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Globally optimal basic design of multiple-unit heat exchangers

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Abstract

A novel approach (Complete Set Trimming) to address the globally optimal design of multiple-unit heat exchangers (Shell and Tube, Double Pipe, Plate, etc.) is presented. Three arrangements: Series, Parallel, Series–Parallel, and Parallel–Series, for minimizing area, CAPEX, or total annualized cost are considered. The geometry of all (equal) units is determined together with the number of units and the fluid allocation. The article illustrates the need to minimize CAPEX explicitly instead of using the minimization of Area as its proxy objective function. In addition, the influence of available pressure drop in the final optimal design is also discussed. Finally, the article shows that solutions obtained by minimizing the Total Annualized Cost (TAC) render different solutions than those obtained by minimizing CAPEX, indicating that pumping costs matter, depending on the balance between operational and capital costs.

1 | INTRODUCTION

Single-phase process-to-process heat exchangers used in the chemical, petrochemical, food, pharmaceutical, and other industries are of various types: double pipe (DPHE), shell and tube (STHE), gasketed plate (GPHE), welded plate (WPHE), spiral plate (SPHE), and so forth, which many times come in structures with N geometrically identical units.

Without loss of generality, we consider four traditional structures: series ($\mathcal{S}$), parallel ($\mathcal{P}$), series–parallel ($\mathcal{SP}$), and parallel–series ($\mathcal{PS}$) (see Figure 1). In these structures, it is assumed that all flows in parallel are equal and all exchanger geometries are the same. We do not consider other configurations that have been proposed (see Supporting Information).

We refer to a "unit" as an individual heat transfer device such that its connection to other units is through flanges and piping. We note that exchangers are not all geometrically symmetric, that is, one side has a different geometry than the other. For example, DPHEs have a "central tube" side and an "annulus" side and STHEs have a "shell" side and a "tube" side. Possible exceptions are GPHEs and WPHEs where there is geometrical symmetry. While the series and parallel structures are clear, the Series–Parallel ($\mathcal{SP}$) and Parallel–Series ($\mathcal{PS}$) need some further explanation. The Series–Parallel ($\mathcal{SP}$) case is described as the hot stream being in series and the cold in parallel, while the opposite holds for the Parallel–Series ($\mathcal{PS}$) case. In the design procedure, each stream can be allocated to any particular "side" (like allocating the cold stream to a tube side in a STHE). Thus, when considering stream allocation one can invert the geometry associated with the choices. In addition, each of these sides may have "passes." The number of passes of a heat exchanger is referred to as the number of times a stream passes through the main unit from inlet to outlet. Also, in Figure 1, we indicate the inlet and outlet

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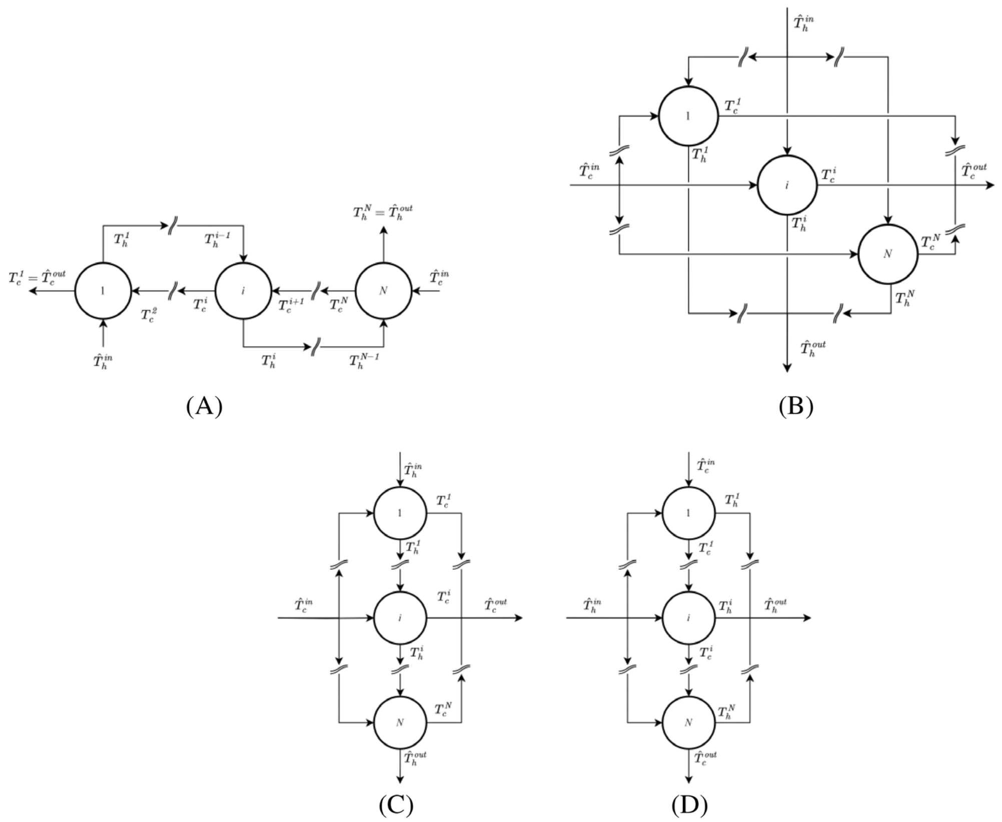

FIGURE 1 N unit structures: (A) series ($\mathcal{S}$), (B) parallel ($\mathcal{P}$), (C) series–parallel (hot stream in Series) ($\mathcal{SP}$), (D) parallel–series (cold stream in Series) ($\mathcal{PS}$).

temperatures associated with each side, which corresponds to the hot or cold stream. The figure does not indicate fluid allocation in exchangers where the sides have different geometries (e.g., hot stream in tubes, cold stream in shell for STHE, hot stream in the annulus, cold stream in the center tube for DPHE, etc.). The nature of the heat exchanger structure ($\mathcal{S}$, $\mathcal{P}$, $\mathcal{SP}$, and $\mathcal{PS}$) and the fluid allocation are decided together during the optimization procedure. Thus, the optimization task is to decide which of the eight possible alternatives is optimal, encompassing four structures and two alternative fluid allocations, together with the number of units and the corresponding dimensions of each unit. Finally, the symbol "^" is used for problem parameters.

In what follows, when something applies to any structure in the same way, we use the superscript "*," and when a single unit is considered, then a superscript "*su*" is used.

As stated above, the flow path within a unit can be organized in one or multiple so-called passes. We denote by M_h the number of passes of the hot stream and by M_c the number of passes of the cold stream, respectively. In STHEs, typical numbers of tube passes are 1, 2, 4, 6, and 8. The number of shell passes is usually one (TEMA *E* shell), but two shell passes within the same unit are also employed (TEMA *F* shell)[1] (other shell types, such as *X*, *G*, and *H* are not discussed here). A common case of STHE with multiple shells corresponds to a heat exchanger with 2 shells with 2 tube passes in each TEMA *E* shell (which is equivalent to a single shell with two shell passes and four tube passes, i.e., a "2–4" exchanger); in our case, this configuration is considered as composed of two units, with one shell pass and two tube passes each. Gasketed plate exchangers, welded-plate heat exchangers (e.g., Compablocs), or plate-fin exchangers can also have different combinations of passes for the streams. Double pipe units composed of one or more "hairpins" do not have passes, that is $M_h = M_c = 1$. Spiral-plate units can be countercurrent or co-current, and share the same description, that is $M_h = M_c = 1$ (alternatively, spiral plates can also present a crossflow pattern, usually found in condensation/vaporization). In turn, the symbol "*al*" refers to the allocation of fluids: tube or shell side for STHE, inner tube or annulus for DPHE, and so forth, when appropriate.

Sizing of exchanger structures consists of determining the dimensions for a given heat transfer task for given temperatures, flow rates, and the total heat load. Applying the *LMTD* approach, the total area required ($A^*_{T,req}$) is given by:

$$A^*_{T,req} = \frac{\widehat{Q}_T}{U^*_{T,al,M_h,M_c}\, F^*_{T,al,M_h,M_c}\, \widehat{LMTD}_T}, \tag{1}$$

where $\widehat{Q}_T$ is the total heat transfer rate, $\widehat{LMTD}_T$ is the logarithmic mean temperature difference of the equivalent countercurrent configuration, both parameters for the design problem. In turn, U^*_{T,al,M_h,M_c} and F^*_{T,al,M_h,M_c} are the overall heat transfer coefficient (which depends on allocation) and the correction factor respectively. We remark that in most cases (STHE, GPHE, WPHE), the correction factor does not depend on allocation. Exceptions exist (SPHE; see reference 2) and for this reason, we keep the dependence on allocation in the notation. The asterisk stands for any of the configurations ($\mathcal{S}, \mathcal{P}, \mathcal{SP}$, and $\mathcal{PS}$).

The overall correction factor for the whole multiple-unit exchanger depends on the choice of the number of passes and, if there are multiple units, it is also affected by the type of structure (Figure 1). Each exchanger type has procedures to obtain this coefficient as a function of the fluid properties, the geometry, and the flow regimes. Several sources cover the correlations needed for individual units ([3,4]; Bell–Delaware developed in the 1960s and explained by[1,5–7]). Additionally, the correction factor also depends on other geometric parameters, such as the number of plates in GPHE.[8] Finally, some exchanger units are stream-allocation symmetric, *that is*, the fluid allocation does not modify the correction factor.[9] Another alternative for a heat exchanger evaluation is the $\varepsilon - NTU$ method, equivalent to the LMTD method.[9] In some cases, like the SPHE, the correction factor can be calculated as a function of the NTU, which is determined from the heat exchanger effectiveness, using the inlet and outlet temperatures.[2,10] In this article, we use the LMTD model.

Because we assume that the properties of the fluids (heat capacity, viscosity, thermal conductivity, and density) do not vary in the range of the inlet and outlet temperatures, the heat transfer coefficient (U^{*}_{T,al,M_h,M_c}) is the same for all N units (they are assumed of equal geometry). When the variation of properties with temperature is mild, the average of the inlet and outlet is sufficient to provide accurate results. Larger variations of properties are not considered in this article.

Expressions of the correction factor have been developed for a single unit of a variety of exchanger types. For STHEs, expressions for one shell and multiple tube passes were developed by several authors.[11–20] Despite the existence of these more accurate options, most design books suggest that the correction factor for one unit with a single shell pass for all cases of different even numbers of tube passes is roughly the same as the one for two passes, that is, $F^{su}_{T,al,1,M_c} \sim F^{su}_{T,al,1,2}$ for $M_c = \{2, 4, 6, \ldots\}$ with $al =$ hot stream in the shell and $F^{su}_{T,al,M_h,1} \sim F^{su}_{T,al,2,1}$ for $h = \{2, 4, 6, \ldots\}$ with $al =$ cold stream in the shell, because for correction factors higher than 0.7 the difference between $F^{su}_{T,al,1,2}$ and $F^{su}_{T,al,1,\infty}$ or $F^{su}_{T,al,2,1}$ and $F^{su}_{T,al,\infty,1}$ are lower than 2%.[21] Other expressions were developed by Gardner,[15] who presents expressions valid for any unlimited even number of passes. Expressions for an odd number of tube passes are also known.[13,14,17,18] Because it is an option rarely used in practice, we leave the uncommon case of an odd number of passes (different from one) for future work. Finally, the effect of the number of baffles on the correction factor of STHEs was studied by Gaddis and Vogelpohl,[22] Shah and Pignotti,[23] Roetzel,[24,25] Gaddis and Schlünder,[73] and Magazoni et al.[26] This correction is relevant when the number of baffles is small and, for the usual number of baffles used in practice, it is ignored. The case of DPHEs does not need review ($F^{su}_{T,al,1,1} = 1$). In turn, spiral exchangers appear to be purely countercurrent because there are two channels with flow running in opposite directions; However, each channel is connected to the other channel, inside and outside of it, both at different temperatures; therefore they depart from pure countercurrent conditions and they need correction factors.[2,27] Finally, in gasketed plate and welded-plate heat exchangers, the heat transfer at end plates introduces deviations.

Correction factors for multiple units $F^{*}_{T,al,1,M_c}$ and $F^{*}_{T,al,M_h,1}$ for selected configurations of STHE, mostly in series also exist[20,28,29] (see Supporting Information). Bowman[11] showed that for several shells in STHEs of equal areas in series, the overall correction factor ($F^{\mathcal{S}}_{T,al,1,M_c}$ and $F^{\mathcal{S}}_{T,al,M_h,1}$) for multiple passes in the tubes is the same as the correction factor of the individual shells i ($F^{\mathcal{S}}_{i,al,1,M_c}$ and $F^{\mathcal{S}}_{i,al,M_h,1}$). However, the proof is valid for any type of exchanger. Because the proof offered by Bowman[11] makes some assumptions, we provide a new derivation and we extend it to a series–parallel structure (for parallel structures, this is trivially true). The calculation of the overall correction factor $\left(F^{*}_{T,al,M_h,M_c}\right)$ as a function of the correction factors of the individual units (F^{*}_{i,al,M_h,M_c}) is also of interest. Gardner[29] treated the series and series–parallel cases and gave an expression for the overall correction factor $\left(F^{\mathcal{SP}}_{T,al,M_h,M_c}\right)$ and its relation to the individual shell (unit) correction factors. Expressions of correction factors for other types of single-unit exchangers exist.[1,3,5,6,30] However, individual DPHEs do not need correction factors.

The consensus among the literature is to increase the number of units only when it is strictly needed, because of maximum size, or because single units show unacceptable temperature crossing (when the cold stream outlet temperature is higher than the hot outlet temperature) rendering them infeasible for multiple passes. The reasons are practical because additional units require more piping connections as well as other fixed costs. For STHEs, several authors have developed procedures to estimate the minimum number of shells in series to address problems related to the temperature cross in multi-pass shells: Trivedi,[31] Ahmad et al.,[32] and Bhatti et al.[28] proposed the "X_p design method." We know of no equivalent method for other arrangement options, although extensions could be made. Gulyani and Mohanty,[33,34] Gulyani,[35] and Gulyani et al.[36] also made use of the X_p design method. This method is based on the arbitrary parameter (usually $X_p = 0.9$; see reference 37). It is based on obtaining the maximum value of the P parameter for a single shell, multiplying such a number by X_p, and using it to obtain an estimate of the number of units in STHE in series. This strategy was used to develop a cost-based strategy by Moita et al.[38] Therefore, it cannot guarantee that the number of shells resulting is optimal, but the answers could be nearly optimal, something that has not been determined. Some more elaborate criteria for selecting the value of X_p have been proposed: Ahmad et al.[32] and Shenoy[39] proposed to pick a value based on a given slope. For the parallel case, the correction factor is straightforward and the same regardless of the number of shells. The only criterion to estimate the minimum number of shells seems to be the maximum size of an individual exchanger. The estimation of the number of shells series–parallel has not been developed to our knowledge. After the number of shells is determined, Vengateson[40] proposed a formal design of multiple shells making several assumptions about the P factor, a contributor to the correction factor $F^{su}_{T,al,1,M_c}/F^{su}_{T,al,M_h,1}$. Some of the above results can be generalized for other types of exchangers. The need to estimate the number of shells is associated with the heat exchanger network synthesis problem, to provide a more accurate assessment of the capital costs. This issue was explored in several works, such as Gulyani et al.,[41] Sun et al.,[42] and Cotrim et al.[43]

The literature on design optimization of heat exchangers is voluminous; however, the algorithms are focused on single units, and most do not guarantee global optimality, except for Gonçalves et al.[44–46] and Lemos et al.[47] The analysis of the optimal design problem considering multiple units and their different arrangements (series, parallel, and series–parallel) was rarely addressed: to our knowledge, aside from the work by Ahmad et al.[32] mentioned above, the unique references that addressed this problem are limited to series structures of STHE. Ponce-Ortega et al.[48] proposed a nonlinear model, solved using a MINLP procedure to design multiple 1–2 exchangers in series, and later, Ponce-Ortega et al.[49] presented a simple algorithm for the design and economic optimization of multiple-pass 1–2 shell-and-tube heat exchangers using mixed-integer nonlinear models, solving it using MINLP procedures that are not guaranteed to be globally optimal unless proper solvers are used (an attempt that was not made by the authors).

This article presents the first systematic globally optimal approach for designing heat exchangers composed of multiple units involving three main arrangements: series, parallel, and two variants of series–parallel without assuming a constant value of the overall heat transfer coefficient by making it a function of the chosen geometry. The rest of the article is organized as follows. The problem statement and some preliminary procedures are first presented, and then we follow with the description of the proposed algorithm. Next, the results are shown, and we end by discussing a roadmap for extensions of the algorithm to the case of fluid properties varying with temperature.

2 | PROBLEM STATEMENT

Given a defined heat transfer task $\widehat{Q}_T$ for the given $\widehat{LMTD}_T$, between a hot and a cold stream, it is desired to obtain: (a) *The type of exchanger unit*: DPHE, STHE, GPHE, WPHE, SPHE, or other, (b) *The arrangement*: single unit, or multiple units in series ($\mathcal{S}$), parallel ($\mathcal{P}$), series–parallel ($\mathcal{SP}$), or parallel–series ($\mathcal{PS}$), with units of equal geometry (same area), (c) *The number of passes for each side*, (d) *The fluid allocation*, when there is no geometrical symmetry, (e) *The set of geometric design variables of each unit*.

As stated, all units have equal area, that is $A_i^* = A_T^*/N$. Therefore, the required area associated with a single unit is given by:

$$A_{req,i}^* = \frac{Q_i^*}{U_{i,al,M_h,M_c}^* F_{i,al,M_h,M_c}^* LMTD_i^*} \quad \forall i. \tag{2}$$

The heat transfer coefficient for each exchanger (U_{i,al,M_h,M_c}^*) has the same value for all units because all units have the same geometry and the flow rates are uniformly distributed among the exchangers for parallel and series–parallel configurations.

Finally, for the basic design of single units, there are several literature approaches. The procedures range from trial and verification,[5,6] to the use of metaheuristics,[50–57] mathematical programming,[44–46,48,58–61] hybrid methods combining metaheuristics and mathematical programming,[62] and Complete Set Trimming.[47] Set trimming was proposed by Costa and Bagajewicz,[63] as a generalization of an idea first presented in the specific context of the design of plate exchangers.[64] Caputo et al.[65] make a critical review, ignoring, unfortunately, the few articles that guarantee global optimality using MILP procedures[44–46] and Set Trimming.[47] Because the majority of the approaches do not guarantee global optimality (some not even local optimality), this article uses Complete Set Trimming, which guarantees global optimality, is robust, that is, presents no need for initial values, and has no convergence problems (it does not iterate). In addition, previous computational studies that addressed the design optimization of single units indicate that Set Trimming is faster than mathematical programming (sometimes by an order of magnitude) and metaheuristic methods.[47] It is also important to remark that all methods, including Set Trimming, may miss good solutions if the search space of geometrical options is not comprehensive enough.

Other important remarks are the following:

a. Expressions for the correction factor of one unit/shell F_{i,al,M_h,M_c}^* are available.
b. In all cases, all the correction factors are equal, that is:

$$F_{1,al,M_h,M_c}^* = \cdots = F_{i,al,M_h,M_c}^* = \cdots = F_{N,al,M_h,M_c}^*. \tag{3}$$

The property has been illustrated in the past and proved in some cases. We provide full proof in Appendix A. Expressions for the correction factor of the overall exchanger (F_{T,al,M_h,M_c}^*) are available for all number of passes. For series arrangements, we have that the correction factor for the overall exchanger is the same as the one for the individual exchangers (see Appendix B):

$$F_{T,al,M_h,M_c}^{\mathcal{S}} = F_{1,al,M_h,M_c}^{\mathcal{S}} = \cdots = F_{i,al,M_h,M_c}^{\mathcal{S}} = \cdots = F_{N,al,M_h,M_c}^{\mathcal{S}}. \tag{4}$$

The same is true for the parallel case, that is:

$$F_{T,al,M_h,M_c}^{\mathcal{P}} = F_{1,al,M_h,M_c}^{\mathcal{P}} = \cdots = F_{i,al,M_h,M_c}^{\mathcal{P}} = \cdots = F_{N,al,M_h,M_c}^{\mathcal{P}}. \tag{5}$$

However, for the other cases ($\mathcal{SP}$ and $\mathcal{PS}$), the correction factors for each unit are not equal to the correction factor for the whole heat exchanger. In addition, for the particular case of STHEs, the correction factor for each unit is the same whether the first pass is arranged in co-current or countercurrent flow (see the Supporting Information for these arrangements). This has been proven by Underwood.[20]
For the series–parallel ($\mathcal{SP}$) arrangement of Figure 1C, there is an expression proposed by Gardner,[29] who does not show its derivation, which is presented in Appendix B:

$$F_{T,al,M_h,M_c}^{\mathcal{SP}} = F_{i,al,M_h,M_c}^{\mathcal{SP}} \frac{\left(\frac{\widehat{R}_T}{N} - 1\right) ln\left(\frac{1-\widehat{P}_T}{1-\widehat{P}_T\widehat{R}_T}\right)}{\left(\widehat{R}_T - 1\right) ln\left(\frac{1-\frac{N}{\widehat{R}_T}\left(1-\left(1-\widehat{P}_T\widehat{R}_T\right)^{\frac{1}{N}}\right)}{1-\left(1-\left(1-\widehat{P}_T\widehat{R}_T\right)^{\frac{1}{N}}\right)}\right)}, \tag{6}$$

where $\widehat{R}_T$ and $\widehat{P}_T$ are the well-known parameters used to calculate the correction factors. Likewise, for the parallel–series ($\mathcal{PS}$) arrangement, the expression is:

$$F^{\mathcal{PS}}_{T,al,M_h,M_c} = F^{\mathcal{PS}}_{i,al,M_h,M_c} \frac{\left(N\widehat{R}_T - 1\right)}{N\left(\widehat{R}_T - 1\right)} \frac{ln\left(\frac{1-\widehat{P}_T}{1-\widehat{P}_T\widehat{R}_T}\right)}{ln\left(\frac{\left(1-\widehat{P}_T\right)^{1/N}}{1-\widehat{R}_T N\left[1-\left(1-\widehat{P}_T\right)^{1/N}\right]}\right)}. \quad (7)$$

c. Without loss of generality, the investment cost of each configuration (C_N) is:

$$C_N = N\left(\widehat{c}_f + \widehat{a}\, A_i^{*\widehat{b}}\right), \quad (8)$$

where N is the number of units, $\widehat{c}_f$ is the fixed cost associated with each unit, and $\widehat{a}$ as well as $\widehat{b}$ are parameters. Note that A_i^* is the area of one unit (all units have the same area). Usually, $\widehat{b} < 1$ due to the economy of scale. However, the value of $\widehat{b}$ is sometimes considered to be $\widehat{b} = 1$, or closer to one.[66] Other more complex costing models can be used.[67]

d. The pumping cost for each exchanger (i) is calculated as follows:

$$PC_N = \widehat{\delta} \begin{cases} \left(\frac{\widehat{m}_h}{\widehat{\rho}_h}\Delta P_h + \frac{\widehat{m}_c}{\widehat{\rho}_c}\Delta P_c\right) - \text{series arrangements } (\mathcal{S}) \\ \left(\frac{\widehat{m}_h/N}{\widehat{\rho}_h}\Delta P_h + \frac{\widehat{m}_c/N}{\widehat{\rho}_c}\Delta P_c\right) - \text{parallel arrangements } (\mathcal{P}) \\ \left(\frac{\widehat{m}_h}{\widehat{\rho}_h}\Delta P_h + \frac{\widehat{m}_c/N}{\widehat{\rho}_c}\Delta P_c\right) - \text{series/parallel arrangements } (\mathcal{SP}) \\ \left(\frac{\widehat{m}_h/N}{\widehat{\rho}_h}\Delta P_h + \frac{\widehat{m}_c}{\widehat{\rho}_c}\Delta P_c\right) - \text{series/parallel arrangements } (\mathcal{PS}) \end{cases}, \quad (9)$$

where $\widehat{\delta}$ is the annual cost per pumping power installed and ΔP_h and ΔP_c are the total pressure drop of the hot and cold stream flow through all units, respectively.

e. Without loss of generality, the TAC is obtained as follows:

$$\text{TAC} = \widehat{af}\, C_N + OC_N, \quad (10)$$

where $\widehat{af}$ is the annualization factor for $\widehat{n}$ years and interest rate $\widehat{ir}$, C_N is the CAPEX and OC_N is the OPEX (pumping costs):

$$\widehat{af} = \frac{\widehat{ir}\left(1+\widehat{ir}\right)^{\widehat{n}}}{\left(1+\widehat{ir}\right)^{\widehat{n}} - 1}. \quad (11)$$

In STHE, the overall heat transfer coefficient increases with the number of tube passes, whereas the introduction of multiple tube passes for a single shell-side pass decreases the correction factor from unity to a smaller value. Moreover, once two passes are introduced, more passes make the correction factor change further (however this difference is small in practice). Sometimes these opposite tendencies resolve in favor of a higher heat transfer, but not always. However, the pressure drop increases with the number of passes.

3 | GLOBALLY OPTIMAL PROCEDURE

Each solution candidate for the design of a multiple-unit heat exchanger is composed of a set of values of the discrete design variables, that is, the number of units (*Nunits*), the type of structure ($struc \in STRUC = \{\mathcal{S},\mathcal{P},\mathcal{SP},\mathcal{PS}\}$), the fluid allocation (*al*) {*al-h= hot stream on a specified geometry*} (*al-h* in STHEs can be shell or tube side), and the variables that define the full geometry of the individual unit (*geom_dim*). In particular, for STHEs with an E-type shell, the independent set of variables *geom_dim* is composed of: tube diameter (outer and inner: *dte and dti*), tube layout (*lay*), tube pitch ratio (*rp*), number of passes in the tube-side (*Npt*), number of baffles (*Nb*), shell diameter (*Ds*), tube length (*L*), and baffle cut (*Bc*). For the case of DPHEs, the independent geometric variables are the internal and external diameters of the annular region and the length of the hairpin (the unit). For GPHEs and WPHES, the independent geometric variables are the dimensions of the plate, the number of plates, and parameters related to the adopted plate corrugation and surface characteristics (for example, for chevron plates it is the corrugation angle). Finally, for SPHEs the independent geometric variables are the spiral angle, the length, and the internal and external radius. We omit details of other exchangers without loss of generality.

The optimal design problem of a heat exchanger can be formulated as the minimization of cost or the minimization of the *TAC*. The minimization of total area is no longer a good substitute for cost in the case of multiple units, as it is in the case of a single unit, as it becomes evident in the results section. We use Complete Set Trimming based on the following sets:

- *Primordial Set*: This is the set of all candidates built using all combinations of the discrete options for each unit (based on the union of the *geom_dim*, *struc*, and *Nunits*).
- *Initial Set*: The dimensions of an individual unit must comply with mechanical and heuristic geometric guidelines.

Next, the *Initial Set* is used to perform the set trimmings for each exchanger for one fluid allocation, updating the incumbent solution after each Set Trimming. The process is then repeated for the other fluid allocation. The Set Trimmings are as follows:

1. Correction Factor F: All candidates with a value of the P_i^* larger than the maximum value are eliminated. For STHEs this is reported by Smith,[37] Appendix E, where the maximum value is equal to X_p P_{max} (we use $X_p = 0.9$, as suggested in the literature), where P_{max} is the value at which the expression for the correction factor tends to $-\infty$.[37] Candidates are also eliminated if the factor is larger than a minimum (0.75 is a value suggested in the literature).
2. Flow velocity: velocities that do not obey the bounds (fouling, erosion, and vibration).
3. Reynolds number: They are limited due to the validity range of the correlations.

4. Pressure drop: Limits are imposed on the whole exchanger, rather than on individual units. When *TAC* is used as the objective function, this set trimming is omitted.
5. Thermal task: This trimming eliminates candidates that do not have enough heat transfer area to fulfill the thermal task, as follows:

$$A_T^* = N A_i^* \geq (1 + Aex) A_{T,req}^* = \frac{(1 + Aex)\widehat{Q}_T}{U_{i,al,M_h,M_c}^* \, F_{T,al,M_h,M_c}^* \, \widehat{LMTD}_T^*}, \tag{12}$$

where F_{T,al,M_h,M_c}^* is obtained from the individual correction factors (Appendix B). In turn, these individual correction factors can be obtained using the values of R_i^* and P_i^*, the former being straightforward and the latter being calculated from the overall values $\widehat{R}_T$ and $\widehat{P}_T$ (see Appendix B).

4 | RESULTS

In this article, without loss of generality, we only show results for STHE. Two examples are presented, and two optimizations are performed for each, one minimizing the *area* and the other minimizing the *TAC*. In calculating TAC, the following parameters are used for capital cost: $\widehat{c}_f = 8500$, $\widehat{a} = 410$, $\widehat{b} = 0.85$; for pumping costs, $\widehat{\delta} = 0.15$ \$/kWh with the network operating 7500 h per year, and a combined motor pump efficiency of around 60% is assumed. The number of years for amortization is $\widehat{n} = 10$ and the adopted interesting rate is $\widehat{i} = 10\%$. For the heat transfer film coefficients, we use the Bell–Delaware model[7] for the shell side and the Gnielinski correlation for the tube-side turbulent flow.[68] Finally, the correction factors of the individual units are calculated using the well-known 1–2 expressions developed by Underwood, and a value of $X_p = 0.9$. For pressure drop, we use the Bell–Delaware method for the shell-side flow and the Darcy–Weisbach for the tube side.[69]

The geometrical options used for the STHE unit structure are shown in Table 1. The excess area is 10%. The thermal conductivity of the tube wall is 50 W/(m·K) and the tube thickness is 1.65 mm (BWG 16). The lower and upper limits on the aspect ratio (*L/D*) are 3 and 15, the baffle-to-baffle distance over shell diameter is set to be between 0.2 and 1, the velocity limits are 1 and 3 m/s for the tubes and 0.5 and 2 m/s for the shell,[37] and the Reynolds number lower and upper limits are zero and $5 \cdot 10^6$ for the tube-side and zero and 10^5 for the shell-side, respectively.

Two systems are investigated. The first system (Examples 1–3) considers methanol and water as hot and cold streams, respectively, and their data are depicted in Table 2. It is assumed that, according to the operating pressure, the streams are liquids. The second system (Example 4) involves two gaseous streams with the same composition (for the sake of simplification, the physical properties of both streams are assumed equal, as reported by Saunders[69]). The maximum pressure drop, sometimes known as "available pressure drop" among designers is for the whole exchanger, independent of the number of units.

A computer with a processor i5-6500 3.2 GHz with 8 GB of RAM memory (HP ProDesk 400 G4 SFF) was used. The sizes of the primordial and initial sets are 8,736,000 and 3,759,840 candidates, respectively, and the average time to solve each case is around 20 s. At the end of the set trimming, the size of the surviving candidates set, before sorting, varies from around 2,000 to 20,000 for CAPEX and Area Minimization. These sizes are smaller when pressure drop limitations are tightened, as expected. For the case of TAC, the final size before sorting varies from 2,000 to 70,000.

TABLE 1 Discrete values of the design variables.

Variable	Values
Ds: Shell diameter (m)	0.2032, 0.254, 0.3048, 0.33655, 0.38735, 0.43815, 0.48895, 0.53975, 0.59055, 0.635, 0.6858, 0.7366, 0.7874, 0.8382, 0.889, 0.9398, 0.9906, 1.0668, 1.143, 1.2192, 1.3716, 1.524, 1.6764, 1.8288, 1.9812, 2.1336, 2.286, 2.4384, 2.7432, 3.048
dte: Outer tube diameter (m)	0.01905, 0.02540, 0.03175, 0.03810, 0.05080
Ntp: Number of tube passes	1, 2, 4, 6, 8
rp: Tube pitch ratio	1.25, 1.33, 1.50
lay: Tube layout	1 (triangular, 30° layout), 2 (squared, 90° layout)
L: Tube length (m)	1.2192, 1.524, 1.8288, 2.1336, 2.4384, 2.7432, 3.048, 3.3528, 3.6576, 3.9624, 4.2672, 4.572, 4.8768, 5.1816, 5.4864, 5.7912, 6.096
Nb: Number of baffles	2, 4, 6, 8, …, 20
Bc: Baffle cut ratio	0.1, 0.15, 0.2, 0,25, 0.3, 0.35, 0.4, 0.45
N: Number of shells	1, 2, 3, 4, 5, 6, 7, 8
Struc: Structures	0 ($\mathcal{S}$: Series), 1 ($\mathcal{P}$: Parallel), 2 ($\mathcal{SP}$: Series – Parallel; Hot in series), 3 ($\mathcal{PS}$: Parallel – Series; Cold in series)

Example 1. The mass flow rate of the methanol is 15 kg/s, and its inlet and outlet temperatures are equal to 120 and 85°C. On the other hand, the water mass flow rate is 9.328 kg/s, and its inlet and outlet temperatures are equal to 40 and 75°C, respectively. Table 3 presents the optimal solution for minimum CAPEX, Area, and TAC, the first two for two sets of available pressure drops, as indicated.

The best configuration is a Single Unit with the hot stream in tubes and 8 passes for CAPEX minimization and TAC minimization, while the Series option with 6 shells and 2 tube passes each is chosen for Area minimization. When limiting the pressure drop of the cold stream to 40 kPa and maintaining the hot stream limiting pressure drop at 100 kPa, the optimal choice for CAPEX minimization reduces the number of tube passes while increasing the area. When restricting the pressure drop of the cold stream to 50 kPa, the optimal choice for AREA minimization increases mildly the total area, reduces the number of units by one and the number of baffles (but increasing the tube

TABLE 2 Streams data.

Stream	Cp $\left(\frac{J}{kg\,K}\right)$	Density $\left(\frac{kg}{m^3}\right)$	Viscosity (Pa s)	Thermal Conductivity $\left(\frac{W}{(m\,K)}\right)$	Fouling factor $\left(\frac{m^2\,K}{W}\right)$	Allowed (Maximum) Pressure Drop (kPa)[a]
Methanol	2600	776	$4.76 \cdot 10^{-4}$	0.122	0.0002	70
Water	4181	992	$5.70 \cdot 10^{-4}$	0.59	0.0002	100
Gaseous stream	2311	17.62	$7.58 \cdot 10^{-6}$	0.03172	0.00035	25

[a]Not used for *TAC*.

TABLE 3 Optimal solution of Example 1.

Case name	Min CAPEX DPhmax = 70 kPa DPcmax = 100 kPa	Min CAPEX DPhmax = 40 kPa DPcmax = 100 kPa	Min AREA DPhmax = 70 kPa DPcmax = 100 kPa	Min AREA DPhmax = 70 kPa DPcmax = 50 kPa	Min TAC DPhmax = ∞ DPcmax = ∞
Configuration	Single	Single	(S): Series	(S): Series	Single
Stream allocation	Hot in tubes	Hot in tubes	Hot in tubes	Hot in tubes	Hot in tubes
Number of shells	1	1	6	5	1
Tube passes	8	6	2	2	4
Area per shell [m^2]	56.93	60.28	7.54	9.12	68.42
Total area [m^2]	57	60	45	46	68
External tube diameter [m]	0.0254	0.01905	0.03175	0.03175	0.01905
Shell diameter [m]	0.5906	0.5906	0.3048	0.3048	0.5906
Tube layout	Square	Triangular	Triangular	Square	Square
Pitch ratio	1.25	1.25	1.33	1.25	1.25
Length [m]	3.0488	2.439	2.439	3.0488	3.0488
Number of baffles	20	16	18	12	20
Baffle cut	0.1	0.1	0.15	0.1	0.35
Number of tubes	234	413	31	30	375
Overall correction factor	0.89	0.89	1.00	1.00	0.89
Area/Areq	1.12	1.11	1.11	1.12	1.12
Tube velocity [m/s]	1.72	1.44	1.96	2.03	1.06
Shell velocity [m/s]	0.52	0.52	0.93	0.61	0.51
ht [W/m^2K]	2897.64	2551.32	3181.78	3277.89	1931.01
hs [W/m^2K]	3282.66	3246.53	4707.70	4410.76	2851.04
U [W/m^2K]	671.64	628.27	747.05	744.81	559.69
Pressure drop in tubes [kPa]	45.56	27.76	63.58	64.14	12.37
Pressure drop in shell [kPa]	6.94	8.73	94.86	49.94	4.28
Operational cost (tube) [USD/year]	$1651	$1006	$2304	$2325	$448
Operational cost (shell) [USD/year]	$122	$154	$1672	$880	$75
Capital cost [USD]	$21,230	$21,865	$64,702	$55,924	$23,384
Annualized capital cost [USD/year]	$3455	$3558	$10,530	$9101	$3806
Total annualized cost [USD/year] ($n = 10$)	$5229	$4718	$14,507	$12,306	$4329

length). Additionally, the tube layout is modified to square. All of these modifications result in a significantly lower pressure drop in the shell side. We also note that the minimum TAC points to a higher area and smaller pumping costs on both sides, compared to the minimum CAPEX solution. None of these changes can be easily obtained by trial and verification: they are too complex. For other types of structures than the optimal, and other allocations the corresponding CAPEX, Area, and Cost are given in Table 4. As observed, some cases are infeasible and many have an area within 10% of the optimal value. When an infeasible structure is reported, the reason for the infeasibility (*F* or Area) is listed, indicating where the set trimming renders an empty set. This reinforces the idea that obtaining the optimum by trial and verification is cumbersome.

Example 2. The mass flow rate of the methanol is 15 kg/s, and its inlet and outlet temperatures are equal

TABLE 4 Optimal solutions of Example 1 when forcing the structure and allocation.

	Min CAPEX DPhmax = 70 kPa	Min CAPEX DPhmax = 40 kPa	Min AREA DPhmax = 70 kPa	Min AREA DPhmax = 70 kPa	Min TAC DPhmax = ∞
Case name	**DPcmax = 100 kPa**	**DPcmax = 100 kPa**	**DPcmax = 100 kPa**	**DPcmax = 50 kPa**	**DPcmax = ∞**
(S): Series—Cold in tubes	Feasible, *N* = 1, Npt = 6, Area = 61.0, CAPEX = 21,999 USD, TAC = 5193 USD/y	Feasible, *N* = 1, Npt = 6, Area = 61.0, CAPEX = 21,999 USD, TAC = 5193 USD/y	Feasible, *N* = 5, Npt = 4, Area = 50.36, CAPEX = 57,101 USD, TAC = 13,039 USD/y	Feasible, *N* = 3, Npt = 4, Area = 52.55, CAPEX = 39,522 USD, TAC = 9662 USD/y	Feasible, *N* = 1, Npt = 8, Area = 68.61, CAPEX = 23,417 USD, TAC = 4560 USD/y
(P): Parallel—Cold in tubes	Feasible, *N* = 2, Npt = 8, Area = 66.56, CAPEX = 33,131 USD, TAC = 6680 USD/y	Feasible, *N* = 2, Npt = 8, Area = 66.56, CAPEX = 33,131 USD, TAC = 6680 USD/y	Feasible, *N* = 2, Npt = 8, Area = 66.56, CAPEX = 33,131 USD, TAC = 6680 USD/y	Feasible, *N* = 2, Npt = 8, Area = 75.32, CAPEX = 34,918 USD, TAC = 6717 USD/y	Feasible, *N* = 2, Npt = 8, Area = 75.32, CAPEX = 34,918 USD, TAC = 6559 USD/y
(SP): Series/parallel/hot in series—Cold in tubes	Feasible, *N* = 2, Npt = 8, Area = 55.47, CAPEX = 30,815 USD, TAC = 7755 USD/y	Feasible, *N* = 2, Npt = 8, Area = 60.43, CAPEX = 31,859 USD, TAC = 7360 USD/y	Feasible, *N* = 3, Npt = 8, Area = 55.29, CAPEX = 40,141 USD, TAC = 9795 USD/y	Feasible, *N* = 3, Npt = 8, Area = 55.29, CAPEX = 40,141 USD, TAC = 9795 USD/y	Feasible, *N* = 2, Npt = 6, Area = 61.74, CAPEX = 32,133 USD, TAC = 6379 USD/y
(PS): Series/parallel/cold in series—Cold in tubes	Feasible, *N* = 2, Npt = 6, Area = 69.19, CAPEX = 33,671 USD, TAC = 6622 USD/y	Feasible, *N* = 2, Npt = 6, Area = 69.19, CAPEX = 33,671 USD, TAC = 6622 USD/y	Feasible, *N* = 2, Npt = 6, Area = 69.19, CAPEX = 33,671 USD, TAC = 6622 USD/y	Feasible, *N* = 2, Npt = 4, Area = 73.13, CAPEX = 34,475 USD, TAC = 6720 USD/y	Feasible, *N* = 2, Npt = 4, Area = 73.13, CAPEX = 34,475 USD, TAC = 6576 USD/y
(S): Series—Hot in tubes	Feasible, *N* = 1, Npt = 8, Area = 56.93, CAPEX = 21,229 USD, TAC = 5228 USD/y	Feasible, *N* = 1, Npt = 6, Area = 60.28, CAPEX = 21,864 USD, TAC = 4718 USD/y	Feasible, *N* = 6, Npt = 2, Area = 45.25, CAPEX = 64,701 USD, TAC = 14,506 USD/y	Feasible, *N* = 5, Npt = 2, Area = 45.62, CAPEX = 55,923 USD, TAC = 12,306 USD/y	Feasible, *N* = 1, Npt = 4, Area = 68.42, CAPEX = 23,383 USD, TAC = 4329 USD/y
(P): Parallel—Hot in tubes	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area
(SP): Series/Parallel/Hot in series—Hot in tubes	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area
(PS): Series/Parallel/Cold in series—Hot in tubes	Feasible, *N* = 2, Npt = 6, Area = 51.45, CAPEX = 29,961 USD, TAC = 7629 USD/y	Feasible, *N* = 2, Npt = 4, Area = 56.05, CAPEX = 30,939 USD, TAC = 6538 USD/y	Feasible, *N* = 5, Npt = 6, Area = 50.18, CAPEX = 57,056 USD, TAC = 12,998 USD/y	Feasible, *N* = 5, Npt = 6, Area = 50.18, CAPEX = 57,056 USD, TAC = 12,647 USD/y	Feasible, *N* = 2, Npt = 6, Area = 62.77, CAPEX = 32,346 USD, TAC = 5984 USD/y

TABLE 5 Optimal solution of Example 2.

Case name	Min CAPEX DPhmax = 70 kPa DPcmax = 100 kPa	Min CAPEX DPhmax = 50 kPa DPcmax = 100 kPa	Min AREA DPhmax = 70 kPa DPcmax = 100 kPa	Min AREA DPhmax = 50 kPa DPcmax = 100 kPa	Min TAC DPhmax = ∞ DPcmax = ∞
Configuration	(S): Series	(S): Series	(S): Series	(S): Series	(S): Series
Stream allocation	Hot in tubes	Cold in tubes	Hot in tubes	Hot in tubes	Hot in tubes
Number of shells	2	2	7	8	2
Tube passes	4	4	2	2	4
Area per shell [m^2]	45.43	48.74	11.56	10.44	54.74
Total area [m^2]	91	97	81	83	109
External tube diameter [m]	0.01905	0.01905	0.03175	0.01905	0.01905
Shell diameter [m]	0.489	0.3874	0.3874	0.3874	0.5906
Tube layout	Square	Triangular	Square	Square	Square
Pitch ratio	1.25	1.25	1.5	1.33	1.25
Length [m]	3.0488	4.8768	3.0488	1.2195	2.439
Number of baffles	18	14	20	10	16
Baffle cut	0.1	0.1	0.1	0.1	0.4
Number of tubes	249	167	38	143	375
Overall correction factor	0.93	0.93	0.99	1.00	0.93
Area/Areq	1.13	1.11	1.12	1.11	1.11
Tube velocity [m/s]	1.59	1.16	1.60	1.39	1.06
Shell velocity [m/s]	0.55	0.70	0.50	0.83	0.52
ht [W/m^2K]	2793.11	7463.30	2645.81	2465.45	1931.01
hs [W/m^2K]	4133.15	1547.06	4168.24	5170.65	2616.17
U [W/m^2K]	673.60	618.04	695.82	669.54	550.00
Pressure drop in tubes [kPa]	52.62	53.79	57.31	44.06	20.90
Pressure drop in shell [kPa]	19.44	48.64	64.42	79.96	6.18
Operational cost (tube) [USD/year]	$1907	$948	$2077	$1597	$758
Operational cost (shell) [USD/year]	$343	$1763	$1136	$1410	$109
Capital cost [USD]	$38,017	$39,311	$82,476	$92,080	$41,624
Annualized capital cost [USD/year]	$6187	$ 398	$ 3,423	$14,986	$6774
Total annualized cost [USD/year] (n = 10)	$8437	$9109	$16,635	$17,992	$7641

to 120 and 75°C, respectively. On the other hand, the water mass flow rate is 9.328 kg/s, and its inlet and outlet temperatures are equal to 40 and 85°C. Table 5 presents the optimal solution for the CAPEX, Area, and TAC minimizations.

In this example, there is a temperature crossing (the cold stream outlet temperature is higher than the hot outlet temperature, as mentioned above). All optimal solutions are exchangers in series. When limiting the pressure drop of the hot stream to 50 kPa the minimum capital cost solution switches to allocating the cold stream in the tubes, increases the area per shell, reduces the shell diameter, and increases the length. In turn, the minimum area solution increases the number of units reducing the length of each unit. The minimum TAC solution uses two units increasing the total area by 20%. For other types of structures than the optimal, and other allocations the corresponding CAPEX, Area, and TAC are given in Table 6.

Example 3. The mass flow rate of methanol is 150 kg/s, and its inlet and outlet temperatures are equal to 180 and 165°C, respectively. In turn, the water mass flow rate is 11.858 kg/s, and its inlet and outlet temperatures are equal to 42 and 160°C.

The results are shown in Table 7. For minimum CAPEX and TAC, the answer is a parallel–series solution structure, with different allocations of fluids. When the pressure drop limitation for the cold stream is dropped to 50 kPa, the minimum CAPEX solution switches to a series solution with different fluid allocations. In turn, when limiting the pressure drop of the hot stream to 40 kPa, the minimum area reduces the number of units, increases the shell diameter, and reduces the tube diameter. For other types of structures than the optimal, and other allocations the corresponding CAPEX, Area, and TAC are given in Table 8.

TABLE 6 Optimal solutions of Example 2 when forcing the structure and allocation.

Case name	Min CAPEX DPhmax = 70 kPa DPcmax = 100 kPa	Min CAPEX DPhmax = 50 kPa DPcmax = 100 kPa	Min AREA DPhmax = 70 kPa DPcmax = 100 kPa	Min AREA DPhmax = 50 kPa DPcmax = 100 kPa	Min TAC DPhmax = ∞ DPcmax = ∞
(S): Series—Cold in tubes	Feasible, N = 2, Npt = 4, Area = 97.48, CAPEX = 39,311 USD, TAC = 9109 USD	Feasible, N = 2, Npt = 4, Area = 97.48, CAPEX = 39,311 USD, TAC = 9109 USD	Feasible, N = 4, Npt = 4, Area = 84.66, CAPEX = 55,959 USD, TAC = 12,934 USD	Feasible, N = 6, Npt = 4, Area = 91.08, CAPEX = 75,833 USD, TAC = 15,532 USD	Feasible, N = 2, Npt = 8, Area = 109.77, CAPEX = 41,679 USD, TAC = 8027 USD
(P): Parallel—Cold in tubes	Infeasible F	Infeasible F	Infeasible F	Infeasible F	Infeasible F
(SP): Series/Parallel/Hot in series—Cold in tubes	Infeasible F	Infeasible F	Infeasible F	Infeasible F	Infeasible F
(PS): Series/Parallel/Cold in series—Cold in tubes	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area
(S): Series—Hot in tubes	Feasible, N = 2, Npt = 4, Area = 90.87, CAPEX = 38,017 USD, TAC = 8436 USD	Feasible, N = 2, Npt = 4, Area = 104.73, CAPEX = 40,714 USD, TAC = 85,017 USD	Feasible, N = 7, Npt = 2, Area = 80.89, CAPEX = 82,475 USD, TAC = 16,635 USD	Feasible, N = 8, Npt = 2, Area = 83.49, CAPEX = 92,079 USD, TAC = 17,992 USD	Feasible, N = 2, Npt = 4, Area = 109.48, CAPEX = 41,624 USD, TAC = 7640 USD
(P): Parallel—Hot in tubes	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area
(SP): Series/Parallel/Hot in series—Hot in tubes	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area
(PS): Series/Parallel/Cold in series—Hot in tubes	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area

TABLE 7 Optimal solution of Example 3.

Case name	Min CAPEX DPhmax = 70 kPa DPcmax = 100 kPa	Min CAPEX DPhmax = 70 kPa DPcmax = 50 kPa	Min AREA DPhmax = 70 kPa DPcmax = 100 kPa	Min AREA DPhmax = 40 kPa DPcmax = 100 kPa	Min TAC DPhmax = ∞ DPcmax = ∞
Configuration	(PS): Hot in parallel and cold in series	(S): Series	(S): Series	(S): Series	(PS): Hot in parallel and cold in series
Stream allocation	Cold in tubes	Hot in tubes	Hot in tubes	Hot in tubes	Hot in tubes
Number of shells	2	2	7	5	2
Tube passes	6	2	1	1	1
Area per shell [m^2]	84.66	87.1	21.9	31.38	107.51
Total area [m^2]	169	174	153	157	215
External tube diameter [m]	0.0254	0.0254	0.0381	0.03175	0.01905
Shell diameter [m]	0.5906	0.6858	0.489	0.5906	0.5906
Tube layout	Square	Triangular	Triangular	Square	Triangular
Pitch ratio	1.33	1.25	1.25	1.33	1.25
Length [m]	6.0976	3.0488	2.439	2.439	3.6585
Number of baffles	12	18	12	16	20
Baffle cut	0.15	0.1	0.1	0.1	0.4
Number of tubes	174	358	75	129	491
Overall correction factor	0.93	0.98	1.00	1.00	1.00
Area/Areq	1.12	1.20	1.11	1.13	1.13
Tube velocity [m/s]	1.07	2.82	2.71	2.36	1.01
Shell velocity [m/s]	1.36	0.51	0.62	0.55	0.54
ht [W/m^2K]	6721.06	4520.62	4195.58	3759.55	1851.77
hs [W/m^2K]	2517.10	3021.03	3243.29	3644.92	2591.00
U [W/m^2K]	737.52	728.40	747.95	742.59	540.92
Pressure drop in tubes [kPa]	60.60	57.58	47.30	30.10	3.00
Pressure drop in shell [kPa]	69.69	17.65	48.00	32.22	12.90
Operational cost (tube) [USD/year]	$1358	$20,870	$17,144	$10,911	$1089
Operational cost (shell) [USD/year]	$25,259	$395	$1076	$722	$ 289
Capital cost [USD]	$52,674	$53,543	$99,053	$80,866	$60,705
Annualized capital cost [USD/year]	$8572	$8714	$16,120	$13,161	$9879
Total annualized cost [USD/year] (n = 10)	$35,190	$29,980	$34,340	$24,793	$11,257

Example 4. The mass flow rate of gas is 15 kg/s, and its inlet and outlet temperatures are equal to 120 and 85°C, respectively. On the other hand, the mass flow rate of the other gas is 15 kg/s, and its inlet and outlet temperatures are equal to 40 and 75°C, respectively. The results are shown in Table 9. In all cases, the solution is one or more units in parallel. When pressure drop limitations for the hot and cold stream are dropped to 5 kPa for the hot stream the area remains the same and the units change the baffle cut. For other types of structures than the optimal, and other allocations the corresponding CAPEX, Area, and Cost are given in Table 10.

5 | ANALYSIS OF THE OPTIMAL USE OF EACH ARRANGEMENT

The examples above were selected in such a manner that each design problem would render optimal solutions with different arrangements:

TABLE 8 Optimal Solutions of Example 3 when forcing the structure and allocation.

Case name	Min CAPEX DPhmax = 70 kPa / DPcmax = 100 kPa	Min CAPEX DPhmax = 70 kPa / DPcmax = 50 kPa	Min AREA DPhmax = 70 kPa / DPcmax = 100 kPa	Min AREA DPhmax = 40 kPa / DPcmax = 100 kPa	Min TAC DPhmax = ∞ / DPcmax = ∞
(S): Series—Cold in tubes	Feasible, *N* = 2, Npt = 8, Area = 217.01, CAPEX = 61,049 USD, TAC = 35,868 USD/y	Infeasible Area	Feasible, *N* = 3, Npt = 6, Area = 188.85, CAPEX = 67,095 USD, TAC = 37,862 USD/y	Infeasible Area	Feasible, *N* = 2, Npt = 8, Area = 217.01, CAPEX = 61,049 USD, TAC = 33,603 USD/y
(P): Parallel—Cold in tubes	Infeasible F	Infeasible F	Infeasible F	Infeasible F	Infeasible F
(SP): Series/Parallel/Hot in series—Cold in tubes	Infeasible Maximum shell velocity	Infeasible Maximum shell velocity	Infeasible Maximum shell velocity	Infeasible Maximum shell velocity	Infeasible Maximum shell velocity
(PS): Series/Parallel/Cold in series—Cold in tubes	Feasible, *N* = 2, Npt = 6, Area = 169.33, CAPEX = 52,674 USD, TAC = 35,189 USD/y	Infeasible Area	Feasible, *N* = 4, Npt = 6, Area = 169.33, CAPEX = 73,582 USD, TAC = 38,709 USD/y	Feasible, *N* = 3, Npt = 8, Area = 170.78, CAPEX = 63,688 USD, TAC = 25,854 USD/y	Feasible, *N* = 2, Npt = 8, Area = 217.01, CAPEX = 61,049 USD, TAC = 15,262 USD/y
(S): Series—Hot in tubes	Feasible, *N* = 2, Npt = 2, Area = 174.19, CAPEX = 53,543 USD, TAC = 29,979 USD/y	Feasible, *N* = 2, Npt = 2, Area = 174.19, CAPEX = 53,543 USD, TAC = 29,979 USD/y	Feasible, *N* = 7, Npt = 1, Area = 153.27, CAPEX = 99,052 USD, TAC = 34,340 USD/y	Feasible, *N* = 5, Npt = 1, Area = 156.92, CAPEX = 80,865 USD, TAC = 24,793 USD/y	Feasible, *N* = 2, Npt = 1, Area = 196.18, CAPEX = 57,429 USD, TAC = 12,612 USD/y
(P): Parallel—Hot in tubes	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area
(SP): Series/Parallel/Hot in series—Hot in tubes	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area	Infeasible Area
(PS): Series/Parallel/Cold in series—Hot in tubes	Feasible, *N* = 2, Npt = 2, Area = 178.23, CAPEX = 54,261 USD, TAC = 21,422 USD/y	Feasible, *N* = 2, Npt = 2, Area = 178.23, CAPEX = 54,261 USD, TAC = 21,422 USD/y	Feasible, *N* = 5, Npt = 4, Area = 155.09, CAPEX = 80,486 USD, TAC = 34,464 USD/y	Feasible, *N* = 6, Npt = 4, Area = 158.81, CAPEX = 90,834 USD, TAC = 30,268 USD/y	Feasible, *N* = 2, Npt = 1, Area = 215.01, CAPEX = 60,704 USD, TAC = 11,257 USD/y

TABLE 9 Optimal solution of Example 4.

Case name	Min CAPEX DPhmax = 20 kPa DPcmax = 20 kPa	Min CAPEX DPhmax = 5 kPa DPcmax = 20 kPa	Min AREA DPhmax = 20 kPa DPcmax = 20 kPa	Min AREA DPhmax = 5 kPa DPcmax = 20 kPa	Min TAC DPhmax = ∞ DPcmax = ∞
Configuration	(P): Parallel	(P): Parallel	(P): Parallel	(P): Parallel	(P): Parallel
Stream allocation	Cold in tubes	Cold in tubes	Cold in tubes	Cold in tubes	Cold in tubes
Number of shells	2	2	4	4	3
Tube passes	1	1	1	1	1
Area per shell [m^2]	118.23	118.23	43.06	43.06	78.82
Total area [m^2]	236	236	172	172	236
External tube diameter [m]	0.01905	0.01905	0.01905	0.01905	0.01905
Shell diameter [m]	0.7874	0.7874	0.5906	0.5906	0.7874
Tube layout	Square	Square	Square	Square	Square
Pitch ratio	1.5	1.5	1.5	1.5	1.5
Length [m]	3.6585	3.6585	2.439	2.439	2.439
Number of baffles	4	4	4	4	4
Baffle cut	0.1	0.3	0.1	0.2	0.45
Number of tubes	540	540	295	295	540
Overall correction factor	1.00	1.00	1.00	1.00	1.00
Area/Areq	1.84	1.66	1.28	1.23	1.21
Tube velocity [m/s]	9.36	9.36	8.56	8.56	6.24
Shell velocity [m/s]	5.03	5.03	5.02	5.02	5.03
ht [W/m^2K]	549.05	549.05	509.49	509.49	390.87
hs [W/m^2K]	522.29	405.38	501.35	454.64	278.78
U [W/m^2K]	202.96	182.50	193.12	185.77	133.49
Pressure drop in tubes [kPa]	1.94	1.94	1.18	1.18	0.65
Pressure drop in shell [kPa]	9.70	4.68	6.84	4.18	2.37
Operational cost (tube) [USD/year]	$7142	$7142	$4341	$4341	$2392
Operational cost (shell) [USD/year]	$35,787	$17,277	$25,261	$15,411	$8761
Capital cost [USD]	$64,385	$64,385	$74,162	$74,162	$75,857
Annualized capital cost [USD/year]	$10,478	$10,478	$12,069	$12,069	$12,345
Total annualized cost [USD/year] ($n = 10$)	$53,408	$34,898	$41,672	$31,821	$23,499

single unit (*su*), series ($\mathcal{S}$), series–parallel ($\mathcal{SP}$), or parallel ($\mathcal{P}$). General quantitative rules that would establish what arrangement is optimal for each set of data are hard to obtain and are a possibility in future work. However, some general guidelines and/or conjectures can be inferred from the optimal results, as discussed below.

Example 1. The optimal solutions considering the minimization of CAPEX or TAC are single-shell alternatives. The fixed cost associated with an additional shell explains why a single shell solution with a higher area than multiple shells in series is cheaper. A single shell is the optimal alternative to the majority of the design problems in practice. However, many design tasks cannot be accomplished using a single shell, as discussed in the other examples. An important message from this set of results is that CAPEX minimization is a more realistic function than Area minimization, which ignores the additional fixed costs associated with multiple shells. As shown, it may yield solutions that are considerably more expensive. In this example, area minimization renders an optimal solution with a large number of shells with 2 passes (instead of 8), smaller shell diameters, and smaller tube lengths, associated with about 20%–30% less area when compared with the solutions for minimum CAPEX. The area reduction stems from a smaller shell diameter and other changes, which increases velocities and, in turn, increases the overall heat transfer coefficient. In addition, a larger heat transfer coefficient and an increase in the number of shells are associated with a reduction in tube length. However, these solutions are considerably more expensive (almost triple CAPEX and also triple TAC). As stated, this illustrates

TABLE 10 Optimal Solutions of Example 4 when forcing the structure and allocation.

Case name	Min CAPEX DPhmax = 20 kPa DPcmax = 20 kPa	Min CAPEX DPhmax = 5 kPa DPcmax = 20 kPa	Min AREA DPhmax = 20 kPa DPcmax = 20 kPa	Min AREA DPhmax = 5 kPa DPcmax = 20 kPa	Min TAC DPhmax = ∞ DPcmax = ∞
(S): Series—Cold in tubes	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 75,754 USD	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 51,855 USD	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 75,754 USD	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 51,855 USD	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 51,855 USD
(P): Parallel—Cold in tubes	Feasible, N = 2, Npt = 1, Area = 236.47, CAPEX = 64,385 USD, TAC = 53,408 USD	Feasible, N = 2, Npt = 1, Area = 236.47, CAPEX = 64,385 USD, TAC = 34,897 USD	Feasible, N = 4, Npt = 1, Area = 172.24, CAPEX = 74,161 USD, TAC = 41,671 USD	Feasible, N = 4, Npt = 1, Area = 172.24, CAPEX = 74,161 USD, TAC = 31,821 USD	Feasible, N = 3, Npt = 1, Area = 236.47, CAPEX = 75,856 USD, TAC = 23,498 USD
(SP): Series/Parallel/Hot in series—Cold in tubes	Feasible, N = 2, Npt = 4, Area = 1485.59, CAPEX = 242,970 USD, TAC = 137,519 USD	Infeasible	Feasible, N = 2, Npt = 4, Area = 1485.59, CAPEX = 242,970 USD, TAC = 137,519 USD	Infeasible	Feasible, N = 2, Npt = 4, Area = 1485.59, CAPEX = 242,970 USD, TAC = 103,944 USD
		Maximum pressure drop		Maximum pressure drop	
(PS): Series/Parallel/Cold in series—Cold in tubes	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 62,173 USD	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 55,716 USD	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 62,173 USD	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 55,716 USD	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 48,576 USD
(S): Series—Hot in tubes	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 75,754 USD	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 75,754 USD	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 75,754 USD	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 75,754 USD	Feasible, N = 1, Npt = 2, Area = 767.89, CAPEX = 124,722 USD, TAC = 75,754 USD
(P): Parallel—Hot in tubes	Feasible, N = 2, Npt = 1, Area = 236.47, CAPEX = 64,385 USD, TAC = 53,408 USD	Feasible, N = 2, Npt = 1, Area = 236.47, CAPEX = 64,385 USD, TAC = 53,408 USD	Feasible, N = 4, Npt = 1, Area = 172.24, CAPEX = 74,161 USD, TAC = 41,671 USD	Feasible, N = 4, Npt = 1, Area = 172.24, CAPEX = 74,161 USD, TAC = 41,671 USD	Feasible, N = 3, Npt = 1, Area = 236.47, CAPEX = 75,856 USD, TAC = 23,498 USD
(SP): Series/Parallel/Hot in series—Hot in tubes	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 62,173 USD	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 62,173 USD	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 62,173 USD	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 62,173 USD	Feasible, N = 3, Npt = 1, Area = 685.33, CAPEX = 149,913 USD, TAC = 62,173 USD
(PS): Series/Parallel/Cold in series—Hot in tubes	Feasible, N = 2, Npt = 4, Area = 1485.59, CAPEX = 242,970 USD, TAC = 137,519 USD	Feasible, N = 3, Npt = 4, Area = 2228.38, CAPEX = 364,455 USD, TAC = 145,346 USD	Feasible, N = 2, Npt = 4, Area = 1485.59, CAPEX = 242,970 USD, TAC = 137,519 USD	Feasible, N = 3, Npt = 4, Area = 2228.38, CAPEX = 364,455 USD, TAC = 145,346 USD	Feasible, N = 2, Npt = 4, Area = 1485.59, CAPEX = 242,970 USD, TAC = 103,944 USD

well the danger of using the area as a proxy for capital costs. Table 4 reveals why a series solution is chosen for area minimization: the parallel, series–parallel, and parallel–series solutions render a similar number of shells, and have almost ∼50%, 20%, and 10% larger area, respectively. CAPEX minimization shows a similar pattern: the parallel, series–parallel, and parallel–series solutions use two shells and exhibit quite similar increases in CAPEX (∼50%, 20%, and 40%, respectively).

Example 2. This example is characterized by a considerable temperature cross. Therefore, single-shell solutions with multiple passes are infeasible.[1,5] Countercurrent single shells do not yield infeasible temperature profiles, but, because there is only a single tube-side pass in this case, tube-side velocities are usually low, which renders small values of heat transfer coefficient. Therefore, these alternatives are frequently nonoptimal. The association of shells in series with multiple passes increases the resultant LMTD correction factor (*F*), which allows the use of shells with multiple passes in the presence of temperature cross. Parallel arrangements do not modify the temperature profiles, therefore, they are affected by the temperature cross in the same way as single units. In the series–parallel and parallel–series alternatives, there is a split of the flow rate among multiple shells, causing a reduction of the flow rate and velocity in each shell, which implies a reduction of the overall heat transfer coefficient. This alternative also yields a higher LMTD correction factor (F) than a single unit alternative, but the increase is lower than the series structure with the same number of shells. This comparative analysis explains why the optimal solution to problems with temperature cross and similar flow rates is usually the series structure. This behavior is observed in Table 5, where all optimal solutions are multiple shells in series, and in Table 6, where all other alternatives, except series, are infeasible because the correction factor is too low in many cases, the *P* parameter is larger than the maximum, or the required area is too high due to a low, yet acceptable value of *F* or a small value of *U*, or a combination thereof. Thus, in an attempt to generalize the results of this example, one can make the conjecture that when the flow rates are similar, and there are no pressure drop limitations, the most likely optimal solution for cases with temperature crossing is the arrangements in series. This pattern is observed in practice in several heat exchangers in the industry. In fact, the utilization of a series arrangement is a classical approach to solving design problems with temperature cross, as discussed in several textbooks.[5,69] Area minimization renders several more shells for the same reason explained in Example 1.

Example 3. This example is associated with a large flow rate difference between the hot and cold streams (the ratio of the flow rates is larger than 10). Consequently, to accommodate such large asymmetry between the flow rates, optimal solutions based on CAPEX and TAC involved a parallel–series alternative, with the hot stream splitting, the one with a larger flow rate. The use of other alternatives is limited in this type of problem, due to the need to fulfill the flow velocity and pressure drop bounds on both streams.

This example suggests the conjecture that the series–parallel or the parallel–series alternatives are likely the optimal solutions when there is a large difference between the flow rates of the streams. Another conjecture that could be made is that the series–parallel and the parallel–series alternatives are expected to be optimal solutions when one of the streams is associated with a severely restricted pressure drop, as mentioned by Gardner.[29] Table 8 illustrates that there are several infeasible cases (some obvious as the Series–parallel with hot in series), or the parallel structures. Table 7 reveals that when the area is minimized, the series structure is preferred, at the cost of increasing the number of units from 2 to 7 with an associated 100% increase in CAPEX. The resulting area is about 10% smaller than the solution for CAPEX minimization. The solution minimizing TAC has the same structure as the minimum CAPEX optimal structure with a significantly lower TAC value (66% reduction from the solution obtained minimizing CAPEX). This illustrates the impact of pumping costs.

Example 4. In this example, the smaller density of the gaseous streams and the relatively large flow rates yield optimal solutions with parallel structures (Table 9), due to pressure drop limitations or the larger energy costs associated with the flow of gaseous streams. Thus, the conjecture can be made that parallel structures are expected to be optimal when there are large flow rates and/or pressure drop limitations in both streams, because the split of the flow rate of both streams among multiple shells reduces the flow velocity and, consequently, the pressure drop, thus avoiding pressure drop restrictions, or large economic penalties associated with the operating costs. The solution corresponding to minimizing TAC shows again the effect of pumping costs. Indeed, it has a 56% smaller TAC than the corresponding solution when CAPEX is minimized. Table 10 indicates that alternative structures are feasible, but they exhibit unreasonably larger costs and areas, thus reinforcing the conjecture above.

6 | ROADMAP FOR CHANGING PROPERTIES WITH TEMPERATURE

Garner and Taborek[70] revised some assumptions about the use of the same value of the overall heat transfer coefficient (*U*) throughout the exchanger area for fluids with significant changes in properties (particularly, viscosity) with temperature, and the existence of by-passes in the shell. Indeed, if one assumes that physical properties change with temperature, the whole LMTD model breaks down because it is based on the hypothesis of a uniform value of the overall heat transfer coefficient. There would be no reason to use the correction factor if this hypothesis is abandoned.

To address the situation, a simple model to take into account the overall heat transfer coefficient dependence on temperature was proposed by Colburn.[71] Assuming the global coefficient is a linear function of the local temperature difference, a log-mean of the product between the global coefficient calculated using the temperatures of the fluids on one side of the exchanger and the temperature difference on the opposite side of the equipment is proposed to replace the product of the mean global coefficient and the log mean temperature difference in the log mean traditional equation. A method using a temperature-dependent overall heat transfer coefficient (*U*) to model each unit usually requires a numerical discretization of the balance equations or surrogate models and has been proven to be needed when large variations of physical properties exist, especially viscosity. In our case, an extension to such a case consists of having some simulation model, based on first principles or surrogate, performing Proxy Set Trimming followed by a Smart Enumeration.[63]

7 | CONCLUSIONS

This article presented a rigorous approach to the design of multi-unit exchangers based on the LMTD model, for the case where all units have the same geometrical dimensions and area. The cases where the correction factor is a function of the geometry aside from the inlet/outlet temperatures (the case of spiral exchangers is one) will be covered in future work.

The global optimization procedure used is the Complete Set Trimming.[63] Suboptimal solutions have been identified and discussed.

Other configurations such as multiple units with equal heat transferred in each unit, unequal number of passes, as well as other types of configurations with unequal area and heat transferred in each unit, are a matter of future work.

Three objective functions, exchanger cost, total area, and total annualized cost are illustrated, and the influence of available pressure drop is discussed. It is shown that minimization of Area as a proxy for CAPEX renders costly and complex designs. Finally, the solutions obtained minimizing TAC sometimes have significantly lower TAC values than the TAC corresponding to the solutions obtained minimizing CAPEX, illustrating the influence and importance of pumping costs in the design optimization.

NOMENCLATURE

Parameters

$\widehat{a}$	cost parameter [USD/m^2]
$\widehat{Aexc}$	excess area [%]
$\widehat{af}$	annualization factor
$\widehat{b}$	cost parameter
$\widehat{c}_f$	fixed cost of a unit [USD]
$\widehat{Cp}$	heat capacity [J/(kg K)]
$\widehat{ir}$	interest rate
$\widehat{m}_h$	mass flowrate hot stream [kg/s]
$\widehat{m}_c$	ass flowrate cold stream [kg/s]
$\widehat{n}$	number of years
$\widehat{T}_h^{in}$	hot stream inlet temperature [°C]
$\widehat{T}_h^{out}$	hot stream outlet temperature [°C]
$\widehat{T}_c^{in}$	cold stream inlet temperature [°C]
$\widehat{T}_c^{out}$	cold stream outlet temperature [°C]
$\widehat{R}$	ratio of flowrates times *Cp*
$\widehat{P}$	temperature difference ratio
$\widehat{Q}$	total heat transfer [W]

Variables

A_T	total area [m^2]
A_i	area of unit *i* [m^2]
C_N	exchanger CAPEX [USD]
D	shell diameter [m]
F	correction factor
L	tube length [m]
LMTD	logarithmic mean temperature difference [°C]
m	mass flowrate [kg/s]
OC_N	pumping cost
Q_i	heat load for unit *i* [W]
T	temperature [°C]
TAC	total annualized cost [USD/yr]
U	overall heat transfer coefficient

Subscripts

al	fluid allocation
c	cold fluid
h	hot fluid
in	inlet
out	outlet
N	number of units
M	number of passes
T	total

Greek letters

$\widehat{\delta}$	pumping cost coefficient ($/kWh)
$\widehat{\rho}$	density [kg/m^3]
ΔP	pressure drop [Pa]

AUTHOR CONTRIBUTIONS

Miguel J. Bagajewicz: Conceptualization; investigation; writing – original draft; methodology; writing – review and editing;

software; supervision. **Andre L. M. Nahes:** Software; formal analysis; conceptualization; writing – original draft; methodology. **Eduardo M. Queiroz:** Conceptualization; writing – original draft; methodology; writing – review and editing. **Diego G. Oliva:** Conceptualization; investigation; methodology; writing – review and editing; software. **Javier A. Francesconi:** Conceptualization; investigation; methodology; writing – review and editing. **André L. H. Costa:** Conceptualization; investigation; writing – original draft; methodology; writing – review and editing.

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DATA AVAILABILITY STATEMENT

The equations presented in this article and the references as well as all the data needed by any knowledgeable reader to build the procedure in the computational platform and language of choice to reproduce our results are included in the article. Access to the use of the algorithm is temporarily available at https://ou.edu/class/che-design/Optihexx-OU.htm.

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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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