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# Globally optimal simultaneous heat exchanger network synthesis and basic heat exchanger design

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## Abstract

In this article, we extend a previously developed globally optimal enumeration methodology for the synthesis of heat exchanger networks (HENs) to include the basic design of heat exchangers (HEXs). The method addresses together all trade-offs between network structure, energy usage, and the basic design of the HEXs. Without loss of generality, we focus on shell-and-tube HEXs. Unlike previous approaches, such as Pinch Analysis, Metaheuristic methods, or Mathematical Programming, our procedure guarantees global optimality. The procedure is not iterative and does not present any convergence challenges. We enumerate HEN structures using a mixed-integer linear programming method and we use Set Trimming followed by sorting for the HEX design. In addition, because some network structures are incompatible with single shell exchangers, we use multiple shell exchangers in series. The comparison of the results of the proposed approach with solutions obtained using two alternative methods extracted from the literature indicates that considerable cost reductions may be obtained.

**KEYWORDS**
decarbonization, global optimization, heat exchangers networks

## 1 | INTRODUCTION

The heat exchanger network (HEN) synthesis problem is a well-researched subject due to the importance of energy recovery in chemical processes. This problem was intensively studied using algorithmic approaches based on thermodynamic principles (i.e., Pinch Analysis and others), which exhibited several limitations. The lack of local (much less global) optimality is the most important of these limitations. Later, Mathematical Programming as well as Metaheuristic methods were also introduced.[1]

There is abundant literature on HEN synthesis: more than 4000 papers and counting.[2] Except for a relatively small number of papers, all research relied on a priori selected fixed film heat transfer coefficient for each of the streams. Such fixed values were widely used for all exchangers between two streams, regardless of the presence of stream splits, and the assumption was considered reasonable. Thus, one can say that the original three-step approach (targeting followed by network design and subsequently performing exchanger design) of the Pinch Design Method, evolved into a two-step approach (network design followed by exchanger design), used by the majority of the Mathematical Programming approaches and to a great extent the Metaheuristic approaches. The limitations of this approach started to be pointed out very early by Polley and Shahi,[3] mainly focusing on the lack of consideration of pressure drop in the synthesis. Other limitations, like solutions with exchangers impossible to build in practice, were seldom discussed, if at all.

Because of the limitations of the conventional HEN synthesis approaches based on fixed values of film heat transfer coefficients, different alternatives were developed for solving the HEN synthesis and the associated heat exchanger (HEX) design problems. In addition, most literature considers shell-and-tube HEXs, the exception being Wang et al.[4] who considered detailed plate HEX design. The review paper by Li et al.[2] discusses this issue and concludes that "HENS design is essentially an mixed-integer nonlinear programing (MINLP) without the guaranteed optimal solution. Optimization with the detailed thermal-hydraulic performance has introduced more discontinue [sic] and nonlinear terms, making the HEN model more difficult to solve." They continue by recognizing that initialization is hard to come by and that although "heuristic" methods are successful, they obtain nothing more than local solutions. They also state that the state of the art is the use of sequential methods of designing the network first and then designing the exchangers, sometimes using some feedback loops to iterate.

In response to the pessimistic view of Li et al.,[2] namely that the PSE community is trapped in a (for now) unsolvable problem of not being capable of solving a large and complex mixed integer nonlinear optimization model (MINLOM) to global optimality, we present in this article an alternative to the use of MINLP procedures, showing that it is possible to solve this problem to global optimality after all. We prefer MINLOM to "MINLP model," a commonly used acronym that we believe mixes the mathematical nature of the model with its solution using mathematical programming, even though it can be solved using other approaches.

Previous papers that addressed the HEN-HEX design optimization can be organized into three different approaches, according to the HEN synthesis technique used: Pinch Analysis, Metaheuristic methods, and Mathematical Programming.

Polley et al.[5] extended the Pinch Analysis to consider pressure drop in the retrofit of HENs, by using a relationship between pressure drop and film heat transfer coefficients that they developed. The concept was extended to HEN grassroots design by Polley and Shahi,[3] where they fixed the pressure drops in the targeting step of Pinch Analysis and obtained the film heat transfer coefficients or vice versa. Liporace et al.[6] used Pinch Analysis to identify the structure of the HEN, followed by the basic design of each exchanger using the procedure proposed by Jegede and Polley.[7] Based on the results, they showed that it is possible to exclude matches using ad hoc criteria and redesign the network. Ravagnani et al.[8] used Pinch Analysis to obtain a HEN associated with maximum energy recovery, followed by a heat load loop-breaking procedure. Once a network is obtained, the basic design of each HEX is performed considering the Bell-Delaware method and tubular exchanger manufacturers association standards. Garcia et al.[9] proposed a hybrid method for the synthesis of HENs and detailed exchanger design. The method combines Pinch Analysis with Mathematical Programming and a Bell-Delaware-based algorithm to design the HEXs. They used decomposition and a recursive algorithm. Akbari et al.[10] proposed a new area targeting based on stream allocation to shells or tubes. The whole methodology incorporates area targeting in a methodology similar to supertargeting of the minimum temperature approach ($\Delta T_{min}$). Zunlong et al.[11] proposed the utilization of Pinch Analysis and exergoeconomic analysis for the determination of the optimal minimum temperature approach, followed by the synthesis using Pinch Analysis and the design of the different HEXs considering the pressure drop distribution among HEXs of each stream. Allen et al.[12] used Pinch Analysis for the HEN synthesis and a genetic algorithm (GA) for the design of HEXs. The procedure is repeated for different values of the minimum temperature approach and the lowest cost solution is then selected. Serna-González and Ponce-Ortega[13] considered a three-way trade-off between utility consumption, network area, and pumping costs. After the network is obtained, the problem is defined as a nonlinear programming problem for a given minimum temperature approach using the Bell-Delaware model to determine the film heat transfer coefficients and pressure drops related to the geometry of HEXs. Sun et al.[14] adapted the targeting procedures of Pinch Analysis to consider multipass exchangers. The approaches based on Pinch Analysis do not use the results of the HEX design problem to optimize the HEN synthesis. This limitation hinders the cost reductions that can be obtained through the connection between HEN synthesis and HEX design.

The utilization of metaheuristic methods for the HEN synthesis together with the HEX design involves the utilization of a stochastic-based algorithm for the HEN structure selection. The evaluation of the objective function of each solution candidate during the search involves the application of a proper design algorithm for the corresponding HEXs. Different Metaheuristic methods were explored, all of them relying on the stage-wise superstructure[15] for the representation of the HEN structure and the Bell-Delaware model for the design of shell-and-tube HEXs. Ponce-Ortega et al.[16] used a GA for generating structures and another GA for the design of HEXs. Silva et al.[17] proposed the generation of the structures using particle swarm optimization and the optimization of HEXs using Mathematical Programming.[18] Ravagnani and Silva[19] used particle swarm for the retrofit of HENs with detailed equipment design. Xiao et al.[20] used a combination of genetic algorithms and simmulated annealing (GA/SA) with solution candidates that represent the network structure and design variables of HEXs. In this case, an inner algorithm is solved to finish the HEX design for each solution candidate. Karimi et al.[21] used particle swarm optimization and considered different material choices concerning corrosion issues. Finally, Farzin et al.[22] presented a hybrid genetic-particle swarm method. These Metaheuristic-based methods are characterized by their efficiency in finding good solutions, but they require parameter tuning that usually demands several runs to adjust them (an aspect rarely reported by the authors of these papers), making them problematic to be used by industry. Therefore, the majority of these methods are not easy to use by practitioners who have no expertise/training in most-of-the-time problem-specific parameter tuning, much less ability or desire to build the codes. Additionally, by construction, these methods do not guarantee global optimality. Therefore, Mathematical Programming, or some form of rigorous optimization where the user does not have to be technically trained on the details of the methodology, is the most appealing viable alternative if global optimality is a more desired goal.

Even if one uses the recently developed mixed-integer linear models for HEX design[23–25] together with HEN superstructure equations, the problem is likely to be cumbersome to solve, especially if global optimality using Mathematical Programming is pursued. Indeed, a set of equations for the design of an exchanger (including the selection of tube and shell side fluid allocation) dedicated to each pair of streams is needed and the logarithmic mean temperature difference (LMTD) as well as the correction factor ($F$) equations, introduce complex nonlinearities, mostly nonconvex. In addition, if one is presented with the prospect of variable physical properties, one can anticipate a problem of very large size. Many researchers recognized the aforementioned difficulties of attempting to solve a large MINLOM. Therefore, they used decomposition as well as iterative procedures that do not guarantee optimality (local or global). Indeed, Frausto-Hernández et al.[26] solved the HEN synthesis with HEX design using a MINLOM applied to the Yee and Grossmann[15] superstructure and the design of HEXs based on a model proposed by Serna[27] with an approximation for the pressure drop in each stage developed by Shenoy.[28] Their main assumption was to build a MINLOM where the maximum allowable pressure drops are used. The MINLOM was solved without the utilization of decomposition schemes, but the authors mentioned convergence problems and local optimality issues. Mizutani et al.[29] proposed using a logic-based outer approximation method to solve the HEN synthesis with a detailed HEX design. It couples the HEX design model presented by Mizutani et al.[30] with the Yee and Grossmann[15] superstructure model for HEN synthesis. Ravagnani and Caballero[18] solved the HEN synthesis and the HEX design problems using two MINLOM formulations, according to a decomposition scheme. The algorithm is iterative between the two models and considers an initial film heat transfer coefficient to find the first HEN and then it calculates the actual film heat transfer coefficients using the design optimization procedure for each exchanger of the HEN; the new film heat transfer coefficients are then used for another HEN synthesis trial. This is performed until the cost becomes larger than the previous one or does not change. Another difficulty is that the film heat transfer coefficients needed for the HEN synthesis step have to be some average of more than one exchanger. The procedure does not guarantee that there will be no solutions featuring better costs. By construction, even if each model is solved to global optimality, this procedure cannot guarantee global optimality. Odejobi et al.[31] proposed adding a choice of intensification for the film heat transfer coefficients, but no detailed design of the exchangers was included. Short et al.[32] used the stage-wise superstructure to generate an initial HEN to later design HEXs from which correction factors related to pressure drop and area are calculated and included in the objective function of the HEN superstructure model, iterating until convergence is obtained. These correction factors have the goal of approximating the areas obtained by the MINLOM to those obtained by the detailed design model. The solution neither guarantees local optimality nor global optimality. A similar approach based on correction factors was used by Short et al.[33] Souza et al.[34] proposed a mixed integer nonlinear model that includes the equipment design and the piping layout. In this model, the classical connections between pressure drop and film heat transfer coefficient are used. Kazi et al.[35] proposed a procedure based on a multistep approach. The structure of the network is determined using a MINLOM based on the stage-wise superstructure of Yee and Grossmann,[15] including a smoothed LMTD approximation. The second step is a continuous nonlinear optimization model associated with nonisothermal mixing. Finally, the individual HEXs are designed by solving a continuous nonlinear optimization model reformulating it as a discretized model based on a small number of geometrical options.[36] The authors did not claim, nor present, any argument that the model gives global optimal results. A variant of the previous paper using a trust region framework was proposed by Kazi et al.,[37] where the decomposition of the problem is still used. Cotrim et al.[38] proposed a bi-level approach that is an improvement of Ravagnani and Caballero,[18] with a new capital cost parameter that is iteratively updated based on the values obtained during the design of the HEXs. Li et al.[39] proposed a MINLOM formulation based on the stage-wise superstructure[15] together with shell-and-tube HEX design equations, including the option of helical baffles. Simplifications in the HEX model allow the solution of the problem in a single step. They used the discrete and continuous optimizer (DICOPT) to solve it, which does not guarantee global optimality. Also, the authors did not report what initialization was used.

Departing from Pinch Analysis, Metaheuristic methods, and Mathematical Programming, Wang et al.[4] used an algorithmic approach: the advanced Grid Diagram, which also considered plate exchangers and does not guarantee global optimality. The grid technique, some mixed-integer linear models, and several Metaheuristic approaches were incorporated into SPIL, a software package.[40]

A feature of most of the above-mentioned papers is that multiple shells are rarely considered. This was recently addressed by Isafiade and Short,[41] but without solving the optimal HEX design problem. We show in this article that some problems require considering multiple shell arrangements due to temperature cross when more than one pass is considered.

This article proposes a new approach focusing on the network enumeration procedure proposed by Chang et al.,[42–44] which is used together with the Set Trimming approach used by Lemos et al.[45] for the design of HEXs. The design model guarantees global optimality and is coupled to the synthesis procedure in a way that also renders global optimality. As discussed above, none of the previous papers that addressed this problem proposed a solution that can guarantee that its optimum is global.

The article is organized as follows: We first discuss the nature of the HEN synthesis problem together with the HEX design and present the HEN synthesis methodology used by Chang et al.,[42–44] discussing where we introduce our changes to extend this approach to include the design task of the HEXs in a single problem and what optimal search algorithm we use. Then, we discuss briefly HEX design models and methods. We finish presenting the results and the conclusions.

## 2 | HEN SYNTHESIS AND HEX DESIGN

The traditional method of HEN synthesis has been presented as one where the film heat transfer coefficient for each stream is constant. The synthesis objective functions almost invariably involved the calculation of the cost of each exchanger, plus the pumping cost, sometimes. The investment cost is connected to the HEX area, through known simplified formulas. These areas are usually expressed by the classical equation of the LMTD method, here shown for an exchanger between a hot stream $i$ and a cold stream $j$:

$$A_{i,j} = \frac{Q_{i,j}}{U_{i,j} LMTD_{i,j}}. \quad (1)$$

In turn, in these models, the film heat transfer coefficient is a parameter as follows:

$$\widehat{U}_{i,j} = \frac{1}{\frac{1}{\widehat{h}_i} + \frac{1}{\widehat{h}_j}}, \tag{2}$$

where the film heat transfer coefficients $\widehat{h}_i$ and $\widehat{h}_j$ presumably include the fouling resistances while the thermal conductive resistance of the wall is neglected. Usually, these models do not discuss fluid allocation or exchanger type. Also, the correction factor is absent, as all exchangers are assumed to simply consist of one unit with a perfect countercurrent flow. Finally, there is no mention of the need for multiple shells in MINLOMs. Only works using Pinch Analysis considered multiple shells.[46]

Despite all its shortcomings, Equation (1) is used under the implicit assumption that the optimal network, whatever "optimal" means for each choice of model (superstructures, isothermal mixing or not, etc.), will have the same economic performance after the exchangers are designed. In other words, a decomposition method is used: first, the HEN structure and utility usage are obtained and then the basic design of the exchangers (shell and tube diameters, number of tubes, number of passes, etc.) are obtained. It is easy to argue that this is incorrect. Indeed, the values of the film heat transfer coefficients adopted during the synthesis step can be considerably different from the actual values determined during the design of the HEXs. This mismatch implies that a suboptimal solution is obtained where the trade-off between operational and capital costs is different, not to mention that the optimal network structure can be different. Additionally, in many cases, multiple shells, each with multiple passes, may be needed, and in such cases the cost of the exchanger as if it had only one shell is misleading. Other disadvantages include the synthesis of networks with exchangers that are very difficult to build, like the case of very different flowrates on the two sides. These difficulties suggest performing the synthesis together with the basic design of HEXs, which guarantees a better assessment of the investment cost, especially when multiple shells are considered, and non-viable exchangers are eliminated by the optimization.

The method we present in this article is an extension of the one proposed by Chang et al.,[42] which guarantees global optimality (provided that the unimodal conjecture is true) and is focused on minimal networks, but their method is based on fixed film heat transfer coefficients. In our extension, we also guarantee global optimality. The concept of minimal network was introduced by Chang et al.[42] It is a HEN structure where the heat loads of all exchangers are unique when the utility usage is fixed. This means that there are no heat load loops, as defined by Pinch Analysis. In our method, we replace the calculation of HEX areas based on fixed film heat transfer coefficients with a HEX design task. We consider the option of multiple shells in series and we solve the optimal energy recovery using a global optimization method. Because all structures are enumerated, topology traps are absent.

For the sake of focusing on the methodology and without loss of generality, all HEXs are of the shell-and-tube type, and process streams do not involve phase change. The same feature is considered for the coolers (e.g., cooling water as cold utility). The heaters use saturated steam, which condenses on the shell side.[47] However, the procedure is flexible: For example, other types of HEXs, such as gasketed-plate HEXs[48] or heaters with phase change[49] can be considered as options in the design of the equipment. Moreover, one can determine the cheapest option among different types of exchangers. The proposed algorithm is shown below:

- Step 0: Initialization—Set the incumbent best upper bound of the global solution (*UBTAC*) to infinity. Select a maximum energy consumption ($\widehat{E}_{hu}^{MAX}$) (this maximum energy consumption prevents looking for poor solutions, see Remark 1). Calculate the estimated minimum number of units: $Nmin =$ number of streams $+1$. Set $N = Nmin$ (see Remark 2). Set a counter that indicates the number of minimal structures identified with $N$ units: $Structure\_Counter_N = 0$.
- Step 1: Structure generation—Obtain a minimal structure (*MSTR*) candidate, limited by $\widehat{E}_{hu}^{MAX}$. This step solves a model, based on Yee and Grossmann,[15] with the number of units equal to $N$. The model is linear (the HEX design equations of the Synheat model are not included), and it uses a dummy objective function. In addition, to avoid solutions with heat duties equal to zero, a constraint is added to limit the heat load to a minimum value $\widehat{\varepsilon}$ (in our examples we use $\widehat{\varepsilon} = 1$ kW) when an exchanger exists. The model also excludes previous solutions using well-known exclusion constraints,[50] often referred to as integer cuts. If this problem is feasible, then go to Step 2, otherwise, go to Step 8.
- Step 2: Structure check—If the structure obtained in Step 1 is minimal (see Remark 2), then make $Structure\_Counter_N \leftarrow Structure\_Counter_N + 1$, and go to Step 3, otherwise, go to Step 1.
- Step 3: Determination of energy consumption bounds—For the chosen *MSTR*, obtain the minimum and the maximum energy consumptions (*Emin*, *Emax*) (see Remark 3).
- Step 4: Utility path check—If $Emin = Emax$, then there are no utility paths (i.e. there is only one possible value of energy consumption), go to Step 5; otherwise, it is possible to optimize the energy consumption, minimizing the total annualized cost (*TAC*), go to Step 6.
- Step 5: *TAC* evaluation when there are no utility paths—For the energy consumption evaluated in Step 4, determine all temperatures and heat loads, determine the global optimal design of all HEXs,[45] evaluate the resultant *TAC*, go to Step 7.
- Step 6: *TAC* optimization when there are utility paths—Apply the Direct method[51] to find the minimum *TAC* for the current structure. Here, the *MSTR* is solved for different fixed energy values according to the need of the search and for each evaluation of the *TAC*, the global optimal design of each HEX is obtained using Set Trimming followed by Sorting.[45] Go to step 7.
- Step 7: Incumbent update—If $TAC \le UBTAC$, then update *UBTAC*. Go to Step 1.
- Step 8: Stop criterion—If $Structure\_Counter_N = 0$, then Stop, *UBTAC* is the global optimum (see Remark 4). Otherwise, reduce the number of units, $N \leftarrow N - 1$, set $Structure\_Counter_N = 0$ and go to Step 1.

*Remark* 1. Because of its combinatorial nature, the HEN synthesis is associated with a large number of possible structures. Indeed, as energy consumption increases, the number of feasible combinations of matches featuring poor energy recovery can drastically increase. It means that the enumeration procedure can generate several structures with low energy recovery, which have a very small probability of being the global optimal solution of the synthesis. Because this set of structures requires a significant computational effort to be evaluated, we introduce a new constraint in the structure generation model to avoid visiting these low-energy recovery structures. The criterion used is maximum energy consumption, or minimum energy recovery, as follows:

$$E_{hu} \leq \widehat{E}_{hu}^{MAX}, \quad (3)$$

where $E_{hu}$ is the hot utility energy consumption and $\widehat{E}_{hu}^{MAX}$ is the maximum energy consumption defined by the user. In our examples, the $\widehat{E}_{hu}^{MAX}$ is equal to three times the minimum energy consumption calculated using Pinch Analysis. Lower values of $\widehat{E}_{hu}^{MAX}$ may reduce the computation time.

*Remark* 2. Minimal structures do not contain heat load loops. Usually, when one uses the minimum number of exchangers (*Nmin*) as defined above, the structures obtained are minimal, but there can exist structures featuring the minimum number of exchangers containing heat load loops. This has been identified in Pinch Analysis. The presence of heat load loops in a structure can be identified by checking the rank of the coefficient matrix of the algebraic linear system of equations of the model associated with the structure obtained where the utility consumption is fixed. If the matrix is singular, there are heat load loops. Otherwise, the structure is minimal.

*Remark* 3. The determination of the minimum and maximum energy consumptions for a given structure can be obtained by solving the linear problem described in Step 1, fixing the binaries associated with the structure, and substituting the objective function with the energy consumption (the resultant problem is a linear problem).

*Remark* 4. The use of exhaustive enumeration and global optimization algorithms allows the identification of the global optimum, as explained below:

1. The combinatorial nature of the problem associated with the different structures is solved by an exhaustive enumeration of structures obtained using the mixed-integer linear optimization model described in Step 1. Previous structures already visited are excluded from the search through the insertion of proper integer cuts, known as exclusion constraints.[50]
2. For a given structure, the optimal tradeoff between capital and operating costs is determined using a global optimization method, which minimizes the *TAC*.
3. The evaluation of the capital costs associated with a given energy consumption is also solved using a global optimization method.

The associated computational effort can be reduced by enumerating all the structures first and distributing their evaluation among several processors.

## 3 | HEX DESIGN OPTIMIZATION PROCEDURE

For the design of HEXs in the network as well as the heaters and coolers, we consider shell-and-tube HEXs with an E-type shell and single segmental baffles. The film heat transfer coefficients without phase change in the tube side and shell side are evaluated using the Gnielinksi correlation for turbulent flow and the Bell-Delaware method, respectively. The film heat transfer coefficient for steam condensation in the shell side is evaluated using the Nusselt model. The complete set of equations for HEX models is available in the open literature.[47,52]

The solution to the global optimal design problem of each HEX of the network is obtained through an extension of the Set Trimming approach presented by Lemos et al.[45] for the design of shell-and-tube HEXs.

Seven design variables represent the dimensions of a HEX shell: number of tube passes (*Npt*), outer tube diameter (*dte*), tube layout (*lay*), tube pitch ratio (*rp*), number of baffles (*Nb*), shell diameter (*Ds*), and tube length (*L*). The inner tube diameter (*dti*) is obtained from standards and is related to pressure. The fluid allocation (shell-side vs. tube-side) and the number of shells in series are also HEX design variables (that were not handled by Lemos et al.[45]), but they are treated separately, as explained later. The search space is represented by the set of solution candidates, each candidate is composed of a given combination of discrete values of the design variables.

The Set Trimming procedure[53] is an algorithm proposed first for equipment design based on the successive application of the problem inequality constraints to eliminate infeasible candidates. Only the remaining candidates from a constraint check are submitted to the next one. Therefore, there is a reduction of the computational effort, because the size of the set of candidates decreases along the search. After the application of all constraints, the remaining set of candidates contains only feasible ones and the global optimum can be obtained through a simple sorting procedure using the corresponding values of the objective function. It is important to observe that the method does not explore single solution candidates, but it operates on a set of candidates. Therefore, the computational efficiency of the algorithm is provided through the utilization of specialized routines for handling large sets of data, instead of using slow conventional loops (e.g., dynamic indices in GAMS, vectorization techniques in Matlab/Scilab or arrays from Numpy in Python).

The set of constraints applied in the solution of the design problem is presented below, considering a given number of shells and fluid allocation (pressure drop constraints are not addressed). Here, the fixed parameters established before the optimization are represented with the symbol "^." The order of the constraints corresponds to the order in which they are applied in the Set Trimming algorithm. The constraints that depend on more complex evaluations are applied at the end of the process to reduce the computational effort because they will be used in inspecting a smaller set of candidates.

## 3.1 | Geometric trimming

These constraints correspond to design recommendations associated with HEX dimensions[54,55]:

$$3\,Ds \leq L \leq 15\,Ds, \tag{4}$$

$$0.2\,Ds \leq lbc \leq 1.0\,Ds, \tag{5}$$

where $lbc$ is the baffle spacing. Additionally, to avoid too large shells related to obstacles for cleaning and maintenance, a maximum shell size is imposed[47]:

$$A_{SS} \leq \widehat{A}_{SS}^{max}, \tag{6}$$

where $A_{SS}$ is the area of a single shell, and $\widehat{A}_{SS}^{max}$ is the upper bound adopted.

## 3.2 | Correction factor trimming

The HEN synthesis algorithm can propose HEXs associated with temperature cross (i.e., the outlet temperature of the cold stream is larger than the outlet temperature of the hot stream). This may hinder the utilization of design alternatives with multiple passes. In these cases, the heat exchange may be impossible or associated with a low value of the LMTD correction factor ($F$), which expresses the departure of the behavior of a given HEX configuration from the countercurrent configuration:

$$\widehat{Q} = U A\, F\, \widehat{LMTD}. \tag{7}$$

Low $F$ values are also related to a steep slope of the $F$ curve, thus a small variation of the problem parameters may cause a large $F$ reduction, that is, it is not safe to design a HEX to work in these zones.[56,57] Then, an additional trimming is added (this trimming also eliminates candidates where the $F$ value cannot be calculated because the heat exchange is impossible for that candidate's configuration):

$$F \geq 0.75. \tag{8}$$

The utilization of multiple shells in series with a multiple pass configuration increases the $F$ factor, therefore the design algorithm considers the number of shells as a design variable.

Instead of using a feasibility criterion based on the $F$ value directly, Ahmad and Smith[46] proposed an alternative constraint:

$$P \leq \widehat{X}_P\, \widehat{P}_{max}, \tag{9}$$

where $P$ is the variable related to the HEX effectiveness for evaluation of $F$, $\widehat{P}_{max}$ is the abscissa corresponding to the asymptotic value of $F$ and $\widehat{X}_P$ is the safety factor imposed to avoid regions where the $F$ slope is steep (e.g., $\widehat{X}_P = 0.9$). This approach is also reported by Smith.[47] The flexibility of the Set Trimming also allows the utilization of this alternative.

## 3.3 | Flow velocity trimming

Lower and upper bounds on tube-side and shell-side velocities are imposed to avoid fouling, erosion, and vibration problems:

$$\widehat{vtmin} \leq vt \leq \widehat{vtmax}, \tag{10}$$

$$\widehat{vsmin} \leq vs \leq \widehat{vsmax}, \tag{11}$$

where $vt$ and versus are the tube-side and shell-side flow velocities, and $\widehat{vtmin}$, $\widehat{vtmax}$, $\widehat{vsmin}$, and $\widehat{vsmax}$ are the corresponding bounds.

Reynolds number trimming: Upper bounds on the tube-side and shell-side Reynolds numbers are imposed according to the interval of the validity of the correlations:

$$Ret \leq 5 \cdot 10^6, \tag{12}$$

$$Res \leq 1 \cdot 10^5, \tag{13}$$

where Ret and Res are the for the tube-side and shell-side Reynolds numbers, respectively.

## 3.4 | Required area trimming

This constraint eliminates candidates whose area does not comply with the minimum excess area required:

$$A \geq \left(1 + \frac{\widehat{Aexc}}{100}\right) Areq, \tag{14}$$

where $A$ is the area of the exchanger, $\widehat{Aexc}$ is the excess area, and $Areq$ is the required area, obtained using Equation (7), where the correction factor is related to the number of tube passes and number of shells, and the overall heat transfer coefficient is obtained using film heat transfer coefficients calculated by proper correlations considering the corresponding values of the design variables, the conductivity of the tube wall and the fouling resistances ($\widehat{Rf}$), which, without loss of generality, are considered as parameters in this work.

After the application of the set of trimmings, only the feasible candidates are left and the optimum is identified through the evaluation of the objective function of the remaining candidates and a sorting to select the candidate with the lowest value of the objective function.

The selection of which stream flows in the tube side or the shell side involves several factors, such as fouling, stream temperatures, pressures, fluid viscosities, and so forth.[47,58–60] In this article, we will assume that this decision is a design variable. The inclusion of the fluid allocation in the solution of the design problem is addressed through the application of the Set Trimming procedure twice. The first run obtains the optimal solution for a given allocation option (i.e., an incumbent is obtained) and the second run uses the opposite choice. The second run includes a first trimming that eliminates solution candidates with objective functions higher than the incumbent.

## 4 | SET TRIMMING FOR HEX DESIGN

For a given fluid allocation and number of shells, the search space of a shell-and-tube exchanger is composed of all possible combinations of the design variables already mentioned: $Npt$, $dt$, $lay$, $rp$, $Nb$, $Ds$, and $L$. This search space is valid for any HEX design problem generated during the HEN synthesis. However, the geometric constraints in Equations (4)–(8) do not depend on any specific data of a given HEX design problem. Therefore, the trimmings related to Equations (4)–(8) are applied to the initial search space, thus yielding a reduced search space composed of geometrically feasible shells. This reduced search space is used as a starting point for all HEX design problems solved during the synthesis. This reduction of the search space decreases the computational effort because it avoids an unnecessary repetition of the geometric trimmings.

Considering that the smaller the number of shells, the lower the cost,[47] the optimization procedure identifies the optimal solution with the lowest number of shells. This goal is attained through a sequential procedure, starting with only one shell, if the Set Trimming procedure

**TABLE 1** Data for design variables.

| Design variable | Options |
|---|---|
| Shell diameter (m) | 0.205, 0.305, 0.387, 0.489, 0.591, 0.686, 0.787, 0.889, 0.9906, 1.143, 1.2192, 1.3716, 1.524 |
| Tube diameter (m) | 0.01905, 0.02540, 0.03175, 0.03810, 0.5080 |
| Number of tube passes | 1, 2, 4, 6 |
| Pitch ratio | 1.25, 1.33, 1.50 |
| Layout | 1 (square), 2 (triangular) |
| Length (m) | 1.2195, 1.8293, 2.4390, 3.0488, 3.6585, 4.8768, 6.0976 |
| Number of baffles | 1, 2, 4, 6, …, 16, 18, 20 |

**TABLE 2** Example 1: Stream data.

| Stream | $\widehat{FCp}$ (kW/K) | $\widehat{Tin}$ (K) | $\widehat{Tout}$ (K) | $\hat{\rho}$ (kg/m$^3$) | $\widehat{Cp}$ (J/(kg K)) | $\hat{\mu}$ (Pa·s) | $\hat{k}$ (W/(m·K)) | $\widehat{Rf}$ (m$^2$·K/W) |
|---|---|---|---|---|---|---|---|---|
| H1 | 80.1 | 465 | 400 | 815 | 2670 | 0.00086 | 0.10 | $2.75 \cdot 10^{-4}$ |
| H2 | 208.53 | 410 | 310 | 876 | 2317 | 0.0028 | 0.11 | $6 \cdot 10^{-4}$ |
| C1 | 126.3 | 315 | 370 | 877 | 2105 | 0.0042 | 0.13 | $6 \cdot 10^{-4}$ |
| C2 | 213.6 | 315 | 400 | 908 | 1780 | 0.0091 | 0.12 | $6 \cdot 10^{-4}$ |
| Hot utility | - | 416 | 416 | 800 | 2000 | 0.00164 | 0.02 | $1 \cdot 10^{-4}$ |
| Cold utility | - | 290 | 300 | 999 | 4180 | 0.001 | 0.6 | $1.75 \cdot 10^{-4}$ |

**TABLE 3** Example 2: Stream data.

| Stream | $\widehat{FCp}$ (kW/K) | $\widehat{Tin}$ (K) | $\widehat{Tout}$ (K) | $\hat{\rho}$ (kg/m$^3$) | $\widehat{Cp}$ (J/(kg K)) | $\hat{\mu}$ (Pa·s) | $\hat{k}$ (W/(m·K)) | $\widehat{Rf}$ (m$^2$·K/W) |
|---|---|---|---|---|---|---|---|---|
| H1 | 44.5 | 465 | 400 | 815 | 2670 | 0.00086 | 0.10 | $2.75 \cdot 10^{-4}$ |
| H2 | 173.2 | 410 | 300 | 876 | 2317 | 0.0028 | 0.11 | $6 \cdot 10^{-4}$ |
| H3 | 80.0 | 454 | 433 | 872 | 2433 | 0.00076 | 0.15 | $2.75 \cdot 10^{-4}$ |
| C1 | 60.4 | 293 | 398 | 877 | 2105 | 0.0042 | 0.13 | $6 \cdot 10^{-4}$ |
| C2 | 52.6 | 293 | 373 | 908 | 1780 | 0.0091 | 0.12 | $6 \cdot 10^{-4}$ |
| C3 | 160 | 293 | 393 | 860 | 2008 | 0.0022 | 0.14 | $6 \cdot 10^{-4}$ |
| Hot utility | - | 416 | 416 | 800 | 2000 | 0.00164 | 0.02 | $1 \cdot 10^{-4}$ |
| Cold utility | - | 290 | 300 | 999 | 4180 | 0.001 | 0.6 | $1.75 \cdot 10^{-4}$ |

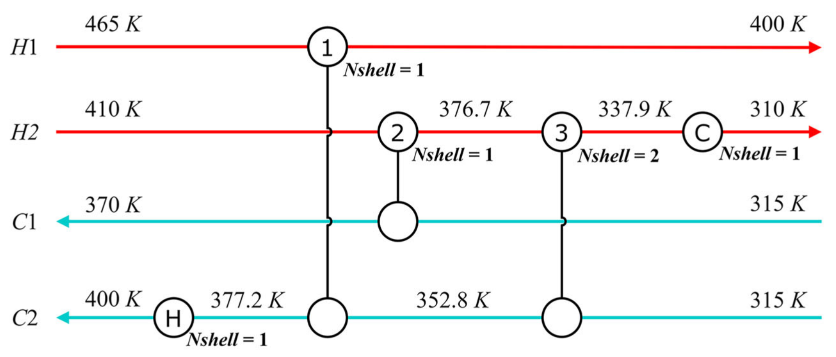


**FIGURE 1** Example 1: Optimal HEN using the Simultaneous Global HEN-HEX approach.

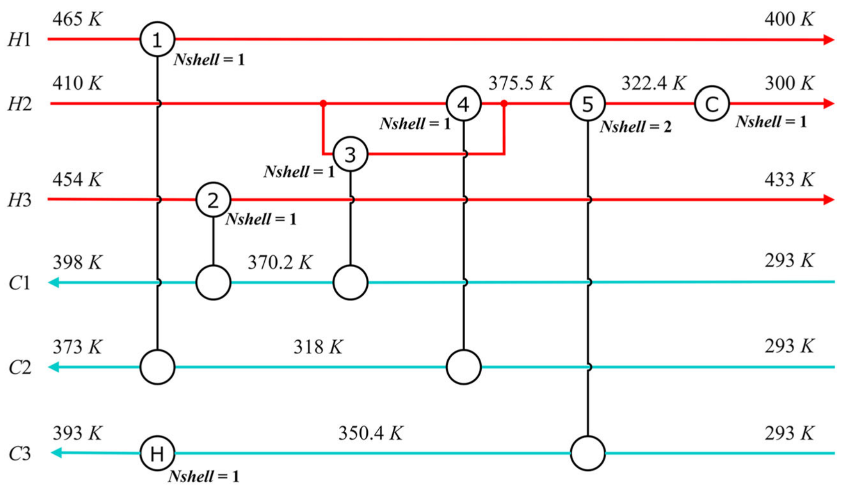


**FIGURE 2** Example 2: Optimal HEN using the Simultaneous Global HEN-HEX approach.

**TABLE 4** Example 1: Optimal HEXs using Simultaneous Global HEN-HEX approach.

| | Heat exchanger | | | | |
|---|---|---|---|---|---|
| | 1 | 2 | 3 | C | H |
| Q (kW) | 5206 | 6946 | 8080 | 5826 | 4869 |
| A ($m^2$) | 249.2 | 738.6 | 1895.4 | 274.1 | 559.8 |
| *dte* (m) | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.01905 |
| *L* (m) | 6.0976 | 6.0976 | 6.0976 | 6.0976 | 6.0976 |
| *Nb* | 14 | 12 | 18 | 18 | 14 |
| *Ntp* | 6 | 6 | 6 | 2 | 6 |
| *rp* | 1.25 | 1.25 | 1.25 | 1.25 | 1.25 |
| *Ds* (m) | 0.7874 | 1.2192 | 1.3716 | 0.7874 | 1.143 |
| *lay* | Triangular | Square | Square | Triangular | Triangular |
| *Ntt* | 683 | 2024 | 2597 | 751 | 1534 |
| Tube-side | Hot stream | Hot stream | Hot stream | Cold stream | Cold stream |
| *ht* ($W/(m^2 \cdot K)$) | 1962.1 | 988.2 | 765.0 | 8994.1 | 737.4 |
| *hs* ($W/(m^2 \cdot K)$) | 990.7 | 653.8 | 719.7 | 1500.0 | 13934.1 |
| *U* ($W/(m^2 \cdot K)$) | 385.4 | 242.9 | 230.8 | 606.4 | 389.9 |
| *Nshell* | 1 | 1 | 2 | 1 | 1 |
| *F* | 0.99 | 0.86 | 0.88 | 0.93 | 1 |

identifies an optimal feasible solution, the procedure stops. Otherwise, a new shell is added, and the procedure is repeated, stopping as soon as an optimal solution is found with multiple shells or the number of shells in series becomes higher than the maximum.

The algorithm is described below:

1. Pick the set of candidates with geometrically feasible shells already identified

2. Set the maximum number of shells $\widehat{Nshell}^{MAX}$ and go to Step 3
3. Run the Set Trimming procedure considering the following set of design variables: {*Npt*, *dt*, *lay*, *rp*, *Nb*, *Ds*, *L*} and the stream allocation, as discussed above. If a solution is achieved, go to Step 6, otherwise go to Step 4.
4. If $Nshell < \widehat{Nshell}^{MAX}$, make $Nshell = Nshell + 1$ and go to Step 3, otherwise go to Step 5
5. Stop: There is no feasible solution
6. Stop, the optimal solution contains the number of shells in series equal to *Nshell*.

If a HEN candidate contains a HEX with no feasible solution, the corresponding objective function is increased with a large penalty value. The absence of a feasible solution for the problem of the design of HEXs usually occurs when the HEN structure contains one or more heat exchanges involving streams with very different flow rates. In these cases, it is not possible to obey both flow velocity limits in the same equipment.

## 5 | RESULTS

Aiming at comparing the performance of the proposed approach with alternative procedures available in the literature, two problems, Example 1 and Example 2, are solved using the following techniques:

- Simultaneous Global HEN-HEX approach: This is our method for performing the globally optimal HEN Synthesis including HEX design. We use the word "simultaneous" to indicate that the structure of the network, the utility usage, and the basic design of multiple-shell HEXs are obtained by considering all tradeoffs simultaneously.
- Traditional approach: HEN synthesis with fixed film heat transfer coefficients, followed by the design of the resultant HEXs.
- Iterative procedure: Traditional HEN synthesis followed by HEX design updating the film heat transfer coefficients. We adopted a typical decomposition approach available in the literature.[18]

The design of HEXs is based on the discrete values of the variables presented in Table 1. It is considered that HEXs are AEL type (one pass shell with a fixed tubesheet and channel heads), with a tube wall thickness and thermal conductivity of 1.65 mm (BWG 16) and 50 W/(m·K), respectively. We also use a 25% baffle cut, a maximum number of shells equal to 5, and a minimum excess area of 10%. The tube count data is based on Kakaç and Liu.[58] The maximum HEX area

**TABLE 6** Film heat transfer coefficient estimators.

| Stream | *h* (W/(m$^2$K)) |
|---|---|
| H1 | 1125 |
| H2 | 275 |
| H3 | 1125 |
| C1 | 500 |
| C2 | 500 |
| C3 | 500 |
| HU | 10,000 |
| CU | 6250 |

**TABLE 5** Example 2: Optimal HEXs using Simultaneous Global HEN-HEX approach.

| | Heat exchanger | | | | | | |
|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | C | H |
| Q (kW) | 2893 | 1680 | 4666 | 1313 | 9187 | 3890 | 6812 |
| *A* (m$^2$) | 133.2 | 75.35 | 475.9 | 59.8 | 1895.4 | 296.3 | 288.0 |
| *dte* (m) | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.0254 |
| *L* (m) | 6.0976 | 3.0488 | 6.0976 | 3.6585 | 6.0976 | 6.0976 | 6.0976 |
| *Nb* | 18 | 14 | 20 | 20 | 20 | 16 | 16 |
| *Ntp* | 6 | 6 | 6 | 6 | 6 | 4 | 6 |
| *rp* | 1.33 | 1.25 | 1.25 | 1.25 | 1.25 | 1.25 | 1.5 |
| *Ds* (m) | 0.5906 | 0.5906 | 0.9906 | 0.489 | 1.3716 | 0.7874 | 1.143 |
| *lay* | Square | Square | Square | Square | Square | Square | Triangular |
| *Ntt* | 365 | 413 | 1304 | 273 | 2597 | 812 | 592 |
| Tube-side | Hot stream | Hot stream | Hot stream | Hot stream | Cold Stream | Cold stream | Cold stream |
| *ht* (W/(m$^2$·K)) | 2033 | 4496.5 | 994.4 | 1331.3 | 891.4 | 11031.0 | 1894.5 |
| *hs* (W/(m$^2$·K)) | 578 | 927.1 | 559.7 | 814.7 | 769.1 | 1178.1 | 11530.0 |
| *U* (W/(m$^2$·K)) | 303.5 | 431.7 | 229.1 | 285.9 | 248.8 | 562.0 | 658.6 |
| *Nshell* | 1 | 1 | 1 | 1 | 2 | 1 | 1 |
| *F* | 0.91 | 0.97 | 0.84 | 0.98 | 0.79 | 0.82 | 1 |

Abbreviations: HEN, heat exchanger network; HEX, heat exchangers.

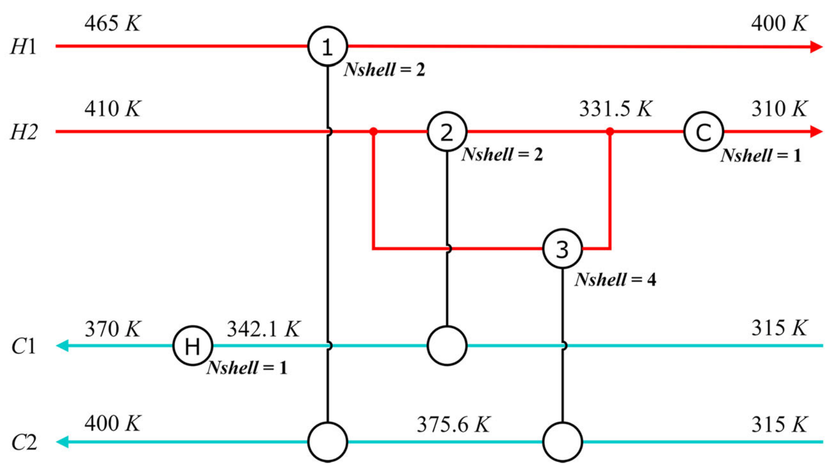


**FIGURE 3** Example 1: Optimal HEN using the traditional HEN-HEX approach.

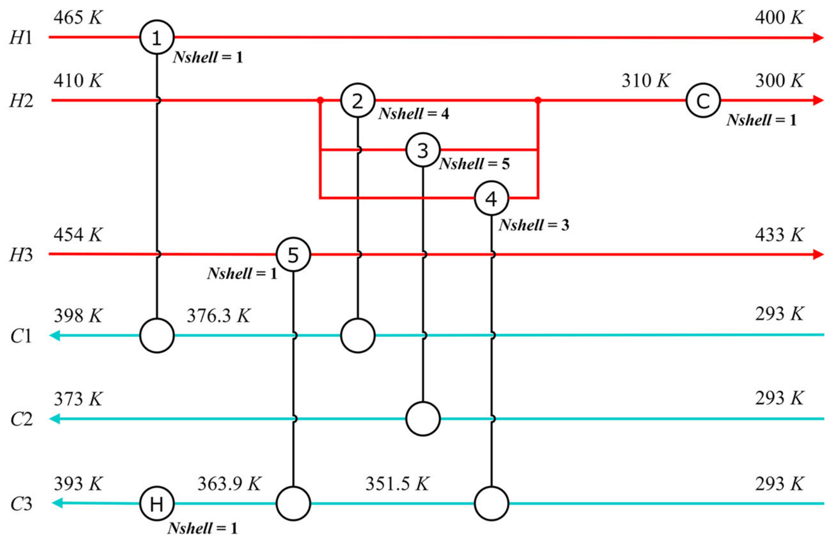


**FIGURE 4** Example 2: Optimal HEN using the traditional HEN-HEX approach.

per shell is 1000 $m^2$. Smith[47] mentions that fixed tubesheet HEXs can have an area per shell up to 4500 $m^2$, but we preferred to explore a more conservative value. The data for Examples 1 and 2 are depicted in Tables 2 and 3, respectively. The physical properties of the process streams are based on typical values of organic streams, hot utility is saturated steam at 2.94 bar, and cold utility is cooling water. Both examples were solved using a computer with a processor i7-8565U 1.8 GHz with 8 GB RAM. The codes were implemented in Python.

## 5.1 | Simultaneous global HEN-HEX approach

The solution of Examples 1 and 2 used the Synheat superstructure with two and three stages, respectively.[15] The identification of the HEN structures used a model coded in Pyomo.[61]

The HEN obtained using our method for Examples 1 and 2 are displayed in Figures 1 and 2, also with the indication of the number of shells of each HEX. The corresponding design of each HEX is given in Tables 4 and 5 (*ht* and *hs* are the film heat transfer coefficients of the tube-side and shell-side streams).

## 5.2 | Traditional approach

This technique corresponds to the solution of the HEN synthesis using fixed film heat transfer coefficients, followed by the final design of each HEX identified in the synthesis step. This procedure in two steps is the current way how the energy integration procedures are applied in practice in a project of a new plant: first, a process flowsheet diagram is created, and then the different equipment is designed, yielding a set of equipment datasheets.

During the synthesis step, all HEXs are assumed countercurrent. If a given HEX in the synthesis presents an area higher than 1000 $m^2$, the evaluation of the capital cost considers the division of the total heat transfer area in a set of identical shells with individual areas lower than 1000 $m^2$.

The HEN synthesis method used is the same as the one presented by Chang et al.,[42] except for the fact that we introduce the consideration of multiple shells in series as explained above. We emphasize that the HEX design procedure used here is the same as the one used in our procedure, thus any difference in the solution is a consequence of the consideration of constant film heat transfer coefficients in this step. To provide a realistic estimation of the film heat transfer coefficients, these data were collected from Bell,[62] a work that presents ranges of film heat transfer coefficients for several classes of streams. The values depicted in Table 6 correspond to the average of the interval.

The HEN obtained in Examples 1 and 2 are displayed in Figures 3 and 4, respectively. The corresponding HEX details for the final design are given in Tables 7 and 8.

## 5.3 | Iterative procedure

This technique is based on the approach proposed by Ravagnani and Caballero[18] to address the HEN synthesis together with the HEX design and it is a typical example of the decomposition approaches usually used to solve this problem in the literature. Instead of solving both problems in a single structure, this technique involves the solution of the HEN synthesis with fixed film

**TABLE 7** Example 1: Optimal HEXs using the traditional HEN-HEX approach.

| | Heat exchanger | | | | |
|---|---|---|---|---|---|
| | 1 | 2 | 3 | C | H |
| Q (kW) | 5206 | 3423 | 12,949 | 4480 | 3523 |
| *A* ($m^2$) | 362.0 | 459.9 | 2585.1 | 155.1 | 115.3 |
| *dte* (m) | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.03175 |
| *L* (m) | 6.0976 | 4.8768 | 6.0976 | 6.0976 | 4.8768 |
| *Nb* | 10 | 18 | 14 | 14 | 10 |
| *Ntp* | 6 | 6 | 6 | 1 | 5 |
| *rp* | 1.25 | 1.25 | 1.25 | 1.25 | 1.25 |
| *Ds* (m) | 0.6858 | 0.7874 | 1.143 | 0.5906 | 0.7874 |
| *lay* | Triangular | Square | Square | Triangular | Triangular |
| *Ntt* | 496 | 788 | 1771 | 425 | 237 |
| Tube-side | Hot stream | Cold stream | Hot stream | Cold stream | Cold stream |
| *ht* (W/($m^2$·K)) | 2628.3 | 1398.6 | 892.0 | 1688.9 | 1390.6 |
| *hs* (W/($m^2$·K)) | 943.9 | 557.8 | 792.2 | 6357.2 | 10879.1 |
| *U* (W/($m^2$·K)) | 401.86 | 248.8 | 251.23 | 613.4 | 588.3 |
| *Nshell* | 2 | 2 | 4 | 1 | 1 |
| *F* | 0.96 | 0.92 | 0.91 | 1 | 1 |

**TABLE 8** Example 2: Optimal HEX using the traditional HEN-HEX approach.

| | Heat exchanger | | | | | | |
|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | C | H |
| Q (kW) | 2893 | 3452 | 4206 | 9665 | 1680 | 1732 | 4655 |
| *A* ($m^2$) | 138.3 | 482.1 | 1045.5 | 1261.2 | 40.6 | 559.8 | 215.6 |
| *dte* (m) | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.0254 | 0.01905 | 0.0254 |
| *L* (m) | 4.8768 | 4.8768 | 6.0976 | 6.0976 | 3.6585 | 6.0976 | 4.8768 |
| *Nb* | 20 | 18 | 14 | 18 | 8 | 20 | 12 |
| *Ntp* | 6 | 6 | 6 | 6 | 4 | 6 | 6 |
| *rp* | 1.25 | 1.25 | 1.25 | 1.33 | 1.33 | 1.25 | 1.33 |
| *Ds* (m) | 0.489 | 0.5906 | 0.6858 | 0.9906 | 0.489 | 1.143 | 0.9906 |
| *lay* | Triangular | Square | Square | Square | Square | Triangular | Triangular |
| *Ntt* | 237 | 413 | 573 | 1152 | 139 | 1534 | 554 |
| Tube-side | Hot stream | Cold stream | Hot stream | Cold stream | Hot stream | Hot stream | Cold stream |
| *ht* (W/($m^2$·K)) | 3016.0 | 1277.6 | 695.6 | 1961.8 | 4379.0 | 1083.1 | 2014.0 |
| *hs* (W/($m^2$·K)) | 1001.1 | 606.8 | 501.7 | 693.3 | 1695.2 | 3562.7 | 11973.6 |
| *U* (W/($m^2$·K)) | 422.1 | 252.7 | 196.3 | 292.3 | 554.4 | 428.4 | 676.1 |
| *Nshell* | 1 | 4 | 5 | 3 | 1 | 1 | 1 |
| *F* | 0.96 | 0.95 | 0.91 | 0.885 | 0.99 | 0.80 | 1 |

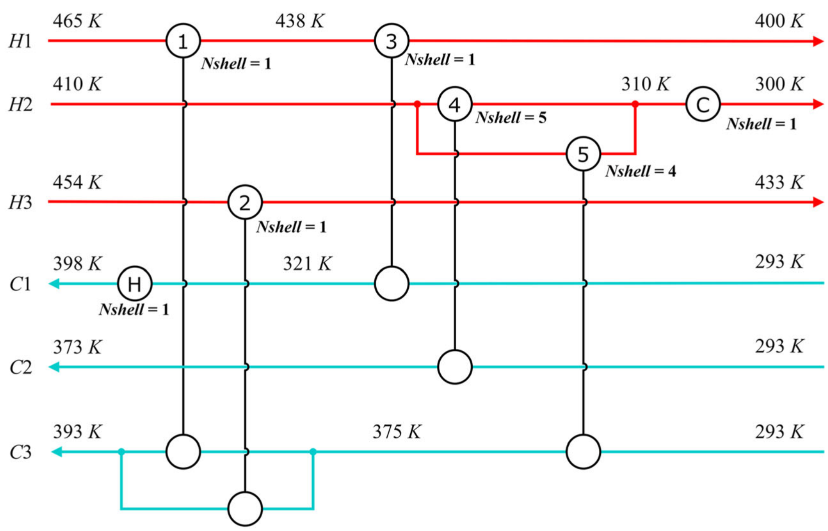


**FIGURE 5** Example 2: Optimal HEN using the iterative HEN-HEX approach.

**TABLE 9** Example 2: Optimal HEXs using the iterative HEN-HEX approach.

| | Heat exchanger | | | | | | |
|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | C | H |
| Q (kW) | 1202 | 1680 | 1691 | 4206 | 13,118 | 1732 | 4654 |
| *A* ($m^2$) | 42.3 | 60.4 | 39.8 | 1045.5 | 2558.8 | 559.8 | 572.3 |
| *dte* (m) | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.01905 | 0.01905 |
| *L* (m) | 4.8768 | 3.0488 | 2.439 | 6.0976 | 6.0976 | 6.0976 | 4.8768 |
| *Nb* | 12 | 16 | 14 | 14 | 18 | 20 | 12 |
| *Ntp* | 4 | 4 | 6 | 6 | 6 | 6 | 6 |
| *rp* | 1.25 | 1.33 | 1.25 | 1.25 | 1.25 | 1.25 | 1.5 |
| *Ds* (m) | 0.3874 | 0.5906 | 0.489 | 0.6858 | 1.2192 | 1.143 | 0.6858 |
| *lay* | Triangular | Triangular | Square | Square | Triangular | Triangular | Triangular |
| *Ntt* | 145 | 331 | 273 | 573 | 1753 | 1534 | 345 |
| Tube-side | Hot stream | Hot stream | Hot stream | Hot stream | Cold stream | Hot stream | Cold stream |
| *ht* ($W/(m^2 \cdot K)$) | 3261.5 | 3807.5 | 2651.2 | 695.6 | 1316.4 | 1083.1 | 1526.2 |
| *hs* ($W/(m^2 \cdot K)$) | 1388.5 | 1637.7 | 1119.5 | 501.7 | 712.6 | 3562.7 | 10777.5 |
| *U* ($W/(m^2 \cdot K)$) | 485.4 | 527.1 | 431.3 | 196.3 | 271.4 | 428.4 | 572.3 |
| *Nshell* | 1 | 1 | 1 | 5 | 4 | 1 | 1 |
| *F* | 0.98 | 0.98 | 0.98 | 0.91 | 0.84 | 0.80 | 1 |

Abbreviation: HEN, heat exchanger network.

**TABLE 10** Comparison of results.

| | Example 1 | | Example 2 | |
|---|---|---|---|---|
| Technique | TAC (US$/year) | Time (s) | TAC (US$/year) | Time (s) |
| One-step global HEN_HEX | 1,156,402 | 451 | 1,311,792 | 18,977 |
| Traditional | 1,280,250 | 9.7 | 1,720,992 | 4946 |
| Iterative | 1,280,250 | 19.1 | 1,653,545 | 14,446 |

Abbreviations: HEN, heat exchanger network; HEX, heat exchangers; TAC, total annualized cost.

heat transfer coefficients followed by the design of the resultant HEXs. Updated film heat transfer coefficients of the streams are generated from the values obtained from the design of the HEXs. Then, the sequence of HEN synthesis followed by HEX design is repeated, until the same HEN, or a worse one is obtained.

Each iteration composed of the HEN synthesis and the HEX design uses equivalent procedures to the other techniques. Therefore, the differences in the results are only related to the limitations of the iterative procedure (which does not guarantee global optimality).

Example 1 is solved in two iterations (the solution obtained in the second iteration is worse than the first one). Thus, the solution using the iterative process is the same as the solution obtained using fixed film heat transfer coefficients. In turn, Example 2 is solved with three iterations (the second iteration is better than the first one, but the third iteration is worse than the second). The obtained HEN is illustrated in Figure 5 and HEX details are given in Table 9.

## 6 | COMPARISON OF RESULTS

Table 10 presents the optimal TAC and the computational time of each technique. Not surprisingly, the proposed approach attains the best solution for both examples, which illustrates the fact that our approach provides the global optimum and the other approaches do not. The traditional approach using fixed film heat transfer coefficients obtained the worst results. The iterative approach proposed by Ravagnani and Caballero[18] obtained the same result of the technique with fixed film heat transfer coefficients in Example 1 and a result with an intermediate value of the objective function in Example 2.

The proposed approach attained an optimal TAC in Example 1 that is almost 10% lower than the TAC obtained using the other techniques. The reductions attained using the proposed approach are even higher in Example 2, larger than 20%. These reductions clearly illustrate the importance of the solution of the HEN synthesis and HEX design problem using a global optimization approach.

## 7 | CONCLUSIONS

This article presents a methodology that addresses the HEN synthesis and HEX design problems together. The HEN synthesis is based on an extension of the enumerative approach proposed by Chang et al.,[42] with the Direct method for the determination of the optimal energy consumption, and the HEX design carried out with Set Trimming followed by sorting. Therefore, despite the strong nonlinearities present in the film heat transfer coefficient models, we included them without convergence problems and with global optimality guaranteed, as well as including multiple shells in series and fluid allocation.

The proposed approach attained the best results in two HEN examples when compared with two other solution techniques. These results show the importance of addressing the HEN synthesis and the HEX design together, departing from the traditional HEN synthesis problem based on fixed film heat transfer coefficients or attempts to integrate both steps using decomposition schemes.

### NOMENCLATURE

| | |
|---|---|
| $\widehat{Aexc}$ | excess area (%) |
| $A_{i,j}$ | heat exchanger area between a hot stream $i$ and cold stream $j$ ($m^2$) |
| $A_{SS}$ | area of a single shell ($m^2$) |
| $\widehat{A}_{SS}^{max}$ | upper bound of a single shell ($m^2$) |
| $Areq$ | required area ($m^2$) |
| $Cp$ | stream specific heat capacity (J/(kg·K)) |
| $Ds$ | shell diameter (m) |
| $dte$ | outer tube diameter (m) |
| $dti$ | inner tube diameter (m) |
| $E_{hu}$ | hot utility energy consumption (kW) |
| $E_{hu}^{MAX}$ | maximum energy consumption defined by the user (kW) |
| $F$ | correction factor |
| $h_i$ | film heat transfer coefficient of a hot stream $i$ (W/($m^2$·K)) |
| $h_j$ | film heat transfer coefficient of a cold stream $j$ (W/$m^2$·K) |
| $\widehat{k}$ | stream thermal conductivity (W/(m·K)) |
| $L$ | tube length (m) |
| $lay$ | tube layout |
| $lbc$ | baffle spacing (m) |
| $LMTD_{i,j}$ | logarithmic mean temperature difference between streams $i$ and $j$ (K) |
| $Nb$ | number of baffles |
| $Npt$ | number of tube passes |
| $Ntt$ | total number of tubes |
| $Nshell$ | number of shells |
| $\widehat{Nshell}^{Max}$ | maximum number of shells |
| $P$ | variable related to the heat exchanger effectiveness for evaluation of $F$ |
| $\widehat{P}_{max}$ | abcissa corresponding to the asymptotic value of $F$ |
| $Q_{i,j}$ | heat load between a hot stream $i$ and cold stream $j$ (kW) |
| $Res$ | shell side Reynolds number |
| $Ret$ | tube side Reynolds number |
| $\widehat{Rf}$ | fouling resistance ($m^2$·K/W) |
| $rp$ | tube pich ratio |
| $TAC$ | total annualized cost (US$/year) |
| $\widehat{U}_{i,j}$ | overall heat transfer coefficient between hot and cold streams $i$ and $j$ (W/($m^2$·K)) |
| $vs$ | Shell side velocity (m/s) |
| $\widehat{vsmax}$ | Upper bound of shell side velocity (m/s) |
| $\widehat{vsmin}$ | Lower bound of shell side velocity (m/s) |
| $vt$ | Tube side velocity (m/s) |
| $\widehat{vtmax}$ | Upper bound of tube side velocity (m/s) |
| $\widehat{vtmin}$ | lower bound of tube side velocity (m/s) |
| $\widehat{X}_P$ | safety factor imposed in parameter $P$ |
| $\widehat{\rho}$ | stream density (kg/$m^3$) |
| $\widehat{\mu}$ | stream viscosity (Pa·s) |
| $\widehat{\varepsilon}$ | minimum heat load for an exchanger (kW) |

### AUTHOR CONTRIBUTIONS

**Diego G. Oliva:** Conceptualization (supporting); investigation (supporting); software (supporting); writing – review and editing (supporting). **Andre L. M. Nahes:** Conceptualization (supporting); methodology (equal); software (lead); writing – review and editing (supporting). **Julia C. Lemos:** Conceptualization (equal); methodology (equal); writing – original draft (equal). **André L. H. Costa:** Conceptualization (lead); methodology (equal); project administration (equal); software (supporting); supervision (lead); writing – review and editing (lead). **Miguel**

**J. Bagajewicz:** Conceptualization (lead); methodology (lead); project administration (lead); software (supporting); supervision (lead); writing – original draft (equal); writing – review and editing (lead).

## DATA AVAILABILITY STATEMENT

Our Supplementary material S1 includes instructions to any knowledgeable reader to build the procedure described above in the computational platform and language of choice to reproduce our results. All data needed to run the global optimization procedure are presented in the body of the article.

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## SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.


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