HEN Optimizations Without Using Logarithmic-Mean-Temperature Difference

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A simple 1-1 shell-and-tube heat-exchanger model without the logarithmic-mean-temperature difference ΔT_{lm} is proposed for heat-exchanger network (HEN) optimizations. The model consists of two algebraic equations and allows to determine hot and cold outlet temperatures independent of each other. HEN optimization problems are classified as feasible- and infeasible-path formulations, and compared with regard to problems originating from the use of ΔT_{lm} in exchanger energy-balance equations. The ΔT_{lm}-free model eliminates numerical failures in computing the logarithmic terms with negative arguments due to possible inconsistent initialization/progress of exchanger interconnection temperatures during HEN optimizations. The ΔT_{lm}-free model does not require inclusion of approach-temperature inequality constraints since positive approach temperatures are guaranteed. It also eliminates iterative solution of nonlinear energy-balance equations in feasible-path formulations and is represented as linear equality constraints in infeasible-path formulations for fixed areas, heat-capacity-flow rates, and bypass flows. As demonstrated with two representative HEN optimization problems, the ΔT_{lm}-free model significantly reduces numerical difficulties and decreases computation time in the optimization phase of synthesis/design, retrofit, and flexibility-analysis of HENs. Thus, it permits handling large HEN problems.

Introduction

Heat-exchanger network (HEN) problems are among the most extensively studied problems in chemical engineering (Furman and Sahinidis, 2001) and involve themes such as synthesis, design, retrofit, flexibility analysis, and control (Gundersen and Naess, 1988; Grossmann et al., 1999). The trend of handling these themes is from heuristic/algorithmic approaches (Nishida et al., 1977; Linnhoff and Flower 1978a,b) to completely automated mathematical-programming (MP) based techniques (Floudas et al., 1986; Floudas and Grossmann, 1986; Yee and Grossmann, 1990a,b; Gundersen et al., 1991; Papalexandri and Pistikopoulos, 1993; Briones and Kokossis, 1999). An important aspect of HEN problems is that they draw attention either directly or as challenging test examples for MP-based synthesis, design, retrofitting, flexibility analysis, and control algorithms (Swaney and Grossmann, 1985; Grossmann and Floudas, 1987; Dolan et al., 1990; Dimitriadis and Pistikopoulos, 1995; Glemmestad et al., 1997; Bansal et al., 2000).

MP approaches to HEN problems involve at least one (or iterative combination) of LP, NLP, MILP, and MINLP formulations (Floudas, 1995). Pure LP or MILP formulations are generally used for the synthesis of minimum-utility HENs and are outside the scope of this work since they do not involve exchanger design equations (nonlinear equality constraints) in which the problematical ΔT_{lm} (logarithmic-mean-temperature-difference) term appears. NLP and MINLP formulations are used for synthesis/design,

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retrofitting, and flexibility analysis of HENs (Papalexandri and Pistikopoulos, 1993; Floudas, 1995) and they require the use of exchanger design equations as nonlinear equality constraints.

In HEN optimizations, the problems due to the ΔT_{lm} term generally are avoided in *ad hoc* fashions; such as by using smooth approximating functions of ΔT_{lm} (even the arithmetic average), and by finding the feasible initial guess values for exchanger interconnection temperatures via trial-and-error procedures. Among the smooth approximations to ΔT_{lm}, the most widely used are the Chen (1987), Paterson (1984), and Underwood (1970) approximations. The Chen approximation has the advantage that when the approach temperature on either side of the exchanger equals zero, the driving force (ΔT_{lm}) is approximated as zero; however, the other two approximations still predict a non-zero value. Furthermore, the Paterson approximation slightly overestimates the ΔT_{lm} (thus, underestimates the exchanger area), whereas the Chen approximation slightly underestimates the ΔT_{lm} (thus, overestimates the exchanger area) (Yee and Grossmann, 1990a).

Therefore, if the problems associated with the use of ΔT_{lm} can be avoided without an approximation, the numerical difficulties, problem dimensions, and computation time in the optimization phase of any MP-based synthesis/design, retrofit design, flexibility analysis, and steady-state-model-based control of HENs can be significantly reduced without the loss of accuracy. Also, the MP formulations can be applied to much larger industrial-size HEN problems.

In this work, for simple 1-1 shell-and-tube heat exchangers, an exact model is disclosed, free of the ΔT_{lm} term, and its advantages are demonstrated especially for use in HEN optimizations. First, the notation and equations of the conventional ΔT_{lm} model and the proposed ΔT_{lm}-free model for a single heat exchanger equipped with bypass streams are presented. It is shown that the proposed ΔT_{lm}-free model is identical to the conventional ΔT_{lm} model. Then, a property is disclosed of the ΔT_{lm}-free model that makes it favorable for use in HEN optimizations. Next, the formulation is disclosed of HEN optimization problems as feasible-path and infeasible-path MP formulations. Then, how the proposed ΔT_{lm}-free model avoids the problems associated with the use of ΔT_{lm} such as consistent initialization of exchanger interconnection temperatures is disclosed, as well as how it eliminates iterative solution of nonlinear energy-balance equations in feasible-path formulations. Finally, the conventional and proposed models are compared with two typical HEN optimization problems (a steady-state HEN control problem and an optimal retrofit design with flexibility targeting problem) in terms of initial-guess dependence, total number of decision variables, number of equality and inequality constraints, and computation time.

Conventional ΔT_{lm} Model

Figure 1 shows a single countercurrent heat exchanger of a HEN equipped with two bypass streams and establishes the notation associated with it. The bypass streams are included on both sides of the exchanger for the sake of generality.

An energy balance around the exchanger (before bypass mixing) gives the following nonlinear set of equations (Konukman et al., 1995a) that relate hot- and cold-side effluent temperatures T^e to input temperatures T^i. The first term of Eq. 2 may also be written in terms of the cold stream. The derivation of Eqs. 1–3, without bypass streams ($u=0$), can be found in standard heat-transfer textbooks

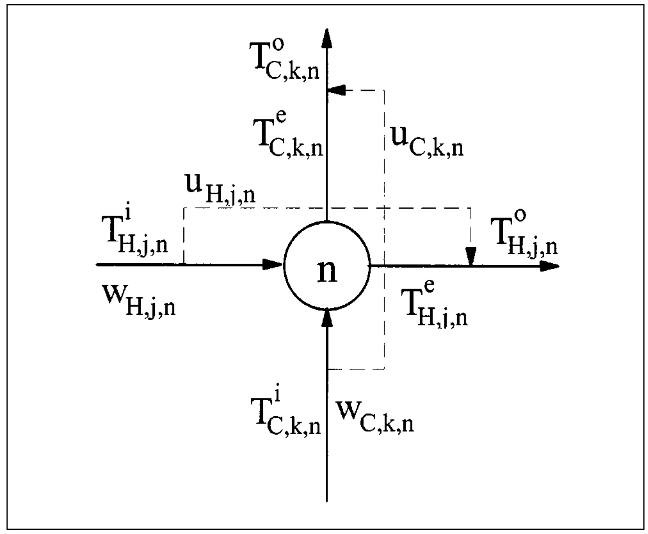

Figure 1. Single heat exchanger with bypass streams and notation.

$$w_{H,j,n}(1-u_{H,j,n})\left(T^i_{H,j,n}-T^e_{H,j,n}\right) - w_{C,k,n}(1-u_{C,k,n})\left(T^e_{C,k,n}-T^i_{C,k,n}\right)=0 \quad (1)$$

$$w_{H,j,n}(1-u_{H,j,n})\left(T^i_{H,j,n}-T^e_{H,j,n}\right)-U_nA_n\Delta T_{lm,n}=0 \quad (2)$$

where

$$\Delta T_{lm,n}=\frac{\left(T^i_{H,j,n}-T^e_{C,k,n}\right)-\left(T^e_{H,j,n}-T^i_{C,k,n}\right)}{\ln\left\{\left(T^i_{H,j,n}-T^e_{C,k,n}\right)/\left(T^e_{H,j,n}-T^i_{C,k,n}\right)\right\}} \quad (3)$$

Energy balances around the bypass-mixing points relate hot- and cold-side output temperatures T^o to input and effluent temperatures with the following set of equations

$$T^o_{H,j,n}=u_{H,j,n}T^i_{H,j,n}+\left(1-u_{H,j,n}\right)T^e_{H,j,n} \quad (4)$$

$$T^o_{C,k,n}=u_{C,k,n}T^i_{C,k,n}+\left(1-u_{C,k,n}\right)T^e_{C,k,n} \quad (5)$$

The exchanger model consists of two equations (Eqs. 1–2), and two unknowns (effluent temperatures) and forms a *nonlinear* algebraic-equation set. Given heat-capacity-flow rates w, inlet temperatures, overall heat-transfer coefficient U, and heat-transfer area A, the effluent temperatures can be calculated by the simultaneous solution of Eqs. 1–2 (such as using a Newton-Raphson (NR) procedure). The outlet temperatures can then be calculated directly from Eqs. 4–5. Alternatively, Eq. 1 can be written in terms of inlet and outlet temperatures as given by Eq. 6

$$w_{H,j,n}\left(T^i_{H,j,n}-T^o_{H,j,n}\right)-w_{C,k,n}\left(T^o_{C,k,n}-T^i_{C,k,n}\right)=0 \quad (6)$$

However, this requires the solution of Eqs. 6, 2, 4, and 5 simultaneously as a four-equation-four-unknown (effluent and outlet temperatures) system.

The numerical/convergence problems for the solution of the model equations of a single heat exchanger are not major. However, initial guesses for the unknowns must be supplied as close to the solution as possible and as consistent with Eq. 3 to avoid the possibility of getting a negative number in the argument of the logarithmic function in the denominator. Therefore, it is better to use a nonlinear-algebraic-equation solver that allows bounds on unknown variables. Additionally, at the limit when $(T_H^i - T_C^e) = (T_H^e - T_C^i)$, the ΔT_{lm} reduces to the arithmetic-mean. This limit, however, cannot be detected automatically during computations and must be remedied by switching from ΔT_{lm} to arithmetic-mean expression, and by using "if-then" programming statements. On the other hand, the problems when using these model equations for a network of heat exchangers are major, and this point will be discussed later.

The ΔT_{lm}-Free Model

For the ΔT_{lm}-free model of a single countercurrent heat exchanger in a HEN, we will start from an unsteady-state distributed-parameter model to make the model terms and coefficients more understandable and proceed through its steady-state solution. It should be mentioned that the ΔT_{lm}-free model can also be obtained from symbolic solution of Eqs. 1–2.

The partial-differential-equation model describing a countercurrent shell-and-tube heat exchanger, where the thermal capacities of the shell-and-tube walls are neglected, is given by Eqs. 7–8 (Friedly, 1972). For the sake of simplicity, we drop the subscripts j, k, and n

$$\frac{\partial T_H}{\partial t} = -\upsilon_H \frac{\partial T_H}{\partial z} - U a_c \frac{(T_H - T_C)}{A_H \rho_H C_{pH}} \tag{7}$$

$$\frac{\partial T_C}{\partial t} = +\upsilon_C \frac{\partial T_C}{\partial z} + U a_c \frac{(T_H - T_C)}{A_C \rho_C C_{pC}} \tag{8}$$

Since Eqs. 7–8 are for the fluids in the tube and shell sides, the linear velocities υ are calculated from the heat-capacity-flow rates w, by taking the bypass fractions into account, as follows

$$\upsilon = \left[w/(A \rho C_p) \right](1-u) \tag{9}$$

The steady-state solution of Eqs. 7–8 obeys the following set of ordinary differential equations

$$\frac{dT_H}{dz} = -\frac{UA}{\omega_H L}(T_H - T_C) \quad \text{at } z=0, T_H = T_H^i \tag{10}$$

$$\frac{dT_C}{dz} = -\frac{UA}{\omega_C L}(T_H - T_C) \quad \text{at } z=L, T_C = T_C^i \tag{11}$$

In going from Eqs. 7–8 to Eqs. 10–11, the following parameters were defined both to simplify the notation and to provide analogy with the ΔT_{lm} model

$$A = a_c L, \quad \omega = \upsilon A \rho C_p = w(1-u) \tag{12}$$

The analytical solution of Eqs. 10–11, when evaluated at $z = L$ for the effluent temperature of the hot stream and at $z = 0$ for the effluent temperature of the cold stream, is given by Eqs. 13–14 (Friedly, 1972; Uztürk, 1996)

$$T_H^e = T_H^i - \Delta T^i \left[\frac{1 - e^r}{1 - \Omega e^r} \right] \tag{13}$$

$$T_C^e = T_C^i + \Delta T^i \left[\frac{\Omega(1 - e^r)}{1 - \Omega e^r} \right] \tag{14}$$

where

$$\Delta T^i = T_H^i - T_C^i \tag{15}$$

$$\Omega = \omega_H / \omega_C \tag{16}$$

$$r = U_0 A_0 \left(\frac{1}{\omega_C} - \frac{1}{\omega_H} \right) \tag{17}$$

If $\omega_H = \omega_C (= \omega)$, then $\Omega = 1$ and $r = 0$. However, the effluent temperatures can be obtained from Eqs. 13–14 by evaluating their limit as $\Omega \to 1$ and $e^r \to 1$. In this case, Eqs. 13–14 can be replaced with the following expressions

$$T_H^e = \frac{T_H^i + [(UA)/\omega] T_C^i}{1 + [(UA)/\omega]} \tag{18}$$

$$T_C^e = \frac{[(UA)/\omega] T_H^i + T_C^i}{1 + [(UA)/\omega]} \tag{19}$$

The exchanger model (Eqs. 13–14) consists of two decoupled equations (*linear* in temperatures), and, thus, contrary to Eqs. 1–2 of the ΔT_{lm} model, the two unknowns (effluent temperatures) can be calculated directly; without numerical/convergence problems. The equivalence of this model to the ΔT_{lm}-based model is proved in Appendix A. As before, energy balances around the bypass-mixing points (Eqs. 4–5) relate hot- and cold-side output temperatures to input and effluent temperatures. Alternatively, the use of only one of the Eqs. 13–14 is sufficient since the other unknown (T_H^e or T_C^e) can be calculated using an overall energy balance (for example, Eq. 1 or Eq. 6). The other advantages of using this ΔT_{lm}-free model for a network of heat exchangers will be disclosed later.

Another important point is that, at the instance when $\omega_H = \omega_C$, the switch from Eqs. 13–14 to Eqs. 18–19 must be done via "if-then" programming statements. However, if the heat-capacity-flow rates w and bypass fractions u are fixed quantities, then the use of "if-then" statements can be avoided by pre-assigning Eqs. 18–19 to the exchangers for which $\omega_H = \omega_C$. On the other hand, the ΔT_{lm}-based model, to avoid the denominator of Eq. 3 becoming zero, requires switching from the logarithmic mean expression (Eq. 3) to the arithmetic mean either when $\omega_H = \omega_C$ or when $(T_H^i - T_C^e) = (T_H^e$

$- T_C^i$) (since each equality implies the other and since Eqs. 1–2 must be solved simultaneously). Therefore, in the ΔT_{lm}-based model, since the effluent temperatures are the unknown variables, the switching problem cannot be avoided (and is coupled with the problem of evading negative arguments in the logarithmic function) even for fixed values of w and u.

A Property of the ΔT_{lm}-Free Model

An important property of the ΔT_{lm}-free model is that it eliminates the necessity of including the minimum-approach-temperature ΔT_a constraints (Eqs. 20–21) in HEN optimizations if the input constraint (Eq. 22) is satisfied for every exchanger in the HEN (nonoverlapping exchanger input temperatures).

The minimum-approach-temperature inequality constraints (MATICs) for exchanger n in the HEN are defined as

$$T_C^i - T_H^e + \Delta T_a \leq 0 \tag{20}$$

$$T_C^e - T_H^i + \Delta T_a \leq 0 \tag{21}$$

The input inequality constraint for exchanger n in the HEN is defined as

$$T_C^i - T_H^i \leq 0 \tag{20}$$

Corollary

If the input constraint (Eq. 22) is satisfied (that is, as long as the inlet temperature of the hot-side fluid is greater than the inlet temperature of cold-side fluid) for an exchanger in the HEN, the ΔT_{lm}-free model (Eqs. 13–14) guarantees that the MATICs (Eqs. 20–21) are satisfied.

Proof

Equations 13–14 can be rearranged as

$$T_H^e - T_C^i = \Delta T^i \lambda_1, \qquad \lambda_1 = e^r\left(\frac{1-\Omega}{1-\Omega e^r}\right) \tag{23}$$

$$T_H^i - T_C^e = \Delta T^i \lambda_2, \qquad \lambda_2 = \left(\frac{1-\Omega}{1-\Omega e^r}\right) \tag{24}$$

Depending on all possible values of Ω (Eq. 16) and r (Eq. 17): (a) If $\Omega > 1$, then $e^r > 1$, so that $\lambda_1,\ \lambda_2 > 0$; (b) If $\Omega < 1$, then $e^r < 1$, so that $\lambda_1,\ \lambda_2 > 0$; (c) If $\Omega = 1$, then $e^r = 1$, so that $\lambda_1,\ \lambda_2 > 0$.

Therefore, given that $\Delta T^i \geq 0$, $\Delta T_a \geq 0$, and since $\lambda_1,\ \lambda_2 \geq 0$ $\forall\ \Omega$ and $\forall\ r$, the inequalities given by Eqs. 25–26, and thus the MATICs, are always true. In other words, even if the minimum-approach-temperature is taken as $\Delta T_a = 0$, as long as $\Delta T^i \geq 0$, it is guaranteed that the crossover of effluent temperatures is not possible. Also, if ΔT_a is specified, then the corresponding requirement for ΔT^i can be calculated

$$T_C^i - T_H^e + \Delta T_a = -\Delta T^i \lambda_1 + \Delta T_a \leq 0 \tag{25}$$

$$T_C^e - T_H^i + \Delta T_a = -\Delta T^i \lambda_2 + \Delta T_a \leq 0 \tag{26}$$

HEN Optimization Formulations

Formulations of HEN optimization problems may be classified as feasible-path (FP) (sequential, modular) and infeasible-path (IP) (simultaneous, equation-oriented).

In FP formulation, the equations describing the energy balances of the exchangers in a HEN are not directly open to the optimizer, and the balance equations are to be satisfied (as the term *feasible* implies) implicitly (such as, in a subroutine) at each iteration of the optimization algorithm. The objective function and the external constraints or variable bounds are the ones that are open to the optimizer. The decision variables in the optimization are the free variables that give extra (positive) degrees of freedom to the problem. In each iteration of the optimization algorithm, the energy balances of the HEN are solved based on the current-iteration values of the decision variables, and the objective function is evaluated based on the feasible solution of the balance equations. The solution of the balance equations in each iteration of the optimizer is done, usually to a high accuracy, in subroutines using algebraic-equation solvers. Thus, the iterative (NR type) solution of the HEN's balance equations is necessary throughout the optimization, including the early stages where the optimizer is far from an optimal or even feasible solution (feasible with respect to external constraints).

In IP formulation, the equations describing the energy balances of the exchangers in a HEN are directly open to the optimizer as equality constraints that are not necessarily satisfied at each iteration of the optimization algorithm (as the term *infeasible* implies). The satisfaction (feasibility) of the balance equations, as well as other constraints, is realized gradually as the optimization algorithm reaches the feasible and optimal solution. The set of decision variables is augmented by the unknowns in the balance equations which are considered as auxiliary decision variables. However, the actual free variables that give the extra degrees of freedom to the problem are still considered to be the original decision variables; the auxiliary variables are consumed in satisfying the balance equations (equality constraints). Thus, in IP formulation, the iterative (NR type) solution of the HEN's balance equations is discarded and replaced by the optimization algorithm's way of handling the equality constraints.

The advantages and disadvantages of the FP and IP formulations with regard to the use of ΔT_{lm}-based and ΔT_{lm}-free models can be discussed with the help of a simple HEN depicted in Figure 2. It should be obvious that an exchanger's inlet temperature T^i is considered (relabeled) the source temperature T^s, if the particular stream is a source stream of the HEN, and that an exchanger's outlet temperature T^o (or, if there is no bypass associated with that stream, effluent temperature T^e) is considered (relabeled) the target temperature T^t, if the particular stream is a target stream of the HEN.

ΔT_{lm}-based model

When the conventional ΔT_{lm}-based exchanger model is used in a FP formulation of a HEN optimization problem, in each iteration of the optimizer, first the nonlinear set of energy-balance equations (Eqs. 1–2) is solved in a subroutine (such as using NR procedure), and then Eqs. 4–5 are used to compute the outlet (target) temperatures. This is done for

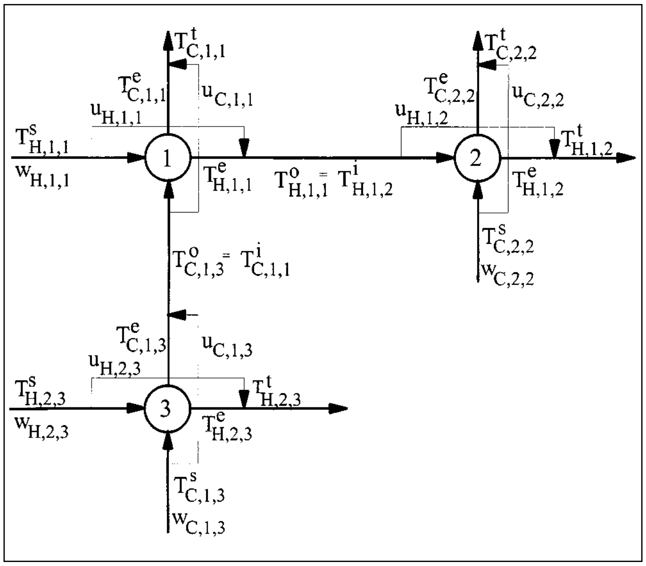

Figure 2. HEN with bypass streams and notation.

each exchanger and in the order of the direction of material flow. With respect to the HEN shown in Figure 2, first for exchanger $n = 3$, Eqs. 1–2 are to be solved simultaneously to calculate the hot and cold effluent temperatures ($T^e_{H,2,3}$ and $T^e_{C,1,3}$); then, Eqs. 4–5 are to be used to compute the hot and cold outlet temperatures ($T^o_{H,2,3} = T^t_{H,2,3}$ and $T^o_{C,1,3} = T^i_{C,1,1}$). Then, the same procedure (subroutine) is applied to exchanger $n = 1$, and finally to exchanger $n = 2$. At each iteration of the optimizer, in the iterative solution of Eqs. 1–2, the initial guesses for the unknowns (effluent temperatures) must be supplied as close to the solution as possible and as consistent with Eq. 3 to avoid the possibility of getting a negative number in the argument of the logarithmic function (such as for exchanger $n = 3$ in Figure 2, $T^e_{C,1,3} < T^i_{H,2,3}$ and $T^e_{H,2,3} > T^s_{C,1,3}$). Alternatively, the exchanger areas may be among the optimization decision variables. In such a case, it may be necessary to include the MATICs for exchangers (Eqs. 20–21) to avoid zero approach temperatures that lead to infinite exchanger areas. However, since Eqs. 20–21 do not contain the decision variables explicitly, the vector of MATICs have to be given implicitly as $\boldsymbol{g}(\boldsymbol{x}) \leq \boldsymbol{0}$ (that is, the outcomes of such inequalities at each iteration depend on the solution of Eqs. 1–2). Furthermore, since most optimization algorithms do not try to satisfy the feasibility of constraints at each iteration, unless remedied with *ad-hoc* "if-then" program statements, the violations of MATICs may lead to failure in computing Eq. 3 due to possible negative argument of the logarithmic function. Thus, it may be necessary to adjust the initial-guess values of the unknowns at each iteration of the optimizer to avoid numerical problems, possibly as dependent on current values of decision variables (such as bypass fractions), and, for instance, for exchanger $n = 2$ in Figure 2, as dependent on the current effluent/outlet temperatures of exchanger $n = 1$. Also, in order to avoid premature termination of optimization, the termination criterion of the optimizer must be larger than the convergence tolerance used for the iterative solution of Eqs. 1–2. Furthermore, at the limit when $(T^i_H - T^e_C) = (T^e_H - T^i_C)$, the shift from ΔT_{lm} to arithmetic-mean must be done smoothly by taking into account the termination criterion of the optimizer, convergence tolerance of the nonlinear solver, and the machine precision.

When the conventional ΔT_{lm}-based exchanger model is used in an IP formulation of a HEN optimization problem, the nonlinear set of energy-balance equations (Eqs. 1–2) and bypass-mixing equations (Eqs. 4–5) are included as equality constraints. Since all equations are handled simultaneously, the direction of material flow in the HEN structure is immaterial. With respect to the HEN shown in Figure 2, besides the original decision variables such as bypass fractions ($u_{H,j,n}$, $u_{C,k,n}$; $j = 1,2$; $k = 1,2$; $n = 1,2,3$), the variables in the balance equations (Eqs. 1–2 and 4–5) are the auxiliary decision variables ($T^e_{H,j,n}$, $T^e_{C,k,n}$, $T^o_{H,j,n}$, $T^o_{C,k,n}$; $j = 1,2$; $k = 1,2$; $n = 1,2,3$). The interconnections may be expressed with equality constraints as well ($T^i_{C,1,1} - T^o_{C,1,3} = 0$ and $T^i_{H,1,2} - T^o_{H,1,1} = 0$). Since all variables in the ΔT_{lm} expression for all exchangers are in the decision-variable set, the initial guesses for these optimization decision variables must be supplied as close to the solution as possible and as consistent with Eq. 3 to avoid getting negative arguments of the logarithmic functions. Besides the initial guesses, to prevent the same problem during optimization, it is also necessary to include the MATICs for exchangers as inequality constraints. However, since most optimization algorithms do not attempt to satisfy the feasibility of constraints at each iteration, it is likely to encounter violations of MATICs and, hence, failure of computations, unless the situation is remedied with *ad-hoc* "if-then" program statements or with the use of approximating expressions for ΔT_{lm}. This is a significant drawback of the ΔT_{lm}-based model, and the difficulties associated with the ΔT_{lm} term is aggravated more when used in HEN optimizations as compared to its use in single-exchanger calculations.

ΔT_{lm}-free model

When the ΔT_{lm}-free exchanger model is used in a FP formulation of a HEN optimization problem, in each iteration of the optimizer, first the linear and decoupled equations (Eqs. 13–14) are used to compute the effluent temperatures within a subroutine, directly without iteration, and then Eqs. 4–5 are used to compute the outlet (target) temperatures. This is done for each exchanger and in the order of the direction of material flow, as explained before. Since the effluent temperatures can be calculated without iteration at every iteration of the optimizer, the initial-guess problems associated with Eq. 3 of the ΔT_{lm}-based model are not present. Also, the inclusion of the MATICs for exchangers are not necessary even if the exchanger areas are among the optimization decision variables since, as proved, given that $\Delta T^i \geq 0$, the MATIC requirements are always satisfied (that is, it is guaranteed that the crossover of effluent temperatures is not possible if $\Delta T^i \geq 0$). Also, given the design specifications (λ_1 and λ_2), it may even be possible to check the feasibility of the posed optimization problem from Eqs. 25–26 before actually solving it. For instance, considering exchanger $n = 3$ in Figure 2, if $T^e_{H,2,3} = T^t_{H,2,3}$ is a hard target (zero variation allowed), then if the specified source-temperature value after disturbance (say $T^s_{C,1,3} = T^i_{C,1,3}$) does not allow satisfaction of Eq. 25 with any value of bypass fraction, then the optimization problem can be concluded as infeasible.

When the ΔT_{lm}-free exchanger model is used in an IP formulation of a HEN optimization problem, the *linear* (with respect to temperatures) and decoupled equations (Eqs. 13–14) and bypass-mixing equations (Eqs. 4–5) are included as equality constraints. The variables in Eqs. 13–14 and 4–5 are the auxiliary decision variables ($T^e_{H,j,n}$, $T^e_{C,k,n}$, $T^o_{H,j,n}$, $T^o_{C,k,n}$; $j=1,2$; $k=1,2$; $n=1,2,3$), and the interconnections may be expressed as equality constraints (that is, $T^i_{C,1,1}-T^o_{C,1,3}=0$ and $T^i_{H,1,2}-T^o_{H,1,1}=0$). However, as opposed to IP formulation with the ΔT_{lm}-based model, where Eq. 2 introduces as many *nonlinear* equality constraints as the number of exchangers in a HEN (even if exchanger areas, flow rates, and bypass fractions are not among the decision variables), Eqs. 13–14 of the ΔT_{lm}-free model introduce the same number of *linear* equality constraints that are more efficiently handled without gradient evaluation by optimization softwares (if exchanger areas, flow rates, and bypass fractions are not among the decision variables). In IP formulation with the ΔT_{lm}-free model, the initial-guess problems associated with Eq. 3 of the ΔT_{lm}-based model are not present. Also, the inclusion of the MATICs for exchangers are not necessary even if the exchanger areas are among the optimization decision variables since, as proved, given that $\Delta T^i \geq 0$, the MATIC requirements are always satisfied (that is, it is guaranteed that the crossover of effluent temperatures is not possible if $\Delta T^i \geq 0$). Therefore, the use of ΔT_{lm}-free model, especially in HEN optimizations, completely eliminates the drawbacks of the conventional ΔT_{lm}-based model and also reduces the number of inequality constraints due to inherent dispensability of the MATICs.

Comparison with Example HEN Optimization Problems

In this section we compare the ΔT_{lm}-based and ΔT_{lm}-free models and demonstrate the advantages of the proposed ΔT_{lm}-free model with two typical HEN optimization problems: a steady-state HEN control problem (Konukman et al., 1995a) and an optimal retrofit design with flexibility targeting problem (Konukman et al., 1995b).

Example 1: steady-state optimal HEN control problem

Figure 3 shows the example HEN with two hot and four cold process streams, five exchangers, four bypass streams, and one split stream. The heat-capacity-flow rates, source- and target-stream temperatures, and exchanger areas shown in the figure correspond to the nominal operating condition of the HEN. The nominal values of the bypass fractions are taken as zero, and the nominal split fraction is 0.4. The overall heat-transfer coefficient U used in the calculations is 500 W/m^2-K for all exchangers. Since the design is fixed (known areas), the minimum-approach temperature ΔT_a was considered to be zero for all exchangers.

The steady-state optimal-control problem is defined as follows: When the HEN experiences source-stream temperature-step disturbances of $+6.5$ K for hot streams and -6.5 K for cold streams, minimize the target-temperature deviations from the nominal values (ΔT^t) and also keep the target-temperatures deviations (ΔT^t) within ± 3 K of the nominal values by the optimal choice of bypass (u) and split (s) fractions.

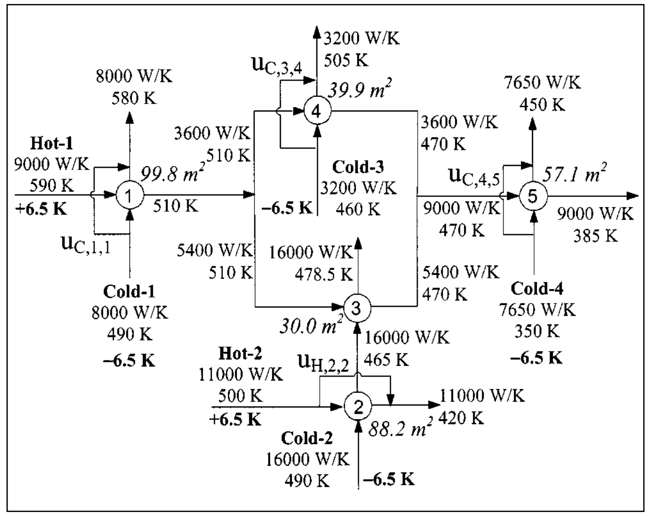

Figure 3. HEN used for steady-state optimal control problem.

The problem was formulated and solved as the IP formulation with ΔT_{lm}-based exchanger model (called P1) and as the FP formulation with ΔT_{lm}-free exchanger model (called P2).

The objective function, identical in both P1 and P2 formulations, was expressed as follows

$$\text{minimize}\left\{\sum_j^2 |\Delta T^t_{H,j,n}| + \sum_k^4 |\Delta T^t_{C,k,n}|\right\} \tag{27}$$

The inequality constraints common in both P1 and P2 are the input constraints for exchangers (Eq. 22), and the following target-temperature range constraints. The target-temperature range constraints were rewritten in standard form $\boldsymbol{g}(\boldsymbol{x}) \leq \mathbf{0}$, and, thus, for each hot and cold target, there were two constraints of the standard form

$$\left(T^i_{H,j,n} - \Delta T^t_{H,j,n}\right) \leq T^o_{H,j,n} \leq \left(T^t_{H,j,n} + \Delta T^t_{H,j,n}\right) \tag{28}$$

$$\left(T^t_{C,k,n} - \Delta T^t_{C,k,n}\right) \leq T^o_{C,k,n} \leq \left(T^t_{C,k,n} + \Delta T^t_{C,k,n}\right) \tag{29}$$

The other inequalities, common in both P1 and P2 and implemented as side constraints (variable bounds), were the bypass and split limits

$$0 \leq u_{H,j,n} \leq 0.95 \tag{30}$$

$$0 \leq u_{C,k,n} \leq 0.95 \tag{31}$$

$$0.05 \leq s \leq 0.95 \tag{32}$$

In P1, there were 15 optimization decision variables ($u_{H,j,n}$, $u_{C,k,n}$, s, $T^e_{H,j,n}$, $T^e_{C,k,n}$). The outlet temperatures ($T^o_{H,j,n}$ and $T^o_{C,k,n}$) were not considered as decision variables since the bypass-mixing equations (Eqs. 4–5) were not used as equality constraints. The number of nonlinear equality constraints in P1 was 10 (Eqs. 1–2 for each exchanger). The total number of inequality constraints in P1 was 27:10 MATICs (Eqs. 20–21 for each exchanger), 5 input constraints (Eq. 22 for each exchanger), and 12 target-temperature range constraints (Eqs. 28–29 for each target stream).

In P2, there were 5 optimization decision variables ($u_{H,j,n}$, $u_{C,k,n}$, s). There were no equality constraints in P2. Since there were no MATICs, the total number of inequality constraints in P2 was 17: 5 input constraint (Eq. 22 for each exchanger), and 12 target-temperature range constraints (Eqs. 28–29 for each target stream).

The optimization problems P1 and P2 were solved using the package ADS (a FORTRAN program for Automated Design Synthesis) (Vanderplaats, 1984) on a PC using double-precision arithmetic and by overriding (tightening) some of the default ADS parameters. The algorithmic options of ADS were selected such that the problems were solved with the exterior-penalty-function technique utilizing the Broyden-Fletcher-Goldfarb-Shanno (BFGS) variable-metric method for unconstrained optimizations and the polynomial interpolation with bounds for one-dimensional (1–D) searches.

The problem P1 (ΔT_{lm}-based model), with 15 decision variables, 10 equality constraints, and 27 inequality constraints, required 5,540 total function (model) evaluations. However, the problem P2 (ΔT_{lm}-free model), with 5 decision variables, no equality constraints, and 17 inequality constraints, required only 595 total function (model) evaluations. Both solutions were identical. Thus, even for this simple problem, the use of the proposed ΔT_{lm}-free model in FP formulation required about 1/9th of the total function evaluations and 1/5th of the execution time as compared to the conventional ΔT_{lm}-based model in IP formulation (with which there were also difficulties associated with supplying good initial guesses consistent with Eq. 3).

Example 2: optimal HEN retrofit design with flexibility targeting problem

The optimal HEN retrofit with flexibility targeting problem (Konukman et al., 1995b) can be defined as follows: given HEN structure, bypass locations, and targeted flexibility, the objectives of the optimal retrofit design are as follows: the design should be a minimum total cost (area plus utility) design; without a disturbance, the retrofit HEN should recover the nominal operating conditions exactly; it should possess maximum flexibility in each disturbance direction; and it should satisfy target-temperature hard/soft constraints for all disturbance directions. The decision variables to achieve these objectives are the bypass fractions (a different set for each disturbance direction) and the increments in heat-exchanger areas (common to each disturbance direction).

As some background information may be needed for this section, a general formulation for the "optimal retrofit/design with flexibility-targeting" problem and its special case "vertex-based formulation" are provided in Appendix B.

The disturbance directions are the vertices of the polyhedral (hypercubical) region of uncertainty in the space of source-stream temperatures. The largest possible distance of the vertices from the centeroid is called the *flexibility index* (Swaney and Grossmann, 1985) that shows the maximum magnitude of the disturbance (identical in all source streams) under which the HEN remains feasible. Therefore, a flexibility target less than the flexibility index specifies the distance of the vertices from the centeroid of the hypercube, and, thus, specifies the magnitude of the disturbance in the source-stream temperatures. In other words, when all source-stream temperatures are perturbed by the same scalar, called the flexibility target, the HEN is required to be feasible and optimal simultaneously at all vertex points) When the uncertainty is in the source-stream temperatures of a HEN, it is known that (Floudas, 1995) the problem is convex, and, thus, if the retrofit HEN is feasible at the targeted flexibility, it will be feasible (operable) for any disturbance that falls anywhere in the hypercubical region. For a HEN problem with NH hot streams and NC cold streams, there are $V = 2^N$ vertices ($N = NH + NC$) (+ and − directed simultaneous disturbance directions) besides the nominal operating point (under no disturbance).

To summarize without the mathematical details, the vertex-based optimal HEN retrofit with flexibility targeting problem formulation requires the equality constraints (energy balances) and inequality constraints (input and MATICs, and bypass limits) to be written for each of the 2^N vertices, as well as for the nominal operating point. The decision variables are the exchanger effluent temperatures and bypass fractions (a different set with dimension $V + 1$: for each vertex direction and for the nominal operating point), and the heat-exchanger areas (unique to all $V + 1$ operating points).

Figure 4 shows the example HEN with two hot and two cold process streams, three process exchangers, one utility exchanger (cooler), and three bypass streams. The heat-capacity-flow rates, source- and target-stream temperatures shown in the figure correspond to the nominal operating condition of the HEN. The overall heat-transfer coefficient U, used in the calculations was 1,000 W/m^2-K for all exchangers. The minimum-approach temperature ΔT_a was considered to be 0 K for all exchangers since the objective function minimizes the exchanger areas. The target temperatures were considered to be hard targets. With $NH = 2$, $NC = 2$, the total number of vertices is $V = 2^{(2+2)} = 16$, and including the nominal point, there are $V + 1 = 17$ operating points.

The problem was formulated and solved as the IP formulation with the ΔT_{lm}-based exchanger model (called P3), and as the IP formulation with ΔT_{lm}-free exchanger model (called P4).

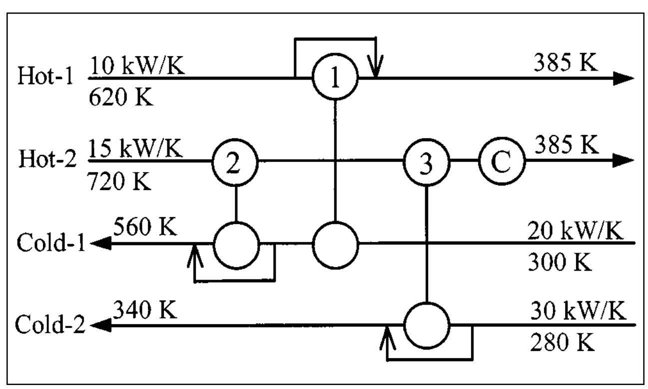

Figure 4. HEN used for optimal retrofit design with flexibility targeting problem.

The objective function, identical in both P3 and P4 formulations, was expressed with Eq. 33 for the particular HEN shown in Figure 4. The fixed cost term includes the areas of the process exchangers only (A_n, $n = 1,2,3$). The constant γ is the annual rate of return factor for the fixed costs, α, β, C_E, are the investment cost coefficients for exchangers, and C_C is the coefficient for the cost of cooling.

$$\underset{\left(\begin{array}{c} u_{H,j,n,d}, u_{C,k,n,d}, \\ T^e_{H,j,n,d}, T^e_{C,k,n,d}, A_n \end{array}\right)}{\text{minimize}} \quad \gamma \sum_{n=1}^{3} \left(C_E + \alpha A_n^{\beta}\right) + \left(C_C Q_{C,d=0}\right) \qquad (33)$$

The utility cost (cost of cooling) was calculated from the heat load of the cooler ($Q_{C,d=0}$) as shown in Eq. 34. The heat load of the cooler is operating point dependent ($V+1$ operating points). However, in the objective function, the heat load only at the nominal operating point ($d = 0$) was used

$$Q_{C,d=0} = w_{H,3,3}\left(T^e_{H,3,3,d=0} - 385\right) \qquad (34)$$

The inequality constraints common in both P3 and P4 are the input constraints for exchangers (Eq. 22). These inequalities are written for all vertices and for the nominal operating point. Since the target temperatures were considered to be hard targets (no variation is allowed), they are fixed at the nominal-operating-point values, and thus no target-temperature range constraints were used. The other inequalities, common in both P3 and P4 and implemented as side constraints (variable bounds), were the bypass and split limits (Eqs. 30–32). These bounds were defined for all vertex points and for the nominal operating point. Additionally, in both P3 and P4, to guarantee that the cooler is functioning properly, the following inequality was written for all vertices and for the nominal operating point

$$385 - T^e_{H,3,3,d} \le 0 \qquad d = 0,...,16 \qquad (35)$$

The equality constraints common in both P3 and P4 were the bypass-mixing equations (Eqs. 4–5). These equalities were written for all vertices and for the nominal operating point. The MATICs were included only in P3, and these inequalities were written for all vertices and for the nominal operating point. Formulation P4 did not include the MATICs. In P3, the equality constraints were the energy-balance equations including the ΔT_{lm} term (Eqs. 1–2). In P4, the equality constraints were the effluent-temperature expressions of the ΔT_{lm}-free model (Eqs. 13–14).

In both P3 and P4, the total number of optimization decision variables were 156; 3×17 bypass fractions ($u_{H,1,1,\mathrm{d}}$ and $u_{C,k,n,d}$; $k = 1,2$; $n = 2,3$, $d = 0,...16$), 6×17 effluent temperatures ($T^e_{H,j,n,d}$, $T^e_{C,k,n,d}$; $j = 1,2$; $k = 1,2$; $n = 1,...,3$, $d = 0,...16$), and three areas (A_n; $n = 1,...,3$). The number of equality constraints in both P3 and P4 was 153; 3×17 bypass-mixing equations (Eqs. 4–5), and 6×17 energy-balance equations (Eqs. 1–2 in P3 or Eqs. 13–14 in P4). The total number of inequality constraints in P3 was 153: 6×17 MATICs (Eqs. 20–21 for each exchanger), 2×17 input constraints (Eq. 24 for each exchanger), and 1×17 cooler constraints (Eq. 35). The total number of inequality constraints in P4 was 51 since no MATICs were necessary. It should also be noted that P3 involves the computation of the ΔT_{lm} term (Eq. 3) in 51 equality constraints (Eq. 2).

The optimization problems P3 and P4 were solved using the widely-used package General Algebraic Modeling System (GAMS) (Brooke et al., 1992), which is a front-end parser for powerful solvers. The NLP solver used with GAMS was CONOPT (based on the GRG algorithm) (Drud, 1994). The values of the constants used were $\gamma = 0.125$, $\alpha = 150$, $\beta = 1$, $C_E = 5{,}500$, and $C_C = 15$. The flexibility target was $\delta = 5$ K. The bypasses were limited as $0.05 \le u \le 0.95$.

When the set of initial guesses for the decision variables were supplied very close to the solution, the problem P3 (ΔT_{lm}-based model: with 156 decision variables, 153 equality constraints, 153 inequality constraints, and 702 non-zero elements in GAMS) consumed about twice the CPU time in CONOPT as compared to problem P4 (ΔT_{lm}-free model: with 156 decision variables, 153 equality constraints, 51 inequality constraints, and 549 non-zero elements in GAMS). Both solutions were identical. When the initial guesses were supplied away from the solution, the problem P3 either required more computational resources or failed due to numerical problems related to the ΔT_{lm} term. On the other hand, the problem P4 was successfully solved even without supplying an initial-guess set.

Additional Comments

The above comparisons, even with relatively simple example problems, disclose the advantages of the proposed ΔT_{lm}-free model over the conventional ΔT_{lm}-based model in terms of total number of function evaluations and execution time, as well as in avoiding difficulties related to supplying initial guesses consistent with the ΔT_{lm} term. The examples presented above required only one time solution of the nonlinear programming (NPL) problems with continuous variables only. The advantages of the proposed ΔT_{lm}-free model should be even more striking when used in large-scale problems involving MINLP formulations which require iterative solution of a primal NLP problem and a master MILP problem. One good example is the multiperiod hyperstructure MINLP formulation of Papalexandri and Pistikopoulos (1993) for the synthesis and retrofit of flexible HENs. In their article, the authors solved, with GAMS using the Generalized Benders Decomposition (GBD) algorithm (Floudas, 1995), a large problem that involved 2,891 constraints, 2,832 continuous variables, and 1,098 structure-determining binary variables. In the NLP primal problem of the GBD, the equality constraints involved nonlinear energy-balance equations containing the ΔT_{lm} term. The entire GBD algorithm was repeated until the flexibility test satisfied the flexibility target. The advantages of using the proposed ΔT_{lm}-free model in such large problems requiring iteration/decomposition should be significant. Another example that requires repetitive solution of steady-state HEN optimization problem is the model predictive control (MPC) of HENs (Akman and Uygun, 1999), where optimal bypass flows were obtained from the steady-state model of a HEN and supplied to the dynamic optimizer as optimal steady-state manipulated-variable targets at each sampling period of the MPC algorithm. The use of ΔT_{lm}-free model in steady-state HEN optimization enables completion of the dynamic and steady-state optimization tasks within restricted sampling periods.

Conclusions

A heat-exchanger model that does not involve ΔT_{lm} term was presented for use in HEN optimizations. The model consists of two algebraic equations and allows the determination of hot- and cold-side outlet temperatures independently. The use of the ΔT_{lm}-free model in HEN optimization problems eliminates, without an approximation, numerical failures in computing the logarithmic terms with negative arguments due to possible inconsistent initializations or progress of exchanger interconnection temperatures during optimization. The proposed ΔT_{lm}-free model: does not require the inclusion of approach-temperature inequality constraints since positive approach temperatures are automatically satisfied, and thus reduces the size of the optimization problems; eliminates iterative solution of nonlinear energy-balance equations in feasible-path formulations; and is represented as linear equality constraints in infeasible-path formulations for fixed heat-capacity-flow rates and bypass flows. The use of the ΔT_{lm}-free model in HEN optimizations reduces problem dimensions and decreases computation time, and thus permits handling of large industrial-size HEN problems.

Acknowledgments

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Notation

a_C = outer surface area of tube per unit length (cold side), m^2/m
A = exchanger overall heat-transfer area, m^2
A_C = shell (cold) side cross sectional area, m^2
A_H = tube (hot) side cross sectional area, m^2
C_C = cost coefficient for cost of cooling, \$/kW-year
C_E = investment cost constant for exchanger area, \$
C_p = heat capacity, J/kg·K
$\boldsymbol{d}$ = vector of design variables
$\boldsymbol{g}(.)$ = vector of inequality constraints
$\boldsymbol{h}(.)$ = vector of equality constraints
L = length of heat exchanger, m
N = total number of process streams
NC = number of cold process streams
NH = number of hot process streams
$\boldsymbol{p}$ = vector of fixed parameters
q = differential amount of heat transferred, W
Q = total heat-transfer rate, W
Q_C = heat load of cooler, W
R = region describing scaled hyperrectangle
s = split fraction
t = time, h
T = temperature, K
ΔT_a = minimum approach temperature, K
ΔT^i = temperature difference between hot and cold inlets, K
ΔT_{lm} = logarithmic mean temperature difference, K
ΔT^t = target-temperature deviation from nominal value, K
u = bypass fraction
$\boldsymbol{u}$ = vector of control/free variables
U = overall heat-transfer coefficient based on tube outside, W/K·m^2
v = velocity, m/h
V = total number of operating points (vertex points)
w = heat-capacity-flow rate, W/K
$\boldsymbol{x}$ = vector of decision variables, vector of state variables
z = axial position, m

Greek letters

α = investment cost coefficient for exchanger area, \$/m^2
β = investment cost exponent for exchanger area
γ = annualization factor, 1/yr
δ = flexibility target
δ^* = flexibility index
θ = vector of uncertain parameters
θ^o = vector of nominal values of uncertain parameters
$\Delta\theta^{\pm}$ = scaled deviations from vector of nominal values of uncertain parameters
ρ = fluid density, kg/m^3
Φ = objective function

Subscripts

C = cold
d = vertex identifier
H = hot
j = cold process stream index
k = hot process stream index
n = exchanger index

Superscripts

d = vertex identifier
e = effluent (before bypass mixing)
i = inlet
o = outlet (after bypass mixing), nominal value
t = target

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Appendix A

The equivalence of the ΔT_{lm}-free and ΔT_{lm}-based models can be proved as follows.

In a single-pass shell-and-tube heat exchanger, the differential energy balance over a differential section is given as

$$dq = \omega_H dT_H = \omega_C dT_C = U(T_H - T_C)dA \tag{A1}$$

Substituting dT_H into the differential equation for the hot fluid (Eq. 10), simplifying with $\Delta T = (T_H - T_C)$ and rearranging gives

$$\frac{dq}{\Delta T} = -\frac{UA}{L}dz \tag{A2}$$

For constant heat-capacity-flow rates, the mixing-cup temperatures are linear with respect to q, and, hence, their difference ΔT is also linear with respect to q. Therefore, the derivative of ΔT with respect to q may be expressed in terms of the overall change in ΔT and total heat-transfer rate Q as follows:

$$\frac{d(\Delta T)}{dq} = \frac{\Delta T_{|z=0} - \Delta T_{|z=L}}{Q} \tag{A3}$$

Rearranging Eq. A3, substituting into Eq. A2, and integrating gives

$$\int_{\Delta T_{|z=0}}^{\Delta T_{|z=L}} \frac{Q}{\Delta T_{|z=0} - \Delta T_{|z=L}} \frac{d(\Delta T)}{\Delta T} = \int_0^L -\frac{UA}{L}dz \tag{A4}$$

$$\frac{Q}{\Delta T_{|z=0} - \Delta T_{|z=L}} \ln\left(\frac{\Delta T_{|z=L}}{\Delta T_{|z=0}}\right) = -UA \tag{A5}$$

$$Q = UA\frac{\Delta T_{|z=0} - \Delta T_{|z=L}}{\ln\left(\frac{\Delta T_{|z=0}}{\Delta T_{|z=L}}\right)} = Q = UA\Delta T_{lm} \tag{A6}$$

Appendix B

The general MP formulation for an optimal retrofit/design with flexibility targeting can be stated as (Swaney and Grossmann, 1985)

$$\min_{\boldsymbol{d},\boldsymbol{x},\boldsymbol{u}} (\boldsymbol{d},\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{\theta}) \tag{B1}$$

$$\text{s.t.} \quad \boldsymbol{h}(\boldsymbol{d},\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{\theta}) = \boldsymbol{0} \tag{B2}$$

$$\boldsymbol{g}(\boldsymbol{d},\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{\theta}) \le \boldsymbol{0} \tag{B3}$$

$$\theta \in R(\delta) = \{\theta | (\theta^\circ - \delta\Delta\theta^-) \le \theta \le (\theta^\circ = \delta\Delta\theta^+)\} \tag{B4}$$

where $\boldsymbol{d}$ is the vector of design variables (exchanger areas), $\boldsymbol{x}$ is the vector of state variables (outlet/effluent temperatures), $\boldsymbol{u}$ is the vector of control/free variables (heater/cooler loads, bypass flows), $\boldsymbol{p}$ is the vector of fixed parameters (heat-transfer coefficients), and $\boldsymbol{\theta}$ is the vector of uncertain parameters (in this work, source-stream temperatures). Equation B1 is the objective function and can be formulated in terms of total annualized cost or total utility consumption. If the vector of states $\boldsymbol{x}$ can be eliminated using Eq. B2, then Eq. B3 can be written as the vector of reduced inequalities. Equation B4 describes the range of the uncertain parameters as deviations from nominal values $\boldsymbol{\theta}^o$, where $\Delta\boldsymbol{\theta}^-$ and $\Delta\boldsymbol{\theta}^+$ are the scaled deviations from $\boldsymbol{\theta}^o$, and the non-negative scalar δ is the targeted flexibility. The region $R(\delta)$ describes the scaled hyperrectangle which is required to be within the feasible region defined by Eqs. B2 and B3. For a fixed HEN design (known $\boldsymbol{d}$), the flexibility index δ^* defined by Swaney and Grossmann (1985) is the maximum of scalar δ. This problem (Eqs. B1 through B4) can be solved indirectly with a two-stage procedure (as iterations between a multiperiod synthesis problem and a flexibility-analysis step) (Papalexandri and Pistikopoulos, 1993). However, this technique requires the solution of large MIPs through, for example, the generalized benders decomposition (Floudas, 1995) in each iteration.

The optimal retrofit design of HENs satisfying a given flexibility target can be accomplished through a one-stage, noniterative formulation with the supposition that the feasible region defined by the reduced inequality constraints is convex in uncertain parameters. Therefore, the optimal solution can be explored on the basis of the vertices of the polyhedral region of uncertainty. For this purpose, the general vertex-based formulation is described by

$$\min_{\boldsymbol{x}^d, \boldsymbol{x}^d} \Phi(\boldsymbol{d}^0, \boldsymbol{x}^0, \boldsymbol{u}^0, \boldsymbol{p}, \boldsymbol{\theta}^0) \qquad d = 0, 1, \ldots, 2^N \tag{B5}$$

$$\text{s.t.} \quad \boldsymbol{h}^d(\boldsymbol{d}^0, \boldsymbol{x}^d, \boldsymbol{z}^0, \boldsymbol{u}^d, \boldsymbol{p}, \boldsymbol{\theta}) = \mathbf{0} \qquad d = 0, 1, \ldots, 2^N \tag{B6}$$

$$\boldsymbol{g}^d(\boldsymbol{d}^0, \boldsymbol{x}^d, \boldsymbol{z}^0, \boldsymbol{u}^d, \boldsymbol{p}, \boldsymbol{\theta}) \le \mathbf{0} \qquad d = 0, 1, \ldots, 2^N \tag{B7}$$

$$\theta - \theta^0 = \mathbf{0} \qquad d = 0 \tag{B8}$$

$$\theta - \theta^0 - \delta\theta^d = \mathbf{0} \qquad d = 1, \ldots, 2^N \tag{B9}$$

$$\theta^d \in R_0(\delta) = \{\theta^d | \theta^d \text{is a vertex of} R(\delta), \quad d = 1, \ldots, 2^N\} \tag{B10}$$

The vertex formulation, described by Eqs. B5 through B10, is a reformulation of the more general nonvertex formulation, described by Eqs. B1 through B4, using the approach named as "Algorithm I" by Halemane and Grossmann (1983). In this case, the feasible region defined by the reduced inequality constraints is convex in uncertain parameters $\boldsymbol{\theta}$, and the formulations described by Eqs. B1 through B4 and Eqs. B5 through B10 are identical (Halemane and Grossmann, 1983; Swaney and Grossmann, 1985). For a HEN problem where the uncertain parameters are considered to be the source-stream temperatures only, the feasible region defined by the reduced inequality constraints is convex (Floudas, 1995). Thus, the critical point that limits the solution lies at a vertex of the polyhedral region of uncertainty, and Eqs. B5 through B10 can be used instead of Eqs. B1 through B4. Equation B5 is the objective function that is evaluated at the nominal operating point $d = 0$. Equations B6 and B7 are the augmented forms of the vector of equality and inequality constraints (Eqs. B2 and B3) that are evaluated at the nominal operating point ($d = 0$), as well as at each vertex ($d = 1, \ldots, 2^N$) simultaneously. The $\boldsymbol{\theta}$ values in Eqs. B6 and B7 are governed by Eqs. B8 and B9. Equation B9 constrains the vector $\boldsymbol{\theta}$ to take only 2^N vertex values $\boldsymbol{\theta}^d$ ($2^N \pm$ directed deviations from the nominal $\boldsymbol{\theta}^o$ values), scaled by the scalar δ, which is the desired flexibility. Equation B8 denotes that at $d = 0$, δ is considered to be zero. The set $R_o(\delta)$ describes the vertices of the scaled hyperrectangle, which is required to be within the feasible region defined by Eqs. B6 and B7. As indicated in Eq. B5, a unique set of design variables $\boldsymbol{d}^o$ applies to all $2^N + 1$ operating points (2^N vertex points plus the nominal operating point). This enforces the optimal design to be valid at all $2^N + 1$ operating points. The state variables $\boldsymbol{x}^d$ (such as the exchanger outlet temperatures), and the control/free variables, $\boldsymbol{u}^d$ (such as heater/cooler and exchanger heat loads, and bypass flows), are defined for all $2^N + 1$ operating points. In this way, the optimal design (which is unique to all operating points) and the optimal values of the operating-point-dependent state and control vectors are obtained simultaneously as the solution of the optimization problem defined by Eqs. B5 through B10.

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