Simultaneous Optimization and Heat Integration of Chemical Processes

A procedure is proposed for simultaneously handling the problem of optimal heat integration while performing the optimization of process flow sheets. The method is based on including a set of constraints into the nonlinear process optimization problem so as to insure that the minimum utility target for heat recovery networks is featured. These heat integration constraints, which do not require temperature intervals for their definition, are based on a proposed representation for locating pinch points that can vary according to every set of process stream conditions (flow rates and temperatures) selected in the optimization path. The underlying mathematical formulations correspond to nondifferentiable optimization problems, and an efficient smooth approximation method is proposed for their solution. An example problem on a chemical process is presented to illustrate the economic savings that can be obtained with the proposed simultaneous approach. The method reduces to simple models for the case of fixed flow rates and temperatures.

M. A. DURAN and I. E. GROSSMANN

Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213

SCOPE

The heat recovery network synthesis problem in process design has received considerable attention in the literature (Nishida et al., 1981). The most recent approaches include the pinch design method of Linnhoff and Hindmarsh (1983), the transportation formulation of Cerda et al. (1983), and the transshipment model of Papoulias and Grossmann (1983a). These methods decompose this synthesis problem into two successive stages: prediction of minimum utility cost, and derivation of a network structure that satisfies the minimum utility cost and involves the fewest number of heat exchange units. Since this strategy is aimed at the reduction of both operating and investment costs of the network, these methods tend to produce very good solutions. However, the definition of the synthesis problem for which these methods apply relies on the assumption that fixed values are given for the flow rates and temperatures of the process streams that are to be integrated in the network. Consequently, these methods for heat integration are sequential in the sense that they can be applied only after the process conditions have been determined.

In the optimization as well as in the synthesis of process flow sheets, the flow rates and temperatures of the process streams are in general unknown since they must be determined so as to define an optimal processing scheme. Since flow rates and temperatures have an important impact in the heat recovery network, the heat integration problem should be considered simultaneously with the optimization and synthesis problems. This would account explicitly for the interactions between the chemical process and the heat recovery network in order to establish proper trade-offs between capital investment, raw material utilization, and energy consumption. However, to make this simultaneous approach possible, the heat integration problem should be formulated so as to allow for variable flow rates and temperatures of the process streams.

Papoulias and Grossmann (1983b) have proposed to take into account the interactions between a chemical process and a heat recovery network by including the linear constraints of their transshipment model for heat integration within a mixed-integer linear formulation for the structural optimization of the chemical process. The actual network structure is derived in a second stage with information obtained from the solution of this optimization problem. An important limitation of this procedure is that while the flow rates of the streams can be treated as variables in the optimization, the temperatures can only assume discrete values in a prespecified set. This is due to the fact that the transshipment model requires fixed temperature intervals, and that the operating conditions that give rise to nonlinearities (e.g. pressures, temperatures) are discretized in order to obtain a mixed-integer linear model for the chemical process.

The objective of this paper is to present a procedure for solving nonlinear optimization and synthesis problems of chemical processes simultaneously with the minimum utility target for heat recovery networks. As will be shown, a set of constraints that are based on a pinch point location method can be formulated for embedding the minimum utility target within the process optimization. Since no temperature intervals are required in the proposed procedure, variable flow rates and temperatures of the process streams can be handled, and thus process nonlinearities can be treated explicitly. An example problem is presented to illustrate the large economic savings that can be obtained with this procedure.

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* Correspondence concerning this paper should be addressed to I. E. Grossmann.
M. A. Duran is presently at Universidad Autonoma Metropolitana-Iztapalapa, Mexico City.

CONCLUSIONS AND SIGNIFICANCE

This paper has presented a procedure for the simultaneous optimization and heat integration of process flow sheets that involve nonlinear models. It was shown that this objective can be accomplished by introducing a special set of constraints into the optimization problem so as to insure that the flow sheet will feature the minimum utility target for heat integration. The unique characteristic in this approach is that variable flow rates and temperatures of the streams can be handled within a nonlinear optimization framework. The procedure is straightforward to apply, and can be used in the optimization of fixed flow sheet structures, as well as in the simultaneous structural and parameter optimization methods for process synthesis. Also, the proposed procedure renders simple models for the standard heat integration case of fixed flow rates and temperatures.

Constraints were developed for the case in which only one heating and one cooling utility are available, as well as for the case of multiple utilities. As was shown, these constraints lead to structural nondifferentiabilities which can be handled efficiently with a proposed smooth approximation procedure. The results of the example problem showed that the proposed simultaneous approach is computationally efficient, and can produce considerable economic savings because of its capability of establishing proper trade-offs between capital investment, raw material utilization, and energy consumption in integrated chemical processes.

INTRODUCTION

This paper addresses the problem of simultaneously considering the minimum utility target for heat recovery networks (Hohmann, 1971; Linnhoff and Flower, 1978) within a nonlinear process optimization framework where temperatures and flow rates of the process streams are continuous variables to be selected by an optimization procedure. The main motivation behind this work lies in establishing proper economic trade-offs between capital investment, raw material utilization, and energy consumption in chemical processes.

Process optimization problems arise either in the determination of optimum sizes and operating conditions of a given flow sheet, or else in the simultaneous structural and parameter optimization approach for synthesizing process flow sheets. The former problem involves the solution of a nonlinear program (Biegler and Hughes, 1982; Stadtherr and Chen, 1984; Berna et al., 1980; Jirapongphan et al., 1980), whereas the latter problem involves the solution of a mixed-integer nonlinear program that is the model for a superstructure of alternative flow sheets (Duran and Grossmann, 1984; Duran, 1984). In either type of optimization problem, the objective function is typically economic in nature involving both investment and operating costs. The effect of the heat integration among process streams is reflected by the heating and cooling utility costs incurred in the heat recovery network.

As is well known, for specified flow rates and inlet and outlet temperatures of the process streams, a near-optimal solution of the heat recovery network synthesis problem features the following characteristics (Hohmann, 1971; Linnhoff and Flower, 1978):

1. Minimum utility consumption (cost).
2. Fewest number of heat exchange units.

For a given minimal temperature approach ΔT_m for heat exchange, the minimum utility requirements can be determined exactly and prior to determining the actual network structure. The minimum number of units also can be estimated a priori. The two objectives listed above impose targets that are to be achieved in the synthesis of heat recovery networks.

Since flow rates and temperatures of process streams are not known in advance in the optimization or synthesis of a chemical process, it becomes a nontrivial problem to account for the heat integration within these problems. The difficulty is that there exists a strong interaction between the chemical process and the heat recovery network (Papoulias and Grossmann, 1983b). This is because the flow rates and temperatures of the process streams affect both the economic performance of the process and the heat integration that can be achieved in the heat recovery network. Therefore the sequential procedure involving first the design of the nonintegrated plant, followed by the heat integration based on the flow rates and temperatures of the process streams that were determined, will in general not properly take into account the economic trade-offs between the process optimization and the heat integration. Hence, this sequential strategy is likely not to lead to the most economic and energy-efficient design for most cases.

In order to account for the interactions between the chemical process and the heat recovery network, ideally both should be optimized simultaneously. However, this rigorous approach would lead to a difficult combinatorial problem. Therefore, in order to simplify this problem, and based on the synthesis targets above, the strategy to be used will consist of optimizing the chemical process simultaneously with the minimum utility target for heat integration of the process streams. In this way the resulting design will exhibit flow rates and temperatures of the streams that guarantee maximum heat integration. The detailed heat recovery network structure could then be developed in a second stage as shown in Figure 1. This approach is similar to the one suggested by Papoulias and Grossmann (1983b) for their mixed-integer linear programming framework for process synthesis.

As will be shown, a set of constraints that are based on a pinch point location method can be formulated for embedding the minimum utility target in the simultaneous nonlinear optimization problem. These heat integration constraints, which allow the treatment of variable flow rates and temperatures as given by the process optimization path, do not require temperature intervals for their definition. The extension to the case in which multiple utilities are available is also presented. In order to handle the structural nondifferentiabilities that arise in the proposed formulations, a smooth approximation procedure is described that allows the use of standard nonlinear programming algorithms. An example problem on a chemical process is presented to illustrate the economic savings that can be obtained with the suggested approach for simultaneous optimization and heat integration.

PROBLEM STATEMENT

The problem addressed in this paper can be stated as follows:

Given is a process flowsheet or a superstructure of flow sheet alternatives that is to be optimized. The specified streams for which heat integration is intended in the process is given by a set of n_H hot process streams $i \in H$, which are to be cooled, and a set of n_C cold process streams $j \in C$, which are to be heated. The

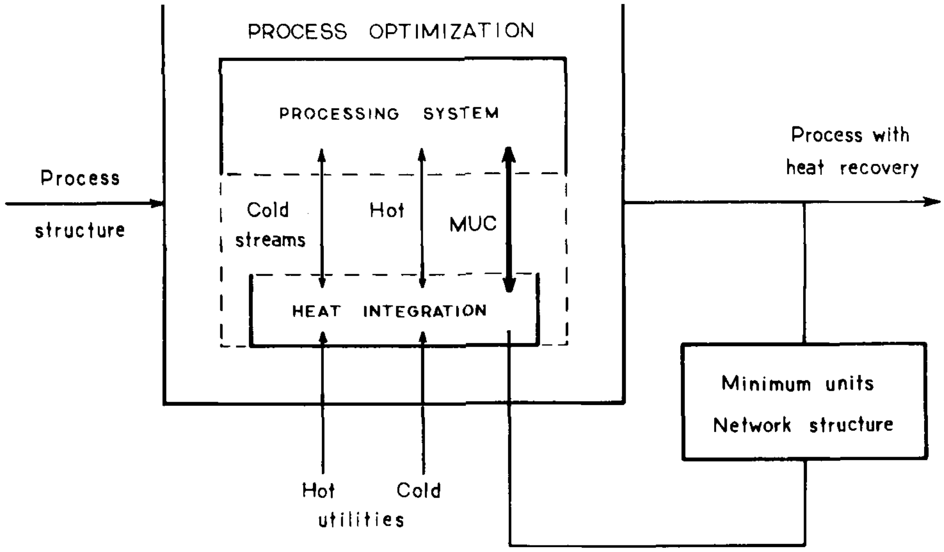

Figure 1. Heat integration in an optimization environment.

objective is to determine an optimal process flow sheet that features minimum utility consumption (cost) for these sets of streams. The flowrates and inlet and outlet temperatures of the hot streams ($F_i, T_i^{in}, T_i^{out}: i \in H$) and cold process streams ($f_j, t_j^{in}, t_j^{out}: j \in C$), must be determined optimally in the feasible space for process optimization and heat integration, given that a set of n_{HU} hot utilities $i \in HU$, and a set of n_{CU} cold utilities $j \in CU$ are available for supplying the heating and cooling requirements.

For the sake of simplicity in the presentation, it will be assumed that the heat capacities ($C_i: i \in H$) and ($c_j: j \in C$), of the hot and cold process streams are constant, and that these streams exhibit a finite difference between inlet and outlet temperatures. Also, fixed inlet temperature levels ($T_H^i: i \in HU$) and ($T_C^j: j \in CU$), are assumed for the hot and cold utilities. As will be discussed in the Remarks section, these assumptions can be relaxed in the proposed method either fully, or to a great extent.

The model for the optimization or synthesis of a chemical process without heat integration among process streams is assumed to be given in the form

$$
\begin{aligned}
\min \phi &= F(w,x) + \sum_{i \in HU} c_H^i Q_H^i + \sum_{j \in CU} c_C^j Q_C^j \\
\text{s.t.} \quad & h(w,x) = 0 \\
& g(w,x) \le 0 \qquad\qquad (P_o) \\
Q_H^i &= r_i^H(x),\ i \in HU \\
Q_C^j &= r_j^C(x),\ j \in CU \\
& Q_H^i, Q_C^j \in R_+^1: i \in HU, j \in CU \\
& w \in W \subset R_+^n,\ x \in X \subset R_+^m
\end{aligned}
$$

The vector of variables w represents process parameters such as pressures, temperatures, flow rates, equipment sizes, or also structural parameters (represented as $0-1$ binary variables) in the case of the synthesis of a processing scheme; the vector of variables $x = (F_i, T_i^{in}, T_i^{out}: \text{all } i \in H; f_j, t_j^{in}, t_j^{out}: \text{all } j \in C)$, represents the flow rates and temperatures of the process streams that are to undergo either cooling or else heating. The variables in w and x belong to the respective sets W and X, which are typically given by known lower and upper bounds (e.g., physical constraints, specifications), and also pure $0-1$ restrictions in the synthesis case. The vectors of constraints h, g, represent material and energy balances, design specifications, or also structural relationships for the synthesis problem. In a nonintegrated process flow sheet, all of the heating and cooling is supplied with utilities that have been preassigned to process streams so as to insure feasible heat exchange. The equations in P_o involving the expressions $r_i^H(x): i \in HU$ and $r_j^C(x): j \in CU$, represent the specific heat balances for calculating the heating and cooling utility requirements, $Q_H^i: i \in HU$ and $Q_C^j: j \in CU$, for the nonintegrated flow sheet.

The objective function ϕ is in general economic in nature involving both investment and operating costs in the term $F(w,x)$; the other terms correspond to the utility costs with $c_H^i: i \in HU$ and $c_C^j: j \in CU$, representing unit costs for the respective heating and cooling utilities.

For the case of an optimal design of a given process flow sheet, problem P_o corresponds to a nonlinear program, as then only continuous variables are involved in the vectors w and x. In the case of the optimal synthesis of a process flow sheet, some of the variables in w are associated with discrete decisions, and can only take $0-1$ values in the simultaneous structural and parameter optimization that defines problem P_o as a mixed-integer nonlinear program (Duran and Grossmann, 1984). The objective of this paper will be to show how the heat balance equations for a nonintegrated flow sheet can be replaced by a set of constraints that will insure that the process streams are heat integrated in the optimized flow sheet so as to feature the minimum utility target.

It should be noted that a simpleminded approach to incorporate the heat integration objective in the nonlinear optimization problem P_o, would be to replace the heat balance equations, involving the expressions r_i^H and r_j^C, by an implicit procedure that calculates the minimum utility target for the flow rates and temperatures determined at each iteration of the optimization. The implicit procedure could be any of the standard methods for fixed stream conditions (e.g., problem table, Linnhoff and Flower, 1978; transportation problem, Cerda et al., 1983; transshipment model, Papoulias and Grossmann, 1983a).

A major difficulty with this approach is that since the flow rates and temperatures will change at each iteration of the optimization, the temperature intervals required for predicting the utility target with these methods would have to be redefined at each iteration. Since this implies making discrete decisions, the implicit procedure would give rise to nondifferentiabilities, and hence cause numerical difficulties to standard nonlinear programming algorithms that rely on the differentiability assumption.

Therefore, what is required is a procedure for heat integration that does not require temperature intervals, which should preferably be expressed in explicit form, and in which, where possible, nondifferentiabilities should easily be identified so as to treat them through a suitable approximation procedure. This is precisely the motivation behind the pinch location method presented below.

PINCH POINT LOCATION METHOD

It will be assumed first that there is only one heating and one cooling utility available to satisfy the utility demands. Further, the inlet temperatures of the utilities are such that they cover the feasible temperature range of the process streams that are considered. The minimum utility consumption for process streams with fixed flow rates and temperatures can then be determined graphically as follows (Hohmann, 1971).

The supercooling curve (composite curve of all hot process streams) and the superheating curve (composite curve of all cold process streams) are plotted on a temperature (T) vs. enthalpy flow (H) diagram (see Figure 2). These curves are then brought together as close as possible via horizontal displacement, but without violating a minimum prespecified temperature driving force (ΔT_m) for heat exchange, as shown in Figure 2. The temperature pair (T^p, $T^p - \Delta T_m$) in the diagram, at which the minimum vertical separation ΔT_m occurs between the composite streams, corresponds to the pinch point T^p that limits the full heat integration. This pinch point separates the system into two parts: one requiring only heating (above pinch), the other requiring only cooling (below pinch). For constant heat capacities this pinch point can only occur at any of the inlet temperatures of the process streams. In Figure 2, inlet temperatures correspond to corner points at which a decrease in slope is present in the direction of the respective superstream. By identifying the pinch point(s), one can then readily determine the minimum heating (Q_H) and minimum cooling (Q_C) for heat integration in a system. These utility requirements correspond to the uncovered portions of the composite curves in Figure 2. The minimum heating utility requirement can be obtained algebraically by performing a heat balance above the pinch, whereas the minimum cooling utility requirement can be obtained by a heat balance below the pinch.

Clearly, there are cases when either only heating or only cooling utility is required for the heat integration (see Figure 3). In these cases no pinch point as defined above may occur with ΔT_m approach in the network. These cases are known as unpinched or threshold problems, and they are identified by the threshold temperature level (T_h, $T_h - \Delta T_h$), where $\Delta T_h > \Delta T_m$. The determination of utility requirements for threshold problems can still be treated within the framework described above. If only cooling is required, the composite curves will be aligned on the side of the highest inlet temperature of the hot streams (Figure 3a), and the heat balance below this temperature yields the cooling requirements. Similarily, if only heating is required, the lowest inlet temperature of the cold streams will define the side for alignment of the composite streams (Figure 3b), and heat balance above this temperature yields the heating requirements.

For convenience in this paper, pinch points will be denoted as those that may actually arise in pinched networks with ΔT_m approach temperature, or else as those associated with the highest and lowest temperatures that determine respectively cooling or heating requirements for unpinched networks. Note that under this definition pinch points will always be associated with inlet temperatures of the streams.

It is proposed to develop a mathematical formulation for predicting the minimum utility target for both pinched and non-

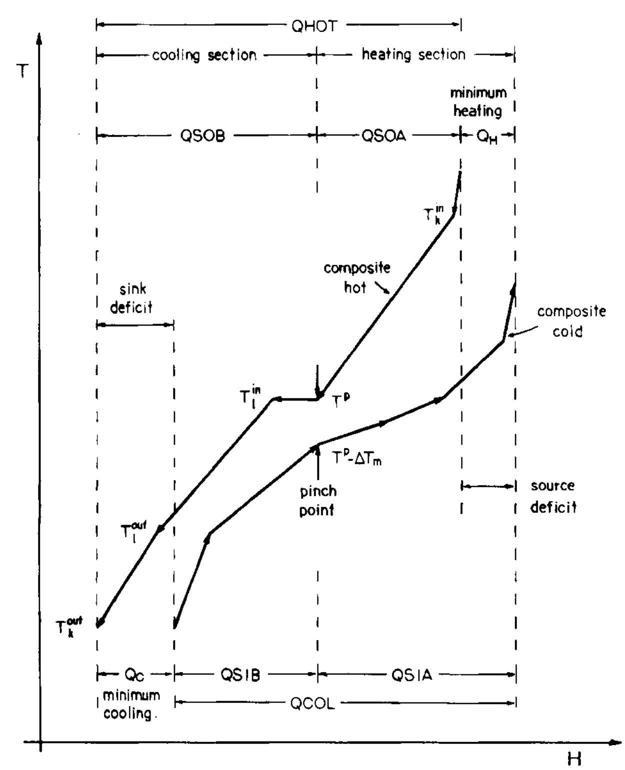

Figure 2. Graphic determination of MUC and definition of deficit functions.

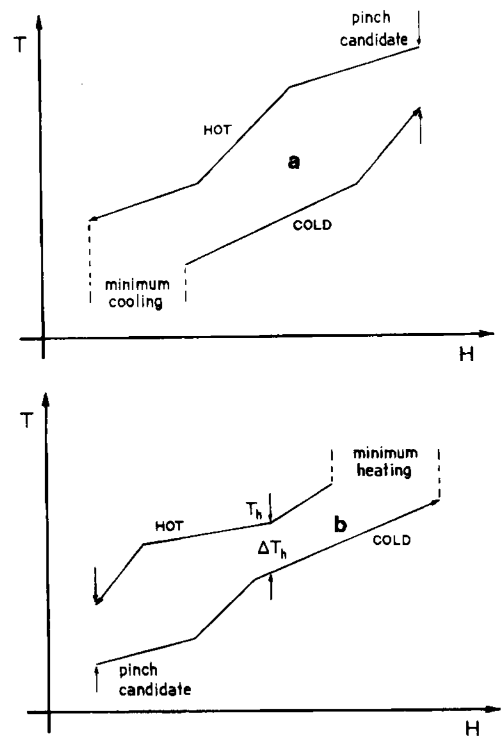

Figure 3. Nonpinched systems: a. only cooling requirements; b. only heating requirements.

pinched networks under conditions of variable flow rates and temperatures of the process streams. This formulation will be based on the above observation that for determining the minimum utility target it suffices to locate the pinch point(s) in the system, since then minimum heating and cooling requirements are given by heat balances above and below the pinch point(s), respectively. The basic idea will be to postulate a set of pinch point candidates that are associated with the inlet temperature of every hot and cold process stream. Heat integration constraints will then be developed for each of the postulated pinch points. As will be shown, these constraints allow identification of true pinch points as defined in this paper.

In order to gain some insight into the proposed pinch point location method for heat integration, it is useful to consider first the case of fixed stream conditions. Figure 4 shows the T vs. H diagrams that would be obtained when each of the four inlet temperatures in the well-known 4SP1 problem is regarded as a pinch point candidate p. When heat balances are performed above and below each pinch point candidate p, to determine the associated minimum heating Q_H^p and cooling Q_C^p requirements respectively, it is easily seen from Figure 4 that the following statements apply:

1. At a true pinch point (Figure 4a) the utility requirements (Q_H^p, Q_C^p) correspond to the actual minimum utility consumption (Q_H, Q_C) for feasible heat integration.
2. Every pinch point candidate not corresponding to a true pinch point (Figures 4b,c,d) leads to infeasible heat exchange due to violation of the ΔT_m constraint. Furthermore, the conjecture that this is a pinch point leads to lower than actual heating utility consumption above the pinch (i.e., $Q_H^p < Q_H$), and also lower cooling utility consumption below the pinch (i.e., $Q_C^p < Q_C$) — in some cases negative values.

Therefore, for fixed flow rates and temperatures, the minimum utility consumption (Q_H, Q_C) that is physically attainable in a network can be determined by locating those pinch points that feature the maximum of both minimum heating, Q_H^p, and minimum cooling, Q_C^p, requirements among all candidate pinch points p. This criterion insures feasible heat exchange and is formulated as

$$Q_H = \max_{p \in P} \{Q_H^p\}$$
$$Q_C = \max_{p \in P} \{Q_C^p\} \tag{1}$$

where $P = H \cup C$ is the index set of the process streams associated with the pinch point candidates. As will be shown in the next section, the statements in Eq. 1 can be expressed as explicit heat integration constraints which insure that the minimum utility target is satisfied.

Problem 4SP1

		FC_p [kW/°C]	T^{in}	T^{out} [°C]
2	H1	8.79	160	93
1	H2	10.55	249	138
4	C1	7.62	60	160
3	C2	6.08	116	260

pinch (249,239 °C)

Q_H=127.7 kW , Q_C=250.1 kW

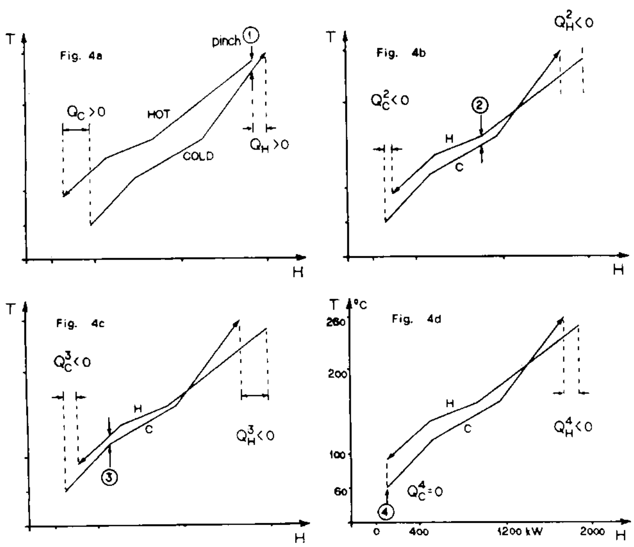

Figure 4. Problem 4SP1: MUC at different pinch point candidate assumption.

Constraints for Fixed Flow Rates and Temperatures

The statements in Eq. 1 underlying the proposed criterion for minimum utility target, can be formulated as a set of explicit constraints in terms of appropriate heat balances among process streams. In particular, since the composite hot stream is a source of heat and the cold is a sink, heating and cooling requirements for heat balance in the system can be interpreted respectively as the deficits in source and sink heat availabilities (see Figure 2).

In the context of the proposed pinch point location method, these source and sink deficits are clearly dependent on the particular pinch point $p \in P$ that is assumed, and they are functions of the process streams flow rates and temperatures, $x = [F_i, T_i^{in}, T_i^{out}: \text{all } i \in H; f_j, t_j^{in}, t_j^{out}: \text{all } j \in C]$. Although process stream conditions will first be considered fixed, the derivation of the equations will be presented in a parameterized manner for a transparent extension to the variable flow rates and temperatures case.

To evaluate the corresponding source and sink deficits, heating and cooling sections can be identified for each pinch point candidate $p \in P$, and the following associated terms for heat availability can be defined (see Figure 2):

- Source above the pinch, $QSOA(x)^p$, which accounts for the contributions of hot process streams to the available heat above the particular pinch candidate.
- Sink above the pinch, $QSIA(x)^p$, which accounts for the heat requirements above the assumed pinch in order for the cold streams to reach their outlet temperatures.
- Source below the pinch, $QSOB(x)^p$, representing the heat below the pinch that hot streams must transfer to reach their outlet temperatures.
- Sink below the pinch, $QSIB(x)^p$, which indicates the capacity of the cold streams to accept heat below the pinch.

Based on these heat availability terms, one can then define the following deficit functions for each pinch candidate $p \in P$:

$$z_H^p(x) = QSIA(x)^p - QSOA(x)^p \tag{2}$$

which corresponds to the heating deficit above the pinch; and

$$z_C^p(x) = QSOB(x)^p - QSIB(x)^p \tag{3}$$

which corresponds to the cooling deficit below the pinch. These heating and cooling deficits have to be satisfied using utilities. The minimum heating and cooling duties, Q_H^p, Q_C^p, for each assumed pinch $p \in P$, are then given by

$$Q_H^p = z_H^p(x) \tag{4}$$

$$Q_C^p = z_C^p(x) \tag{5}$$

This implies that the actual minimum heating, Q_H, and minimum cooling, Q_C, utility requirements as given by Eq. 1 can be expressed as

$$Q_H = \max_{p \in P} \{z_H^p(x)\} \tag{6}$$

$$Q_C = \max_{p \in P} \{z_C^p(x)\} \tag{7}$$

These minimum utility requirements must clearly satisfy a total heat balance that also involves the heat contents of the process streams for which heat integration is intended. That is,

$$\Omega(x) + Q_H - Q_C = 0 \tag{8}$$

where $\Omega(x) = QHOT(x) - QCOL(x)$, represents the difference between the total heat content of the hot and cold process streams (see Figure 2).

According to Eqs. 6 and 7, the actual minimum utility requirements will be determined by those pinch point candidate(s) $q \in P$ for which the maximum of the deficit functions is attained. It is known that for maximum heat recovery no heat transfer across the pinch must occur. Therefore, since the pinch separates the system into two independent parts that are in full heat balance, one of the equations among Eqs. 6, 7, and 8 is redundant. Thus, the problem of determining the minimum utility consumption can be formulated either in terms of Eqs. 6 and 7, or else in terms of any of these two equations together with Eq. 8. In this paper, for convenience, Eqs. 6 and 8 will be selected. That is, the equations that express the minimum utility consumption (MUC) target for fixed process streams flow rates and temperatures can be given by,

$$Q_H = \max_{p \in P} \{z_H^p(x)\} \tag{9}$$

$$Q_C = \Omega(x) + Q_H \tag{10}$$

It should be noted that when the process stream data x (flow rates and temperatures) are being regarded as fixed, the terms $z_H^p(x)$: all $p \in P$, and $\Omega(x)$ in Eqs. 9 and 10 are constants that can be computed a priori. Therefore, the heat integration problem of determining the minimum utility consumption for fixed stream conditions reduces to solving the simple algebraic system given by Eqs. 9 and 10 in the two unknowns Q_H and Q_C. Notice that the only decision involved in this procedure occurs in Eq. 9, where the selection of the heating deficit of largest value among all possible pinch candidates has to be made. Further, those heating deficit(s) $z_H^q(x)$, $q \in P$, for which this largest value is attained defines the location of the actual pinch point(s) q. A small example problem is presented in Appendix B to illustrate the application of this formulation.

As will be shown in the next section, Eqs. 9 and 10, which guarantee the minimum utility target for any set of fixed conditions x, can readily be extended to consider the case of variable flow rates and temperatures of the process streams, i.e., variable conditions x.

Constraints for Variable Flow Rates and Temperatures

In a process optimization problem, the flow rates, as well as the inlet and outlet temperatures of the process streams, are not known a priori since these are variables whose values will change throughout the optimization procedure. Equations 9 and 10, however, hold for any conditions x in the feasible region of the process optimization problem P_o. For the case of single heating and cooling utilities, problem P_o involves only Q_H and Q_C as utility duties and there are only two heat balance equations to define them. Thus, to guarantee the minimum utility target in a process optimization problem, all that it is required is to replace the heat balance equations involving Q_H and Q_C in problem P_o by Eqs. 9 and 10, which underlie the criterion for heat integration. This defines the following problem for the optimization of a flow sheet that will feature minimum utility consumption.

$$\begin{aligned} \min\ \phi &= F(w,x) + c_H Q_H + c_C Q_C \\ \text{s.t.}\quad & h(w,x) = 0 \\ & g(w,x) \le 0 \\ & Q_H = \max_{p \in P} \{z_H^p(x)\} \\ & Q_C = \Omega(x) + Q_H \\ & Q_H \ge 0,\ Q_C \ge 0 \\ & w \in W,\ x \in X \end{aligned} \tag{P_1}$$

where the equality constraint defining the minimum heating for each x is the maximum value among the series of heating deficit functions $z_H^p(x)$: all $p \in P$. These heating deficits and the term $\Omega(x)$ are obviously not constant, and their values change according to the optimization path followed for solving problem P_1. Therefore, to determine the value of these terms at every stream conditions point x, expressions with definite functionality must be derived that account for the appropriate heat contributions.

From Eq. 2, each heating deficit function $z_H^p(x)$, $p \in P$, involves two terms: $QSOA(x)^p$ that accounts for the heat content of the hot streams above the assumed pinch $p \in P$, and $QSIA(x)^p$ that accounts for the heating requirements of the cold streams above the same pinch temperature level. For an assumed pinch $p \in P$ with associated temperatures $(T^p, T^p - \Delta T_m)$, these terms are given by the following expressions involving functions in the flow rates and temperatures of the process streams:

$$QSOA(x)^p = \sum_{i \in H} F_i C_i [\max\{0, T_i^{in} - T^p\} - \max\{0, T_i^{out} - T^p\}] \tag{11}$$

$$QSIA(x)^p = \sum_{j \in C} f_j c_j [\max\{0, t_j^{out} - (T^p - \Delta T_m)\} - \max\{0, t_j^{in} - (T^p - \Delta T_m)\}] \tag{12}$$

The set of candidate pinch temperatures $T^p : p \in P$, in expressions 11 and 12 is given by the assignments

$$\{T^p = T_i^{in} : \text{all } p = i \in H;\ T^p = (t_j^{in} + \Delta T_m) : \text{all } p = j \in C\} \tag{13}$$

according to the assumption that pinch points can only occur at inlet temperatures of the process streams considered for heat integration. As inferred from Eq. 13, locations of potential pinch points change as stream conditions change.

It should be noted that the *max*{.} expressions in Eqs. 11 and 12 have the global effect of including only the relevant portion of the heat content of each process stream as contribution above the assumed pinch temperatures $(T^p, T^p - \Delta T_m)$ (see Figure 2). This is accomplished without the need to know in advance the relative location of inlet, outlet, and pinch temperatures, thus avoiding the definition of prespecified temperature intervals. As an illustration, consider in Eq. 11 the expression for taking into account the appropriate temperature difference associated with the heat contribution, above the assumed pinch temperature level, of a given hot stream k (see Figure 2):

$$[\max\{0, T_k^{in} - T^p\} - \max\{0, T_k^{out} - T^p\}] \tag{14}$$

This expression handles properly all of the possible cases, namely,

- The hot stream k is located entirely above the pinch candidate; this implies $T_k^{in} > T_k^{out} \ge T^p$, which reduces Eq. 14 to $[T_k^{in} - T_k^{out}]$ as the temperature difference associated with the heat contribution, i.e., all of the heat content.
- The hot stream k crosses the pinch; this implies $T_k^{in} > T^p > T_k^{out}$, which reduces Eq. 14 to $[T_k^{in} - T^p]$, i.e., only a fraction of total heat content.
- The hot stream k is located entirely below the pinch; this implies $T^p \ge T_k^{in} > T_k^{out}$, which reduces Eq. 14 to [0], i.e., no heat contribution.

Thus, the *max* expressions in Eq. 14 have the effect of including only the relevant temperature difference associated with the heat contribution of the hot stream k to the heat available above the assumed pinch point. Similarly, it can be verified that Eq.

12 includes only the appropriate portions of each cold stream as contributions to the heat required above the assumed pinch temperature level. The term $\Omega(x)$, which represents the process stream's part in the heat integration balance, can be expressed directly in terms of process streams conditions.

Since problem P_1 is a minimization problem, and the variables Q_H and Q_C appear in the objective function with positive cost coefficients, the pointwise maximum constraint in this problem can be expressed as an equivalent set of inequality constraints. The rigorous proof for this equivalence is presented in Appendix A. Qualitatively, Appendix A shows that for any feasible set of stream conditions x, for both pinched and unpinched problems, at least one of the heating deficit constraint inequalities $z_H^p(x) - Q_H \leq 0$: all $p \in P$, is active for the associated minimum utility requirements.

Thus, if the maximum constraint in problem P_1 is replaced by its equivalent set of heating deficit inequality constraints, an optimal integrated process flow sheet featuring minimum heating (Q_H) and minimum cooling (Q_C) requirements can then be determined by solving the following nonlinear program,

$$\begin{aligned} \min \phi &= F(w,x) + c_H Q_H + c_C Q_C \\ \text{s.t.} \quad & h(w,x) = 0 \\ & g(w,x) \leq 0 \\ & z_H^p(x) - Q_H \leq 0\} \quad \text{all } p \in P \\ & \Omega(x) + Q_H - Q_C = 0 \\ & Q_H \geq 0,\ Q_C \geq 0 \\ & w \in W,\ x \in X \end{aligned} \qquad (P_2)$$

where $\Omega(x)$ and $z_H^p(x) : p \in P$, are given respectively by the explicit expressions

$$\Omega(x) = \sum_{i \in H} F_i C_i (T_i^{in} - T_i^{out}) - \sum_{j \in C} f_j c_j (t_j^{out} - t_j^{in}) \qquad (15)$$

$$\begin{aligned} z_H^p(x) = & \sum_{j \in C} f_j c_j [\max\{0,\ t_j^{out} - (T^p - \Delta T_m)\} \\ & - \max\{0,\ t_j^{in} - (T^p - \Delta T_m)\}] \\ & - \sum_{i \in H} F_i C_i [\max\{0,\ T_i^{in} - T^p\} \\ & - \max\{0,\ T_i^{out} - T^p\}] \end{aligned} \qquad (16)$$

and the heating deficits $z_H^p(x)$: all $p \in P$, $P = H \cup C$, are dependent on the set of pinch point candidates

$$\{T^p = T_i^{in} : \text{all } p = i \in H;\ T^p = (t_j^{in} + \Delta T_m) : \text{all } p = j \in C\}$$

Problem P_2 allows then the simultaneous optimization and heat integration of chemical processing systems. The solution to this problem will be a process featuring the optimal minimum utility consumption (Q_H, Q_C).

Note that incorporation of the minimum utility target into the process flow sheet optimization framework does not introduce any additional variables for the definition of problem P_2. It only introduces the $[n_H + n_C + 1]$ heating deficit inequality constraints for heat integration in place of the heat balances in P_0 to determine the utility requirements for the nonintegrated process. However, the price one has to pay is that one has to deal with the structural nondifferentiabilities (see Figure 6) inherent to the functions *max*{.} involved in the expression in Eq. 16 that defines the heating deficit functions $z_H^p(x)$: all $p \in P$. These nondifferentiabilities are potentially many and arise for instance when $T_i^{in} = T^p$ or when $t_j^{out} = (T^p - \Delta T_m)$. Thus, the nonlinear program one has to solve for the simultaneous process optimization and heat integration corresponds to a nondifferentiable optimization problem. Before addressing issues related to the solution of such a problem, it is worth considering first the extension of problem P_2 to the case in which multiple utilities are available to satisfy the minimum utility requirements for a process.

MULTIPLE UTILITIES

The proposed pinch point location method is not necessarily restricted to a single heating and a single cooling utility, but can be extended to the case when several hot and cold utilities are available, e.g., fuel, hot gases, steam at various pressures, cooling water, refrigerants. For the case of multiple utilities, a selection among them has to be made for their feasible and economic use to satisfy the utility demands. In Figure 5 a graphic representation is given of the composite hot and cold curves for heat integration when both process streams and multiple utilities are considered. From this figure it is clear that pinch points may also arise due to the presence of utilities whose inlet temperatures fall within the temperature range of the process streams. Therefore, additional deficit constraints must be included in the pinch point location model to insure feasible heat exchange for these "intermediate" utilities whenever they are selected. For the sake of simplicity in the presentation, it will be assumed that neither prespecified nor optimally determined outlet temperatures are to be considered for utilities acting over a temperature range. This assumption allows the utilities to be represented as variables associated with heat loads rather than as explicit enthalpy expressions (i.e., flow rates, temperatures). Within this framework, suitable flow rate selection will allow outlet temperatures for utilities to be determined in a second stage based on feasibility and/or economic considerations. The Remarks section discusses the relaxation of the above assumption.

To make more transparent the transition between the single and the multiple utilities cases, consider first the case of fixed flow rates and temperatures for the process streams, i.e., fixed variables x. The heat loads of the different hot and cold utilities are represented by the variables $u = \{Q_H^i : i \in HU,\ Q_C^j : j \in CU\}$,

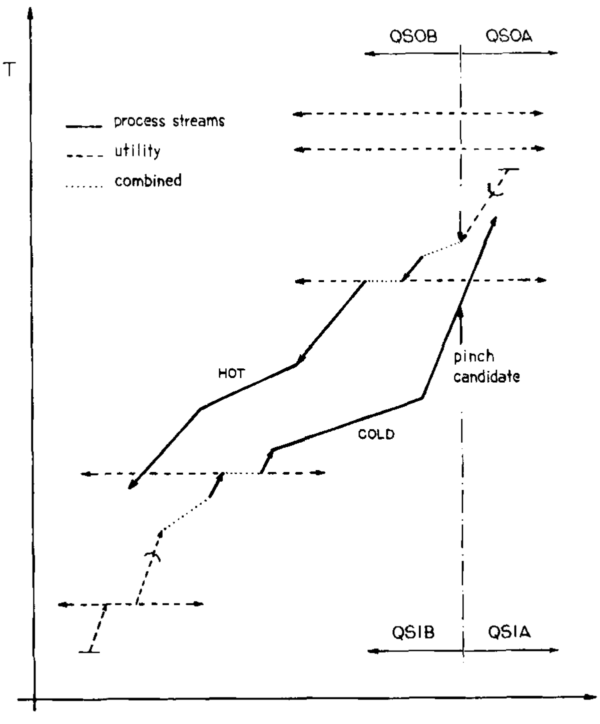

Figure 5. Generalized (process + utility streams) composite curves.

where HU and CU are the respective hot and cold utilities index sets. For given sets of utilities, the hot utility $h \in HU$ with highest inlet temperature, and the cold utility $c \in CU$ with lowest inlet temperature, can be identified such that they bound the entire feasible range of temperatures for heat integration. These utilities can be regarded as the hot and cold utilities in the single utility case discussed previously, but now as applied to the composite hot and cold curves of Figure 5. The remaining utilities can therefore potentially lead to pinch points. These sets of intermediate hot and cold utilities will be denoted by the sets $HU' = HU \backslash \{h\}$ and $CU' = CU \backslash \{c\}$, respectively.

According to the proposed pinch point location method, the inlet temperatures of both intermediate utilities and the process streams will then define the candidates for pinch points in the multiple utility case. Furthermore, the criterion to guarantee the minimum utility target (Eq. 6) holds naturally for the *multiple* utilities case if heating deficit constraints are also derived for pinch points associated with intermediate utilities. The criterion for multiple utilities, however, involves degrees of freedom since more than single utilities are considered. Hence, the utilities have to be considered individually, as in general there is no unique feasible assignment. Thus, expressing the corresponding pointwise maximum constraint of Eq. 6 in terms of its equivalent set of heating deficit inequality constraints, one can easily show that for fixed process stream conditions (i.e., fixed x), incorporation of the minimum utility target in the presence of multiple utilities yields the following optimization program for the standard minimum utility cost problem,

$$\begin{aligned} \min \; & \sum_{i \in HU} c_H^i Q_H^i + \sum_{j \in CU} c_C^j Q_C^j \\ \text{s.t.} \; & z_H^p(x,u) - Q_H^h \le 0 \} \quad \text{all } p \in P' \qquad (P_3) \\ & \Omega(x,u) + Q_H^h - Q_C^c = 0 \\ & u = \{Q_H^i : i \in HU, Q_C^j : j \in CU\} \in R_+^{m_U} \end{aligned}$$

where $m_U = [n_{HU} + n_{CU}]$, and $\{Q_H^h, h \in HU; Q_C^c, c \in CU\} \in u$. In this case the streams index set P' of candidate pinch points is given by $P' = H \cup C \cup HU' \cup CU'$, that is by both all of the process streams and all of the intermediate utilities. For fixed $x = [F_i, T_i^{\text{in}}, T_i^{\text{out}} : \text{all } i \in H; f_j, t_j^{\text{in}}, t_j^{\text{out}} : \text{all } j \in C]$, the process streams parts of the terms $\Omega(x,u)$ and $z_H^p(x,u)$ in problem P_3 are *clearly constant* and identical to expressions 15 and 16. The general expression for $\Omega(x,u)$ can then be obtained from Eq. 15 by also considering the utility heat loads, that is,

$$\Omega(x,u) = \sum_{i \in H} F_i C_i (T_i^{\text{in}} - T_i^{\text{out}}) - \sum_{j \in C} f_j c_j (t_j^{\text{out}} - t_j^{\text{in}}) + \sum_{i \in HU'} Q_H^i - \sum_{j \in CU'} Q_C^j \qquad (17)$$

The heating deficit functions $z_H^p(x,u)$: all $p \in P'$, are defined similarly, as in Eq. 2, by

$$z_H^p(x,u) = QSIA(x,u)^p - QSOA(x,u)^p \qquad (18)$$

The expressions for the heat availability terms in Eq. 18 are straightforward extensions of those in Eqs. 11 and 12, and can be obtained by simply including terms to account for the heat contributions of the intermediate utilities. Recall that outlet temperatures for utilities are assumed to be neither specified nor variables to be determined. Therefore, since pinch locations change along the optimization, to allocate utility heat contributions to the heat contents in the appropriate side of a given pinch point candidate, it will be assumed that utility streams undergo a fictitious finite temperature change. This temperature change is somewhat arbitrary (see the Remarks section), and for simplicity in the presentation is assumed to be 1 K. Hence, the general form for the heat availability terms in Eq. 18 can be expressed by extending Eqs. 11 and 12 to yield,

$$\begin{aligned} QSOA(x,u)^p = & \sum_{i \in H} F_i C_i [\max\{0, T_i^{\text{in}} - T^p\} - \max\{0, T_i^{\text{out}} - T^p\}] \\ & + \sum_{i \in HU'} Q_H^i [\max\{0, T_H^i - T^p\} - \max\{0, T_H^i - 1 - T^p\}] \qquad (19) \end{aligned}$$

$$\begin{aligned} QSIA(x,u)^p = & \sum_{j \in C} f_j c_j [\max\{0, t_j^{\text{out}} - (T^p - \Delta T_m)\} - \max\{0, t_j^{\text{in}} - (T^p - \Delta T_m)\}] \\ & + \sum_{j \in CU'} Q_C^j [\max\{0, T_C^j + 1 - (T^p - \Delta T_m)\} - \max\{0, T_C^j - (T^p - \Delta T_m)\}] \qquad (20) \end{aligned}$$

where the candidate pinch temperatures are given by

$$\begin{aligned} \{T^p = T_i^{\text{in}} : p = i \in H, \; T^p = T_H^i : p = i \in HU', \\ T^p = (t_j^{\text{in}} + \Delta T_m) : p = j \in C, \\ T^p = (T_C^j + \Delta T_m) : p = j \in CU'\} \qquad (21) \end{aligned}$$

Since utility temperatures are given, it is clear that for fixed process stream conditions (i.e., fixed x) the terms defining $\Omega(x,u)$ and $z_H^p(x,u)$: all $p \in P'$, in problem P_3 are either constants, or else involve the variables $\{Q_H^i : i \in HU', Q_C^j : j \in CU'\} \in u$, acting in a linear manner. Thus, for fixed stream data x, the problem of determining the minimum utility cost in the presence of multiple utilities corresponds to the linear programming program P_3. This program involves $[n_{HU} + n_{CU}]$ variables and $[n_H + n_{HU} + n_C + n_{CU} - 1]$ constraints. Appendix B presents a small example problem to illustrate the formulation P_3.

For the case of variable flow rates and temperatures of the streams, the functions $z_H^p(x,u)$: all $p \in P'$ and $\Omega(x,u)$ defined above are neither linear nor parameterized expressions. However, they apply for any set of process conditions and are suitable to be embedded in an optimization *framework*. Thus, replacing the utility heat balances in program P_0 by the constraints in problem P_3, yields the following nonlinear program as the model for the case when the minimum utility cost target is to be considered simultaneously in the process optimization problem P_0:

$$\begin{aligned} \min \phi = & F(w,x) + \sum_{i \in HU} c_H^i Q_H^i + \sum_{j \in CU} c_C^j Q_C^j \\ \text{s.t.} \; & h(w,x) = 0 \\ & g(w,x) \le 0 \qquad (P_4) \\ & z_H^p(x,u) - Q_H^h \le 0 \} \quad \text{all } p \in P' \\ & \Omega(x,u) + Q_H^h - Q_C^c = 0 \\ & u = \{Q_H^i : i \in HU, Q_C^j : j \in CU\} \in R_+^{m_U} \\ & w \in W, x \in X \end{aligned}$$

where $z_H^p(x,u)$: all $p \in P'$, and $\Omega(x,u)$ are given by Eqs. 18, 19, 20, and 17. An optimal solution to problem P_4 will then determine an economic process flow sheet that will feature optimal heat integration in the presence of multiple utilities. Note that as in the case of problem P_2, structural nondifferentiabilities arise in problem P_4 due to the *max* functions in the expressions that define the heating deficits. The next section presents a procedure to handle this particular class of nondifferentiabilities. This procedure will allow the use of standard nonlinear programming algorithms for the solution of problems P_2 and P_4.

NONDIFFERENTIABLE OPTIMIZATION: SMOOTH APPROXIMATION

The nonlinear programming programs P_2 and P_4, which have been proposed for the simultaneous optimization and heat in-

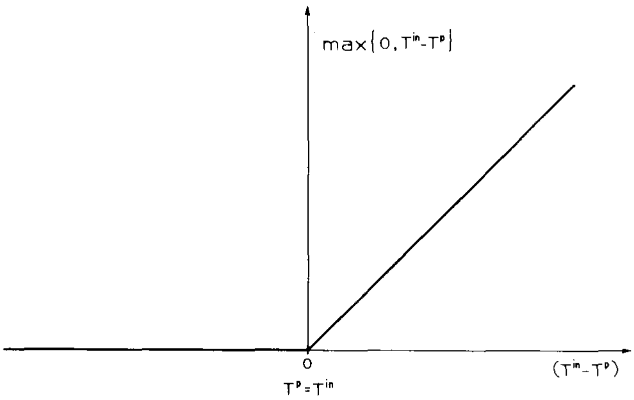

Figure 6. Kink: noncontinuously differentiable function.

tegration of chemical processes, correspond to nondifferentiable optimization problems; hence the following considerations must be taken into account for their solution. First, efficient algorithms for nonlinear programming (NLP) require in general derivative information, or at least rely on the differentiability assumption. Second, the optimal solutions to problems P_2 and P_4 are likely to occur at nondifferentiable points. This is because, as shown in Appendix A, at the optimum at least one deficit constraint will be active, and that corresponds to the condition that at least one of the equalities $T^p = T_i^{in}$ or $T^p = (t_j^{in} + \Delta T_m)$ will hold. At points like these, which define pinch points, single *max*{.} functions in Eq. 16 or in Eqs. 19 and 20 have a value of zero and the derivative is not continuous, as shown in Figure 6. If a standard NLP algorithm were to be used for the solution, these discontinuities on the gradients could cause convergence to a nonoptimum point due to jamming, or numerical failures could happen. Therefore, it is clear that special provisions must be made to handle nondifferentiabilities of the special class arising in functions of the general form: $\max\{0, f(x)\}$.

It should be pointed out that a number of special-purpose algorithms have been proposed for nondifferentiable optimization (Balinski and Wolfe, 1975; Fletcher, 1982). However, some of these methods either are applicable only to special classes of problems, or otherwise they may have very slow convergence properties. Therefore, to handle the nondifferentiabilities in problems P_2 and P_4, a recent approximation procedure proposed by Duran and Grossmann (1985) will be used. This method is based on obtaining continuity of the derivative by replacing the structural nondifferentiabilities with a suitable

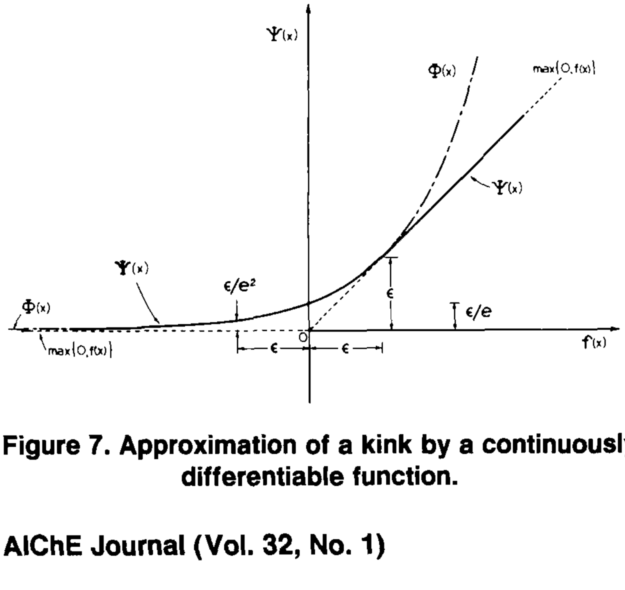

Figure 7. Approximation of a kink by a continuously differentiable function.

smooth approximation function. The simple general function $\max\{0, f(x)\}$, which arises in the proposed models, is commonly called a kink, and has the graph shown in Figures 6 and 7. Even when $f(x)$ is continuously differentiable, it is clear that the derivative of a kink is not continuous at $f(x) = 0$. Since this type of source of nondifferentiability is due to the form of the function and can be identified readily, it is denoted as structural.

The basic idea in the approach by Duran and Grossmann consists of replacing each kink, $\max\{0, f(x)\}$, by an approximation function $\Psi(x)$ that is everywhere continuously differentiable. Assuming that $f(x)$ is continuously differentiable, the only nondifferentiability of the kink arises at $f(x) = 0$. To eliminate this discontinuity on the derivative, a smooth function $\Phi(x)$ can be determined to approximate the kink for values of $f(x)$ in an ϵ-neighborhood around $f(x) = 0$ (see Figure 7). For $\Phi(x)$ to be a suitable approximation function, it must satisfy the two following conditions for a sufficiently small $\epsilon > 0$:

$$\text{i) At } f(x) = \epsilon : \Phi(x) = f(x) \quad \text{and} \quad \frac{d\Phi(x)}{dx} = \frac{df(x)}{dx}$$

$$\text{ii) For } f(x) \le \epsilon : \Phi(x) \ge 0 \quad \text{and} \quad \frac{d\Phi(x)}{dx} \to 0 \quad \text{as} \quad \Phi(x) \to 0$$

The first condition insures continuity of both function and derivative at $f(x) = \epsilon$, while the second condition insures that the smooth function $\Phi(x)$ follows closely both the value and the derivative of the kink, so as to have small approximation error for $f(x) \le \epsilon$. A convenient choice for the smooth function $\Phi(x)$ is the exponential function $\Phi(x) = \beta \exp\{f(x)/\epsilon\}$, where $\beta = \epsilon/\exp(1)$ (Figure 7). This function can then be used to define a function $\Psi(x)$ that is continuously differentiable everywhere, and that approximates the kink $\max\{0, f(x)\}$ according to (Figure 7):

$$\Psi(x) = \begin{Bmatrix} f(x), & \text{if } f(x) \ge \epsilon, \dfrac{df(x)}{dx} \\ \Phi(x) = \beta \exp\{f(x)/\epsilon\}, & \text{otherwise}, \dfrac{\Phi(x)}{\epsilon}\dfrac{df(x)}{dx} \end{Bmatrix} = \frac{d\Psi(x)}{dx} \tag{22}$$

Good approximation to a kink can be obtained typically with values of ϵ in the range $0.0001 \le \epsilon \le 0.01$. Also, the approximation error at any point can be determined readily, and the maximum error with Eq. 22, which occurs at $f(x) = 0$, is given by $\beta = \epsilon/\exp(1)$. Clearly, no significant errors occur with the suggested values of ϵ above. Therefore, by replacing each kink function in Eqs. 16, 19, and 20 with the information of the continuously differentiable function $\Psi(x)$, the solution to problems P_2 and P_4 can then be obtained using standard nonlinear programming algorithms.

REMARKS

As for the assumptions and limitations of the proposed method, the following remarks can be made. First, the assumption of a finite difference temperature between inlet and outlet temperatures for process streams can be fully relaxed. That is, single-component streams condensing or vaporizing, and therefore present at a single source point temperature ($T^{in} = T^{out}$), can also readily be handled. The heat capacity flow rates (FCp) for such streams correspond to heat contents, and expressions similar to the ones for the utilities, in Eqs. 19 and 20, can be derived to allocate the corresponding heat contributions to the heat content in the proper side of a given pinch point candidate.

The assumption of constant heat capacities (Cp) can be relaxed to a great extent by supplying enthalpy information. One way of treating general correlations for enthalpy is by defining equivalent heat capacity flow rates (FCp_e) as follows. For streams with finite inlet and outlet temperature difference, ΔT, [$\Delta T = T_i^{in} - T_i^{out} : i \in H$ or $\Delta T = t_j^{out} - t_j^{in} : j \in C$], the equivalent heat capacity flow rate can be defined as

$$FCp_e = \frac{F\,\Delta H}{\Delta T} \tag{23}$$

where ΔH is the enthalpy difference between the two temperature states as predicted by any correlation. For streams condensing or vaporizing at a constant temperature, the FCp_e can be defined as

$$\begin{aligned} FCp_e &= F\,\Delta H_{vap} \\ FCp_e &= F\,\Delta H_{cond} \end{aligned} \tag{24}$$

where ΔH_{vap}, ΔH_{cond}, are the heats of vaporization and condensation. For multicomponent streams undergoing both phase and sensible heat changes, the heat content can be partitioned as given by a set of streams with equivalent heat capacity flow rates according to the several stages.

Note that defining the FCp_e as in Eqs. 23 and 24 does not require additional constraints in the proposed formulations, and they can readily be accommodated in the expressions for the heating deficits and heat balances. It should be pointed out that general correlations for enthalpy could be considered explicitly in the proposed method by simply defining the models in terms of specific enthalpies rather than in terms of temperatures. However, it is clear that this could lead to complex expressions.

The limitation there is in dealing with arbitrary nonlinear correlations for enthalpy in any manner, is that pinch points may not necessarily correspond to the inlet temperatures of the process streams (see Figure 8). At present there does not seem to be a simple procedure to handle pinch point candidates different from the inlet temperatures, except by linear piecewise approximation of the enthalpy curves for process streams.

The fictitious 1 K temperature change assumed in Eqs. 19 and 20 was adopted for convenience, but actually is rather arbitrary as far as the coefficients for the heat capacity flow rates are adjusted to reflect the scale of the finite temperature difference assumed. This applies to the handling of intermediate utilities when only inlet temperatures are specified, and the handling of single temperature point process streams and streams represented by Eq. 24. The only limitation on the assumed temperature change is that it must be smaller than the smallest temperature difference expected between inlet temperatures for the streams.

With respect to outlet temperatures for the utilities [$T_H^{i,out} : i \in HU'$, $T_C^{j,out} : j \in CU'$], whenever they are specified, and also are to be different from the given inlet temperatures [$T_H^{i,in} : i \in HU'$, $T_C^{j,in} : j \in CU'$], they can still be accommodated within the formulations P_3 and P_4 in terms of only utility duties. In this case, feasible heat exchange can be insured by defining appropriate coefficients for the utility duties so as to take into account only the feasible portions with respect to an assumed pinch point candidate. This can be accomplished with the following coefficients for the utility duties in Eqs. 19 and 20,

$$\begin{aligned} &[T_H^{i,in} - \max\{T^p, T_H^{i,out}\}]/(T_H^{i,in} - T_H^{i,out}),\ i \in HU' \\ &[\min\{T^p - \Delta T_m, T_C^{j,out}\} - T_C^{j,in}]/(T_C^{j,out} - T_C^{j,in}),\ j \in CU' \end{aligned} \tag{25}$$

where T^p is the only variable for nonfixed process stream conditions. An alternative representation to consider specified utility outlet temperatures would be to formulate the expressions in Eqs. 19 and 20 for the utilities in terms of temperatures and flow rates as for the process streams. Utility flow rates would then be variables to be determined in problems P_3 and P_4. For the case when optimal outlet temperatures have to be determined, problem P_4 would also involve them as variables subject to given upper bounds.

Finally, one limitation of the proposed procedure is that since the structure of the heat recovery network is not known, the cost of the actual heat exchangers cannot be included as part of the simultaneous optimization and heat integration. A model to consider the network configuration would involve discrete decisions and would correspond to a complex mixed-integer nonlinear program. At present, to account in the optimization for the investment cost of heat exchangers, a unit cost for total heat exchanged is considered. However, note that a way to partly circumvent this problem is by solving the simultaneous optimization problem for different values of the temperature approach ΔT_m. In this way the network structures could be developed for each ΔT_m value to size and cost the exchangers. The investment cost of the exchangers could then be added the optimal objective function value so as to select the ΔT_m solution with minimum total cost.

EXAMPLE

To illustrate the application of the proposed procedure for simultaneous optimization and heat integration, the flow sheet shown in Figure 9 is considered. The feed consists of the three

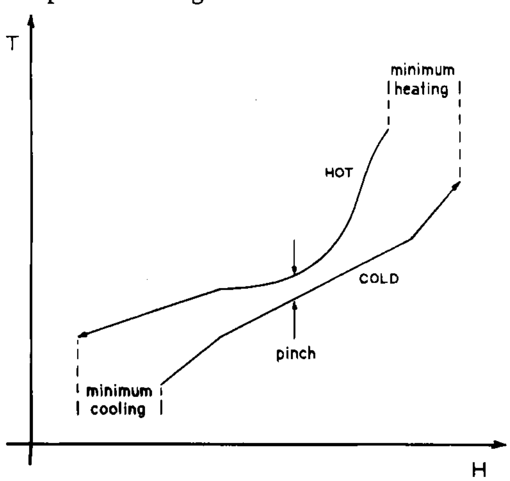

Figure 8. Pinch points due to curvature of enthalpy curve.

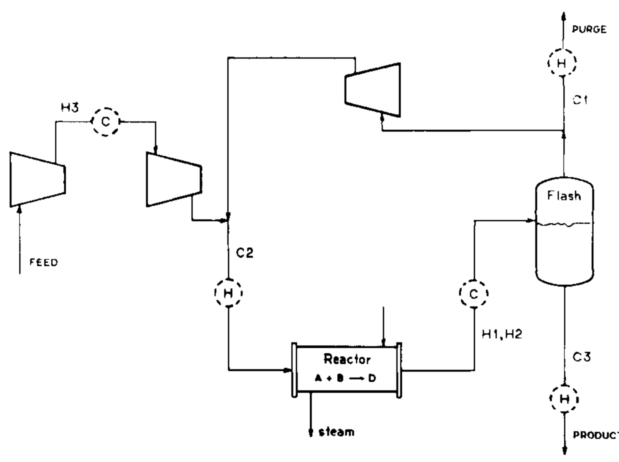

Figure 9. Example: simultaneous process optimization and heat integration.

components A, B, and C, where C is an inert component. The pressure of the feed is raised with a two-stage centrifugal compressor with intermediate cooling. The feed is mixed with the recycle, and the resulting stream is then preheated at the inlet of the reactor where components A and B react to produce product D. Since the reaction is exothermic, steam is raised with the heat released by the reaction. Depending on the conditions and amount of generated steam, the operation of the reactor could be anywhere in the range from adiabatic to isothermal. The effluent of the reactor is cooled and sent to a flash unit where most of the product is recovered in the liquid stream. This stream is heated so as to deliver the required product as saturated vapor. A fraction of the vapor stream from the flash unit is recompressed for recycle to the reactor. The remaining of the vapor stream is purged to avoid the accumulation of the inert C in the recycle. This purge stream is heated so as to deliver it at a fixed temperature value.

The basic process specifications, data, unit operating costs, investment cost expressions, particular models, and main constraints in the process are given in Table 1. The reactor has been modeled with a simple nonlinear correlation in which the reactor volume increases with higher conversion per pass, inlet temperature, and inert concentration; it decreases with higher pressure. The phase equilibrium in the flash is predicted with ideal model, while isentropic compression corrected by efficiency factors is assumed for the compressors. Constant heat capacities were assumed for the process streams.

TABLE 1. SPECIFICATIONS FOR EXAMPLE PROBLEM IN FIGURE 9

Design basis	Cost
Working time: 8,376 h/yr	
Payout time factor: 0.3/yr	
Product: 0.36169 kmol/s (1,000 metric ton/d) of saturated vapor with 98 mol % D	\$3.81/kmol
Feedstock: gas at 2 atm and 310 K with composition: 45% A, 50% B, 5% C (inert), and 0% D	\$0.75/kmol
Purge: gas at 670 K	\$0.55/kmol
Generated steam	\$1.8537 × 10^{-5}/kJ
Utilities	
Cooling water: 294.2 K supply temperature, 322.0 K max return temperature	\$2.4642 × 10^{-6}/kJ
Heating: fuel at 700 K	\$5.5613 × 10^{-5}/kJ
Purchased electric power	\$0.025/kWhr
Demineralized water	\$2.3400 × 10^{-3}/kmol
Compressors: isentropic and adiabatic. $\gamma = 1.4$, efficiencies: $\eta_m = 0.9$, $\eta_c = 0.8$	\$4,685.04 $(HP)^{0.796}$
Heat exchanged: $\Delta T_m = 15$ K	\$53.9075/kW
Reactor: exothermic reaction: $A + B \rightarrow D$ operation: from adiabatic to isothermal. conversion x (%): (T, P at inlet conditions)	\$27,015$(V)^{0.41}(P)^{0.31}$

$$x = 50 \exp(-0.002T)\left[\frac{V}{V+10}\right] P[y_A y_B/(1 + y_C + y_D)]$$

Flash: isothermal, equilibrium: ideal model	\$19.11 $(\mu)^{0.66}(P)^{0.79}$

Antoine constants (P: mm Hg)

Comp.	a	b	c
A	13.6333	164.90	3.19
B	14.3686	530.22	−13.15
C	15.2243	897.84	−7.16
D	18.5875	3626.55	−34.29

T(K), P(atm), V(m^3), μ(gmol/s), HP(kW), y_i: mol fraction

Constraints

Reactor	Other
$T_{outlet} \geq T_{inlet}$	$320 \text{ K} \leq T_{flash} \leq 380$ K
$T_{outlet} \leq 690$ K	$0 \leq$ purge $\leq 100\%$
$450 \text{ K} \leq T_{inlet} \leq 670$ K	product $D \geq$ product × (0.98)
5 m^3 ≤ volume ≤ 80 m^3	
9 atm ≤ pressure ≤ 29 atm	
$0 \leq x \leq 100\%$	

SI conversions: kPa = mm Hg × 0.133; kPa = atm × 101.325.

The flow sheet in Figure 9 involves three process streams requiring cooling and three streams requiring heating. The effluent of the reactor has been partitioned into two hot streams: $H1$ represents the cooling of the effluent to the dew point, while $H2$ represents the cooling from the dew point to the flash temperature. Hot stream $H3$ is associated with the intercooler between the two stages of the feed compressor. Cold stream $C2$ represents the preheat to the reactor, while streams $C1$ and $C3$ correspond to the heating of the purge and the product, respectively. Only one heating utility (fuel at 700 K) and one cooling utility (cooling water at 294.2 K) have been assumed for this problem. The minimum temperature approach ΔT_m selected was 15 K.

The optimal design of the process flow sheet involves selecting the equipment sizes as well as the operating conditions so as to maximize the total annual profit. Major decisions involve the pressure of the reaction loop, the reactor design (volume, conversion per pass, outlet temperature), and the purge rate, which has a great influence on the overall conversion of the raw materials as it determines the amount of recycle. When no heat integration is considered (i.e., all heating and cooling requirements are satisfied with utilities), the optimal design of the flow sheet can be formulated as a nonlinear program that has the form of problem P_0. For the example in this paper, problem P_0 involves 40 variables in 36 equations, one inequality, and the eight sets of lower and upper bound constraints in Table 1. When the proposed heating deficit constraints for heat integration are incorporated into the above nonlinear program, it takes the form of problem P_2. The problem then involves 40 variables in 35 equations, seven inequalities, and eight lower and upper bound constraints. The difference in the number of equations arises because the two heat balance equations that define the heating and cooling utilities in problem P_0 are replaced by the total heat balance (Eq. 8) in P_2. Also, there are six more inequality constraints in problem P_2 because they correspond to the heating deficit constraints derived for the six pinch point candidates associated with the three hot and three cold process streams that are considered for heat integration.

To demonstrate the potential of the proposed procedure for simultaneous optimization and heat integration, results were also obtained with the sequential procedure of optimizing first the nonintegrated process, followed by the heat integration using the flow rates and temperatures obtained from the optimization. The corresponding nonlinear programs P_0 and P_2 of the two approaches were solved with the computer code MINOS/AUGMENTED (Murtagh and Saunders, 1980); the smooth approximation procedure discussed in a previous section was used to handle the nondifferentiabilities that arise in problem P_2. A value of $\epsilon = 0.0001$ for the parameter ϵ was used, and no ill-conditioning was observed during the optimization. The solution of the nonlinear program P_2 for the simultaneous optimization and heat integration took 29.22 s of CPU time (DEC-20 computer system). The solution of the nonintegrated process optimization (problem P_0) took 10.38 s. The time to predict the minimum utility consumption for this solution was negligible. The results with the two approaches are shown in Table 2. The annual profits shown in this table correspond to the integrated designs with cost of all major equipment items, incomes, and expenses included.

Clearly the striking feature of the results in Table 2 is that with the proposed simultaneous procedure the annual profit is 90.7% higher than with the sequential procedure (19.2645 M\$/yr vs. 10.1005 M\$/yr). The main reasons for this difference is that the simultaneous procedure yields a design with higher overall conversion of raw material A (81.7 vs. 75.1%), and with

TABLE 2. RESULTS FLOW SHEET OPTIMIZATION AND HEAT INTEGRATION

	Simultaneous	Sequential
	Economic	
Expenses ($\$ \times 10^6$/yr)		
Feedstock	22.6717	26.4166
Capital investment	3.7596	3.9108
Electricity compress	2.3774	2.4871
Heating utility	2.8244	14.4586
Cooling utility	0.7900	0.7247
Earnings ($\$ \times 10^6$/yr)		
Product	41.5300	41.5300
Purge	4.5169	6.8242
Generated steam	5.6407	9.7441
Annual Profit	19.2645	10.1005
	Technical	
Overall conversion A	81.68	75.13%
Pressure reactor	12.10	13.87 atm
Conversion per pass	30.43	37.53%
Temp. inlet reactor	450.00	450.00 K
Temp. outlet reactor	502.65	450.00 K
Steam generated	10,119.12	17,479.60 kW
Pressure in flash	9.10	10.87 atm
Temperature flash	320.00	339.88 K
Purge rate	9.66	19.66%
Power compressors	11,353.60	11,877.44 kW
Heating utility	1,684.27	8,622.04 kW
Cooling utility	10,632.04	9,752.77 kW
Total heat exchanged	31,962.20	28,720.61 kW

a much lower heating utility consumption (1,684 vs. 8,622 kW). There were no large differences in the total capital investment and in the selection of the pressure.

It is interesting to note that in both cases the highest reactor volume was selected (80 m^3). However, as seen in Table 2, in the case of the simultaneous procedure the conversion per pass in the reactor was lower (30.4 vs. 37.5%). This was due to the higher outlet temperature in the reactor (502.7 vs. 450 K), and to the larger amount of inerts since the purge rate was smaller (9.7 vs. 19.7%). In fact, for these reasons the sequential procedure derived higher incomes from the purge and from the steam that was generated. However, these gains were offset by a higher cost of raw material and heating utility costs as can be seen in Table 2.

It is also worth noting that although in the simultaneous solution the total heat exchanged was greater (31,962 vs. 28,721 kW), the selection of proper operating conditions allowed a more efficient heat integration. This can clearly be seen in Figures 10 and 11, where the temperature-enthalpy diagrams are plotted for the resulting flow rates and temperatures obtained with the two approaches (see Table 3). Note in Figure 10 that in the simultaneous procedure there are two pinch points. The one at (383.7, 368.7 K) corresponds to the inlet stream ($C2$) of the reactor preheater; the one at (502.7, 487.7 K) corresponds to the effluent ($H1$) of the reactor. By setting the temperature of this stream at 502.7 K and reducing the flow in the purge stream, it is clear that more heat integration is achieved. On the other hand, in Figure 11 the sequential procedure gave rise to only one pinch point at (363.1, 348.1 K), which corresponds to the dew temperature of the reactor effluent ($H2$). In this case the temperature of $H1$ was set to the lower value of 450 K, presumably to generate more steam in the reactor and because the sequential procedure does not have the information on the implications of selecting proper temperatures for efficient heat integration. Information about matches for minimum number of heat exchangers was determined with the MILP model of Papoulias and Grossmann [1983a]. The network configurations for both cases were then derived, and they are shown in Figures 12 and 13.

DISCUSSION

The example that has been presented shows very clearly the advantages of simultaneously optimizing the chemical process and performing heat integration that guarantees the minimum utility target. The proposed procedure leads to designs that are both economic and energy efficient since it accounts explicitly for the strong interactions between the processing system and the heat recovery network. This allows one to establish proper economic trade-offs between capital investment, raw material utilization, and energy consumption. Furthermore, the computational effort with the suggested procedure is not greatly increased with respect to the sequential approach.

The results of this example show that the proposed procedure is superior to the sequential approach consisting of first optimizing a nonintegrated process followed by standard heat

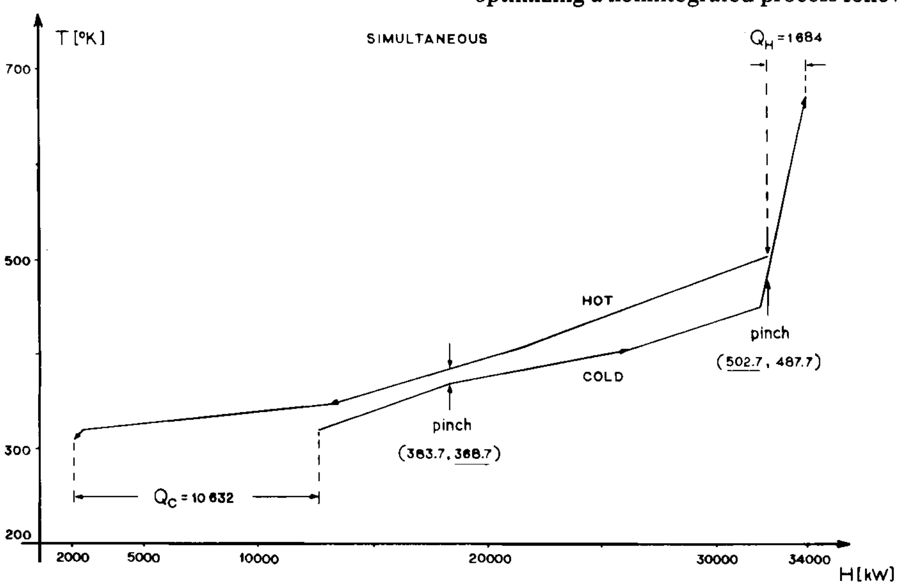

Figure 10. *T* vs. *H* diagram: simultaneous approach.

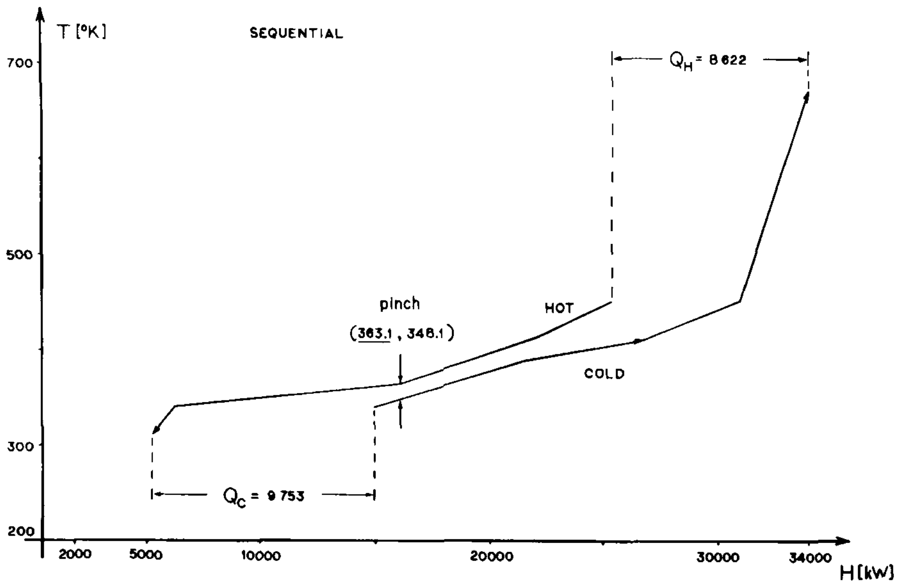

Figure 11. *T* vs. *H* diagram: sequential approach.

Table 3. Resulting Flow Rates and Temperatures of Process Streams

Stream	*F* kmol/s	Cp_s kJ/kmol·K	T^{in} K	T^{out} K	*Q* kW
		Simultaneous			
*H*1	3.1826	35.1442	502.65	347.41	17,363.58
*H*2	3.1826	115.4992	347.41	320.00	10,075.58
*H*3	1.0025	29.6588	405.48	310.00	2,838.90
*C*1	0.2724	33.9081	320.00	670.00	3,232.80
*C*2	3.5510	31.8211	368.72	450.00	9,184.37
*C*3	0.3617	297.7657	320.00	402.76	8,913.40
		Sequential			
*H*1	2.4545	35.1438	450.00	363.08	7,497.76
*H*2	2.4545	158.6957	363.08	339.88	9,036.83
*H*3	1.1681	29.6596	412.87	310.00	3,563.97
*C*1	0.4115	33.9116	339.88	670.00	4,606.69
*C*2	2.8494	31.8188	387.33	450.00	5,681.95
*C*3	0.3617	340.8035	339.88	410.30	8,680.58

integration for fixed stream conditions. Qualitatively, the reason for the superiority of the simultaneous approach vs. the sequential approach is as follows. In the sequential approach too much weight is given to the utility costs in the process optimization, since at this stage it is assumed that the duties of the process streams are satisfied exclusively by utilities that have been preassigned. While this will tend to have the effect of reducing the total heat exchanged between the streams, this does not mean that utility consumption and utility selection will be optimized when performing the heat integration after the process optimization is completed. The example problem showed very clearly that it is far more important to select proper operating conditions to achieve efficient heat integration than to minimize the total heat exchanged. Furthermore, by not anticipating the heat integration at the process optimization stage in the sequential approach, this can have the effect of distorting the economic trade-off between raw material conversion and energy consumption. Since the simultaneous approach does account for efficient heat integration, it will give

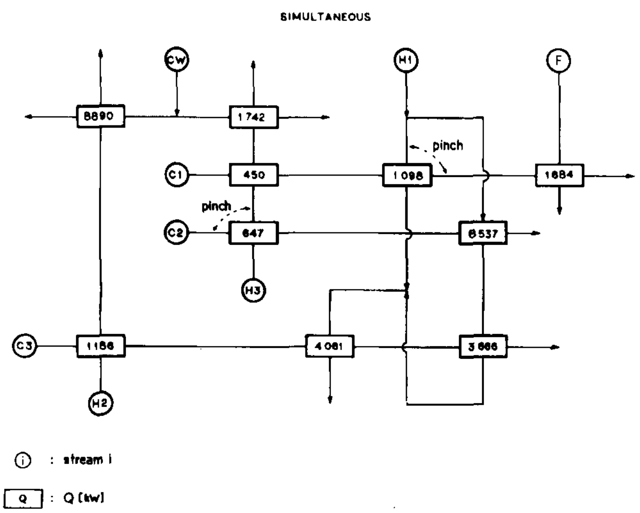

Figure 12. Network configuration: simultaneous approach.

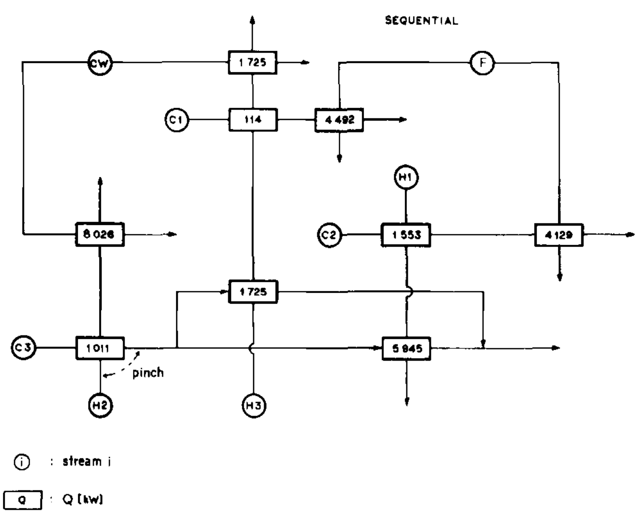

Figure 13. Network configuration: sequential approach.

the appropriate weight to the utility costs; hence it will have the tendency of producing designs with higher raw material conversion, as was shown in the example.

It should be pointed out that the proposed procedure can be applied to the optimal design of given flow sheet structures, as well as to the optimal synthesis of chemical processes. In the former case the procedure can easily be implemented in any of the flow sheet optimization techniques, whether in the equation-oriented approach (Berna et al., 1980) or in the simultaneous modular approach (Biegler and Hughes, 1982; Jirapongphan et al., 1980; Stadtherr snd Chen, 1984). In the synthesis case the procedure can be implemented within a mixed-integer nonlinear programming optimization framework, as has been discussed by Duran (1984).

It is also worth noting than an interesting application of the method suggested in this paper would be in the energy retrofit of existing chemical plants. In this case the flow rates and temperatures of the process streams could be optimized to indicate the maximum heat integration that can be achieved. This optimization could be performed when all or part of the existing heat exchanger network is replaced.

Another interesting point in this work is that for the case of fixed flow rates and temperatures of the process streams, the proposed pinch point location method provides very efficient formulations for the standard heat integration problems. The minimum utility consumption problem reduces to solving an algebraic system of two equations (Eqs. 9 and 10) in the two unknowns corresponding to the minimum heating and cooling requirements. For the case of multiple utilities, the minimum utility cost problem corresponds to the linear programming problem P_3, which involves as variables only the utility duties. Therefore, for fixed stream conditions, the formulations presented in this paper are simpler and require fewer variables than optimization models propered previously in the literature.

The suggested procedure, to the authors' knowledge, is the first systematic procedure proposed for simultaneous nonlinear flow sheet optimization and heat integration. This work constitutes a different representation and view of the heat integration problem, and with minor conceptual refinements can be used as part of procedures for dealing with other important process design problems.

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NOTATION

c = index cold utility at lowest temperature
c_c^j = unit cost cooling utility j
c_H^i = unit cost heating utility i
C = index set cold process streams
c_j, C_i = heat capacity cold stream j, hot stream i
CP_e = equivalent heat capacity
CU = index set cooling utilities
f_j, F_i = flowrate cold stream j, hot stream i
$g(w,x)$ = vector of inequality constraints
h = index hot utility at highest temperature
$h(w,x)$ = vector of equality constraints
H = index set hot process streams
HU = index set heating utilities
n_C = number of cold process streams
n_{CU} = number of cooling utilities
n_H = number of hot process streams
n_{HU} = number of heating utilities
p = index for candidate pinch at inlet of stream p
P = index set for candidate pinch points
q = index for actual pinch point(s)
Q_H, Q_C = duties of heating, cooling utilities
Q_H^i, Q_C^j = duties of heating utility i, cooling utility j
Q_H^p = duty of heating utility at candidate pinch p
Q_C^p = duty of cooling utility at candidate pinch p
$QHOT(x)$ = heat content of hot process streams
$QCOL(x)$ = heat content of cold process streams
$QSOA(x)^p$ = heat source above candidate pinch p
$QSIA(x)^p$ = heat sink above candidate pinch p
$QSOB(x)^p$ = heat source below candidate pinch p
$QSIB(x)^p$ = heat sink below candidate pinch p
t_j^{in}, t_j^{out} = inlet, outlet temperatures cold stream j
T_i^{in}, T_i^{out} = inlet, outlet temperatures hot stream i
T^p = temperature of candidate pinch p
T_C^j, T_H^i = temperature cooling utility j, heating utility i
w = vector of process parameters
x = vector of flowrates and temperatures of process streams
$z_H^p(x)$ = heating deficit above candidate pinch p
$z_C^p(x)$ = cooling deficit below candidate pinch p

Greek Letters

ΔT_m = minimum temperature approach
ΔH = enthalpy change
ϵ = tolerance for smooth approximation
ϕ = objective function
$\Omega(x)$ = difference of heat content between hot and cold process streams

APPENDIX A: LOCATION OF PINCH POINTS—ACTIVITY OF DEFICIT CONSTRAINTS

To identify actual pinch points in both pinched and nonpinched systems, problem P_2 involving fixed stream flow rates and temperatures (i.e., fixed x) can serve as a basis for analysis. That is, the optimality conditions can be analyzed for the following problem,

$$\begin{aligned} \min \quad & c_H Q_H + c_C Q_C \\ \text{s.t.} \quad & z_H^p(x) - Q_H \leq 0 \leftarrow \lambda_p \} \quad \text{all } p \in P \\ & \Omega(x) + Q_H - Q_C = 0 \leftarrow \mu \\ & Q_H \geq 0 \leftarrow \rho_H \\ & Q_C \geq 0 \leftarrow \rho_C \end{aligned} \tag{A}$$

where $z_H^p(x)$ and $\Omega(x)$ are constants for fixed x; c_H and c_C are constant positive unit costs; and λ_p: all $p \in P$, μ, ρ_H, and ρ_C, are the associated multipliers for the dual formulation of problem A. The Lagrangean function is then given by,

$$L = c_H Q_H + c_C Q_C + \sum_{p \in P} \lambda_p [z_H^p(x) - Q_H] + \mu[\Omega(x) + Q_H - Q_C] - \rho_H Q_H - \rho_C Q_C$$

which has the following associated Karush-Kuhn-Tucker optimality conditions,

$$\frac{\partial L}{\partial Q_H} = 0 \Rightarrow c_H - \sum_{p \in P} \lambda_p + \mu - \rho_H = 0 \tag{a}$$

$$\frac{\partial L}{\partial Q_C} = 0 \Rightarrow c_C - \mu - \rho_C = 0 \tag{b}$$

$$\lambda_p[z_H^p(x) - Q_H] = 0 \quad \text{all } p \in P \tag{c}$$

$$\lambda_p \geq 0,\ z_H^p(x) - Q_H \leq 0 \quad \text{all } p \in P \tag{d}$$

$$\Omega(x) + Q_H - Q_C = 0 \tag{e}$$

$$\rho_H Q_H = 0,\ \rho_H \geq 0,\ Q_H \geq 0 \tag{f}$$

$$\rho_C Q_C = 0,\ \rho_C \geq 0,\ Q_C \geq 0 \tag{g}$$

Therefore, a pair (Q_H, Q_C) of minimum heating and cooling utilities has to satisfy the above conditions to be an optimal solution to the minimum utility consumption problem *A*. It has been shown in this paper that this solution will be given by,

$$Q_H = \max_{p \in P} \{z_H^p(x)\} \tag{h}$$

$$Q_C = \max_{p \in P} \{z_C^p(x)\} \tag{i}$$

Further, according to the definition of the heating $z_H^p(x)$ (Eq. 2) and cooling $z_C^p(x)$ (Eq. 3) deficit functions, the difference between the total heat content of the hot and cold process streams (see Figure 2) $\Omega(x) = QHOT(x) - QCOL(x)$ can be expressed as,

$$\Omega(x) = z_C^p(x) - z_H^p(x) \tag{j}$$

The location of pinch points in the pinched and unpinched cases, and corresponding implications can then be analyzed as follows.

Pinched Case: $Q_H > 0$, $Q_C > 0$

For this case, conditions (f) and (g) above imply $\rho_H = \rho_C = 0$, which in turn defines the stationary conditions (b) and (a) as,

$$\mu = c_C > 0,\ \sum_{p \in P} \lambda_p = c_H + c_C > 0$$

which imply that there exist scalars μ and $\lambda_p : p \in P$, and at least one λ_p is strictly greater than zero. Thus, according to the complementary slackness condition (c), this result implies that at least one of the deficit constraints must be active at the solution, i.e., $z_H^p(x) - Q_H = 0$. As given by the definition of the deficit functions, to be active for feasible (Q_H, Q_C) means that the system is in exact heat balance above and below the associated temperature. Thus, the actual pinch points in the system will be given by the corresponding deficit constraints active at the solution of problem P_3, or P_4 when multiple utilities are considered.

Nonpinched cases

a) *Only heating requirements:* $Q_H > 0$, $Q_C = 0$

The conditions for this case lead to the following relations with respect to the Lagrange multipliers,

$$\rho_H = 0,\ \rho_C > 0,\ \mu = c_C - \rho_C,\ \sum_{p \in P} \lambda_p = c_H + c_C - \rho_C$$

which do not necessarily imply the existence of positive multipliers λ_p: $p \in P$. However, Eq. (i) implies that there exists a pinch candidate p' for which the maximum $Q_C = z_C^{p'} = 0$ is attained. For that particular p', Eqs. (j) and (e) imply,

$$z_H^{p'}(x) - Q_H = 0$$

which together with optimality conditions (c) and (d) imply that the corresponding multiplier is positive, i.e., $\lambda_{p'} > 0$, and hence the associated deficit constraint will be active at the solution. In particular, p' will be associated with the lowest stream inlet temperature value considered as potential pinch point.

b) *Only cooling requirements:* $Q_H = 0$, $Q_C > 0$

This case determines the following relations,

$$\rho_H > 0,\ \rho_C = 0,\ \mu = c_C > 0,\ \sum_{p \in P} \lambda_p = c_H + c_C - \rho_H$$

This again does not necessarily imply that at least one deficit constraint must be active. However, Eq. (h) implies that there exists a pinch candidate p' for which the maximum is attained, i.e., $Q_H = z_H^{p'}(x) = 0$. Complementary slackness in (c) implies then that for that particular pinch point p' the associated multiplier must be such that, $\lambda_{p'} > 0$. This pinch point will correspond to the highest value inlet temperature among streams that are being considered. The corresponding deficit constraint will therefore be active at the solution, this then defining the location of the pinch point.

The proof for the mixed case, $Q_H = 0$, $Q_C = 0$, follows from the proofs above.

APPENDIX B: EXAMPLES—HEAT INTEGRATION FOR FIXED FLOW RATES AND TEMPERATURES

1. Minimum Utility Consumption: Single Heating and Cooling.

PROBLEM: 4SP1

	FC_p kW/°C	T^{in} °C	T^{out} °C
*H*1	8.79	160	93
*H*2	10.55	249	138
C1	7.62	60	160
C2	6.08	116	260
	$\Delta T_m = 10$°C		

CALCULATIONS

p	T^p	$QSIA(x)^p$	$QSOA(x)^p$	$z_H^p = QSIA(x)^p - QSOA(x)^p$ kW
*H*1	160	745.00	938.95	−193.95
⇒ *H*2	249	127.68	0.0	127.68 ⇐ $\max_{p \in P} \{z_H^p\}$
C1	70	1,637.52	1,759.98	−122.46
C2	126	1,210.80	1,469.91	−259.11
$\Omega(x) = QHOT(x) - QCOL(x) = 1{,}759.98 - 1{,}637.52 = 122.46$ kW				

Solution: Algebraic problem of two equations in two variables (see Eqs. 9 and 10)

$$Q_H = \max\{z_H^{H1}, z_H^{H2}, z_H^{C1}, z_H^{C2}\} = z_H^{H2} = 127.68 \text{ kW}$$

⇒ pinch point = (249°C, 239°C): stream *H*2

$$\Omega(x) + Q_H - Q_C = 0 \Rightarrow Q_C = \Omega(x) + Q_H = 250.14 \text{ kW}$$

If heating: steam at 280°C, $c_H = 70$ \$/kWyr

If cooling: water at 21°C, $c_C = 20$ \$/kWyr

Utilities cost:

$$c_H Q_H + c_C Q_C = 13{,}940.40 \text{ \$/yr.}$$

2. Minimum Utility Cost: Multiple Utilities

PROBLEM

	FC_p kW/K	T^{in} °K	T^{out} °K
$H1$	1	450	350
$H2$	2	400	280
$C1$	2	320	480

$\Delta T_m = 10$ K

Utilities: Single Temperature

$HU1$: HP steam at 500 K, $c_H^{HU1} = 70$ \$/kWyr

$HU2$: LP steam at 430 K, $c_H^{HU2} = 50$ \$/kWyr

$CU1$: Cooling at 300 K, $c_C^{CU1} = 20$ \$/kWyr

$CU2$: Refrigerant 270 K, $c_C^{CU2} = 120$ \$/kWyr

CALCULATIONS

p	T^p	$QSIA(x,u)^p$	$QSOA(x,u)^p$	$z_H^p = QSIA(x,u)^p - QSOA(x,u)^p$ kW
$H1$	450	80	0.0	80
$H2$	400	180	$50 + Q_H^{HU2}$	$130 - Q_H^{HU2}$
C1	330	320	$240 + Q_H^{HU2}$	$80 - Q_H^{HU2}$
$HU2$	430	120	20	100
$CU1$	310	$320 + Q_C^{CU1}$	$280 + Q_H^{HU2}$	$40 + Q_C^{CU1} - Q_H^{HU2}$

$\Omega(x,u) = QHOT(x,u) - QCOL(x,u) = 340 + Q_H^{HU2} - 320 - Q_C^{CU1} = 20 + Q_H^{HU2} - Q_C^{CU1}$

Formulation: Linear Programming Problem

$$\min \quad 70Q_H^{HU1} + 50Q_H^{HU2} + 20Q_C^{CU1} + 120Q_C^{CU2}$$

$$\text{s.t.} \quad Q_H^{HU1} \geq 80$$

$$Q_H^{HU2} + Q_H^{HU1} \geq 130$$

$$Q_H^{HU2} + Q_H^{HU1} \geq 80$$

$$Q_H^{HU1} \geq 100$$

$$Q_H^{HU2} + Q_H^{HU1} - Q_C^{CU1} \geq 40$$

$$Q_H^{HU2} + Q_H^{HU1} - Q_C^{CU1} - Q_C^{CU2} = -20$$

$$Q_H^{HU2}, Q_H^{HU1}, Q_C^{CU1}, Q_C^{CU2} \geq 0$$

Solution

$$Q_H^{HU1} = 100 \text{ kW}, Q_H^{HU2} = 30 \text{ kW}$$

$$Q_C^{CU1} = 90 \text{ kW}, Q_C^{CU2} = 60 \text{ kW}$$

Minimum utility cost: 17,500 \$/yr.

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