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Alternative Mixed-Integer Linear Programming Formulations for Shell and Tube Heat Exchanger Optimal Design

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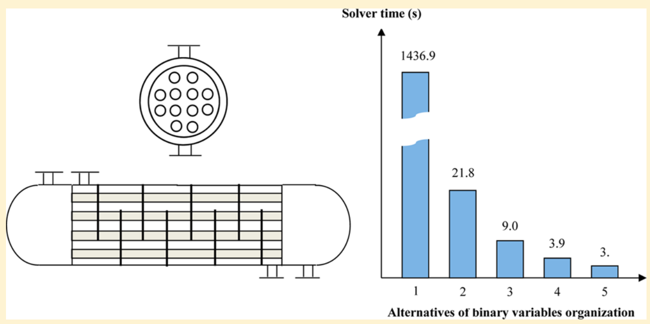
Supporting Information

ABSTRACT: In a recent article (Gonçalves et al., *AIChE J.* **2017**. DOI: 10.1002/aic.15556), we presented a mixed-integer linear programming formulation for the detailed design of shell and tube heat exchangers based on the Kern approach (Kern, D. Q. *Process Heat Transfer*; McGraw Hill, 1950). The formulation relies on the use of standardized values for several mechanical parts, which we express in terms of discrete choices. Because we aim at having this model used as part of more complex models (i.e., heat exchanger networks synthesis), we identified a need to improve its computational efficiency. In this article, we explore several different modeling options to speed up solutions. These options are based on different alternatives of aggregation of the discrete values in relation to the set of binary variables. Numerical results show that these procedures allow large computational effort reductions.



1. INTRODUCTION

Heat exchangers are equipment responsible for the modification of the temperature or physical state of process streams. They are a considerable fraction of the hardware of process industries, where a large process plant (e.g., a refinery) may involve the design of several hundreds of heat exchangers.[3]

The traditional approach for the design of heat exchangers involves the direct intervention of a skilled engineer in a trial-and-error procedure. Most often, the main target is the identification of a feasible heat exchanger candidate just able to fulfill the desired thermal service, not necessarily in an optimal manner. Since, for a given thermal task, there are different feasible alternatives, the quality of the design is highly dependent on the experience of the engineer. This aspect becomes even more important in a scenario of generational transition, where engineering teams were reduced and thermal specialists became rare in chemical and oil companies.[4] Modern textbooks present algorithms for the solution of the design problem, where some level of optimization is included, but these schemes keep the same trial-and-error logic.[5]

By aiming at circumventing the limitations of the traditional design approach, several papers formulate the design problem as an optimization problem.[6] The objective function is usually the minimization of the heat exchanger area restricted by allowable pressure drops or the minimization of the total annualized cost including capital and operating costs in a yearly basis.[7] The main constraints are the thermal and hydraulic equations of the heat exchanger model.

In general, the computational techniques employed for the solution of the design problem can be classified into three categories: heuristic, metaheuristic, and mathematical programming. The heuristic methods explore the search space based on thermo-fluid dynamic relations with the support of graphics[8] or screening tools.[9] Metaheuristic methods consist of randomized algorithms for the search of the optimal solution such as simulated annealing,[10] genetic algorithms,[11] particle swarm optimization,[12] among others. Our article is inserted into the category of mathematical programming. Mathematical programming techniques involve the utilization of deterministic algorithms, where the solution can be found based on formal optimality conditions (local or global). Newer mathematical programming solutions for the design of heat exchangers consider the discrete nature of the design variables and thus yield mixed-integer nonlinear programming (MINLP) problems.[13−15] An important aspect of MINLP alternatives is their nonconvexity, which may present nonconvergence problems and multiple local optima.

Recently, we proposed a mixed-integer linear programming (MILP) formulation for the design problem[1] aimed at the minimization of the heat transfer area. The model is based on the utilization of standard values for several mechanical parts expressed in terms of discrete choices together with one simple hydraulic and thermal model.[2] For example, tube diameters come only in certain discrete values, and their wall thickness is

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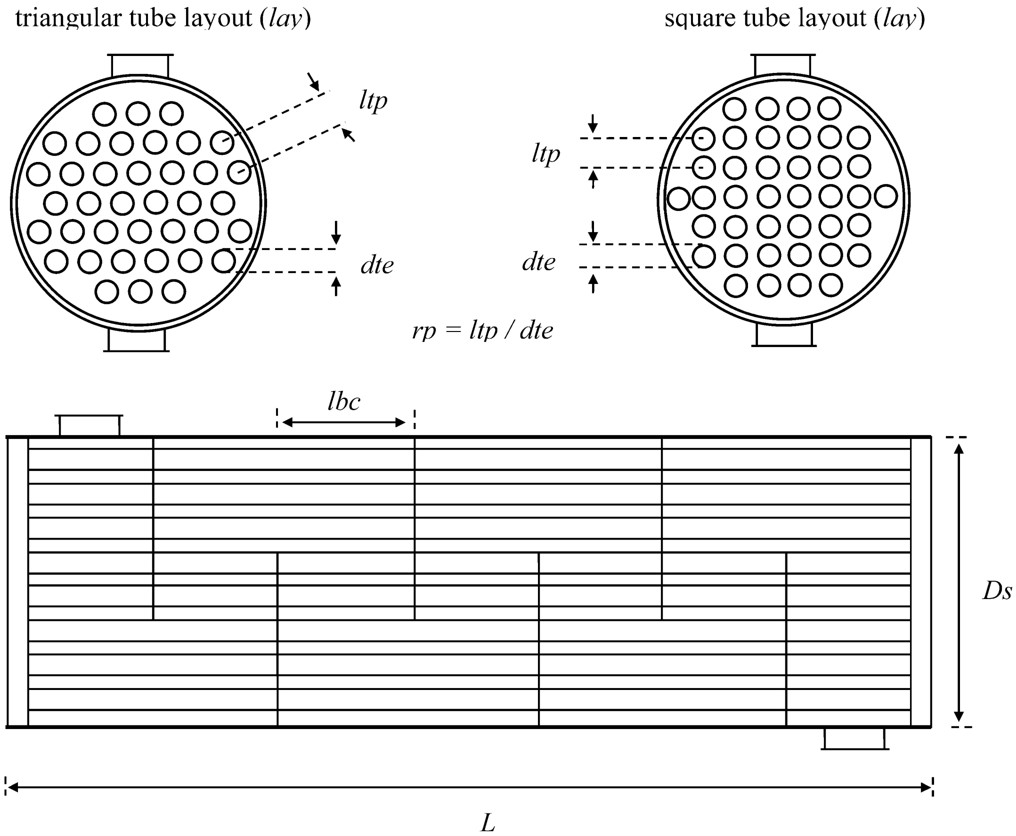

Figure 1. Design variables representation.

dictated by a BWG scale. The same goes for shell diameters, tube length, etc.

The model presented by Gonçalves et al.[1] makes use of several binary variables, representing the discrete options of the geometric parameters. When using these discrete representations together with the nonlinear equations corresponding to the calculation of heat transfer coefficients (shell, tube, and overall), and the pressure drop on both tube and shell sides, the resulting model is a MINLP. We attempted to solve this MINLP model and obtained local minima in several cases. However, when the discrete variables are substituted and several algebraic conversions are made, the resulting model is rigorously linear. Work is underway to apply this methodology to more modern hydraulic and thermal models (e.g., Bell-Delaware and stream analysis).

Despite the MILP superiority in relation to the reduction of the objective function and convergence when compared to the MINLP version, computational times employed are high. Because we want to use this model as part of more complex models (i.e., HEN synthesis), there is a need to improve computational efficiency. Therefore, the focus of this paper is to present alternative MILP formulations for reducing the computational effort.

For each standard value of a design variable, Gonçalves et al.[1] used a corresponding binary variable in their MILP model. The same direct relation between design and binary variables was also employed in Mizutani et al.[13] There are, however, some alternatives in the literature. Ravagnani and Caballero[15] used heat exchanger counting tables to describe some of the discrete values, where each combination of geometric parameters, corresponding to a counting table row, is associated with a single binary variable.

This paper investigates modifications of the arrangement of the set of binary variables for the design of shell-and-tube heat exchangers, in relation to different aggregation options of the discrete values, to improve the computational performance of the MILP solution algorithm.

The article is organized as follows. For completion, we first present the MINLP model as presented by Gonçalves et al.,[1] which is used as starting point to the MILP formulation development. We then discuss the alternative representations of the discrete variables and use one option to present the resulting linear model. Finally, we discuss the computational performance results obtained using different options and the corresponding conclusions.

2. HEAT EXCHANGER MODEL

2.1. Scope. Our optimization problem corresponds to the design of shell and tube heat exchangers with a single E-type shell with single segmental baffles, applied for services without phase change in turbulent flow. There are seven design variables: number of tube passes (*Npt*), tube diameter (outer and inner: *dte* and *dti*), tube layout (*lay*), tube pitch ratio (*rp*), number of baffles (*Nb*), shell diameter (*Ds*), and tube length (*L*). The fluid allocation is assumed to be established by the designer and is not included in the optimization. Figure 1 illustrates the organization of the design variables along the heat exchanger.

The next subsections present the nonlinear model of the heat exchanger design problem that is employed as starting point for the development of all linear formulations compared in this paper. Here, the fixed parameters established prior the optimization are represented with the symbol "^".

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2.2. Shell-Side Thermal and Hydraulic Equations. The convective heat transfer coefficient is evaluated using the Kern model,[2] relating Nusselt (Nus), Reynolds (Res), and Prandtl numbers ($\widehat{Prs}$):

$$Nus = 0.36Res^{0.55}\widehat{Prs}^{1/3} \tag{1}$$

$$Nus = \frac{hsDeq}{\widehat{ks}} \tag{2}$$

$$Res = \frac{Deqvs\widehat{\rho s}}{\widehat{\mu s}} \tag{3}$$

$$\widehat{Prs} = \frac{\widehat{Cps}\widehat{\mu s}}{\widehat{ks}} \tag{4}$$

where hs is the shell-side convective heat transfer coefficient, vs is the flow velocity, and Deq is the equivalent diameter. The thermophysical properties are density, $\widehat{\rho s}$, heat capacity, $\widehat{Cps}$, dynamic viscosity, $\widehat{\mu s}$, and thermal conductivity, $\widehat{ks}$.

The evaluation of the equivalent diameter depends on the tube layout:

$$Deq = \frac{4ltp^2}{\pi dte} - dte \text{ (Square pattern)} \tag{5}$$

$$Deq = \frac{3.46ltp^2}{\pi dte} - dte \text{ (Triangular pattern)} \tag{6}$$

where ltp is the tube pitch.

The expression of the shell-side flow velocity is

$$vs = \frac{\widehat{ms}}{\widehat{\rho s}Ar} \tag{7}$$

where $\widehat{ms}$ is the mass flow rate. The flow area in the shell-side flow is given by

$$Ar = DsFARlbc \tag{8}$$

where lbc is the baffle spacing. The expression of the free-area ratio, FAR, is

$$FAR = \frac{ltp - dte}{ltp} = 1 - \frac{1}{rp} \tag{9}$$

The head loss in the shell-side flow is also based on the Kern model:[2]

$$\frac{\Delta Ps}{\widehat{\rho s}\hat{g}} = fs\frac{Ds(Nb + 1)}{Deq}\left(\frac{vs^2}{2\hat{g}}\right) \tag{10}$$

where ΔPs is the shell-side pressure drop, and fs is the shell-side friction factor.

The shell-side friction factor is given by

$$fs = 1.728Res^{-0.188} \tag{11}$$

The relation between the number of baffles and the baffle spacing is

$$Nb = \frac{L}{lbc} - 1 \tag{12}$$

2.3. Tube-Side Thermal and Hydraulic Equations. The convective heat transfer coefficient is evaluated using the Dittus-Boelter correlation,[16] which relates Nusselt (Nut), Reynolds (Ret), and Prandtl numbers ($\widehat{Prt}$) of the tube-side flow:

$$Nut = 0.023Ret^{0.8}\widehat{Prt}^{n} \tag{13}$$

$$Nut = \frac{htdti}{\widehat{kt}} \tag{14}$$

$$Ret = \frac{dtivt\widehat{\rho t}}{\widehat{\mu t}} \tag{15}$$

$$\widehat{Prt} = \frac{\widehat{Cpt}\widehat{\mu t}}{\widehat{kt}} \tag{16}$$

where ht is the convective heat transfer coefficient, vt is the flow velocity, $\widehat{\rho t}$ is the density, $\widehat{Cpt}$ is the heat capacity, $\widehat{\mu t}$ is the dynamic viscosity, $\widehat{kt}$ is the thermal conductivity, and the parameter n is equal to 0.4 for heating and 0.3 for cooling.

The expression of the flow velocity in the tube-side is

$$vt = \frac{4\widehat{mt}}{Ntp\pi\widehat{\rho t}dti^2} \tag{17}$$

where $\widehat{mt}$ is the mass flow rate, and Ntp is the number of tubes per pass.

The head loss in the tube-side flow is given by[17]

$$\frac{\Delta Pt}{\widehat{\rho t}\hat{g}} = \frac{ftNptLvt^2}{2\hat{g}dti} + \frac{KNptvt^2}{2\hat{g}} \tag{18}$$

where ft is the tube-side friction factor. The parameter K, associated with the head loss in the heads, is equal to 0.9 for one tube pass and 1.6 for two or more tube passes.

The Darcy friction factor for turbulent flow is given by[17]

$$ft = 0.014 + \frac{1.056}{Ret^{0.42}} \tag{19}$$

2.4. Heat Transfer Rate Equation and Overall Heat Transfer Coefficient. On the basis of the LMTD method, and considering a design margin ("excess area", $\widehat{Aexc}$), the heat transfer area must obey the following relation:

$$UA \geq \left(1 + \frac{\widehat{Aexc}}{100}\right)\frac{\hat{Q}}{\widehat{\Delta Tlm}F} \tag{20}$$

where U is the overall heat transfer coefficient, A is the heat transfer area, $\hat{Q}$ is the heat load, $\widehat{\Delta Tlm}$ is the logarithmic mean temperature difference (LMTD), and F is the LMTD correction factor.[16]

The area of the heat exchanger (A) depends on the total number of tubes (Ntt):

$$A = Ntt\pi dteL \tag{21}$$

The expression for the evaluation of the overall heat transfer coefficient (U) is

$$U = \frac{1}{\frac{dte}{dtiht} + \frac{\widehat{Rft}dte}{dti} + \frac{dte\ln\left(\frac{dte}{dti}\right)}{2\widehat{ktube}} + \widehat{Rfs} + \frac{1}{hs}} \tag{22}$$

where $\widehat{ktube}$ is the thermal conductivity of the tube wall, and $\widehat{Rft}$ and $\widehat{Rfs}$ are the tube-side and shell-side fouling factors.

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The LMTD correction factor is equal to 1 for one tube pass and is equal to the following expression for an even number of tube passes:

$$F = \frac{(\hat{R}^2 + 1)^{0.5} \ln\left(\frac{(1-\hat{P})}{(1-\hat{R}\hat{P})}\right)}{(\hat{R} - 1) \ln\left(\frac{2-\hat{P}(\hat{R}+1-(\hat{R}^2+1)^{0.5})}{2-\hat{P}(\hat{R}+1+(\hat{R}^2+1)^{0.5})}\right)} \quad (23)$$

where

$$\hat{R} = \frac{\widehat{Thi} - \widehat{Tho}}{\widehat{Tco} - \widehat{Tci}} \quad (24)$$

$$\hat{P} = \frac{\widehat{Tco} - \widehat{Tci}}{\widehat{Thi} - \widehat{Tci}} \quad (25)$$

2.5. Bounds on Pressure Drops, Flow Velocities, and Reynolds Numbers. The lower and upper bounds on pressure drops, velocities, and Reynolds numbers are represented by

$$\Delta Ps \leq \widehat{\Delta Psdisp} \quad (26)$$

$$\Delta Pt \leq \widehat{\Delta Ptdisp} \quad (27)$$

$$vs \geq \widehat{vsmin} \quad (28)$$

$$vs \leq \widehat{vsmax} \quad (29)$$

$$vt \geq \widehat{vtmin} \quad (30)$$

$$vt \leq \widehat{vtmax} \quad (31)$$

$$Res \geq 2 \times 10^3 \quad (32)$$

$$Ret \geq 10^4 \quad (33)$$

2.6. Geometric Constraints. Design recommendations impose the following set of constraints:[18,19]

$$lbc \geq 0.2Ds \quad (34)$$

$$lbc \leq 1.0Ds \quad (35)$$

$$L \geq 3Ds \quad (36)$$

$$L \leq 15Ds \quad (37)$$

2.7. Objective Function. The objective function of the optimization is the minimization of the heat transfer area:

$$\min A \quad (38)$$

2.8. Discrete Variables. As anticipated above, several variables can only adopt discrete values according to engineering practice[18] and TEMA standards.[20] They are inner and outer tube diameter (dti and dte), tube length (L), number of baffles (Nb), number of tube passes (Npt), pitch ratio (rp), shell diameter (Ds), and tube layout (lay). Thus, we substitute the following expressions in the above presented model:

$$x = \sum_i \widehat{xd}_i y_i \quad (39)$$

$$\sum_i y_i = 1 \quad (40)$$

where x represents a generic discrete variable, $\widehat{xd}_i$ the value of option i for this variable, and y_i a binary variable that is used to make the model choose one and only one option.

2.9. MILP Model. After the substitution of the discrete variables is made, the model results in a complex mixed integer nonlinear programming (MINLP) model that contains products of binaries and continuous variables. In our previous contribution,[1] we converted this rigorous MINLP model into a rigorous linear model (MILP), making no simplifying assumptions. Thus, a rigorous solution of the MILP is also a rigorous solution of the MINLP. Moreover, because of its linearity, the MILP model renders a global solution. As we have shown in our previous paper, solving the MINLP model using local solvers many times rendered a nonglobal local solution.

2.10. MILP Model Performance. After testing several options of binary variable prioritizations in the MILP branch and bound, we came up with one option that rendered solutions in the range from 153−2824 s, with an average of 1458 s for 10 test problems (computer with a processor Intel Core i7 3.40 GHz with 12.0 GB RAM memory). This performance time is more than acceptable for a stand-alone run, even if the number of geometric options is increased. However, this computational time is high when, for example, repeated runs are needed to handle uncertainty and when the model becomes a submodel of others, like the simultaneous design of a heat exchanger network with detailed heat exchanger design. We now explore different rigorous alternatives of binary variable aggregation, all having different computational efficiency still rendering the same result.

3. ALTERNATIVES OF BINARY VARIABLES ORGANIZATION

We present five different aggregations of binary variables leading to MILP formulations, which render the same result each with its own computational efficiency.

3.1. Alternative 1. In this alternative, each set of binary variables corresponds to a discrete variable referred to as seen in the work of Gonçalves et al.[1] Therefore, yd_{sd} corresponds to the variable representing the tube diameter, yDs_{sDs} corresponds to shell diameter, yL_{sL} corresponds to tube length, $ylay_{slay}$ corresponds to tube layout, yNb_{sNb} corresponds to number of baffles, $yNpt_{sNpt}$ corresponds to number of tube passes, and yrp_{srp} corresponds to tube pitch ratio.

3.2. Alternative 2. A counting table structure can be employed to organize the discrete values of the shell diameter, tube diameter, tube layout, number of tube passes, and tube pitch ratio, where only one set of binary variables, $yrow_{srow}$, is employed to represent these discrete values. In this context, $srow$ is a multi-index set, that is, $srow = (sd, sDs, slay, sNpt, srp)$. The tube length and the number of baffles remain represented by the original sets of binary variables yL_{sL} and yNb_{sNb}.

3.3. Alternative 3. This alternative represents the discrete values in two tables. The first one corresponds to the counting table, as shown in the previous alternative, where the corresponding set of binaries is $yrow1_{srow1}$ with $srow1 = (sd, sDs, slay, sNpt, srp)$. The second table contains all pairs of discrete values of tube length and number of baffles. The set of binaries that represents these discrete values is $yrow2_{srow2}$ with $srow2 = (sNb, sL)$.

3.4. Alternative 4. Another possible combination was the use of two set of binary variables: $yrow1_{srow1}$ with $srow1 = (sd, sDs, slay, sNpt, srp, sL)$, representing all variables but the number of baffles, which is represented by the original binary yNb_{sNb}.

3.5. Alternative 5. The last alternative investigated in this work is the use of a unique set of binary variables, $yrow_{srow}$, which corresponds to all discrete variables, $srow = (sd, sDs, slay, sNpt, srp, sL, sNb)$.

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Table 1. Alternatives Investigated of Binary Variables

alternative	binary variable {original discrete variable}
1	$yd_{sd}\{dt\}$, $yDs_{sDs}\{Ds\}$, $ylay_{slay}\{lay\}$, $yNpt_{sNpt}\{Npt\}$ $yrp_{srp}\{rp\}$, $yL_{sL}\{L\}$, $yNb_{sNb}\{Nb\}$
2	$yrow_{srow}\{dt, Ds, lay, Npt, rp\}$, $yL_{sL}\{L\}$, $yNb_{sNb}\{Nb\}$
3	$yrow1_{srow1}\{dt, Ds, lay, Npt, rp\}$, $yrow2_{srow2}\{L, Nb\}$
4	$yrow_{srow}\{dt, Ds, lay, Npt, rp, L\}$, $yNb_{sNb}\{Nb\}$
5	$yrow_{srow}\{dt, Ds, lay, Npt, rp, L, Nb\}$

Table 1 contains an overview of the different combinations between binary variables and the original discrete variables.

4. DEVELOPMENT OF THE MILP FORMULATIONS

The new MILP formulations are built starting from the MINLP model (eqs 1−38) through three main steps: the organization of the data table of the discrete variables, the model reformulation, and the conversion to a linear model. For reasons of space and because the procedure is very similar when aggregates of binary variables is made, we only illustrate Alternative 5 in detail (this alternative is associated with the highest reduction of the computational time consumed by the MILP solver, as it will be shown in the results). Alternative 1 is identical of the proposal of Gonçalves et al.,[1] and the equations of Alternatives 2, 3, and 4 can be found in the Section 1 of the Supporting Information.

4.1. Organization of Data Table of Discrete Variables.

The original relation between the discrete variables and the corresponding binaries is given by (as it is employed in Alternative 1):

$$dte = \sum_{sd=1}^{sdmax} \widehat{pdte}_{sd} yd_{sd} \tag{41}$$

$$dti = \sum_{sd=1}^{sdmax} \widehat{pdti}_{sd} yd_{sd} \tag{42}$$

$$Ds = \sum_{sDs=1}^{sDsmax} \widehat{pDs}_{sDs} yDs_{sDs} \tag{43}$$

$$lay = \sum_{slay=1}^{slaymax} \widehat{play}_{slay} ylay_{slay} \tag{44}$$

$$Npt = \sum_{sNpt=1}^{sNptmax} \widehat{pNpt}_{sNpt} yNpt_{sNpt} \tag{45}$$

$$rp = \sum_{srp=1}^{srpmax} \widehat{prp}_{srp} yrp_{srp} \tag{46}$$

$$L = \sum_{sL=1}^{sLmax} \widehat{pL}_{sL} yL_{sL} \tag{47}$$

$$Nb = \sum_{sNb=1}^{sNbmax} \widehat{pNb}_{sNb} yNb_{sNb} \tag{48}$$

with the following equations needed to guarantee only one choice among many:

$$\sum_{sd=1}^{sdmax} yd_{sd} = 1 \tag{49}$$

$$\sum_{sDs=1}^{sDsmax} yDs_{sDs} = 1 \tag{50}$$

$$\sum_{slay=1}^{slaymax} ylay_{slay} = 1 \tag{51}$$

$$\sum_{sNpt=1}^{sNptmax} yNpt_{sNpt} = 1 \tag{52}$$

$$\sum_{srp=1}^{srpmax} yrp_{srp} = 1 \tag{53}$$

$$\sum_{sL=1}^{sLmax} yL_{sL} = 1 \tag{54}$$

$$\sum_{sNb=1}^{sNbmax} yNb_{sNb} = 1 \tag{55}$$

According to the aggregation strategy employed in the development of the new MILP formulations, the parameters that represent the discrete values can be grouped in one or more tables. Therefore, several discrete values of the design variables are identified by the same index (a multi-index related to the corresponding original indices). For example, in Alternative 5, the multi-index *srow* represents the discrete values of all design variables. The corresponding set of parameters that compose the table are defined from the original ones, as follows:

$$\widehat{Pdte}_{srow} = \widehat{pdte}_{sd} \tag{56}$$

$$\widehat{Pdti}_{srow} = \widehat{pdti}_{sd} \tag{57}$$

$$\widehat{PDs}_{srow} = \widehat{pDs}_{sDs} \tag{58}$$

$$\widehat{Play}_{srow} = \widehat{play}_{slay} \tag{59}$$

$$\widehat{PNpt}_{srow} = \widehat{pNpt}_{sNpt} \tag{60}$$

$$\widehat{Prp}_{srow} = \widehat{prp}_{srp} \tag{61}$$

$$\widehat{PL}_{srow} = \widehat{pL}_{sL} \tag{62}$$

$$\widehat{PNb}_{srow} = \widehat{pNb}_{sNb} \tag{63}$$

Consequently, different discrete variables become associated with the same set of binaries. In Alternative 5, all discrete variables are described by the set of binaries $yrow_{srow}$, thus yielding

$$dte = \sum_{srow} \widehat{Pdte}_{srow} yrow_{srow} \tag{64}$$

$$dti = \sum_{srow} \widehat{Pdti}_{srow} yrow_{srow} \tag{65}$$

$$Ds = \sum_{srow} \widehat{PDs}_{srow} yrow_{srow} \tag{66}$$

$$lay = \sum_{srow} \widehat{Play}_{srow} yrow_{srow} \tag{67}$$

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$$Npt = \sum_{srow} \widehat{PNpt}_{srow} yrow_{srow} \tag{68}$$

$$rp = \sum_{srow} \widehat{Prp}_{srow} yrow_{srow} \tag{69}$$

$$L = \sum_{srow} \widehat{PL}_{srow} yrow_{srow} \tag{70}$$

$$Nb = \sum_{srow} \widehat{PNb}_{srow} yrow_{srow} \tag{71}$$

$$\sum_{srow} yrow_{srow} = 1 \tag{72}$$

4.2. Model Reformulation. In this step, the model equations are modified through the substitution of the discrete variables by their binary representation. This reformulation step also involves a procedure for the organization of the resultant expressions containing binary variables, as described in the following paragraphs.

As stated, the relation between a design variable x and their discrete values $\widehat{xd}_i$, using binary variables y_i, is expressed by eqs 39 and 40, where i can be a multi-index.

The substitution of a set of discrete variables $p, q, \cdots, z$ by its binary representation in the heat exchanger model yields terms of the form $p^{n1}q^{n2}\cdots z^{nm}$ that are substituted as follows:

$$p^{n1}q^{n2}\cdots z^{nm} = [\sum_i \widehat{pd}_i yp_i]^{n1}[\sum_j \widehat{qd}_j yq_j]^{n2}[\sum_k \widehat{zd}_k yz_k]^{nm} \tag{73}$$

Because all binary variables are equal to 1 only once in the corresponding set, this equation is equivalent to

$$p^{n1}q^{n2}\cdots z^{nm} = \sum_{i,j,..k} \widehat{pd}_i^{\,n1}\widehat{qd}_j^{\,n2}\cdots..\widehat{qd}_k^{\,nm} yp_i yq_j \cdots yz_k \tag{74}$$

After the application of this procedure, the reformulated model becomes composed of several expressions containing multiple summations of products of binary variables.

4.3. Conversion to a Linear Model. The product of binaries obtained from the discrete variable substitution can be reorganized in equivalent linear expressions, as discussed below.

Let the product of binaries be substituted by a nonnegative variable $w_{i,j,\cdots,k}$:

$$p^{n1}q^{n2}\cdots z^{nm} = \sum_{i,j,..k} \widehat{pd}_i^{\,n1}\widehat{qd}_j^{\,n2}\cdots..\widehat{qd}_k^{\,nm} w_{i,j,\cdots k} \tag{75}$$

where:

$$w_{i,j,\cdots,k} = yp_i yq_j \cdots yz_k \tag{76}$$

However, the nonlinearity existent in this equation can be eliminated through the substitution of this expression by the equivalent set of linear inequality constraints:

$$w_{i,j,\cdots,k} \le yp_i \tag{77}$$

$$w_{i,j,\cdots,k} \le yq_j \tag{78}$$

$$w_{i,j,\cdots,k} \le yz_k \tag{79}$$

...

$$w_{i,j,\cdots,k} \ge yp_i + yq_j + \cdots + yz_k - (m-1) \tag{80}$$

where m is the number of binary variables in the product. Since Alternative 5 contains only one set of binary variables (in fact, it is an integer linear programming, ILP), this step is not necessary in its development, but it is fundamental to the other alternatives with lower aggregation levels.

5. FORMULATION WITH A SINGLE SET OF BINARIES

This section presents the complete linear formulation of the optimal heat exchanger design problem based on a unique set of binary variables to represent the discrete options of the design variables (Alternative 5).

5.1. Binary Variables Equality Constraints. This constraint imposes that only one design alternative must be chosen:

$$\sum_{srow} yrow_{srow} = 1 \tag{81}$$

5.2. Heat Transfer Rate Equation. The expressions of all heat transfer coefficients and the heat transfer area are inserted into the heat transfer equation, thus yielding

$$\begin{aligned} &\hat{Q}\Bigg(\sum_{srow} \frac{\widehat{Pdte}_{srow}}{\widehat{Pht}_{srow}\widehat{Pdti}_{srow}} yrow_{srow} + \widehat{Rft}\sum_{srow}\frac{\widehat{Pdte}_{srow}}{\widehat{Pdti}_{srow}} yrow_{srow} \\ &+ \frac{\sum_{srow}\widehat{Pdte}_{srow} yrow_{srow}\ln\left(\frac{\widehat{Pdte}_{srow}}{\widehat{Pdti}_{srow}}\right)}{2\widehat{ktube}} + \widehat{Rfs} + \sum_{srow}\frac{1}{\widehat{Phs}_{srow}} yrow_{srow}\Bigg) \\ &\le \left(\frac{100}{100 + \widehat{Aexc}}\right)\left(\pi\sum_{srow}\widehat{PNtt}_{srow}\widehat{Pdte}_{srow}\widehat{PL}_{srow} yrow_{srow}\right)\widehat{\Delta Tlm}\hat{F}_{srow} \end{aligned} \tag{82}$$

where $\widehat{PNtt}_{srow}$ is the total number of tubes, and

$$\widehat{Pht}_{srow} = \frac{\widehat{kt}0.023\left(\frac{4\widehat{mt}}{\pi\widehat{\mu t}}\right)^{0.8}\widehat{Prt}^{\,n}}{\widehat{Pdti}_{srow}^{\,1.8}}\left(\frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow}}\right)^{0.8} \tag{83}$$

$$\widehat{Phs}_{srow} = \frac{\widehat{ks}0.36\left(\frac{\widehat{ms}}{\widehat{\mu s}}\right)^{0.55}\widehat{Prs}^{\,1/3}}{\widehat{PDeq}_{srow}^{\,0.45}}\left(\frac{(\widehat{PNb}_{srow}+1)}{\widehat{PDs}_{srow}\widehat{PFAR}_{srow}\widehat{PL}_{srow}}\right)^{0.55} \tag{84}$$

$$\widehat{PFAR}_{srow} = 1 - \frac{1}{\widehat{Prp}_{srow}} \tag{85}$$

$$\widehat{pDeq}_{srow} = \frac{\widehat{aDeq}_{srow}\widehat{Prp}_{srow}^{\,2}\widehat{Pdte}_{srow}^{\,2}}{\pi\widehat{Pdte}_{srow}} - \widehat{Pdte}_{srow} \tag{86}$$

$$\widehat{aDeq}_{srow} = \begin{cases} 4 & \text{if } \widehat{Play}_{srow} = 1 \\ 3.46 & \text{if } \widehat{Play}_{srow} = 2 \end{cases} \tag{87}$$

$$\hat{F}_{srow} = \begin{cases} \dfrac{(\hat{R}^2+1)^{0.5}\ln\left(\frac{(1-\hat{P})}{(1-\hat{R}\hat{P})}\right)}{(\hat{R}-1)\ln\left(\frac{2-\hat{P}(\hat{R}+1-(\hat{R}^2+1)^{0.5})}{2-\hat{P}(\hat{R}+1+(\hat{R}^2+1)^{0.5})}\right)} & \text{if } \widehat{PNpt}_{srow} \ne 1 \\ 1 & \text{if } \widehat{PNpt}_{srow} = 1 \end{cases} \tag{88}$$

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5.3. Bounds on Pressure Drops, Flow Velocities, and Reynolds Numbers. The bounds on the shell-side and tube-side pressure drops are expressed by

$$\sum_{srow} \widehat{P\Delta Ps}_{srow} yrow_{srow} \leq \widehat{\Delta Ps}disp \tag{89}$$

$$\sum_{srow} \widehat{P\Delta Ptturb1}_{srow} yrow_{srow} + \sum_{srow} \widehat{P\Delta Ptturb2}_{srow} yrow_{srow} + \sum_{srow} \widehat{P\Delta Ptcab}_{srow} \hat{K}_{srow} yrow_{srow} \leq \widehat{\Delta Pt}disp \tag{90}$$

where

$$\widehat{P\Delta Ps}_{srow} = 0.864 \frac{\widehat{ms}^{1.812} \widehat{\mu s}^{0.188}}{\widehat{\rho s}} \left(\frac{(\widehat{PNb}_{srow} + 1)^{2.812}}{\widehat{PDs}_{srow}^{0.812} (\widehat{PFAR}_{srow} \widehat{PL}_{srow})^{1.812} (\widehat{PDeq}_{srow})^{1.188}} \right) \tag{91}$$

$$P\Delta \widehat{Ptturb1}_{srow} = \left(\frac{0.112 \widehat{mt}^2}{\pi^2 \rho t} \right) \left(\frac{\widehat{PNpt}_{srow}^{3} \widehat{PL}_{srow}}{\widehat{PNtt}_{srow}^{2} \widehat{Pdti}_{srow}^{5}} \right) \tag{92}$$

$$P\Delta \widehat{Ptturb2}_{srow} = (0.528) \left(\frac{4^{1.58} \widehat{mt}^{1.58} \widehat{\mu t}^{0.42}}{\pi^{1.58} \widehat{\rho t}} \right) \frac{\widehat{PNpt}_{srow}^{2.58} \widehat{PL}_{srow}}{\widehat{PNtt}_{srow}^{1.58} \widehat{Pdti}_{srow}^{4.58}} \tag{93}$$

$$P\Delta \widehat{Ptcab}_{srow} = \left(\frac{8 \widehat{mt}^2}{\pi^2 \widehat{\rho t}} \right) \frac{\widehat{PNpt}_{srow}^{3}}{\widehat{PNtt}_{srow}^{2} \widehat{Pdti}_{srow}^{4}} \tag{94}$$

The bounds on the shell-side and tube-side flow velocities are

$$\widehat{vs}min \leq \frac{\widehat{ms}}{\widehat{\rho s}} \sum_{srow} \frac{(\widehat{PNb}_{srow} + 1)}{\widehat{PDs}_{srow} \widehat{PFAR}_{srow} \widehat{PL}_{srow}} yrow_{srow} \tag{95}$$

$$\widehat{vs}max \geq \frac{\widehat{ms}}{\widehat{\rho s}} \sum_{srow} \frac{(\widehat{PNb}_{srow} + 1)}{\widehat{PDs}_{srow} \widehat{PFAR}_{srow} \widehat{PL}_{srow}} yrow_{srow} \tag{96}$$

$$\widehat{vt}min \leq \frac{4\widehat{mt}}{\pi \widehat{\rho t}} \sum_{srow} \frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow} \widehat{Pdti}_{srow}^{2}} yrow_{srow} \tag{97}$$

$$\widehat{vt}max \geq \frac{4\widehat{mt}}{\pi \widehat{\rho t}} \sum_{srow} \frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow} \widehat{Pdti}_{srow}^{2}} yrow_{srow} \tag{98}$$

The bounds on the Reynolds numbers are

$$\frac{\widehat{ms}}{\widehat{\mu s}} \sum_{srow} \frac{\widehat{PDeq}_{srow} (\widehat{PNb}_{srow} + 1)}{\widehat{PDs}_{srow} \widehat{PFAR}_{srow} \widehat{PL}_{srow}} yrow_{srow} \geq 2.10^3 \tag{99}$$

$$\frac{4\widehat{mt}}{\pi \widehat{\mu t}} \sum_{srow} \frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow} \widehat{Pdti}_{srow}} yrow_{srow} \geq 10^4 \tag{100}$$

5.4. Geometric Constraints. The maximum and minimum baffle spacing constraints are

$$\sum_{srow} \frac{\widehat{PL}_{srow}}{(\widehat{PNb}_{srow} + 1)} yrow_{srow} \leq 1.0 \sum_{srow} \widehat{PDs}_{srow} yrow_{srow} \tag{101}$$

$$\sum_{srow} \frac{\widehat{PL}_{srow}}{(\widehat{PNb}_{srow} + 1)} yrow_{srow} \geq 0.2 \sum_{srow} \widehat{PDs}_{srow} yrow_{srow} \tag{102}$$

The constraints related to the ratio between the tube length and the shell diameter are

$$\sum_{srow} \widehat{PL}_{srow} yrow_{srow} \leq 15 \sum_{srow} \widehat{PDs}_{srow} yrow_{srow} \tag{103}$$

$$\sum_{srow} \widehat{PL}_{srow} yrow_{srow} \geq 3 \sum_{srow} \widehat{PDs}_{srow} yrow_{srow} \tag{104}$$

5.5. Objective Function. The expression of the objective function in relation to the binary variables is given by

$$\min \pi \sum_{srow} \widehat{PNtt}_{srow} \widehat{Pdte}_{srow} \widehat{PL}_{srow} yrow_{srow} \tag{105}$$

5.6. Additional Constraints for the Reduction of the Search Space. These extra sets of constraints aim to accelerate the search and are derived from the bounds on velocities, shell-side pressure drop, and tube length/shell diameter ratio. A lower bound on the heat transfer area is also included based on maximum flow velocities (see Gonçalves et al.[1] for further details).

Flow Velocities Bounds:

$$yrow_{srow} = 0 \quad \text{for } srow \in (Svsmin\ out \cup Svsmax\ out) \tag{106}$$

$$yrow_{srow} = 0 \quad \text{for } srow \in (Svtmin\ out \cup Svtmax\ out) \tag{107}$$

The sets *Svsminout*, *Svsmaxout*, *Svtminout*, and *Svtmaxout* are given by

$$Svsminout = \left\{ srow / \frac{\widehat{ms}}{\widehat{\rho s}} \frac{(\widehat{PNb}_{srow} + 1)}{\widehat{PDs}_{srow} \widehat{PFAR}_{srow} \widehat{PL}_{srow}} \leq \widehat{vs}min - \varepsilon \right\} \tag{108}$$

$$Svsmaxout = \left\{ srow / \frac{\widehat{ms}}{\widehat{\rho s}} \frac{(\widehat{PNb}_{srow} + 1)}{\widehat{PDs}_{srow} \widehat{PFAR}_{srow} \widehat{PL}_{srow}} \geq \widehat{vs}max + \varepsilon \right\} \tag{109}$$

$$Svtminout = \left\{ srow / \frac{4\widehat{mt}}{\pi \widehat{\rho t}} \frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow} \widehat{Pdti}_{srow}^{2}} \leq \widehat{vt}min - \varepsilon \right\} \tag{110}$$

$$Svtmaxout = \left\{ srow / \frac{4\widehat{mt}}{\pi \widehat{\rho t}} \frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow} \widehat{Pdti}_{srow}^{2}} \geq \widehat{vt}max + \varepsilon \right\} \tag{111}$$

where ε is a small positive number.

Shell-Side Pressure Upper Bound:

$$yrow_{srow} = 0 \quad \text{for } srow \in SDPsmaxout \tag{112}$$

where the set *SDPsmaxout* is given by

$$SDPsmaxout = \{ srow / \widehat{P\Delta Ps}_{srow} \geq \widehat{\Delta Ps}disp + \varepsilon \} \tag{113}$$

Baffle Spacing:

$$yrow_{srow} = 0 \quad \text{for } srow \in (SLNbminout \cup SLNbmaxout) \tag{114}$$

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where the sets $SLNbminout$ and $SLNbmaxout$ are given by

$$SLNbminout = \left\{ srow / \frac{\widehat{PL}_{srow}}{\widehat{PNb}_{srow} + 1} \leq 0.2\widehat{PDs}_{srow} - \varepsilon \right\} \tag{115}$$

$$SLNbmaxout = \left\{ srow / \frac{\widehat{PL}_{srow}}{\widehat{PNb}_{srow} + 1} \geq 1.0\widehat{PDs}_{srow} + \varepsilon \right\} \tag{116}$$

Tube Length/Shell Diameter Ratio:

$$yrow_{srow} = 0 \text{ for } srow \in (SLDminout \cup SLDmaxout) \tag{117}$$

where the sets $SLDminout$ and $SLDmaxout$ are given by

$$SLDminout = \{srow / \widehat{PL}_{srow} \leq 3\widehat{PDs}_{srow} - \varepsilon\} \tag{118}$$

$$SLDmaxout = \{srow / \widehat{PL}_{srow} \geq 15\widehat{PDs}_{srow} + \varepsilon\} \tag{119}$$

Heat Transfer Area:

$$yrow_{srow} = 0 \quad \text{for } srow \in SAminout \tag{120}$$

where the set of heat exchangers with area lower than the minimum possible is

$$SAminout = \{srow / \pi \widehat{PNtt}_{srow} \widehat{Pdte}_{srow} \widehat{PL}_{srow} \leq \widehat{Amin} - \varepsilon\} \tag{121}$$

The lower bound on the heat transfer area can be determined by

$$\widehat{Amin} = \frac{\hat{Q}}{\widehat{Umax}\ \widehat{\Delta Tlm}} \tag{122}$$

$$\widehat{Umax} = \frac{1}{\frac{1}{\widehat{htmax}}\widehat{drmin} + \widehat{Rft}\cdot\widehat{drmin} + \frac{\widehat{Pdte}_{srow}\ln(\widehat{drmin})}{2\widehat{ktube}} + \widehat{Rfs} + \frac{1}{\widehat{hsmax}}} \tag{123}$$

$$\widehat{htmax} = max(\widehat{Pht}_{srow}) \tag{124}$$

$$\widehat{hsmax} = max(\widehat{Phs}_{srow}) \tag{125}$$

$$\widehat{drmin} = min(\widehat{Pdte}_{srow} / \widehat{Pdti}_{srow}) \tag{126}$$

6. RESULTS

The five aggregation alternatives of the discrete variables were applied to the sample of ten thermal tasks proposed by Gonçalves et al.[1] involving different heating and cooling services. The complete description of each problem is available at the Section 2 of the Supporting Information material (Tables S1, S2, and S3). The standard values of the discrete variables employed in the solutions are shown in Table 2, related to a fixed tubesheet type exchanger with tube thickness of 1.65 mm (BWG 16) and thermal conductivity of the tube wall equal to 50 W/m K. The minimum excess area is 11%, and the tube count data are based on Kakaç et al.[21]

These problems were solved using the five alternatives of MILP formulations described in Table 1, implemented in the optimization software GAMS using the solver CPLEX.

The comparison of the solution time demanded by each alternative (elapsed time) and the time consumed by the solver itself are shown in Table 3, together with the optimal value of the objective function (since all alternatives are MILP problems, the solution found is always the same, corresponding to the global optimum). The computational times were measured using a computer with a processor Intel Core i7 3.40 GHz with 12.0 GB RAM memory. The details of each design solution are available at the Section 3 of the Supporting Information material (Tables S4, S5, S6, and S7).

The solution times in Table 3 for the Alternative 1 differ slightly from those reported by Gonçalves et al.[1] due to eventual computer performance fluctuations (the registered times are wall times from new independent runs conducted in this paper for the same problems).

The analysis of Table 3 indicates that the proposed procedure of aggregation of the binary variables (Alternatives 2−5) allows large reductions of the computational effort in relation to the original formulation (Alternative 1). The average time consumed by the solver is associated with reductions ranging from 98.50−99.79%. The corresponding reductions of the total elapsed time are similar, ranging from 98.10−99.33%.

By comparing the time consumed by the solver in the different alternatives, it is possible to observe that there is a reduction

Table 2. Standard Values of the Discrete Design Variables

variable	values
outer tube diameter $\widehat{pdte}_{sd}$ (m)	0.019, 0.025, 0.032, 0.038, 0.051
tube length, $\widehat{pL}_{sL}$ (m)	1.220,1.829,2.439, 3.049, 3.659, 4.877, 6.098
number of baffles, $\widehat{pNb}_{sNb}$	1, 2, ⋯, 20
number of tube passes, $\widehat{pNpt}_{sNpt}$	1, 2, 4, 6
tube pitch ratio, $\widehat{prp}_{srp}$	1.25, 1.33, 1.50
shell diameter, $\widehat{pDs}_{sDs}$ (m)	0.787, 0.838, 0.889, 0.940,0. 991, 1.067, 1.143, 1.219, 1.372, 1.524
tube layout, $\widehat{play}_{slay}$	1 = square, 2 = triangular

Table 3. Performance Comparison

example	heat transfer area (m^2)	solution time (s) solver time (s) 1	2	3	4	5
1	624	1730	19	13	11	12
		1726	13	6	4	3
2	319	1574	44	12	10	11
		1571	39	6	4	3
3	199	212	10	11	9	11
		208	5	5	3	3
4	872	139	11	11	9	12
		136	5	5	3	3
5	144	869	19	11	10	12
		865	13	6	4	3
6	332	2755	49	12	9	11
		2751	44	6	4	3
7	207	2535	15	12	9	12
		2532	9	5	4	3
8	914	173	11	13	9	12
		169	6	7	3	3
9	287	2077	53	31	11	12
		2073	47	25	6	3
10	327	2342	43	25	10	12
		2338	37	19	4	3
average		1440.6	27.4	15.1	9.7	11.7
		1436.9	21.8	9.0	3.9	3.0

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trend from Alternative 1 to Alternative 5, that is, the increase of the binary variables aggregation decreases the solver time. The behavior of the total elapsed time is similar, but the demand for processing larger data sets associated with the variable aggregation procedure implies in slightly higher computing times before the solver starts in these alternatives. Therefore, the lowest solver time is associated with the Alternative 5, but the lowest elapsed time corresponds to Alternative 4 (however, the difference is only 2 s).

7. CONCLUSIONS

This paper presented an investigation aiming at the reduction of the computational effort for the solution of the MILP problem for the design of shell and tube heat exchangers. Several MILP formulations were proposed based on different alternatives of aggregation of the discrete values of the design variables in relation to the binary variables.

In the original paper of Gonçalves et al.,[1] where the MILP formulation was proposed, each discrete value corresponds to a binary variable. The alternatives developed in this paper tried to aggregate the discrete alternatives in tables, where each group of discrete values becomes an individual binary variable.

The results showed that the aggregation of the binary variables allows a considerable reduction of the computational effort to solve the MILP problem. Considering a sample of 10 design problems, the best aggregation alternative demanded only 0.21% of the total solver time in comparison of the original MILP.

This performance gain is important because allows further investigations for the inclusion of this model into more complex problems such as the insertion of the detailed heat exchanger design into the heat exchanger network synthesis problem.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.iecr.6b04950.

> Complete description of Alternatives 2, 3, and 4; description of heat exchanger design tasks; details of design of each heat exchanger solution (PDF)

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Notes

The authors declare no competing financial interest.

■ NOMENCLATURE

Sets

sd = tube diameter, 1, ..., $sdmax$
sDs = shell diameter, 1, ..., $sDsmax$
sL = tube length, 1, ..., $sLmax$
$slay$ = tube layout, 1, ..., $slaymax$
sNb = number of baffles, 1, ..., $sNbmax$
$sNpt$ = number of tube passes, 1, ..., $sNptmax$
srp = tube pitch ratio, 1, ..., $srpmax$
$srow$ = multi-index

Parameters

$\widehat{Aexc}$ = excess area, %
$\widehat{cp}$ = heat capacity, J/kg K
$\hat{F}_{srow}$ = correction factor to logarithmic mean temperature difference
$\hat{g}$ = gravity acceleration, m/s^2
$\hat{k}$ = thermal conductivity, W/m K
$\hat{m}$ = mass flow rate, kg/s
$\hat{n}$ = 0.4 for heating services; 0.3 for cooling services
$\hat{P}$ = LMTD correction factor parameter
$\widehat{PDeq}_{srow}$ = equivalent diameter, m
$\widehat{PDs}_{srow}$ = shell diameter, m
$\widehat{Pdte}_{srow}$ = outer tube diameter, m
$\widehat{Pdti}_{srow}$ = inner tube diameter, m
$\widehat{PL}_{srow}$ = tube length, m
$\widehat{Play}_{srow}$ = tube layout
$\widehat{PNb}_{srow}$ = number of baffles
$\widehat{PNpt}_{srow}$ = number of tube passes
$\widehat{PNtt}_{srow}$ = total number of tubes
$\widehat{Prp}_{srow}$ = tube pitch ratio
$\widehat{Pr}$ = Prandtl number
$\hat{Q}$ = heat duty, W
$\hat{R}$ = LMTD correction factor parameter
$\widehat{Rf}$ = fouling factor, m^2 K/W
$\hat{T}$ = temperature, °C
$\hat{\rho}$ = density, kg/m^3
$\hat{\mu}$ = viscosity, Pa·s
$\widehat{\Delta Pdisp}$ = available pressure drop, Pa
$\widehat{\Delta Tlm}$ = log-mean temperature difference

Binary Variables

yd_{sd} = variable representing the tube diameter
yDs_{sDs} = variable representing the shell diameter
yL_{sL} = variable representing the tube length
$ylay_{slay}$ = variable representing the tube layout
yNb_{sNb} = variable representing the number of baffles
$yNpt_{sNpt}$ = variable representing the number of tube passes
yrp_{srp} = variable representing the tube pitch ratio
$yrow_{srow}$ = variable representing the set of variables

Continuous Variables

A = area, m^2
Ar = flow area in the shell side, m^2
d = tube diameter, m
Deq = equivalent diameter, m
Ds = shell diameter, m
f = friction factor
FAR = free-area ratio
h = convective heat transfer coefficient, W/m^2 K
K = pressure drop parameter
L = tube length, m
lbc = baffle spacing, m
ltp = tube pitch, m
Nb = number of baffles
Npt = number of tube passes
Ntp = number of tubes per passes
Ntt = total number of tubes
Nu = Nusselt number
Re = Reynolds number
rp = tube pitch ratio

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U = overall heat transfer coefficient, W/m^2 K
v = velocity, m/s
ΔP = pressure drop, Pa

Subscripts

c = cold fluid
h = hot fluid
i = inlet
o = outlet
s = shell-side
t = tube-side
$tube$ = heat exchanger tube variable
max = maximum value
min = minimum value

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