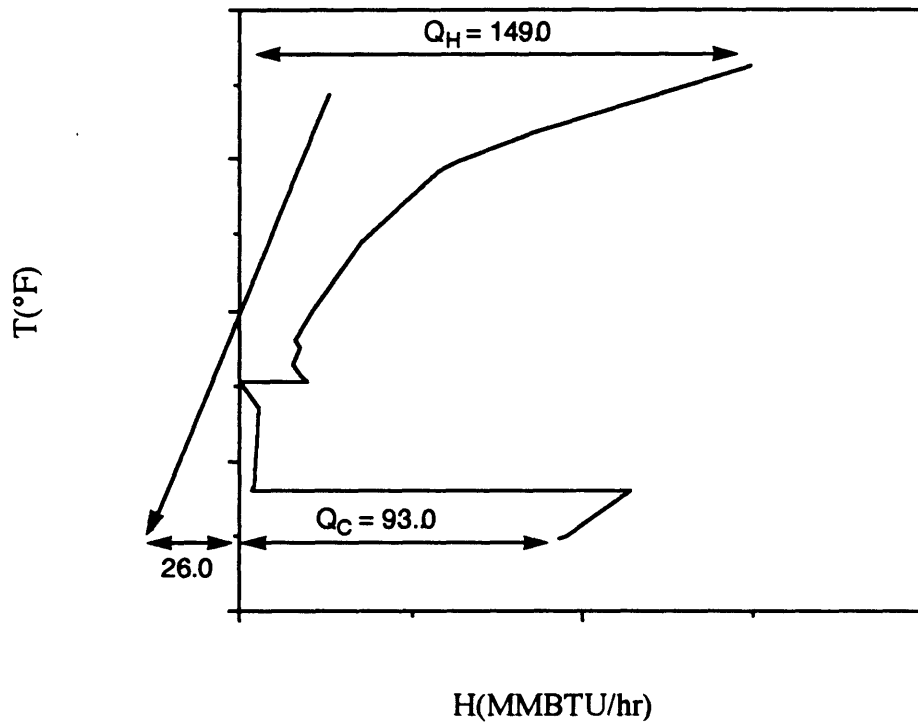
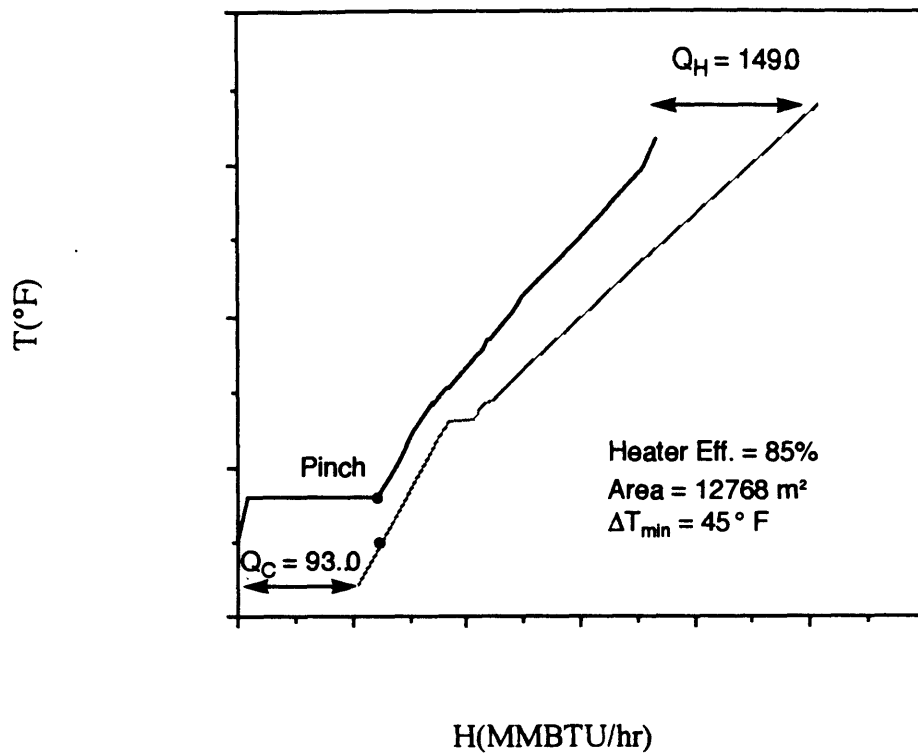


FIGURE 6.4 The composite and grand composite curves of the solution to the atmospheric petroleum crude tower optimization problem obtained with Lang, Biegler, and Grossmann's (1988) method.

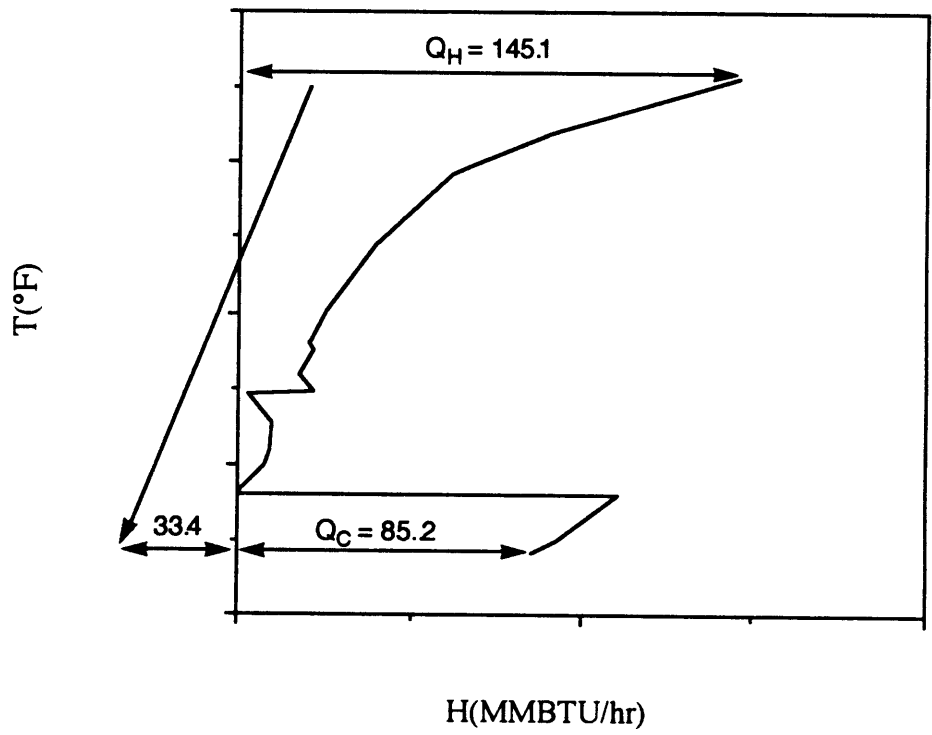
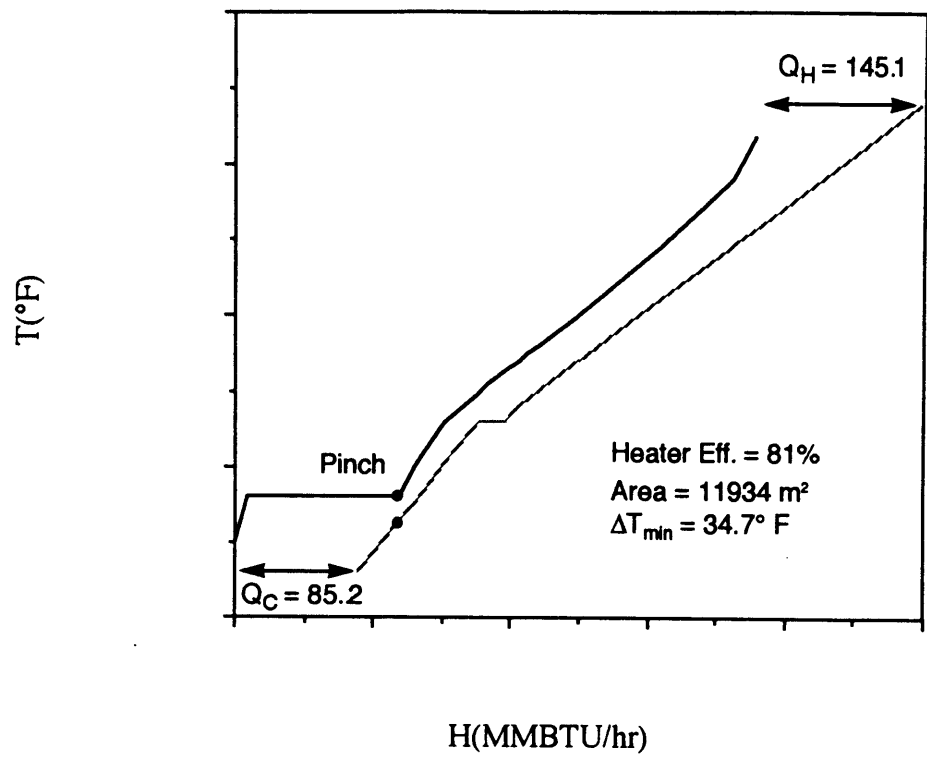


FIGURE 6.5 The composite and grand composite curves of the solution to the atmospheric petroleum crude tower optimization problem obtained with the simultaneous method.

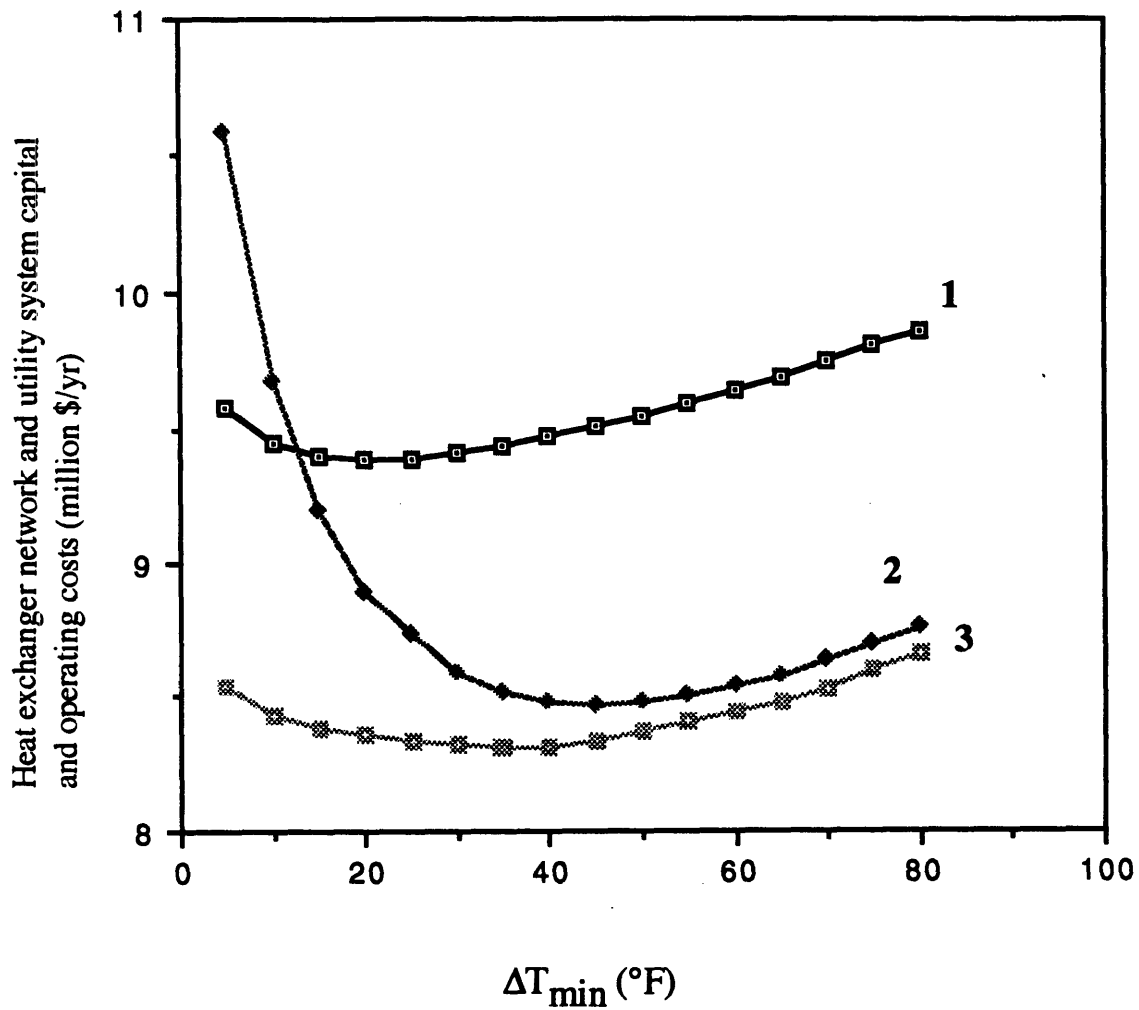
The reason the simultaneous method obtained lower total costs than the sequential approach and Lang, Biegler and Grossmann's method is that all major subsystem heat interaction were considered in the optimization step. The simultaneous method anticipates heat integration and its effects on the capital costs of the heat exchanger network and on the performance and costs of the utility system (furnace). Therefore, the plus/minus rules are followed only if there is a net decrease in total system cost through further process heat integration.

When solving the atmospheric petroleum crude tower optimization problem with the simultaneous method the optimizer had no trouble converging and finding the minimum cost solution. The same solution was obtained from various starting points. Multiple solutions were not encountered.

The sensitivity of the heat exchanger network and utility system capital and operating costs (chemical process costs are constant) of all three methods with  $\Delta T_{\min}$  is illustrated in Figure 6.6. At low values of  $\Delta T_{\min}$  the capital costs of the heat exchanger network dominate and, at high values of  $\Delta T_{\min}$  the utility system costs dominate. The sensitivity analysis on  $\Delta T_{\min}$  is very similar to the one dimensional optimization of  $\Delta T_{\min}$  in the sequential approach and is the same thing as the one dimensional optimization of  $\Delta T_{\min}$  in Lang, Biegler, and Grossmann's method.

The sequential approach does not anticipate process heat integration in its optimization step (solving NLP P0) and, as a result, outlet hot process streams are not fully utilized to provide heat. The cost targeting step of the sequential approach (one dimensional optimization of  $\Delta T_{\min}$ ) compensates for the lack of process heat integration by obtaining a low optimum value for  $\Delta T_{\min}$ . Nevertheless, the solutions with the sequential approach give the highest total costs except at very low values of  $\Delta T_{\min}$ . This is expected, since the sequential approach ignores process heat integration and, in this optimization problem, process heat integration is important.





- 1 Sequential Approach
- 2 Lang, Biegler and Grossmann's (1988) method
- 3 The Simultaneous Optimization Method

FIGURE 6.6 The sensitivity of the solutions to the atmospheric petroleum crude tower optimization problem with  $\Delta T_{\min}$ .

At low values of  $\Delta T_{\min}$  Lang, Biegler, and Grossmann's method gives the highest total costs and, at high values of  $\Delta T_{\min}$  it obtains relatively low total costs. This occurs because the capital cost of the heat exchanger network is not included in their optimization step (solving NLP P1). At low values of  $\Delta T_{\min}$  the capital cost of the heat exchanger network dominates while at high values it's not very important.

The simultaneous method obtains lower total costs at all values of  $\Delta T_{\min}$ . The solutions obtained using the simultaneous method have very shallow or flat optima. This can increase iterations in the optimizer since the error tolerance needs to be decreased but, shallow optima can increase design flexibility.

## 6.1 Summary

The sequential approach, Lang, Biegler and Grossmann's method, and the simultaneous method were implemented in a process simulator and used to solve the atmospheric petroleum crude tower optimization problem. The simultaneous method obtained lower total costs and required no iterations in the optimization of the subsystem's operating conditions and parameters for process heat or utility system integration ( $\Delta T_{\min}$ ,  $\Delta T_{\text{ummin}}$ ). In sequential approach and Lang, Biegler and Grossmann's method  $\Delta T_{\min}$  was optimized in a one dimensional search and  $\Delta T_{\text{ummin}}$  was fixed.

Since not all heat interactions between the subsystems are included in the sequential approach and in Lang, Biegler, and Grossmann's method, ambiguities occurred in their NLP's objective functions. These ambiguities caused both methods to have multiple solutions. Lang, Biegler and Grossmann's method also had two pinches which slowed down the optimizer and caused it trouble converging. Sensitivity analysis further illustrated the drawbacks of these methods. The sequential approach gives the highest total costs except at very low values of  $\Delta T_{\min}$ . This occurs because this method ignores process heat integration and, in this optimization problem, process heat integration is important. At low values of

$\Delta T_{\min}$  Lang, Biegler, and Grossmann's method gives the highest total costs. This occurs because this method ignores the capital costs of the heat exchanger network in the optimization step and, at low values of  $\Delta T_{\min}$ , the capital costs of the heat exchanger network are important.

The simultaneous method had no trouble converging and found the same optimal solution from various starting points. In this example, the simultaneous method did not encounter multiple solutions. Sensitivity analysis demonstrated that the simultaneous method always obtains the lowest total system cost and that its solutions have very shallow optima.

### **Notations used in Chapter 6**

$Q_c$	minimum cold utility demand
$Q_H$	minimum hot utility demand
$\Delta T_{\min}$	minimum approach temperature for process heat integration
$\Delta T_{\min}$	minimum approach temperature for flue gas integration

## **CHAPTER 7 : THE COLD END OF AN ETHYLENE PLANT OPTIMIZATION PROBLEM**

The sequential approach, Lang, Biegler and Grossmann's (1988) method, and the simultaneous method were implemented in a process simulator and used to solve the cold end of an ethylene plant optimization problem. This chapter compares and analyses their results.

The simulation of the cold end of the ethylene plant was based on information for similar plants (Zdonik, Green, and Hallee, 1970; EPRI 1989). Figure 7.1 illustrates the flowsheet for the cold end of the ethylene plant optimization problem. A hydrocarbon feedstock is compressed (to separation pressure) and separated into various products. Purity specifications for ethylene, propylene, and the four carbon products are given. The separation towers are modeled using Aspen Plus' rigorous separation model Radfrac, except for the C2 and C3 splitters. Since the C2 and C3 splitters required a large number of trays (125 and 225 respectively), the calculation time was reduced by using the Winn-Underwood-Gilliland short cut method. As expected, the short cut method obtained the same reboiler and condenser temperatures as the rigorous method, but their thermal duties varied slightly. A correction factor to match the condenser and reboiler duties of both columns to the rigorous model was used. The physical properties were calculated using the Redlich-Kwong-Soave equation of state for both liquid and vapor phases.

The selection of the utility system's structure for this example was discussed in subsection 4.2.2. The utility system contains a cascade refrigeration system with three levels of ethylene refrigeration in the low temperature cycle and four levels of propylene refrigeration in the high temperature cycle. It also provides low temperature steam from a steam turbine and cooling water from a cooling tower.

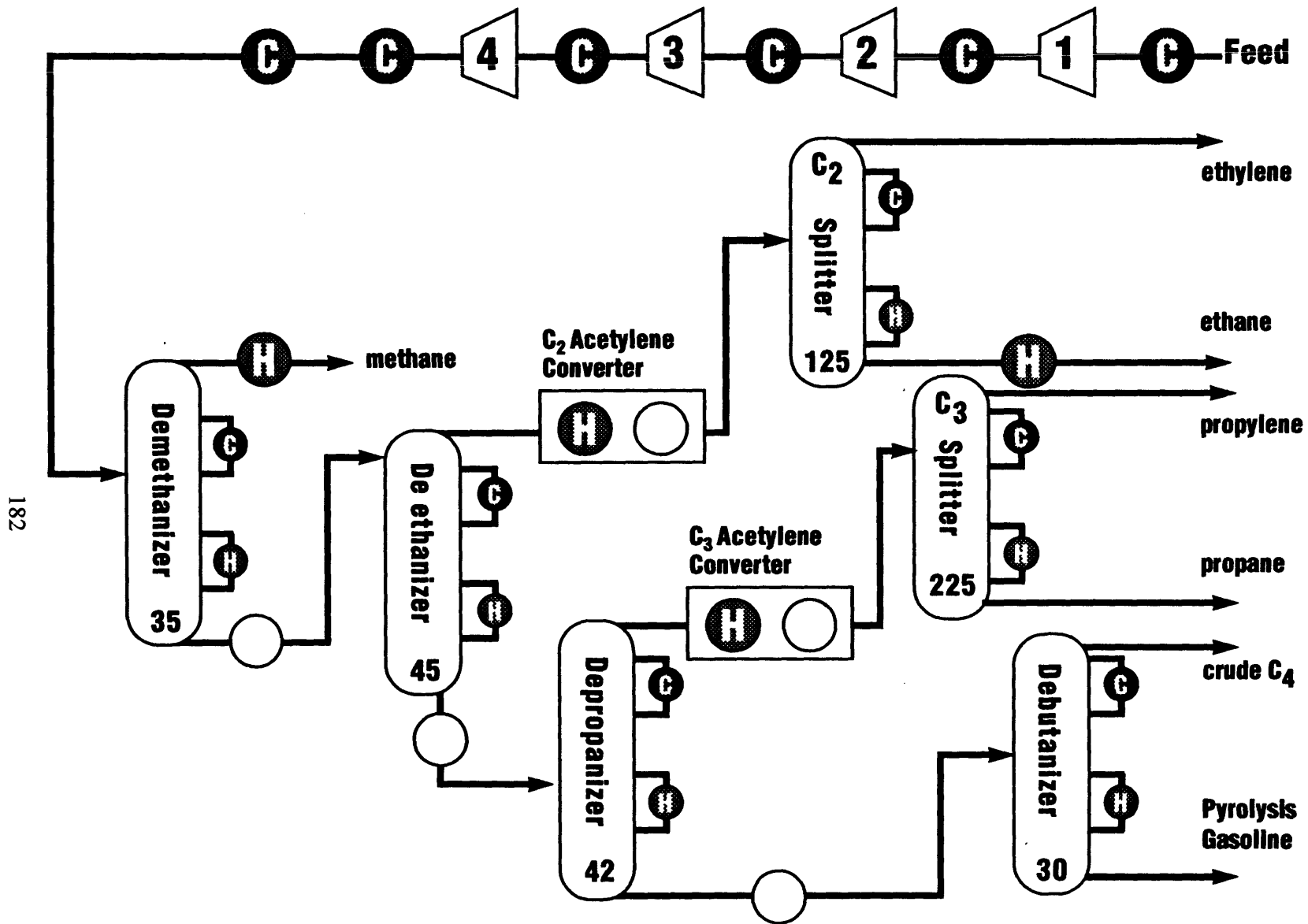


FIGURE 7.1 The flowsheet for the cold end of an ethylene plant optimization problem.

This optimization problem was chosen because the decisions that lead to lower total process costs revolve around the optimization of the utility system. Figure 7.2 illustrates composite curves and grand composite curve for the cold end of a typical ethylene plant. From the large amount (and wide temperature range) of subambient cooling duty required, it is clear that heat and work integration of the refrigeration system is very important to obtain the minimum total cost solution. An optimization problem where heat and work integration of utility systems is important was desirable to explore the simultaneous optimization method's ability to account for heat and work interactions of utility systems.

Table 7.1 contains a summary of the cost data for the cold end of an ethylene plant optimization problem. In the sequential approach and Lang, Biegler and Grossmann's method some of the heat and work interactions with the utility system are fixed by assuming the temperature levels of the utilities present and their unit costs for thermal energy. The temperatures and unit costs for thermal energy of cooling water, low temperature steam, and seven refrigeration utilities are given in Table 7.1. The unit costs for refrigeration were obtained by calculating the amount of work needed to provide a unit amount of refrigeration (MMBTU) at a given refrigeration utility temperature in the cascade refrigeration system. In order to maintain consistency with the simultaneous method, the refrigeration performance equations were used to calculate the unit costs of thermal energy for the refrigeration utilities.

Since the simultaneous method accounts for the heat and work interactions of all subsystems, the utility temperature levels can be optimization variables. Utilities unit costs for thermal energy are not necessary. Instead, the simultaneous method can target for the capital and operation cost of the utility system.

In this example, as discussed in subsection 4.2.2, the utility system has important heat and work interactions. Therefore, both heat and work interactions must be accounted for in order to predict utility system's capital and operating costs. The heat interactions are accounted for by

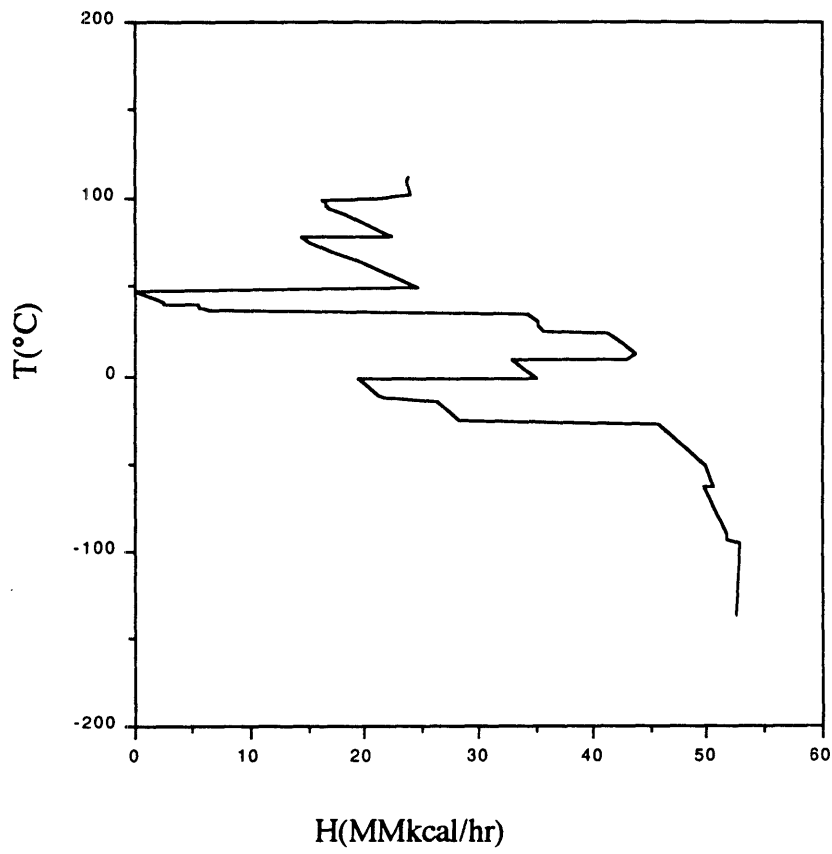
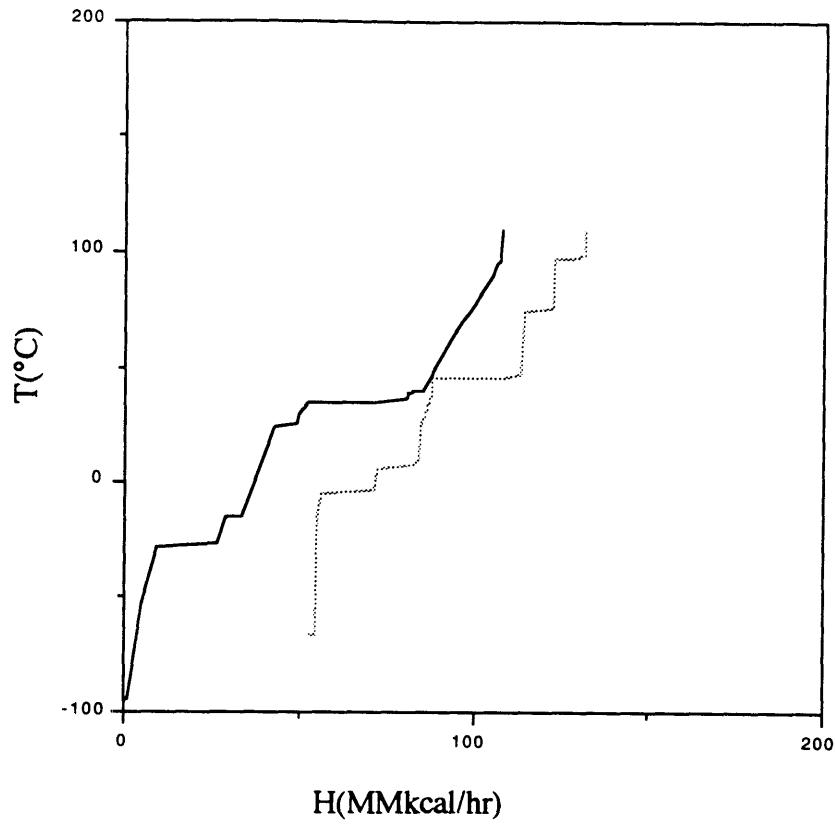


FIGURE 7.2 The composite and grand composite curves for the cold end of a typical ethylene plant.



**TABLE 7.1 Cost data for the cold end of a ethylene plant optimization problem.**

**A) Installed Columns**

$$3.5*(Cb*Fm+Nt*Cbt*Ftm*Ftt*Fnt+Cpl)$$

$$Cb = f(Ws,D,Lt,Tb,Tp)$$

$$Cbt = f(D)$$

$$Cpl = f(D,Lt)$$

**B) Installed Compressors (\$)**

$$8,215*(HP)^{7.3}$$

**C) Installed Exchanger Capital Cost (\$)**

$$25,000 + 600 A \text{ (m}^2\text{)}$$

**D) Utility Cost (\$)**

$$\text{Steam}_{130} = 1.50 / \text{MMBTU}$$

$$\text{CoolW}_{130} = 0.10 / \text{MMBTU}$$

$$\text{ElectricP} = 20.00 / \text{MMBTU}$$

$$\text{Prop-15} = 1.56 / \text{MMBTU}^*$$

$$\text{Prop-5} = 3.14 / \text{MMBTU}^*$$

$$\text{Prop-25} = 7.52 / \text{MMBTU}^*$$

$$\text{Prop-45} = 12.32 / \text{MMBTU}^*$$

$$\text{Eth-65} = 18.54 / \text{MMBTU}^*$$

$$\text{Eth-85} = 24.57 / \text{MMBTU}^*$$

$$\text{Eth-105} = 29.49 / \text{MMBTU}^*$$

**E) Capital Annualization Factor**

$$0.20$$

**F) Plant Operates**

$$8,300 \text{ hr /yr}$$

\*Not needed in the simultaneous method.

fitting the utilities in the grand composite curve to determine their thermal duties. The work interactions are accounted for with the refrigeration performance equations. The refrigeration performance equations allow the quick prediction of the work consumption by each individual compressor in the refrigeration system without a rigorous simulation of the cascade refrigeration system. From the utilities thermal duties, the work demand by each individual compressor in the cascade refrigeration system, and the cost correlations of Table 7.1, the capital and operating costs of the utility system can be predicted.

In Table 7.1 the cooling water and low temperature steam's supply and target temperatures are fixed and per unit costs of thermal energy are given. These models for the cooling tower and steam turbine are used in all three method. The simultaneous method could define more detailed models where the degree of integration of the above ambient temperature section of the utility system can change, but this is not necessary since the cooling water and steam costs are very low when compared with refrigeration costs.

In the simultaneous method, the degree of integration of the below ambient section of the utility system is not fixed. Therefore, a new optimization variable is defined, the minimum approach temperature for the integration of the refrigeration section of the utility system ( $\Delta T_{\min}$ ). A given  $\Delta T_{\min}$  and the shape of the grand composite curve determines the cooling duties of a given set of refrigeration utilities.  $\Delta T_{\min}$  can be very different than the minimum approach temperature for heat exchange ( $\Delta T_{\min}$ ) defined earlier.

The decision variables for the cold end of an ethylene plant optimization problem are given in Table 7.2. The results and solution vectors obtained using the sequential approach, Lang Biegler and Grossmann's method, and the simultaneous method are given in Table 7.3. The sequential approach solution is obtained by first solving the nonintegrated flowsheet problem, NLP P0. The stream data of the solution to NLP P0 and a variation of Linhoff and Ahmad's (1990) cost

**TABLE 7.2** The decision variables in the cold end of an ethlene plant optimization problem.

<b>Demethanizer Pressure</b>	30-35 atm
<b>Deethanizer Pressure</b>	23-30 atm
<b>C2 Splitter Pressure</b>	15-23 atm
<b>Depropanizer Pressure</b>	5-15 atm
<b>C3 Splitter Pressure</b>	8-20 atm
<b>Debutanizer Pressure</b>	3-7 atm
$\Delta T_{\min}$	.5-8°C
$\Delta T_{r\min}$	.5-8 °C
<b>4 levels of propylene refrigeration</b>	> -45°C
<b>3 levels of ethylene refrigeration</b>	> -105°C

TABLE 73 The results and solution vectors of the cold end of an ethylene plant optimization problem obtained with the sequential approach, Lang, Biegler and Grossmann's (1988) method and the simultaneous method.

<b>Decision Variables</b>	<b>Sequential Solution</b>	<b>LBG's Solution</b>	<b>Simultaneous Solution</b>
<b>Demethanizer Pressure</b>	31.33	30*	30.62
<b>Deethanizer Pressure</b>	23*	23.20	26.92
<b>C2 Splitter Pressure</b>	23*	20.82	22.09
<b>Depropanizer Pressure</b>	9.01	5.26	11.19
<b>C3 Splitter Pressure</b>	12.20	8*	15.50
<b>Debutanizer Pressure</b>	3.72	3.90	4.61
<b><math>\Delta T_{\min}</math> (°C)</b>	2.2***	1.5+	2.25
<b><math>\Delta T_{r\min}</math> (°C)</b>	1.0***	1.5+	1.53
<b>Propylene 1 Temperature</b>	15**	15**	13.74
<b>Propylene 2 Temperature</b>	-5**	-5**	0.01
<b>Propylene 3 Temperature</b>	-25**	-25**	-21.29
<b>Propylene 4 Temperature</b>	-45**	-45**	-39.34
<b>Ethylene 1 Temperature</b>	-65**	-65**	-53.42
<b>Ethylene 2 Temperature</b>	-85**	-85**	-79.48
<b>Ethylene 3 Temperature</b>	-105**	-105**	-97.03
<b>COSTS (x10E6)</b>			
<b>Columns</b>	4.91	4.56	5.44
<b>Feed Comp. (Capital)</b>	3.01	2.98	2.99
<b>Feed Comp. (Operating)</b>	10.00	9.87	9.93
<b>Ref. Comp. (Capital)</b>	5.07	5.15	4.41
<b>Ref. Comp. (Operating)</b>	17.26	17.39	11.69
<b>Heat Exchangers</b>	3.18	3.53	3.91
<b>Steam</b>	1.00	.49	1.17
<b>Cooling Water</b>	.25	.22	.23
<b>Total Cost</b>	44.68	44.19	39.77

\* Value at end of range

\*\* Not optimized

\*\*\* Optimized in two dimensional search

+ Optimized with successive one dimensional searches

targeting method are used to optimize  $\Delta T_{\min}$  and  $\Delta T_{\min}$  (in a two dimensional search) and target for the capital costs of the heat exchanger network and the utilities thermal duties. Finally, the utilities thermal duties and the performance equations are used to target for the capital and operating costs of the utility system. Lang Biegler and Grossmann's (1988) solution is obtained by solving NLP P1 at various  $\Delta T_{\min}$ s followed by the addition of the capital and operating costs of the heat exchanger network and utility system. To be consistent,  $\Delta T_{\min}$  was optimized in a one dimensional search when adding the capital and operating costs of the heat exchanger network and the utility system. The simultaneous solution was obtained by solving NLP P3.

The sequential approach optimized  $\Delta T_{\min}$  and  $\Delta T_{\min}$  with a two dimensional search. Lang, Biegler and Grossmann's method optimized  $\Delta T_{\min}$  and  $\Delta T_{\min}$  with successive one dimensional searches. The simultaneous method optimized  $\Delta T_{\min}$  and  $\Delta T_{\min}$  with the rest of the optimization variables for the three subsystems. In the sequential approach and Lang, Biegler and Grossmann's method, the optimization of  $\Delta T_{\min}$  and  $\Delta T_{\min}$  is time consuming. This extra effort was spent to minimize cost differences with the simultaneous method except those due to a better work integrated utility system.

The solution obtained with the sequential approach has an objective function value of 44.68 million \$/yr. It requires 49.35 MMKcal/hr of cooling duty, utilizes 24,428 m<sup>2</sup> of heat transfer area, has a  $\Delta T_{\min}=2.2$  °C, a  $\Delta T_{\min}=1.0$  °C, and the pinch is at 38.9 °C. The composite curves and grand composite curve corresponding to this solution are given in Figure 7.3.

The main reason the sequential approach obtained a suboptimal solution is that it does not take account for all the heat and work interactions with the utility system. This solution and its corresponding composite and grand composite curves are similar to the ones obtained using the simultaneous method. The main difference is that the pocket that occurs between 26 °C and -1 °C is smaller and cannot be used to fit economizers. Process modifications to fit economizers

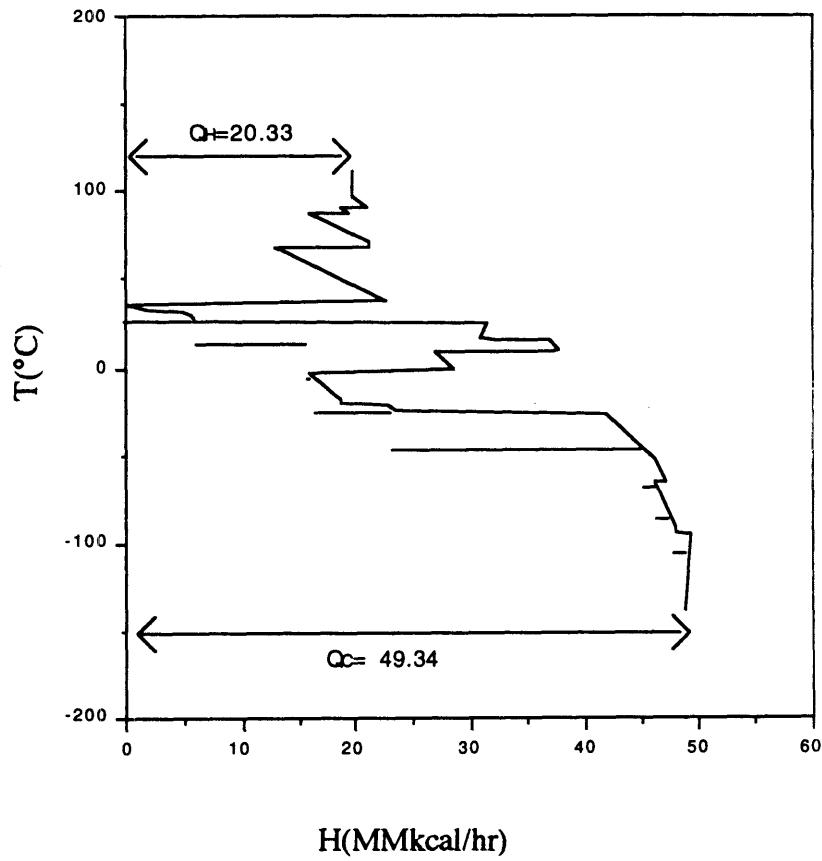
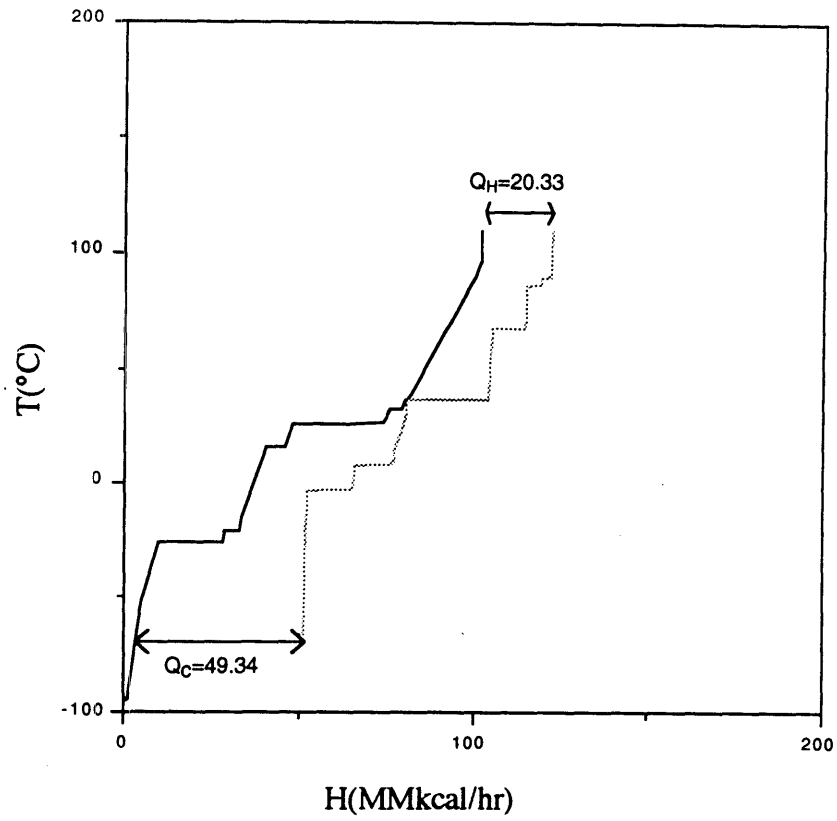


FIGURE 7.3 The composite and grand composite curve for the cold end of a typical ethylene plant.

using pinch or exergy analysis could be attempted to try and improve the solution. Again, this will require many sequential iterations and its success in finding the minimum cost solution cannot be guaranteed.

Another problem with the sequential approach in this example is that of multiple stationary points. Depending on the initial guesses, at least three different stationary points to NLP P0 were found. The solution presented here had the lowest objective function value and was obtained by using the simultaneous solution as the initial guess. If the initial guess is near Lang, Biegler, and Grossmann's solution, problem P0 finds a stationary point similar to the solution obtained using their method.

In this example, the decision variables that have significant effects on process heat integration were not optimized. Therefore, the sequential approach's inability to anticipate process heat integrations was not a major drawback. This was done to minimize cost differences in all three methods except those due to better work integration in the utility system.

For example, the methane and ethane products streams exit the demethanizer and the C2 splitter very cold. If heat integration is anticipated, they would be used to provide refrigeration to the rest of the chemical process and reduce the cooling load (and work demand) of the refrigeration system. If heat integration is not anticipated (sequential approach) then they would be kept as cold as possible and not fully utilized to reduce refrigeration demands. This would occur because the sequential approach assumes all heating of cold process streams would be done with steam. Therefore, heating an outlet cold process stream beyond its lower temperature limit will always increase the objective function value of NLP P0 by increasing the total steam demand.

The solution obtained with Lang, Biegler and Grossmann's method has an objective function value of 44.19 million \$/yr. It requires 39.25 MMKcal/hr of cooling duty, utilizes 29,508 m<sup>2</sup> of heat transfer area, has a  $\Delta T_{\min}=1.5$  °C, a  $\Delta T_{\min}=1.5$  °C, and the pinch is at 20.8 °C. The

composite curves and grand composite curve corresponding to this solution are given in Figure 7.4.

The reason Lang, Biegler and Grossmann's method obtained a suboptimal solution was that NLP P1 does not consider the effects of process conditions on the capital cost of the heat exchanger network and on the performance of the utility system (refrigeration system). Here, as in the atmospheric petroleum crude tower optimization problem, Lang, Biegler and Grossmann's method performs excessive process heat integration.

Their solution has a highly constrained region between 20.8 °C and -5.6 °C, and a near pinch at 9.9 °C (Figure 7.4). There is a small pocket between 9.9 °C and -6.2 °C, but it is too small and the region too constrained to fit economizers. Although this method has the lowest capital cost of the chemical process and the lowest total utility requirements, the constrained region causes high area requirements for the heat exchanger network and poor opportunity of integration with the utility system. The result is a higher total cost than the simultaneous method. The pinch and the near pinch also caused the optimizer to be slow and have trouble converging.

The solution obtained with the simultaneous method has an objective function value of 39.77 million \$/yr. It requires 52.13 MMKcal/hr of cooling duty, utilizes 30,494 m<sup>2</sup> of heat transfer area, has a  $\Delta T_{\min}=2.3$  °C, a  $\Delta T_{\min}=1.5$  °C, and the pinch is at 48.1 °C. The composite curves and grand composite curve corresponding to this solution are given in Figure 7.5.

The reason the simultaneous method obtained lower total costs than the sequential approach or Lang, Biegler and Grossmann's method is that all major heat and work interactions between the subsystems were considered in the optimization step. The simultaneous method anticipates heat integration and its costs as well as the effects of process conditions on the performance of the utility system.



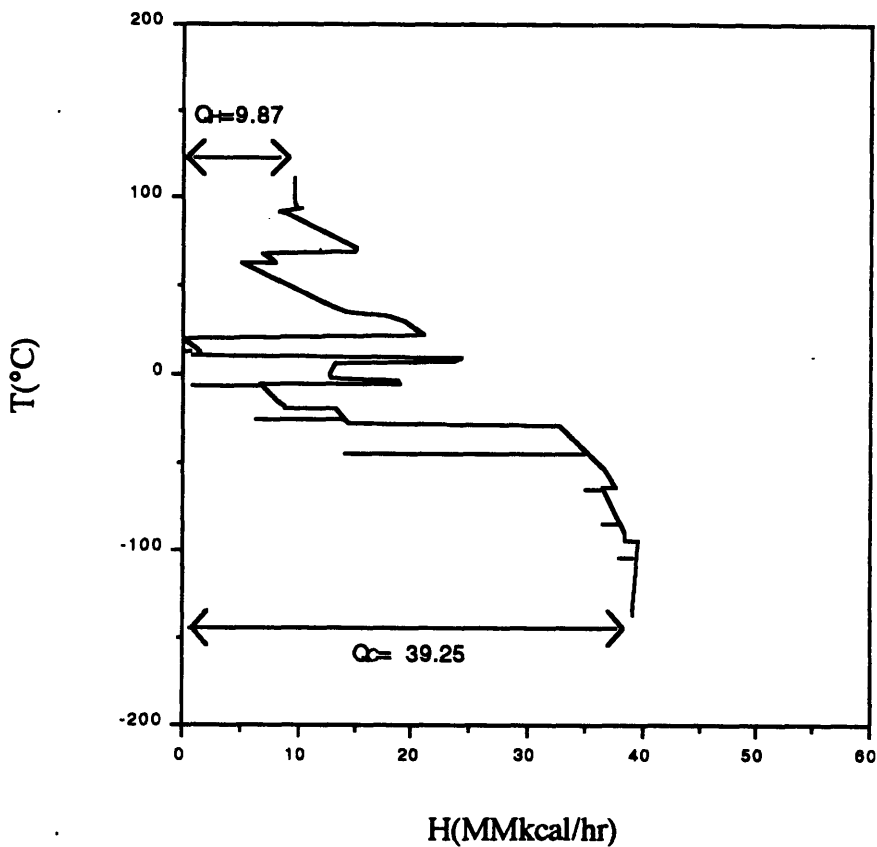
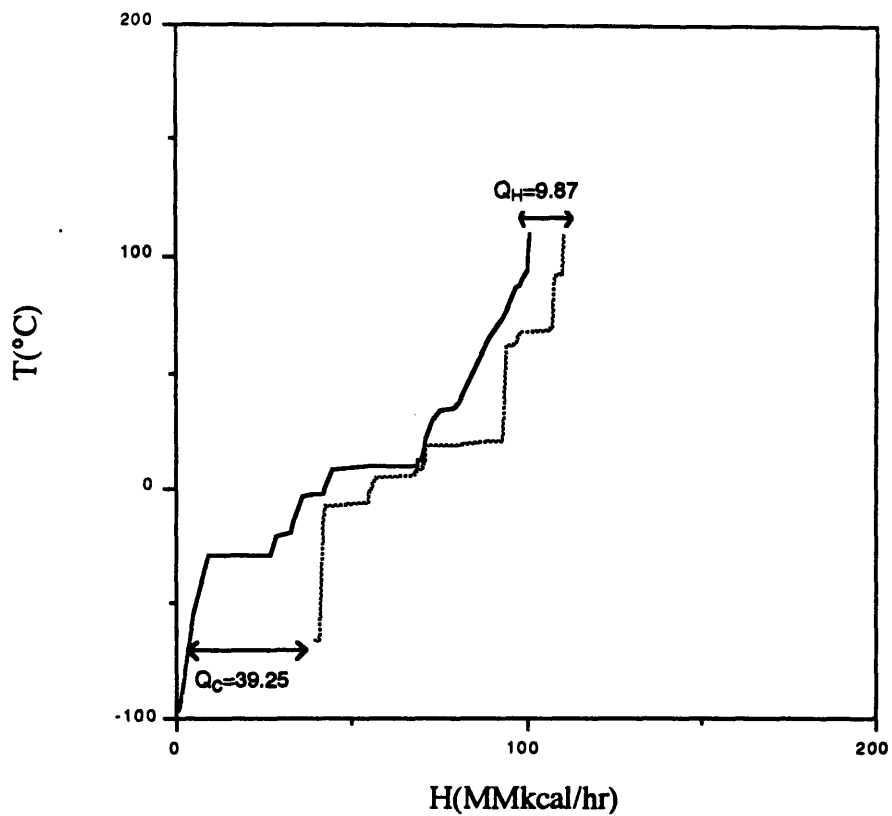


FIGURE 7.4 The composite and grand composite curves of the solution to the cold end of an ethylene plant optimization problem obtained with Lang, Biegler, and Grossmann's (1988) method.

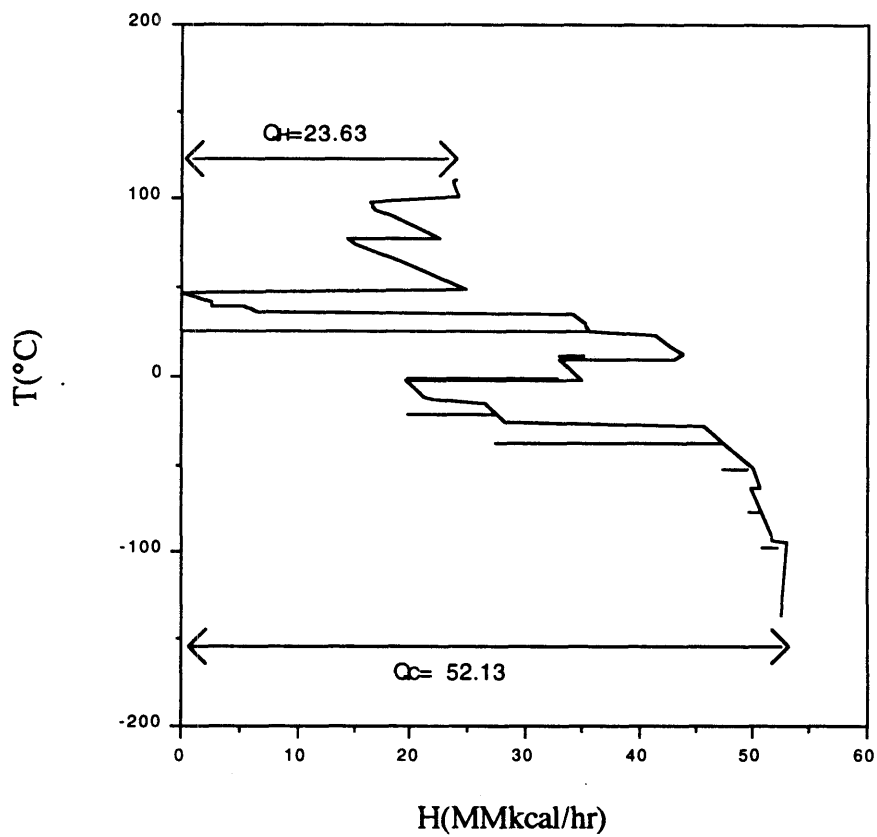
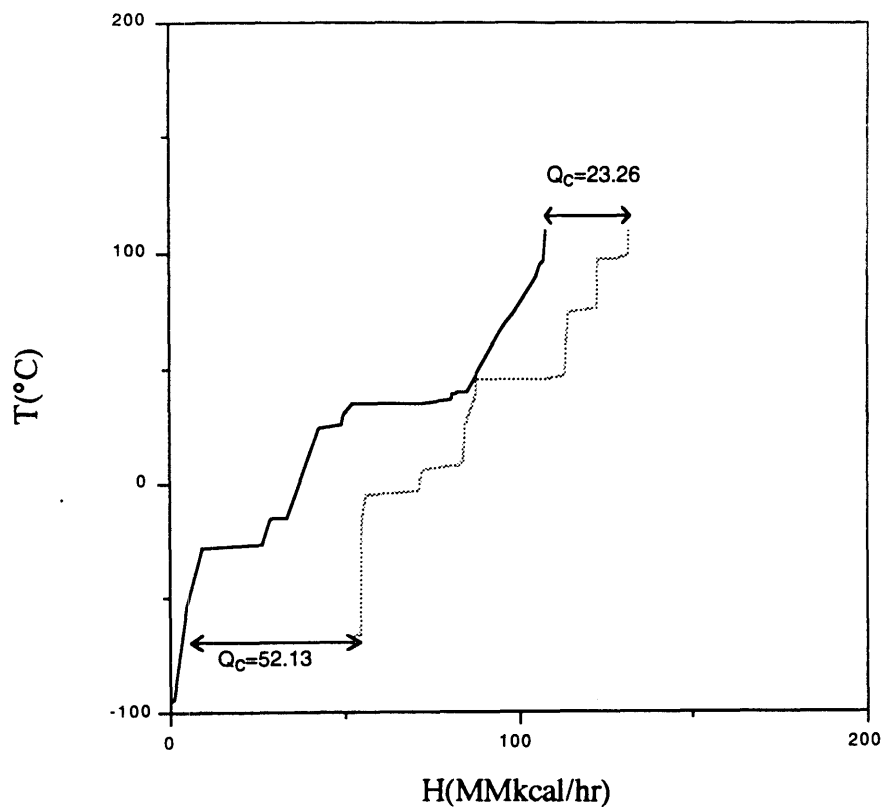


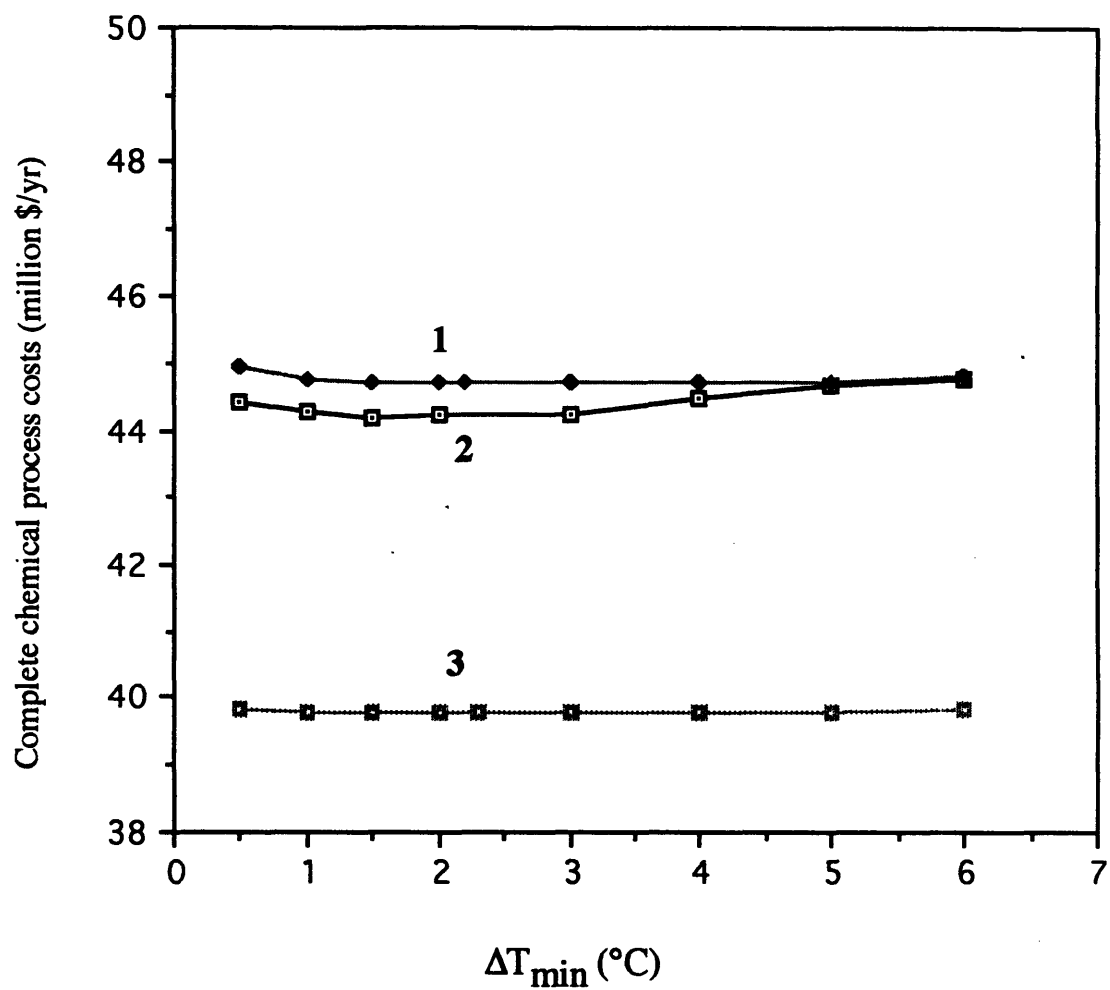
FIGURE 7.5 The composite and grand composite curves of the solution to the cold end of an ethylene plant optimization problem obtained with the simultaneous method.

The simultaneous solution has a large pocket between 35.9 °C and -2.5 °C. This pocket is used to fit economizers and reduce the work demanded by the refrigeration system. Creating and utilizing the large pocket causes the simultaneous method to have the highest capital cost for the chemical process and the heat exchanger network as well as the highest total utility requirements. Nevertheless, the use of the pocket (with economizers) leads to very good work integration with the refrigeration system. The savings in the capital and operating costs of the refrigeration system outweigh heavily the extra costs associated with creating and utilizing the pocket.

When solving the cold end of an ethylene plant optimization problem with the simultaneous method the optimizer had no trouble converging and finding the minimum cost solution. The same solution was obtained from various starting points. Multiple solutions were not encountered.

The sensitivity of the complete chemical process cost of all three methods with  $\Delta T_{\min}$  is illustrated in Figure 7.6. At low values of  $\Delta T_{\min}$  the capital costs of the heat exchanger network dominate and, at high values of  $\Delta T_{\min}$  the utility system costs dominate. When performing this sensitivity analysis for the sequential approach and Lang, Biegler, and Grossmann's method  $\Delta T_{\min}$  was kept at its optimal value.

The solutions obtained with the sequential approach had the highest total costs at all values of  $\Delta T_{\min}$ . This was due to the sequential approach's inability to anticipate process heat integration or account for the heat and work interactions of the utility system. Since the effects of not anticipating process heat integration were minimized in this example, the sequential approach solutions had similar total costs to the solutions obtained with Lang, Biegler and Grossmann's method.



- 1** Sequential Approach
- 2** Lang, Biegler and Grossmann's (1988) method
- 3** The Simultaneous Optimization Method

FIGURE 7.6 The sensitivity of the solutions to the cold end of an ethylene plant optimization problem with  $\Delta T_{\min}$ .

Lang, Biegler, and Grossmann's method suffered the same major drawback as the sequential approach. It ignored the important heat and work interactions with the refrigeration system that occur in this complete process. As a result, their method performed slightly better than the sequential approach but much worse than the simultaneous method.

The simultaneous method obtained much lower total costs at all values of  $\Delta T_{\min}$ . The simultaneous method was able to account for the important heat and work interactions with the refrigeration system. Sensitivity analysis demonstrated that, in this example, the other two methods can't compete with the simultaneous method. Again, the solutions obtained using the simultaneous method have very shallow or flat optima. This can increase iterations in the optimizer since the error tolerance needs to be decreased but, shallow optima can increase design flexibility.

## 7.1 Summary

The sequential approach, Lang, Biegler and Grossmann's method, and the simultaneous method were implemented in a process simulator and used to solve the cold end of an ethylene plant optimization problem. The simultaneous method obtained lower total costs and required no iterations in the optimization of the subsystem's operating conditions and parameters for process heat or utility system integration ( $\Delta T_{\min}$ ,  $\Delta T_{\min}$ ). In sequential approach the utility temperatures were fixed and  $\Delta T_{\min}$  and  $\Delta T_{\min}$  were optimized in a two dimensional search. In Lang, Biegler and Grossmann's method the utility temperatures were also fixed and  $\Delta T_{\min}$  and  $\Delta T_{\min}$  were optimized in successive one dimensional searches.

In this example, the sequential approach again had multiple solutions. The reason for the existence of multiple solutions is not clear; but it is probably due to ambiguities in NLP PO's

objective function. This ambiguities probably occur because not all heat and work interactions between the subsystems are included in the optimization step.

This time, multiple solutions were not found when using Lang, Biegler, and Grossmann's method. However, the solutions obtained with their method always had a pinch and a near pinch. This slowed the optimizer and caused convergence problems.

Sensitivity analysis further illustrated the drawbacks of these two methods. They both ignored the significant heat and work interactions with the refrigeration system that occurred in this process. As a result, both method always obtained solutions with much higher complete process costs than the simultaneous method.

The simultaneous method had no trouble converging and found the same optimal solution from various starting points. In this example, the simultaneous method did not encounter multiple solutions. Sensitivity analysis demonstrated that the simultaneous method always obtains much lower complete process costs and that its solutions have very shallow optima.

### Notations used in Chapter 7

$Q_c$	minimum cold utility demand
$Q_H$	minimum hot utility demand
$\Delta T_{\min}$	minimum approach temperature for process heat integration
$\Delta T_{\min}$	minimum approach temperature for flue gas integration

## CHAPTER 8 : CONCLUSIONS AND FUTURE WORK

### 8.1 Conclusions

A strategy for the simultaneous optimization of a chemical process, its heat exchanger network, and the utility system using was presented. The complete process optimization was accomplished by incorporating the heat and work interactions between the subsystems in the optimization. The simultaneous optimization method was developed by analyzing and providing new insights into the heat and work interactions between subsystems, proposing and developing mathematical models to account for these interactions, and implementing the mathematical models in a rigorous sequential process simulator.

The plus/minus rules (Linnhoff and Vredeveld, 1984) were used to understand some of the heat and work interactions between a chemical process and its heat exchanger network and the appropriate placement rules (Townsend and Linnhoff, 1983a,b) to understand some of the heat and work interactions between the heat exchanger network and the utility system. In Section 3.3 a new insight into the heat and work interactions between a chemical process and the utility system was introduced. This observation stated that the efficiency of the utility system is improved if the chemical process' operating conditions are changed to lower the pinch temperature. The problem with these observations was that they only improved the heat or work integration of the total system. It was recognized that changing process conditions to follow any of these principles could cause inefficient use of capital and raw materials and higher total system cost.

Mathematical methods that incorporate the subsystem's heat and work interactions were proposed and later developed. The expansion on Duran and Grossmann's [1986] pinch location method to not only account for heat integration but also to target for the capital cost of the heat exchanger network was identified as a method that incorporates heat and work interactions between a chemical process and its heat exchanger network. A superstructure



for the design and optimization of integrated utility systems that accounted for the heat and work interactions between heat exchanger networks and utility systems was also identified. Unfortunately, it required solving a very large and difficult MINLP. This superstructure was not solved in the thesis but, it was used as a guideline to develop a new method predict the capital and operating costs of utility systems without their rigorous design.

NLP P2 was presented as a mathematical model that accounted for the heat and work interactions between a chemical process and its heat exchanger network. This NLP was a simple expansion of Duran and Grossmann's (1986) pinch location method to target for the capital costs of the heat exchanger network. Later, NLP P3 was introduced as a strategy that also accounted for the heat and work interactions with the utility system. NLP P3 was obtained by incorporating the new method to target for the capital and operating costs of utility systems (by accounting for their heat and work interactions) in NLP P2. The simultaneous optimization method (the main objective of the thesis) was obtained by implementing NLP P3 in a rigorous sequential process simulator.

The simultaneous optimization method, the sequential approach, and Lang, Biegler, and Grossmann's (1988) method were used to solve two complete process optimization problems. The atmospheric petroleum crude tower optimization problem was chosen because the decisions that lead to lower total cost solutions revolve around the optimization of the heat exchanger network. An optimization problem where heat recovery is important was desirable to explore the effects of adding the target for capital costs of the heat exchanger network to Lang, Biegler and Grossmann's (1988) method. The cold end of an ethylene plant optimization problem was chosen because the decisions that lead to lower total cost solutions revolve around the optimization of the utility system. An optimization problem where heat and work integration of utility systems is important was desirable to explore the simultaneous optimization method's ability to account for the heat and work interactions of utility systems.

Since the sequential approach and Lang, Biegler and Grossmann's method fixed some of the heat and work interactions between subsystems, they could not simultaneously optimize the complete process' decision variables. Some decision variable were either fixed permanently (the supply and target temperatures of the utilities) while others required post-optimization (the parameters for process heat and utility system integration). On the other hand, the simultaneous method simultaneously optimized all three subsystem's operating conditions together with their parameters for process heat and utility system integration (because all subsystems' heat and work interactions are included in the optimization). This significantly reduces the total time required to optimize the complete system.

In the atmospheric petroleum crude tower optimization problem process heat integration is very important to obtain low total cost solutions. The sequential approach initially ignores process heat integration. Therefore, it is not surprising that it obtained the solution with the highest total system cost. Lang, Biegler, and Grossmann's method accounts for heat integration and it obtained a low total cost solution. In this example, both of these methods had multiple solutions. This was attributed to their inability to account for all the subsystems' heat and work interactions.

In the cold end of an ethylene plant optimization problem heat and work integration with the refrigeration system is crucial to obtain low total cost solutions. The sequential approach and Lang, Biegler, and Grossmann's method fix the heat and work interactions with the utility system. Their solutions have a much higher total system cost than the simultaneous method. As in the previous example, the sequential approach had multiple solutions. Again, this is probably due because many subsystems' heat and work interactions are ignored.

In both problems Lang, Biegler, and Grossmann's method had difficulty converging. This occurred because, as a result of ignoring the capital cost of the heat exchanger network in the optimization, their solutions have essentially two pinches. Two near pinches can cause the

pinch to change from one iteration to the next and create problems calculating derivatives for the optimization.

The simultaneous optimization method always obtained the lowest total system cost. It had a unique optimum and it required no iterations in the optimization of all the operating conditions. All these advantages are attributed to its ability to account for all the heat and work interactions between a chemical process, its heat exchanger network and the utility system.

## **8.2 Future Work**

The simultaneous optimization method was successfully applied to an atmospheric petroleum crude tower and the cold end of an ethylene plant. In the first problem the optimization of the heat exchanger network is important while in the second, the optimization of the utility system dominates. It would be interesting to solve an optimization problem where the optimization of the chemical processing steps determines the total system cost.

The refrigeration performance equations proved to be useful in optimizing refrigeration systems. They allowed the targeting of the refrigeration system's capital and operating cost without a rigorous design of the entire system. This saved valuable computer time. Developing performance equations for the above ambient temperature section of the utility system could be very useful. Perhaps, since the very simple performance equations would replace the material and energy balances, the superstructure for the design and optimization of integrated utility systems given in Chapter 3 could be solved. Solving this superstructure can be useful for many practical problems.

With a few alterations, the superstructure could be used to design and optimize utility systems for 'Total Sites'. 'Total Sites' are several chemical process linked and serviced by a central utility system (Dhole and Linnhoff, 1992). The components in the superstructure

would remain the same, but there are several process heat sinks and process heat sources to integrate with the utility system.

Finally, the superstructure has potential applications in retrofit. A very interesting case is to retrofit an existing utility system during the addition of a new plant to a 'Total Site'. If the chemical plants are not allowed to be reoptimized, the utility system superstructure for the 'Total Site' could solve this problem by allowing the pieces of equipment that already exist in the utility system to exist at no cost. Lower cost solutions could be obtained if the chemical plants are allowed to be reoptimized. This will require solving the superstructure together with all the models for the chemical plants.

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