

# 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 to the simultaneous synthesis of the network and the basic design of Heat Exchangers. Our procedure guarantees global optimality, unlike previous approaches, such as Pinch Technology, metaheuristics, or mathematical programming that do not guarantee it and sometimes do not even guarantee local optimality. The procedure is not iterative, and does not present any convergence issues. To enumerate HEN structures, we use linear methods and for the HEX design we use Set Trimming followed by sorting. 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 two solution alternatives from the literature in two different problems indicates that considerable cost reductions may be obtained.

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## ***ABSTRACT***

In this article, we extend a previously developed globally optimal enumeration methodology for the synthesis of Heat Exchanger Networks (HEN) to the simultaneous synthesis of the network and the basic design of Heat Exchangers (HEX). Without loss of generality, we focus on shell-and-tube heat exchangers. Our procedure guarantees global optimality, unlike previous approaches, such as Pinch Technology, metaheuristics, or mathematical programming that do not guarantee it and sometimes they do not even guarantee local

optimality. The procedure is not iterative, and does not present any convergence issues. To enumerate HEN structures, we use linear methods and for the HEX design, we use Set Trimming followed by sorting. In addition, because some network structures are incompatible with single shell exchangers, without loss of generality, we use multiple shell exchangers in series. The comparison of the results of the proposed approach with two solution alternatives from the literature in two different problems indicates that considerable cost reductions may be obtained.

## **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 Technology and others), which exhibited several limitations, among which the lack of local (much less global) optimality was one. Later, mathematical programming as well as metaheuristics were also introduced (Furman and Sahinidis, 2002).

There is abundant literature on HEN synthesis: more than 4,000 papers and counting (Li et al, 2022a). Except for a relatively small number of papers, all research relied on a-priori selected fixed convective heat transfer coefficient for each of the streams. Such fixed value was 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 by 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 (1991), 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 heat transfer coefficients, different alternatives were developed for solving the HEN synthesis and the associated HEX design problems. In addition, most literature considers shell-and-tube heat exchangers, the exception being Wang et al. (2022) who considered detailed plate heat exchanger design. The review paper by Li et al. (2022a) discusses this issue and concludes that “HENS design is essentially an MINLP without the guaranteed optimal solution. Optimisation with the detailed thermal-hydraulic performance has introduced more discontinuous and nonlinear terms, making the HEN model more difficult to solve.” They continue recognizing that initialization is hard to come by and that although “heuristic” methods are successful in obtaining nothing more than local solutions. They also point out that the state of the art is the use of sequential methods of designing the network first and then designing the exchangers, with some feedback loops.

In response to the pessimistic view of Li et al. (2022a) 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 (MINLON) 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.

Previous papers that addressed the simultaneous HEN-HEX design optimization can be organized into three different approaches, according to the employed HEN synthesis technique: Pinch Technology, metaheuristic methods, and mathematical programming.

Polley et al. (1990) extended Pinch Technology to consider pressure drop in the retrofit of HEN, by using a relationship between pressure drop and heat transfer coefficients that they developed. The concept was extended to HEN grassroots design by Polley and Shahi (1991), where they fix the pressure drops and obtain the heat transfer coefficients or viceversa in the

targeting step of Pinch Technology. Liporace et al. (1999) employed Pinch Technology to identify the structure of the HEN, followed by the basic design of each exchanger using the procedure proposed by Jegede and Polley (1992). Based on the results, they showed that it is possible to exclude matches using ad-hoc criteria and re-design the network. Ravagnani et al. (2003) used Pinch Technology to obtain a HEN associated with maximum energy recovery; then they followed with a loop-breaking procedure. Once a network is obtained, the basic design of each heat exchanger is performed considering the Bell-Delaware method and TEMA standards. Garcia et al. (2006) proposed a hybrid method for the synthesis of heat exchanger networks and detailed exchanger design. The method combines pinch design with mathematical programming and a Bell-Delaware-based algorithm to design the heat exchangers. They use decomposition and a recursive algorithm. Ravagnani et al. (2003) also used pinch technology for the HEN synthesis, with a special loop-breaking procedure and the detailed design of the heat exchangers using the Bell-Delaware model. Akbari et al. (2008) 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 approach ( $\Delta T_{\min}$ ). Zunlong et al. (2008) proposed the utilization of Pinch Technology and exergoeconomic analysis for the determination of the optimal minimum temperature difference, followed by the synthesis using Pinch Technology and the design of the different heat exchangers considering the pressure drop distribution among the heat exchangers of a same stream. Allen et al. (2009) employed Pinch Technology for the HEN synthesis and a Genetic Algorithm (GA) for the design of the heat exchangers. The procedure is repeated for different values of the minimum temperature difference and the lowest cost solution is then selected. Serna-González and Ponce-Ortega (2011) 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 (NLP) problem for a given minimum temperature difference with the Bell-Delaware model in the heat exchanger design

to determine the heat transfer coefficients and pressure drops related to the heat exchangers geometry. Sun et al. (2015) adapted the pinch technology targeting to consider multipass exchangers. The approaches based on Pinch Technology do not employ 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 the stochastic 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 heat exchangers. Different metaheuristics methods were explored, all of them relying on the stages model (Yee and Grossmann, 1990) for the representation of the HEN structure and the Bell-Delaware model for the design of shell-and-tube heat exchangers. Ponce-Ortega et al. (2007) used a GA for generating structures and another GA for the design of the heat exchangers. Silva et al. (2008) proposed the generation of the structures using PSO and the optimization of the heat exchangers using mathematical programming (Ravagnani and Caballero, 2007). Ravagnani and Silva used particle swarm for the retrofit of heat exchanger networks with detailed equipment design. Xiao et al. (2019) used a GA/SA with solution candidates that represent the network structure and design variables of the heat exchangers. In this case, an inner algorithm is solved to finish the HEX design for each solution candidate. Karimi et al. (2020) used particle swarm optimization and considered different material choices concerning corrosion issues. Finally, Farzin et al. (2021) presented a hybrid genetic-particle swarm method. These metaheuristics 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 for end industrial applications. 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, due to its nature, these methods cannot guarantee global optimality. Therefore, we conclude that 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 sought after.

In the case of the use of mathematical programming, even if one uses the recently developed linear models for heat exchanger design (Gonçalves et al., 2017a, 2017b, 2019) 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 LMTD as well as the correction factor ( $F$ ) equations, introduce severe nonlinearities. In addition, if one is presented with the prospect of variable physical properties, one can anticipate a problem of larger size and a larger number of complex nonlinearities. 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). Frausto-Hernández et al. (2003) solved the HEN synthesis with HEX design through a MINLP procedure using the Yee and Grossmann (1990) superstructure and the heat exchanger design based on a model proposed by Serna (1999) and an approximation for the pressure drop in each stage developed by Shenoy (1995). The main assumption to build the MINLP is that maximum allowable pressure drops are used. The MINLP is solved without the utilization of decomposition schemes, but the authors mentioned convergence problems and local optimality issues. Mizutani et al. (2003b) proposed using a logic-based outer approximation method to solve the HEN synthesis with a detailed heat exchanger design. It couples the heat exchanger design model presented by Mizutani et al. (2003a) with the Yee and Grossmann (1990) superstructure model for HEN synthesis. Ravagnani and Caballero (2007) solved the

HEN synthesis and the HEX design problems using two MINLP formulations, according to a decomposition scheme. The algorithm is iterative between the two models and considers an initial film coefficient to find the first HEN and then it calculates the actual film coefficients using the design optimization procedure for each exchanger of the HEN; the new 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 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. Odejebi et al. (2015) proposed adding a choice of intensification for the heat transfer coefficients, but no detailed design of the exchangers was included. Short et al. (2016a) used the stage-wise superstructure to generate an initial HEN to later design the heat exchangers from which correction factors related to pressure drop and area are calculated and included in the objective function of the HEN superstructure model. The iterative procedure goes on until convergence is obtained. These correction factors have the goal of approximating the areas obtained by the MINLP model 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. (2016b). Souza et al. (2016) 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 heat transfer coefficient are used. Kazi et al. (2020b) proposed a procedure based on a multistep approach. The structure of the network is determined using a MINLP based on the stage-wise superstructure of Yee and Grossmann (1990), including a smoothed LMTD approximation. The second step is a NLP problem associated with nonisothermal mixing, with and without by-passes. Finally, the individual heat exchangers are designed by solving a NLP using a discretized model based on a small number of geometrical options (Kazi et al., 2020a). The

authors did not claim or present any indication that the model gives global optimal results. A variant of the previous paper using a trust region framework was proposed by Kazi et al. (2021), where the decomposition of the problem is still used. Cotrim et al. (2021) proposed a bi-level approach that is an improvement of Ravagnani and Caballero (2007), with a new capital cost parameter that is iteratively updated based on the heat exchanger design solutions. Li et al. (2022b) proposed a MINLP formulation based on the stage-wise superstructure of Yee and Grossmann (1990) together with shell-and-tube heat exchanger design equations, including the alternative of helical baffles. Some simplifications in the heat exchanger model allow the solution of the problem in a single step. They used DICOPT, which does not guarantee global optimality and the authors do not report what initialization was used.

Departing from pinch technology, metaheuristics, and mathematical programming Wang et al. (2022) used an algorithmic approach: the advanced Grid Diagram and considered plate exchangers. The grid technique, some MILP models, and several metaheuristics approaches were incorporated into SPIL, a software package (Chin et al., 2022).

A feature of most of the above-mentioned papers is that multiple shells are rarely considered. As we shall show in this article, some problems require considering multiple shell arrangements due to temperature cross when more than one pass is considered.

The present paper proposes a new approach focusing on the network enumeration procedure proposed by Chang et al. (2020a, 2020b, 2021), which is used together with the Set Trimming approach used by Lemos et al. (2020) for the design of the heat exchangers. 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 associated with the HEX design and present the HEN synthesis methodology used by Chang et al. (2020a, 2020b, 2021), discussing where we introduce our changes to extend this

approach to include the heat exchanger design task in a single problem. Then, we discuss briefly the heat exchanger design models and methods. We finish presenting the results and the conclusions.

## **SIMULTANEOUS HEN SYNTHESIS AND HEAT EXCHANGER DESIGN**

The traditional method of HEN synthesis has been presented as one where the 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 heat exchanger 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 heat transfer coefficient is a parameter as follows:

$$\hat{U}_{i,j} = \frac{1}{\frac{1}{\hat{h}_i} + \frac{1}{\hat{h}_j}} \quad (2)$$

where the heat transfer coefficients  $\hat{h}_i$  and  $\hat{h}_j$  presumably include the fouling resistances of the streams and the thermal conductive resistance of the wall is dismissed. Usually, these models do not discuss fluid allocation or exchanger type. Also absent in the expression is the correction factor, as all exchangers are assumed to be one unit with a perfect countercurrent flow. Finally, there is no mention of the need for multiple shells.

Equation (1) with all its shortcomings is used under the implicit assumption that the optimal network, whatever optimal means for each choice of model (superstructures, isothermal mixing or not, etc.) is made, will have the same performance after the exchangers are designed. In other words, a decomposition method is used: first, the HEN structure and the 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 because 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 both sides. These difficulties suggest performing the synthesis simultaneously with the basic design of the heat exchangers, which guarantees a better assessment of the investment cost, especially when multiple shells are considered, and non-viable exchangers are weeded out by the optimization.

The method we present in this article achieves the goal of global optimality. The method is an extension of the one proposed by Chang et al. (2020a), which is based on fixed heat transfer coefficients that guarantee global optimality (provided that the unimodal conjecture is true). In our method, we replace the calculation of area using fixed heat transfer coefficients with a heat exchanger design and we consider the option of multiple shells in series. The assumption of unimodality is still used and because all structures are enumerated, topology traps are absent.

The main idea behind the method is that the total annualized cost (TAC) of a given network changes with the energy consumption and this relation gives us a convex function where the minimum value of the TAC is easily obtained by using a traditional search algorithm, like the Golden Ratio Search. All the demonstration of the TAC behavior is displayed in the original paper (Chang et al., 2020a).

The algorithm proposed by Chang et al. (2020a) was modified to include the heat exchanger design. The original algorithm's main steps are shown next without further explanation.

- Step 0: Initialization – Set the incumbent  $UBTAC$ , the best upper bound so far, to infinity. Set the initial minimum number of units ( $N$ ).

- Step 1: Obtain the first viable minimal structure (*MSTR*). This step solves a model based on the Yee and Grossmann (1990) model with the number of units equal to  $N$ , being linear, and using a dummy objective function.
- Step 2: If Step 1 is feasible, then go to Step 3, otherwise go to Step 8.
- Step 3: For the chosen *MSTR* obtain the minimum energy consumption ( $E_{min}$ ).
- Step 4: For the chosen *MSTR* obtain the maximum energy consumption ( $E_{max}$ ).
- Step 5: Check if the function is monotone, if yes, then the minimum is at  $E_{min}$  or  $E_{max}$ , determine the minimum, calculate TAC using the conventional HEX design model (Equations 1 and 2), and go to Step 7. Otherwise, go to Step 6.
- Step 6: Apply Golden Ratio Search to find the minimum TAC for the current structure (the *MSTR* is solved for different fixed energy values according with the need of the search).
- Step 7: If  $TAC \leq UBTAC$ , then update  $UBTAC$ .
- Step 8: Obtain another *MSTR* with the same number of units, if it is infeasible make (number of units), if it continues to be infeasible go to Step 9. Otherwise, go to Step 3.
- Step 9:  $UBTAC$  is the global optimum.

Every time a TAC must be calculated, the design problem is solved by using an extension of the approach proposed by Lemos et al. (2020), which is globally optimal, so its use in the algorithm presented by Chang et al. (2020a) also guarantees the global optimum for the HEN + HEX synthesis and design optimization problem. Thus, to our knowledge, our proposed method is the first one to guarantee global optimality for this problem.

This direct connection between the HEN synthesis algorithm and HEX design method in a computationally effective way explores the following aspects of each approach:

- 1) The enumeration approach for the HEN synthesis problem is flexible, the design of the heat exchangers is only run for evaluation of the TAC, instead of being part of a complex superstructure problem; and

- 2) The HEX design method is fast, so it can be run many times during the search without implying a large computational burden.

For the sake of simplification and without loss of generality, all heat exchangers are of the shell-and-tube type and we take into account utility heat exchangers (coolers and heaters) without phase change streams, e.g. cooling water and thermal oil as cold and hot utilities, respectively. However, the flexibility of the procedure can also consider other types of heat exchangers, such as gasketed-plate heat exchangers (Nahes et al., 2021) or heat exchangers with phase change (Sales et al., 2021).

In addition, due to its combinatorial nature, 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:

$$E_{hu} \leq E_{hu}^{MAX} \quad (3)$$

where  $E_{hu}$  is the hot utility energy consumption and  $E_{hu}^{MAX}$  is the maximum energy consumption defined by the user. In our examples, the  $E_{hu}^{MAX}$  is equal to two times the minimum energy consumption calculated by the Pinch Technology.

## **HEAT EXCHANGER DESIGN OPTIMIZATION PROCEDURE**

For the design of the heat exchangers in the network as well as the heaters and coolers, we consider shell-and-tube heat exchangers with an E-type shell and single segmental baffles. The heat transfer coefficients of the streams that flow in the tube-side and shell-side are

evaluated using the Gnielinski correlation for turbulent flow and Bell-Delaware method, respectively. The complete equations for the heat exchanger models are available in the open literature (Taborek, 2008a,b).

The solution to the global optimal design problem of each heat exchanger of the network is obtained through an extension of the Set Trimming approach presented by Lemos et al. (2020) for the design of shell-and-tube heat exchangers.

Seven design variables represent the dimensions of a heat exchanger shell: number of tube passes ( $N_{pt}$ ), tube diameter (outer and inner:  $d_{te}$  and  $d_{ti}$ ), tube layout ( $lay$ ), tube pitch ratio ( $rp$ ), number of baffles ( $N_b$ ), shell diameter ( $D_s$ ), and tube length ( $L$ ). The fluid allocation (shell-side vs tube-side) and the number of shells in series are also heat exchanger design variables (that were not handled by Lemos et al. (2020)), 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 (Costa and Bagajewicz, 2019) is an algorithm employed 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 “ $\wedge$ ”. 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 employed for a smaller set of candidates.

Geometric trimming: These constraints correspond to design recommendations associated with the heat exchanger dimensions (Taborek, 2008):

$$3 D_s \leq L \leq 15 D_s \quad (4)$$

$$0.2 D_s \leq lbc \leq 1.0 D_s \quad (5)$$

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 (Smith, 2005):

$$A_{SS} \leq \hat{A}_{SS}^{max} \quad (6)$$

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

Correction factor trimming: The HEN synthesis algorithm can propose heat exchangers 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 detachment of the behavior of a given heat exchanger configuration from the countercurrent configuration:

$$\hat{Q} = UA \widehat{LMTD} F \quad (7)$$

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, i.e. it is not safe to design a heat exchanger to work in these zones (Serth, 2007; Cao, 2010). 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):

$$F \geq 0.75 \quad (8)$$

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 et al. (1988) proposed an alternative constraint based on the  $P$  parameter:

$$P \geq X_P P_{max} \quad (9)$$

where  $P_{max}$  is the abscissa corresponding to the asymptotic value of  $P$  and  $X_P$  is the safety factor imposed to avoid regions where the  $F$  slope is steep (e.g.  $X_P = 0.9$ ). This approach is also reported by Smith (2005). The flexibility of the Set Trimming also allows the utilization of this alternative.

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

$$\widehat{vtmin} \leq vt \leq \widehat{vtmax} \quad (10)$$

$$\widehat{vsmín} \leq vs \leq \widehat{vsmax} \quad (11)$$

where  $vt$  and  $vs$  are the tube-side and shell-side flow velocities, and  $\widehat{vtmin}$ ,  $\widehat{vtmax}$ ,  $\widehat{vsmín}$ , 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:

$$Ret \leq 5 \cdot 10^6 \quad (12)$$

$$Res \leq 1 \cdot 10^5 \quad (13)$$

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

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

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

where  $A$  is the area of the thermal surface,  $\widehat{Aexc}$  is the excess area, and  $Areq$  is the required area, obtained using Eq. (7), with the evaluation of the heat transfer coefficients associated with the corresponding values of the design variables.

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, etc. (Saunders, 1988; Kakaç and Liu, 2002; Smith, 2005; Raza, 2013). In the current paper, 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 employs the opposite choice. The second run includes a first trimming that eliminates solution candidates with objective functions higher than the incumbent.

As the nature of the design problem is discrete, since the geometric variables have commercial discrete values, the TAC is not a continuous variable anymore. However, this change does not impact the HEN+HEX problem solution, because one can still assume that the function of TAC vs. energy is quasi-convex allowing the golden search algorithm to identify the optimum.

## **SET TRIMMING FOR HEX DESIGN**

For a given fluid allocation and number of shells, the search space of a single shell and tube exchanger is composed of all possible combinations of the design variables already mentioned:  $N_{pt}$ ,  $dt$ ,  $lay$ ,  $rp$ ,  $Nb$ ,  $Ds$ , and  $L$ . This search space is valid for any heat exchanger design problem generated during the HEN synthesis. However, the geometric constraints in

Eqs. (4-8) do not depend on any specific data of a given HEX design problem. Therefore, the trimmings related to Eqs. (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 employed as a starting point for all heat exchanger 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 (Smith, 2005), 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 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  $N_{shell}^{MAX}$  and go to Step 3
3. Run the Set Trimming procedure considering the following set of design variables:  $\{N_{pt}, dt, lay, rp, Nb, Ds, L\}$  and the stream allocation, as discussed above. If a solution is achieved, go to Step 6, otherwise go to Step 4.
4. If  $N_{shell} < N_{shell}^{MAX}$ , make  $N_{shell} = N_{shell} + 1$  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  $N_{shell}$ .

If a HEN candidate contains a heat exchanger with no feasible solution, the corresponding objective function is increased with a large penalty value. The absence of a feasible solution for the heat exchanger design problem 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.

## 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:

Technique 1: Simultaneous HEN synthesis and HEX design (proposed approach)

Technique 2: HEN synthesis with fixed heat transfer coefficients, followed by the design of the resultant heat exchangers (traditional approach).

Technique 3: HEN synthesis and HEX design solved by adapting a typical decomposition approach available in the literature (Ravagnani and Caballero, 2007).

The design of the heat exchangers is based on the discrete values of the variables presented in Table 1. It is considered that the heat exchangers are fixed tubesheet AEL type with tube wall thickness of 1.65 mm (BWG 16), tube wall thermal conductivity equal to 50 W/(m·K), baffle cut 25% and maximum number of shells equal to 5. The minimum excess area is 10%. The tube count data is based on Kakaç and Liu (2002). The maximum heat exchanger area per shell is 1000 m<sup>2</sup> (Smith (2005) mentions that fixed tubesheet heat exchangers can be an area per shell up to 4500 m<sup>2</sup>, but we preferred to explore a more conservative value).

**Table 1.** Design variable data

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

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The data for the Example 1 are depicted in Table 2. In addition, the physical properties and the fouling factor are depicted in Table 3. The physical properties of the process streams are based on typical values of organic streams, the hot utility is based on a kerosene stream and the cold utility on cooling water. Tables 4 and 5 show the equivalent information for the Example 2.

**Table 2.** Example 1 – Stream Data

Stream	$F C_p$ (kW/K)	$T_{in}$ (K)	$T_{out}$ (K)
H1	80.1	465	400
H2	208.53	410	310
C1	126.3	315	370
C2	213.6	315	400
Hot Utility	-	420	400
Cold Utility	-	290	300

**Table 3.** Example 1 – Physical properties and fouling factor of the streams

Stream	$\rho$ (kg/m <sup>3</sup> )	$C_p$ (J/(kg K))	$\mu$ (Pa·s)	$k$ (W/(m·K))
H1	815	2670	0.00086	0.10
H2	876	2317	0.0028	0.11
C1	877	2105	0.0042	0.13
C2	908	1780	0.0091	0.12
Hot utility	800	2000	0.00164	0.02
Cold utility	999	4180	0.001	0.6

**Table 4.** Example 2 – Stream Data

Stream	$F C_p$ (kW/K)	$T_{in}$ (K)	$T_{out}$ (K)
H1	44.5	465	400
H2	173.2	410	300
H3	80.0	454	433
C1	60.4	293	398
C2	52.6	293	373
C3	160	293	393
Hot utility	-	420	400

Cold utility	-	290	300
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**Table 5.** Example 2 – Physical properties and fouling factor of the streams

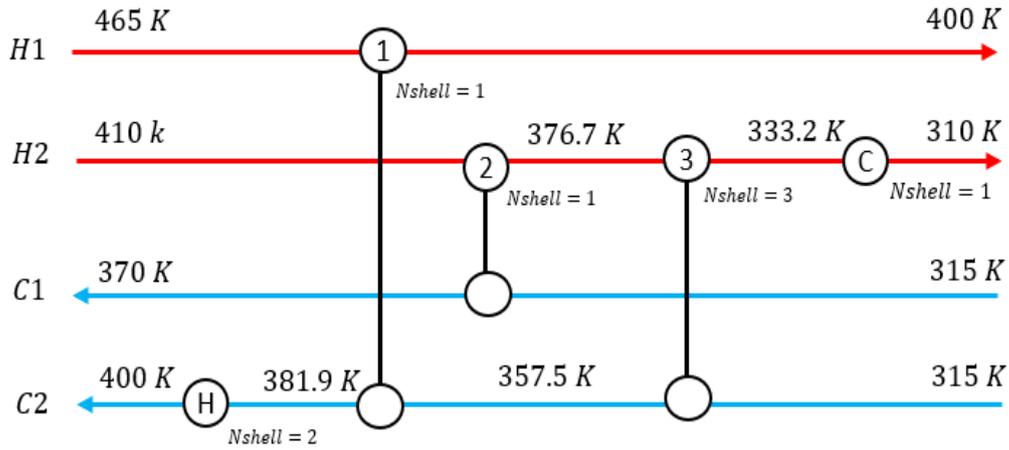
Stream	$\rho$ (kg/m <sup>3</sup> )	$C_p$ (J/(kg K))	$\mu$ (Pa·s)	$k$ (W/(m K))
H1	815	2670	0.00086	0.10
H2	876	2317	0.0028	0.11
H3	872	2433	0.00076	0.15
C1	877	2105	0.0042	0.13
C2	908	1780	0.0091	0.12
C3	860	2008	0.0022	0.14
Hot utility	800	2000	0.00164	0.02
Cold utility	999	4180	0.001	0.6

Both examples were solved using a computer with a processor i7-8565U 1.8GHz with 8 GB RAM memory. The codes were implemented in Python.

## TECHNIQUE 1

The solution of Examples 1 and 2 using the proposed approach employed the Synheat superstructure with 2 and 3 stages, respectively (Yee and Grossmann, 1990). The identification of the HEN structures employed a model coded using Pyomo (Bynum et al., 2021).

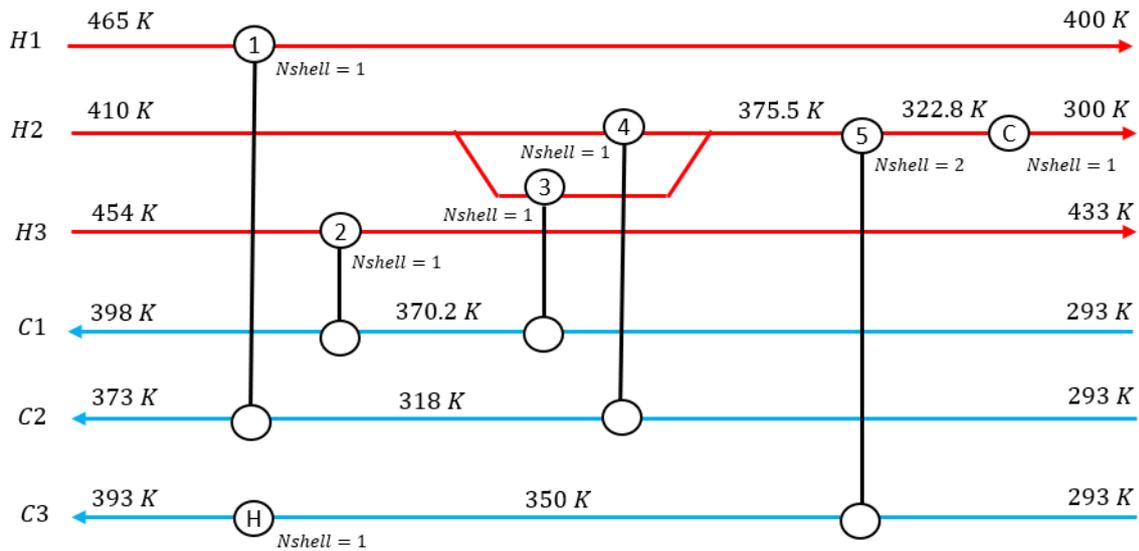
The HEN obtained using our method for Examples 1 and 2 are displayed in Figures 1 and 2, also with the indication of the number of shells of each heat exchanger. The corresponding design of each heat exchanger is shown in Tables 6 and 7 ( $ht$  and  $hs$  are the convective heat transfer coefficients of the tube-side and shell-side streams).



**Figure 1.** Example 1 – Technique 1 – Optimal HEN

**Table 6.** Example 1 – Technique 1 – Optimal heat exchangers

	Heat exchanger				
	1	2	3	C	H
$Q$ (kW)	5206	6946	9075	4831	3874
$A$ (m <sup>2</sup> )	287.2	738.6	2511.4	236.1	951.7
$dte$ (m)	0.01905	0.01905	0.01905	0.01905	0.01905
$L$ (m)	6.0976	6.0976	6.0976	4.8768	6.0976
$Nb$	18	12	18	16	10
$Ntp$	6	6	6	4	6
$rp$	1.33	1.25	1.33	1.33	1.25
$Ds$ (m)	0.889	1.2192	1.3716	0.889	0.9906
$lay$	Triangular	Square	Square	Triangular	Square
$Ntt$	787	2024	2294	809	1304
Tube-side	Hot stream	Hot stream	Hot stream	Cold stream	Hot stream
$ht$ (W/(m <sup>2</sup> K))	1722.7	988.2	870.2	13227.7	694.4
$hs$ (W/(m <sup>2</sup> K))	922.5	653.8	716.4	1292.2	804.4
$U$ (W/(m <sup>2</sup> K))	363.0	242.9	241.1	583.7	252.9
$Nshell$	1	1	3	1	2
$F$	0.92	0.86	0.89	0.93	0.96



**Figure 2.** Example 2 – Technique 1 – Optimal HEN

**Table 7.** Example 2 – Technique 1 – Optimal heat exchangers

	Heat exchanger						
	1	2	3	4	5	C	H
$Q$ (kW)	2893	1680	4666	1313	9120	3958	6880
$A$ (m <sup>2</sup> )	133.2	75.35	475.9	59.8	1895.4	296.3	947.7
$dte$ (m)	0.01905	0.01905	0.01905	0.01905	0.01905	0.01905	0.01905
$L$ (m)	6.0976	3.0488	6.0976	3.6585	6.0976	6.0976	6.0976
$Nb$	18	14	20	20	12	18	12
$Ntp$	6	6	6	6	6	4	6
$rp$	1.33	1.25	1.25	1.25	1.25	1.25	1.25
$Ds$ (m)	0.5906	0.5906	0.9906	0.489	1.3716	0.7874	1.3716
$lay$	Square	Square	Square	Square	Square	Square	Square
$Ntt$	365	413	1304	273	2597	812	2597
Tube-side	Hot stream	Hot stream	Hot stream	Hot stream	Cold Stream	Cold stream	Hot stream
$ht$ (W/(m <sup>2</sup> K))	2033	4496.5	994.4	1331.3	891.4	11031.0	623.9
$hs$ (W/(m <sup>2</sup> K))	578	927.1	559.7	814.7	698.7	1216.9	869.0
$U$ (W/(m <sup>2</sup> K))	303.5	431.7	229.1	285.9	241.0	562.0	246.4
$Nshell$	1	1	1	1	2	1	1
$F$	0.91	0.97	0.84	0.98	0.81	0.82	0.88

## TECHNIQUE 2

This technique corresponds to the solution of the HEN synthesis using fixed heat transfer coefficients, followed by the final design of each heat exchanger 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 (PFD) is created, and then the equipment are designed, yielding a set of equipment datasheets.

During the synthesis step, all heat exchangers are assumed countercurrent. If a given heat exchanger area in the synthesis presents an area higher than 1000 m<sup>2</sup>, 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<sup>2</sup>.

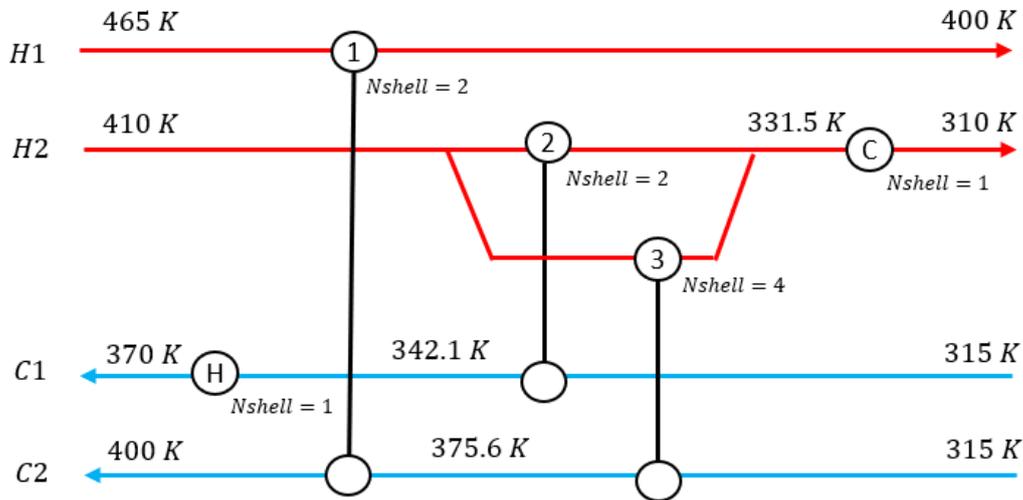
The HEN synthesis method used is the same as the one presented by Chang et al. (2020a), except for the fact that we introduce the consideration of multiple shells in series as explained above. We emphasize that the procedure guarantees global optimality, thus any difference in the solution is a consequence of the consideration of constant heat transfer coefficients and the absence of a more rigorous heat exchanger design in this step. The heat exchanger design is based on the same algorithm employed in the proposed approach already described above.

Aiming at providing realistic estimations of heat transfer coefficients, these data were collected from Taborek (2008), which presents ranges of heat transfer coefficients for several classes of streams. The values depicted in Table 8 correspond to the average of the interval.

**Table 8.** Heat transfer coefficient estimation

Stream	$h$ (W/(m <sup>2</sup> K))
H1	1125
H2	275
H3	1125
C1	500
C2	500
C3	500
HU	1125
CU	6250

The HEN obtained in Examples 1 and 2 using Technique 2 are displayed in Figures 3 and 4, respectively. The corresponding heat exchanger details obtained after the final design are shown in Tables 9 and 10.

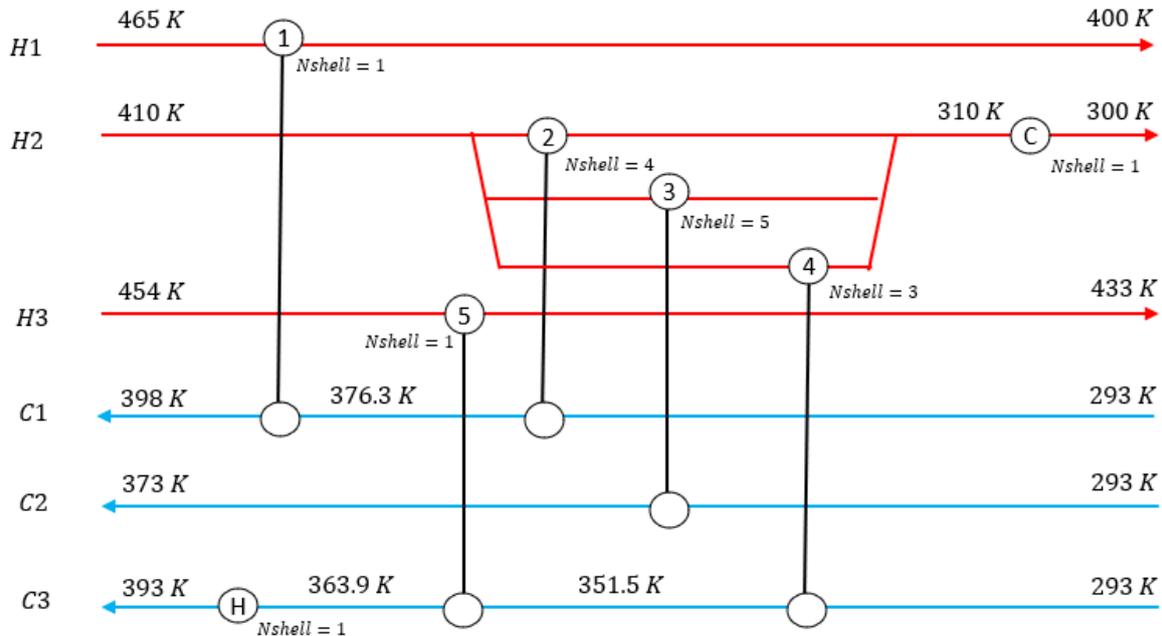


**Figure 3.** Example 1 – Technique 2 – Optimal HEN

**Table 9.** Example 1 – Technique 2 – Optimal heat exchangers

	Heat exchanger				
	1	2	3	C	H
$Q$ (kW)	5206	3423	12949	4480	3523
$A$ (m <sup>2</sup> )	362.0	459.9	2585.1	155.1	295.2
$dte$ (m)	0.01905	0.01905	0.01905	0.01905	0.01905
$L$ (m)	6.0976	4.8768	6.0976	6.0976	6.0976
$Nb$	10	18	14	14	20
$Ntp$	6	6	6	1	4
$rp$	1.25	1.25	1.25	1.25	1.33
$Ds$ (m)	0.6858	0.7874	1.143	0.5906	0.889

<i>lay</i>	Triangular	Square	Square	Triangular	Triangular
<i>Ntt</i>	496	788	1771	425	809
Tube-side	Hot stream	Cold stream	Hot stream	Cold stream	Hot stream
<i>ht</i> (W/(m <sup>2</sup> K))	2628.3	1398.6	892.0	1688.9	679.6
<i>hs</i> (W/(m <sup>2</sup> K))	943.9	557.8	792.2	6357.2	878.6
<i>U</i> (W/(m <sup>2</sup> K))	401.86	248.8	251.23	613.4	257.3
<i>Nshell</i>	2	2	4	1	1
<i>F</i>	0.96	0.92	0.91	1	0.97



**Figure 4.** Example 2 – Technique 2 – Optimal HEN

**Table 10.** Example 2 – Technique 2 – Optimal heat exchangers

	Heat exchanger						
	1	2	3	4	5	C	H
<i>Q</i> (kW)	2893	3452	4206	9665	1680	1732	4655
<i>A</i> (m <sup>2</sup> )	138.3	482.1	1045.5	1261.2	40.6	559.8	820.7
<i>dte</i> (m)	0.01905	0.01905	0.01905	0.01905	0.0254	0.01905	0.01905
<i>L</i> (m)	4.8768	4.8768	6.0976	6.0976	3.6585	6.0976	6.0976
<i>Nb</i>	20	18	14	18	8	20	20
<i>Ntp</i>	6	6	6	6	4	6	6
<i>rp</i>	1.25	1.25	1.25	1.33	1.33	1.25	1.25

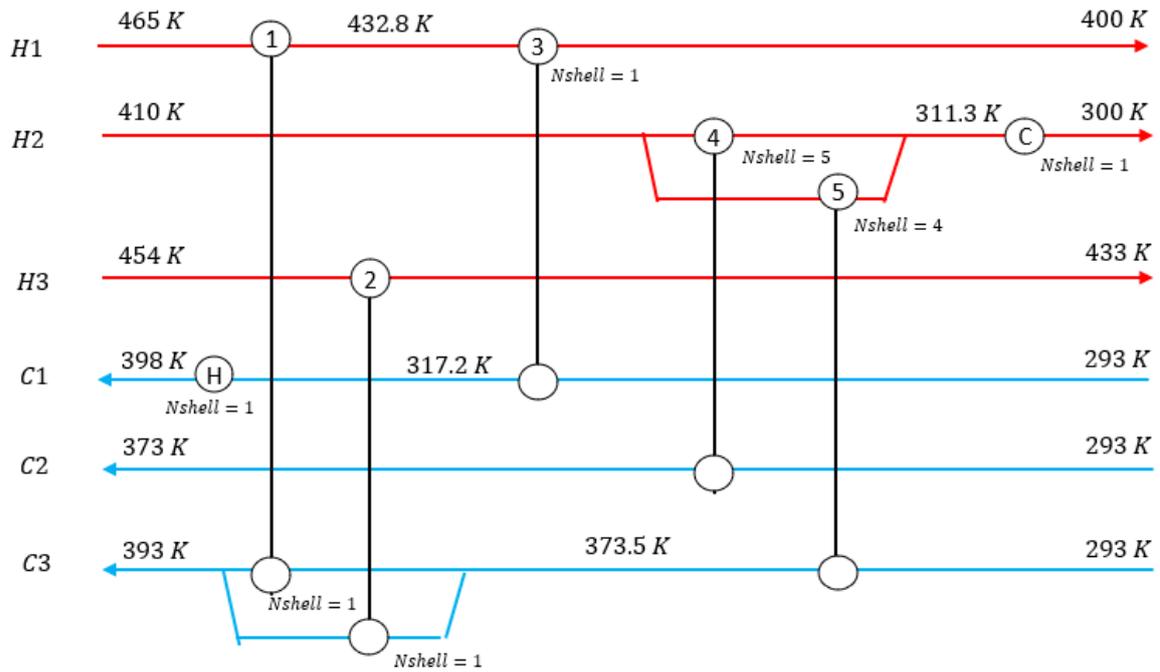
<i>Ds</i> (m)	0.489	0.5906	0.6858	0.9906	0.489	1.143	1.3716
<i>lay</i>	Triangular	Square	Square	Square	Square	Triangular	Triangular
<i>Ntt</i>	237	413	573	1152	139	1534	2249
Tube-side	Hot stream	Cold stream	Hot stream	Cold stream	Hot stream	Hot stream	Hot stream
<i>ht</i> (W/(m <sup>2</sup> K))	3016.0	1277.6	695.6	1961.8	4379.0	1083.1	494.7
<i>hs</i> (W/(m <sup>2</sup> K))	1001.1	606.8	501.7	693.3	1695.2	3562.7	995.8
<i>U</i> (W/(m <sup>2</sup> K))	422.1	252.7	196.3	292.3	554.4	428.4	226.3
<i>Nshell</i>	1	4	5	3	1	1	1
<i>F</i>	0.96	0.95	0.91	0.885	0.99	0.80	0.89

### TECHNIQUE 3

This technique is based on the approach proposed by Ravagnani and Caballero (2007) to address the HEN synthesis together with the HEX design and it is a typical example of the decomposition approaches usually employed 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 heat transfer coefficients followed by the design of the resultant heat exchangers. Updated heat transfer coefficients of the streams are generated from the values obtained in the design of the heat exchangers. Then, the sequence HEN synthesis followed by HEX design is repeated. The procedure stops if a worse solution or the same HEN is obtained.

Each iteration composed of the HEN synthesis and the HEX design employs the same procedures employed in the other techniques. Therefore, the differences in the results are only related to the limitations of the iterative process (that does not guarantee global optimality).

Example 1 is solved using Technique 3 in two iterations (the solution obtained in the second iteration is worse than the first one). Thus, the solution of Technique 3 is the same as Technique 2. 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 the heat exchanger details are shown in Table 11.



**Figure 5.** Example 2 – Technique 3 – Optimal HEN

**Table 11.** Example 2 – Technique 3 – Optimal heat exchangers

	Heat exchanger						
	1	2	3	4	5	C	H
$Q$ (kW)	1431	1680	1462	4206	12889	1961	4884
$A$ (m <sup>2</sup> )	51.9	60.4	31.7	923.3	2239.2	639.7	570.2
$dte$ (m)	0.01905	0.01905	0.01905	0.01905	0.01905	0.01905	0.01905
$L$ (m)	3.6585	3.0488	3.6585	6.0976	6.0976	6.0976	6.0976
$Nb$	12	16	16	18	18	18	18
$Ntp$	6	4	4	6	6	6	4
$rp$	1.25	1.33	1.25	1.33	1.25	1.25	1.25
$Ds$ (m)	0.489	0.5906	0.3874	0.6858	1.143	1.2192	0.889
$lay$	Triangular	Triangular	Triangular	Square	Triangular	Triangular	Square
$Ntt$	237	331	145	506	1534	1753	586
Tube-side	Hot stream	Hot stream	Hot stream	Hot stream	Cold stream	Hot stream	Hot stream
$ht$ (W/(m <sup>2</sup> K))	3016.0	3807.5	3261.5	804.4	1496.6	947.6	645.9
$hs$ (W/(m <sup>2</sup> K))	1535.6	1637.7	1231.5	520.6	734.4	3561.6	558.4
$U$ (W/(m <sup>2</sup> K))	494.8	527.1	464.7	208.9	283.13	400.9	221.2
$Nshell$	1	1	1	5	4	1	1
$F$	0.97	0.98	0.99	0.92	0.87	0.80	0.96

## COMPARISON

Tables 12 displays the optimal TAC and the computational time of each technique.

**Table 12.** Comparison of the solution results

Technique	Example 1	Example 2
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	TAC (US\$/yr)	Time (s)	TAC (US\$/yr)	Time (s)
1	1,278,612	116	1,224,448	5,269
2	1,303,053	6	1,675,231	2,641
3	1,303,053	19	1,592,619	8,553

The analysis of Table 12 indicates that the proposed approach (Technique 1) attains the best solution for both examples. The traditional approach (Technique 2) obtained the worst results. The approach proposed by Ravagnani and Caballero (2007) (Technique 3) obtained the same result of Technique 2 in Example 1 and a result with an intermediate value of the objective function in Example 2.

The difference between the proposed approach and the other techniques is small in the first example, with an objective function reduction lower than 2%. However, the difference in the second example is very pronounced, where our proposed approach has a solution with an optimal value of the objective function that is 37% smaller than Technique 2, and 30% smaller than Technique 3, which clearly illustrates the importance of the simultaneous HEN synthesis and HEX design using a global optimization approach.

## **DATA AVAILABILITY AND REPRODUCIBILITY STATEMENT**

Our supplemental material 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 described above are presented in the body of the article.

## **CONCLUSIONS**

This paper presented a methodology that addresses the HEN synthesis and HEX design problems simultaneously. The HEN synthesis is based on the enumerative approach proposed by Chang et al. (2020a), and the HEX design is carried out with Set Trimming followed by sorting. Therefore, despite the strong nonlinearities present in the 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 heat transfer coefficients or attempts to integrate both steps using decomposition schemes.

## NOMENCLATURE

$\widehat{A_{exc}}$	Excess area
$A_{i,j}$	Heat exchanger area between a hot stream $i$ and cold stream $j$
$A_{SS}$	Area of a single shell
$\hat{A}_{SS}^{max}$	Upper bound of a single shell
$A_{req}$	Required area
$C_p$	Stream heat capacity
$D_s$	Shell diameter
$d_{te}$	Outer tube diameter
$d_{ti}$	Inner tube diameter
$E_{hu}$	Hot utility energy consumption
$E_{hu}^{MAX}$	Maximum energy consumption defined by the user
$F$	Correction factor
$h_i$	Convective heat transfer coefficient of a hot stream $i$
$h_j$	Convective heat transfer coefficient of a cold stream $j$
$HEN$	Heat exchanger network
$HEX$	Heat exchanger
$k$	Stream thermal conductivity
$L$	Tube length
$lay$	Tube layout
$lbc$	Baffle spacing
$LMTD_{i,j}$	Logarithmic mean temperature difference between streams $i$ and $j$
$Nb$	Number of baffles
$N_{pt}$	Number of tube passes
$N_{shell}$	Number of shells
$N_{shell}^{MAX}$	Maximum number of shells

$P$	Model parameter
$P_{max}$	Abcissa corresponding to the asymptotic value of $P$
$Q_{i,j}$	Heat load between a hot stream $i$ and cold stream $j$
$Res$	Shell side Reynolds number
$Ret$	Tube side Reynolds number
$rp$	Tube pitch ratio
$TAC$	Total annualized cost
$U_{i,j}$	Overall heat transfer coefficient between hot and cold streams $i$ and $j$
$vs$	Shell side velocity
$\widehat{vsmax}$	Upper bound of shell side velocity
$\widehat{vsmin}$	Lower bound of shell side velocity
$vt$	Tube side velocity
$\widehat{vtmax}$	Upper bound of tube side velocity
$\widehat{vtmin}$	Lower bound of tube side velocity
$X_p$	Safety factor imposed in parameter $P$
$\rho$	Stream density
$\mu$	Stream viscosity.

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