Article

An Automated Approach for the Optimal Design of Heat Exchangers

Prosenjit D. Chaudhuri, Urmila M. Diwekar, and Jefferey S. Logsdon

Ind. Eng. Chem. Res., **1997**, 36 (9), 3685-3693• DOI: 10.1021/ie970010h • Publication Date (Web): 02 September 1997

An Automated Approach for the Optimal Design of Heat Exchangers

Prosenjit D. Chaudhuri[†] **and Urmila M. Diwekar***

Center for Energy and Environmental Studies, Department of Engineering and Public Policy, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213-3890

Jefferey S. Logsdon[‡]

Amoco Corporation, Process Engineering Cape Group, Naperville, Illinois 60563

This paper presents an efficient strategy based on simulated annealing (SA), an algorithmic procedure for large-scale combinatorial optimization problems, for the optimal design of heat exchangers. The general heat exchanger design problem can be posed as a large-scale discrete optimization problem, and SA was found to be well suited for this type of heat exchanger design problem. A methodology based on a command procedure has been developed to run the HTRI design program coupled to the annealing algorithm, iteratively. At first, initial runs were made using the command procedure developed to determine the key annealing parameters. These parameters were then used to study several test cases pertaining to the general heat exchanger design problem involving infeasible configurations and vibration constraints. The analyses were performed using two different objective functions namely, total heat transfer area and a linearized purchased cost index. Lastly, the variable set governing the different configurations was extended to incorporate a larger set of design variables. It was observed that, in almost all cases, the optimum designs obtained using the simulated annealing algorithm yielded better performance or cost functions compared to the base case (Amoco) designs. It has also been shown that an improvement in heat exchanger designs is achievable by extending the variable set to include a larger set of design alternatives. Simulated annealing offers great computational savings (in terms of CPU time) as a search strategy and has been found to be a robust technique for the optimal design of heat exchangers subject to process infeasibilities and vibration constraints.

1. Introduction

Computer software marketed by companies such as HTRI, HTFS, and B-JAC International are extensively used in the thermal design and rating of heat exchangers. Such organizations develop and continue to support design programs for the various classes of heat transfer equipment, namely shell-and-tube exchangers, condensers, reboilers, air-cooled exchangers, and plate-type exchangers. Tubular exchanger manufacturers association (TEMA) have classified shell-and-tube exchangers into three classes, and for each class several variations are possible (Amoco Report, 1994). A design engineer can choose between the several *discrete* alternatives that are available by varying the tube length, tube diameter, tube pitch, shell type, shell orientation, baffle type, and tube pattern, etc., to obtain a design configuration of the heat exchanger. A primary objective in heat exchanger design is the estimation of the minimum heat transfer area required for a given duty, as it governs the overall cost of the heat exchanger (Peters and Timmerhaus, 1980). However, since the possible design configurations of heat transfer equipment are numerous, an exhaustive search procedure for the optimal design is computationally intensive.

The objective of attaining the minimum heat transfer surface area or the minimum fixed cost of a heat exchanger for a given duty can be posed as a large-scale discrete optimization problem. Traditionally, pure-integer programming techniques (e.g., cutting plane, branch and bound) were used to handle such problems. However, strategies based on the branch and bound enumeration procedure, which is widely used to solve pure-integer programming problems, rely on good estimates of the bounds to yield significant computational savings. These estimates are based on heuristics and expert judgments, which may be difficult to obtain in certain cases. Further, since branch and bound requires the solution of a linear program for the pure-integer programming problem at each node (Reklaitis et al., 1983), it is not suited for black-box models such as the HTRI design program (ST-5), where explicit relationships for the constraints are not available. Alternative to the mathematical programming approach is simulated annealing (SA), a probabilistic-based optimization technique used to address combinatorial optimization problems in many diverse areas in the recent past. In this paper, the advantage of simulated annealing to obtain the minimum heat transfer area or the minimum cost of a heat exchanger is illustrated. The program (ST-5) is primarily intended for the design and rating of heat exchangers involved in sensible heat transfer on the basis of given design variables related to the configurations (e.g., shell type, baffle type, tube length, tube diameter, etc.). In order to facilitate the coupling of the simulated annealing algorithm with the external ST-5 program, a command procedure has been created. Figure 1 illustrates the generalized procedure for the optimal design of heat exchangers with ST-5 (the executable HTRI design program). In Figure 1, the annealer (optimization algorithm based on SA) decides the design (decision) variables. The ST-5 program generates the heat transfer area and provides indica-

* Author to whom correspondence should be addressed. Tel: 412-268-3003. Fax: 412-268-3757. E-mail: urmila@cmu.edu.

[†] Present address: The BOC Group, 100 Mountain Avenue, Murray Hill, NJ 07974. E-mail: prosenjit.chaudhuri@us.gtc.boc.com.

[‡] E-mail: jlogsdon@amoco.com.

S0888-5885(97)00010-9 CCC: $14.00

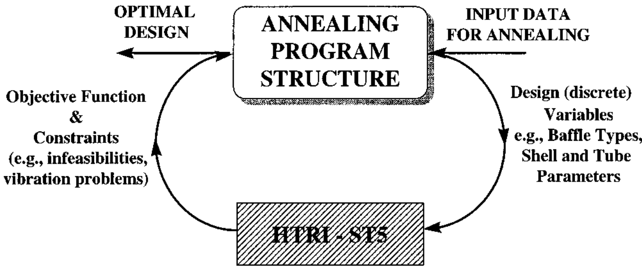

Figure 1. Generalized procedure for the optimal design of heat exchangers with the black-box design program (ST-5).

tions of vibration problems and infeasibilities associated with any given configuration. This information is translated in the form of objective function and constraints and transferred to the annealer. The annealer uses this information to predict new design variables, and the process continues until the optimality criteria defined by the SA algorithm is satisfied. In the next section, a brief overview of simulated annealing is presented. A detailed illustration of the program structure and how the command procedure was customized for the general heat exchanger design problem is discussed in a later section. This is followed by an illustration of several test cases analyzed to ascertain the efficiency of the algorithmic procedure. The cases studied pertain to the following design scenarios, and their purposes are listed as follows:

(1) Case Study A: The primary goal of this case study was to determine the simulated annealing parameters. The objective function in this case was the total heat transfer area. The search space was derived from 3564 design configurations. Since the main aim of this case study was to estimate the key annealing parameters, detailed analyses involving the constraints to ascertain the presence of acoustic and tube vibrations were neglected.

(2) Case Study B: This case involved the same search space of 3564 combinations. The objective function in this case was the total heat transfer area. However, in this case the objective function was subjected to vibration constraints, a practical concern faced by engineers in heat exchanger design. The program structure for the base case scenario was modified to take into consideration vibration constraints and infeasible configurations. The optimal design configuration was compared with the base case design to illustrate the deviation of the optimal design from the base case design.

(3) Case Study C: Same as Case Study B, except that the objective function was changed to reflect the purchased cost of the heat exchanger set. The cost function was the linearized purchased cost of the heat exchanger set, which depends on the total heat transfer area and the number of shells.

(4) Case Study D: This case involved an extended set of variables giving rise to an increased number of possible design configurations. The search space involved 165888 combinations. As in Case Study C, the purchased cost of the heat exchanger set was minimized subject to process infeasibilities and vibration constraints.

In the next section, the general simulated annealing algorithm is described followed by the study performed to determine the key annealing parameters used in the analyses of the several test cases. It was found, on the basis of the analysis with a smaller set of design alternatives, that the functional topology for the heat transfer area is usually flat in sections, having many local optima. The functional topology offers a challenge to the simulated annealing algorithm, which allows random uphill moves to overcome local minima. Usually, on an average, the optima obtained were within 5% of the global optima. Computationally, significant savings in CPU time was achieved by allowing simulated annealing to identify the optimum compared to an exhaustive search procedure. Simulated annealing proved to be an efficient, reliable search tool in determining the optimal design of heat exchangers.

2. Simulated Annealing—An Overview

Simulated annealing is a heuristic approach for solving combinatorial optimization problems involving many variables. In recent years, simulated annealing has been employed in many diverse areas such as VLSI chip floor planning, the traveling salesman problem, image processing, and physical design of computers, to name a few. It is a probabilistic method based on ideas from statistical mechanics (Kirkpatrick et al., 1983), which deals with the behavior of systems having many degrees of freedom in thermal equilibrium at finite temperatures. Systems involving liquid metals freeze and crystallize or cool and anneal. At high temperatures, the molecules of liquid metals exhibit greater thermal mobility. If such a system is cooled slowly (i.e., *annealed*), the atoms orient themselves to form a pure crystal, thus attaining the lowest energy state of the system. On the contrary, if the liquid metal is cooled quickly (i.e., *quenched*) it does not reach this minimum energy state, but rather attains a polycrystalline or amorphous state possessing high energy.

The behavior of atoms in the presence of a heat bath is governed by the temperature. At each temperature, the system is allowed to attain thermal equilibrium. The probability (Pr) of such a system of being in a state with energy E is given by the Boltzmann distribution:

$$\mathrm{Pr}(E) = \frac{1}{Z_t} \exp\left(\frac{-\Delta E}{K_b T}\right)$$

where K_b is the Boltzmann's constant (1.3806×10^{-23} J/K) and $1/Z_t$ is a normalization factor (Collins et al., 1988). In simulated annealing, the objective function (usually cost) is analogous to the energy of the system. The aim of such a problem then is to minimize the cost/energy denoted by $f(\bar{X})$, where $\bar{X} = (X_1, X_2, ..., X_N)$ represents a particular configuration of the system. To observe the behavior of the system, the system is perturbed from its present state to another state. These individual perturbations are referred to as *neighborhood moves*.

The behavior of a system subject to such a neighborhood move is determined from an observation of the objective function. If the configuration results in a lower energy state, the move is accepted. However, if the move results in a higher energy state, the move is *still* accepted according to Metropolis criteria [i.e., accepted with a probability $\exp(-\Delta E/K_b T)$]. Thus, at high temperatures, a large percentage of uphill moves are accepted. The system is allowed to reach thermal equilibrium at each temperature; the temperature is then lowered, and the annealing process continues until the system reaches a temperature corresponding to a certain "freezing" temperature. The general simulated annealing algorithm is described as follows:

Initialize variables
T_{initial}, accept and reject limits or N (number of moves at a given temperature), initial configuration S and Obj(S).
while $T > T_{\mathrm{freeze}}$ do
while $i < N$ do
Generate a random move S' by perturbing S
$\Delta\mathrm{Obj} = \mathrm{Obj}(S') - \mathrm{Obj}(S)$
If $\Delta\mathrm{Obj} \leq 0$ or random (0, 1) $< \exp(-\Delta\mathrm{Obj}/T)$ then accept S'
$S = S'$
update number of accepts, rejects until equilibrium is reached at T (when $i = \mathrm{N}$)
update T: $T_{\mathrm{new}} = \alpha T$ $(0.8 < \alpha < 0.98)$
until $T < T_{\mathrm{freeze}}$

where Obj signifies the objective function, while T, α, and N refer to the key annealing parameters namely, temperature, temperature decrement factor, and number of allowable moves at a temperature level, respectively. It must be realized that, in the physical annealing process, the temperature is real. On the other hand, in simulated annealing, the term "temperature" is *only* analogous to the real temperature in the physical annealing process and has the units of the cost or the objective function. The initialization temperature for the simulated annealing procedure is usually given by T_{start} such that $\exp(\Delta\mathrm{Cost}/T_{\mathrm{start}}) \leq 0.8$, where the ΔCost is obtained by evaluating the change in the objective function for a large number (e.g., 100) of *neighborhood moves*.

Simulated annealing combines standard iterative improvement and random uphill jumps to ensure that the system is not confined to a local minimum. In other words, moves which are highly probable can be rejected, and very improbable moves can be accepted occasionally. By successfully lowering the temperature and applying the Metropolis' algorithm, it is possible to simulate the system attaining equilibrium at each newly reduced temperature and thus simulate the physical annealing process. Simulated annealing can be applied to nonconvex objective functions, does not require gradient information (which may be unobtainable or difficult to compute), and offers the alternative of a random uphill move which enables the system to "jump out" of a local minimum toward a global minimum.

Simulated annealing, however, is not a panacea for all combinatorial optimization problems. The convergence of the annealing algorithm is guaranteed *asymptotically*, if the move sequences are Markov chains. This implies that if one makes infinitely many moves, then the probability of attaining the global minimum can be made as close to one. Computationally, this does *not* provide a practical guarantee of convergence in a real problem. The basic structure of the particular configuration space—its landscape of multidimensional hills and valleys—determines the reliability of the simulated annealing algorithm (Rutenbar, 1989). In other words, a functional landscape that is mostly smooth with gradually flowing hills and valleys is relatively easy to anneal than a flat landscape with several, densely packed gopher holes. Therefore, annealing can be regarded as a promising technique for solving a large class of combinatorial optimization problems, "superior to some approaches for some problems, inferior to others" (Rutenbar, 1989). The major advantage of annealing, however, arises owing to its practical usefulness in solving a wide spectrum of optimization problems, requiring no assumptions in the form of the objective functions and the constraints.

The heat exchanger design problem addressed here is well suited for simulated annealing, since the baffle types, number of shells, number of tubes passes, tube lengths, tube layout patterns, tube o.d., and tube pitch etc., presents a large number of discrete configurations. Similar problems in other areas have suggested a probabilistic-based approach such as simulated annealing to be an apt methodology to ascertain the optimal design in such cases. The equivalent "temperature" (objective function) in the case of the design of heat exchangers is the total surface area or the purchased cost of the heat exchangers. The following section describes the key annealing parameters and illustrates how simulated annealing was able to identify the optimal/near-optimal solutions for different key annealing parameters and initial configurations for the simplest case—the heat exchanger design problem involving a reduced set of design variables for the unconstrained case.

3. Case Study A: Determination of the Annealing Parameters

The objective of this case study was to customize simulated annealing for the heat exchanger design problem. This step is essential, since it determines the annealing parameters for the subsequent case studies. The initial runs performed to determine the annealing parameters involved the objective of minimizing the total heat transfer area, without taking into consideration any constraints in the problem. It was assumed that the following alternatives were available:

(1) Three types of baffle choices involving "type" and "no-tubes-in-the-window" (corresponding to the integer variable, $L = 1-3$).

(2) Nine types of shell choices involving "number of shells in series" and "number of tube passes" (corresponding to the integer variable, $K = 1-9$).

(3) Twelve choices of tube data from set no. 1 involving "tube length" and "tube layout pattern" (corresponding to the integer variable, $J = 1-12$).

(4) Eleven choices of tube data from set no. 2 involving "tube o.d." and "tube pitch" (corresponding to the integer variable, $I = 1-11$).

The critical annealing parameters for any annealing schedule are the initial value of the control parameter or temperature, number of temperature levels, temperature decrement factor (α), and the number of temperature moves at a particular temperature (vanLaarhoven and Aarts, 1987). These parameters govern the implementation of the algorithm to real-life optimization problems and must be determined *a priori* before the procedure is applied to any given problem.

The number of scenarios possible based on the set of alternatives gave rise to $3 \times 9 \times 12 \times 11$ (or 3564) combinations. This set is referred to as the reduced-variable set as opposed to the extended-variable set which is discussed in Case Study D involving a larger set of alternatives.

Program Structure. As mentioned previously, the program ST-5 which computes the heat transfer area for a given duty is a black-box as far as the annealer is concerned. In other words, for a given configuration (as specified by the user), it can compute the heat transfer area for a given duty. Since the ST-5 program needs to be run repeatedly during annealing, an elegant and efficient program structure was developed to manipulate

Table 1. Dependence of the Optimal Design on the Initial Temperature, Temperature Decrement Factor (α), and the Initial Configuration for Case test 1

init conf (*L*, *K*, *J*, *I*)	glob soln (area, aq ft) α = 0.9	glob soln (area, aq ft) α = 0.97	final opt soln (area, sq ft) α = 0.9	final opt soln (area, sq ft) α = 0.97
		Initial Temperature = 100.0		
1, 2, 3, 4	403 (1, 8, 10, 10)	409 (1, 7, 3, 1)	436 (2, 8, 10, 8)	428 (3, 7, 4, 4)
3, 8, 11, 9	415 (2, 4, 12, 5)	393 (1, 6, 6, 2)	415 (2, 4, 12, 5)	403 (1, 7, 10, 4)
2, 5, 6, 7	403 (1, 7, 10, 4)	393 (1, 6, 6, 2)	415 (2, 4, 12, 5)	403 (1, 7, 10, 4)
1, 6, 6, 8	409 (1, 7, 3, 1)	409 (1, 7, 3, 1)	409 (1, 7, 3, 1)	428 (3, 7, 4, 4)
		Initial Temperature = 50.0		
1, 2, 3, 4	415 (2, 8, 9, 5)	403 (1, 7, 10, 4)	415 (2, 8, 9, 5)	403 (1, 7, 10, 4)
3, 8, 11, 9	415 (2, 8, 9, 5)	403 (1, 7, 10, 4)	415 (2, 8, 9, 5)	415 (2, 4, 12, 5)
2, 5, 6, 7	393 (1, 6, 6, 2)	403 (1, 7, 10, 4)	393 (1, 6, 6, 2)	415 (2, 4, 12, 5)
1, 6, 6, 8	415 (2, 4, 12, 5)	415 (1, 8, 9, 6)	415 (2, 4, 12, 5)	428 (3, 7, 4, 4)
		Initial Temperature = 25.0		
1, 2, 3, 4	393 (1, 6, 6, 2)	403 (1, 7, 10, 4)	403 (1, 7, 10, 4)	415 (1, 9, 1, 6)
3, 8, 11, 9	415 (1, 9, 1, 6)	415 (1, 9, 1, 6)	415 (1, 9, 1, 6)	415 (1, 9, 1, 6)
2, 5, 6, 7	393 (1, 6, 6, 2)	403 (1, 7, 10, 4)	403 (1, 7, 10, 4)	415 (1, 9, 1, 6)
1, 6, 6, 8	415 (2, 8, 9, 5)	403 (1, 8, 10, 10)	415 (2, 8, 9, 5)	436 (2, 8, 10, 8)

[a] The numbers within the parentheses indicates the integer variables corresponding to the different design configurations.

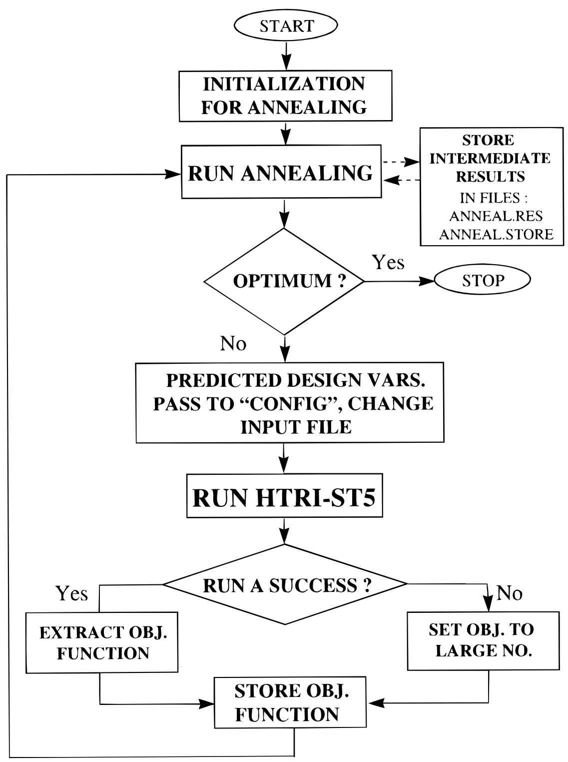

Figure 2. A schematic diagram of the program structure to determine the key annealing parameters.

the intermediate files which needs to be created during execution of the program. The sequence of the various steps in the entire program was controlled by this command procedure which initializes counters, initiates the annealing procedure, assigns specific files to the key input and output HTRI data files, and runs ST-5 with the design variables predicted by the annealer. The annealer computes ΔObj (the change in the objective function), decides to accept or reject the move on the basis of the Metropolis' algorithm, and predicts a new configuration for the computation of a new heat transfer area. The design (decision) variables predicted by the annealer results in the assignment of specific data related to the geometry of the heat exchanger in the module CONFIG. This data was passed on to another subroutine, which changes the current HTRI input data file. The ST-5 executable was then run with this modified data file to determine the heat transfer area for the new set of design variables. It must be noted here that, for some configurations, ST-5 failed to compute the heat transfer area. The command procedure accounted for these cases by setting the objective to a higher value to signify an infeasible configuration. The command procedure also controlled the flags governing the various stages of the algorithms and stored intermediate results in a data file. A flow chart of the various steps of the program structure is presented in Figure 2.

Results. The annealing parameters were determined using the input data for test 1 by performing multiple runs involving three choices of the initial temperature, two choices of the temperature decrement factor (α), and four choices of the starting configurations. This set of the annealing parameters were based on common heuristics in simulated annealing literature and is not elaborated here for the sake of brevity. The parameters determined through this exercise were found to be equally applicable for other test cases. The recommended annealing parameters used in subsequent case studies are listed as follows:

$$\text{initial starting temperature} = 50.0$$

$$\text{number of temperature levels} = 50$$

$$\text{temperature decrement factor} = 0.97$$

$$\text{number of moves at a temperature level} = 60$$

Apart from the "final" minimum obtained from the annealing procedure, a record of the configuration which gave the "global" minimum was also maintained, as the algorithm explored the functional topology through random jumps during annealing runs. The global optimum obtained in each case and the final optimal solution are illustrated in Table 1. Table 2 compares the design variables for the base case design with the optimum design obtained using the annealing procedure. The case for the best solution obtained is represented in Figure 3, where the objective function is plotted against the annealing temperature to show the progress of the annealing procedure. It is realized that although the annealer makes random uphill moves in the initial stages of the procedure and encounters infeasible configurations during its search, it does not

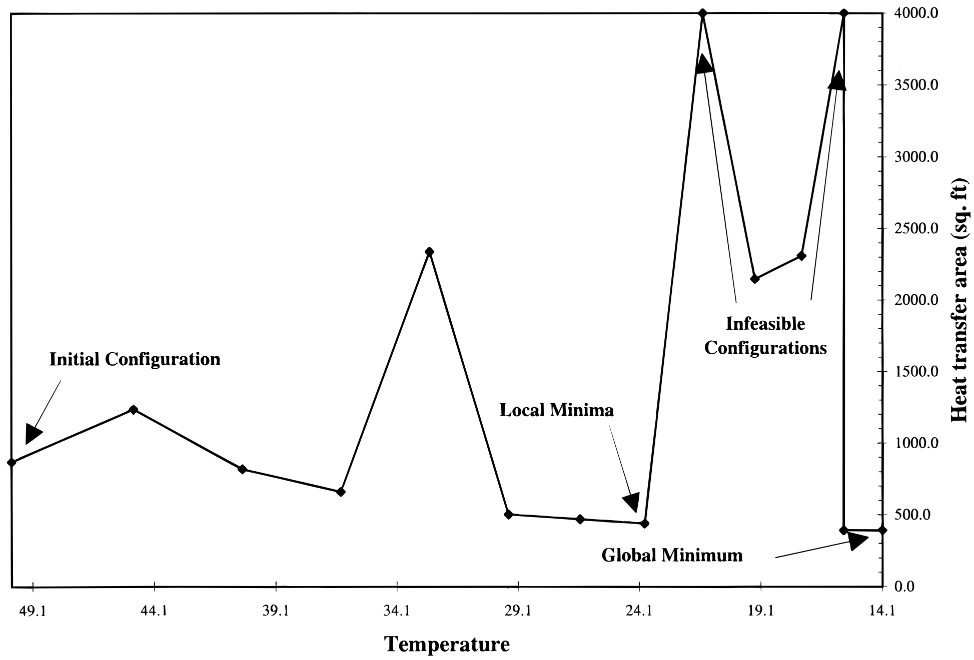

Figure 3. Objective function (heat transfer area) as a function of the annealing temperature for the "global" optimal solution for case test 1. Note: For certain configurations, ST-5 was unable to predict the heat transfer areas corresponding to those configurations. The program accounts for these infeasible configurations by setting the heat transfer area to 4000 sq ft.

Table 2. Optimal Solution Obtained for test 1 and a Comparison between the Base Case Design with the Optimal Design for this Design Problem (unconstrained case). An Exhaustive Search Demands 7.5 h of CPU Time on a VAX-4000

design variables	base case design	optimal design (unconstrained case)
baffle type	1-seg, TIW	1-seg, TIW
no. of shells in series	2	4
no. of tube passes	2	1
tube length (ft)	25.0	24.0
tube layout pattern (deg)	30	30
tube o.d. (in.)	0.625	0.625
tube pitch (in.)	0.781	0.812
area (sq ft)	426.0	393.0
vibration problems	no	possibly yes

get trapped in regions of local minima and is able to converge on the global optimum for certain choices of the initial temperature, initial configuration, and the temperature decrement factor.

The probability of obtaining the global optimum is 1/3564 or 0.0003. Simulated annealing overcame the major hurdle of being trapped in regions of local minima, identified the global optimum, and in most cases was able to obtain an optimal solution within 5% of the global optimum. In order to appreciate the reliability of simulated annealing, consider Figures 4 and 5, which plot the heat transfer aea obtained for all the feasible configurations as a frequency polygon to show the distribution of the different designs for cases test 1 and test 3 respectively. From the figures, it is evident that there are some heat transfer areas which have a high probability of occurrence, since they are estimated from many feasible configurations. Simulated annealing was able to navigate through these local "troughs" (regions of local minima of high probability) and identify the global minimum as well. The global optimum solution found in some scenarios (e.g., test 3) was found to have 84% less area than that of the base case (Amoco) design.

4. Case Study B: Optimal Design of Heat Exchangers (Based on Total Surface Area) Subject to Vibration Constraints

This case involved the optimal design of heat exchangers for a given duty on the basis of the total heat transfer area requirement, subject to the vibration constraints. The entire search space was derived from the same number of design configurations as in Case Study A (i.e., 3564 combinations). The program structure was modified to incorporate checks for process infeasibilities and vibration constraints. The modified program structure is presented in the next section.

Generalized Program Structure for the Optimal Design of Heat Exchangers. The overall framework for the generalized program structure is similar to the one presented previously where vibration considerations were neglected. However, in order to incorporate checks for process infeasibilities (which usually caused the HTRI ST-5 design program to write a "fatal error" message in the report file) and vibration constraints, the program structure was modified significantly. In this case, the output or the report file was analyzed by the module FATALERR to determine if fatal error was encountered (Figure 5). If any fatal error messages were encountered, control was transferred to the annealer, which was then prompted to predict a new configuration. On the contrary, if fatal error messages were not encountered, the control was transferred to the module VIBRATION, which then checked for violations in acoustic and tube vibration constraints. The vibration problem associated with heat exchangers and how it was taken into consideration in order to determine the optimal design is discussed in the following section.

Incorporation of Vibration Constraints. Large heat exchangers with increased shellside flow velocities improve heat transfer and reduce fouling. However, increased flow velocities, on the other hand, induce large shellside pressure drops, which can be minimized to a certain extent by reducing the number of baffles. This results in acoustic and tube vibrations. HTRI provides guidelines that allows designers to check for acoustic

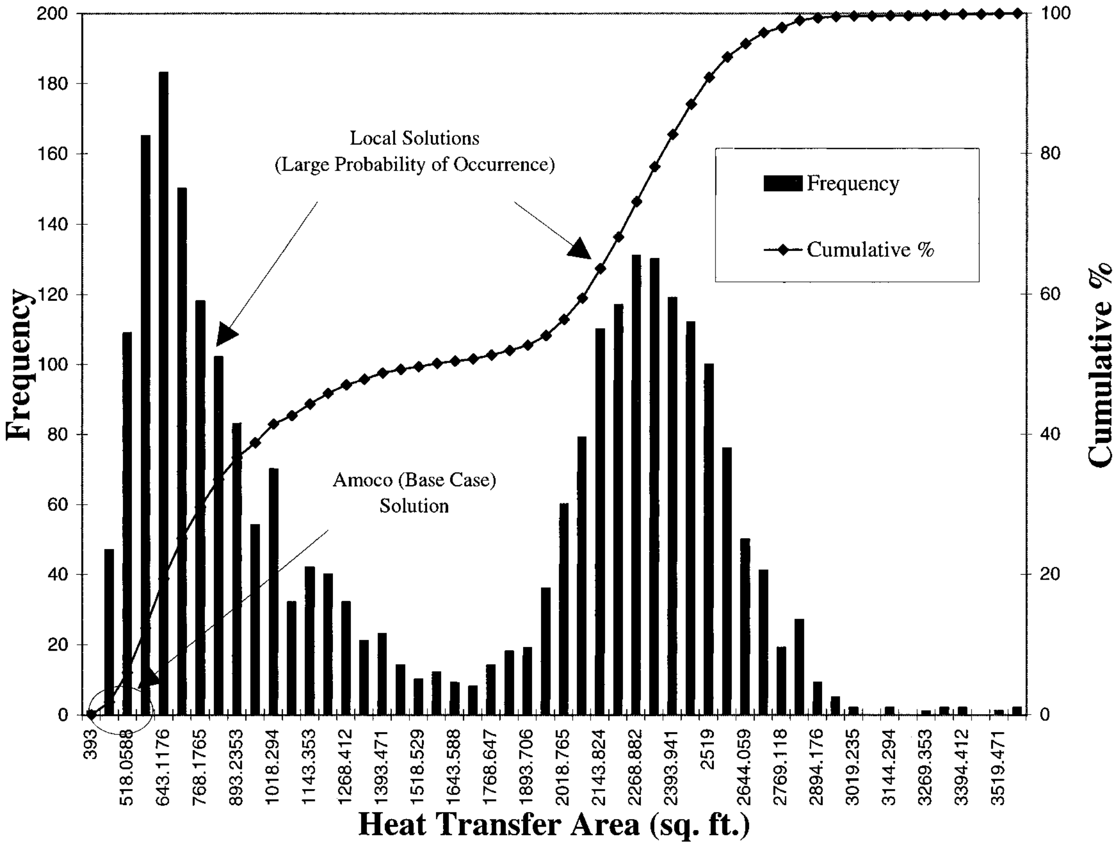

Figure 4. Distribution of the heat transfer area for all feasible configurations (test 1).

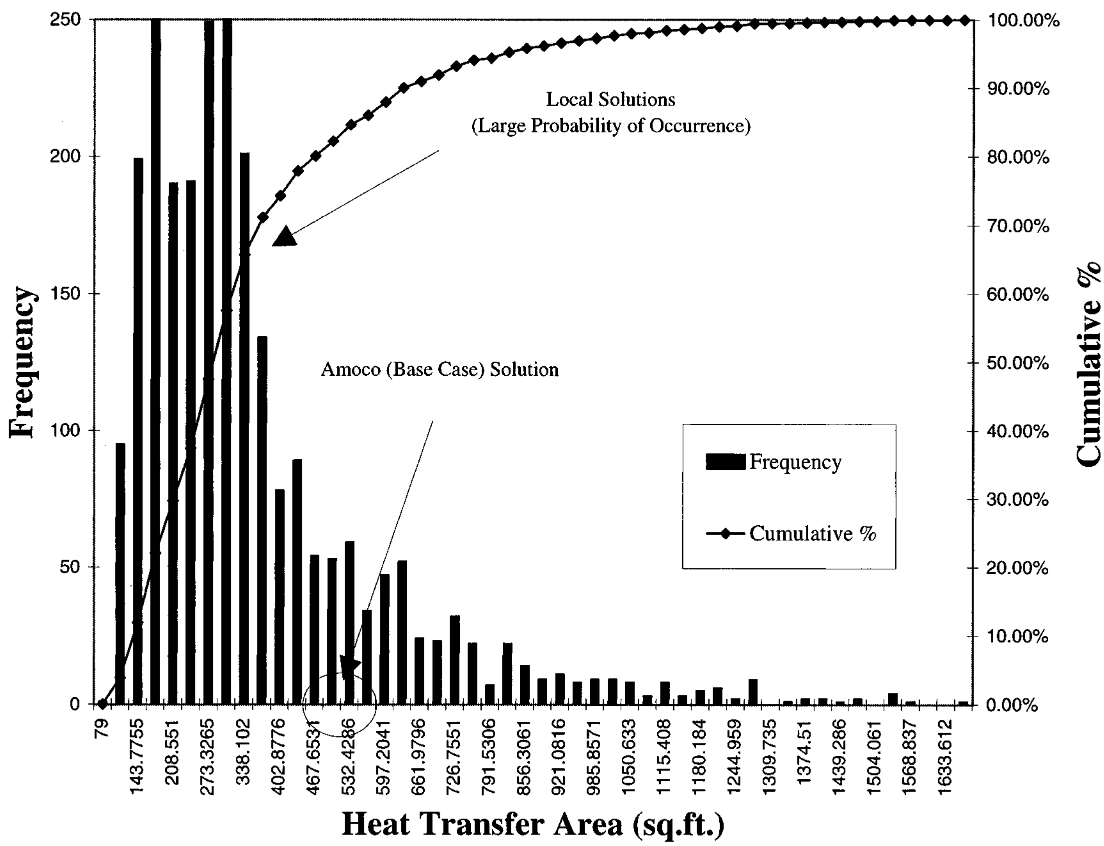

Figure 5. Distribution of the heat transfer area for all feasible configurations (test 3).

and tube vibrations (Amoco Report, 1994). The guidelines follow a step-by-step procedure and uses the output data listed in the section "Flow-Induced Vibration Analysis" in the HTRI ST-5 report file to determine whether acoustic or tube vibrations are possible with a particular design. The outcome of the analysis usually results in one of the three scenarios: possible vibration problem, probable vibration problem, or no vibration problem for a given design. In this study, the objective function is penalized for "possible" and "probable"

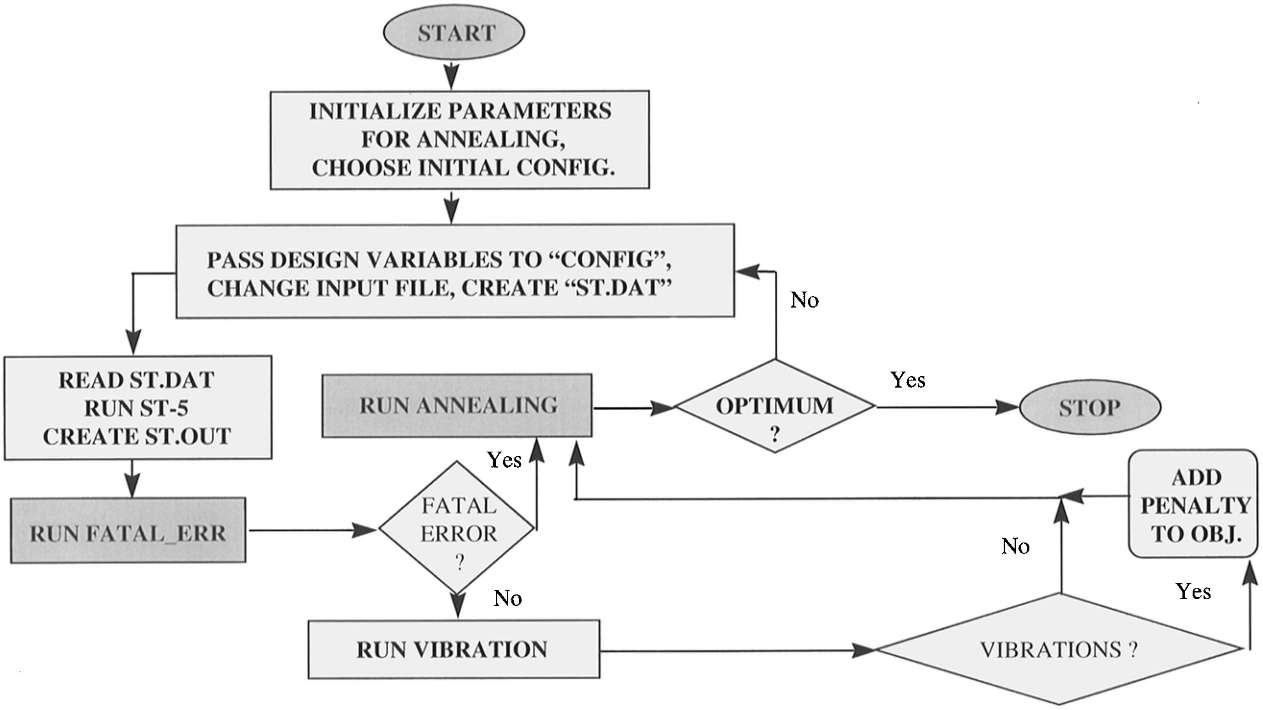

Figure 6. Generalized program structure for optimal design of heat exchangers.

Table 3. Deviation of the Optimal Design from the Base Case Design (Based on Total Heat Transfer Area)

	test 1	test 2	test 3	test 4	test 5
design variables			base case configuration (total surface area)		
baffle type	1-seg, TIW	1-seg, TIW	1-seg, NTIW	2-seg, NTIW	2-seg, NTIW
no. of shells in series	2	1	4	1	1
no. of shells in parallel	1	1	1	1	1
no. of tube passes	2	2	1	2	2
tube length (ft)	25.0	28.0	20.0	41.9961	41.9961
tube layout pattern (deg)	30	30	30	90	90
tube o.d. (in.)	0.625	0.625	0.750	0.750	0.750
tube pitch (in.)	0.781	0.875	1.000	1.062	1.062
vibration problems	no	yes	no	yes	no
total surface area (sq ft)	426.0	6644.0	519.0	1848.0	3101.0
design variables			optimal design configuration (total surface area)		
baffle type	1-seg, NTIW	2-seg, TIW	1-seg, NTIW	1-seg, NTIW	2-seg, TIW
no. of shells in series	2	4	4	2	4
no. of shells in parallel	1	1	1	1	1
no. of tube passes	4	2	2	4	4
tube length (ft)	16.0	24.0	8.00	16.0	10.0
tube layout pattern (deg)	90	90	90	90	90
tube o.d. (in.)	0.750	1.000	0.625	0.625	0.625
tube pitch (in.)	0.938	1.312	0.875	0.875	0.812
vibration problems	no	no	no	no	no
total surface area (sq ft)	440.0	5027.0	84.0	2105.0	1938.0
savings in area		24%	84%		38%

acoustic or tube vibrations as follows:

$$\text{Penalized Objective} = \text{Real Objective} + \text{wgt}_{\text{pos}}\,(\text{Real Objective})$$

(possible vibration problem)

$$\text{Penalized Objective} = \text{Real Objective} + \text{wgt}_{\text{prob}}\,(\text{Real Objective})$$

(probable vibration problem)

The weights for the "possible" (wgt_{pos}) and the "probable" (wgt_{prob}) vibration problem scenarios encountered are user-defined and stored in a data file (WEIGHTS.DAT), which is read by the routine analyzing vibration data. The penalized objective function (as opposed to th real objective function in the unconstrained case) is analyzed by the annealer to predict new design variables. A large (penalized) objective function implies an infeasible design configuration; the annealing algorithm selectively eliminates those infeasible configurations, thereby narrowing down the search space.

Table 4. Optimal Designs with and without Incorporating Vibration Constraint Considerations

test cases	no vibration check	vibration check
test 3	84.0 (2, 4, 7, 3)	84.0 (2, 7, 7, 3)
test 4	1506.0 (3, 2, 11, 3)	2105.0 (2, 5, 10, 3)
test 5	1508.0 (1, 7, 9, 4)	1938.0 (3, 9, 8, 2)

Results. The objective in this case study was to ascertain the minimum heat transfer area required subject to the vibration constraints and process infeasibilities (i.e., fatal errors associated with the ST-5 design

Table 5. Deviation of the Optimal Design from the Base Case Design (Based on the Purchased Cost of the Heat Exchanger)

	test 1	test 2	test 3	test 4	test 5
design variables			base case configuration (purchased cost)		
baffle type	1-seg, TIW	1-seg, TIW	1-seg, NTIW	2-seg, NTIW	2-seg, NTIW
no. of shells in series	2	1	4	1	1
no. of shells in parallel	1	1	1	1	1
no. of tube Passes	2	2	1	2	2
tube length (ft)	25.0	28.0	20.0	41.9961	41.9961
tube layout pattern (deg)	30	30	30	90	90
tube o.d. (in.)	0.625	0.625	0.750	0.750	0.750
tube pitch (in.)	0.781	0.875	1.000	1.062	1.062
area (aq ft)	426.0	6644.0	519.0	1848.0	3101.0
vibration problems	no	yes	no	yes	no
purchased cost ($)	10947	38844	20165	13957	24827
design variables			optimal design configuration (purchased cost)		
baffle type	1-seg, NTIW	1-seg, NTIW	1-seg, NTIW	1-seg, NTIW	2-seg, TIW
no. of shells in series	2	2	1	1	2
no. of shells in parallel	1	1	1	1	1
no. of tube Passes	3	4	1	1	3
tube length (ft)	20.0	16.0	20.0	24.0	20.0
tube layout pattern (deg)	90	90	90	30	90
tube o.d. (in.)	0.625	0.750	0.625	0.625	0.625
tube pitch (in.)	0.812	0.938	0.781	0.781	0.812
area (sq ft)	446.0	5417.0	158.0	2239.0	1597.0
vibration problems	no	no	no	no	no
purchased cost ($)	11050	36845	5188	15986	17023
savings in cost		5%	74%		31%

program). Five test cases were analyzed; in each case, the vibration constraints and the fetal errors related to infeasible configurations in ST-5 were treated in the manner outlined in the previous section. The design configurations predicting the heat transfer areas are mentioned within the parentheses. Table 3 shows the deviation of the base case (Amoco) design from the optimal design. The technique adopted in this proposed approach predicted lower heat transfer areas for all the test cases, except for Test 1, compared to the base case designs. This is attributed to the fact that the base case design configuration for test 1 was not part of the larger set, which defines the search space from which the optimal configuration is selected. A percentage savings in the heat transfer area can be defined by comparing the base case (Amoco) design with the optimal design as follows:

$$\%\text{ savings (in area)} = (\text{area corresponding to base case (Amoco) design} - \text{global minimum area})/(\text{area corresponding to base case (Amoco) design}) \times 100$$

On the basis of the above formulation, the percentage savings in the heat transfer area are also reported in Table 3. The percentage savings were not calculated for test 1 and test 4 cases. The reason for this is as follows: for test 1, the base case configuration is not part of the larger set of configurations considered in the first place, and for test 4, the base configuration is infeasible due to vibration problems associated with the design. However, it must be noted that starting from different initial configurations, savings of up to 84% was achieved by the optimal design predicted by the annealing algorithm. Finally, Table 4 shows that vibration check is critical for determining the optimal design. Optimal design for test cases test 4 and test 5 yielded lower bounds for the total heat transfer area when no vibration considerations were taken into account.

5. Case Study C: Optimal Design of Heat Exchangers Subject to Vibration Constraints (Based on Purchased Cost)

In this case, the determination of the optimal design of heat exchangers was undertaken keeping in view the purchased cost as the objective function, subject to the vibration constraints and process infeasibilities. The purchased cost is a more realistic index for the optimal design than the total heat transfer area, since the total heat transfer area as well as the number of shells affect the cost of the heat exchanger set for a given duty. The purchased cost of the heat exchanger was based on a linearized cost function typical of fixed-tube-sheet heat exchangers (Peters and Timmerhaus, 1980):

$$\text{purchased cost (\$)} = 4368.0(n_{\text{series}} n_{\text{parallel}}) + 5.189 \left(\frac{\$}{\text{sq ft}}\right)(\text{total surface area (sq ft)})$$

where

n_{series}: no. of shells in series

n_{parallel}: no. of shells in parallel

Results. This case study was similar to Case Study B, except that the objective function reflected the purchased cost of the heat exchanger set. The method of analysis was therefore similar to Case Study B. Deviation of the optimal design from the base case (Amoco) design is reported in Table 5. The base case designs were more cost intensive as opposed to the optimal design configurations obtained using the annealing approach. The percentage savings in the purchased cost can be achieved according to a similar formulation mentioned previously:

$$\%\text{ savings (in cost)} = (\text{purchased cost corresponding to base design} - \text{minimum cost (global)})/(\text{purchased cost corresponding to base case (Amoco) design}) \times 100$$

Table 6. Deviation of the Optimal Design from the Base Case Design for the Extended Variable Set (Based on the Purchased Cost of the Heat Exchanger)

	test 1	test 2	test 3
	base case configuration (purchased cost)		
design variables			
baffle type	1-seg, TIW	1-seg, TIW	1-seg, NTIW
shell type	BEM	BEM	BEM
shell orientation (deg)	0	0	0
no. of shells in series	2	1	4
no. of shells in parallel	1	1	1
no. of tube Passes	2	2	1
tube length (ft)	25.0	28.0	20.0
tube layout pattern (deg)	30	30	30
tube o.d. (in.)	0.625	0.625	0.750
tube pitch (in.)	0.781	0.875	1.000
area (sq ft)	426.0	6644.0	519.0
vibration problems	no	yes	no
purchased cost ($)	10947	38844	20165
	optimal design configuration (purchased cost)		
design variables			
baffle type	1-seg, NTIW	1-seg, NTIW	1-seg, TIW
shell type	BEM	BEM	BEM
no. of shells in series	2	2	1
no. of shells in parallel	1	1	1
no. of tube Passes	4	4	1
tube length (ft)	16.0	24.0	24.0
tube layout pattern (deg)	90	90	90
tube o.d. (in.)	0.750	1.000	0.625
tube pitch (in.)	1.062	1.375	0.781
area (sq ft)	440.0	5278.0	114.0
vibration problems	no	no	no
purchased cost ($)	11019	36124	4960
savings in cost		7%	76%

The percentage savings in the purchased cost for the optimal design obtained by the annealing approach relative to the base case designs are also illustrated in Table 5. The optimal design configuration for the extended set of design variables is presented in the next section.

6. Case Study D: Optimal Design of Heat Exchangers (Based on Purchased Cost) Subject to Vibration Constraints—Extended Variable Set

An extended set of design variables was incorporated to include a larger set of alternatives. The tube data pertaining to o.d., pitch and wall thickness was extended to include five more discrete scenarios. The number of shells in parallel was varied between 1 and 4. It was also possible to define two layouts for the shell orientation: 0 and 90°. Further, the shell types "BEM" and "BJM" were included in the set of design variables, and for single-segmental, NTIW baffle types, there were four types of "vibs" record that were incorporated in the set of decision variables. The total number of combinations is given by ($6 \times 9 \times 12 \times 16 \times 4 \times 2 \times 2 \times$) or 165888 combinations.

Results. The optimal design configurations for the extended set of variables are listed in Table 6. The percentage savings in the cost are also presented in Table 6. The computational savings based on the number of enumerations by the annealer can be expressed as a percentage of the total number of combinations as follows:

$$\text{computational savings} = \frac{165888 - \text{no. of enumerations by the annealer}}{165888} \times 100$$

The computational savings for all the test cases considered were above 98%. This showed that simulated annealing coupled to ST-5 is a potential tool for the optimal design of heat exchangers.

7. Conclusions

Simulated annealing has been shown to be a promising tool for the optimal design of heat exchangers. Since the ST-5 program represents a black-box model, an efficient procedure was developed so that the annealer was able to interact with the ST-5 program. Simulated annealing was able to attain a optimal solution within 5% of the global optimum in most cases and was also able to obtain the global optimum which has an extremely low probability of occurrence. Considerable savings in the objective functions—area (84%) and cost (74%)—were obtained for the reduced-variable cases using simulated annealing. Furthermore, this procedure eliminated designs with vibration problems or infeasible process configurations. The computational savings for the extended variable was approximately 99% with equally promising results. Consequently, simulated annealing represents a viable, robust, favorable technique for the optimal design of heat exchangers and provides a tool to optimize systems of large-scale, black-box models with numerous combinations.

Literature Cited

Amoco Training Course on the Design and Rating of Heat Exchangers—Sensible Heat Transfer and Condensation, Amoco Report, Amoco Chemical Company, Naperville, Illinois, 1994.

Collins, N. E.; Eglese, R. W.; Golden, B. L. Simulated Annealing—An Annotated Bibliography. *Am. J. Math. Sci.* **1988**, *8*, 209.

Kirkpatrick, S.; Gelatt, C.; Vecchi, M. Optimization by Simulated Annealing. *Science* **1983**, *220*, 670.

Peters, M. S., Timmerhaus, K. D. *Plant Design and Economics for Chemical Engineers*, 3rd ed.; McGraw-Hill Book Company: New York, 1980.

Reklaitis, G. V.; Ravindran, A.; Ragsdell, K. M. *Engineering Optimization: Methods and Applications*; Wiley & Sons: New York, 1983.

Rutenbar, R. A. Simulated Annealing Algorithms: An Overview *IEEE Circuits Devices Magazine* **1989**, *100*, 19.

vanLaarhoven, P. J. M.; Aarts, E. H. L. *Simulated Annealing: Theory and Applications*; Reidel Publishing Co.: Holland, 1987.

Received for review January 2, 1997
Revised manuscript received May 5, 1997
Accepted May 6, 1997[⊗]

IE970010H

[⊗] Abstract published in *Advance ACS Abstracts,* August 1, 1997.