

# Optimal Design Refinements To Accommodate HEN Cleaning Schedules

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**Supporting Information** 

**ABSTRACT:** Due to severe fouling in the heat-transfer units, the target temperatures of process streams in a heat exchanger network (HEN) may not always be achievable after a sufficiently long period of operation. To circumvent this practical problem, the conventional cost-optimal HEN design should be modified to accommodate online cleaning operations via proper allocation of area margins, bypasses, spares, and auxiliary heaters/ coolers. For the purpose of facilitating solution convergence of the corresponding optimization problem, the candidate units for incorporating margins and the corresponding bypasses are identified on the basis of test



runs in this study and, also, extra constraints on the spares formulated according to a set of heuristic rules to further reduce the search space. A solvable MINLP model can then be constructed by including these test findings and heuristic constraints. From the optimum solution, one could then obtain the proper refinements to any given design to facilitate implementation of an optimal cleaning schedule. Finally, the optimization results of extensive case studies are also presented in this article to demonstrate the feasibility and effectiveness of the proposed approach.

## 1. INTRODUCTION

Efficient energy recovery is an important objective of process design not only for cost reduction but also for emission minimization, while a heat exchanger network (HEN) can be configured to facilitate these purposes for almost any chemical plant. After putting all heat exchangers in service, the solid impurities in process streams may be deposited continuously on their heat-transfer surfaces and, thus, the overall performance of HEN tends to deteriorate over time. This fouling problem can be abated by cleaning the heat transfer units as a part of the general maintenance (or checkup) program during the planned shutdown. However, since it is also possible to clean some of them when the normal production is still in progress, a proper scheduling strategy must be developed to maximize the implied cost saving.

A programming approach has often been adopted in the past to produce the aforementioned cleaning schedules. To this end, Smaili et al.<sup>1</sup> first developed a mixed integer nonlinear programming (MINLP) model for the thin-juice preheat train in a sugar refinery. Since its global solution cannot always be obtained, several additional studies have been carried out to overcome the convergence problems. Georgiadis et al.<sup>2</sup> tried to build a mixed integer linear program (MILP) via linearization of the nonlinear constraints so as to produce the near-optimum schedules efficiently, while Georgiadis and Papageorgiou<sup>3</sup> later proposed improved solution strategies of the MINLP models. Alle et al.<sup>4</sup> then solved several example problems with the outer approximation algorithm, while Smaili et al.5 made use of the simulated annealing, threshold accepting, and backtracking threshold accepting algorithms. Again for the purpose of reaching the global optimum efficiently, Lavaja and Bagajewicz<sup>6</sup>

formulated a new MILP model for the schedule synthesis problem. Markowski and Urbaniec<sup>7</sup> applied a graphic method to analyze the effects of fouling and the corresponding cleaning schedules. Assis et al.<sup>8</sup> proposed to apply heuristic rules to roughly predict the performance of each heat exchanger before solving the mathematical programs so as to avoid trapping in the local optimum, while Gonçalves et al.<sup>9</sup> also adopted recursive heuristics to facilitate effective convergence.

Other than the above studies on solution strategies, a few practical issues in realistic applications were also addressed. Sanaye and Niroomand<sup>10</sup> produced the optimal HEN cleaning schedule for the urea and ammonia units by minimizing the operating cost. In a grass-root design, Xiao et al.<sup>11</sup> developed a programming approach to generate both a HEN structure and the corresponding cleaning schedule by minimizing the total annual cost. Ishiyama et al.<sup>12</sup> synthesized the cleaning schedule for the crude preheating train with special emphasis on maintaining a stable feed temperature of the desalting unit, while Ishiyama et al.<sup>13</sup> considered different cleaning models for fouling and aging on the heat-transfer surface.

Although a cleaning schedule generated with any of the existing methods could be used to effectively reduce the additional utility costs caused by fouling, a defouling operation still calls for temporary removal of one or more online units for a considerable amount of time. The missing heat duties may be compensated online with several operational techniques, i.e.,

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Figure 1. A fictitious stream structure in HEN.

- (a) Replacing the removed unit with a spare one.
- (b) Adjusting the heat duties in the available units by making use of area margins and bypasses.
- (c) Raising the hot and cold utility consumption rates in the existing heaters and coolers and/or extra auxiliary units.

Although Cheng and Chang<sup>14</sup> developed a MINLP model to generate the HEN cleaning schedule and spare replacement schedule simultaneously, virtually no studies have been performed for systematic implementation of the other options mentioned above. On the other hand, it should be noted that these added features in HEN, i.e., margins, bypasses, and auxiliary units, were quite useful for enhancement of system operability and controllability during normal operation<sup>15,16</sup> and also for retrofit designs.<sup>17</sup> It can be expected that they should also be effective for energy minimization in the defouling operations. Since the aforementioned design refinements were only considered partially in the existing schedule synthesis strategy, there are incentives to modify the available model<sup>14</sup> to optimally allocate spares, margins, bypasses, and auxiliary heats/coolers for implementing an effective and energy efficient cleaning schedule.

#### 2. TIME HORIZON PARTITION

In this work, the maximum length of time horizon that can be considered for schedule synthesis (say  $t_f$ ) is the duration in months between the ending and beginning instances of two consecutive planned plant shutdowns. To simplify calculation, the entire duration of a cleaning schedule for a given HEN is set to be coincided with this time interval. This schedule horizon  $[0,t_f]$  is partitioned into  $n_v$  different periods and each is further divided into two intervals for performing the cleaning and heatexchange operations, respectively. The existing equal-length assumption concerning the above time periods<sup>14</sup> is still adopted in the present study, i.e.,  $t_f = n_p \tau$ , where  $n_p$  is the total number of time periods and  $\tau$  is a given constant denoting the period length. It is also assumed that the durations of all subperiods required for defouling  $(f_c)$  are the same and their values can be determined in advance. Thus, within each partitioned period, four time points should also be identified to facilitate accurate presentation of the proposed model, i.e., bcp (beginning of cleaning subperiod), ecp (end of cleaning subperiod), bop (beginning of operation subperiod), and eop (end of operation subperiod). Note that time point ecp represents the instance

just before bop. To produce concise model formulation, let us introduce the following two label sets to characterize the periods and time points, respectively:

$$\mathbf{P} = \{1, 2, \cdots, n_{\mathbf{P}}\}$$

 $TP = \{bcp, ecp, bop, eop\}$ 

## 3. REPRESENTATION OF HEN STRUCTURE

It is assumed that, before applying the proposed method, a preliminary HEN design should be made available a priori. In principle, this design can be produced with any traditional HEN synthesis procedure, e.g., Papoulias and Grossmann<sup>18</sup> or Yee and Grossmann.<sup>19</sup> To characterize this given structure, let us first introduce the following two label sets to collect and classify the process streams:

 $I = \{i \mid i \text{ is the label of a hot stream in a given HEN} \}$ 

 $J = \{j \mid j \text{ is the label of a cold stream in a given HEN} \}$ 

Since the HEN design is known, each set can be further divided into two subsets as follows:

$$I = I_a \cup I_b$$
$$J = J_a \cup J_b$$

where,  $I_a$  is a set of hot streams which are cooled without utilities and  $I_b = I/I_a$ ;  $J_a$  is a set of cold streams which are heated without utilities and  $J_b = J/J_a$ . In addition, the matches in HEN can be expressed mathematically with a function, i.e., a mapping from the set of heat exchangers between process steams (EX) to the set of matches (MA), i.e., *f*: EX  $\rightarrow$  MA The units in the given HEN are represented with labels in the former set, i.e.,

 $EX = \{e \mid e \text{ denotes an existing unit in the given HEN}\}$ 

The corresponding matches are stored in the latter set, i.e.,

$$MA = \{(i, j)|(i, j) \text{ denotes an existing match between} \\ \text{streams } i \in I \text{ and } i \in I \}$$

Notice that f(e) = (i,j) is known for all  $e \in EX$ . In addition, the HEN structure can be described more clearly by defining the following subsets of EX:

 $EX_{i'} = \{e_{i'} \mid e_{i'} \in EX \text{ denotes a unit on hot stream } i'\}$ 

 $\text{EX}_{j'} = \{e_{j'} \mid e_{j'} \in \text{EX} \text{ denotes a unit on hot stream } j'\}$ 

where,  $i' \in I$  and  $j' \in J$  Since the units on each process stream may be placed in series and/or in parallel, they can be classified according to the "mixing points" as follows:

 $\text{EX}_{i'}^m = \{e_{i'}^m | e_{i'}^m \text{ denotes a unit just before } m^{\text{th}}\}$ 

mixing points on hot stream i'}

 $\text{EX}_{j'}^n = \{e_{j'}^n | e_{j'}^n \text{ denotes a unit just before } n^{\text{th}} \}$ 

mixing points on hot stream j'

where,  $EX_{i'} = U_{m=1}^{Mi'} EX_{i'}^m$  and  $M_{i'}$  is the total number of mixing points on hot stream i';  $EX_{j'} = U_{n=1}^{N_{j'}} EX_{j'}^n$  and  $N_{j'}$  is the total number of mixing points on cold stream j'. To further clarify this notation, let us consider the bullets (i.e., mixing points) in the fictitious structure in Figure 1. One can identify that

- $M_{i'} = 2$ ,  $EX_{i'}^1 = \{1,2\}$ , and  $EX_{i'}^2 = \{3\}$  on hot steam i'.
- $N_{j'} = 3$ ,  $EX_{j'}^1 = \{4,5\}$ ,  $EX_{j'}^2 = \{6,7\}$ , and  $EX_{j'}^3 = \{8\}$  on cold stream j'.

Notice that it is also assumed that a bypass may join the output streams from heat exchangers at each mixing point.

Finally, let us group all spares into another set to make model notation consistent:

 $S = \{s \mid s \text{ is label of a spare}\}$ 

## 4. BINARY VARIABLES AND LOGIC CONSTRAINTS

The selections of exchangers to be cleaned can be expressed with the following binary variables:

$$Y_{e,p} = \begin{cases} 1 \text{ if heat exchanger } e \text{ is cleaned in period } p \\ 0 \text{ otherwise} \end{cases}$$
(1)

where,  $e \in EX$  and  $p \in P$ . To facilitate formulation simplicity, let us introduce an additional parameter in the proposed model, i.e.,

$$Y_{e,0} = 0$$
 (2)

Notice that  $e \in EX$  and  $0 \notin P$ .

On the other hand, it is clear that the decision to use a spare to replace unit *e* in period *p* can only be made after determining whether this unit should be removed and cleaned in the same period. All such logic constraints can be represented with another set of binary variables  $X_{e,p,p}$  i.e.,

$$(1 - Y_{e,p}) + \sum_{s \in S} X_{e,p,s} \le 1$$
 (3)

where,  $e \in EX$ ,  $p \in P$  and

$$X_{e,p,s} = \begin{cases} 1 \text{ if heat exchanger } e \text{ is replaced with spare } s \\ \text{ in period } p \\ 0 \text{ otherwise} \end{cases}$$
(4)

Obviously, spare s can be used to replace at most one unit in period p, i.e.,

$$\sum_{e \in \mathrm{EX}} X_{e,p,s} \le 1 \tag{5}$$

For the entire horizon, it is necessary to make use of the following inequality constraint to summarize the connection between every pair of unit and spare:

$$\sum_{p \in \mathcal{P}} X_{e,p,s} \le n_{\mathcal{P}} \Gamma_{e,s} \tag{6}$$

where,  $e \in \text{EX}$ ;  $s \in S$ ;  $n_p$  is the total number of periods;  $\Gamma_{e,s} \in \{1,0\}$  is used to reflect whether or not spare *s* is used in at least one period to replace unit *e*. If a particular unit can only be replaced with the same spare, then the corresponding constraint should be

$$\sum_{s \in \mathcal{S}} \Gamma_{e,s} \le 1 \tag{7}$$

where,  $e \in EX$ . If, on the other hand, a particular spare can be shared by at most a given number (say NS<sub>s</sub>) of units over the entire horizon, then the corresponding constraint should be

$$\sum_{e \in \mathrm{EX}} \Gamma_{e,s} \le \mathrm{NS}_s \tag{8}$$

where,  $s \in S$ . Finally, in order to calculate the total capital cost of spares, it is necessary to determine whether or not spare *s* is utilized in at least one period, i.e.,

$$\sum_{e \in \mathrm{EX}} \Gamma_{e,s} \le n_{\mathrm{E}} Z_s \tag{9}$$

where,  $s \in S$ ;  $n_E$  is the total number of heat exchangers in the given HEN;  $Z_s \in \{1,0\}$  is used to reflect whether or not spare *s* is needed to facilitate implementation of the cleaning schedule.

## 5. OVERALL HEAT TRANSFER COEFFICIENTS

As a result of fouling, the overall heat-transfer coefficient of every exchanger in HEN may decrease with time during operation and this behavior can be sufficiently described with the following model: $^{6}$ 

$$U_{e}(t) = \left[\frac{1}{\eta_{cl}U_{e}^{cl}} + r_{e}(t)\right]^{-1}$$
(10)

where,  $e \in EX$ ;  $U_e(t)$  denotes the overall heat-transfer coefficient of exchanger e at time t and  $U_e^{cl}$  is a corresponding constant value when the heat-transfer surface is completely clean;  $\eta_{cl}$  is the cleaning efficiency. Notice that  $\eta_{cl}U_e^{cl}$  represents the overall heat-transfer coefficient of unit e at a time immediately after defouling. Under the assumption that every exchanger can be thoroughly cleaned before operating the given HEN,  $\eta_{cl}$  should be set to 1 at time point  $b_{cp}$  in the first period (p = 1) but updated to a less-than-1 constant (say 0.99) after any cleaning operation. Notice also that the time function  $r_e(t)$ is the fouling resistance of exchanger e at time t, which can be expressed with either an exponential or a linear model.<sup>6</sup> Since the former is in general more realistic, let us consider only the corresponding model formulations for the sake of brevity. Specifically, the exponential fouling model can be written as

$$r_{e}(t) = r_{e}^{\infty} [1 - \exp(-K_{e}t)]$$
(11)

where,  $r_e^{\infty}$  is the asymptotic maximum fouling resistance and  $K_e$  is the characteristic fouling speed.

On the other hand, it should be pointed out that exactly four scenarios should be considered for modeling the overall heat-transfer coefficient of unit e at the aforementioned four time points in period p of a cleaning schedule:

- (i) Exchanger e is not cleaned during period p (p ≥ 2), but in at least one of the prior periods a defouling operation has been performed, i.e., Y<sub>e,p</sub> = 0 and Π<sup>p - 1</sup><sub>k=1</sub>(1 − Y<sub>e,k</sub>) = 0 for p = 2,3,..., n<sub>p</sub>.
- (ii) Exchanger *e* is cleaned and replaced with a spare in period p ( $p \ge 1$ ), i.e.,  $Y_{e,p} = 1$  and  $\sum_{s \in S} X_{e,p,s} = 1$  for  $p = 1, 2, \dots, n_p$ .
- (iii) Exchanger *e* is cleaned but not replaced with a spare in period *p* ( $p \ge 1$ ), i.e.,  $Y_{e,p} = 1$  and  $\sum_{s \in S} X_{e,p,s} = 0$  for  $p = 1, 2, \dots, n_p$ .
- (iv) Exchanger *e* has never been cleaned since period 1, i.e.,  $Y_{e,1} = Y_{e,2} = \cdots = Y_{e,p} = 0$  for  $p = 1,2, \dots, n_p$ .

Furthermore, it is also assumed that

- Any spare used during period p in scenario (ii) is always taken offline at time point ecp in the same period and then cleaned offline with efficiency  $\eta_{\rm cl}$ .
- Each heat exchanger cleaned during period *p* in scenario (ii) or (iii) is always put back online at time point bop in the same period.

Specific formulas of the overall heat transfer coefficients at all time points in all scenarios are presented below.

5.1. Overall Heat Transfer Coefficient in Cleaning Subperiod. The overall heat-transfer coefficient of exchanger e at time points bcp and ecp during period p in the aforementioned scenarios can be expressed with four corresponding terms on the right-hand side of the following equation

$$U_{e,p}^{E,\text{tp}} = \sum_{k=0}^{p-1} \left[ a_{e,k,p}^{E,\text{tp}} Y_{e,k} \prod_{\nu=k+1}^{p} (1 - Y_{e,\nu}) \right] + b s_{e,p}^{E,\text{tp}}$$
$$Y_{e,p} \sum_{s \in S} X_{e,p,s} + 0 + c_{e,p}^{E,\text{tp}} \prod_{z=0}^{p} (1 - Y_{e,z})$$
(12)

where  $e \in EX$ ;  $p \in P$ ;  $tp \in \{bcp, ecp\}$ ;  $U_{e,p}^{E,tp}$  denotes the overall heat-transfer coefficient determined according to exponential fouling model for exchanger *e* at time point tp in period *p*;  $a_{e,k,p}^{E,\text{tp}}$ denotes the corresponding overall heat-transfer coefficient at time point tp during period p ( $p \ge 2$ ) in scenario (i) if exchanger *e* is last cleaned during period k ( $1 \le k < p$ );  $bs_{e,p}^{E,tp}$  is the corresponding overall heat-transfer coefficient at time point tp during period p in scenario (ii) if a spare is adopted to replace exchanger e; 0 is the value of overall heat-transfer coefficient in scenario (iii) since exchanger e is taken out of service without any replacement;  $c_{e,p}^{E,tp}$  is the corresponding overall heat-transfer coefficient in scenario (iv). From eq 3, one can deduce that  $\sum_{s \in S} X_{e,p,s} = 0$  in the first and fourth scenarios due to  $Y_{e,p} = 0$ . On the other hand, notice that  $\sum_{s \in S} X_{e,p,s} = 1$  in scenario (ii) and  $\sum_{s \in S} X_{e,p,s} = 0$  in scenario (iii) by definition. Note also that, when p = 1, the first term in eq 12 vanishes because of the permanent setting  $Y_{e,0} = 0$  in eq 2.

The aforementioned overall heat transfer coefficients at time points bcp and ecp can be written explicitly according to the exponential fouling model as follows:

• At time point bcp

$$a_{e,k,p}^{E,\text{bop}} = \frac{1}{\frac{1}{\eta_{c}U_{e}^{cl}} + r_{e}^{\infty} \left[1 - \exp\left[-K_{e}((\tau_{k} - f_{c}) + \sum_{w=k+1}^{p-1} \tau_{w})\right]\right]}$$
(13)

$$bs_{\epsilon,p}^{\mathrm{E,bcp}} = \eta_{\mathrm{cl}} U_{\mathrm{sp}}^{\mathrm{cl}} \tag{14}$$

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$$c_{e,p}^{E,bcp} = \frac{1}{\frac{1}{U_e^{d}} + r_e^{\infty} [1 - \exp(-K_e \sum_{w=0}^{p-1} \tau_w)]}$$
(15)

At time point ecp

$$\begin{aligned} a_{\epsilon,k,p}^{\text{E,ecp}} &= \\ \frac{1}{\frac{1}{\eta_{cl}U_{\epsilon}^{cl}} + r_{\epsilon}^{\infty} \left[1 - \exp\left[-K_{\epsilon}\left((\tau_{k} - f_{c}) + \sum_{w=k+1}^{p-1} \tau_{w} + f_{c}\right)\right]\right]} \end{aligned}$$
(16)

$$b_{e,p}^{E,ecp} = \frac{1}{\frac{1}{\eta_{d} U_{sp}^{d}} + r_{e}^{\infty} [1 - \exp(-K_{d}f_{c})]}$$
(17)

$$c_{e,p}^{E,ecp} = \frac{1}{\frac{1}{U_e^{cl}} + r_e^{\infty} [1 - \exp(-K_e(\sum_{w=0}^{p-1} \tau_w + f_c))]}$$
(18)

To ensure the validity, generality, and conciseness of the above formulas, it is necessary to assume at the outset that  $\tau_0 = 0$ . Thus, from eqs 2, 12, and 15, one could deduce that  $U_{e,1}^{\text{E,bcp}} = C_{e,1}^{\text{E,bcp}} = U_e^{\text{cl}}$  if no cleaning takes place in period 1 (p = 1), i.e., scenario (iv) and  $Y_{e,1} = 0$ . On the other hand, if heat exchanger e is nonetheless cleaned in period 1, this same coefficient may assume two alternative constant values at time point bcp, i.e.,  $\eta_{\text{cl}}U_{\text{sp}}^{\text{cl}}$  or 0, depending upon whether or not a spare is chosen to take its place, i.e., scenario (ii) or (iii). The corresponding values of  $U_{e,1}^{\text{E,ccp}}$  in scenarios (ii) and (iv) can be obtained according to eqs 17 and 18, respectively, while that in scenario (iii) should still be zero.

In cases when  $p \ge 2$ , all four scenarios are possible and exactly one of corresponding terms in eq 12 remains after fixing the values of  $Y_{e,p}$  and  $\sum_{s\in S} X_{e,p,s}$ . Again for the sake of generality and conciseness, it is necessary to set  $\sum_{w=p}^{p-1} \tau_w = 0$  in eqs 13 and 16 for scenario (i) to incorporate the possibility of performing the defouling operation in period p - 1.

5.2. Overall Heat Transfer Coefficient in Operation Subperiod. The overall heat-transfer coefficient of exchanger e at time points bop and eop during period p in the aforementioned scenarios can be expressed with three corresponding terms as follows

$$U_{e,p}^{\mathrm{E},\mathrm{tp}} = \sum_{k=0}^{p-1} \left[ a_{e,k,p}^{\mathrm{E},\mathrm{tp}} Y_{e,k} \prod_{\nu=k+1}^{p} (1 - Y_{e,\nu}) \right] + b_{e,p}^{\mathrm{E},\mathrm{tp}} Y_{e,p} + c_{e,p}^{\mathrm{E},\mathrm{tp}} \prod_{z=0}^{p} (1 - Y_{e,z})$$
(19)

where  $e \in EX$ ;  $p \in P$ ;  $tp \in \{bop, eop\}$ . It should be noted first that the second term on the right side can be used to represent the overall heat-transfer coefficient in both scenarios (ii) and (iii). This formulation is due to the fact that the defouling operation is called for in both cases and, also, due to the previous assumption that a cleaned heat exchanger is always immediately put back into service at time point bop. Consequently,  $b_{e,p}^{E,tp}$  in eq 19 denotes the overall heat-transfer coefficient at time point tp during period p for both scenarios without considering whether or not a spare is adopted. On the other hand, the first and third terms in eq 19 are associated with scenarios (i) and (iv) respectively and the definitions of  $a_{e,kp}^{E,tp}$  and  $c_{e,p}^{E,tp}$  should be the same as before.

For representing the overall heat-transfer coefficients at time points bop and eop in the above three different cases, two sets of formulas have been developed and they are presented below:

• At time point bop

$$\begin{aligned} a_{e,k,p}^{E,\text{bop}} &= \\ \frac{1}{\frac{1}{\eta_{cl}U_{e}^{cl}} + r_{E}^{\infty} \left[1 - \exp\left[-K_{e}\left((\tau_{k} - f_{c}) + \sum_{w=k+1}^{p-1} \tau_{w} + f_{c}\right)\right]\right]} \end{aligned}$$
(20)

$$b_{e,p}^{\mathrm{E,bop}} = \eta_{\mathrm{cl}} U_e^{\mathrm{cl}} \tag{21}$$

$$c_{e,p}^{E,\text{bop}} = \frac{1}{\frac{1}{U_e^{d}} + r_e^{\infty} [1 - \exp(-K_e(\sum_{w=0}^{p-1} \tau_w + f_c))]}$$
(22)

• At time point eop

$$a_{e,k,p}^{E,eop} = \frac{1}{\frac{1}{\frac{1}{\eta_{cl}U_{e}^{cl}} + r_{e}^{\infty} \left[1 - \exp[-K_{e}((\tau_{k} - f_{c}) + \sum_{w=k+1}^{p} \tau_{w})]\right]}}$$
(23)

$$b_{e,p}^{E,eop} = \frac{1}{\frac{1}{\eta_{d}U_{e}^{cl}} + r_{e}^{\infty}[1 - \exp(-K_{e}(\tau_{p} - f_{c}))]}$$
(24)

$$c_{e,p}^{E,eop} = \frac{1}{\frac{1}{U_e^{d}} + r_e^{\infty} [1 - \exp(-K_e \sum_{w=0}^p \tau_w)]}$$
(25)

Note that, since exchanger *e* is not cleaned during period *p* in scenarios (i) and (iv), the corresponding overall heat-transfer coefficients at time points ecp and bop should be the same. Specifically, from eqs 16, 18, 20, and 22, one can see that  $a_{e,k,p}^{\text{E,ecp}} = a_{e,k,p}^{\text{E,bop}}$ , and  $c_{e,p}^{\text{E,ecp}} = c_{e,p}^{\text{E,bop}}$ . From eq 21, one can also see that  $b_{e,p}^{\text{E,ecp}}$  is a constant that represents the overall heat-transfer coefficient just after cleaning. Finally, notice that the formulas for representing the overall heat-transfer coefficient of exchanger *e* at time point eop during period *p*, i.e., eqs 23–25, can be obtained by introducing additional fouling resistance increased since time point bop into eqs 20–22, respectively.

## 6. TEMPERATURE ADJUSTMENTS ALONG PROCESS STREAMS

It is assumed that the initial and target temperatures of every process stream in a HEN are fixed a priori and these input and output conditions must be kept unchanged throughout the entire horizon despite disturbances caused by fouling and/or cleaning operations. Since the temperature of each stream is adjusted with heat exchangers, coolers/heaters and perhaps also mixers according to the structure described in Figure 1, it is imperative to determine the intermediate temperatures at critical locations and time points along every stream and check if they satisfy thermodynamic and/or operational constraints.

By assuming counter-current flow, let us first consider the energy-transfer rate achieved in heat exchanger e at time point tp in period  $p(Q_{en}^{tp})$ :

$$Q_{e,p}^{\text{tp}} = \mu_e A_e U_{e,p}^{\text{E,tp}} \text{LMTD}_{e,p}^{\text{tp}}$$
(26)

where,  $e \in EX$ ; tp  $\in$  TP;  $p \in P$ ;  $A_e$  denotes the given heattransfer area of unit e in the original HEN design;  $\mu_e = A_e^M/A_e$  is a decision variable used to represent design margin and  $A_e^M$ denotes the enlarged heat-transfer area of unit e; LMTD<sup>p</sup><sub>e,p</sub> is the log-mean temperature difference of heat exchanger e at time point tp in period p. In the proposed model, the margin ratios of heat exchangers are bounded between 1 and 2, i.e.,  $1 \le \mu_e \le 2$ , to avoid having unreasonably large units in the final design. The corresponding energy balance can be expressed as follows

$$Q_{e,p}^{tp} = Fcp_i^H \phi_{e,p}^{H,tp} (Ti_{e,p}^{H,tp} - To_{e,p}^{H,tp})$$
$$= Fcp_j^C \phi_{e,p}^{C,tp} (To_{e,p}^{C,tp} - Ti_{e,p}^{C,tp})$$
(27)

where  $\text{tp} \in \text{TP}$ ;  $p \in \text{P}$ ;  $i \in \text{I}$ ;  $j \in \text{J}$ ;  $e \in \text{EX}$ ;  $f(e) = (i,j) \in \text{MA}$ ;  $\text{Fcp}_i^{\text{H}}$  and  $\text{Fcp}_j^{\text{C}}$ , respectively, denote the heat-capacity flow rates (kW/K) of hot stream *i* and cold stream *j*;  $\text{Ti}_{e,p}^{\text{H,tp}}$  and  $\text{To}_{e,p}^{\text{H,tp}}$ , respectively, denote the inlet and outlet hot stream temper atures of unit *e* at time point tp;  $\text{Ti}_{e,p}^{\text{C,tp}}$  and  $\text{To}_{e,p}^{\text{C,tp}}$ , respectively, denote the inlet and outlet cold stream temperatures of unit *e* at time point tp in period p;  $\phi_{e,p}^{\text{H,tp}}$  is the fraction of flow rate of hot stream passing through unit *e* at time point tp in period p;  $\phi_{e,p}^{\text{C,tp}}$  is the fraction of flow rate of cold stream passing through unit *e*  at time point tp in period *p*. In the above two equations, all quantities are time-dependent variables except  $\text{Fcp}_i^{\text{H}}$  and  $\text{Fcp}_i^{\text{C}}$ .

To facilitate further understanding of the above notations, let us use mixing point m on hot stream i and mixing point n on



Figure 2. Stream structures at mixing points in a fictitious example.

cold stream j in the fictitious structure in Figure 2 as examples. The corresponding mass balances can be written as

$$\tilde{\phi}_{i,p}^{m,\mathrm{tp}} + \sum_{e \in \mathrm{EX}_i^m} \phi_{e,p}^{\mathrm{H},\mathrm{tp}} = 1$$
(28)

$$\tilde{\phi}_{j,p}^{n,\mathrm{tp}} + \sum_{e \in \mathrm{EX}_{j}^{n}} \phi_{e,p}^{C,\mathrm{tp}} = 1$$
(29)

where tp  $\in$  TP;  $p \in$  P;  $i \in$  I;  $j \in$  J  $\tilde{\phi}_{i,p}^{m,\text{tp}}$  denotes the flow fraction of bypass joining mixing point m on hot stream i at time point tp in period p;  $\tilde{\phi}_{j,p}^{n,\text{tp}}$  denotes the flow fraction of bypass joining mixing point n on hot stream j at time point tp in period p.

Since the log-mean temperature of heat exchanger e at time point tp in period p can be expressed as

$$LMTD_{e,p}^{tp} = \frac{(Ti_{e,p}^{H,tp} - To_{e,p}^{C,tp}) - (To_{e,p}^{H,tp} - Ti_{e,p}^{C,tp})}{\ln[(Ti_{e,p}^{H,tp} - To_{e,p}^{C,tp})/(To_{e,p}^{H,*} - Ti_{e,p}^{C,*})]}$$
(30)

From eqs 26, 27, and 30, one can derive an expression for the outlet hot stream temperatures of unit e at time point tp, i.e.,

$$\mathrm{To}_{e,p}^{\mathrm{H,tp}} = \frac{(R_{e,p}^{\mathrm{tp}} - 1)\mathrm{Ti}_{e,p}^{\mathrm{H,tp}} + \left\{ \exp\left[\frac{U_{e,p}^{\mathrm{E,tp}}A_{e,p}}{\mathrm{Fer}_{f}^{\mathsf{C}}Q_{e,p}^{\mathsf{C},\mathrm{tp}}}(R_{e,p}^{\mathrm{tp}} - 1)\right] - 1 \right\} R_{e,p}^{\mathrm{tp}}\mathrm{Ti}_{e,p}^{\mathsf{C,tp}}}{R_{e,p}^{\mathrm{tp}}\mathrm{exp}\left[\frac{U_{e,p}^{\mathrm{E,tp}}A_{e,p}}{\mathrm{Fer}_{f}^{\mathsf{C}}Q_{e,p}^{\mathsf{C,tp}}}(R_{e,p}^{\mathrm{tp}} - 1)\right] - 1}$$
(31)

where tp  $\in$  TP;  $p \in$  P;  $i \in$  I;  $j \in$  J;  $e \in$  EX;  $f(e) = (i,j) \in$  MA;  $R_{e,p}^{\text{tp}}$  is defined as

$$R_{e,p}^{\text{tp}} = \frac{\operatorname{Fcp}_{j}^{C} \phi_{e,p}^{C,\text{tp}}}{\operatorname{Fcp}_{i}^{H} \phi_{e,p}^{H,\text{tp}}}$$
(32)

To simplify model formulation, let us define two additional variables  $d_{e,p}^{\text{tp}}$  and  $ds_{e,p}^{s,\text{tp}}$ :

$$d_{e,p}^{\rm tp} = \frac{A_e \mu_e}{\text{Fcp}_j^C \phi_{e,p}^{C,\text{tp}}} (R_{e,p}^{\rm tp} - 1)$$
(33)

$$ds_{e,p}^{s,tp'} = \frac{As_s}{Fcp_j^C \phi_{e,p}^{C,tp'}} (R_{e,p}^{tp'} - 1)$$
(34)

where, tp  $\in$  TP;  $tp' \in \{bcp, ecp\}$ ;  $p \in P$ ;  $i \in I$ ;  $i \in J$ ;  $e \in EX$ ;  $f(e) = (i,j) \in MA$ ;  $s \in S$ ; As is the heat-transfer area of spare s.

After substituting eqs 12, 19, 33, and 34 into eq 31, one can then obtain the following two formulas to determine the outlet hot stream temperatures of a heat exchanger  $e \in EX$  and  $f(e) = (i,j) \in MA$  at time point tp  $\in$  TP in period  $p \in P$ :

$$To_{e,p}^{H,p'} = Y_{e,p} T_{e,p'}^{H,p'} \left( 1 - \sum_{z \in S} X_{e,p,z} \right)$$

$$+ Y_{e,p} \sum_{s \in S} X_{e,p,z} \frac{\left( R_{e,p}^{s'} - 1 \right) TI_{e,p}^{H,p'} + R_{e,x}^{s'} TI_{e,p}^{C,p'} \left( \exp\left( ds_{e,p}^{s,p'} bs_{e,p}^{E,p'} \right) - 1 \right)}{R_{e,p}^{s} \exp\left( ds_{e,p}^{s',p'} bs_{e,p}^{E,p'} \right) - 1}$$

$$+ \left( 1 - Y_{e,p} \right) \times \left\{ \left[ \left( R_{e,p}^{s'} - 1 \right) TI_{e,p}^{H,p'} - R_{e,p}^{s'} TI_{e,p}^{C,p'} \right] \times \left[ \sum_{k=0}^{p-1} \frac{Y_{e,k} \prod_{z \neq k}^{p-1} \left( 1 - Y_{e,z} \right)}{R_{e,p}^{s'} \exp\left( ds_{e,p}^{s',p'} bs_{e,p}^{E,p'} \right) - 1} + \frac{\prod_{z \neq k}^{p-1} \left( 1 - Y_{e,z} \right)}{R_{e,p}^{s'} \exp\left( ds_{e,p}^{s',p'} ds_{e,p}^{E,p'} \right) - 1} + \frac{\prod_{z \neq k}^{p-1} \left( 1 - Y_{e,z} \right)}{R_{e,p}^{s'} \exp\left( ds_{e,p}^{s',p'} ds_{e,p}^{E,p'} \right) - 1} + \frac{\prod_{z \neq k}^{p-1} \left( 1 - Y_{e,z} \right)}{R_{e,p}^{s'} \exp\left( ds_{e,p}^{s',p'} ds_{e,p}^{E,p'} \right) - 1} + \frac{\sum_{z \neq k}^{p-1} \left( 1 - Y_{e,z} \right) \exp\left( ds_{e,p}^{s',p'} ds_{e,p}^{E,p'} \right) - 1}{R_{e,p}^{s'} \exp\left( ds_{e,p}^{s',p'} \exp\left( ds_{e,p}^{s',p'} ds_{e,p}^{E,p'} \right) - 1} + \frac{\sum_{z \neq k}^{p-1} \left( 1 - Y_{e,z} \right) \exp\left( ds_{e,p}^{s',p'} ds_{e,p}^{E,p'} \right) - 1}{R_{e,p}^{s'} \exp\left( ds_{e,p}^{s',p'} \exp\left( ds_{e,p}^{s',p'} ds_{e,p}^{E,p'} \right) - 1} \right] \right\}$$

$$(35)$$

where  $tp' \in \{bcp, ecp\}$ .

$$To_{e,p}^{H,p^{*}} = \left[ \left( R_{e,p}^{tp^{*}} - 1 \right) Ti_{e,p}^{H,p^{*}} - R_{e,p}^{tp^{*}} Ti_{e,p}^{C,tp^{*}} \right] \times$$

$$\begin{bmatrix} \sum_{s=0}^{n-1} \frac{Y_{e,r}\prod(1-Y_{e,r})}{R_{e,p}^{pr}\exp\left(d_{e,r}^{pr}d_{e,k,p}^{E,pr}\right) - 1} + \frac{Y_{e,r}}{R_{e,p}^{pr}\exp\left(d_{e,r}^{pr}d_{e,k,p}^{E,pr}\right) - 1} + \frac{\prod(1-Y_{e,r})}{R_{e,p}^{pr}\exp\left(d_{e,r}^{pr}d_{e,k,p}^{E,pr}\right) - 1} \end{bmatrix}$$

$$+ R_{e,r}^{pr}T_{e,p}^{C,pr}\left[\sum_{s=0}^{p-1} \frac{Y_{e,s}\prod(1-Y_{e,s})\exp\left(d_{e,r}^{pr}d_{e,k,p}^{E,pr}\right) - 1}{R_{e,r}^{pr}\exp\left(d_{e,r}^{pr}d_{e,k,p}^{E,pr}\right) - 1} + \frac{Y_{e,r}\exp\left(d_{e,r}^{pr}d_{e,p}^{E,pr}\right) - 1}{R_{e,r}^{pr}\exp\left(d_{e,r}^{pr}d_{e,k,p}^{E,pr}\right) - 1} + \frac{Y_{e,r}\exp\left(d_{e,r}^{pr}d_{e,p}^{E,pr}\right) - 1}{R_{e,r}^{pr}\exp\left(d_{e,r}^{pr}d_{e,r}^{E,pr}\right) - 1} \end{bmatrix}$$

$$(36)$$

$$+ \frac{r}{R_{e,r}^{pr}}T_{e,r}^{C,pr}\left[\sum_{s=0}^{p-1} \frac{Y_{e,s}\prod(1-Y_{e,s})\exp\left(d_{e,r}^{pr}d_{e,r}^{E,pr}\right) - 1}{R_{e,r}^{pr}\exp\left(d_{e,r}^{pr}d_{e,r}^{E,pr}\right) - 1} \right]$$

where,  $tp'' \in \{bop, eop\}$ .

On the other hand, the outlet temperatures of cold stream at different time instances can be determined according to eqs 27 and 32, i.e.,

$$To_{e,p}^{C,tp} = Ti_{e,p}^{C,tp} + \frac{Ti_{e,p}^{H,tp} - To_{e,p}^{H,tp}}{R_{e,p}^{tp}}$$
(37)

where tp  $\in$  TP;  $p \in$  P;  $i \in$  I;  $i \in$  J;  $e \in$  EX;  $f(e) = (i,j) \in$  MA. Let us next consider the energy balances around the mixing

points. For mixing point *m* on hot stream *i*, one can write

$$T_{m,i,p}^{\mathrm{H,tp}} = \tilde{\phi}_{i,p}^{m,\mathrm{tp}} T_{m-1,i,p}^{\mathrm{H,tp}} + \sum_{e \in \mathrm{EX}_{i}^{m}} (\phi_{e,p}^{\mathrm{H,tp}} To_{e,p}^{\mathrm{H,tp}})$$
(38)

where  $tp \in TP$ ;  $p \in P$ ;  $i \in I$ ;  $m = 1, 2 \cdots, M_i$ . Note that this mixing point temperature should also be the inlet temperature of hot stream entering the heat exchangers before the next mixing point, i.e.

$$Ti_{e,p}^{\mathrm{H,tp}} = T_{m,i,p}^{\mathrm{H,tp}}$$

$$\tag{39}$$

where tp  $\in$  TP;  $p \in$  P;  $i \in$  I;  $e \in \text{EX}_i^{m+1}$ ;  $m = 0, 1, 2, \dots, M_i - 1$ . Notice that  $T_{0,i,p}^{\text{H},\text{tp}} = \text{TI}_i^{\text{H}}$  and  $\text{TI}_i^{\text{H}}$  denotes the initial temperature of hot stream *i*, which is a given parameter.

The mixing point temperatures on the cold streams can be described with a similar approach. Specifically, for tp  $\in$  TP;  $p \in$  P;  $j \in$  J and  $n = 1, 2 \cdots, N_p$ , these temperatures are

$$T_{n,j,p}^{C,\text{tp}} = \tilde{\phi}_{j,p}^{n,\text{tp}} T_{n-1,j,p}^{C,\text{tp}} + \sum_{e \in \text{Ex}_{j}^{n}} (\phi_{e,p}^{C,\text{tp}} T o_{e,p}^{C,\text{tp}})$$
(40)

And they are also subject to similar constraints, i.e.,

$$\operatorname{Ti}_{e,p}^{\mathrm{C},\mathrm{tp}} = T_{n,j,p}^{\mathrm{C},\mathrm{tp}}$$

$$\tag{41}$$

where  $e \in EX_j^{n+1}$  and  $n = 0, 1, 2 \cdots, N_j - 1$ . Notice that  $T_{0,j,p}^{C,tp} = TI_j^C$  and  $TI_j^C$  denotes the initial temperature of cold stream *j*, which is also a given model parameter.

## 7. ADDITIONAL INEQUALITY CONSTRAINTS

Two types of extra inequalities are included in the proposed model to ensure feasibility and operability of the final HEN design. They are detailed in the following subsections:

**7.1. Bypass Constraints.** The bypasses are included in a HEN design to enhance operability. As mentioned previously, the bypass line(s) may be installed on the hot and/or cold streams of a heat exchanger. Since either option may be selected to adjust the amount of exchanged heat effectively, only one of them is allowed in the proposed model. The corresponding constraints can be written as

$$\sum_{p \in \mathbb{P}} \sum_{\mathbf{t} p \in \mathrm{TP}} \tilde{\phi}_{i,p}^{m, \mathrm{tp}} \le 4n_{\mathrm{p}} \xi_{e}^{\mathrm{H}}$$
(42)

$$\sum_{p \in \mathcal{P}} \sum_{\mathbf{t} p \in \mathrm{TP}} \tilde{\phi}_{j,p}^{n,\mathbf{t}} \le 4n_{\mathrm{P}} \xi_{e}^{\mathrm{C}}$$
(43)

$$\xi_e^{\mathrm{H}} + \xi_e^{\mathrm{C}} \le 1 \tag{44}$$

where  $i \in I$ ;  $j \in J$ ;  $m = 1, 2 \cdots, M_i$ ;  $n = 1, 2 \cdots, N_j$ ;  $e \in EX_i^m \cap EX_j^n$ and  $f(e) = (i,j) \in MA$ ;  $\xi_e^H \in \{1,0\}$  denotes whether or not the bypass on unit *e* is located on the hot-stream side;  $\xi_e^C \in \{1,0\}$ denotes whether or not the bypass on unit *e* is located on the cold-stream side.

**7.2. Temperature Constraints.** To ensure that the heat transfer in every unit in HEN is consistent with the laws of

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thermodynamics at all time points over the entire horizon, additional temperature constraints on the corresponding inlet and outlet temperatures are included in the proposed model. Specifically,

$$\mathrm{Ti}_{e,p}^{\mathrm{H},\mathrm{tp}} \ge \mathrm{To}_{e,p}^{\mathrm{C},\mathrm{tp}} \tag{45}$$

$$\mathrm{To}_{e,p}^{\mathrm{H},\mathrm{tp}} \geq \mathrm{Ti}_{e,p}^{\mathrm{C},\mathrm{tp}} \tag{46}$$

where tp  $\in$  TP;  $p \in$  P;  $e \in$  EX. On the other hand, it is also reasonable to require that the mixing point temperatures on each process stream must increase or decrease monotonically, i.e.,

$$T_{m,i,p}^{\rm H,tp} \le T_{m-1,i,p}^{\rm H,tp}$$
 (47)

$$T_{n,j,p}^{C,\text{tp}} \ge T_{n-1,j,p}^{C,\text{tp}}$$

$$\tag{48}$$

where tp  $\in$  TP;  $p \in$  P;  $i \in$  I;  $j \in$  J;  $m = 1, 2..., M_i$ ;  $n = 1, 2..., N_j$ . Finally, it is implied in the given stream data of any HEN design problem that the following inequalities should be valid:

$$T_{M_i,i,p}^{\mathrm{H},\mathrm{tp}} \ge TT_i^{\mathrm{H}} \tag{49}$$

$$T_{N_j,j,p}^{C,\mathrm{tp}} \le TT_j^C \tag{50}$$

where tp  $\in$  TP;  $p \in$  P;  $i \in$  I;  $j \in$  J;  $TT_i^{\text{H}}$  and  $TT_j^{\text{C}}$  denote the target temperatures of hot stream i and cold stream j, respectively, and they are both given model parameters. Since the above target constraints often cause convergence difficulties, they are reformulated in this study to relieve the computation burden. Specifically, each constraint is relaxed by introducing two fictitious variables as follows

$$TT_{i}^{\rm H} - T_{M_{i},i,p}^{\rm H,tp} = \mathrm{po}_{i,p}^{\rm H,tp} - \mathrm{ne}_{i,p}^{\rm H,tp}$$
(51)

$$T_{N_{j},j,p}^{C,tp} - TT_{j}^{C} = po_{j,p}^{C,tp} - ne_{j,p}^{C,tp}$$
 (52)

where tp  $\in$  TP;  $p \in$  P;  $i \in$  I;  $j \in$  J;  $\text{po}_{i,p}^{\text{H,tp}}$ ,  $\text{po}_{i,p}^{\text{C,tp}}$ ,  $\text{ne}_{i,p}^{\text{H,tp}}$ , and  $\text{ne}_{j,p}^{\text{C,tp}}$  are nonnegative and real. The first two fictitious variables (i.e.,  $\text{po}_{i,p}^{\text{H,tp}}$  and  $\text{po}_{j,p}^{\text{C,tp}}$ ) should be viewed as the degrees of constraint violation, while the others (i.e.,  $\text{ne}_{i,p}^{\text{H,tp}}$  and  $\text{ne}_{j,p}^{\text{C,tp}}$ ) the degrees of conformity. Thus, it is imperative to force the right sides of eqs 51 and 52 negative or zero. Furthermore, these variables should satisfy the following equality constraints:

$$po_{i,p}^{\mathrm{H,tp}}ne_{i,p}^{\mathrm{H,tp}} = 0$$
(53)

$$p o_{j,p}^{C,tp} n e_{j,p}^{C,tp} = 0 (54)$$

In other words, although all fictitious variables may be zero, only one out of the two in eq 53 and another in eq 54 can be positive. Clearly, the HEN cleaning schedule is infeasible if  $\mathrm{po}_{i,p}^{\mathrm{H},\mathrm{tp}} > 0$  or  $\mathrm{po}_{i,p}^{\mathrm{C},\mathrm{tp}} > 0$  In order to avoid violating the target constraints, a penalty term ( $\Psi$ ) can be added to the traditional objective function (e.g., TAC) and this penalty may be expressed in terms of the undesired violation variables as follows

$$\Psi = \omega \left( \sum_{i \in I} \max_{tp \in TP, p \in P} po_{i,p}^{H,tp} + \sum_{j \in J} \max_{tp \in TP, p \in P} po_{j,p}^{C,tp} \right)$$
(55)

#### 8. UTILITY CONSUMPTION RATES

A straightforward computation can be performed to determine the utility consumption rate needed to bring the final temperature of each process stream to its target value at time point tp in period p.

$$Qu_{j,p}^{H,\psi} = Fcp_j^{C}ne_{j,p}^{C,\psi}$$
(56)

$$Qu_{i,p}^{C,tp} = Fcp_i^H ne_{i,p}^{H,tp}$$
(57)

where tp  $\in$  TP;  $p \in$  P;  $i \in$  I;  $j \in$  J;  $Qu_{jp}^{H,tp}$  is the hot utility consumption rate needed by cold stream j at time point tp in period p;  $Qu_{ip}^{C,tp}$  is the cold utility consumption rate needed by hot stream i at time point tp in period p. Consequently, one can estimate the total amounts of utilities consumed respectively by cold stream j and hot stream i in period p according to the following formulas:

$$\operatorname{Eu}_{j,p}^{\mathrm{H}} = \frac{\operatorname{Qu}_{j,p}^{\mathrm{H,bep}} + \operatorname{Qu}_{j,p}^{\mathrm{H,eep}}}{2} f_{\mathrm{c}} + \frac{\operatorname{Qu}_{j,p}^{\mathrm{H,bep}} + \operatorname{Qu}_{j,p}^{\mathrm{H,eep}}}{2} (\tau - f_{\mathrm{c}})$$
(58)

$$\mathrm{Eu}_{i,p}^{C} = \frac{\mathrm{Qu}_{i,p}^{C,\mathrm{bep}} + \mathrm{Qu}_{i,p}^{C,\mathrm{eep}}}{2} f_{\mathrm{c}} + \frac{\mathrm{Qu}_{i,p}^{C,\mathrm{bop}} + \mathrm{Qu}_{i,p}^{C,\mathrm{eop}}}{2} (\tau - f_{\mathrm{c}})$$
(59)

where,  $p \in P$ ;  $i \in I$ ;  $j \in J$ ;  $Eu_{j,p}^{H}$  is the estimated amount of hot utility consumed by cold stream *j* in period *p*;  $Eu_{i,p}^{C}$  is the estimated amount of cold utility consumed by hot stream *i* in period *p*.

## 9. HEAT TRANSFER AREAS OF UTILITY USERS

As mentioned before, some of the process streams in the original HEN design do not require utilities and these hot and cold streams are grouped into sets  $I_a$  and  $J_a$  respectively. Although the corresponding utility users may not be needed at the starting time of the given horizon, it is possible that  $ne_{i_{ab}p'}^{\prime\,\mathrm{H,tp}\,\prime}$ > 0 ( $\exists i'_a \in I_a, \exists tp' \in TP, \exists p' \in P$ ) and/or ne<sup>"C,tp"</sup> > 0 ( $\exists j''_a$ )  $\in J_{a'} \exists tp'' \in TP, \exists p'' \in P)$  and, thus, extra auxiliary coolers and/or heaters should be added to bring the final temperatures of the corresponding hot and cold streams to their respective targets at all such instances. On the other hand, for the process streams that are equipped with utility users in the original HEN design, it is also possible that  $ne_{i_bp'}^{\prime H, i_{p'}} (\exists i_b' \in I_b, \exists i_{p'} \in TP, \exists$  $p' \in P$ ) and/or ne<sup>"C,tp"</sup> ( $\exists j_b" \in J_b$ ,  $\exists tp" \in TP$ ,  $\exists p" \in P$ ) are larger than those adopted in the given design specifications. In these cases, area margins should be introduced into the corresponding coolers and heaters.

The largest heat duties of the above two types of utility users can be expressed in the following general formulas:

$$\bar{Q}_{j}^{\mathrm{HT}} = \max_{\mathrm{tp}\in\mathrm{TP}, p\in\mathrm{P}} \mathrm{Qu}_{j,p}^{\mathrm{H},\mathrm{tp}}$$
(60)

$$\bar{Q}_{i}^{\text{CL}} = \max_{\text{tp}\in\text{TP}, p\in\text{P}} \text{Qu}_{i,p}^{\text{C,tp}}$$
(61)

where,  $i \in I$ ;  $j \in J$ . The corresponding log-mean temperature differences should be

$$\overline{\text{LMTD}}_{j}^{\text{HT}} = \frac{(\text{Ti}^{\text{HU}} - TT_{j}^{\text{C}}) - (\text{To}^{\text{HU}} - \min_{\text{tp}\in\text{TP},p\in\text{P}} T_{N_{j},j,p}^{\text{C},\text{tp}})}{\ln(\text{Ti}^{\text{HU}} - TT_{j}^{\text{C}})/(\text{To}^{\text{HU}} - \min_{\text{tp}\in\text{TP},p\in\text{P}} T_{N_{j},j,p}^{\text{C},\text{tp}})}$$
(62)

where  $\omega$  is a positive constant.

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where  $i \in I$ ;  $j \in J$ .

The heat-transfer areas of the auxiliary heaters and coolers can be approximated with the following formulas:

$$A_{j_a}^{\text{AHT}} \approx \frac{\bar{Q}_{j_a}^{\text{HT}}}{\hat{U}_{j_a}^{\text{AHT}} \overline{\text{LMTD}}_{j_a}^{\text{HT}}}$$
(64)

$$A_{i_a}^{\text{ACL}} \approx \frac{\bar{Q}_{i_a}^{\text{CL}}}{\hat{U}_{i_a}^{\text{ACL}} \overline{\text{LMTD}}_{i_a}^{\text{CL}}}$$
(65)

where  $i_a \in I_a$ ;  $j_a \in J_a$ ;  $A_{j_a}^{AHT}$  denotes the heat-transfer area of auxiliary heater on cold stream  $j_a$  and  $\hat{U}_{j_a}^{AHT} \approx \left[\frac{1}{U_{AHT,j_a}^d} + r_{AHT,j_a}^{\infty}\right]^{-1}$  is a conservative estimate of

overall heat-transfer coefficient of the corresponding heater, which can be obtained according to eqs 10 and 11 as  $t \to \infty$ ;  $A_{i_a}^{ACL}$  denotes the heat-transfer area of auxiliary cooler on cold

stream  $i_a$  and  $\hat{U}_{i_a}^{\text{ACL}} \approx \left[\frac{1}{U_{\text{ACL},i_a}^{\text{cl}}} + r_{\text{ACL},i_a}^{\infty}\right]^{-1}$  is a conservative

estimate of overall heat-transfer coefficient of the corresponding cooler, which can also be obtained according to eqs 10 and 11 as  $t \rightarrow \infty$ .

On the other hand, the area margins of existing heaters and coolers can be estimated according to the following equations:

$$\mu_{j_b}^{\mathrm{HT}} \approx \frac{\bar{Q}_{j_b}^{\mathrm{HT}}}{\hat{U}_{j_b}^{\mathrm{HT}} A_{j_b}^{\mathrm{HT}} \overline{LMTD}_{j_b}^{\mathrm{HT}}}$$
(66)

$$\mu_{i_b}^{\text{CL}} \approx \frac{\bar{Q}_{i_b}^{\text{CL}}}{\hat{U}_{i_b}^{\text{CL}} A_{i_b}^{\text{CL}} \overline{\text{LMTD}}_{i_b}^{\text{CL}}}$$
(67)

where  $i_b \in I_b$ ;  $j_b \in J_b$ ;  $\mu_{jb}^{\text{HT}}$  represents the margin ratio of heater on cold stream  $j_b$ ;  $A_{jb}^{\text{HT}}$  denotes the given heat-transfer area of the existing heater on cold stream  $j_b$  in the original HEN design and  $\hat{U}_{j_b}^{\text{HT}} \approx \left[\frac{1}{U_{\text{HT},j_b}^{\text{d}}} + r_{\text{HT},j_b}^{\infty}\right]^{-1}$  is a conservative estimate of overall heat-transfer coefficient of the corresponding heater, which can be obtained according to eqs 10 and 11 as  $t \to \infty$ ;  $\mu_{i_b}^{\text{CL}}$  represents the margin ratio of cooler on hot stream  $i_b$ ;  $A_{i_b}^{\text{CL}}$ denotes the given heat-transfer area of the existing cooler on hot stream  $i_b$  in the original HEN design and  $\hat{U}_{i_b}^{\text{CL}} \approx \left[\frac{1}{U_{\text{CL},i_b}^{\text{d}}} + r_{\text{CL},i_b}^{\infty}\right]^{-1}$  is a conservative estimate of overall heat-transfer coefficient of the corresponding cooler, which can be obtained according to eqs 10 and 11 as  $t \to \infty$ .

#### **10. OBJECTIVE FUNCTION**

As mentioned before, the maximum length of time horizon allowed for schedule synthesis is chosen to be the duration between the ending and beginning instances of two consecutive planned shutdowns, i.e.,  $t_{\rm f}$ . The total annual cost (TAC) associated with operating and cleaning a given HEN can be

approximated by summing the total annualized capital cost (TACC) and the average value of the total annual operating cost (TAOC), i.e.,

$$TAC = TACC + \overline{TAOC}$$
(68)

The former consists of three components: (1) the purchase costs of spares (CC<sub>1</sub>), (2) the capital cost increases caused by introducing area margins into the existing heat exchangers and utility users (CC<sub>2</sub>), and (3) the capital costs of auxiliary units (CC<sub>3</sub>). Specifically, these three components can be expressed as follows

$$CC_{1} = C_{fix}^{SP} \sum_{s \in S} Z_{s} + C_{M}^{SP} \sum_{s \in S} Z_{s} (As_{s})^{\alpha}$$

$$(69)$$

$$CC_{2} = C_{M} \sum_{e \in EX} [(\mu_{e}^{)\alpha} - 1](A_{e}^{)\alpha} + C_{M}^{HT} \sum_{j \in J_{b}} [(\mu_{j}^{HT})^{\alpha} - 1](A_{j}^{HT})^{\alpha} + C_{M}^{CL} \sum_{i \in I_{b}} [(\mu_{i}^{CL})^{\alpha} - 1](A_{i}^{CL})^{\alpha}$$
(70)

$$CC_{3} = C_{\text{fix}}^{\text{AHT}} \sum_{j \in J_{a}} Z_{j}^{\text{AHT}} + C_{M}^{\text{AHT}} \sum_{j \in J_{a}} Z_{j}^{\text{AHT}} (A_{j}^{\text{AHT}})^{\alpha} + C_{\text{fix}}^{\text{ACL}} \sum_{i \in I_{a}} Z_{i}^{\text{ACL}} + C_{M}^{\text{ACL}} \sum_{i \in I_{a}} Z_{i}^{\text{ACL}} (A_{i}^{\text{ACL}})^{\alpha}$$
(71)

where  $C_M^{\text{SP}}$ ,  $C_{M}$ ,  $C_M^{\text{HT}}$ ,  $C_M^{\text{CL}}$ ,  $C_M^{\text{AHT}}$ , and  $C_M^{\text{ACL}}$  are variable cost coefficients;  $C_{\text{fix}}^{\text{SP}}$ ,  $C_{\text{fix}}^{\text{AHT}}$ , and  $C_{\text{fix}}^{\text{ACL}}$  are the fixed cost coefficients. Notice that all other parameters and variables in the above three formulas have already been defined previously except the two binary variables in eq 72, i.e.,  $Z_j^{\text{AHT}} \in \{1,0\}$  ( $j \in J_a$ ) and  $Z_i^{\text{ACL}} \in \{1,0\}$  ( $i \in I_a$ ). They reflect whether or not auxiliary heater on cold stream j and auxiliary cooler on hot stream i are present, respectively. The following inequality constraints should be imposed to determine their values

$$0 \le \bar{Q}_{j}^{\text{HT}} \le Z_{j}^{\text{AHT}} \text{QCL}_{j}$$
(72)

$$0 \le \bar{Q}_i^{\text{CL}} \le Z_i^{\text{ACL}} \text{QHL}_i \tag{73}$$

where  $i \in I_a$ ;  $j \in J_a$ ; QHL<sub>i</sub> and QHL<sub>j</sub> denote the given heat loads of hot stream *i* and cold stream *j*, respectively.

On the other hand, the total annual operating cost is approximated simply by taking the arithmetic average of total operating cost ( $\overline{TAOC}$ ) in the schedule horizon, i.e.,

$$\overline{\text{TAOC}} = \overline{\text{TAUC}} + \overline{\text{TACLC}}$$
(74)  
$$\overline{\text{TAUC}} = \frac{12}{t_{f}} \left( \frac{C_{HU}}{\eta^{H}} \sum_{p \in P} \sum_{i \in J} \text{Eu}_{i,p}^{H} + \frac{C_{CU}}{\eta^{C}} \sum_{p \in P} \sum_{i \in I} \text{Eu}_{i,p}^{C} \right)$$
(75)  
$$\overline{\text{TACLC}} = \frac{12}{t_{f}} \left( C_{+} \sum_{p \in P} \sum_{i \in J} Y_{+} + C_{+}^{\text{SP}} \sum_{p \in P} \sum_{i \in I} X_{+} \right)$$

$$\overline{\text{TACLC}} = \frac{12}{t_{\rm f}} \left( C_{\rm cl} \sum_{p \in \mathcal{P}} \sum_{e \in \mathrm{EX}} Y_{e,p} + C_{\rm cl}^{\rm SP} \sum_{p \in \mathcal{P}} \sum_{e \in \mathrm{EX}} \sum_{s \in \mathrm{S}} X_{e,p,s} \right)$$
(76)

where, TAUC and TACLC denote the arithmetic averages of total annual utility cost and total annual cleaning cost, respectively;  $C_{\rm HU}$  and  $C_{\rm CU}$  denote the unit costs of heating and cooling utilities;  $\eta^{\rm H}$  and  $\eta^{\rm C}$  denote the heat-transfer efficiencies in heater and cooler respectively;  $C_{\rm cl}$  and  $C_{\rm cl}^{\rm SP}$ 



Figure 3. Network structure of a given HEN design.

represent the costs of cleaning a heat exchanger and a spare, respectively.

Finally, the objective function of the proposed MINLP model is

$$obj = TAC + \Psi$$
 (77)

where, the penalty term  $\Psi$  has been defined in eq 55.

#### **11. SUPERSTRUCTURE FOR EFFECTIVE REFINEMENTS**

Since the aforementioned comprehensive formulation may result in overwhelmingly heavy computational burden in solving the proposed MINLP model, it is desirable to first produce a HEN superstructure to incorporate only the effective design refinements. This superstructure is then used as the basis for constructing a solvable model by limiting the search space that facilitates easier convergence. More specifically, before solving the optimization problem at hand, it is important to first determine candidate locations of the bypasses, the margined heat exchangers and utility users and, also, the auxiliary heaters and coolers in the given HEN structure.

On the basis of eqs 60, 61, 72, and 73, one can see that every cold stream  $j \in J_a$  may require the heating utility and every hot stream  $i \in I_a$  may need the cooling utility. Thus, the candidate auxiliary units should be placed on all such streams in the superstructure. On the other hand, over the entire horizon of a cleaning schedule, the area margin in any heat exchanger and the corresponding bypasses are utilized primarily for the purpose of reducing the overall utility consumption level in two different scenarios. In particular,

- They may be manipulated to make up the difference between the target heat duty of this unit and a lower value caused by fouling;
- (2) They may be used to make up the lost capacity in other unit(s) by shifting loads along a path or a loop in HEN. This lost duty may be due to a cleaning operation or simply due to fouling.

A series of test runs are carried out in this study to determine the effects of introducing margin into each unit on the minimum average total annual utility cost ( $\overline{TAUC}$ ). The most effective ones are then chosen in the superstructure. Let us use a fictitious example to illustrate this heuristic approach,. The given HEN design in this example is shown in Figure 3 (network structure), Table 1 (stream data), and Table 2 (unit

Tab	le 1.	Stream	Data	of a	Given	HEN	Design
-----	-------	--------	------	------	-------	-----	--------

stream no.	TI/TT (K)	Fcp (kW/K)
C1	330/360	30
C2	366/411	43.9
C3	411/422	48.44
H1	470/419	28
H2	522/410	40.55
H3	544/478	42.56
H4	500/532	44.77
CU	293/298	
HU	600/600	

Table 2. Unit Specifications of a Given HEN Design

е	$U_e^{ m cl}$ (kW/m <sup>2</sup> K)	$A_e (m^2)$	${\mathop{\rm Ti} olimits_e^{\rm C}}/{\mathop{\rm To} olimits_e^{\rm C}}$	${\mathop{\rm Ti} olimits_e^{ m H}/ m To}_e^{ m H}$ $(K)$	Qe (kW)
HE1	0.85	135.62	366/426	470/376	2634
HE2	0.85	122.32	411/434	446/421	1136
HE3	0.85	27.51	330/410	500/446	2400
HE4	0.85	86.83	434/452	466/444	860
HE5	0.85	284.54	452/524	544/462	3479
HE6	0.85	64.28	426/478	522/466	2282
CL1	0.5	7.243	293/298	376/360	445.2
CL2	0.5	12.13	293/298	444/411	1358
CL3	0.5	13.08	293/298	462/422	1711.8
CL4	0.5	0.85	293/298	421/419	89.5
HT3	0.5	6.28	524/532	600/600	384.6

specifications). Since the exponential fouling model is adopted for the present purpose, the corresponding asymptotic maximum fouling resistance  $(r_e^{\infty})$  and characteristic fouling speed  $(K_e)$  are chosen to be 0.8 m<sup>2</sup>K/kW and 0.07 month<sup>-1</sup>, respectively. The unit costs of hot and cold utilities are assumed to be 3.86 × 10<sup>-5</sup> USD/kJ and 7.72 × 10<sup>-6</sup> USD/kJ respectively. The margin ratio of the unit under consideration  $(\mu_e)$  is fixed at 1.5 in every test run. The other model

parameters are selected as follows:  $t_f = 18 \pmod{; \tau = 1 \pmod{; \tau = 1 \pmod{; \tau = 1}}$  $f_c = 0.2 \pmod{; \eta^H = 1; \eta^C = 1.$ 

A slightly modified version of the aforementioned mathematical programming model is solved in each test run. The modified formulations and the corresponding results are described in the sequel:

**11.1. Scenario 1.** Since cleaning is not considered in this case, it is necessary to impose the following constraints:

$$Y_{e,p} = 0 \tag{78}$$

where  $e \in EX$  and  $p \in P$ . By setting  $t_f = 18$  and  $\mu_e = 1.5$  for a distinct heat exchanger in six separate test runs, one can produce the results in Table 3. One can see that, if the HEN is

Table 3. Test Run Results Obtained without Cleaning

margined unit	TAUC <sup>min</sup> (10 <sup>6</sup> \$/yr)	hot-stream bypasses	cold-stream bypasses
HE1	2.21	HE3,HE6	HE2
HE2	2.33	HE3	HE2,HE4
HE3	2.02	HE3	HE2
HE4	2.30	HE3	
HE5	2.06	HE3	
HE6	2.00	HE3,HE6	HE2

operated without cleaning, introducing area margin into HE6, HE3, or HE5 results in a somewhat lower minimum  $\overline{\text{TAUC}}$ . Notice also that, in order to achieve any of these desired levels of heat recovery, it is required to place the corresponding bypasses at locations suggested in the last column of this table.

**11.2. Scenario 2.** When a particular heat exchanger in HEN is removed for cleaning purpose and no spare is used to take its place, the most appropriate margin location may also be identified by minimizing the corresponding TAUC with proper bypasses. To facilitate the test runs in scenario 2, it is necessary to change the length of every cleaning subinterval in the proposed model to be  $f_c = \tau = 1$  mon. In other words, the designated unit in a text run is assumed to be offline

throughout the entire horizon. Thus, a total of six different test runs should be performed to cover all heat exchangers in Figure 3. In any test run, if a particular unit  $e' \in EX$  in HEN is removed for cleaning, then the additional binary settings in model should be

$$Y_{e,p} = \begin{cases} 1 \text{ if } e = e' \\ 0 \text{ if } e \in EX/\{e'\} \end{cases}$$

$$\tag{79}$$

Also, since cleaning is not allowed, all corresponding binary variables should be zero, i.e.,

$$X_{e',p,s} = 0 \tag{80}$$

where  $p \in P$ ;  $s \in S$ . Finally, the corresponding test run results are given in Supporting Information for the sake of brevity.

Note that every test run in the above two scenarios yields a unique ranking in terms of  $\overline{TAUC}^{min}$ . Since the effectiveness of a margined unit for compensating the lost duties in HEN is indirectly reflected in  $\overline{TAUC}^{min}$ , the following two heuristic rules are adopted in this study for choosing the candidate margin and bypass locations:

- (a) Identify the higher-ranked units in each run, and then use the most overlapped ones as the candidate units in superstructure.
- (b) Identify bypasses that facilitate the compensation functions of the above candidate units, and then include all of them in the superstructure.

If the first three in each ranking is selected (see Table 3 and Tables S1–S6 in Supporting Information), one can deduce that HE3, HE5, and HE6 should be the candidate units and the corresponding bypasses should be on the cold streams of HE2, HE4, and HE5 and on the hot streams of HE3 and HE6. The resulting superstructure is presented in Figure 4. Note that the auxiliary utility users, the candidate heat exchangers for incorporating margins, and the chosen locations of bypasses are all marked with dashed line in this figure. Finally, if there is still a need to further limit the total number of candidate units after applying the aforementioned heuristic rules, then the



Figure 4. Superstructure.



Figure 5. Refined HEN design obtained in Case 1.

following constraints can be imposed in the programming model:

$$\sum_{e \in \mathrm{EX}} Z_e^M \le \mathrm{NM}$$
(81)

where NM is a given model parameter denoting the maximum allowable number of margined heat exchangers;  $Z_e^M \in \{1,0\}$  reflects whether or not unit *e* is margined and this binary value can be determined by incorporating the following inequality:

$$\mu_e - 1 \le Z_e^M \tag{82}$$

## **12. ALLOCATION OF SPARES**

...

As mentioned before, the heat duty of a heat exchanger in HEN may be taken over by a spare when the former is removed for defouling. Since this function can usually be fulfilled if the equipment specifications of the two are similar, it is beneficial to include the corresponding binary settings to further reduce the search space. As an example, let us consider the heat exchangers listed in Table 2. It can be observed that their heat transfer areas can be roughly divided into two groups, i.e., {HE1, HE2, HE5} and {HE3, HE4, HE6}, and two different spares can be assigned to these two groups, respectively. Specifically, one can set  $X_{1,p,2} = X_{2,p,2} = X_{5,p,2} = 0$  to avoid using the second spare (s = 2) in the first group and  $X_{3,p,1} = X_{4,p,1} = X_{6,p,1} = 0$  to avoid using the first spare (s = 1) in the second group.

On the other hand, if the heat-transfer area of a particular heat exchanger in the given design is exceptionally large, it may be difficult to compensate its duty with a margined unit when it is taken offline for cleaning. Since a spare is clearly the best solution in this situation, the corresponding inequality in eq 5 may have to be replaced with an equality constraint instead. For example, since the heat-transfer area of HE5 in Table 2 is considerably larger than those of the other units, one can impose the corresponding constraint as  $(1 - Y_{5,p}) + \sum_{s \in S} X_{5,p,s} = 1$ .

## 13. CASE STUDIES

On the basis of a given HEN design, all above formulations have been utilized to construct a comprehensive MINLP model for producing the optimal refinements and the corresponding spare-supported cleaning schedules. Starting from randomly generated initial guesses, the model was solved repeatedly (say 500 runs) in every application with solver SBB in GAMS 23.9.5 so as to ensure solution quality. It should be noted that all such computations were carried out on a PC equipped with Intel core i7-4790 3.6 GHz. Notice also that, although the proposed model has been shown to be feasible and effective in extensive case studies for several examples,<sup>20</sup> this section only reports the optimization results obtained from the preliminary design specified in Table 1, Table 2, and Figure 3 for the sake of brevity. Following is a list of additional model parameters needed to carry out the corresponding computations.

- The cleaning cost of an online exchanger is assumed to be 4000 USD, while that of a spare is 1000 USD. The cleaning efficiency was fixed at  $\eta^{cl} = 0.99$ .
- The annualized fixed capital cost coefficients are all set at the same value, i.e.,  $C_{fix}^{SP} = C_{fix}^{AHT} = C_{fix}^{ACL} = 5500 \frac{USD}{yr}$ , while the annualized variable capital cost coefficients are also assumed to be the same, i.e.,  $C_M = C_M^{HT} = C_M^{CL} = C_M^{SP}$  $= C_M^{AHT} = C_M^{ACL} = 550 \text{ USD/yr} \cdot m^{2\alpha} (\alpha = 0.6).$
- The set of spares is denoted as  $S = \{1,2,3\}$ . Each of the first two is shared by at most 3 heat exchanges during the schedule horizon, i.e.,  $NS_1 = NS_2 = 3$  while the third is unlimited, i.e.,  $NS_3 = 6$ .
- The estimated overall heat-transfer coefficients of the auxiliary utility users are assumed to be  $\hat{U}_i^{\text{AHT}} = \hat{U}_i^{\text{ACL}} = 0.5 \frac{\text{kW}}{2}$ .

$$U_{j_a} = U_{j_a} = 0.5 \frac{1}{m^2 K}.$$

**13.1. Base Case.** The maximum allowable number of margined heat exchangers can be set at any value which is smaller than  $n_E$ , i.e., 6. As a first attempt, let us consider the case when NM = 1 in eq 81 and it is referred to as Case 1 in this article. By solving the proposed mathematical programming model, one can find the optimal refinements in Figure 5 and the corresponding spare-supported cleaning schedule in Table 4. It can be observed that the margined heat exchanger is

Κ

		month																
unit	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
HE1					1								1			1		
HE2		1								0				1				
HE3			2				2				2			2			2	
HE4						2				2						2		
HE5			1							1							1	
HE6													2					

Table 4. Spare-Supported Cleaning Schedule in Case 1<sup>a</sup>





Figure 6. Time profiles of last mixing point on stream C2 in Case 1.



Figure 7. Time profile of bypass flow fraction on stream H2 of unit HE6 in Case 1.

chosen to be HE6 in this refined design and its heat-transfer area is enlarged from the original area of 64.28 m<sup>2</sup> in Table 2 to 93.15 m<sup>2</sup> ( $\mu_6 = 1.449$ ). Notice that cold stream C1 calls for the extra auxiliary heater AHT1 with a heat-transfer area of 1.78 m<sup>2</sup>, while C2 is supposed to be brought to its target temperature via heat exchanges with the hot process streams only. Notice also that the margin ratios of the existing heaters and coolers are all specified under the corresponding utility users in Figure 5. Specifically, the heat-transfer areas of these margined units in the refined design are increased from their original values in Table 2 to those listed below

- CL1:17.75 m<sup>2</sup> ( $\mu_1^{\text{CL}} = 2.45$ );
- CL2:21.11 m<sup>2</sup> ( $\mu_2^{CL} = 1.74$ );
- CL3:22.76 m<sup>2</sup> ( $\mu_3^{\text{CL}} = 1.74$ );
- CL4:19.98 m<sup>2</sup> ( $\mu_4^{\text{CL}} = 23.5$ );
- HT3:17.08 m<sup>2</sup> ( $\mu_3^{\text{HT}} = 2.72$ ).

The selected bypass locations are essentially the same as those adopted in superstructure, i.e., the cold-stream sides of HE2, HE4, and HE5 and the hot-stream sides of HE3 and HE6. From Table 4, one can also see that two spares should be purchased. Spare 1 supports HE1, HE2, and HE5 with a heat-transfer area of 90 m<sup>2</sup>, while spare 2 supports HE3, HE4, and HE6 with an area of 71.34 m<sup>2</sup>.

Let us next take a closer look at the end temperatures of cold streams C1 and C2 over the whole horizon. Such details are important because, in the original design, these two streams are not equipped with heaters and thus should be difficult to control under disturbances. Since C2 in the refined HEN deisgn (i.e., Figure 5) is still without an auxiliary heater, maintaining its target temperature is considered to be one of the most critical task in the corresponding HEN operation. Therefore, let us examine the dynamic behavior of temperature at the last mixing point on C2 in the optimum solution (see Figure 6). According to the Gantt chart presented in Table 4, HE6 is supposed to be operated continuously in the first 12 months without cleaning and the defouling operation is performed only in the 13th month with a spare. It can be oberved from Figure 6 that the design target of C2 can nontheless be achieved approximately throughout the entire horizon by adjusting the bypass flow on HE6. To facilitate further understanding of the corresponding compensation





mechanism, the time profile of bypass flow fraction on the hotstream side of HE6 is also plotted in Figure 7. On the other hand, since there are no margined heat exchangers on C1 and HE3 is scheduled to be cleaned and replaced with a large enough spare in the third, seventh, 11th, 14th, and 17th month, the design target of C1 may not be reachable at the last mixing point (see Figure 8). As a result, an auxiliary heater (AHT1) must be installed on C1 to make up the difference between the targeted and actual heat exchange rates of HE3 in the months when cleaning is not performed.

The cost estimates of three distinct scenarios in Case 1 can be found in Table 5. First, it can be observed that a 36.9%

Table 5. Cost Estimates in Case 1

		without margins, bypasses, and cleaning	spare- supported cleaning without margins	spare- supported cleaning with HEN refinements
TAOC (million \$/year)	TAUC (hot)	1.06	0.99	0.59
	TAUC (cold)	1.42	1.12	0.89
	TACLC		0.04	0.06
TACC	$CC_1$		0.04	0.02
(million \$/year)	$CC_2$			0.005
	$CC_3$	0.02	0.02	0.007
TAC (million \$/yes	ar)	2.49	2.20	1.57
computation time (	sec)	46	139	659

reduction in the total annual cost (TAC) is achievable by applying the spare-supported cleaning schedule together with the proposed design refinements. Notice that a less significant 11.6% saving is realized with only the spare-supported clean operations (but without the desig refinements). This is due to the fact that incorporation of the proposed design changes clearly drives the total annual utility cost to a much lower level. More specifically, the added margins, bypasses and auxiliary units enhance the system flexibility considerably and enable effective heat load shifts on the paths and loops embedded in the given HEN. Finally, it should be noted that the proposed supperstructure (see Figure 4) is really indispensable for all optimization runs in the present case. Without it, all locations of margins and bypasses must be considered and the corresponding computations cannot converge.

**13.2.** Additional Cases. Let us next raise the maximum number of margined units in HEN to 2, i.e., NM = 2 (which is referred to as Case 2). By solving the proposed mathematical programming model based on the superstructure in Figure 4,

one can produce the optimal refinements in Figure 9 and the corresponding spare-supported cleaning schedule in Table 6. It can be observed that the margined units in this case are switched to HE3 and HE5 instead and their heat-transfer areas are required to be increased from the original values in Table 2 to 41.27 m<sup>2</sup> ( $\mu_3 = 1.5$ ) and 426.8 m<sup>2</sup> ( $\mu_5 = 1.5$ ), respectively. Notice that the extra auxiliary heater AHT2 is now placed on cold stream C2, while C1 is without any auxiliary unit. The heat-transfer area of AHT2 is 21.2 m<sup>2</sup>. Again, the margin ratios of the existing heaters and coolers are specified under the corresponding utility users in Figure 9 and the selected bypass locations are essentially the same as those adopted in superstructure. The heat-transfer areas of the margined coolers and heater in the refined design are raised from their original values in Table 2 to those listed below

- CL1:52.46 m<sup>2</sup> ( $\mu_1^{\text{CL}} = 7.63$ ).
- CL2:32.39 m<sup>2</sup> ( $\mu_2^{\text{CL}} = 2.67$ ).
- CL3:24.46 m<sup>2</sup> ( $\mu_3^{CL} = 1.87$ ).
- CL4:18.11 m<sup>2</sup> ( $\mu_4^{\text{CL}} = 21.3$ ).
- HT3:18.21 m<sup>2</sup> ( $\mu_3^{\text{HT}} = 2.9$ ).

One can also observe from Table 6 that only one spare is needed in this case, i.e., spare 3, which is used to support HE1, HE4, HE5, and HE6 with a heat-transfer area of  $284 \text{ m}^2$ .

Figures 10 and 11 show the last mixing-point temperatures on cold streams C1 and C2, respectively. Since C1 in Figure 9 is without an auxiliary heater, its target temperature should be maintained by manipulating the bypass flow on the margined unit HE3. According to the Gantt chart presented in Table 6, HE3 can be operated continuously in the entire 18 months without cleaning. Although fouling may gradually reduce its overall heat-transfer coefficient during operation, HE3 should still be able to carry the same heat load by diverting more flow from bypass to the heat exchanger. This general downturn can be observed in the time profile of bypass flow fraction on HE3 in Figure 12. On the other hand, since there are no margined heat exchangers on C2, its design target is not always reachable at the last mixing point (see Figure 11) and, thus, the auxiliary heater AHT2 must be made available for bringing the end temperature of C2 to the designated value.

Although the same computations have been repeated for NM = 3 (Case 3), the corresponding results are not included in this paper for the sake of brevity. Instead, the cost estimates of all three cases are compared in Table 7. By comparing with the reference scenario in which the given HEN is operated without spares, margins, bypasses, and cleaning (see Table 5), the TAC savings in Case 2 and Case 3 are further increased to 46 and 50%, respectively. The lower TAC is primarily due to the lower



Figure 9. Refined HEN design obtained in Case 2.

Table 6. Spare-Supported Cleaning Schedule in Case  $2^{a}$ 

									1	month								
unit	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
HE1		0			0					3					0			
HE2		0								0					0			3
HE3																		
HE4					0			3					3					0
HE5		3			3							3			3			
HE6							(3)							(3)				

 $^{a}$ O: Regular cleaning operation; 3: cleaning operation supported by spare 3.



Figure 10. Time profiles of last mixing point on stream C1 in Case 2.

operating costs realized with with a larger number of margined units.

## 14. CONCLUSIONS

An improved mathematical programming model has been proposed in this work to synthesize the optimal sparesupported cleaning schedule and the corresponding design refinements for any given heat exchanger network. For the purpose of ensuring solution convergence in the optimization runs, a systematic procedure has been developed to perform preliminary test runs for identifying candidate locations of margins and bypasses. The candidate refinements can be incorporated into a superstructure for use as a template to build the aforementioned MINLP model. In addition, a set of heuristic rules have also been adopted to impose extra constraints on the spares to further reduce the search space. The effectiveness of this approach has been verified in extensive case studies. It can be observed from the optimization results that spares, margins, bypasses, and auxiliary units are viable options for reducing the extra amount of utility consumption caused by fouling and/or temporarily removing online heat exchangers for cleaning purpose.



Figure 11. Time profiles of last mixing point on stream C2 in Case 2.



Figure 12. Time profile of bypass flow fraction on stream H4 of unit HE3 in Case 2.

#### Table 7. Comparison of Cost Estimates in All Cases

case no. 1		1	2	3
TAOC (million \$/year)	TAUC (hot)	0.59	0.51	0.33
	TAUC (cold)	0.89	0.86	0.83
	TACLC	0.06	0.054	0.046
TACC (million \$/year)	$CC_1$	0.02	0.02	0.02
	$CC_2$	0.005	0.009	0.012
	$CC_3$	0.007	0.007	0.008
TAC (million \$/year)		1.57	1.46	1.24
computation time $(sec)$		659	738	628

## ASSOCIATED CONTENT

## **S** Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.iecr.7b04098.

Test run results for scenario 2 in example problem (PDF)

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## Notes

The authors declare no competing financial interest.

#### NOMENCLATURE

#### Sets

EX = Set of all exchangers in the given HEN I = Set of all hot streams in the given HEN

 $I_a$  = Set of hot streams which are cooled without utilities

 $I_b^{"}$  = Set of hot streams that are partially cooled with utilities

J = Set of all cold streams in the given HEN

 $J_a$  = Set of cold streams which are heated without utilities

 $J_b$  = Set of cold streams that are partially heated with utilities

- MA = Set of all matches in the given HEN
- P = Set of all periods in the given time horizon
- S = Set of all spares

TP = Set of all time points, i.e., {bcp,ecp,bop,eop}

#### Variables

 $A_e^{\text{M}}$  = Heat-transfer area of margined heat exchanger  $e \in \text{EX}$  $A_{j_a}^{\text{AHT}}$ ,  $A_{i_a}^{\text{ACL}}$  = Heat-transfer areas of auxiliary heater on cold stream  $j_a \in J_a$  and auxiliary cooler on hot stream  $i_a \in I_a$  $As_s$  = Heat-transfer area of spare  $s \in S(m^2)$ 

 $a_{e,kp}^{\text{fm},\text{tp}} = \text{Overall heat-transfer coefficient of exchanger } e \in \text{EX}$ determined according to fouling model fm  $\in \{L, E\}$  at time point tp  $\in$  TP during period  $p \in \text{P}$  ( $p \ge 2$ ) in scenario (i) if exchanger  $e \in \text{EX}$  is last cleaned during period k and  $1 \le k < p$  (kW/m<sup>2</sup>K)

 $c_{e,p}^{\text{fm},\text{tp}} = \text{Overall heat-transfer coefficient determined according to fouling model fm } \in \{L, E\}$  at time point tp  $\in$  TP during period  $p \in P$  in scenario (iv) (kW/m<sup>2</sup>K)

 $\mathbf{E}\mathbf{u}_{j,p}^{H}$ ,  $\mathbf{E}\mathbf{u}_{i,p}^{C}$  = Estimates of the total hot and cold utility consumption levels needed respectively by cold stream  $j \in \mathbf{J}$ and hot stream  $i \in \mathbf{I}$  in period  $p \in \mathbf{P}$  (kW-mon)

LMTD<sup>ip</sup><sub>*e,p*</sub> = Log-mean temperature difference of heat exchange  $e \in EX$  at time point tp  $\in$  TP in period  $p \in P(K)$ 

 $ne_{i,v}^{H,tp}$ ,  $ne_{i,v}^{C,tp}$  = Fictitious nonnegative variables showing conformity levels of target temperatures of hot stream  $i \in I$ and cold stream  $i \in J$ , respectively, at time point tp  $\in TP$ during period  $p \in P(K)$ 

 $po_{i,p}^{H,tp}$ ,  $po_{i,p}^{C,tp}$  = Fictitious nonnegative variables showing violation levels of target temperatures of hot stream  $i \in I$  and cold stream  $j \in J$ , respectively, at time point tp  $\in$  TP during period  $p \in P(K)$ 

 $Q_{e,p}^{\text{tp}}$  = Heat-transfer rate achieved in heat exchanger  $e \in \text{EX}$ at time point tp  $\in$  TP in period  $p \in$  P (kW)

 $Qu_{i,p}^{H,tp}Qu_{i,p}^{C,tp}$  = Hot and cold utility consumption rates needed respectively by cold stream  $j \in J$  and hot stream  $i \in I$ at time point tp  $\in$  TP in period  $p \in$  P (kW)

 $R_{en}^{tp}$  = Ratio between the heat capacity flow rates of cold and hot streams in heat exchanger  $e \in EX$  at time point tp  $\in TP$ during period  $p \in P$ 

 $r_e$  = Fouling resistance of heat exchanger  $e \in \text{EX} (\text{m}^2\text{K}/\text{kW})$  $T_{m,i,v}^{\mathrm{H,tp}}$  = Temperature at mixing point *m* on hot stream *i*  $\in$  I at time point tp  $\in$  TP during period  $p \in$  P (K)

 $T_{n,i,p}^{C,tp}$  = Temperature at mixing point *n* on hot stream *j*  $\in$  J at time point tp  $\in$  TP during period  $p \in$  P (K)

 $\operatorname{Ti}_{e,p}^{H,tp}$ ,  $\operatorname{To}_{e,p}^{H,tp}$  = Inlet and outlet hot stream temperatures of unit  $e \in EX$  at time point tp  $\in$  TP during period  $p \in P(K)$  $\operatorname{Ti}_{e,v}^{C,tp}$ ,  $\operatorname{To}_{e,v}^{C,tp}$  = Inlet and outlet cold stream temperatures of unit  $e \in EX$  at time point tp  $\in$  TP during period  $p \in P(K)$  $U_{e,n}^{\text{fm,tp}}$  = Overall heat-transfer coefficients of exchanger  $e \in \text{Ex}$ at time point tp  $\in$  TP in period  $p \in$  P determined according to fouling model fm  $\in \{L, E\}$  (kW/m<sup>2</sup>K)

 $X_{e,p,s}$  = A binary variable used to denote whether or not spare  $s \in S$  is adopted to replace exchanger  $e \in EX$  during period p  $\in P$ 

 $Y_{e,p}$  = A binary variable used to denote whether or not exchanger  $e \in EX$  is cleaned during period  $p \in P$ 

 $Z_s$  = A binary variable used to reflect whether or not spare s  $\in$  S is needed to facilitate implementation of the cleaning schedule

 $Z_e^{\rm M}$  = A binary variable used to reflect whether or not unit *e* is margined

 $Z_i^{AHT}$ ,  $Z_i^{ACL}$  = Binary variables used to reflect whether or not auxiliary heater on cold stream  $i \in J_a$  and auxiliary cooler on hot stream  $i \in I_a$  are present, respectively

 $\Gamma_{e,s}$  = A binary variable denoting whether or not exchanger *e*  $\in$  EX is replaced with spare  $s \in$  S in at least one period  $\mu_e$  = Margin ratio of heat exchanger  $e \in EX$ 

 $\mu_{j_b}^{\text{HT}}$ ,  $\mu_{i_b}^{\text{CL}}$  = Margin ratios of existing heater on cold stream  $j_b$  $\in$  J<sub>b</sub> and existing cooler on hot stream  $i_b \in$  I<sub>b</sub>

 $\phi_{en}^{\rm H,tp}$  = Fraction of flow rate of hot stream passing through unit  $e \in EX$  at time point tp  $\in$  TP during period  $p \in P$  $\phi_{e,p}^{C,tp}$  = Fraction of flow rate of cold stream passing through unit  $e \in EX$  at time point tp  $\in$  TP during period  $p \in P$  $\tilde{\phi}_{i,p}^{m,\text{tp}}$  = Flow fraction of bypass joining mixing point *m* on hot stream  $i \in I$  at time point tp  $\in$  TP during period  $p \in$  P  $ilde{\phi}^{n, ext{tp}}_{i,p}$  = Flow fraction of bypass joining mixing point n on hot stream  $j \in J$  at time point tp  $\in$  TP during period  $p \in$  P  $\xi_e^{\rm H}$  = A binary variable denoting whether or not the bypass on unit  $e \in EX$  is located on the hot-stream side  $\xi_e^{\rm C}$  = A binary variable denoting whether or not the bypass

on unit  $e \in EX$  is located on the cold-stream side

## $\Psi$ = Penalty term in the objective function

#### Parameters

 $A_e$  = Heat-transfer area of exchanger  $e \in EX$  in the given HEN  $(m^2)$ 

 $A_{i_{b}}^{\text{HT}}$ ,  $A_{i_{b}}^{\text{CL}}$  = Heat-transfer areas of the existing heater on cold stream  $j_h \in J_h$  and the existing cooler on hot stream  $i_h \in I_h$  in the original HEN design

 $b_{e,n}^{\text{fm,tp}}$  = The overall heat-transfer coefficient of exchanger  $e \in$ EX determined according to fouling model fm  $\in \{L,E\}$  at time point tp  $\in$  {*bop,eop*} during period *p*  $\in$  P in scenarios (ii) and (iii)  $(kW/m^2K)$ 

 $bs_{e,p}^{fm,tp}$  = The overall heat-transfer coefficient determined according to fouling model fm  $\in \{L,E\}$  at time point tp  $\in$ {bcp,ecp} during period  $p \in P$  in scenario (ii) if a spare is adopted to replace exchanger  $e \in EX (kW/m^2K)$ 

 $C_{\text{fix}}^{\text{SP}}$ ,  $C_{\text{fix}}^{\text{AHT}}$ ,  $C_{\text{fix}}^{\text{ACL}}$  = Fixed costs of installing a spare, an auxiliary heater and an auxiliary cooler respectively (\$/yr)

 $C_{\rm M}^{\rm SP}$ ,  $C_{\rm M}^{\prime}$ ,  $C_{\rm M}^{\rm HT}$ ,  $C_{\rm M}^{\rm CL}$ ,  $C_{\rm M}^{\rm AHT}$ ,  $C_{\rm M}^{\rm ACL}$  = Variable cost coefficients for purchasing a spare, an existing heat exchanger, an existing heater, an existing cooler, an auxiliary heater, and an auxiliary cooler, respectively  $(\$/m^{1.6}yr)$ 

 $C_{HU}$ ,  $C_{CU}$  = Unit costs of heating and cooling utilities (\$/kJ)  $C_{cl}$ ,  $C_{cl}^{SP}$  = Unit cleaning costs of a heat exchanger and a spare respectively (\$/cleaning)

 $C_{\rm sp}$  = Annualized cost coefficient for the capital cost of heat exchanger (\$/m<sup>1.6</sup>yr)

 $f_c$  = Duration of a defouling subperiod (mon)

 $Fcp_i^H$ ,  $Fcp_i^C$  = Heat-capacity flow rates (kW/K) of hot stream  $i \in I$  and cold stream  $j \in J$ 

 $K_e$  = Characteristic fouling speed of exchanger  $e \in EX$  $(mon^{-1})$ 

NM = Maximum allowable number of margined heat exchangers

 $NS_s = Maximum$  number of units supported by spare  $s \in S$ over the entire horizon

 $n_{\rm E}$  = Total number of heat exchangers in the given HEN

 $n_n$  = Total number of periods  $\dot{Q}HL_i$ ,  $QCL_i$  = Heat loads of hot stream  $i \in I$  and cold

stream  $i \in J$ , respectively

 $\dot{r}_e$  = Constant fouling rate of exchanger  $e \in EX$  (m<sup>2</sup> K/mon kW)

 $r_e^{\infty}$  = Asymptotic maximum fouling resistance of exchanger e  $\in$  EX (m<sup>2</sup> K/kW)

 $TI_i^{\rm H}$ ,  $TI_i^{\rm C}$  = Initial temperatures of hot stream  $i \in {\rm I}$  and cold stream  $j \in J$ , respectively (K)

 $t_{\rm f}$  = Time horizon (mon)

 $TT_i^{\rm H}$ ,  $TT_i^{\rm C}$  = Target temperatures of hot stream  $i \in I$  and cold stream  $j \in J$ , respectively

 $U_e^{\rm cl}$ ,  $U_{\rm sp}^{\rm cl}$  = Overall heat-transfer coefficients of exchanger  $e \in$ EX and spare  $s \in S$  when the heat-transfer surface is clean

 $(kW/m^2 \tilde{K})$  $\hat{U}_{j_a}^{AHT}$ ,  $\hat{U}_{i_a}^{ACL}$  = Estimates of overall heat-transfer coefficients of the auxiliary heater on cold stream  $j_a \in J_a$  and auxiliary cooler on hot stream  $i_a \in I_a$ 

 $\hat{U}_{i_h}^{\text{HT}}$ ,  $\hat{U}_{i_h}^{\text{CL}}$  = Estimates of overall heat-transfer coefficients of the existing heater on cold stream  $j_h \in J_h$  and existing cooler on hot stream  $i_b \in I_b$ 

 $\tau_p$  = Length of period  $p \in P \pmod{p}$ 

 $\eta_{cl}^{H}$  = Efficiency of cleaning operation  $\eta^{H}$ ,  $\eta^{C}$  = Heat-transfer efficiencies in heater and cooler respectively

 $\omega$  = A positive constant

#### Superscripts:

bcp = The time point at the beginning of cleaning subperiod bpp = The time point at the beginning of operation subperiod

ecp = The time point at the end of cleaning subperiod

eop = The time point at the end of operation subperiod

- E = The exponential fouling model
- L = The linear fouling model

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