

# Heat and Power Integration of Chemical Processes

An efficient nonlinear programming strategy is presented for integration of heat engines and heat pumps with chemical processes. The strategy utilizes the temperature interval method and shows how to use negative heat deficits to obtain lower cost designs. Two important situations are presented in which the resulting designs are less costly when the heat engines and heat pumps are integrated with temperature intervals having negative heat deficits.

**T. R. Colmenares, W. D. Seider**

Department of Chemical Engineering  
University of Pennsylvania  
Philadelphia, PA 19104

## Introduction

The rapid escalation of oil costs in the mid-1970's led process engineers to develop new strategies for retrofitting chemical plants and designing new processes. Much emphasis was placed on heat integration, with the primary target of reducing the cost of utilities for heating and cooling. Linnhoff and Flower (1978) popularized the temperature interval method; Umeda et al. (1978), Linnhoff and Turner (1981), and Linnhoff and Hindmarsh (1983) introduced the pinch concept; and Papoulias and Grossmann (1983b) formalized a mixed-integer linear program to configure a network of the fewest heat exchangers having minimum utilities.

More recently, methods for the synthesis of utility systems have been presented. Papoulias and Grossmann (1983a) set up a superstructure of a utilities system including steam turbines and a gas turbine. They introduced a mixed-integer linear program to select, from among predesignated pressure levels, an optimal configuration for specified steam and power demands. When coupled with their mixed-integer linear programs for the heat exchanger network and the remainder of the process, this achieved a high degree of heat and power integration (Papoulias and Grossmann, 1983c). Petroulas and Reklaitis (1984) introduced a superstructure including steam turbines, a gas turbine, steam requirements for process heat exchange, and raw steam for process needs (such as steam stripping). They utilized a linear programming strategy coupled with dynamic programming to locate an optimal configuration for specified steam and power demands.

Meanwhile, Townsend and Linnhoff (1983a) introduced qualitative guidelines for positioning heat engines and heat pumps to improve the efficiency of processes having minimum utilities for heating and cooling. Their guidelines, or rules, are based upon thermodynamic principles and upon their observa-

tions that it is inefficient (utilities are increased or work is converted to heat) to operate heat engines across the pinch temperature and heat pumps entirely above or below the pinch temperature. To minimize the utilities for heating and cooling, the power cycles are permitted to transmit heat to the temperature intervals above the pinch temperature and extract heat from the temperature intervals below the pinch temperature. However, in a complementary article (Townsend and Linnhoff, 1983b), when considering "reentrant process source/sink profiles," the efficient exchange of exhaust heat from a heat engine with a temperature interval below the pinch temperature, contrary to their initial guidelines, is shown. Another counterexample, a process with which it is more efficient to integrate a heat pump entirely below the pinch temperature, is presented by Linnhoff et al. (1982). In the present paper, two additional processing situations, believed to be of greater practical significance, are demonstrated for which the initial Townsend and Linnhoff (1983a) guidelines lead to less efficient designs.

Furthermore, while these guidelines for positioning heat engines and heat pumps are well illustrated graphically using temperature-enthalpy diagrams, they do not address the optimization problem given fixed power demands. In this paper, a nonlinear programming (NLP) strategy is introduced to identify the optimal selection of working fluids and the best temperature intervals for the integration of heat engines and heat pumps with the process. The strategy is presented in two stages, first, when the initial Townsend and Linnhoff (1983a) rules apply, and second, extended when these rules lead to suboptimal designs. Two examples are provided to demonstrate the utility of the algorithms. Due to space limitations, the methodology and examples for integration with cascades of heat pumps in low-temperature refrigeration processes could not be included. These are presented in another paper (Colmenares and Seider, 1986). Their extension to combined cycles of heat engines is underway.

## Model for Heat and Power Integration

Chemical processes convert raw materials into valuable products. To accomplish this, energy in different forms is supplied and removed from the process. Often the heat recovery network and the utility system are designed and analyzed as separate subsystems, with close ties to the remainder of the chemical process (another subsystem—the so-called chemical plant), as illustrated in Figure 1. The chemical plant is a collection of reactors, separators, compressors, etc., which exhibit demands to be satisfied by the heat recovery network and the utility system. Also, the heat recovery network provides both energy resources for and demands to the utility system.

The NLP model presented herein was designed to achieve a high degree of integration between the three subsystems, to be compact for efficient optimization with widely used algorithms, and to reduce the search space by appropriate placement of the heat engines and heat pumps relative to the pinch temperature  $T_p$ . Given the demands of the chemical plant for heating, cooling, and power, a selection is made from among the available utilities (e.g., steam, fuel, electricity, water, air) and power cycles to minimize some combination of energy and capital costs. The model can be extended with little effort to design the utility system while integrating the power cycles; that is, to adjust the pressure levels of the steam headers to achieve a more optimal design for the entire chemical process. However, due to space limitations, this aspect is not illustrated in this paper.

To formulate the model, the flow rate, enthalpy, and supply and target temperatures of each process stream must be given. Also, the power and raw steam demands are specified. Addi-

tional data are the temperature levels and costs of the available utilities and the correlations of capital costs for equipment in the heat engines and heat pumps.

The solution is carried out in a three-step procedure:

1.  $T_p$  is determined (Umeda et al. 1978; Linnhoff and Turner, 1981; Papoulias and Grossmann, 1983b)
2. The NLP model is set up to minimize an objective function
3. A feasible configuration of the heat exchanger network, coupled with the heat engines and heat pumps, is identified. This can be accomplished using the pinch design method of Linnhoff and Hindmarsh (1983) and the mixed-integer linear programming (MILP) formulation of Papoulias and Grossmann (1983b).

When implementing the rules of Townsend and Linnhoff (1983a), the model for the integration of heat engines is shown schematically in Figure 2, and that for heat pumps in Figure 3. Following the temperature interval (TI) method of Linnhoff and Flower (1978), the cascade on the left represents the exchange of energy between the hot and cold streams in each temperature interval. To assign the temperature intervals, the supply and target temperatures of the hot streams and hot utilities are decreased by the minimum approach temperature  $\Delta T_{min}$ , and, together with the supply and target temperatures of the process cold streams and cold utilities, are listed in descending order. The heat flux from external hot sources in an interval  $n$  above the pinch temperature  $T_p$  is

$$D_n^H + R_n - R_{n-1} \quad n = 1, \dots, p \quad (1)$$

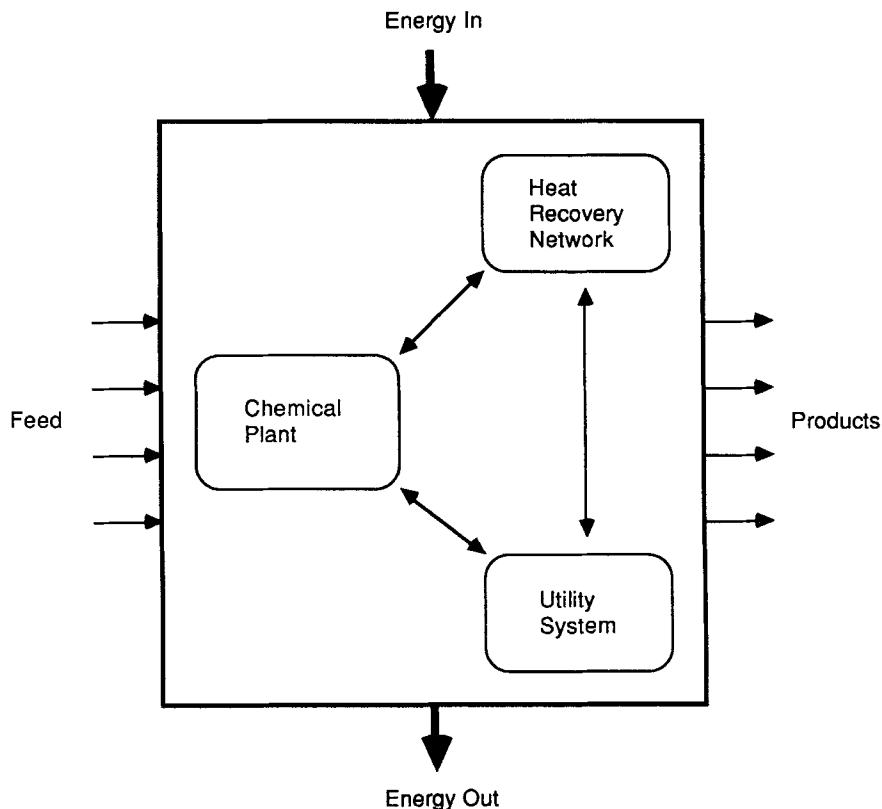


Figure 1. Three subsystems of a chemical process.

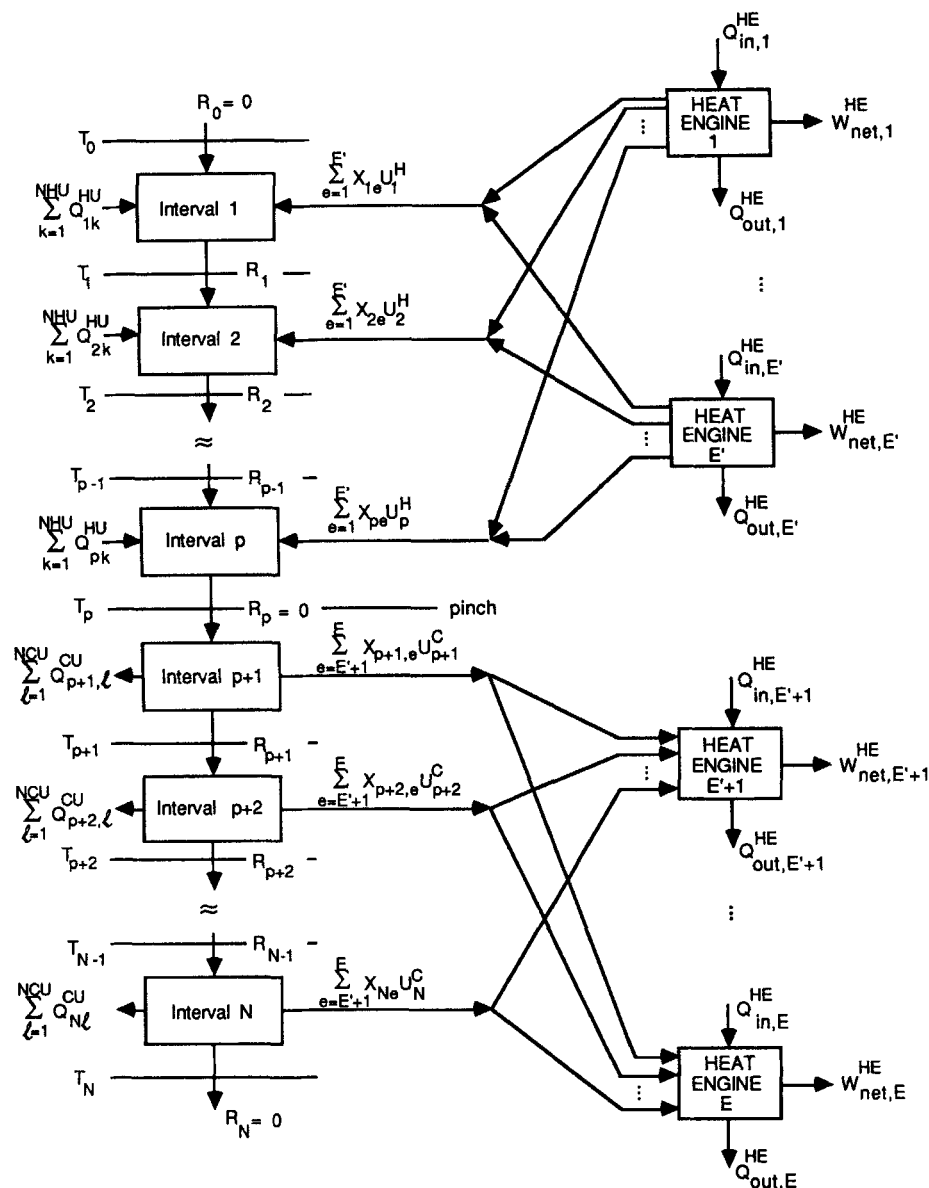


Figure 2. Heat integration diagram for heat engines following rules of Townsend and Linnhoff (1983a).

where  $D_n^H$  is the "hot deficit" in interval  $n$ ,

$$D_n^H = \sum_{j=1}^{NC} Q_{nj}^C - \sum_{i=1}^{NH} Q_{ni}^H \quad n = 1, \dots, p \quad (2)$$

$R_n$  is the residual heat transferred from interval  $n$  to interval  $n + 1$  ( $R_p = 0$  at  $T_p$ );  $Q_{nj}^C$  is the heat load of cold stream  $j$  in interval  $n$ ;  $Q_{ni}^H$  is the heat load of hot stream  $i$  in interval  $n$ ;  $NC$  is the number of cold streams; and  $NH$  is the number of hot streams. Similarly, the heat released to the external cold sinks (below  $T_p$ ) is

$$D_n^C + R_{n-1} - R_n \quad n = p + 1, \dots, N \quad (3)$$

where  $D_n^C$  is the "cold deficit" in interval  $n$ ,

$$D_n^C = \sum_{i=1}^{NH} Q_{ni}^H - \sum_{j=1}^{NC} Q_{nj}^C \quad n = p + 1, \dots, N \quad (4)$$

and  $N$  is the number of intervals.

### Lumping temperature intervals

The number of intervals obtained with the TI method can be very large, which directly affects the size of the model and the efficiency of obtaining a solution. When implementing the rules of Townsend and Linnhoff (1983a), the integration of heat engines and heat pumps is permitted only in those intervals in which the hot deficit (above  $T_p$ ) or the cold deficit (below  $T_p$ ) is positive. Townsend and Linnhoff (1983b) and Linnhoff et al. (1982) have identified two situations where integration with intervals having negative deficits is desirable. In this paper, two additional situations are introduced. However, the placement

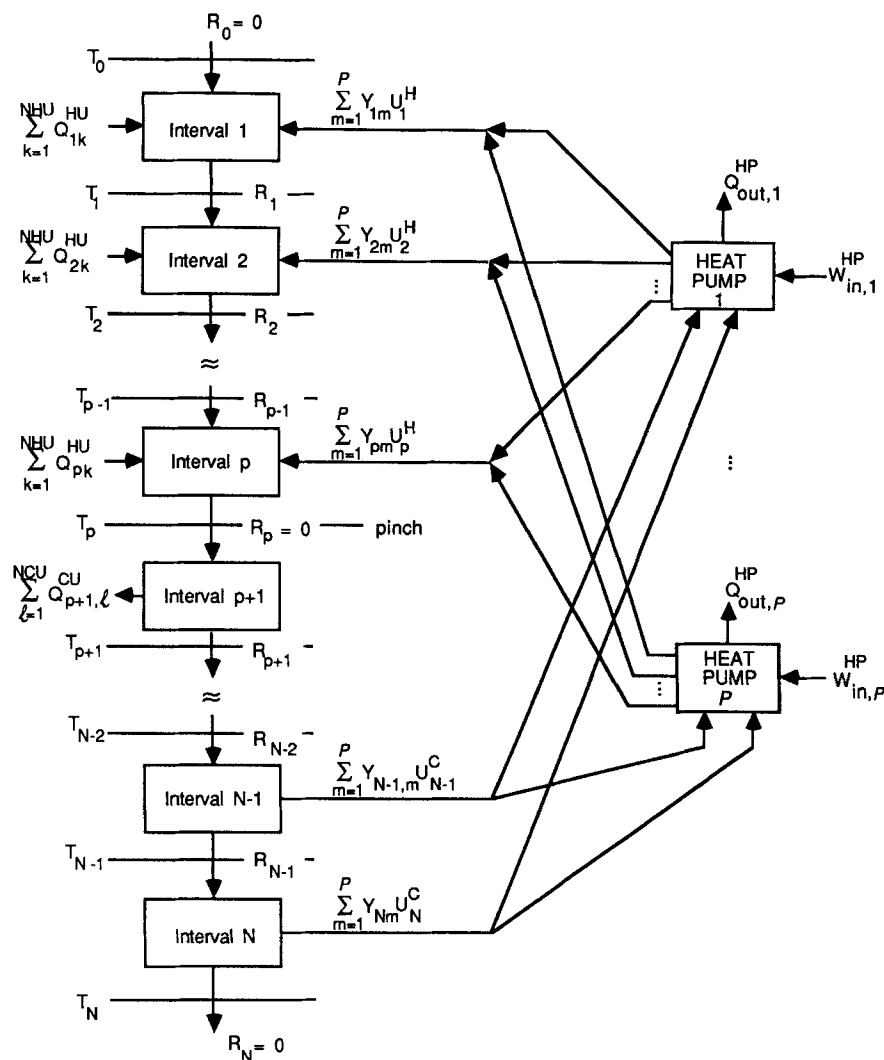


Figure 3. Heat integration diagram for heat pumps following rules of Townsend and Linnhoff (1983a).

rules of Townsend and Linnhoff (1983a) often apply and, when applicable, the fraction of the intervals having positive deficits (available for integration) is usually small.

For these situations, a lumping procedure is introduced, as follows. Above  $T_p$ , intervals with negative hot deficits provide residual heat to satisfy the positive deficits of intervals located below in the cascade. Similarly, below  $T_p$  intervals with negative cold deficits remove heat from intervals higher in the cascade. Therefore, when negative deficits occur in interval  $i$  above  $T_p$ , these are added to the highest temperature interval  $n$  with a positive deficit, where  $n > i$ , and below  $T_p$ , to the lowest temperature interval  $n$  with a positive deficit, where  $n < i$ . The resulting lumped partition includes only intervals for heat and power integration based on the process requirements and defines the bounds on the operating temperatures for the heat engines and heat pumps when integration is attempted. This lumping significantly reduces the model size and usually does not eliminate important alternatives for integration.

### Integration of heat engines

With this lumping, the heat engines must reject energy to the process above  $T_p$  and remove energy from the process below  $T_p$ .

While this strategy minimizes the utilities for heating and cooling the process streams, it does not permit the efficient utilization of high-temperature process heat to drive the heat engines, as suggested by Townsend and Linnhoff (1983b), who introduce steam below the pinch temperature to generate work. Later in this section it will be shown that a high-cost hot utility, such as fuel (for the heat engine), can be replaced by a low-cost hot utility, such as steam (for the process), through the use of high-temperature process heat to drive the heat engine. First, a model is presented for integration with the lumped temperature intervals before it is extended to obtain better designs when it is less expensive to exchange a low-cost hot utility for a high-cost hot utility.

**Cumulative Heat Deficits.** To begin, cumulative heat deficits are introduced to permit integration of a single heat engine with two or more temperature intervals, thereby enabling optimal designs to have fewer heat engines than would be required for condensation at the temperature level of each interval. This is particularly important when it is less costly for one heat engine to satisfy two or more small loads over a larger temperature interval.

For heat engines above  $T_p$ , the heat delivered from heat

engine  $e$  to temperature interval  $n$  is a fraction,  $X_{ne}$ , of  $U_n^H$ , the cumulative hot deficit for intervals between interval  $n$  and  $T_p$ , where:

$$U_n^H = \sum_{k=n}^p D_k^H \quad n = 1, \dots, p \quad (5)$$

$U_n^H$  is the maximum heat at the temperatures in interval  $n$  that can be supplied by the heat engine. The heat rejected to heat engine  $e$  below  $T_p$  is a fraction,  $X_{ne}$ , of  $U_n^C$ , the cumulative cold deficit for intervals between  $T_p$  and interval  $n$ ,

$$U_n^C = \sum_{k=p+1}^n D_k^C \quad n = p+1, \dots, N \quad (6)$$

$U_n^C$  is the maximum heat at the temperatures in interval  $n$  that can be used for power generation. In the NLP model, the variables  $X_{ne}$ ,  $n = 1, \dots, N$  and  $e = 1, \dots, E$ , are adjusted to minimize the objective function and indicate the degree of integration. Note that  $\sum_e X_{ne} \leq 1$ ,  $n = 1, \dots, N$ .

**Rankine Cycles.** Often, simple Rankine cycles are adequate for the heat engines. One cycle, shown in Figure 4, has the design variables  $P_{be}$  (boiler pressure) and  $P_{ce}$  (condenser pressure) which, with the choice of working fluid, influence the tem-

peratures at which heat is absorbed and released and the efficiency of the heat engine. Note that for integration to occur

$$T_{4e} \geq T_{n-1} + \Delta T_{min} \quad e = 1, \dots, E' \quad (7)$$

$$T_{2e} \leq T_n \quad e = E' + 1, \dots, E \quad (8)$$

where  $T_{4e}$  and  $T_{2e}$  are the temperatures out of the condenser and pump of heat engine  $e$ ;  $T_n$  and  $T_{n-1}$  are the lowest and highest temperatures of the composite cold streams in interval  $n$ ;  $E'$  is the number of heat engines operating above  $T_p$ ; and  $E$  is the number of heat engines. The inequality in Eq. 8 permits utilization of the positive cold deficits below  $T_p$  for preheating the boiler feed in low-temperature heat engines.

Next, the energy balances for each leg of the Rankine cycle are expressed as nonlinear functions of  $P_{be}$  and  $P_{ce}$ . These are accompanied by the energy balances for heat integration which express, by difference, the heat removed by the cold utilities or added from the hot utilities for each heat engine.

The condenser operates at saturation with heat duty

$$Q_{ce}^{HE} = M_e^{HE} \Delta h_e^{vap}\{P_{ce}\} \quad e = 1, \dots, E \quad (9)$$

where  $M_e^{HE}$  is the mass flow rate of the working fluid, and  $\Delta h_e^{vap}$

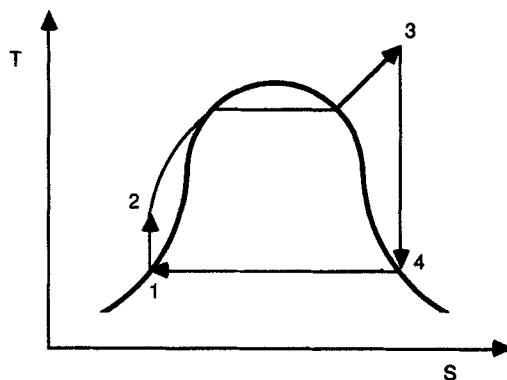
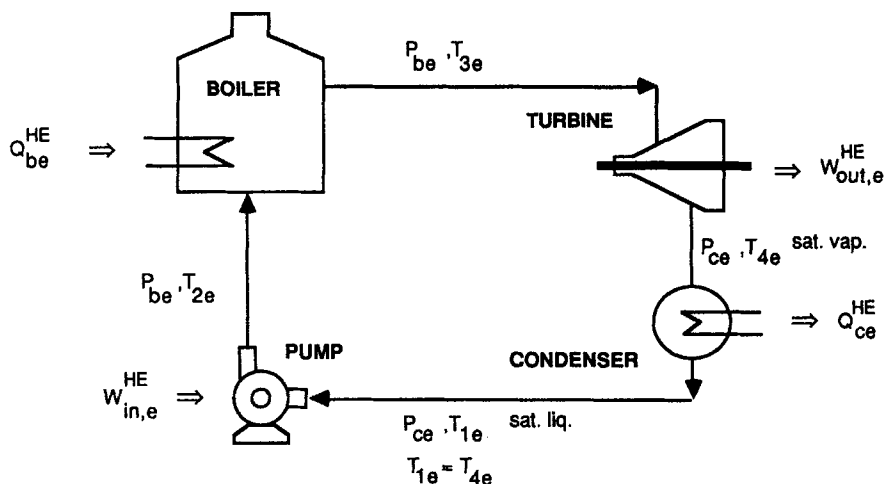


Figure 4. Simple Rankine cycle.

its latent heat of vaporization. For heat engines operating above  $T_p$ , the heat removed by cold utilities is

$$Q_{out,e}^{HE} = Q_{ce}^{HE} - \sum_{n=1}^p X_{ne} U_n^H \quad e = 1, \dots, E' \quad (10)$$

and for those operating below  $T_p$

$$Q_{out,e}^{HE} = Q_{ce}^{HE} \quad e = E' + 1, \dots, E \quad (11)$$

where  $Q_{out,e}^{HE}$  is the heat released to the external cold utilities (normally, cooling water).

Turning to the boiler, its heat duty is

$$Q_{be}^{HE} = M_e^{HE} (h\{P_{be}, T_{3e}\} - h\{P_{be}, T_{2e}\}) \quad e = 1, \dots, E \quad (12)$$

where  $T_{2e}$  and  $T_{3e}$  are the inlet and outlet temperatures. For heat engines operating above  $T_p$ , the heat supplied by hot utilities is

$$Q_{in,e}^{HE} = Q_{be}^{HE} \quad e = 1, \dots, E' \quad (13)$$

and for those operating below  $T_p$

$$Q_{in,e}^{HE} = Q_{be}^{HE} - \sum_{n=p+1}^N X_{ne} U_n^C \quad e = E' + 1, \dots, E \quad (14)$$

where  $Q_{in,e}^{HE}$  is the heat entering heat engine  $e$  from the hot utilities (normally fuel).

The work produced by the turbine,  $W_{out,e}^{HE}$ , is determined by a heat balance across the turbine

$$W_{out,e}^{HE} = M_e^{HE} (h\{P_{be}, T_{3e}\} - h\{P_{ce}, T_{4e}\}) \quad e = 1, \dots, E \quad (15)$$

and that required by the pump,  $W_{in,e}^{HE}$ , is given by

$$W_{in,e}^{HE} = M_e^{HE} (h\{P_{be}, T_{2e}\} - h\{P_{ce}, T_{4e}\}) \quad e = 1, \dots, E \quad (16)$$

Therefore, the net work produced by heat engine  $e$ ,  $W_{net,e}^{HE}$ , is

$$W_{net,e}^{HE} = W_{out,e}^{HE} - W_{in,e}^{HE} \quad e = 1, \dots, E \quad (17)$$

In summary, in the model for integration of the Rankine cycles, the decision variables for heat engine  $e$  (working fluid specified) are the pressure levels  $P_{be}$  and  $P_{ce}$ , the working fluid flow rate  $M_e^{HE}$ , and the  $X_{ne}$  variables. The constraints for heat engine  $e$  are the nonlinear energy balances for each unit in the cycle, plus inequality constraints to set lower and upper bounds on the decision variables; that is, bounds on the pressure levels and power integration variables  $X_{ne}$ . In addition, it is required that:

$$Q_{out,e}^{HE} \geq 0 \quad e = 1, \dots, E' \quad (18)$$

An upper bound on  $P_{be}$  is imposed when capital cost is not included in the objective function; otherwise, this constraint is usually inactive due to high capital costs at high pressures. For heat engines operating below  $T_p$ , the highest interval temperature,  $T_{n-1}$ , at which integration is attempted imposes a constraint on the amount of heat available for power generation:

$$M_e^{HE} (h\{P_{be}, T_{n-1}\} - h\{P_{be}, T_{2e}\}) - \sum_{n=p+1}^N X_{ne} U_n^C \geq 0 \quad (19)$$

which is accompanied by

$$Q_{in,e}^{HE} \geq 0 \quad (20)$$

for each heat engine. The inequality in Eq. 19 bounds the process heat removed by the heat engine by the maximum amount thermodynamically feasible, and the inequality in Eq. 20 requires that the residual boiler duty (not satisfied by process heat) be supplied with hot utilities. Note that a separate heat engine is postulated for each potential working fluid to be integrated at each temperature interval  $n$ .

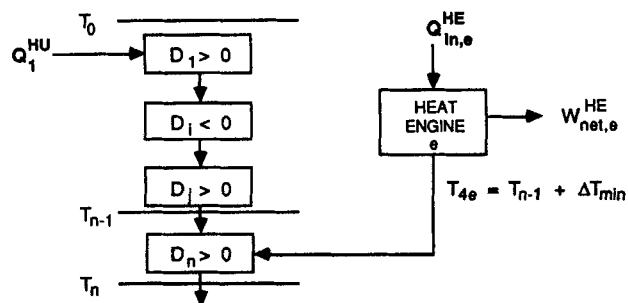
Since the efficiency of the heat engine increases as  $P_{ce}$  decreases, the limiting factor bounding  $P_{ce}$  is the highest interval temperature in which the integration is attempted. With each potential heat engine assigned to a specific temperature interval  $n$ ,  $P_{ce}$  is no longer a decision variable; that is, it is the vapor pressure at  $T_{4e} = T_{n-1} + \Delta T_{min}$ . To provide the alternative of no integration, a heat engine is included for each working fluid with  $P_{ce}$  at atmospheric pressure. Below  $T_p$ , with steam as the working fluid,  $P_{ce}$  is at atmospheric pressure. In both cases, the decision variables are the flow rate of the working fluid, the boiler pressure, and the integration variables.

Since the model permits more than one heat engine above and below  $T_p$ , heat engines with different working fluids and pressure levels can be evaluated competitively. Furthermore, constraints involving the  $X_{ne}$  variables can favor the utilization of particular heat engines in certain temperature intervals.

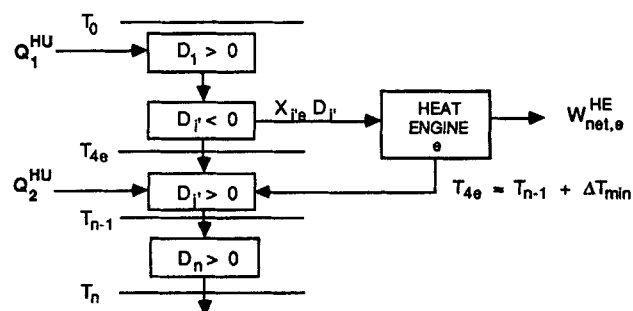
**Complex Power Cycles.** Early in the optimization, emphasis is placed on the selection of the working fluid and pressure levels using the simple Rankine cycle in Figure 4. Once an optimal combination of working fluids and integration levels is obtained, more efficient and complex cycles can be introduced and the NLP resolved. The first step usually identifies, with relatively few calculations, a good starting point for the more rigorous optimization. Alternatively, a rigorous optimization is accomplished in one step by including heat engines with complex configurations. The loss of computation time depends on the NLP algorithm and other factors. For large-scale problems, a step-by-step approach is often preferred.

**Multiple Hot Utilities.** The strategy of lumping, to eliminate temperature intervals with negative hot deficits, can lead to suboptimal designs for the system in Figure 5 when more than one hot utility is available. With just a single hot utility ( $T^{HU} > T_o + \Delta T_{min}$ ), Figure 5a shows a typical result, with the same hot utility (e.g., fuel) providing heat for the heat engine and satisfying the hot deficit in temperature interval 1. However, with a second hot utility at lower temperature, available at lower cost, the integration in Figure 5b is often more efficient. Here,  $Q_{be}^{HE}$  is provided by the negative hot deficit in interval  $i'$ , and the second hot utility provides the hot deficit for interval  $j'$ .

To locate the optimal design, the model must be extended to permit the heat engines to remove heat from the process above  $T_p$ . For each temperature interval  $n$  with a positive hot deficit, a heat engine is considered to satisfy the hot deficit by supplying a fraction of its heat of condensation. To maximize the efficiency of the heat engine, the condenser temperature is set such that  $T_{4e} = T_{n-1} + \Delta T_{min}$ , and  $P_{ce}$  is the vapor pressure at  $T_{4e}$ . Furthermore,  $T_{4e}$  is the lowest temperature for removal of heat from intervals with negative hot deficits; hence,  $T_{4e}$  must be added to the cascade of temperature intervals (when not previously present). In the revised cascade, all temperature intervals above  $T_{4e}$



(a) Partial integration following rules of Townsend and Linnhoff (1983a).



(b) Full integration.

Figure 5. Heat integration diagram for heat engines.

with negative hot deficits become candidates to provide heat for heat engine  $e$ , with adjacent intervals sharing the same sign lumped to reduce the size of the model without eliminating important options for integration. Figure 5b shows a typical revised cascade with the potential heat exchanges for this heat engine. In this integration  $Q_{2,2}^{HU}$ , the low-cost hot utility, replaces the high-cost hot utility  $Q_{in,e}^{HE}$  in Figure 5a. Since heat from the temperature intervals with negative hot deficits can preheat the feed to the boiler of heat engine  $e$ ,  $P_{be}$  can be adjusted to minimize the objective function.

To permit this integration, the constraint set is modified. For heat engine  $e$ , Eq. 13 is replaced by

$$Q_{in,e}^{HE} = Q_{be}^{HE} + \sum_{n=1}^P X_{ne} D_n^H \quad e = 1, \dots, E' \quad (13a)$$

with  $X_{ne}$  included for interval  $n$  where  $D_n^H < 0$ . The highest interval temperature that bounds a negative hot deficit,  $T_{max}$ , also imposes a constraint in the quality and quantity of heat to be used for power generation:

$$M_e^{HE} (h(P_{be}, T_{max}) - h(P_{be}, T_{2e})) + \sum_{n=1}^P X_{ne} D_n^H \geq 0 \quad e = 1, \dots, E' \quad (21)$$

This extension is especially effective as the number of hot util-

ities increases over an extended range of temperatures. As demonstrated in the Process Examples section below, it leads to more optimal designs due to increased integration between the process and the heat engines.

### Integration of heat pumps

With the temperature intervals lumped as shown in Figure 3, the heat pumps must accept energy from the process at temperatures below  $T_p$  and release energy to the process at temperatures above  $T_p$ . This strategy minimizes the utilities for heating and cooling the process streams, but can lead to impractically high compression loads, especially when  $T_p$  is above the ambient temperature. In these cases, the preferred alternative often is to condense with a cold utility, such as cooling water, rather than to integrate with the process above  $T_p$ . Furthermore, the lumped intervals do not permit the efficient utilization of low-temperature cold deficits to remove the heat of condensation, in exchange for additional cold utilities at high temperature (e.g., low-cost cooling water), rather than high-cost compression to reject the heat of condensation to cold utilities at the ambient temperature.

In this section, a model is first presented for integration with the lumped temperature intervals before it is extended to obtain better designs when it is less costly to satisfy the negative cold deficits with the heat of condensation from the heat pumps. The model permits several heat pumps,  $m = 1, \dots, P$ , having different working fluids, to be evaluated competitively to satisfy the demands for refrigeration at many different temperatures (e.g., in olefin plants).

When heat is released by heat pump  $m$  to temperature interval  $n$  above  $T_p$ , it is a fraction  $Y_{nm}$  of the cumulative hot deficit  $U_n^H$ . When temperatures are below  $T_p$  (the temperature below which refrigeration is required), the cold deficits must be eliminated by refrigeration. The heat released to heat pump  $m$  in temperature interval  $n$  ( $n \geq r$ , where  $T_{n-1} < T_p$ ) is a fraction  $Y_{nm}$  of the cumulative cold deficit  $U_n^C$ .  $Y_{nm}$  is adjusted to minimize the objective function, which includes the work of compression required by heat pump  $m$ ,  $W_{in,m}^{HP}$ , and the heat rejected to external cold utilities,  $Q_{out,m}^{HP}$ . As with the heat engines, the cumulative cold deficit  $U_n^C$  permits integration of a single heat pump with two or more temperature intervals, an important alternative when it is less costly for one heat pump to handle two or more small loads over a larger temperature interval.

**Simple Refrigeration Cycle.** The simple refrigeration cycle in Figure 6 is often adequate for integration. As for the Rankine cycle,  $P_{bm}$  and  $P_{cm}$ , and the choice of the working fluid, are the design variables. Its model is comprised of energy balances for each leg of the cycle and for integration with the temperature intervals of the process. These are nonlinear functions of  $P_{bm}$  and  $P_{cm}$  and are expressed below, beginning with the boiler heat duty:

$$Q_{bm}^{HP} = \sum_{n=r}^N Y_{nm} U_n^C \quad m = 1, \dots, P \quad (22)$$

from which the mass flow rate of the working fluid can be determined by a heat balance across the boiler

$$M_m^{HP} = Q_{bm}^{HP} / (h(P_{bm}, T_{1m}) - h(P_{bm}, T_{4m})) \quad m = 1, \dots, P \quad (23)$$

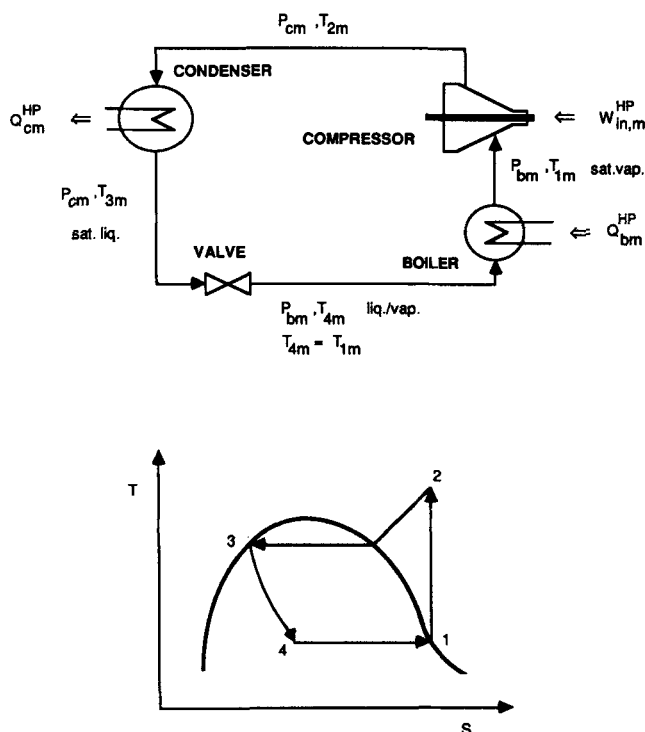


Figure 6. Simple refrigeration cycle.

The condenser heat duty is

$$Q_{cm}^{HP} = M_m^{HP} (h\{P_{cm}, T_{2m}\} - h\{P_{cm}, T_{3m}\}) \quad m = 1, \dots, P \quad (24)$$

and the compression work is

$$W_{in,m}^{HP} = M_m^{HP} (h\{P_{cm}, T_{2m}\} - h\{P_{cm}, T_{1m}\}) \quad m = 1, \dots, P \quad (25)$$

When integration with the process is incomplete, some of the heat of condensation is rejected to a cold utility, such as cooling water. This heat duty depends upon the degree of integration and is

$$Q_{out,m}^{HP} = Q_{cm}^{HP} - \sum_{n=1}^P Y_{nm} U_n^C \quad m = 1, \dots, P \quad (26)$$

Note that later in this section Eq. 26 will be altered to permit the rejection of heat to temperature intervals below  $T_p$ , when it is desirable; see Eq. 26a below.

In summary, in the model for integration of the simple refrigeration cycles, there are at most two degrees of freedom for cycle  $m$ ,  $P_{bm}$  and  $P_{cm}$ , in addition to the choice of working fluid. When heat is rejected to the heat pump in only one temperature interval  $n$ , a common situation,  $P_{bm}$  is the vapor pressure of the fluid at  $T_n$ , and  $P_{cm}$  is the only degree of freedom. In the general case, however, the decision variables for each heat pump are the pressure levels and the  $Y_{nm}$  variables. The constraints for heat pump  $m$  are the nonlinear energy balances, plus inequality constraints setting operating limits on the pressure levels and  $Y_{nm}$  variables. Also, above  $T_p$

$$T_{2m} - T_{n-1} - \Delta T_{min} \geq 0 \quad m = 1, \dots, P \quad (27)$$

$$Q_{out,m}^{HP} \geq 0 \quad m = 1, \dots, P \quad (28)$$

are included. Similarly, below  $T_p$ ,

$$T_n - T_{4m} \geq 0 \quad m = 1, \dots, P \quad (29)$$

guarantees that the evaporator temperature is sufficiently low to remove heat from the process. Finally, when several heat pumps compete to remove heat below  $T_p$ , the inequality constraint

$$\sum_{m=1}^P Y_{nm} \geq D_n^C / U_n^C \quad (30)$$

must be included to assure that the interval cold deficit is satisfied. Note that a separate heat pump is postulated for each potential working fluid to be integrated between two temperature intervals. Consequently, heat pumps with different working fluids and pressure levels can be evaluated competitively. Furthermore, constraints involving the  $Y_{nm}$  variables can favor the utilization of particular heat pumps in certain temperature intervals. In the initial stages of the optimization, emphasis is placed on selecting the working fluid and pressure levels using the simple refrigeration cycle in Figure 6. Once a good starting point is obtained, the cycle configuration can be improved and the NLP resolved. As in the integration of the heat engines, a more rigorous optimization can be attempted initially.

**Condensation Using the Temperature Intervals Below  $T_p$ .** When  $T_p$  is high (typically above ambient temperature), designs based upon integration with temperature intervals above  $T_p$  as illustrated in Figure 3, or based upon heat rejection to a cold utility, as illustrated in Figure 7a, are often more costly than those with heat pumps whose heat of condensation satisfies the negative cold deficits of temperature intervals below  $T_p$ . Unavoidably, this integration increases the requirement for external cooling below  $T_p$ , but the increase is in the temperature intervals above  $T_p$ , where cold utilities such as cooling water are relatively inexpensive. The increase in the cost of the low-priced cold utilities is often offset by the increased efficiency of the heat pump, which requires less high-priced power.

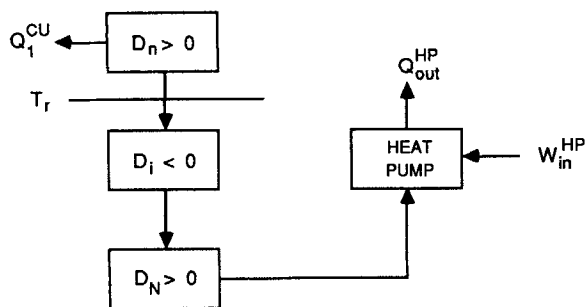
To locate the optimal design, the model was extended to permit the heat pumps to reject heat to temperature intervals with negative cold deficits below  $T_p$ . When this integration is considered, the intervals with negative cold deficits are normally not lumped with the intervals having positive cold deficits below  $T_p$ , unless the difference of temperatures ( $T_{n-1} - T_n$ ) is small. Here, adjacent intervals with cold deficits that share the same sign can be lumped to reduce the size of the model without eliminating important possibilities for integration. Above  $T_p$ , however, there is no advantage to transferring heat to intervals with negative cold deficits, and lumping is accomplished where possible. To allow the rejection of heat below  $T_p$ , for heat pump  $m$  Eq. 26 is replaced by:

$$Q_{out,m}^{HP} = Q_{cm}^{HP} + Y_{nm} D_n^C \quad (26a)$$

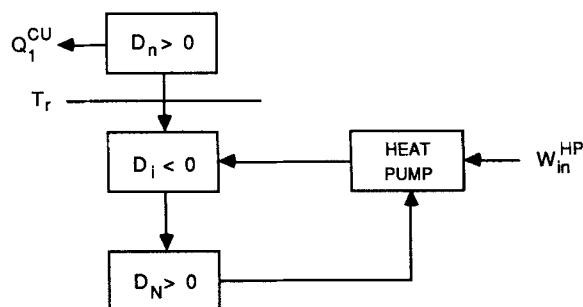
with  $Y_{nm}$  included for interval  $n$  where  $D_n^C < 0$ .

In summary, this model leads to better designs when the trade-offs between the cost of the cold utilities and the cost of compression favor the rejection of heat below  $T_p$ . Since  $T_p$  is high in most chemical processes, integration above  $T_p$  is far from optimal due to high compression ratios, and the rejection of heat





(a) Energy rejected to a cold utility (e.g., cooling water) or intervals above  $T_p$  (not shown).



(b) Energy rejected to intervals below  $T_p$ .

**Figure 7. Heat integration diagram for heat pumps.**

below  $T_r$  is the best alternative—often better than rejecting the heat of condensation to a cold utility above  $T_r$ .

### Combined heat engines and heat pumps

Some complex plants involve both heat engines and heat pumps, with the former providing the compression work for the latter. This often occurs when the products of an exothermic reaction require refrigeration; for example, in coal gasification where the exothermic shift conversion step at approximately 400°C is followed by acid gas removal using the Selexol process. When heat engines and heat pumps compete to reject their heats of condensation to temperature intervals above  $T_p$ , the constraints must be generalized

$$\sum_{e=1}^{E'} X_{ne} + \sum_{m=1}^P Y_{nm} \leq 1 \quad n = 1, \dots, p \quad (31)$$

Also, the power demand to be satisfied by the heat engines must include the compression work for each of the heat pumps under consideration. In general, a constraint is included to assure that the heat engines, heat pumps, and process power requirements are satisfied either by electrical work,  $W_{elec}$ , or turbine shaft work:

$$\sum_{e=1}^E W_{net,e}^{HE} - \sum_{m=1}^P W_{in,m}^{HP} + W_{elec} = W_{spec} \quad (32)$$

where  $W_{spec}$  is the power demand for the process.

### Objective function

The complete NLP model includes an economic objective function subject to a set of linear and nonlinear equality and inequality constraints. There are two choices for the objective function: the cost of external utilities, and the annualized cost of the utility system.

The first sums the annual cost of the utilities used in the process. For example, when heat engines and heat pumps are evaluated competitively, the function includes six terms:

$$C_{util} = \sum_{n=1}^P \sum_{k=1}^{NHU} c_k^{HU} Q_{nk}^{HU} + \sum_{n=p+1}^N \sum_{l=1}^{NCU} c_l^{CU} Q_{nl}^{CU} \\ + \sum_{m=1}^P C_{out,m}^{HP} Q_{out,m}^{HP} + \sum_{e=1}^E C_{in,e}^{HE} Q_{in,e}^{HE} \\ + \sum_{e=1}^E C_{out,e}^{HE} Q_{out,e}^{HE} + C_{elec} W_{elec} \quad (33)$$

where  $NHU$  is the number of hot utilities,  $NCU$  is the number of cold utilities,  $Q_{nk}^{HU}$  is the heat load of hot utility  $k$  in interval  $n$ ,  $Q_{nl}^{CU}$  is the heat load of cold utility  $l$  in interval  $n$ , and the  $c$ 's are the cost coefficients for the different utilities.

The annualized cost of the power systems,

$$C_{ann} = \text{Rate of return} \times C_{equip} + C_{util} \quad (34)$$

accounts for capital costs and therefore better represents the capital-energy trade-offs.  $C_{equip}$  is the cost of the equipment, which depends on the pressure levels and the configuration selected for the heat engines and heat pumps.

Note that minimization of  $C_{util}$  is often adequate for heat integration with heat pumps, where the overriding costs are for power to drive the compressors, as illustrated in the Distillation Sequence example, below. For integration of heat engines,  $C_{util}$  gives impractically high pressures,  $P_{be} = P_{max}$ , and  $C_{ann}$ , which accounts for the high cost of equipment at elevated pressures, provides more realistic designs. Here, however,  $C_{util}$  provides a lower bound on the energy requirements as the heat engines operate at  $P_{be} = P_{max}$ , with the maximum efficiency permitted by the  $P_{max}$  specification.

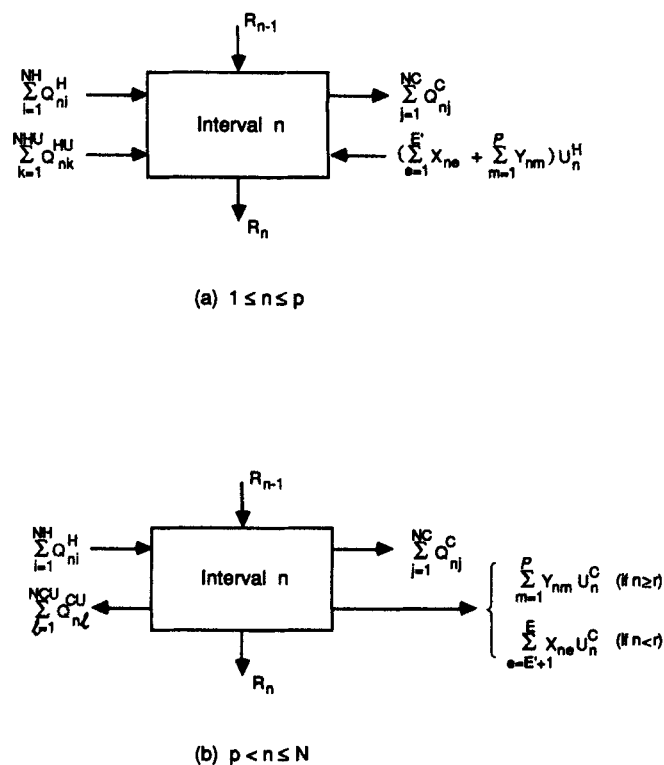
### Temperature interval heat balances

Having defined the heat balances and operating limits and biases on  $X_{ne}$  and  $Y_{nm}$  for the heat engines and heat pumps, it remains to set down the heat balances in each temperature interval. For integration with lumped temperature intervals (having positive hot and cold deficits), these constraints are summarized in Figure 8. For each temperature interval  $n$  in the cascade where  $T_n \geq T_p$ , the energy balance is

$$R_{n-1} - R_n + \sum_{k=1}^{NHU} Q_{nk}^{HU} \\ + \left( \sum_{e=1}^{E'} X_{ne} + \sum_{m=1}^P Y_{nm} \right) U_n^H = \sum_{j=1}^{NC} Q_{nj}^C - \sum_{i=1}^{NH} Q_{ni}^H \quad (35)$$

and with  $T_n < T_p$ ,

$$R_{n-1} - R_n - \sum_{l=1}^{NCU} Q_{nl}^{CU} - Q_{int,n} = \sum_{j=1}^{NC} Q_{nj}^C - \sum_{i=1}^{NH} Q_{ni}^H \quad (36)$$



**Figure 8. Heat balances for temperature interval  $n$  with positive hot deficit ( $1 \leq n \leq p$ ) and positive cold deficit ( $p < n \leq N$ ).**

where  $Q_{int,n}$  is the rate of heat integration with heat engines or heat pumps in interval  $n$  below  $T_p$ . Note that for intervals in which  $T_n \geq T_p$  ( $n < r$ ),

$$Q_{int,n} = \sum_{e=E'+1}^E X_{ne} U_n^C \quad (37)$$

and when  $T_n < T_p$  ( $n \geq r$ ),

$$Q_{int,n} = \sum_{m=1}^P Y_{nm} U_n^C \quad (38)$$

For integration with temperature intervals having negative hot deficits when  $T_n \geq T_p$ , the energy balance is:

$$R_{n-1} - R_n + \sum_{k=1}^{NHU} Q_{nk}^{HU} + \left( \sum_{e=1}^{E'} X_{ne} + \sum_{m=1}^P Y_{nm} \right) U_n^H + \sum_{e=1}^{E'} X_{ne} D_n^H = \sum_{j=1}^{NC} Q_{nj}^C - \sum_{i=1}^{NH} Q_{ni}^H \quad (35a)$$

where

$$D_n^H = \begin{cases} D_n^H & D_n^H < 0 \\ 0 & D_n^H \geq 0 \end{cases}$$

and for integration with intervals having negative cold deficits

when  $T_n < T_p$ ,

$$R_{n-1} - R_n - \sum_{i=1}^{NCU} Q_{ni}^{CU} - Q_{int,n} - \sum_{m=1}^P Y_{nm} D_n^C = \sum_{j=1}^{NC} Q_{nj}^C - \sum_{i=1}^{NH} Q_{ni}^H \quad (36a)$$

where

$$D_n^C = \begin{cases} D_n^C & D_n^C < 0 \\ 0 & D_n^C \geq 0 \end{cases}$$

and  $Q_{int,n}$  is defined as before.

### Properties of NLP model

**Flexibility.** The NLP model is sufficiently flexible to be adapted to situations ranging from grass-roots designs to retrofits. A specific objective function can be defined for each situation. For example, when heat engines and heat pumps are to be integrated, terms accounting for the cost of the hot and cold utilities are included. However, when a utility system is to be designed, an annualized cost objective function is used, which includes the capital costs for a steam generator and the cost of fuel. In all cases, care must be taken in the assignment of the cost coefficients.

**Process Pressure Levels.** The NLP model optimizes the pressure levels in heat engines and heat pumps, but does not optimize the pressure levels of the process. In process design, the algorithm would be used to position heat engines and heat pumps for each potential pressure distribution, with the optimal distribution selected based on the minimum cost criterion.

To expand upon this, the NLP model requires that the engineer set the power and refrigeration requirements as well as the location of the pinch temperature. The latter is accomplished, with knowledge of the supply and target temperatures of the process streams, utilizing the pinch methods referred to earlier (Umeda et al., 1978; Linnhoff and Turner, 1981; Papoulias and Grossmann, 1983b). The power requirements of the process depend upon the pressure increases, with credits taken for pressure decreases when turbine work is available for pumping and compression. Clearly, the pressure levels strongly affect the power requirements and, in turn, the minimum utilities for heating and cooling and the pinch temperature. Hence, for each potential pressure distribution and configuration of pumps, compressors, and turbines, the NLP model must be reformulated.

Consider, for example, a process gas stream at high temperature and pressure, the product of a chemical reactor, to be delivered to a separator at low temperature and pressure. When a heat exchanger and valve are used, the heat integration (minimum utilities and pinch temperature) is unaltered. However, when the stream produces turbine work, it has less energy available for heat exchange and the heat integration is altered. In the latter case, a modified NLP model must be optimized. Here, the turbine work is credited against the power requirements for the process excluding the turbine.

**Raw Steam Demand.** When steam is required as a reactant or mass separating agent, it must be accounted for in the NLP model for the integration of heat engines and heat pumps. One

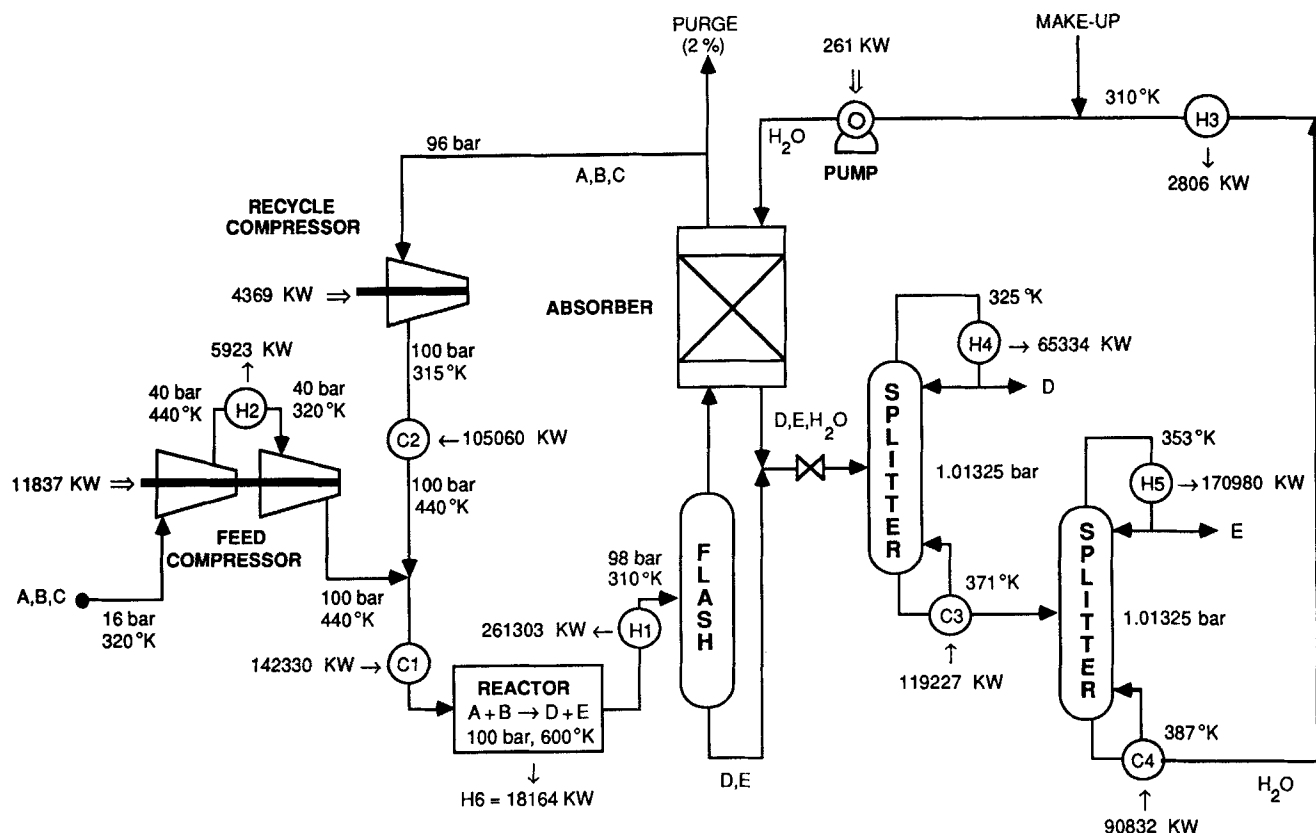


Figure 9. ABCDE process (Papoulias and Grossmann, 1983c).

possibility is to set lower bounds on utility steam at the temperature level  $n$  required. For example,  $Q_{nl}^{HU} \geq Q_{raw}$  would require that the heat load of hot utility 1 (steam) at temperature  $T_n$  be greater than the raw steam required at  $T_n$ .

**Interval Partitions.** The temperature intervals, with or without lumping, establish bounds upon the boiler and condenser temperatures of the power cycles. When large temperature differences occur across an interval, it may be desirable to decompose the interval into intervals with smaller temperature differences and consider many additional combinations of power cycles for integration. In the limit, an infinite number of intervals would give the global optimum. However, in practice a small finite number closely approximates the global optimum. Convergence can be checked by repeated interval reduction.

Table 1. Heating and Cooling Demands for ABCDE Process

Stream	$T_c$ K	$T_h$ K	$Q$ kW	$C$ kW/K
H1	600	310	261,303	901.045
H2	440	320	5,923	49.358
H3	387	310	2,806	36.442
H4	325	325	65,334	—
H5	353	353	170,980	—
H6	600	600	18,164	—
C1	440	600	142,330	889.563
C2	315	440	105,060	840.480
C3	371	371	119,227	—
C4	387	387	90,832	—

## Process Examples

### ABCDE process

To demonstrate the utility of the NLP model, two processes are considered. The first, shown in Figure 9, is the optimal solution obtained by Papoulias and Grossmann (1983c) using their MILP model for process synthesis. A gas mixture of A, B, and C, at 320 K and 16 bar (kPa = bar  $\times$  100), is compressed and

Table 2. Utilities Data\*

Steam cost per year					
Press.	$T$ K	$P$ bar	$\$/\text{ton}$	$h$ kJ/kg	$c^{HU}$ \$/kW
High	672.4	68.95	6.5	1895.2	103.7146
Medium	605.4	17.24	5.4	2227.2	73.3190
Low	411.0	3.45	4.0	2149.0	56.2866
Cooling water					
$T_{in} = 300$ K, $T_{out} = 322$ K, 0.07\$/1,000 gal					
$c^{CU} = c_{out}^{HE} = c_{out}^{HP} = 6.011$ \$/kW					
Electricity					
0.05\$/kWhr					
$c_{elec} = 420.0$ \$/kW					
Fuel					
$\Delta h_c = 43,950$ kJ/kg, 143\$/ton					
$c_{in}^{HE} = 109.3242$ \$/kW					

\*All costs based on 8,400 operating h/yr

°K	Interval deficit, KW	
662.4	0	
600	4092	4092
595.4	4804	4804
590 <sup>+</sup>	-18164	
590 <sup>-</sup>	-478	
548.4	-923	
468	-322	65613
440	-606	
430	-3188	
401 <sup>+</sup>	0	
401 <sup>-</sup>	-1539	
387 <sup>+</sup>	90832	
387 <sup>-</sup>	-1099	
377	-878	117250
371 <sup>+</sup>	119227	
371 <sup>-</sup>	4098	pinch
343 <sup>+</sup>	170980	
343 <sup>-</sup>	3078	
322	1024	
315 <sup>+</sup>	65334	
315 <sup>-</sup>	4934	
310	9375	
300		

Figure 10. Temperature intervals for ABCDE process.

mixed with a recycle stream before entering a high pressure reactor. The reaction,  $A + B \rightarrow D + E$ , is exothermic at 600 K and 100 bar. The reactor products, at 600 K and 100 bar, are cooled to 310 K and 98 bar and sent to a flash separator where unreacted  $A$ ,  $B$ , and inert  $C$  are recovered. The vapor stream is scrubbed with water to recover  $D$  and  $E$ . Two percent of the lean

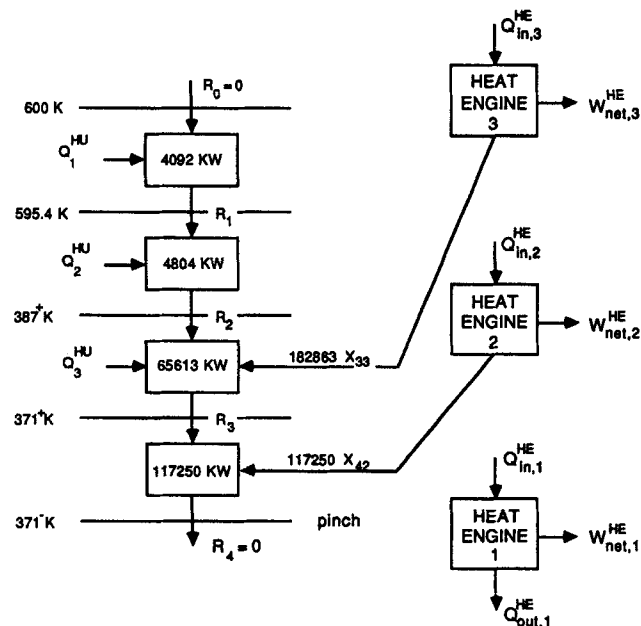


Figure 11. Heat engine integration diagram for ABCDE process with lumped temperature intervals.

Table 3. Solutions for ABCDE Process with Lumped Temperature Intervals

	Case 1*	Case 2**
$X_{33}$	0	0
$X_{42}$	0.23521	0.30203
$P_{b2}^{HE}$ , bar	120	59.91
$P_{c2}^{HE}$ , bar	1.263	1.263
$Q_1^{HU}$ , kW	4092	4092
$Q_2^{HU}$ , kW	4804	4804
$Q_3^{HU}$ , kW	155,285	147,451
$Q_{in,2}^{HE}$ , kW	44,045	51,879
$W_{net,2}^{HE}$ , kW	16,467	16,467
$W_{elec}$ , kW	0	0
$C_T$ , \$	—	10,675,530
$C_P$ , \$	—	54,170
$C_B$ , \$	—	10,567,470
$C$ , \$/yr	14,332,300	17,942,300

\*Utility cost

\*\*Annualized cost

vapor is purged, to remove  $C$ , and the remainder is recirculated to the reactor. The rich water is mixed with liquid from the flash separator and sent to the first of two atmospheric distillation columns. In the first column,  $D$  is removed in the distillate, and the bottoms stream is sent to the second column, where  $E$  is recovered in the distillate. The bottoms stream, mainly water, is pumped back to the absorber. Figure 9 shows the temperatures and pressures of all streams. Cold streams to be heated are labeled  $C\#$  and hot streams to be cooled are labeled  $H\#$ , with heat duties and heat capacity flow rates given in Table 1. The needs for compression work are also annotated in Figure 9.

Following the procedure previously described for heat and power integration, the first step is the determination of the pinch temperature for the network of heat exchangers. Applying the method of Linnhoff and Turner (1981), with  $\Delta T_{min} = 10$  K, the pinch temperature is 371 K.

Next, the NLP model is formulated. First, the temperature

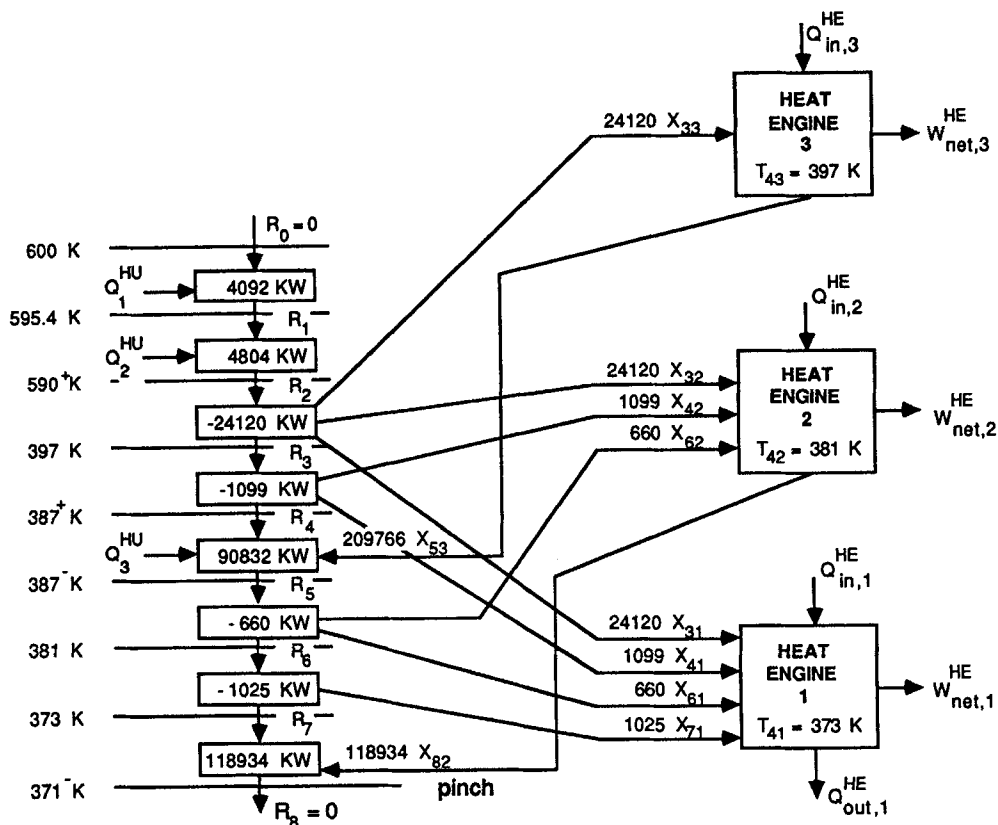
Table 4. Solutions for ABCDE Process with Extended Formulation†

	Case 1*	Case 2**
$X_{n2}$ ( $n \neq 8$ )	1	1
$X_{82}$	0.23188	0.29786
$P_{b2}^{HE}$ , bar	120	59.86
$P_{c2}^{HE}$ , bar	1.263	1.263
$Q_1^{HU}$ , kW	4092	4092
$Q_2^{HU}$ , kW	4804	4804
$Q_3^{HU}$ , kW	181,163	173,316
$Q_{in,2}^{HE}$ , kW	18,167	26,014
$W_{net,2}^{HE}$ , kW	16,467	16,467
$W_{elec}$ , kW	0	0
$C_T$ , \$	—	10,675,500
$C_P$ , \$	—	54,160
$C_B$ , \$	—	10,561,220
$C$ , \$/yr	12,959,700	16,569,600

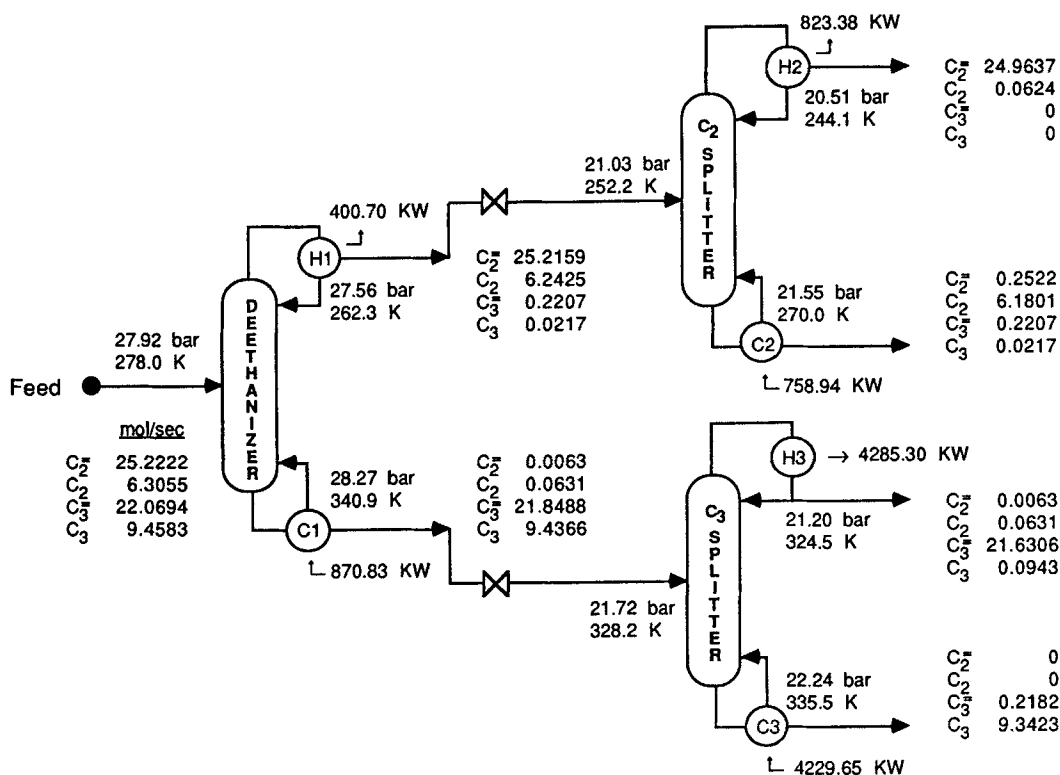
†Potential integration with temperature intervals having negative hot deficits

\*Utility cost

\*\*Annualized cost



**Figure 12. Heat engine integration diagram for ABCDE process.**  
Potential integration with temperature intervals having a negative hot deficit.



**Figure 13. Cold tray distillation sequence.**

°K	Interval deficit, KW	
340.9 <sup>+</sup>		
340.9 <sup>-</sup>	870.83	870.83
335.5 <sup>+</sup>	0	
335.5 <sup>-</sup>	4229.65	4229.65
321.7 <sup>+</sup>	0	pinch
321.7 <sup>-</sup>	4285.30	
270.0 <sup>+</sup>	0	3526.37
270.0 <sup>-</sup>	-758.94	
259.5 <sup>+</sup>	0	400.70
259.5 <sup>-</sup>	400.70	
241.3 <sup>+</sup>	0	823.38
241.3 <sup>-</sup>	823.38	

Figure 14. Temperature intervals for cold tray distillation sequence.

intervals are assigned, after the hot stream temperatures are reduced by  $\Delta T_{min} = 10$  K. These include the temperatures of high-, medium-, and low-pressure steam available from the utility system, as given in Table 2. The heat deficits for each interval are shown on the left in Figure 10. Note that the temperature intervals for isothermal heating and cooling at  $T_n$  are bounded by  $T_n^+$  and  $T_n^-$ .

In this example, heat pumps are not considered since all heat is removed above ambient temperature. However, a steam engine that dumps energy above  $T_p$  is a fine candidate for this process. Heat available below  $T_p$  could drive a subatmospheric steam engine, but too inefficiently to be a reasonable alternative.

Table 5. Heating and Cooling Demands for Cold Tray Distillation Sequence

Stream	$T_h$ K	$T_c$ K	$Q$ kW
H1	262.3	262.3	400.70
H2	244.1	244.1	823.38
H3	324.5	324.5	4,285.30
C1	340.9	340.9	870.83
C2	270.0	270.0	758.94
C3	335.5	335.5	4,229.65

Therefore, only temperature intervals above  $T_p$  are included in the model.

First, the temperature intervals are lumped, eliminating intervals with negative hot deficits. Far fewer temperature intervals result, as shown in Figures 10 and 11, with three alternatives for the steam engine. Note that the cumulative hot deficits  $U_n^H$ , defined in Eq. 5, are multiplied by  $X_{ne}$  to give the heat transferred from heat engine  $e$  to interval  $n$ . Also, hot utilities 1, 2, and 3 are high-, medium-, and low-pressure steam, respectively.

Two objective functions are considered, using the costs of utilities in Table 2, the equations for the cost of equipment in the Appendix, and a 15% rate of return on investment. In each case, the size of the model is reduced, using the equality constraints, by substitution for the state variables in terms of the decision variables. The enthalpies and vapor pressures are estimated using the Peng-Robinson equation. The gradients required by the optimization algorithm are determined analytically.

The first objective is to minimize the cost of utilities. In this

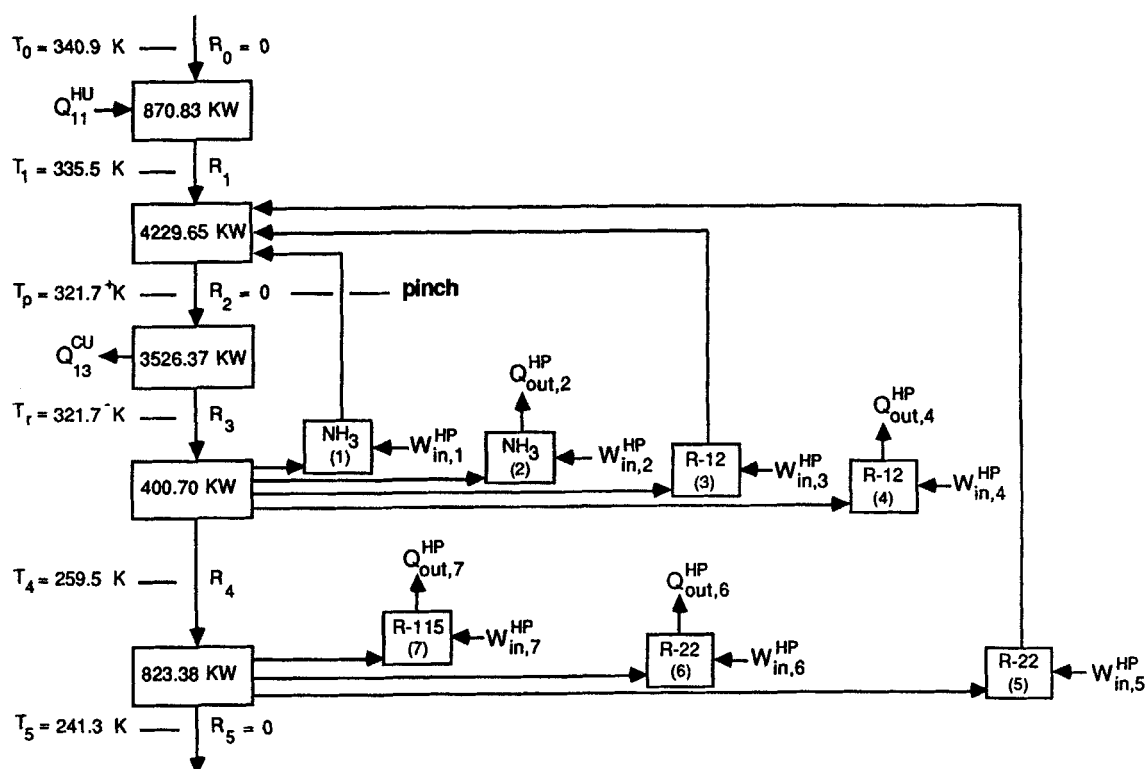


Figure 15. Heat pump integration diagram for cold tray distillation with lumped temperature intervals.

case, the decision variables are the pressure levels of the steam engine, the steam flow rate, and the integration variables  $X_{ne}$ . The model has 19 variables and 11 constraints and was solved using MINOS (Murtagh and Saunders, 1983). The solution in Table 3, case 1, shows integration at interval 4, with the steam engine providing all of the power required by the process. No cooling water is required by the steam engine and the condenser pressure is adjusted to supply heat to the interval. However, the boiler pressure is at the upper bound, 120 bar, as expected, since capital cost is not included in the objective function. The CPU time for this case is 7.22 s on a VAX-11/750 computer.

In the second case, the annualized cost, Eq. 34, is minimized (including the capital costs for only the heat engine). Its solution, in Table 3, shows integration at interval 4. No cooling water is required by the steam engine and the pressure levels are more realistic. The condenser pressure permits steam to condense at 397 K and the boiler pressure is significantly reduced due to the high cost of the equipment at high pressures. In this case, the CPU time is 9.14 s.

As shown in Figure 10, there are a number of intervals with negative hot deficits that can potentially drive the steam engine above  $T_p$ . To account for this possibility, the model was extended, with the resulting integration diagram shown in Figure 12. The model has 31 variables and 21 constraints and was solved using MINOS for the two objective functions. The solutions are presented in Table 4. In each case, the new designs save approximately \$1.4 million per year due to greater integration

between the process and the steam engine. The CPU times for these cases are 11.3 and 13.04 s, respectively.

The final step is the synthesis of the heat exchanger network for each case. This can be accomplished by the methods referred to earlier (Linnhoff and Hindmarsh, 1983; Papoulias and Grossmann, 1983b).

### Distillation sequence

The second example involves the cold tray distillation sequence shown in Figure 13. A gas stream containing ethylene, ethane, propylene, and propane is compressed to 27.92 bar and 278 K and sent to a deethanizer column. The vapor product is flashed across a valve and fed to a  $C_2$  splitter to obtain high-purity ethylene and ethane products. The deethanizer bottoms, after pressure reduction across a valve, is processed in a  $C_3$  splitter where propylene and propane products are recovered. The cold streams to be heated are labeled  $C\#$  and hot streams to be cooled are labeled  $H\#$ , with the heat duties given in Table 5. Note that hot streams  $H1$  and  $H2$  require refrigeration.

With  $\Delta T_{min} = 2.78$  K,  $T_p = 119.42$  K. There are 11 temperature intervals, with four above  $T_p$ , as shown in Figure 14. In interval 5, the cold deficit can be satisfied with cooling water. Intervals 9 and 11 require refrigeration, and hence the NLP model is formulated with alternative heat pumps using ammonia and refrigerant 12, 22, and 115, as the working fluids. For the working fluids, the enthalpies and vapor pressures are computed using the Peng-Robinson equation.

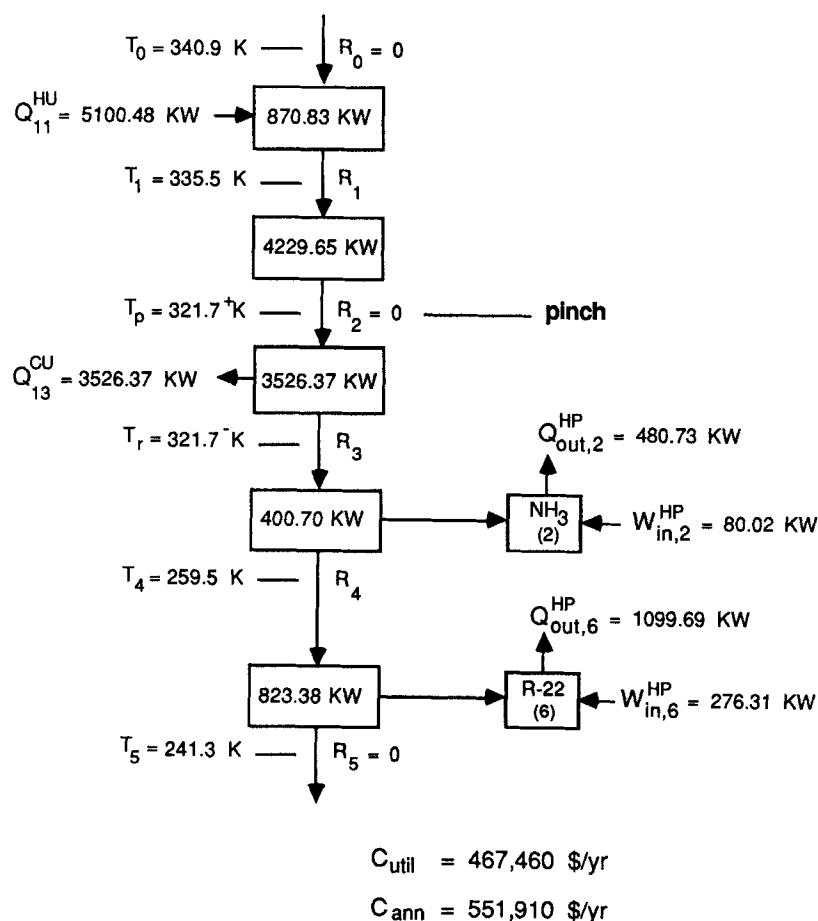


Figure 16. Optimal solutions for cold tray distillation with lumped temperature intervals.

First, the temperature intervals are lumped, eliminating the negative deficit in interval 7, and the NLP model is formulated attempting integration across  $T_p$ . Figure 15 shows the integration diagram. The model has 36 variables and 15 constraints. The optimal solutions in Figure 16 were obtained using the economic data in Table 2 and the equations in the Appendix. With both objective functions, at the optimum, no integration occurs between the heat pumps and the process above  $T_p$ , an ammonia heat pump is integrated with interval 4, and a refrigerant 22 heat pump with interval 5. As expected, the configuration is unchanged since the compression work has the highest cost in both minimizations. The CPU times are 37.48 and 37.78 s when minimizing utility costs and capital costs, respectively.

As shown in Figure 14, the negative cold deficit in interval 5 can potentially absorb the heat of condensation of the heat pumps. To allow this, the NLP model was reformulated with the integration diagram in Figure 17. This model has 53 variables and 22 constraints. Again, optimal solutions were obtained for both objective functions, with the results shown in Figure 18. In both cases, a refrigerant 22 heat pump is positioned to reject its heat of condensation to the negative cold deficit in interval 4. Optimal designs are obtained with savings of 13% and 17% in the two cases. The CPU times are 68.36 and 70.14 s when minimizing utility costs and capital costs, respectively.

## Conclusions and Significance

It is concluded that:

1. When multiple hot utilities are available, the optimal integration of heat engines above the pinch temperature often

involves driving the heat engine with heat from a temperature interval having a negative hot deficit. This violates the initial guidelines of Townsend and Linnhoff (1983a) and is successful when a low-cost hot utility can replace high-priced fuel to drive a heat engine.

2. Below the refrigeration temperature,  $T_r$ , the optimal integration of heat pumps often involves delivering the heat of condensation to temperature intervals with negative cold deficits. This also violates the initial guidelines of Townsend and Linnhoff (1983a), but adopts the qualitative recommendation on page 112 of the book by Linnhoff et al. (1982), and is successful when the cost of compression to condense the working fluid with cooling water exceeds the added cost of cooling water due to heat transfer to the process below  $T_r$ .

3. An efficient nonlinear programming model has been formulated that follows the initial guidelines of Townsend and Linnhoff. It lumps the temperature intervals and introduces cumulative heat deficits to permit one heat engine or heat pump to be integrated with more than one temperature interval.

4. The nonlinear programming strategy has been extended to permit integration with temperature intervals having negative hot and cold deficits. In this extension, the temperature intervals are not lumped, leaving the intervals with negative deficits as candidates for integration with the heat engines or heat pumps.

## Notation

$c$  = cost coefficient  
 $C$  = cost, \$; heat capacity flow rate, kW/K  
 $C_{ann}$  = annualized cost, \$/yr

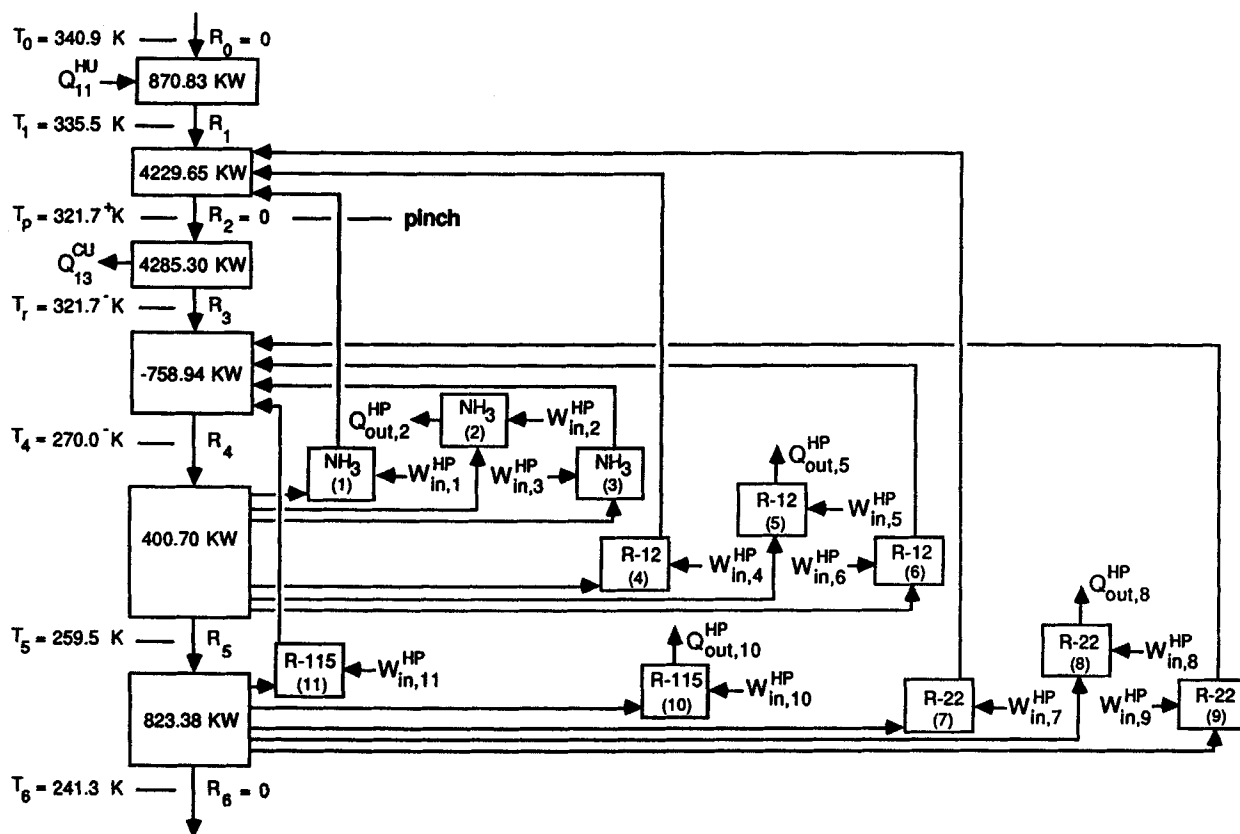
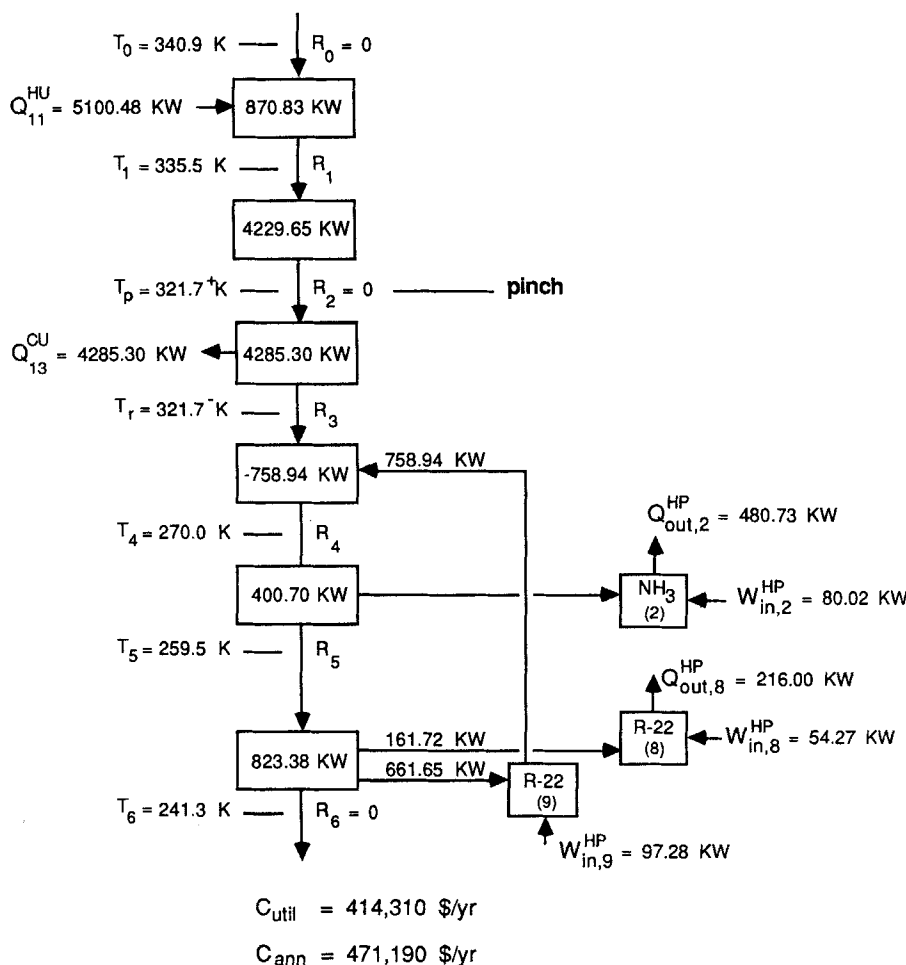


Figure 17. Heat pump integration diagram for cold tray distillation allowing integration with interval 4, having a negative cold deficit below  $T_r$ .





**Figure 18. Optimal solutions for cold tray distillation allowing integration with interval 4, having a negative cold deficit below  $T_p$ .**

$C_b$  = boiler cost, \$  
 $C_c$  = compressor cost, \$  
 $C_{equip}$  = equipment cost, \$  
 $C_p$  = pump cost, \$  
 $C_t$  = turbine cost, \$  
 $C_{util}$  = utilities cost, \$/yr  
 $D_n^C$  = cold deficit in interval  $n$ , kW  
 $D_n^H$  = hot deficit in interval  $n$ , kW  
 $E$  = number of heat engines  
 $E'$  = number of heat engines above  $T_p$   
 $h$  = enthalpy, kJ/kg  
 $\Delta h_e^{vap}$  = latent heat of vaporization of working fluid in heat engine  $e$ , kJ/kg  
 $M$  = mass flow rate of working fluid in boiler, kg/s  
 $M_e^{HE}$  = mass flow rate of working fluid in heat engine  $e$ , kg/s  
 $M_m^{HP}$  = mass flow rate of working fluid in heat pump  $m$ , kg/s  
 $N$  = number of temperature intervals  
 $NC$  = number of cold streams  
 $NCU$  = number of cold utilities  
 $NH$  = number of hot streams  
 $NHU$  = number of hot utilities  
 $P$  = number of heat pumps  
 $P_b$  = boiler pressure, bar  
 $P_{be}$  = boiler pressure in heat engine  $e$ , bar  
 $P_{bm}$  = boiler pressure in heat pump  $m$ , bar  
 $P_{ce}$  = condenser pressure in heat engine  $e$ , bar  
 $P_{cm}$  = condenser pressure in heat pump  $m$ , bar  
 $P_{in}$  = pump inlet pressure, bar  
 $Q_{be}^{HE}$  = boiler heat duty of heat engine  $e$ , kW  
 $Q_{bm}^{HP}$  = boiler heat duty in heat pump  $m$ , kW

$Q_{ce}^{HE}$  = condenser heat duty in heat engine  $e$ , kW  
 $Q_{cm}^{HP}$  = condenser heat duty in heat pump  $m$ , kW  
 $Q_{in,e}^{HE}$  = heat entering heat engine  $e$  from hot utilities, kW  
 $Q_{in,n}$  = heat removed by heat engines and heat pumps in interval  $n$ , kW  
 $Q_{nj}^C$  = heat load of cold stream  $j$  in interval  $n$ , kW  
 $Q_{ni}^H$  = heat load of hot stream  $i$  in interval  $n$ , kW  
 $Q_{nl}^{CU}$  = heat load of cold utility  $l$  in interval  $n$ , kW  
 $Q_{ni}^{HU}$  = heat load of hot utility  $i$  in interval  $n$ , kW  
 $Q_{out,e}^{HE}$  = heat removed by cold utilities from heat engine  $e$ , kW  
 $Q_{out,m}^{HP}$  = heat removed by cold utilities from heat pump  $m$ , kW  
 $Q_{raw}$  = heat load of raw steam demand, kW  
 $R_n$  = residual heat from interval  $n$  to interval  $n + 1$ , kW  
 $T^{HU}$  = temperature of hot utility, K  
 $T_{in}$  = cooling water inlet temperature, K  
 $T_{max}$  = highest interval temperature bounding a negative hot deficit, K  
 $\Delta T_{min}$  = minimum approach temperature, K  
 $T_n$  = interval boundary temperature (smallest temp. in interval  $n$ ), K  
 $T_{out}$  = cooling water outlet temperature, K  
 $T_p$  = pinch temperature, K  
 $T_r$  = temperature at which refrigeration is needed, K  
 $T_s$  = stream supply temperature, K  
 $\Delta T_s$  = superheat, K  
 $T_i$  = stream target temperature, K  
 $T^{sat}$  = saturated temperature, K  
 $T_{2e}$  = boiler inlet temperature in heat engine  $e$ , K  
 $T_{3e}$  = boiler outlet temperature in heat engine  $e$ , K  
 $T_{4e}$  = condenser temperature in heat engine  $e$ , K

$T_{1m}$  = boiler outlet temperature in heat pump  $m$ , K  
 $T_{2m}$  = condenser inlet temperature in heat pump  $m$ , K  
 $T_{3m}$  = condenser outlet temperature in heat pump  $m$ , K  
 $T_{4m}$  = boiler inlet temperature in heat pump  $m$ , K  
 $U_n^C$  = cumulative cold deficit at interval  $n$ , kW  
 $U_n^H$  = cumulative hot deficit at interval  $n$ , kW  
 $W_{elec}$  = electrical work, kW  
 $W_{in}$  = pump work, kW; compression work, kW  
 $W_{in}^{HE}$  = pump work in heat engine  $e$ , kW  
 $W_{HP}^{in,m}$  = compression work in heat pump  $m$ , kW  
 $W_{net,e}^{HE}$  = net work produced by heat engine  $e$ , kW  
 $W_o$  = turbine work, kW  
 $W_{out,e}^{HE}$  = turbine work in heat engine  $e$ , kW  
 $W_{spec}$  = power demand for the process, kW  
 $X_{ne}$  = fraction of cumulative hot or cold deficit exchanged between heat engine  $e$  and interval  $n$   
 $Y_{nm}$  = fraction of cumulative hot or cold deficit exchanged between heat pump  $m$  and interval  $n$

## Subscripts

$e$  = heat engine counter  
 $i$  = hot stream counter  
 $j$  = cold stream counter  
 $k$  = hot utility counter; interval counter  
 $l$  = cold utility counter  
 $m$  = heat pump counter  
 $n$  = interval counter  
 $p$  = interval bounded from below by  $T_p$   
 $r$  = first interval in which refrigeration is required

## Superscripts

$C$  = cold stream  
 $CU$  = cold utility  
 $H$  = hot stream  
 $HU$  = hot utility  
 $HE$  = heat engine  
 $HP$  = heat pump  
 $+$  = saturated vapor  
 $-$  = saturated liquid

## Appendix

The equations for the cost of equipment were derived from the graphical data in Ulrich (1984). The installed cost of turbines as a function of the shaft work is given by

$$C_T = 173,495 (W_o)^{0.424} \quad (A1)$$

where  $W_o$  is in kilowatts.

The installed cost of pumps is correlated as a function of the inlet pressure (for the materials factor) and the shaft work

$$C_P = 3,120 [2 + 0.96 (P_{in})^{0.383}] (W_{in})^{0.368} \quad (A2)$$

where  $W_{in}$  is in kilowatts and  $P_{in}$  is in bar.

The installed cost of boilers is a function of the steam mass

flow rate,

$$C_B = 349,600 f_i f_p M^{0.82}$$

where

$$f_i = 1 - 6.1 \times 10^{-4} \Delta T_s + 1.3 \times 10^{-5} (\Delta T_s)^2$$

$$f_p = 1.0187 - 2.724 \times 10^{-3} P_b + 9.865 \times 10^{-5} (P_b)^2$$

and  $\Delta T_s = T - T^{sat}$  = superheat in K, and  $P_b$  is the boiler pressure in bar.

Finally, the installed cost of compressors as a function of the compression work is computed by

$$C_C = 1,925 (W_{in})^{0.963} \quad (A4)$$

where  $W_{in}$  is in kilowatts.

## Literature cited

- Colmenares, T. R., and W. D. Seider, "Synthesis of Cascaded Refrigeration Systems," *Proc. World Cong. III Chem. Eng.*, Tokyo (Sept., 1986).
- Linnhoff, B., and J. R. Flower, "Synthesis of Heat Exchanger Networks. I: Systematic Generation of Energy Optimal Networks," *AIChE J.*, **24**, 633 (1978).
- Linnhoff, B., and E. Hindmarsh, "The Pinch Design Method for Heat Exchanger Networks," *Chem. Eng. Sci.*, **38**, 745 (1983).
- Linnhoff, B., and J. A. Turner, "Heat Exchanger Network Design: New Insights Yield Big Savings," *Chem. Eng.*, **56**, (Nov., 1981).
- Linnhoff, B., D. W. Townsend, D. Boland, G. F. Hewitt, B. E. A. Thomas, A. R. Guy, and R. H. Marsland, *User Guide on Process Integration For the Efficient Use of Energy*, Inst. Chem. Eng. (England), dist. by Pergamon Press (1982).
- Murtagh, B., and M. Saunders, *MINOS 5.0 User's Guide*, Systems Optimization Lab., Stanford Univ. (1983).
- Papoulias, S., and I. Grossmann, "A Structural Optimization Approach in Process Synthesis—Utility Systems," *Comp. Chem. Eng.*, **7**, 695 (1983a).
- , "A Structural Optimization Approach in Process Synthesis—Heat Recovery Networks," *Comp. Chem. Eng.*, **7**, 707 (1983b).
- , "A Structural Optimization Approach in Process Synthesis—Total Processing Systems," *Comp. Chem. Eng.*, **7**, 723 (1983c).
- Petroulas, T., and G. V. Reklaitis, "Computer-Aided Synthesis and Design of Plant Utility Systems," *AIChE J.*, **30**, 69 (1984).
- Townsend, D. W., and B. Linnhoff, "Heat and Power Networks in Process Design. I: Criteria for Placement of Heat Engines and Heat Pumps in Process Networks," *AIChE J.*, **29**, 742 (1983a).
- , "II: Design Procedure for Equipment Selection and Process Matching," *AIChE J.*, **29**, 748 (1983b).
- Ulrich, G. D., *A Guide to Chemical Engineering Process Design and Economics*, 1st ed., Wiley, New York (1984).
- Umeda, T., J. Itoh, and K. Shiroko, "Heat Exchange System Synthesis," *Chem. Eng. Prog.*, **70** (July, 1978).

Manuscript received Aug. 25, 1986, and revision received Dec. 8, 1986.