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pubs.acs.org/IECR

Optimization of Heat-Integrated Crude Oil Distillation Systems. Part II: Heat Exchanger Network Retrofit Model

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* Supporting Information

ABSTRACT: This is the second part of a series that applies optimization to maximize the productivity and minimize operating costs of existing heat-integrated crude oil distillation systems. This paper presents a two-level retrofit approach for heat exchanger networks. In the first level, simulated annealing proposes topology modifications to the existing network (e.g., adding, removing, and relocating heat exchangers; changing the heat loads of heat exchangers, adding and removing stream splitters, and changing the split fraction of stream splitters). In the second level, a repair algorithm addresses the violation of constraints. These constraints consider the minimum temperature approach, stream enthalpy balances, and existing heat transfer areas. The repair algorithm is formulated as a nonlinear least-squares problem. Temperature-dependent thermal properties are considered in this work for the accurate prediction of stream temperatures. Two case studies illustrate the application of the proposed methodology to decrease total annualized costs.

1. INTRODUCTION

This series presents a new approach to optimize existing heat-integrated crude oil distillation systems (i.e., distillation process and heat exchanger network). In the proposed approach, optimization is applied to find the operating conditions for the overall distillation system and retrofit modifications for the heat exchanger network (HEN) that maximize overall profit. In this paper, challenges related to the modeling and retrofit of heat exchanger networks are addressed, such as the consideration of temperature-dependent thermal properties; the consideration of heat transfer area constraints; the implementation of structural constraints that can account for practical issues such as plant layout and safety, etc.

Part I[1] presents a new approach to model crude oil distillation units. Artificial neural networks are used to obtain accurate and robust models that include the main operational variables of the distillation process (e.g., flow rates of distillation products and stripping steam, pump-around duties, and temperature drops, etc.).

This second part of the series presents a new approach to retrofit heat exchanger networks of crude oil distillation units. The proposed retrofit approach considers structural (e.g., location of heat exchangers and stream splitters in the network) and operational variables (e.g., heat loads, stream split fractions, temperatures, etc.) of the heat exchanger network. Constraints (e.g., HEN structure constraints, minimum temperature approach constraints, heat transfer area constraints, etc.) are included to ensure that solutions are industrially acceptable and practicable. In Part III[2] of the series, the distillation and HEN models described in Parts I[1] and II, respectively, are incorporated into a framework that optimizes the distillation process and HEN simultaneously for net profit improvement.

This paper is organized as follows. A review of previous HEN retrofit approaches is presented first. Then, the HEN simulation model used to calculate stream flow rates and temperatures is described. The two-level retrofit approach is then introduced. Two case studies illustrate the application of the proposed retrofit approach to reduce the total annualized cost of a heat exchanger network. Finally, conclusions highlighting the advantages and limitations of the proposed approach are presented.

2. PREVIOUS WORK ON HEAT EXCHANGER NETWORK RETROFIT

The engineering of heat exchanger networks is carried out in a range of contexts. If a heat exchanger network is needed, the engineering involves its grass-roots design, where the matches between hot and cold streams are selected and the duties, heat transfer areas, and corresponding temperatures are determined. When conditions change, for example, heating needs or energy costs, operational optimization may be needed to determine the most appropriate heat and material flows and corresponding duties within the existing HEN. In this case, the fixed connections and heat exchanger areas constrain the extent to which flows can be changed. Instead, it may be appropriate to retrof it the HEN, where configurational changes related to

Received: September 25, 2014
Revised: March 13, 2015
Accepted: March 23, 2015
Published: March 23, 2015

DOI: 10.1021/ie503804u
Ind. Eng. Chem. Res. 2015, 54, 5001−5017

connections between exchangers and stream splits, and operational changes related to heat and material flows as well as modifications to individual exchangers, are considered. Heat exchanger modifications include the addition and enhancement of the heat transfer area, installation of new heat exchangers, and repiping connections between heat exchangers.

This paper focuses on retrofit of crude oil heat exchanger networks. The reason for this is that, from the total of grass-roots and retrofit projects implemented in industry, approx-imately 70% of these projects are revamps.[3] Operational optimization is even more frequently implemented than grass-roots and retrofit projects. While operational optimization can be applied relatively easily in both the distillation unit and the HEN as no changes in the structure of equipment are made, it is more common to retrofit the HEN than the distillation unit. Structural changes related to the distillation unit (e.g., installation of a preflash, change of column internals, etc.) are more complex, requiring more capital investment and installation time, than structural changes related to the heat exchanger network (e.g., installation of new heat exchangers and stream splitters, repiping existing heat exchangers, etc.). Increased productivity, changes in feedstock conditions, and increased energy costs are some reasons that motivate the implementation of retrofit projects and operational optimiza-tion.

2.1. HEN Design Methodologies. In this paper, HEN design refers to grass-roots, retrofit, and operational optimiza-tion design approaches for heat exchanger networks. These approaches can be divided into methodologies that use pinch analysis, methodologies that employ optimization algorithms, or methodologies that combine both, as noted in a recent comprehensive review of HEN retrofit methodologies.[4] Optimization-based HEN design methodologies can either employ deterministic or stochastic optimization algorithms. The former employs first and second-order derivatives to find solutions, while the latter also uses random numbers in the search procedure.

Pinch analysis includes the pinch design method, which was introduced in ref 5 for the synthesis of energy-efficient heat exchanger networks. This method combines thermodynamic principles and engineering judgment to develop HEN designs with minimum energy consumption (i.e., energy targets). Recent examples of the application of pinch analysis to retrofit HENs are presented by Bulasara et al.[6] and Al-Mutairi and Babaqi.[7] Bulasara et al. [6] considered networks with streams from a crude oil distillation unit and a delayed coking unit, while Al-Mutairi and Babaqi[7] considered streams from an atmospheric unit and a vacuum distillation unit. In these approaches,[6,7] the grand composite curve is used to identify the pinch and to determine energy targets. Then, the pinch design method is applied to retrofit the HEN. The main advantage of these approaches[6,7] is that they are simple and do not require complex algorithms to find solutions. However, as they rely in strong user interaction, optimal solutions cannot be guaranteed. Another disadvantage is that the grand composite curve may fail to provide accurate estimations of energy requirements when compared to detailed HEN models.

Optimization-based methodologies to retrofit heat exchanger networks usually divide the retrofit problem into two or more problems. These problems are also known as stages or levels. Typically, the first stage proposes topology modifications (e.g., adding new heat exchangers, removing or relocating existing heat exchangers, adding or removing stream splitters) that potentially lead to a more cost-effective HEN (e.g., reduced energy consumption, reduced annualized costs, etc.), compared to the original HEN configuration. Then, the HEN with the selected topology modifications is further optimized (e.g., heat loads, heat transfer areas, etc.) in the following stages to improve the HEN performance. A smaller number of retrofit approaches have been formulated as single-stage optimization problems.[8] In these single-stage problems, the discrete (i.e., HEN topology) and continuous variables (e.g., heat loads, stream split fractions) are optimized simultaneously. Solving a multistage HEN retrofit problem is more computationally efficient than solving a single-stage problem. It is easier to solve various simpler, less nonlinear optimization problems than to solve a single complex large-scale problem.

Various HEN retrofit frameworks using deterministic optimization algorithms have been developed.[9−13] However, the main shortcoming of these retrofit approaches is that they usually employ superstructure models,[9,10,12,13] which introduce structural inflexibilities that bias the search process.[14] A superstructure is a stage-wise representation where predefined heat transfer matches between hot and cold streams can occur within each stage.[15] These inflexibilities arise from the predefinition of the number and location of exchanger matches and splitters in each superstructure stage. Zhu and Asante[11] present a retrofit methodology that does not use superstructure models. Instead, the network pinch concept, mixed-integer linear programming and user interaction are used to provide a set of retrofit options (e.g., adding, relocating heat exchangers, adding stream splitters), from which one is selected. The proposed methodology[11] does not guarantee HENs with minimum cost since the selection of retrofit modifications is based on energy demands instead of costs.

Stochastic optimization algorithms have been used to overcome these limitations. Commonly used algorithms to design HENs are simulated annealing[8,14,16] (SA), genetic algorithms,[17,18] tabu search, [19] and differential evolution.[20] Dolan et al.[8] were the first to use stochastic optimization, namely SA, for the synthesis of HENs. Starting from an initial design, the SA algorithm randomly selects structural modifications at random positions within the HEN. In the approach of Dolan et al.,[8] the continuous and discrete variables of the HEN are optimized by solving a single-stage optimization problem. A two-level approach using SA and nonlinear programming (NLP) is presented by Athier et al.[14] In their methodology, topology modifications are performed using SA, while NLP is used to optimize the continuous variables of the HEN. The approaches of Dolan et al.[8] and Athier et al.[14] were originally developed for grass-roots design of HENs. However, the principles used to perform structural modifica-tions can be applied to retrofit as long as practical constraints relevant to the HEN retrofit problem (e.g., constraints on the type and number of structural modifications) are considered.

Rodrıguez[21] presents a simulated annealing-based design methodology to mitigate HEN fouling. A HEN simulation model is developed to predict fouling over a period of time, while a retrofit model using SA is developed to propose HEN structural modifications that potentially reduce fouling. The retrofit approach is similar to that of Athier et al.[14] SA is employed to perform structural modifications (e.g., adding, removing, relocating heat exchangers; adding, removing stream splitters). As a subproblem, deterministic optimization is used to balance the exchanger heat loads so as to meet minimum temperature approach constraints and enthalpy balance

DOI: 10.1021/ie503804u
Ind. Eng. Chem. Res. 2015, 54, 5001−5017

constraints. Although fouling is the main scope of the work in ref 21, the simulation and retrofit models of ref 21 have been used to optimize HENs in terms of energy consumption and total annualized costs.[16,22,23]

Chen and co-workers[16,23] present a design approach applying the models of ref 21 for grass-roots design and retrofit of crude oil heat exchanger networks. Both approaches[16,23] employ SA to perform modifications to the initial HEN, although the approach of Smith et al.[23] applies the network pinch concept [11] to facilitate the identification of retrofit options. Then, NLP is used to calculate the heat loads that regain feasibility (i.e., avoid violating constraints) of the HEN. This SA formulation[16,23] can handle various objectives, such as minimizing energy consumption, minimizing capital investment, or minimizing total costs.

Frameworks based on stochastic optimization can approach the HEN design problem as grand canonical problems.[8] In grand canonical problems, the number of elements vary as the optimization progresses, where the elements include the number of heat exchangers, splitters, and variables associated with these units (e.g., heat loads, heat transfer areas, split fractions). Thus, the size of the optimization problem increases or decreases as the HEN evolves to an improved design. This feature represents an advantage over superstructure-based approaches, where a considerable number of heat exchangers and splitters are predefined even though these units may not exist in the final design.

Stochastic optimization has the ability of performing a more thorough exploration of the search space than deterministic optimization, due to its ability to escape local optima.[24] In particular, SA is advantageous when dealing with discrete optimization variables and highly combinatorial problems,[8,24] such as the HEN retrofit problem. On the other hand, deterministic optimization reaches the optimum with more precision and more quickly than stochastic optimization. It is recommended[24] to combine both stochastic and deterministic optimization algorithms during the search for a global optimum. While most of the approaches mentioned above employ some sort of problem decomposition,[9−14,16,21,23] relatively few approaches follow this recommendation.[14,16,21,23]

The retrofit approach developed by Chen[16] includes the main structural modification options that are relevant to the retrofit problem and models stream enthalpy as a function of temperature. Furthermore, the work of Chen[16] combines stochastic and deterministic optimization to exploit the advantages of each method, where appropriate. That is, SA is used to handle discrete variables and to overcome local minima in the main optimization problem. In the resulting structure, deterministic optimization is employed to quickly optimize the continuos variables of the HEN so as to restore feasibility. Following this rationale, the methodology developed by Chen[16] is extended in this work to perform retrofit of crude oil heat exchanger networks.

2.2. Approaches Used to Simplify the HEN Design Problem.

Grass-roots design and retrofit of heat exchanger networks are classified as NP-hard problems.[20,25] That is, there are no computationally efficient, exact solution algorithms for these problems.[25] The main feature that makes HEN design a NP-hard problem is that many combinations of structural arrangements can be proposed.[26] To reduce this complexity, simplifying assumptions or problem decomposition are often implemented. Although more computationally efficient, the disadvantage of these approaches is that solutions are more likely to be inaccurate, when compared to the real process, or suboptimal.

Some simplifying assumptions relate to the HEN structure and the calculation of stream properties. Examples of simplifying assumptions for the HEN topology include the use of the network pinch concept to identify retrofit modifications,[11,13,23] neglecting certain types of structural modifications, e.g. relocation of heat exchangers[8] or the installation of stream splitters,[9] and the use of superstructure models.[9,10,12,13] Since the HEN grass-roots and retrofit problems are highly combinatorial, to define a superstructure that is manageable in size necessitates the omission of some design options, which can lead to suboptimal solutions.

Other simplifying assumptions relate to the estimation of stream properties, such as heat capacities and heat transfer coefficients. The approaches developed by Zhu and Asante,[11] Chen and co-workers,[16,23] and Sreepathi and Rangaiah[27] consider the temperature dependence of heat capacities. It was shown in Part I[1] of the series, and also by Chen,[16] that energy requirements and stream temperatures may be significantly underestimated when heat capacities are assumed constant. Therefore, the consideration of temperature-depend-ent heat capacities is adopted in this work to provide more realistic estimations of energy requirements, stream temper-atures, and heat transfer areas.

This paper presents a new retrofit approach for heat exchanger networks. HEN simulation and retrofit models are developed to improve the total annualized cost of the HEN. The retrofit model of Chen[16] is extended to include constraints on heat transfer areas and utility consumption, and a more flexible method to handle temperature-dependent heat capacities. The simulation model used by Chen[16] is replaced by a model formulated using principles of graph theory, which explicitly addresses network connectivity in its equations and facilitates the manipulation of the HEN structure by the optimization algorithm.

3. HEN SIMULATION MODEL

Given a fixed HEN structure and specifications (e.g., heat loads, heat capacity flow rates, etc.), the simulation model used in this work calculates the inlet and outlet temperatures for each heat exchanger and splitter, and required heat transfer areas. This information is used in the HEN retrofit methodology to calculate energy and heat transfer area requirements, and to assess the feasibility of the HEN. The implementation of this model into the HEN retrofit methodology is described in section 4. The HEN simulation model is based on the model of de Oliveira Filho et al.,[28] which uses graph theory to describe the HEN topology. One advantage of the simulation model of de Oliveira Filho et al.[28] is that the HEN structure can be easily manipulated using this formulation. Another advantage is that the solution of the model equations is straightforward, since they are formulated as two systems of linear equations.

Key extensions of the model of de Oliveira Filho et al.[28] relate to the use of unit operations relevant to crude oil distillation systems (e.g., desalters) and the energy balance for unit operations and heat exchangers specified in terms of heat loads. For the sake of continuity, the model of de Oliveira Filho et al.[28] and the new extensions are described in sections 3.1 to 3.3. The strategy to simulate HENs for streams with temperature-dependent heat capacities is presented in section 3.4.

DOI: 10.1021/ie503804u
Ind. Eng. Chem. Res. 2015, 54, 5001−5017

3.1. Network Structure. The HEN structure can be represented by a directed graph or digraph. A digraph is composed by points called vertices and edges that connect the vertices. In a directed graph, the edges indicate the direction in which the vertices are connected. The HEN grid diagram is a digraph where the vertices represent the following elements: external units (i.e., supply and demand units), heat exchangers, splitters, mixers, and unit operations. The edges represent the stream segments that connect each element of the HEN.[28]

Figure 1 shows the grid diagram of a simple HEN consisting of two hot process streams, two cold process streams, three heat exchangers, one splitter (s1), one mixer (m1), and one unit operation (P). Unit operations are introduced in this work as devices that modify either the enthalpy or the temperature of a stream. These units are represented in a simplistic manner in this HEN simulation model: no details of the behavior of the unit operation are provided, and the cooling or heating medium are not represented in the overall energy balance. An important example of a unit operation is a crude oil desalter. In this unit, the temperature of the crude oil decreases while no significant change in material flow takes place.

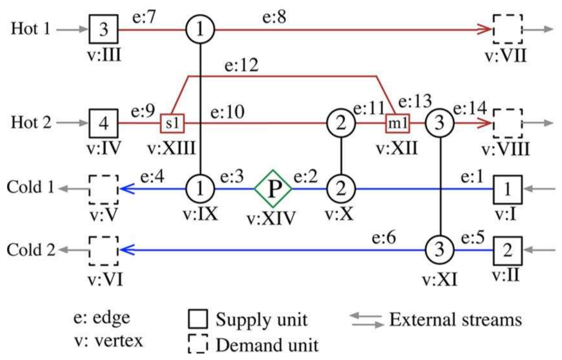

Figure 1. Grid diagram of a simple HEN.

Each stream has one supply unit and one demand unit (i.e., the external units), which indicate the beginning and the end of the stream passing through the HEN. Each external unit is associated with an external stream that represents the material flow entering a supply unit or the material flow leaving a demand unit. These external streams relate to material flows of associated processes (e.g., crude oil distillation). Thus, the HEN depicted in Figure 1 consists of 14 elements (i.e., N vertices) connected by 14 edges (i.e., S edges). External streams are not included in the grid diagram although they are illustrated in Figure 1 for clarity.

Every digraph, and thus the HEN grid diagram, can be described using an incidence matrix. In an incidence matrix M, each row i represents one element of the HEN and each column j represents one edge. If the element i is directed to edge j, then M = −1; if the element i is directed from edge j, $M_{ij} = 1$. If there is no link between element i and edge j, then $M_{ij} =$ 0. Figure 2 shows the incidence matrix corresponding to the HEN presented in Figure 1, where, for clarity, zero values are left blank.

The incidence matrix can be arranged according to de Oliveira Filho et al.[28] into a group of submatrices, as shown in eq 1 (in Figure 2). In this equation, superscripts PS and PD refer to supply and demand units, HE to heat exchangers, MX to mixers, SP to splitters, and PR to unit operations, respectively. Subscripts c and h refer to the cold and hot streams. The dashed lines in Figure 2 indicate the partition of matrix M.

The dimension of matrix M is N × S, where N is the total number of elements ($N = N^{PS} + N^{PD} + N^{HE} + N^{MX} + N^{SP} + N^{PR}$) and S is the total number of edges ($S = S_c + S_h$). The dimensions of submatrices in eq 1 are described in Table S1 (see Supporting Information).

The incidence matrix facilitates the formulation of mass and energy balances for the HEN. Following the procedure proposed by de Oliveira Filho et al.,[28] HEN simulation requires solving two systems of linear equations. The first set of linear equations is a mass balance that calculates the mass flow rates for each edge of the HEN. The second system of linear equations is an energy balance that provides the temperatures for each edge. The mass and energy balances for each type of element will be presented in sections 3.2 and 3.3, respectively.

3.2. Mass Balance. Mass flow rates for each edge of the HEN are represented by vector m (dimension S × 1), which can be divided in cold and hot subvectors $m^T = [m^T{}_c\ m^T{}_h]$. On the other hand, vector n (dimension $N^P \times 1$, where $N^P = N^{PS} + N^{PD}$) represents the mass flow rates of the external streams. This vector can be divided into vectors for the supply and demand units: $n^T = [(n^{PS})^T\ (n^{PD})^T]$.

Each process stream that enters the HEN at the supply units has a known flow rate, since each of these streams comes from the distillation process. These known flow rates are HEN specifications represented by vector $(n^{PS})^*$.

Supply and Demand Units. The expression $m_k - n_k = 0$ represents the mass balance for the supply unit k. The same

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}^{PS} \\ \mathbf{M}^{PD} \\ \mathbf{M}^{HE} \\ \mathbf{M}^{MX} \\ \mathbf{M}^{SP} \\ \mathbf{M}^{PR} \end{bmatrix} = \begin{bmatrix} \mathbf{M}_c^{PS} & \mathbf{M}_h^{PS} \\ \mathbf{M}_c^{PD} & \mathbf{M}_h^{PD} \\ \mathbf{M}_c^{HE} & \mathbf{M}_h^{HE} \\ \mathbf{M}_c^{MX} & \mathbf{M}_h^{MX} \\ \mathbf{M}_c^{SP} & \mathbf{M}_h^{SP} \\ \mathbf{M}_c^{PR} & \mathbf{M}_h^{PR} \end{bmatrix} \quad (1)$$

	1	2	3	4	5	6	7	8	9	1	11	12	13	14
I	-1													
II					-1									
III							-1							
IV									-1					
V				1										
VI						1								
VII								1						
VIII														1
IX			1	-1			1	-1						
X	1	-1								1	-1			
XI					1	-1							1	-1
XII											1	1	-1	
XIII									1	-1		-1		
XIV		1	-1											

Figure 2. Incidence matrix: (left) general formulation (eq 1); (right) incidence matrix corresponding to Figure 1.

DOI: 10.1021/ie503804u
Ind. Eng. Chem. Res. 2015, 54, 5001−5017

expression is applicable to the demand units. Equation 2 shows the matrix representation of the mass balance for these units:

$$\begin{bmatrix} \mathbf{M}^{PS} \\ -\mathbf{M}^{PD} \end{bmatrix} \mathbf{m} + \mathbf{n} = 0 \tag{2}$$

Heat Exchangers. The mass balance for the cold and hot sides of heat exchanger k is described by eq 3 and 4, respectively:

$$m_{k,\mathrm{c,in}} - m_{k,\mathrm{c,out}} = 0 \tag{3}$$

$$m_{k,\mathrm{h,in}} - m_{k,\mathrm{h,out}} = 0 \tag{4}$$

where subscripts in and out refer to the inlets and outlets. For the full set of heat exchangers in the network, the incidence matrix allows eq 3 and 4 to be written as

$$\mathbf{M}_c^{HE} \mathbf{m}_c = 0 \tag{5}$$

$$\mathbf{M}_h^{HE} \mathbf{m}_h = 0 \tag{6}$$

Mixers and Splitters. To model mixers and splitters, it is assumed in this work that only two stream branches are allowed per splitter. However, it is possible to divide a stream into any number of branches by combining various splitters.

Mixer k combines two inlet streams into a single outlet stream, which can be expressed by eq 7:

$$m_{k,\mathrm{in},1} + m_{k,\mathrm{in},2} - m_{k,\mathrm{out}} = 0 \tag{7}$$

where subscripts 1 and 2 are used to differentiate between the inlet streams. Equation 8 shows the matrix formulation of eq 7:

$$\mathbf{M}^{MX} \mathbf{m} = 0 \tag{8}$$

Splitter l divides one inlet stream into two outlet streams. This can be represented by the following equations (eq 9 and 10):

$$m_{l,\mathrm{in}} - m_{l,\mathrm{out},1} - m_{l,\mathrm{out},2} = 0 \tag{9}$$

$$\alpha_l m_{l,\mathrm{in}} - m_{l,\mathrm{out},1} = 0 \tag{10}$$

where α is the fraction of the inlet stream that flows into stream 1. The matrix representation for eq 9 and 10 is presented by eq 11 and 12, respectively:

$$\mathbf{M}^{SP} \mathbf{m} = 0 \tag{11}$$

$$[\mathrm{diag}(\alpha)\, \mathbf{M}_{+}^{SP} - \mathbf{SP}]\mathbf{m} = 0 \tag{12}$$

Vectors α (dimension $N^{SP} \times 1$), a (dimension $N^{SP} \times 1$) and matrix SP (dimension $N^{SP} \times S$) are introduced to express eq 10 in terms of the incidence matrix. Here, α contains the split fraction specifications for each stream splitter. Vector a indicates the edges for which the split fractions are specified. SP is a matrix such that $SP_{ij} = 1$ if $a_i = j$; otherwise $SP_{ij} = 0$. The subscript plus indicates that only the positive elements of the matrix (i.e., the inlets) are taken into account, while the negative elements are discarded. The operator diag transforms a vector into a diagonal matrix.

Unit Operations. The modeling of unit operations was not considered in the work of de Oliveira Filho et al.,[28] and thus its consideration constitutes one of the contributions of this work. The mass balance for unit operation k is expressed by eq 13:

$$m_{k,\mathrm{in}} - m_{k,\mathrm{out}} = 0 \tag{13}$$

using the incidence matrix (eq 14):

$$\mathbf{M}^{PR} \mathbf{m} = 0 \tag{14}$$

Mass Flow Rate Specifications. Finally, the mass flow rate specifications are

$$\mathbf{n}^{PS} - (\mathbf{n}^{PS})^* = 0 \tag{15}$$

Mass Balance Model. Equations 2, 5, 6, 8, 11, 12, 14, and 15 form the system of linear equations that represents the mass balance of the HEN. This system can also be described as

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{16}$$

where

$$\mathbf{x} = \begin{bmatrix} \mathbf{m} \\ \mathbf{n} \end{bmatrix} = \begin{bmatrix} \mathbf{m}_c \\ \mathbf{m}_h \\ \mathbf{n}^{PS} \\ \mathbf{n}^{PD} \end{bmatrix} \tag{17}$$

$$\mathbf{b} = \begin{bmatrix} 0 \\ (\mathbf{n}^{PS})^* \end{bmatrix} \tag{18}$$

The structure of matrix A is described in Figure 3. Equation 16 is solved to find the values of the mass flow rates for each edge of the HEN.

$$\begin{array}{c} \overbrace{\hphantom{\mathrm{diag}(\boldsymbol{\alpha})\,\mathbf{M}_{+}^{SP} - \mathbf{SP}}}^{S \text{ columns}} \; \overbrace{\hphantom{\mathbf{I}^{PS}\;\; -\mathbf{I}^{PD}}}^{N^P \text{ columns}} \\ \left[\begin{array}{cc|cc} \multicolumn{2}{c|}{\mathbf{M}^{PS}} & \mathbf{I}^{PS} & 0 \\ \hline \multicolumn{2}{c|}{\mathbf{M}^{PD}} & 0 & -\mathbf{I}^{PD} \\ \hline \mathbf{M}_c^{HE} & 0 & \multicolumn{2}{c}{0} \\ \hline 0 & \mathbf{M}_h^{HE} & \multicolumn{2}{c}{0} \\ \hline \multicolumn{2}{c|}{\mathbf{M}^{MX}} & \multicolumn{2}{c}{0} \\ \hline \multicolumn{2}{c|}{\mathbf{M}^{SP}} & \multicolumn{2}{c}{0} \\ \hline \multicolumn{2}{c|}{\mathrm{diag}(\boldsymbol{\alpha})\,\mathbf{M}_{+}^{SP} - \mathbf{SP}} & \multicolumn{2}{c}{0} \\ \hline \multicolumn{2}{c|}{\mathbf{M}^{PR}} & \multicolumn{2}{c}{0} \\ \hline \multicolumn{2}{c|}{0} & \mathbf{I}^{PS} & 0 \end{array}\right] \end{array}$$

Figure 3. Structure of matrix A in eq 16

3.3. Energy Balance. Similar to the mass balance, the system of linear equations for the energy balance is used to find the values of the temperatures at each edge of the HEN. In this case, the temperatures for each edge are represented by vector T, which is divided into cold and hot subvectors: $\mathbf{T}^T = [\mathbf{T}_c^T\ \mathbf{T}_h^T]$. The temperatures of the external streams are represented by vector v (dimension $N^P \times 1$), which is divided into subvectors for the supply and demand units: $\mathbf{v}^T = [(\mathbf{v}^{PS})^T\ (\mathbf{v}^{PD})^T]$.

The temperatures are known for the external streams that enter the HEN at the supply units. These supply temperatures are specifications represented by vector $(T_s)^*$ (dimension $N^{PS} \times 1$).

Supply and Demand Units. The equations for the supply and demand units are presented in eq 19 and 20, respectively:

$$\mathbf{M}^{PS}\mathbf{T} + \mathbf{v}^{PS} = 0 \tag{19}$$

$$\mathbf{M}^{PD}\mathbf{T} - \mathbf{v}^{PD} = 0 \tag{20}$$

Heat Exchangers Specified in Terms of Heat Loads. The energy balance for the cold and hot sides of heat exchanger k can be expressed by eq 21 and eq 22, respectively:

DOI: 10.1021/ie503804u
Ind. Eng. Chem. Res. 2015, 54, 5001−5017

$$\overline{CP}_{k,c}(T_{k,c,\text{out}} - T_{k,c,\text{in}}) = q_k \quad (21)$$

$$\overline{CP}_{k,h}(T_{k,h,\text{in}} - T_{k,h,\text{out}}) = q_k \quad (22)$$

where q is the duty of the heat exchanger and $\overline{CP}$ represents the average heat capacity flow rate ($\overline{CP}$ = m$\overline{CP}$, where $\overline{CP}$ is the average heat capacity for the interval [T_{in},T_{out}]). Equation 21 and eq 22 can be expressed in terms of the incidence matrix:

$$-[(\overline{\mathbf{CP}}_c\mathbf{1}) \circ \mathbf{M}_c^{HE}]\mathbf{T}_c = \mathbf{q} \quad (23)$$

$$[(\overline{\mathbf{CP}}_h\mathbf{1}) \circ \mathbf{M}_h^{HE}]\mathbf{T}_h = \mathbf{q} \quad (24)$$

here $\overline{\mathbf{CP}}^T = [\overline{\mathbf{CP}}_c^T\ \overline{\mathbf{CP}}_h^T]$. $\overline{\mathbf{CP}}_c$ and $\overline{\mathbf{CP}}_h$ (dimensions $N^{HE} \times 1$) are vectors that contain the average heat capacity flow rates for the cold and hot streams, respectively, in each heat exchanger. Vector q (dimension $N^{HE} \times 1$) represents the heat loads of the heat exchangers. The open circle operator indicates the Hadamard multiplication, otherwise referred to as element-to-element multiplication, and 1 is a vector of ones (dimension $1 \times N^{HE}$).

Mixers and Splitters. Equation 25 describes the energy balance for a mixer k, while eq 26 and 27 describe the energy balance for a splitter l:

$$CP_{k,\text{in},1}T_{k,\text{in},1} + CP_{k,\text{in},2}T_{k,\text{in},2} - CP_{k,\text{out}}T_{k,\text{out}} = 0 \quad (25)$$

$$CP_{l,\text{in}}T_{l,\text{in}} - CP_{l,\text{out},1}T_{l,\text{out},1} - CP_{l,\text{out},2}T_{l,\text{out},2} = 0 \quad (26)$$

$$T_{l,\text{in}} - T_{l,\text{out},1} = 0 \quad (27)$$

where CP represents the heat capacity flow rate of the streams entering or leaving the mixer or splitter (CP = mCp, where Cp is the heat capacity). Equation 25 to 27 can be expressed using the incidence matrix:

$$\mathbf{M}^{MX}[\text{diag}(\mathbf{CP})]\mathbf{T} = 0 \quad (28)$$

$$\mathbf{M}^{SP}[\text{diag}(\mathbf{CP})]\mathbf{T} = 0 \quad (29)$$

$$[\mathbf{M}_+^{SP} - \mathbf{SP}]\mathbf{T} = 0 \quad (30)$$

where $\mathbf{CP}^T = [\mathbf{CP}_c^T\ \mathbf{CP}_h^T]$ (dimension S × 1) is a vector that contains the values of the heat capacity flow rates for each edge of the HEN.

Unit Operations. For a unit operation k, the specification is the temperature change ΔT^{PR} of the stream passing through the unit. The energy balance can be written as follows:

$$T_{k,\text{in}} - T_{k,\text{out}} = \Delta T_k^{PR} \quad (31)$$

Using a matrix representation:

$$\mathbf{M}^{PR}\mathbf{T} = \Delta\mathbf{T}^{PR} \quad (32)$$

where $\Delta\mathbf{T}^{PR}$ (dimension $N^{PR} \times 1$) is a vector that contains the temperature change specifications for each unit operation.

Supply Temperature Specifications. For supply units, the temperatures of the external streams are equal to the outlet streams. Therefore, the specification is indicated by vector $(\mathbf{T}_s)^*$:

$$\mathbf{v}^{PS} - (\mathbf{T}_s)^* = 0 \quad (33)$$

Energy Balance Model. Equation 19, 20, 23, 24, eq 28 to 30, eq 32 and 33 comprise the system of linear equations for the energy balance. This set of equations can be arranged into the following equation:

$$\mathbf{Cz} = \mathbf{d} \quad (34)$$

where

$$\mathbf{z} = \begin{bmatrix} \mathbf{T} \\ \mathbf{v} \end{bmatrix}, \quad \mathbf{T} = \begin{bmatrix} \mathbf{T}_c \\ \mathbf{T}_h \end{bmatrix}, \quad \mathbf{v} = \begin{bmatrix} \mathbf{v}^{PS} \\ \mathbf{v}^{PD} \end{bmatrix} \quad (35)$$

$$\mathbf{d} = \begin{bmatrix} 0 \\ \mathbf{q} \\ \mathbf{q} \\ 0 \\ \Delta\mathbf{T}^{PR} \\ (\mathbf{T}_s)^* \end{bmatrix} \quad (36)$$

The structure of matrix C is shown in Figure 4, where I indicates an identity matrix. Equation 34 is solved after eq 16 to calculate the temperatures for each edge of the HEN.

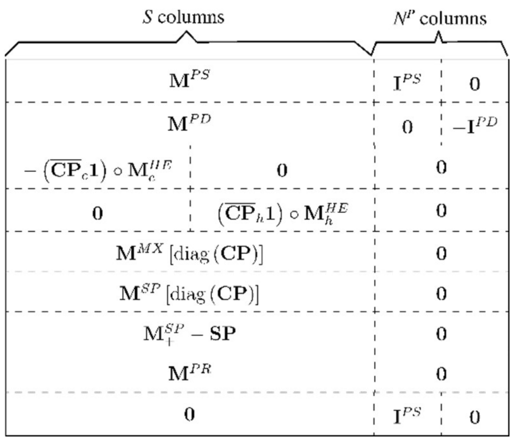

Figure 4. Structure of matrix C in eq 34.

3.4. Simulation Considering Temperature-Dependent Thermal Properties.

It was shown by Chen[16] and in Part I[1] of the series that energy requirements and stream temperatures for a heat-integrated distillation system may be substantially underestimated when thermal properties are assumed constant. This assumption of constant thermal properties may be valid for streams that do not experience considerable changes in temperature and pressure, or phase change. However, this is not the case for stream temperature changes in crude oil distillation. In particular, the crude oil feed undergoes a temperature increase of more than 300 °C, with partial vaporization taking place; while the temperatures of bottom distillation products may be decreased by more than 100 °C. Therefore, it is important to consider temperature-dependent thermal properties when simulating the HEN to obtain more realistic estimations of energy requirements and stream temperatures.

The strategy used in this work to simulate the HEN considering temperature-dependent properties is the one proposed by de Oliveira Filho et al.[28] and is illustrated in Figure 5. The equations developed in Part I[1] of the series to model temperature-dependent heat capacities are used to calculate the values of vectors $\overline{\mathbf{CP}}$ and CP. A similar approach

DOI: 10.1021/ie503804u
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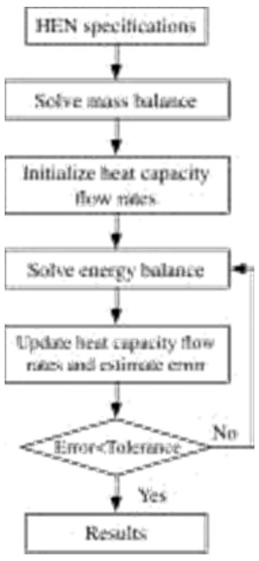

Figure 5. Procedure to simulate HENs considering temperature-dependent heat capacities.

could be used to model other temperature-dependent proper-ties, such as heat transfer coefficients. The strategy starts by solving the mass and energy balances in eq 16 and 34. Then, the values of CP and CP are updated using the temperatures calculated with eq 34. The energy balance is repeatedly solved until the error between the heat capacity flow rates calculated in the previous and current iterations is less than a specified tolerance. This tolerance is selected depending on the order of magnitude of the heat capacity flow rates and the desired accuracy. In this work, the error is calculated as error = $\sum^{S}_{i}|CP_{i,new} - CP_{i,old}|$; the specified tolerance is 1×10^{-6} kW/°C. Typically, around 10 iterations are needed to reach convergence. Note that this iterative procedure is not needed when thermal properties are assumed constant.

3.5. Calculation of Heat Transfer Area.

The heat transfer area A_{calc} for a heat exchanger k can be calculated with the following design equation:

$$A_{calc,k} = \frac{q_k}{U_k F_{T_k} \mathrm{LMTD}_k} \qquad (37)$$

where U_k is the overall heat transfer coefficient, F_{T_k} is the correction factor and LMTD_k is the log mean temperature difference of the heat exchanger k. The value of F_T depends on the type of heat exchanger and can be calculated using correlations (e.g., ref 29 p. 325). The value of LMTD can be calculated with eq 38:

$$\mathrm{LMTD}_k = \frac{(T_{k,h,in} - T_{k,c,out}) - (T_{k,h,out} - T_{k,c,in})}{\ln\left(\frac{T_{k,h,in} - T_{k,c,out}}{T_{k,h,out} - T_{k,c,in}}\right)}$$

4. HEAT EXCHANGER NETWORK RETROFIT MODEL

In general, the following information provides inputs to the HEN design problem:

Given:

- a set of hot streams that need to be cooled from a supply temperature to a target temperature
- a set of cold streams that need to be heated from a supply temperature to a target temperature
- enthalpy change for each hot and cold stream
- heat transfer coefficients for each heat exchanger
- a set of constraints for HEN design (e.g., minimum temperature approach, maximum number of heat exchangers per stream, maximum heat transfer area, etc.)
- heat exchanger network cost data (e.g., utility prices, heat exchanger modification costs, etc.)

Then, the objective is to design (e.g., grass-roots design, retrofit, operational optimization) a cost-effective heat ex-changer network. Cost-effectiveness of a HEN can be described in terms of operating costs (i.e., utility consumption) and required capital investment. For grass-roots design projects, the capital investment is significant, as it includes the purchase and installation of all the equipment in the HEN. Retrofit projects require less capital investment than grass-roots projects. Retrofit only considers the cost of modifying existing equipment and sometimes the installation of some additional equipment. On the other hand, operational optimization consists of real-time modifications to operating variables without altering the configuration of installed equipment. Therefore, operational optimization does not require any capital investment: cost-effectiveness is measured only in terms of operating costs. This section focuses on retrofit of the HEN, where modifications include structural changes (e.g., add, remove, or relocate heat exchangers, add or remove stream splitters) and operational changes (e.g., changes in heat loads and split fractions).

The HEN retrofit framework presented in this work is divided in two levels. The first level proposes modifications to the heat exchanger network. These modifications include: adding a new heat exchanger, deleting an existing heat exchanger, changing the heat load of a heat exchanger, repiping or resequencing a heat exchanger, adding a new stream splitter, removing an existing stream splitter, and varying the split fraction of a stream splitter. The modified HEN is then simulated to check that no constraints are violated. These constraints consider the minimum temperature approach (ΔT_{min}), stream enthalpy balances, installed heat transfer areas, additional heat transfer areas, and utility consumption. If any of these constraints is violated, the second level optimizes the heat loads and split fractions that regain HEN feasibility.

The first level employs SA to propose structural modifications to the HEN. The second level uses the Levenberg−Marquardt algorithm as a repair algorithm. The role of this repair algorithm is to ensure that constraints are met.

The retrofit approaches of Rodrıguez[21] and Chen[16] are extended in this work to include constraints on heat transfer areas[38] and utility consumption, and to use more simple and flexible models for the estimation of temperature-dependent thermal properties. The HEN simulation model extended from the approach of de Oliveira Filho et al.[28] (described in section 3) is implemented in the proposed retrofit approach to calculate mass flow rates and temperatures, which are used to check HEN constraints.

4.1. First Level: Retrofit Modifications Using Simu-lated Annealing. As discussed in section 2, simulated annealing is a stochastic optimization technique particularly well suited for large-scale combinatorial problems. In addition, SA is reported to be more effective for problems that consider discrete variables, compared to other stochastic optimization techniques.[24] Some important features of simulated annealing

DOI: 10.1021/ie503804u
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include the following. (i) The ability to overcome local minima: Trial solutions that deteriorate the objective function may be accepted during the search process. This capability is helpful for escaping local minima, especially for highly nonconvex problems. (ii) Because of the random nature of SA, the search for an optimal solution is independent of the starting point. (iii) Simulated annealing can handle nondifferentiable or discontin-uous objective functions and constraints, since it does not require the calculation of first- and second-order derivatives.
(iv) Simulated annealing allows the formulation of grand canonical problems, where the number of variables changes as the optimization progresses. This feature is useful for the HEN retrofit problem, since it allows adding or deleting elements as the HEN evolves to a more cost-effective design.

The basic formulation and parameters of the simulated annealing algorithm, such as the acceptance criteria, cooling schedule, Markov chain length, initial annealing temperature, termination criteria, etc., used in this work are described in section S2 (see Supporting Information). The implementation of the SA algorithm to perform HEN retrofit is presented next.

4.1.1. Objective Function. In this work, the cost-effectiveness of a HEN is described in terms of operating and capital costs. Operating costs include utility costs (e.g., costs of cooling water and fired heating), while capital costs include the costs of installing additional area to existing heat exchangers, adding new heat exchangers to the existing HEN, repiping and resequencing existing heat exchangers, etc. Thus, the objective function is to minimize the total annualized cost of the HEN, defined as

$$\mathrm{TAC} = \mathrm{OC} + \mathrm{ACC} \tag{39}$$

$$\mathrm{OC} = \sum_{n=1}^{N_{\mathrm{util}}} C_{\mathrm{util},n} F_{\mathrm{util},n} \tag{40}$$

where TAC, OC, and ACC represent the total annualized cost, operating costs, and annualized capital costs, respectively. C and F refer to unit prices and flow rates of the utility streams (util), respectively. N_{util} is the total number of utilities. The annualized capital cost is equal to $\mathrm{ACC} = \mathrm{CC}(i(1 + i)^y)/((1 + i)^y - 1)$, where CC represents the total capital cost, i is the interest rate, and y is the project life (in years).

The simulated annealing algorithm and the simulation of the process are completely decoupled. The SA algorithm proposes new trial points, for which the process, in this case the HEN, is simulated. This simulation returns the value of the objective function to the SA algorithm. The SA algorithm treats the process model as a black box; thus all types of equations and objective functions are allowed. This capability facilitates the implementation of simpler or more complex objective functions than the one described in eq 39. Simpler objective functions may only consider operating costs. More complex objective functions can consider the internal geometry of the heat exchangers, heat exchanger fouling, etc. However, even though the SA algorithm is decoupled from the process model, the computational performance of the optimization is affected by the robustness of the process model and how quickly the model equations are solved.

4.1.2. Constraints on HEN Topology. The SA optimization framework presented in this work allows the imposition of constraints on the HEN topology. Structural constraints are set to avoid solutions that will be impractical or excessively complex to implement. For instance, constraints may relate to process economics, plant layout, safety considerations, etc. The SA framework is formulated so that the following constraints can be specified:

- number and type of modifications that can be implemented in the heat exchanger network
- number and type of modifications that can be implemented to each process stream
- types of modification that can be implemented to each existing heat exchanger and splitter
- forbidden heat exchanger matches

These constraints are applied to the HEN elements (e.g., process streams, heat exchangers, splitters) to select the candidates for each retrofit modification. The specification of structural constraints is very flexible, and it allows the user various alternatives to define the extent of HEN modifications in various ways. Moreover, the designer can specify that a certain type of modification cannot be implemented in a particular HEN element. The implementation of structural constraints is facilitated by the use of tags that identify each element in the HEN, and counters that keep track of the number and type of modifications that are implemented in each element and in the overall HEN.

4.1.3. Simulated Annealing Moves. The simulated anneal-ing algorithm performs alterations to trial solutions in order to find new solutions that improve the objective function. A move represents the various types of alterations that can be carried out. These moves account for the optimization variables of the problem under study. The move tree used for the heat exchanger network retrofit problem is presented in Figure 6.

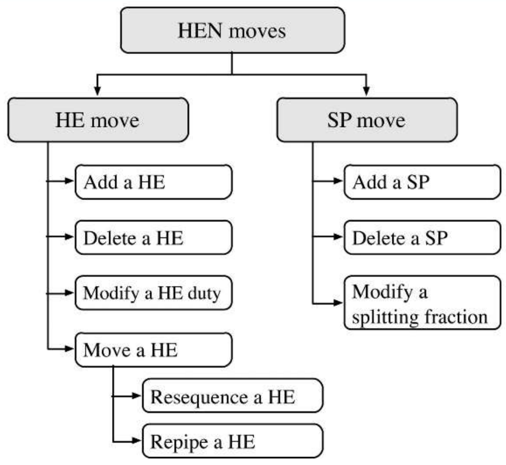

Figure 6. Simulated annealing move tree for HEN retrofit.[16] HE, heat exchanger; SP, stream splitter.

Two types of moves are considered for HEN retrofit: structural and continuous moves. Structural moves include adding a new heat exchanger (HE), deleting an existing heat exchanger, resequencing and repiping a heat exchanger, and adding and removing a stream splitter (SP). Continuous moves include varying the heat loads of the heat exchangers and split fractions of streams. Each splitter creates two outlet streams from a single stream. A sequence of splitters can effectively split a single inlet stream into any number of outlet streams.

The SA algorithm selects the move to be implemented using a random number, generated at each iteration, and the probability assigned to each move. These probabilities are used to bias the search process to focus more on those moves that have a dominant effect on the objective function. Hence, a

DOI: 10.1021/ie503804u
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high probability can be assigned to those moves that are most influential to the problem under study. These probabilities can also be used to prioritize moves based on practical criteria, such as the difficulty and time required to implement a certain type of topology modification.

The move probabilities have a substantial impact on the computational performance of the SA algorithm, since they dictate how the search space is explored. However, how to decide on the values of these move probabilities is not clear. The impact of the moves on the objective function is case-dependent, and the probabilities are usually chosen based on experience, practical considerations, or trial and error.[16]

Eight different moves are considered for the HEN retrofit problem. The sum of all move probabilities must be 1, while the random number must have a value between 0 and 1. Only one move is implemented at each iteration of the SA algorithm. A description of the way each move is implemented in the HEN is presented below, which is based on the work of Rodrıguez.́[21]

(1) Add a heat exchanger. This move adds a heat exchanger at a random position of the heat exchanger network. Heat exchanger can refer to process-to-process heat exchangers, heaters (hot utility heat exchangers), or coolers (cold utility heat exchangers). To ensure that the new network topology is feasible, only thermodynamically feasible matches are taken into account. That is, matches in which the difference between the supply temperature of the hot and cold streams is greater than the minimum temperature approach (T_{min}), as shown in eq 41:[21]

$$T_{s,k,h} - T_{s,k,c} \geq T_{min} \tag{41}$$

where T_s relates to the supply temperatures of the hot and cold streams passing through heat exchanger k. In other words, T_s is the temperature specification for the external stream of a supply unit and is equal to the outlet temperature of this supply unit (see section 3).

This move is implemented by first selecting the pairs of streams for which a match is feasible, according to eq 41. Forbidden stream matches (specified by the user as constraints) are also removed from this selection. Then, a pair of streams is randomly selected. The streams (edges) where the new heat exchanger is inserted are also randomly chosen. The insertion of a new heat exchanger (i.e., a new element) creates two new edges and consequently increases the dimensions of variables in eq 16 and eq 34 used to carry out the material and energy balances within the HEN. Figure 7a illustrates the insertion of a heat exchanger.

Finally, a heat load and overall heat transfer coefficient are assigned to the new heat exchanger. The heat load is set as a random value between zero and the minimum total enthalpy change of both streams; for example, if the total enthalpy changes of the hot and cold streams connected to the new exchanger are 6 MW and 10 MW, respectively, the new heat load is a random number between zero and 6 MW. The overall heat transfer coefficient can be calculated using the heat transfer coefficients of the hot and cold streams, thermal conductivity values for the metal in the exchanger, fouling resistance values, etc., which need to be previously specified.

(2) Remove a heat exchanger. This move randomly chooses a heat exchanger and removes it from the network. Candidate heat exchangers must be selected from streams that have more than one heat exchanger installed. That is, heat exchangers that are unique to a stream must not be removed. Otherwise, if a stream is left without any heat exchanger, it would be

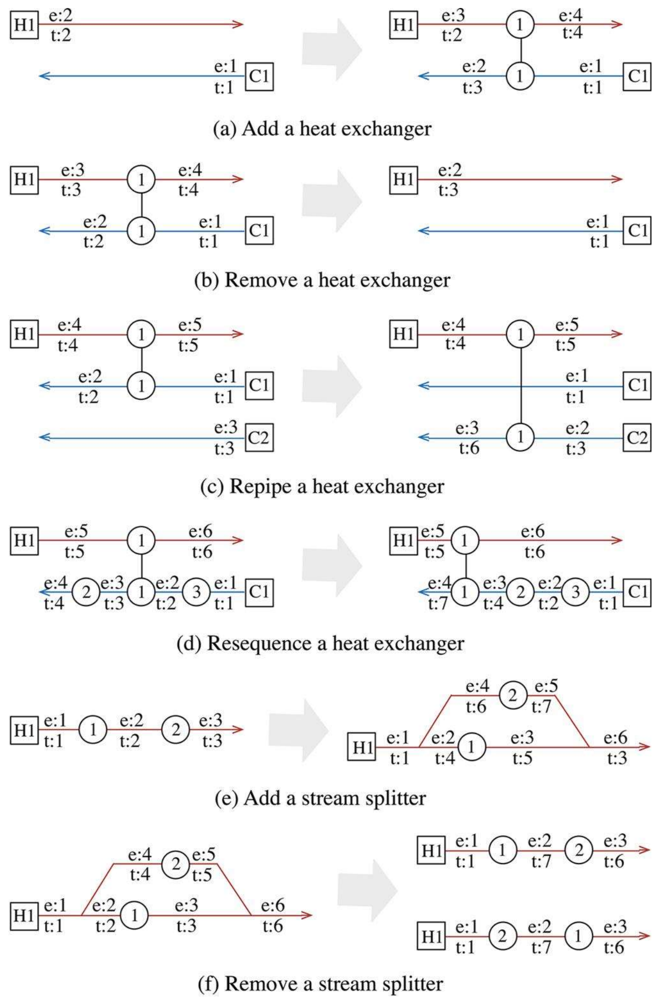

Figure 7. HEN retrofit modifications: e, edge; t, edge tag.

impossible to reach its target temperature. The user can also specify which heat exchangers cannot be removed. These heat exchangers are also excluded from the list of candidates.

This move randomly selects the exchanger to be removed from the list of candidates. The heat exchanger is attached to four stream segments (edges); after the heat exchanger is deleted, the edges related to the outlets are removed, as illustrated in Figure 7b. As a consequence, the dimensions of variables in eq 16 and eq 34 are reduced.

(3) Change the heat load of a heat exchanger. For this move, the prospective heat exchangers are selected from those streams with more than one heat exchanger. It is not possible to modify the duty of a heat exchanger that is unique to a stream, since its duty is defined by the total enthalpy change of that stream. The heat exchanger is randomly selected from the list of candidates. The new duty is a random number between zero and the minimum total enthalpy change of the streams passing through the heat exchanger.

(4) Repipe a heat exchanger. This move randomly chooses a heat exchanger and reconnects its cold or hot side to a different stream, which is selected at random. The side of the heat exchanger that is repiped (i.e., cold or hot side), the destination stream, and the position of the exchanger in the stream (edge) are randomly selected. Equation 41 is also applied in this case to screen candidate matches between streams. Similarly to the "delete a heat exchanger" move, it is

DOI: 10.1021/ie503804u
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not permitted to leave a stream without any heat exchanger. Depending on the context (e.g., plant layout, repiping costs, etc.), the user can also specify if a particular side of a heat exchanger cannot be repiped.

In the case of repiping, neither the number of HEN elements nor the number of stream segments (edges) is modified. However, the "repipe" move involves removing one edge, that is, the edge related to the outlet stream of the side that is to be repiped. It also requires the partition of the destination edge into two edges: the new inlet and outlet streams of the repiped heat exchanger, as shown in Figure 7c.

(5) Resequence a heat exchanger. This move is a special case of the "repipe" move, except that in this case, the heat exchanger is relocated to a different position in the same stream. The same criteria as for the "repipe" move are used to select the heat exchanger, stream side, and destination edge. It is not necessary to use eq 41, since the stream matches do not change. Figure 7d illustrates how the edges are updated for this move.

(6) Add a stream splitter. This move randomly selects two heat exchangers in series in a stream. The move then splits the stream into two parallel branches and relocates each heat exchanger in a branch. The two streams leaving the heat exchangers are then mixed together. The user can specify those streams for which stream splitting is not permitted due to practical reasons such as installation costs, operability of heat exchangers, etc.

This move introduces two HEN elements, namely a stream splitter and a mixer. The number of streams (edges) is increased by three. The edge related to the inlet of the first heat exchanger in series becomes the inlet edge of the splitter, as shown in Figure 7e. The outlet of the second heat exchanger becomes the outlet of the mixer. The edge that used to connect the heat exchangers in series is replaced by four new edges. These four edges serve to connect the heat exchangers now in parallel with the two outlets of the splitter and the two inlets of the mixer.

(7) Delete a stream split. This moves selects a random splitter and the associated mixer, and removes them from the network. To perform this move, the two stream branches from the selected splitter, once arranged in parallel, are instead arranged in series. The decision of which branch is placed first in the series is made at random. The user can specify the streams splitters that cannot be removed.

This move removes two HEN elements, namely a splitter and the associated mixer. As a consequence, three edges are removed. The inlet edge of the splitter and the outlet edge of the mixer are kept. The former edge is connected to the first element of the first branch placed in series, while the latter edge is connected now from the last element of the second branch placed in series. Note that element may refer here to heat exchangers, splitters, and mixers, as a stream branch can have several heat exchangers, splitters, or mixers placed in series. The edges from the outlets of the splitter and the inlets of the mixer are replaced by one single edge, which connects the two branches arranged in series. Figure 7f illustrates this procedure.

(8) Change the split fraction of a stream splitter. This move changes the split fraction of a randomly selected stream splitter. The new split fraction is a random number with a value between 0 and 1.

Constraints are used to limit the number of times each type of move is applied to the HEN so as to produce designs with a minimum number of modifications. However, the application of a move is always enabled for all new heat exchangers and new stream splitters, as this allows any change to the HEN structure to be reversible. The algorithm developed to perform these modifications uses tags to identify each element in the HEN, which allows the identification of new heat exchangers and splitters. Also, counters assigned to each type of move keep track of the times each modification has been implemented in the HEN. The counters are updated depending on whether the move is implemented in an existing element or new element. For example, the counter of the "add a HE" move is increased by one each time a new exchanger is created; the counter of the "remove a HE" move is increased by one only if the move is applied to an existing exchanger, otherwise the counter related to the "add a HE" move is decreased by one. The counters are only updated if the related move is accepted by the SA algorithm.

On the other hand, when a counter related to a particular HEN element and modification type reaches its maximum allowed value, the corresponding HEN element is removed from the list of candidates for the corresponding modification type (e.g., if a stream has reached its maximum number of additional heat exchangers, this stream is removed from the list of candidates when performing the "add a heat exchanger" move). Similarly, to prevent the implementation of certain types of modifications to HEN elements, the designer can set to zero the maximum allowed values of the associated counters.

The HEN simulation model used in this work facilitates the modification of the HEN structure by the SA algorithm. The SA moves change the HEN structure through the incidence matrix, which describes in a simple manner the connectivity between the elements of the HEN. Rows of the incidence matrix are associated with elements of the HEN (e.g., heat exchangers, stream splitters), while columns are associated with stream segments (edges). Elements are added or removed from the HEN by inserting or deleting rows and columns from the incidence matrix. Tags, counters, and associated vectors (e.g., vectors related to heat loads, temperatures, split fractions) are updated in dimensions and values according to changes made to the incidence matrix.

4.2. Second Level: Repair Algorithm. Only constraints related to the SA moves are incorporated in the first level of the retrofit framework. The second level, that is, the repair algorithm, takes into account constraints that describe the feasibility of the heat exchanger network. These constraints consider the minimum temperature approach (T_{min}), stream enthalpy balances, utility consumption (e.g., furnace capacity), and heat transfer areas.

After a move is implemented by the SA algorithm, the feasibility of the heat exchanger network is evaluated. If any constraint is violated, the HEN retrofit procedure calls a feasibility solver (i.e., the repair algorithm) to calculate the heat loads and split fractions that regain feasibility.

Various aspects can be considered to assess the feasibility of a heat exchanger network. These aspects are related to essential features of the HEN and to practical considerations. Essential features include fundamental phenomena, such as conservation of energy, etc., and must never be neglected. Practical considerations, although not fundamental, serve to provide solutions that could actually be implemented in real projects. Practical aspects for the HEN retrofit problem may include available heat transfer area, allowed pressure drop in heat exchangers, availability of utilities, permitted heat exchanger matches related to site geography, safety, etc., among many

DOI: 10.1021/ie503804u
Ind. Eng. Chem. Res. 2015, 54, 5001−5017

others. These practical constraints are included depending on the criteria of the designer and are case-dependent. Practical constraints should be imposed keeping in mind that increasing their number may have a detrimental effect on the performance of the repair algorithm.

In this work, the feasibility of the HEN is evaluated considering the following issues:

- minimum temperature approach
- stream enthalpy balances
- available heat transfer area of each heat exchanger
- total and individual heat transfer area that can be added
- availability of utilities, especially crude oil furnace

These constraints are formulated in such a way that the user can easily enable or disable each type of constraint. The approach proposed by Chen[16] only considered constraints on the minimum temperature approach and on stream enthalpy balances. The present work extends the methodology developed by Chen[16] to include constraints on heat transfer area and crude oil furnace capacity.

The repair algorithm employed by Chen[16] is formulated as a nonlinear least-squares problem, which is solved using the Levenberg−Marquardt algorithm.[30,31] This formulation is also employed in the present work and is described in section 4.2.5 with the extended features.

4.2.1. Minimum Temperature Approach Constraints. The minimum temperature approach (T_{min}) represents the minimum driving force for heat transfer and is a very important design parameter, as it affects the cost of the heat exchanger network. Increasing T_{min} reduces heat transfer area require-ments at the expense of increasing energy requirements; the opposite takes place when T_{min} decreases. Experience, rules of thumb, and sensitivity studies can be used to account for capital-energy trade-offs and select a suitable T_{min} value. The minimum temperature approach constraints for heat exchanger k can be formulated as follows:

capacity

$$(T_{k,h,\mathrm{in}} - T_{k,c,\mathrm{out}}) - T_{\min} \geq 0 \tag{42}$$

$$(T_{k,h,\mathrm{out}} - T_{k,c,\mathrm{in}}) - T_{\min} \geq 0 \tag{43}$$

4.2.2. Stream Enthalpy Balance Constraints. Stream enthalpy balance constraints guarantee that the target temperatures of process streams are met. For a stream k, this constraint can be written as

$$T_{t,k} - (T_t)^{*}_{k} = 0 \tag{44}$$

available heat transfer areas and to control the new area that can be added to each heat exchanger.

The calculated heat transfer area of a heat exchanger, if no extra heat transfer area is to be added, should not exceed its installed heat transfer area. This can be represented as

$$A_{\mathrm{inst},k} - A_{\mathrm{calc},k} \geq 0 \tag{45}$$

where A_{inst} represents the existing heat transfer area of heat exchanger k in the HEN, and A_{calc} is the area required for heat transfer calculated by the simulation model (eq 37).

In addition, a lower bound for the calculated heat transfer area is defined for each heat exchanger. This constraint includes the operability limits of the heat exchanger. If a heat exchanger is to be kept in the HEN, its "used" heat transfer area (the area that is required for heat transfer) should be greater than a lower bound:

$$A_{\mathrm{calc},k} - A^{\mathrm{lb}}_{\mathrm{inst},k} \geq 0 \tag{46}$$

where A_{inst}^{lb} represents the lower bound for the calculated heat transfer area of exchanger k.

Lower and upper bounds (eq 47 and 48) are defined to constrain the amount of heat transfer area that can be added to a exchanger. Implementing additional area with a value below the lower bound would be troublesome without any substantial improvement in heat recovery. On the other hand, additional areas greater than the upper bound may not be accommodated in the existing heat exchangers. These constraints can be expressed as

$$A_{\mathrm{add},k} - A^{\mathrm{lb}}_{\mathrm{add},k} \geq 0 \tag{47}$$

$$A^{\mathrm{ub}}_{\mathrm{add},k} - A_{\mathrm{add}} \geq 0 \tag{48}$$

where

$$A_{\mathrm{add},k} = A_{\mathrm{calc},k} - A_{\mathrm{inst},k} \tag{49}$$

Equations 47 to 49 are only applicable if $A_{calc,k} > A_{inst,k}$. Variables A_{add}, A^{lb}_{add}, A^{ub}_{add} represent the calculated additional area for exchanger k and their lower and upper bounds, respectively.

It is not easy to define the values of the lower and upper bounds in eq 46 to eq 48. These values are case-dependent and can be decided based on engineering judgment, rules of thumb, or correlations, such as the ones presented in ref 32. Note that these constraints on heat transfer area (eq 45 to eq 48) can be imposed on all exchangers in the HEN or on particular heat exchangers.

where $(T_t)^*$ represents the target temperature specification and T_t is the target temperature calculated with the simulation model. T_t is also referred to as the inlet temperature of a demand unit (see section 3).

4.2.3. Constraints on Heat Transfer Area. Adding heat transfer area to existing heat exchangers requires capital investment and labor cost. Moreover, it also requires the unit to be shut down, which may cause production to be lost. It is preferred to obtain a retrofit design with the least amount of modifications in order to reduce cost and implementation time. It would be impractical to obtain a retrofit design in which the heat transfer area of each exchanger needs to be increased. Moreover, if additional heat transfer area is not constrained, solutions could contain additional heat transfer areas that cannot be accommodated in the existing heat exchangers. For these reasons, constraints are applied to take into account

The maximum total heat transfer area (A_{max}) that can be added in the HEN can also be constrained using eq 50:

$$A_{\max} - \sum_{i=1}^{N_{\mathrm{HE}}} A_{\mathrm{add},i} \geq 0 \tag{50}$$

4.2.4. Constraints on Utility Consumption. Constraints on the maximum utility consumption can be expressed as

$$F_{\mathrm{util},k}^{\mathrm{ub}} - F_{\mathrm{util},k} \geq 0 \tag{51}$$

where F_{util} and F_{util}^{ub} represent the flow rates of utility k and their upper bounds, respectively.

4.2.5. Repair Algorithm Problem Formulation. HEN constraints are described in sections 4.2.1 to 4.2.4. These constraints relate to the minimum temperature approach (eq 42 and eq 43), enthalpy balance (eq 44), heat transfer area requirements (eq 45 to eq 50), and utility consumption (eq

DOI: 10.1021/ie503804u
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51). When eq 42 to 48 and eq 50 to 51 are combined, the feasibility of the network can be evaluated with eq 52:

$$
\begin{aligned}
f(\mathbf{q},\alpha) = {} & \vartheta_1 \sum_{i=1}^{N_{HE}} \min(T_{i,h,\mathrm{in}} - T_{i,c,\mathrm{out}} - T_{\min}, T_{i,h,\mathrm{out}} - T_{i,c,in} - T_{\min}, 0)^2 + \vartheta_2 \sum_{j=1}^{N_{PD}} (T_{t,j} - (T_t)^*_j)^2 \\
& + \vartheta_3 \sum_k \min(A_{\mathrm{calc},k} - A^{\mathrm{lb}}_{\mathrm{inst},k}, 0)^2 \\
& + \vartheta_4 \sum_l \min(A_{\mathrm{add},l} - A^{\mathrm{lb}}_{\mathrm{add},l}, 0)^2 \\
& + \vartheta_5 \sum_l \min(A^{\mathrm{ub}}_{\mathrm{add},l} - A_{\mathrm{add},l}, 0)^2 \\
& + \vartheta_6 \min(A_{\max} - \sum_{m=1}^{N_{HE}} A_{\mathrm{add},m}, 0)^2 \\
& + \vartheta_7 \sum_{n=1}^{N_{\mathrm{util}}} \min(F^{\mathrm{ub}}_{\mathrm{util},n} - F_{\mathrm{util},n}, 0)^2 = 0
\end{aligned}
\qquad (52)
$$

where f is the objective function for the feasibility solver. The optimization aims to minimize f, so that all of the active constraints are not violated or violated as little as possible. Index k refers to those heat exchangers for which the required area is less or equal to the installed area ($A_{calc} \leq A_{inst}$), and index l refers to those heat exchangers that require additional area ($A_{calc} > A_{inst}$). Parameter ϑ_i (i = 1,...,7) is used to activate ($\vartheta_i = 1$) or deactivate ($\vartheta_i = 0$) each type of constraint. The values in ϑ are predefined by the designer.

As shown in eq 52, the heat loads and split fractions are the variables of the problem that can be manipulated to minimize f, that is, to achieve feasible solutions. The formulation of eq 52 corresponds to a nonlinear least-squares problem. The Levenberg−Marquardt (LM) algorithm[30,31] is a standard method for solving nonlinear least-squares problems and is selected in this work to restore HEN feasibility.

Figure 8 illustrates the implementation of the HEN simulation model and repair algorithm into the SA optimization framework. Note that heat loads are optimization variables for both the SA and LM algorithms. However, these variables are treated differently by each algorithm. In the SA framework, the 'change the heat load of a heat exchanger' move performs a perturbation to the heat load of a randomly chosen exchanger. The modified HEN is then simulated to check for violation of constraints. If any constraint is violated, the repair algorithm is called to balance the heat loads so as to regain feasibility. If this is the case, the perturbation proposed by the SA algorithm is replaced by the new heat loads calculated by the LM algorithm. The SA algorithm automatically rejects HEN designs for which the repair algorithm has failed, as shown in Figure 8.

5. CASE STUDIES

The methodology described in the previous sections is applied to decrease the total annualized cost of a crude oil preheat train. The existing HEN structure used in this case study corresponds to a design developed by Chen,[16] which was optimized for the existing column operating conditions described in Part I.[1]

The simulation and retrofit models, and the simulated annealing algorithm presented in this paper were coded in MATLAB.[33] The Optimization Toolbox in MATLAB was used

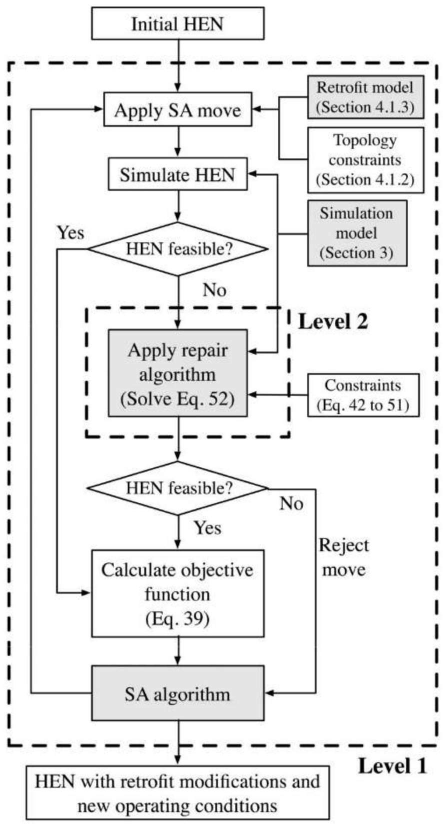

Figure 8. Flowchart for the HEN retrofit procedure.

to solve eq 52. The computer used for these calculations has an Intel Core processor of 3.40 GHz and 8.00 GB of installed RAM.

The objective of the case studies is to minimize the total annualized cost of the heat exchanger network. The optimization of the operating conditions of the distillation column is not considered at this point. Two optimization scenarios will be presented. The first case study (Case 1) considers only constraints on the minimum temperature approach (eq 42 and 43) and stream enthalpy balances (eq 44). Constraints on heat transfer area (eq 45 to 50) are not included. The second case study (Case 2) considers constraints on the temperature approach, stream enthalpy balances, and heat transfer area. The case studies are compared in terms of energy consumption, capital costs, additional heat transfer area requirements and retrofit modifications needed.

Stream information for the existing HEN is presented in Table S2 (see Supporting Information). This table corresponds to the base case operating conditions of the distillation column presented in Part I,[1] in which only the column was modeled. The process stream information remains fixed for both case studies. The equations employed to calculate the heat capacity flow rates of process streams as a function of temperature[1] are presented in section S3.2 (see Supporting Information).

The HEN structure is illustrated in Figure 9. The network consists of 13 process-to-process heat exchangers, 7 coolers, and a process furnace (represented by units 14 and 15) with a calculated required heat transfer area of 5754 m^2. This value is also taken as the installed heat transfer area. The heat transfer areas of units 14 and 15 are not calculated in the case studies, as the design equation of a furnace is very different from that of a shell and tube heat exchanger, a reboiler, or a condenser. It is

DOI: 10.1021/ie503804u

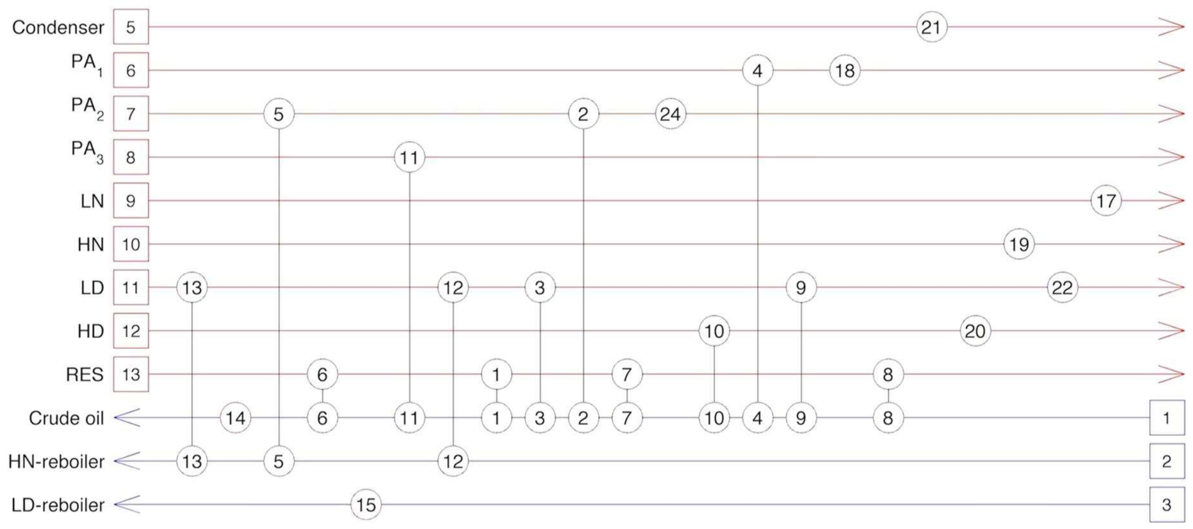

Figure 9. Structure of existing heat exchanger network.

assumed that the existing heat transfer area requirement for the furnace is met. Table S3 (see Supporting Information) presents the heat transfer areas, heat loads, overall heat transfer coefficients, and LMTD values for each heat exchanger. Table S4 (see Supporting Information) shows the inlet and outlet temperatures for each heat exchanger, which were determined with the simulation model described in section 3. The calculation of pressure drops is not considered in these case studies, and heat transfer coefficients are assumed constant for each heat exchanger, even if stream temperatures, flow rates, and properties change.

The minimum temperature approach of the network is 25 °C. The calculated hot and cold utility requirements of the existing heat exchanger network are 60.82 MW and 67.05 MW, respectively. The estimated total operating cost is 9.5 M$/y (millions of US) per year). Fired heating is used as the hot utility while cooling water is used as the cold utility.

Table 1 presents the costs of modifying heat exchangers and utility costs.[16] The maximum number of new heat exchangers

Table 1. Utility and Exchanger Modification Costs[16]

item	value
exchanger additional area ($)	1530 × (additional area, m^2)$^{0.63}$
new exchanger unit ($)	13 000 + 1530 × (exchanger area, m^2)$^{0.63}$
exchanger repiping ($)	60 000
exchanger resequencing ($)	35 000
fired heating (1500−800 °C) ($/kWy)	150
cooling water (10−40 °C) ($/kWy)	5.25
stripping steam (260 °C, 4.5 bar) ($/kmol)	0.14

in the HEN is two; the maximum number of new stream splitters in the HEN is also two; only one existing heat exchanger may be removed from the HEN, and only one repiping and one resequencing modification of existing heat exchangers is allowed in the HEN. There are no limits on the number of 'modify a heat exchanger heat load' moves that can be proposed. For the case when heat transfer areas are constrained, the lower bound for the calculated heat transfer areas (A^{lb}_{inst}) is 10 m^2 for each heat exchanger. For simplicity, it is assumed that the lower and upper bounds for additional heat transfer areas (A^{lb}_{add}, A^{ub}_{add}) are equal to 10% and 40% of the existing installed area. However, different values can be specified for each heat exchanger. Annualized capital cost is calculated assuming a 2-year project life with 5% interest rate. The operating time is 8600 h per year.

Table 2 shows the move probabilities used in the optimization; these values were selected considering that heat exchanger moves have more chances of improving energy recovery than stream splitter moves.[13] A higher probability was assigned to the 'modify a heat exchanger heat load' move, compared to the rest of the heat exchanger moves, due to its potential of improving heat recovery without requiring any HEN topology modifications.

Table 2. Move Probabilities

move decisions	probability
heat exchanger (HE) move; splitter move	0.8; 0.2
HE move: add a HE move; remove a HE move; modify heat load move; relocate a HE move	0.2; 0.1; 0.45; 0.25
HE relocation move: resequence move; repipe move	0.5; 0.5
splitter move: add a splitter move; remove a splitter move; modify split fraction move	0.3; 0.3; 0.4

Table 3 lists the simulated annealing parameters used in these case studies. Tests were carried out to verify that these values were appropriate for the case studies presented in this work. Ten optimization runs were performed for each case study to gain confidence in the optimal solutions. Each optimization took around 15 min to run. The HEN designs with the lowest costs were selected from these runs. For Case 1, the SA algorithm performed 252 iterations, of which 187 were feasible HEN designs (i.e., constraints were met and the

Table 3. Simulated Annealing Parameters

parameter	value
initial annealing temperature	1×10^5
final annealing temperature	1×10^{-4}
markov chain length	30
cooling parameter	0.05
acceptance criteria	Metropolis[34]

DOI: 10.1021/ie503804u
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objective function, eq 39, was calculated). For Case 2, 322 iterations were performed, of which 132 were feasible HEN designs. The feasibility solver was executed for all the iterations of the SA algorithm.

Table 4 summarizes the energy and capital costs for the optimized heat exchanger networks. Heat transfer area constraints are not taken into account in Case 1 (i.e., ϑ_3, ϑ_4, ϑ_5, ϑ_6 are all zero), while for Case 2 these constraints are active. The median and highest costs for the 10 runs of Case 1 are 9.21 M$/y and 9.33 M$/y; while for Case 2 these costs are 9.31 $/y and 9.34 M$/y, respectively. Figures 10 and 11 show the structures of the modified HENs from Cases 1 and 2, respectively. The breakdown of heat loads, heat transfer areas, and inlet and outlet temperatures for the optimized HEN designs are presented in Tables S5 to S8 (see Supporting Information).

Table 4. Optimization Results

item[a]	base case	case 1	case 2
Utility Consumption			
hot utility (MW)	60.82	56.05 (−8%)	58.68 (−4%)
cold utility (MW)	67.05	62.58 (−7%)	65.00 (−3%)
Utility Costs			
hot utility (M$/y)	9.12	8.41 (−8%)	8.80 (−4%)
cold utility (M$/y)	0.35	0.33 (−7%)	0.34 (−3%)
Capital Costs			
new HE area ($)			37 923
additional area ($)		256 667	185 764
repiping ($)		60 000	
resequencing ($)		35 000	35 000
total capital costs ($)		429 732	258 688
ACC (M$/y)		0.19	0.14
TAC (M$/y)	9.47	8.93 (−6%)	9.28 (−2%)

[a] M$ denotes millions of dollars.

In Case 1, the coil inlet temperature of the furnace increased from 265 °C to 274 °C. This increase in temperature reduces the hot and cold utility consumption by 8% and 7%, respectively, with only 0.4 M$ of capital investment. The total annualized cost for this optimized network is reduced by 6%. The HEN design in Case 1 proposes removing heat exchanger 13, repiping heat exchanger 24, and adding a splitter in the crude oil stream. In the optimized split, 0.26 of the stream flows through heat exchanger 3 and the remainder through exchanger 1. The number of proposed modifications is within specified limits.

Table 5 compares the heat transfer areas of the base case and optimized networks. The total additional area required for the optimized network in Case 1 is 1070 m^2. It can be seen in Table 5 that the new required areas for exchangers 3, 6, and 24 in Case 1 are considerably greater than their base case values. In contrast, heat exchanger 11 requires additional area equivalent to only 2% of its installed area. Modifying this heat exchanger would require significant engineering and installation resources and introduce extensive logistical and safety issues, yet it is likely to make little contribution to the improvement of energy recovery. A reduction of 83% in area requirements is observed for exchangers 12 and 17, which suggests that modifications to the configuration of these exchangers should be made.

In Case 2, constraints on additional area are imposed, in an attempt to generate a more practical solution. After optimization, the coil inlet temperature increases by only 2 °C. Hot and cold utility requirements are decreased by 4% and 3% from their base case values, respectively. Required capital investment equals 0.3 M$, which is less investment than for Case 1. The total annualized cost for the optimized network is 9.3 M$/y. This represents a reduction in the total annualized cost of only 2%, which is less than the 6% reduction obtained in Case 1. An inspection of the calculated areas for Case 2 (Table 5) shows more conservative area values than for Case 1. It can also be seen in Table 5 that area requirements in Case 2 are within their specified lower and upper bounds.

As summarized in Figure 11, the HEN design in Case 2 proposes installing a new heat exchanger (unit 26), removing heat exchanger 24, resequencing heat exchanger 12, and adding two stream splitters in the crude oil stream. The split factions for the splitters located in the crude oil and LD streams are 0.22 (to exchanger 3) and 0.66 (to exchanger 13), respectively. The number of proposed modifications is within specified limits.

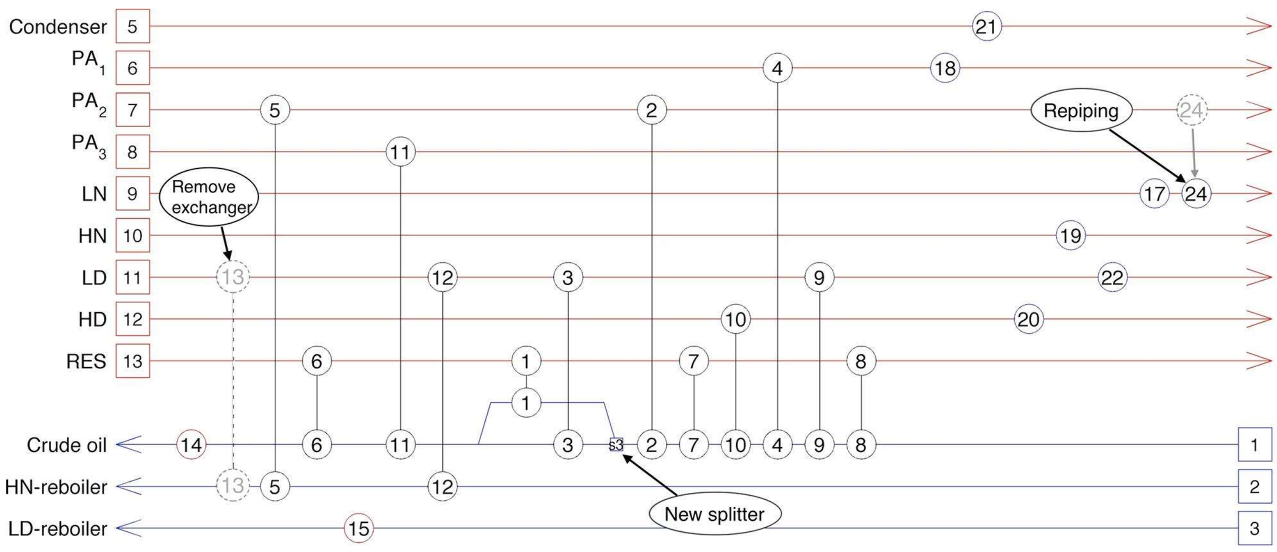

Figure 10. Proposed retrofit modifications. Unconstrained area.

DOI: 10.1021/ie503804u
Ind. Eng. Chem. Res. 2015, 54, 5001−5017

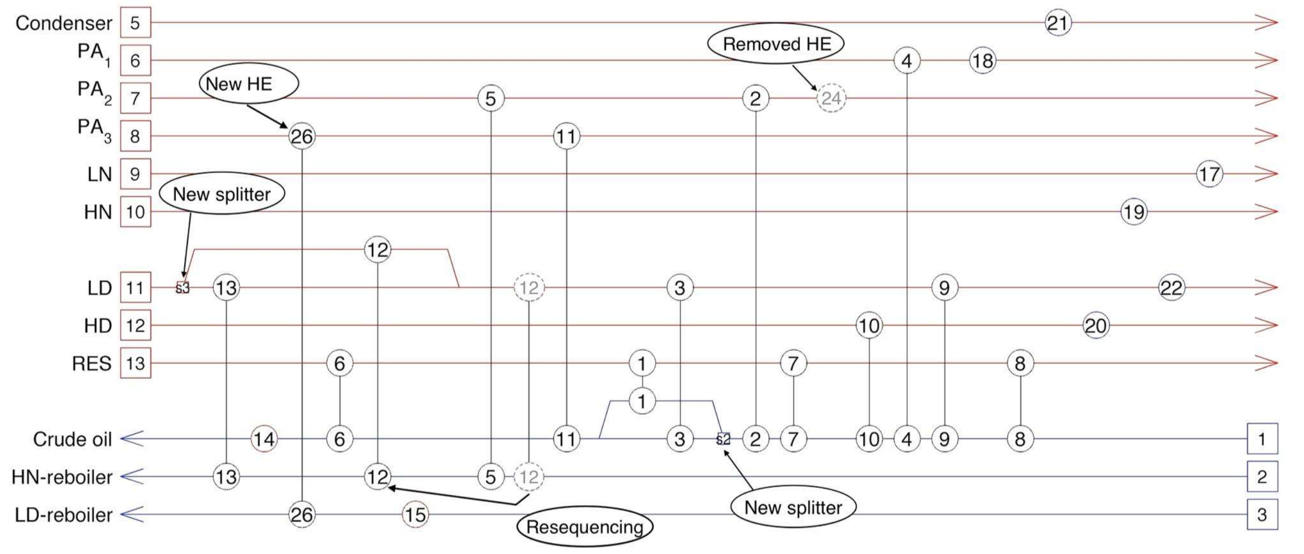

Figure 11. Proposed retrofit modifications. Constrained area.

Table 5. Heat Transfer Areas for Base Case and Optimized Cases with and without Considering Constraints on Heat Transfer Area

	calculated areas (m^2)				
exchanger no.	base case	case 1		case 2	
1	1018	1011	(−1%)	1133	(+11%)
2	808	991	(+23%)	958	(+19%)
3	110	356	(+223%)	143	(+30%)
4	298	391	(+31%)	389	(+31%)
5	95	145	(+52%)	88	(−7%)
6	117	341	(+192%)	144	(+23%)
7	465	671	(+44%)	619	(+33%)
8	255	203	(−20%)	204	(−20%)
9	347	334	(−4%)	160	(−54%)
10	78	104	(+33%)	105	(+34%)
11	558	569	(+2%)	521	(−7%)
12	23	4	(−83%)	17	(−23%)
13	10			12	(+21%)
17^{CU}	48	8	(−83%)	48	
18^{CU}	71	41	(−42%)	31	(−57%)
19^{CU}	103	103		103	
20^{CU}	48	43	(−9%)	42	(−11%)
21^{CU}	1169	1169		1169	
22^{CU}	122	111	(−9%)	163	(+34%)
24^{CU}	10	42	(+310%)		
26				84	
total area	5754	6638	(+15%)	6135	(+7%)
additional area		1070		640	
new HE area				84	

6. CONCLUSIONS

This paper presents a new approach to retrofit heat exchanger networks. The main contributions of this work consist of (1) the incorporation of a simulation model, formulated using principles of graph theory, into the HEN retrofit optimization framework, (2) the use of linear and nonlinear equations to model heat capacity as a function of temperature, and (3) the consideration of constraints on the heat transfer area that can be added to each existing heat exchanger.

The simulation model employed in this work facilitates the manipulation of the HEN structure by the optimization algorithm. Moreover, this model is flexible and simple as it can be used to simulate streams with temperature-dependent properties while keeping the linearity of the model equations. On the other hand, the consideration of temperature-dependent heat capacities adopted in this work provides more accurate estimations of energy requirements and temperatures than using constant heat capacity values.

In this work, operating and capital costs were considered in the optimization framework to select the most attractive design option. Operating costs include hot and cold utility consumption, while capital costs include the investment required to add new heat exchangers, relocate heat exchangers, and increase the heat transfer area of existing heat exchangers. The main advantage of the proposed methodology is that constraints on HEN structure and heat transfer areas can be easily specified by the designer. This allows more realistic designs to be generated, since issues such as plant layout and safety, can be addressed.

The case studies presented in this paper showed that the proposed methodology produced HEN designs with reduced energy consumption, requiring a relatively small investment to retrofit the HEN. Furthermore, the optimization approach proposed minimal topology modifications to the HEN to reduce energy requirements. As expected, the constraints imposed reduced the magnitude of the benefits in terms of energy savings. Future work to progress the application of this methodology includes the calculation of furnace heat transfer areas, the consideration of pressure drops in heat exchangers, and the calculation of heat transfer coefficients considering fouling, temperature, flow rate, viscosity, etc.

ASSOCIATED CONTENT

* Supporting Information

Additional data and results for the heat exchanger networks presented in the case studies. This material is available free of charge via the Internet at http://pubs.acs.org.

DOI: 10.1021/ie503804u
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Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

The authors thank the Mexican National Council of Science and Technology (CONACYT, no. 204362/308621) and the Roberto Rocca Education Program (RREP) for the financial support granted for the development of this work.

NOMENCLATURE

A = matrix of coefficients for the mass balance
CP = vector of average heat capacity flow rates
CP = vector of heat capacity flow rates
C = matrix of coefficients for the energy balance I = identity matrix
M = incidence matrix SP
= split fraction matrix
T = vector of streams temperatures in the heat exchanger network
T_s = vector of temperature specifications for external streams of supply units
a = vector of the indices of outlet streams related to the split fraction
b = vector of solutions for the mass balance d
= vector of solutions for the energy balance
m = vector of mass flow rates for streams in the heat exchanger network
n = vector of mass flow rates for external streams
q = vector of heat loads for exchangers in the network v
= vector of temperatures for external streams
x = vector of variables for the mass balance z
= vector of variables for the energy balance
ACC = annualized capital investment
A = heat transfer area
CC = capital cost
CP = average heat capacity flow rate CP = heat capacity flow rate
Cp = average heat capacity
Cp = heat capacity
C = unit price
F = flow rate
F_T = temperature correction factor LMTD
= log mean temperature difference M = element of the incidence matrix
N = number of elements or streams OC = operating costs
SP = element of split fraction matrix
S = number of edges in the incidence matrix TAC = total annualized cost
T_s = supply temperature
T_t = target temperature
U = overall heat transfer coefficient
f = objective function for the repair algorithm i = interest rate
m = mass flow rate
n = mass flow rate of an external stream
q = heat load of a heat exchanger
y = project life

Greek Letters

T = vector of temperature change specifications
T = temperature change specification
T_{min} = minimum temperature approach
α = vector of split fractions
α = split fraction
ϑ = vector of parameters of the repair algorithm
ϑ = parameter of the repair algorithm

Subscripts

\+ = matrix of positive elements
add = additional heat transfer
area calc = calculated heat
transfer area c = cold stream
h = hot stream
inst = installed heat transfer
area in = inlet
i = matrix index; element index
j = matrix index; element index
k = index for elements
l = index for elements
max = maximum additional heat transfer
area m = index for elements
n = index for
utilities out = outlet
util = utility

Supercripts

* = variable specification
value HE = heat exchanger
MX = mixer
PD = demand unit
PR = unit operation
PS = supply unit P
= external unit SP
= splitter
lb = lower bound
ub = upper bound
T = transpose

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