# Shell and Tube Heat Exchanger Design Using Mixed-Integer Linear Programming

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The design of heat exchangers, especially shell and tube heat exchangers was originally proposed as a trial and error procedure where guesses of the heat transfer coefficient were made and then verified after the design was finished. This traditional approach is highly dependent of the experience of a skilled engineer and it usually results in oversizing. Later, optimization techniques were proposed for the automatic generation of the best design alternative. Among these methods, there are heuristic and stochastic approaches as well as mathematical programming. In all cases, the models are mixed integer non-linear and non-convex. In the case of mathematical programming solution procedures, all the solution approaches were likely to be trapped in a local optimum solution, unless global optimization is used. In addition, it is very well-known that local solvers need good initial values or sometimes they do not even find a feasible solution. In this article, we propose to use a robust mixed integer global optimization procedure to obtain the optimal design. Our model is linear thanks to the use of standardized and discrete geometric values of the heat exchanger main mechanical components and a reformulation of integer nonlinear expressions without losing any rigor. © 2016 American Institute of Chemical Engineers AIChE J, 63: 1907–1922, 2017

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#### Introduction

In its classical book,<sup>1</sup> Kern presents the design of shell and tube heat exchangers, as a guess-and-verify procedure where the overall heat transfer coefficient is guessed first and the design is performed in such a way that the final resulting heat transfer coefficient is at least larger than the one that has been guessed. Modern textbooks<sup>2-4</sup> also presents in essence the same trial-and-error design procedure: first an initial tentative heat exchanger is proposed, then the heat exchanger is rated, and the results are checked to verify if the heat exchanger is acceptable, considering the excess area and the allowable pressure drop. If the proposed heat exchanger does not satisfy the task demands, alterations in the design must be conducted and followed by a new rating and further examination. The procedure must be repeated until an acceptable solution is found. This traditional approach involves the direct intervention of a skilled engineer and remained somewhat unaltered for a long time. Alternatively, algorithms based on heuristic rules, which could be implemented in a computer code, were also proposed for the identification of a design solution.<sup>3,4</sup> However, the heuristic nature of these schemes does not guarantee that the area or the cost are optimal.

More recently, heat exchanger design was considered as an optimization problem with cost being minimized. However, for a given heat transfer task, an accurate assessment of the heat exchanger capital cost would require elaborate costing of parts as well as assembly costs. For this reason, previous works usually employed some substitutes: heat exchanger area or a simplified cost function in relation to the area. Therefore, the objective function used normally is the minimization of the heat exchanger area or the total annualized cost, including capital (area based) and operating costs (pumping costs).

The techniques for design optimization of shell and tube heat exchangers can be organized in three mains classes: heuristic rules based on thermofluidynamic relations, metaheuristic methods, and mathematical programming.

The utilization of heuristic rules involves different techniques for the exploration of the search space, such as, graphical analysis and systematic screening of the counting table. Muralikrishna and Shenoy<sup>5</sup> proposed the analysis of the feasible region of the design problem through a pressure drop graph using geometrical and operational constraints. The insertion of objective function curves in the proposed graph allowed the identification of the best design alternative. Ravagnani et al.<sup>6</sup> proposed the application of an heuristic algorithm to a crescent sequence of shell diameters in the counting table aiming to identify the smallest heat exchanger according to the pressure drop constraints. Eryener<sup>7</sup> presented several graphs associated to the baffle spacing aiming to identify the optimal value of

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this design parameter. Costa and Queiroz<sup>8</sup> applied a systematic screening of the counting table, based on discrete alternatives, seeking to identify the heat exchanger with the smallest area for a given thermal task.

Different metaheuristic algorithms were used to solve the optimal design problem: simulated annealing,<sup>9</sup> genetic algorithms,<sup>10–12</sup> particle swarm,<sup>13,14</sup> imperialist competitive algorithm,<sup>15</sup> cuckoo-search algorithm,<sup>16</sup> firefly algorithm,<sup>17</sup> etc. However, there is a lack of organized comparative studies that allow a clear assessment of the best options among the existent alternatives. In addition, none of these techniques guarantees global optimality.

The utilization of mathematical programming based on a more rigorous treatment of optimality conditions was also investigated. Because of the nature of the problem variables, involving continuous (e.g., heat transfer coefficients, pressure drops, etc.) and discrete variables (e.g., tube diameter, number of the tubes, etc.), and the nonlinearity of the thermal and hydraulic model equations, all works use a mixed-integer nonlinear optimization (MINLP) formulation. Mizutani et al.18 formulated the design optimization based on general disjunctive programming, which structure is organized as a MINLP problem. The objective function encompasses capital and operating costs, and the heat exchanger model is based on the Bell-Delaware method.<sup>19</sup> Ponce-Ortega et al.<sup>20</sup> employed an MINLP formulation to the design of series of shell and tube heat exchangers with 1 shell pass and 2 tube passes. The dimensioning of the heat exchanger components, however, is not discussed. Ravagnani et al.<sup>21</sup> organized the MINLP problem describing the set of heat exchanger design variables associated to the mechanical components according to their corresponding discrete values and the remaining model variables as continuous ones. A common feature of all mathematical programming papers in the literature of heat exchanger design is the nonconvexity of the formulations proposed, which does not guarantee global optimality when using local solvers. An exception of all these string of articles in mathematical programming is the early work of Jegede and Polley,<sup>22</sup> who propose a simplified model consisting of three equations involving the heat transfer coefficients of both tube and shell side and the area, as well as the pressure drops on both sides. For fixed pressure drops these equations can be solved and then other parameters can be obtained. Unfortunately, some parameters as the number of tubes may not be integers. In addition, if the diameters of tubes and lengths are standardized and limited to discrete values, the procedure may also render values that do not match these discrete options. There is no procedure suggested as of how large are these mismatches and how they ought to be handled. When pressure drops are to be optimized in addition to area, the procedure includes pumping/compression costs. Finally, if the pressure drops are to be subject just to a maximum limit, the procedure ought to be different.

In this article, we focus on a mathematical programming optimization procedure, where each solution candidate is described by a set of standard values of the design variables, coherent with industrial practice (TEMA, ASME, or ASTM) and convert all the resulting MINLP model into a linear one. Starting from typical thermal and hydraulic model equations (Kern model), proper mathematical transformations are applied to organize the heat exchanger model in relation to the proposed set of integer design variables. The resultant optimization problem is a mixed-integer linear programming problem (MILP). A significant additional advantage stems from our approach: because it is linear the solution is the global optimum, as opposed to the MINLP formulations recently presented in the literature. In addition, the procedure is based on the use of standardized sizes of tube and shell diameters as well as lengths avoiding any trial and error procedure that could be devised by procedures like the ones proposed by Jegede and Polley.<sup>22</sup> In addition, our MILP model can be an excellent tool to use when embedded as part of bigger system designs, i.e., simultaneous synthesis of heat exchanger networks and design of heat exchangers.

The article is organized as follows. We start presenting the thermal and hydraulic model equations employed in the design in its original form. We then discuss the reformulation of the original equations using binary variables, which represent the discrete nature of the design variables of shell and tube heat exchangers. We then show how the reformulated model can be transformed into a linear one, without losing and rigor, i.e., without making any approximations. We finally illustrate the procedure and compare with other solution procedures.

#### **Heat Exchanger Model**

The analysis is focused on shell and tube heat exchanger without phase change. We use an E-shell type and the service must be executed in a single shell without loss of generality. The flow regime considered is a turbulent one, as it is common in industrial equipment. The physical properties are assumed constant, according to average values. Because we are focusing on the design procedure and not on the model, we chose the simpler Kern formulation for the shell-side equations<sup>1</sup> and the Dittus-Boelter as well as the Darcy-Weisbach for the tube-side.<sup>23,24</sup> The proposed approach can also be extended for more complex thermo-fluid dynamic models, such as the Bell-Delaware and the Stream Analysis methods.<sup>2,4,19,23</sup> We expect that these changes will help fine tuning the designs obtained. We also believe that they will not alter substantially the computational performance.

In this section, the problem parameters, which are fixed prior the optimization, are represented with the symbol "".

## Fluid allocation

The selection of the tube-side and shell-side streams depends on several factors, e.g., fouling, temperature, pressure, flow rate, etc. Therefore, it will be considered that the stream allocation is established prior the optimization. Thus, the values of the physical properties in the tube-side and shellside streams are fixed parameters. Extensions to consider this allocation as a variable will be done in future work.

#### Shell-side thermal and hydraulic equations

The flow velocity in the shell-side (vs) depends on the flow area between adjacent baffles (Ar):

$$vs = \frac{\widehat{ms}}{\widehat{\rho s} Ar} \tag{1}$$

where  $\widehat{ms}$  and  $\widehat{\rho s}$  are the shell-side stream flow rate and density, respectively.

This flow area corresponds to the area delimited by the shell diameter (Ds) and baffle spacing (lbc) multiplied by the free area ratio (FAR):

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$$Ar = Ds \ FAR \ lbc \tag{2}$$

The FAR between baffles is given by:

$$FAR = \frac{(ltp - dte)}{ltp} = 1 - \frac{dte}{ltp} = 1 - \frac{1}{rp}$$
(3)

where *ltp* is the tube pitch, *dte* is the outer tube diameter, and *rp* is the ratio between the tube pitch and the tube diameter.

The Reynolds number associated to the shell-side velocity (*Res*) is given by:

$$Res = \frac{Deq \ vs \ \hat{\rho s}}{\hat{\mu s}} \tag{4}$$

where Deq is the equivalent diameter, and  $\hat{\mu s}$  is the shell-side stream viscosity.

The equivalent diameter present in the Reynolds number depends on the tube layout. For a square and triangular pattern, respectively:

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

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

The Nusselt number for the shell-side flow (*Nus*) is a function of the Reynolds and Prandtl numbers (*Res* and  $\widehat{Prs}$ )<sup>1</sup>:

$$Nus = 0.36 \ Res^{0.55} \widehat{Prs}^{1/3} \tag{7}$$

where the dimensionless groups Nusselt and Prandtl are defined by:

$$Nus = \frac{hs \ Deq}{ks} \tag{8}$$

$$\widehat{Prs} = \frac{\widehat{Cps}\ \widehat{\mu s}}{\widehat{ks}} \tag{9}$$

where *hs* is the shell-side convective heat transfer coefficient,  $\hat{ks}$  is the thermal conductivity, and  $\hat{Cps}$  is the heat capacity.

The head loss in the shell-side flow, dismissing nozzle pressure drop, can be calculated by<sup>1</sup>:

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

where  $\Delta Ps$  is the shell-side stream pressure drop, *fs* is the shell-side friction factor and *Nb* is the number of baffles.

The expression for evaluation of the shell-side friction factor is:

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

The number of baffles is directly related to the baffle spacing and tube length:

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

$$vt = \frac{4 \ mt}{Ntp \ \pi \ \rho t \ dti^2}$$
(13)

where  $\widehat{mt}$  and  $\widehat{\rho t}$  are the tube-side stream flow rate and density, respectively.

The equation of the Reynolds number related to the tubeside flow rate (Ret) is:

$$Ret = \frac{dti \ vt \ \hat{\rho t}}{\mu t} \tag{14}$$

where *dti* is the inner tube diameter, and  $\hat{\mu t}$  is the tube-side stream viscosity.

The Prandtl number for the tube-side stream  $(\widehat{Prt})$  is:

$$\widehat{Prt} = \frac{Cpt \ \widehat{\mu t}}{\widehat{kt}}$$
(15)

where  $\hat{kt}$  and  $\hat{Cpt}$  are the tube-side stream thermal conductivity, and heat capacity, respectively.

The Reynolds and Prandtl numbers allow the evaluation of the tube-side Nusselt number (*Nut*) through the Dittus-Boelter correlation<sup>24</sup>:

$$Nut = 0.023 \ Ret^{0.8} \widehat{Prt}^n \tag{16}$$

where the parameter n is equal to 0.4 for heating services and 0.3 for cooling services.

The definition of the Nusselt number is:

$$Nut = \frac{ht \ dti}{kt} \tag{17}$$

where ht is the tube-side convective heat transfer coefficient.

The head loss in the tube-side flow, dismissing nozzle pressure drop, and the variation of the physical properties, is given by  $^{23}$ :

$$\frac{\Delta Pt}{\rho t \ \hat{g}} = \frac{ft \ Npt \ L \ vt^2}{2 \ \hat{g} \ dti} + \frac{K \ Npt \ vt^2}{2 \ \hat{g}}$$
(18)

where  $\Delta Pt$  is the tube-side stream pressure drop, and ft is the tube-side friction factor. The first term in the RHS corresponds to the head loss in the tube bundle and the second corresponds to the head loss in the front and rear headers. The parameter K is equal to 0.9 for one tube pass and 1.6 for two or more tube passes.

The expression for the Darcy friction factor for turbulent flow can be expressed by  $^{23}$ :

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

## **Overall heat transfer coefficient**

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

$$U = \frac{1}{\frac{dte}{dti}ht + \frac{\widehat{Rft}}{dti}} + \frac{dteln\left(\frac{dte}{dti}\right)}{2 \ ktube} + \widehat{Rfs} + \frac{1}{hs}}$$
(20)

## Tube-side thermal and hydraulic equations

The flow velocity in the tube-side (vt) depends on the number of tubes per pass (Ntp) and the inner tube diameter (dti):

where the ktube is the thermal conductivity of the tube wall, and Rft and Rfs are the fouling factors of the tube-side and shell-side streams, respectively.

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### Heat transfer rate equation

According to the logarithmic mean temperature difference (LMTD) method, the heat transfer rate expression is:

$$\widehat{Q} = UAreq \ \Delta Tlm \ F \tag{21}$$

where  $\widehat{Q}$  is the heat load, *Areq* is the required area,  $\Delta \widehat{Tlm}$  is LMTD, and *F* is the LMTD correction factor.

The LMTD is given by:

$$\Delta \widehat{Tlm} = \frac{\left(\widehat{Thi} - \widehat{Tco}\right) - \left(\widehat{Tho} - \widehat{Tci}\right)}{\ln\left(\frac{\left(\widehat{Thi} - \widehat{Tco}\right)}{\left(\widehat{Tho} - \widehat{Tci}\right)}\right)}$$
(22)

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:

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

where:

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

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

The heat transfer area (A) is represented by the sum of the area of the surface of each tube:

$$A = Ntt \ \pi \ dte \ L \tag{26}$$

where *Ntt* is the total number of tubes.

To guarantee an adequate design margin, the exchanger area must be higher than the required area according to a certain "excess area"  $(\widehat{Aexc})$ , specified by the design engineer:

$$A \ge \left(1 + \frac{\widehat{Aexc}}{100}\right) * Areq \tag{27}$$

Therefore, the heat transfer rate equation is reorganized using actual heat exchanger area:

$$UA \ge \left(1 + \frac{\widehat{Aexc}}{100}\right) \frac{\widehat{Q}}{\widehat{\Delta Tlm} \ F}$$
(28)

# Bounds on pressure drops, flow velocities, and Reynolds numbers

During the process design, allowable pressure drops are imposed according to the pressure profile of the unit. These parameters are related to a trade-off between capital and operating costs. The corresponding constraints are:

$$\Delta Ps \le \Delta Ps disp \tag{29}$$

$$\Delta Pt \le \Delta \widehat{Ptdisp} \tag{30}$$

Additionally, lower and upper bounds on flow velocities are also established:

$$vs \ge vsmin$$
 (31)

$$vs \le vsmax$$
 (32)

$$vt > v\widehat{tmin}$$
 (33)

$$vt \le vt \widehat{\max}$$
 (34)

Flow velocity lower bounds seek to avoid fouling susceptible conditions. Corresponding upper bounds aims to avoid erosional conditions that could damage the heat exchanger during its operational life.

According to the application range of the convective heat transfer coefficient correlations, there are bounds on the Reynolds numbers in the shell-side and tube-side:

$$Res \ge 2 \cdot 10^3 \tag{35}$$

$$Ret \ge 10^4 \tag{36}$$

#### Geometric constraints

The baffle spacing must be limited between 20 and 100% of the shell diameter<sup>25</sup>:

$$lbc \ge 0.2 Ds$$
 (37)

$$lbc < 1.0 Ds$$
 (38)

The ratio between the tube length and shell diameter must be between 3 and  $15^{26}$ :

$$L \ge 3 Ds$$
 (39)

$$L \le 15 \ Ds \tag{40}$$

#### **Objective** function

The optimization problem seeks to minimize the heat transfer area, which has a direct impact in the exchanger cost:

min 
$$A$$
 (41)

Other objective functions can be constructed. Normally, capital cost is monotone with area, so minimizing area is somehow equivalent to minimizing the capital cost. However, cost can also be expressed in terms of other variables (weight, materials of different parts, engineering, labor needed, etc.). Such level of granularity, including other mechanical stress-related and material-related considerations, as well as better thermal and hydraulic modeling will certainly improve results. We leave all these extensions to future work, as our main purpose in this article is to present the MILP methodology.

## Model Reformulation Using Discrete Variables

In the proposed problem formulation, the set of discrete design variables that characterize each discrete variable (*x*) are represented according to their respective standard indexed values. That is, *x* is now represented by several discrete options  $x\hat{d}_i$ , of which one and only one will be chosen. Thus, we introduce a set of binary variables  $y_i$ , and write *x* as follows:

$$x = \sum_{i} x \widehat{d}_{i} y_{i} \tag{42}$$

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$$\sum_{i} y_i = 1 \tag{43}$$

According to the engineering practice and TEMA standards,<sup>25,27</sup> these design variables 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*).

Therefore, for our discrete variables, we write:

$$dte = \sum_{sd=1}^{sd\max} \widehat{pdte}_{sd} \ yd_{sd}$$
(44)

$$dti = \sum_{sd=1}^{sd\max} \widehat{pdti}_{sd} \ yd_{sd}$$
(45)

$$\sum_{sd=1}^{sd\max} yd_{sd} = 1 \tag{46}$$

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

$$\sum_{sL=1}^{sLmax} yL_{sL} = 1 \tag{48}$$

$$Nb = \sum_{sNb=1}^{sNbmax} \widehat{pNb}_{sNb} \ yNb_{sNb}$$
(49)

$$\sum_{sNb=1}^{sNbmax} yNb_{sNb} = 1$$
(50)

$$Npt = \sum_{sNpt=1}^{sNptmax} \widehat{pNpt}_{sNpt} \quad yNpt_{sNpt}$$
(51)

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

$$rp = \sum_{srp=1}^{srpmax} \widehat{prp}_{srp} yrp_{srp}$$
(53)

$$\sum_{srp=1}^{srpmax} yrp_{srp} = 1$$
(54)

$$Ds = \sum_{sDs=1}^{sDsmax} \widehat{pDs}_{sDs} \ yDs_{sDs}$$
(55)

$$\sum_{sDs=1}^{sDsmax} yDs_{sDs} = 1$$
(56)

$$lay = \sum_{slay=1}^{slaymax} \widehat{play}_{slay} \quad ylay_{slay} \quad (57)$$

$$\sum_{slay=1}^{slaymax} ylay_{slay} = 1$$
(58)

Instead of leaving these discrete representation as additional equations to the model, we substitute them in the rest of the equations. After the substitution of the discrete variables by its binary representation, the mathematical expressions in the heat exchanger model we get terms of the form  $p^{n1}q^{n2}\cdots z^{nm}$  that are substituted as follows:

$$p^{n1}q^{n2}\cdots z^{nm} = \left[\sum_{i} \widehat{pd}_{i} yp_{i}\right]^{n1} \left[\sum_{j} \widehat{qd}_{j} yq_{j}\right]^{n2} \left[\sum_{k} \widehat{zd}_{k} yz_{k}\right]^{nm}$$
(59)

Because all binary variables assume a value 1 only once in the corresponding set (see Eq. 43), Eq. 59 it is easy to see that one can write:

$$p^{n1}q^{n2}\cdots z^{nm} = \sum_{i,j,k} \widehat{pd}_i^{n1} \widehat{qd}_j^{n2} \cdots \widehat{qd}_k^{nm} yp_i yq_j \cdots yz_k$$
(60)

Therefore, the reformulated model is now composed by several expressions containing multiple summations of products of binary variables and a few continuous variables. We now show the reformulated model.

## Shell-side thermal and hydraulic equations

The expression of the shell-side flow velocity obtained from Eq. 1 is:

$$v_{S} = \frac{\widehat{ms}}{\widehat{\rho s} \sum_{sDs=1}^{sDsmax} \sum_{srp=1}^{srpmax} \sum_{sL=1}^{sLmax} \sum_{sNb=1}^{sNbmax} \frac{\widehat{\rho Ds}_{sDs} \widehat{\rho FAR}_{srp} \widehat{\rho L}_{sL}}{(pNb_{sNb}+1)} yDs_{sDs} yrp_{srp} yL_{sL} yNb_{sNb}}$$
(61)

This equation is derived through the following expression of the flow area originally present in Eq. 2:

$$Ar = \sum_{sDs=1}^{sDsmax} \sum_{srp=1}^{srpmax} \sum_{sL=1}^{sLmax} \sum_{sNb=1}^{sNbmax} \frac{\widehat{pDs}_{sDs}\widehat{pFAR}_{srp}\widehat{pL}_{sL}}{(pN\widehat{b}_{sNb}+1)} yDs_{sDs}yrp_{srp}yL_{sL} yNb_{sNb}$$
(62)

where:

$$p\widehat{FAR}_{srp} = 1 - \frac{1}{\widehat{prp}_{srp}}$$
(63)

The equivalent diameter corresponding to Eqs. 5 and 6 is given by:

$$Deq = \sum_{srp=1}^{srpmax} \sum_{sd=1}^{sdmax} \sum_{slay=1}^{slaymax} p\widehat{Deq}_{srp,sd,slay} yrp_{srp} yd_{sd} ylay_{slay}$$
(64)

where:

$$p\widehat{Deq}_{srp,sd,slay} = \frac{aDeq_{slay}\widehat{prp}_{srp}^2\widehat{pdte}_{sd}^2}{\pi \widehat{pdte}_{sd}} - \widehat{pdte}_{sd}$$
(65)

$$aDeq_{slay} = 4$$
 if  $slay = 1$  (square pattern) (66)

$$aDeq_{slay} = 3.46$$
 if  $slay = 2$  (triangle pattern) (67)

The Reynolds number equation, associated to the shell-side flow velocity and equivalent diameter, becomes, after reformulation of Eq. 4:

$$Res = \frac{\widehat{ms}}{\widehat{\mu s}} \left( \sum_{srp=1}^{srpmax} \sum_{sd=1}^{sdmax} \sum_{slay=1}^{slaymax} p\widehat{Deq}_{srp,sd,slay}yrp_{srp}yd_{sd}ylay_{slay} \right) \\ \cdot \left( \sum_{sDs=1}^{sDsmax} \sum_{srp=1}^{srpmax} \sum_{sL=1}^{sLmax} \sum_{sNb=1}^{sNbmax} \frac{(pN\widehat{b}_{sNb}+1)}{\widehat{pDs}_{sDs}p\widehat{FAR}_{srp}\widehat{pL}_{sL}} yDs_{sDs}yrp_{srp}yL_{sL} yNb_{sNb} \right)$$
(68)

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Substituting the expression above of the Reynolds number in Eq. 68, the reformulated form of the Nusselt number for the shell-side flow becomes:

$$Nus = 0.36 \left(\frac{\widehat{ms}}{\widehat{\mu s}}\right)^{0.55} SNus_{srp,sd,slay,sDs,sL,sNb} \widehat{Prs}^{1/3}$$
(69)

where *SNus<sub>srp,sd,slay,sDs,sL,sNb*</sub> represents the following sum of binary variables:

$$SNus_{srp,sd,slay,sDs,sL,sNb} = \sum_{srpmax} \sum_{sdmax} \sum_{sd=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{sDs=1}^{sLmax} \sum_{sL=1}^{slbmax} \sum_{sNb=1}^{slbmax} \sum_{sNb=1}^{slaymax} \left( \frac{p\widehat{Deq}}{srp,sd,slay} \left( p\widehat{Nb}_{sNb} + 1 \right)}{p\widehat{Ds}_{sDs}p\widehat{FAR}_{srp}p\widehat{L}_{sL}} \right)^{0.55} yrp_{srp} + yd_{sd}ylay_{slay}yDs_{sDs}yL_{sL} yNb_{sNb}$$

$$(70)$$

The substitution of Eq. 69 in the definition of the Nusselt number in Eq. 8 yields the following equation related to the shellside heat transfer coefficient:

$$hs = \frac{\widehat{ks0.36} \left(\frac{\widehat{ms}}{\widehat{\mu s}}\right)^{0.55} SNus_{srp,sd,slay,sDs,sL,sNb} \widehat{Prs}^{1/3}}{\sum_{srp=1}^{srpmax} \sum_{sd=1}^{sdmax} \sum_{slay=1}^{slaymax} \widehat{pDeq}_{srp,sd,slay} yrp_{srp} yd_{sd} ylay_{slay}}}$$
(71)

The reformulation of Eq. 10 of the head loss in the shell-side flow yields:

$$\Delta Ps = \sum_{sDs=1}^{sDsmax} \sum_{sNb=1}^{sNbmax} \sum_{srp=1}^{srpmax} \sum_{sL=1}^{sLmax} \sum_{sd=1}^{srpmax} \sum_{sd=1}^{srpmax} \sum_{slay=1}^{srpmax} p\widehat{\Delta Ps}_{sDs,sNb,srp,sL,sd,slay} yDs_{sDs} yNb_{sNb}$$
(72)  
 $\cdot yrp_{srp}yL_{sL}yd_{sd}ylay_{slay}$ 

where:

$$p\widehat{\Delta Ps}_{sDs,sNb,srp,sL,sd,slay} = 0.864 \frac{\widehat{ms}^{1.812}\widehat{\mu s}^{0.188}}{\widehat{\rho s}} \left(\frac{\widehat{\mu s}}{\widehat{\mu w}}\right)^{-0.14} \\ \left(\frac{\widehat{(pNb}_{sNb}+1)^{2.812}}{\widehat{pDs}_{sDs}^{0.812} (\widehat{pFAR}_{srp}\widehat{pL}_{sL})^{1.812} (\widehat{pDeq}_{srp,sd,slay})^{1.188}}\right)$$
(73)

## Tube-side thermal and hydraulic equations

The reformulation of the flow velocity in the tube-side is obtained from Eq. 13:

$$vt = 4 \ \widehat{mt} / \left( \pi \ \widehat{\rho t} \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} \frac{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay}\widehat{pdti}_{sd}^2}{\widehat{pNpt}_{sNpt}} \right)$$

$$(74)$$

$$yDs_{sDs} \ yd_{sd}yNpt_{sNpt} \cdot yrp_{srp}ylay_{slay}$$

The Reynolds number expression (Eq. 14) is now as follows:

$$Ret = \frac{4 \ \widehat{mt}}{\pi \ \widehat{\mu t}} \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{srpmax} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay}\widehat{pdti}_{sd}} yDs_{sDs} \ yd_{sd}$$

$$\cdot yNpt_{sNpt}yrp_{srpy}lay_{slay}$$
(75)

The insertion of Eq. 75 into Eq. 16 yields the reformulated form of the Nusselt number for tube-side flow:

$$Nut = 0.023 \left(\frac{4 \ \widehat{mt}}{\pi \ \widehat{\mu t}}\right)^{0.8} SNut_{srp,sd,slay,sDs,sNpt} \widehat{Prt}^n$$
(76)

where *SNut<sub>srp,sd,slay,sDs,sNpt*</sub> represents a sum of binary variables:

$$SNut_{srp,sd,slay,sDs,sL,sNb} = \sum_{srp=1}^{srpmax} \sum_{sd=1}^{sdmax} \sum_{slay=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{sDs=1}^{sLmax} \sum_{sL=1}^{sNbmax} \left( \frac{p\widehat{Npt}_{sNpt}}{p\widehat{Ntt}_{sDs,sd,sNpt,srp,slay}\widehat{pdti}_{sd}} \right)^{0.8} yDs_{sDs} yd_{sd} \cdot yNpt_{sNpt}yrp_{srp}ylay_{slay}$$

$$(77)$$

According the definition of the Nusselt number in Eq. 17, the tube-side heat transfer coefficient equation becomes:

$$ht = \frac{\widehat{kt0.023} \left(\frac{4 \ \widehat{mt}}{\pi \ \widehat{\mu t}}\right)^{0.8} SNut_{srp,sd,slay,sDs,sNpt} \widehat{Prt}^n}{\sum_{sd=1}^{sdmax} \widehat{pdti}_{sd} yd_{sd}}$$
(78)

The reformulation of Eq. 18 of the head loss in the tube-side flow yields:

$$\Delta Pt = \frac{\widehat{\rho t} \sum_{sNpt=1}^{sNptmax} \widehat{pNpt}_{sNpt} yNpt_{sNpt} \sum_{sL=1}^{sLmax} \widehat{pL}_{sL} yL_{sL}}{2 \sum_{sd=1}^{sdmax} \widehat{pdti}_{sd} yd_{sd}} \left( 0.014 + 1.056 \cdot \left( \frac{4 \widehat{mt}}{\pi \widehat{\mu t}} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay} \widehat{pdti}_{sd}} \right)^{-0.42}}{2 \sum_{sd=1}^{sdmax} \widehat{pdti}_{sd} yd_{sd}} \left( 0.014 + 1.056 \cdot \left( \frac{4 \widehat{mt}}{\pi \widehat{\mu t}} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay} \widehat{pdti}_{sd}} \right)^{-0.42}} \right)^{2}$$

$$\sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} yDs_{sDs} yd_{sd} \cdot yNpt_{sNpt} yrp_{srp} ylay_{slay}} \right) \cdot \left( \frac{4 \widehat{mt}}{\pi \widehat{\rho t}} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay} \widehat{pdti}_{sd}}^{2} \right)^{2}$$

$$+ \frac{\widehat{\rho t} \left( \widehat{K1P} yNpt_{sNpt1} + \widehat{KMP} \left( 1 - yNpt_{sNpt1} \right) \right) \sum_{sNpt=1}^{sNptmax} \widehat{pNpt}_{sNpt} yNpt_{sNpt}} \widehat{pNpt}_{sNpt} yNpt_{sNpt}} \cdot \left( \frac{4 \widehat{mt}}{\pi \widehat{\rho t}} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay} \widehat{pdti}_{sd}}^{2} \right)^{2}$$

$$+ \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} yDs_{sDs} yd_{sd} \cdot yNpt_{sNpt} yNpt_{sNpt}} \sum_{sDs=1}^{d} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay} \widehat{pdti}_{sd}}^{2} \right)^{2}$$

$$+ \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{snptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} yDs_{sDs} yd_{sd} \cdot yNpt_{sNpt} yrp_{srp} ylay_{slay}} \sum_{sDs=1}^{d} \widehat{pNpt}_{sNpt} \sum_{sNpt=1}^{d} \widehat{pNtt}_{sDs,sd,sNpt,srp,slay} \widehat{pdti}_{sd}^{2} \right)^{2}$$

$$+ \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{snptmax} \sum_{srp=1}^{slaymax} \sum_{slay=1}^{slaymax} yDs_{sDs} yd_{sd} \cdot yNpt_{sNpt} yrp_{srp} ylay_{slay}} \sum_{sDs=1}^{d} \widehat{pNtt}_{sDs,sd,sNpt,srp,slay} \widehat{pdti}_{sd}^{2} \right)^{2}$$

## **Overall heat transfer coefficient**

The reformulation of the overall heat transfer coefficient in Eq. 20 yields:

$$\frac{1}{U} = \frac{1}{\left(\sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} \widehat{pht}_{sDs,sd,sNpt,srp,slay} yDs_{sDs} yd_{sd}yNpt_{sNpt}yrp_{srp}ylay_{slay}\right)}{\left(\sum_{sd=1}^{sdmax} \widehat{pdte}_{sd} yd_{sd} + \widehat{Rft} \sum_{sd=1}^{sdmax} \widehat{pdte}_{sd} yd_{sd} + \frac{\sum_{sd=1}^{sdmax} \widehat{pdte}_{sd} yd_{sd}}{\sum_{sd=1}^{sdmax} \widehat{pdti}_{sd} yd_{sd}} + \frac{\sum_{sd=1}^{sdmax} \widehat{pdte}_{sd} yd_{sd} \ln\left(\sum_{sd=1}^{sdmax} \widehat{pdte}_{sd} yd_{sd}\right)}{2 Ktube}} \right) (80)$$

$$+ \widehat{Rfs} + \frac{1}{\left(\sum_{srp=1}^{srpmax} \sum_{sd=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{sDs=1}^{sDsmax} \sum_{sl=1}^{sLmax} \sum_{sNb=1}^{slmax} \widehat{phs}_{srp,sd,slay,sDs,sL,sNb} yrp_{srp}yd_{sd}ylay_{slay}yDs_{sDs}yL_{sL} yNb_{sNb}\right)}$$

## Heat transfer rate equation

The heat transfer area related to Eq. 26 is given by:

$$A = \pi \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} \sum_{sL=1}^{sLmax} \widehat{pNtt}_{sDs,sd,sNpt,srp,slay}$$

$$\cdot \widehat{pdte}_{sd}\widehat{pL}_{sL} \ yDs_{sDs} \ yd_{sd}yNpt_{sNpt}yrp_{srp}ylay_{slay}yL_{sL}$$
(81)

The correction factor of the LMTD assumes the following form:

$$F = yNpt_{sNpt1} + \widehat{FMP} \left(1 - yNpt_{sNpt1}\right)$$
(82)

where  $\widehat{FMP}$  is the value of the correction factor of the LMTD for a configuration with a single shell pass and an even number of

tube passes (Eq. 23).

The substitution of these expressions in Eq. 28 yields the reformulated form of the heat transfer rate equation:

$$\frac{1}{\left(\sum_{sDs=1}^{sDsmax}\sum_{sd=1}^{sdmax}\sum_{sNpt=1}^{sNptmax}\sum_{srp=1}^{srpmax}\sum_{slay=1}^{slaymax}\widehat{pht}_{sDs,sd, sNpt, srp, slay} yDs_{sDs} yd_{sd}yNpt_{sNpt}yrp_{srp}ylay_{slay}\right)}$$

$$\cdot \frac{\sum_{sd=1}^{sdmax}\widehat{pdte}_{sd} yd_{sd}}{\sum_{sd=1}^{sdmax}\widehat{pdte}_{sd} yd_{sd}} + \widehat{Rft} \sum_{sd=1}^{sdmax}\widehat{pdte}_{sd} yd_{sd}}{\sum_{sd=1}^{sdmax}\widehat{pdti}_{sd} yd_{sd}} + \frac{\sum_{sd=1}^{sdmax}\widehat{pdte}_{sd} yd_{sd}}{2 ktube}$$

$$+ \widehat{Rfs} + \frac{1}{\left(\sum_{srp=1}^{srpmax}\sum_{sd=1}^{sdmax}\sum_{slay=1}^{slaymax}\sum_{sDs=1}^{sDsmax}\sum_{sl=1}^{slmax}\sum_{sNb=1}^{sNbmax}\widehat{pht}_{slay,sDs,sL,sNb}yrp_{srp}yd_{sd}ylay_{slay}yDs_{sDs}yL_{sL} yNb_{sNb}\right)}$$

$$\leq \frac{1}{\widehat{Q}\left(1 + \frac{\widehat{Aexc}}{100}\right)} \left(\pi \sum_{sDs=1}^{sDsmax}\sum_{sd=1}^{sdmax}\sum_{sNpt=1}^{sNptmax}\sum_{srp=1}^{srpmax}\sum_{slay=1}^{slaymax}\sum$$

## Bounds on pressure drops, flow velocities, and Reynolds numbers

These inequality constraints become:

$$\sum_{sDs=1}^{sDsmax} \sum_{sNb=1}^{sNbmax} \sum_{srp=1}^{srpmax} \sum_{sL=1}^{sLmax} \sum_{sd=1}^{srpmax} \sum_{slay=1}^{slaymax} p\widehat{\Delta Ps}_{sDs,sNb,srp,sL,sd,slay} yDs_{sDs} yNb_{sNb} \cdot yrp_{srp} yL_{sL} yd_{sd} ylay_{slay} \leq \Delta \widehat{Psdisp}$$
(84)

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$$\begin{aligned} \frac{\widehat{\mu}}{2} & \left( 0.014 + 1.056 \cdot \left( \frac{\pi}{4} \frac{\widehat{\mu}}{10t} \sum_{dd=1}^{dd_{logend}} \sum_{dd_{logend}}^{dd_{logend}} \sum_{dd_{logend}^{dd_{logend}}} \sum_{dd_{logend}^{dd_{logend}}}^{dd_{logend}^{dd_{logend}}} \sum_{dd_{logend}^{dd_{logend}}}^{dd_{logend}^{dd_{logend}}} \sum_{dd_{logend}^{dd_{logend}}}^{dd_{logend}^{dd_{logend}}} \sum_{dd_{logend}^{dd_$$

## Geometric constraints

These constraints are modified according to the discrete nature of the design variables:

$$\frac{\sum_{sL=1}^{sL\max} \widehat{pL}_{sL} \ yL_{sL}}{\sum_{sNb=1}^{sNb\max} \widehat{pNb}_{sNb} \ yNb_{sNb} + 1} \ge 0.2 \sum_{sDs=1}^{sDs\max} \widehat{pDs}_{sDs} \ yDs_{sDs}$$
(92)

$$\frac{\sum_{sL=1}^{sL_{max}} \widehat{pL}_{sL} \ yL_{sL}}{\sum_{sNb=1}^{sNb_{max}} \widehat{pNb}_{sNb} \ yNb_{sNb} + 1} \le 1.0 \sum_{sDs=1}^{sD_{smax}} \widehat{pDs}_{sDs} \ yDs_{sDs}$$
(93)

$$\sum_{sL=1}^{sL\max} \widehat{pL}_{sL} \quad yL_{sL} \ge 3 \quad \sum_{sDs=1}^{sDs\max} \widehat{pDs}_{sDs} \quad yDs_{sDs}$$
(94)

$$\sum_{sL=1}^{sL\max} \widehat{pL}_{sL} \quad yL_{sL} \leq 15 \quad \sum_{sDs=1}^{sDs\max} \widehat{pDs}_{sDs} \quad yDs_{sDs}$$
(95)

## **Objective function**

The objective function in relation to the binary variables assumes the following form:

$$\begin{array}{l} \operatorname{Min} \pi \sum_{slaymax} \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \\ \sum_{slay=1}^{slaymax} \sum_{sL=1}^{sLmax} \widehat{pNtt}_{sDs,sd,sNpt,srp,slay} \\ \cdot \ \widehat{pdte}_{sd} \widehat{pL}_{sL} \ yDs_{sDs} \ yd_{sd}yNpt_{sNpt}yrp_{srp}ylay_{slay}yL_{sL} \end{array}$$
(96)

## **Conversion to a Linear Model**

The above reformulation of the heat exchanger model using binary variables contains several expressions with products of binaries. Therefore, at this stage, the problem is a nonlinear one, which could present multiple local optima with different values of objective function.

Aiming at providing a linear formulation of the optimization problem, thus suppressing the nonconvexity drawback, a rigorous linear alternative for these binary expressions is used, according to the procedure shown below. It is important to mention that the proposed procedure does not involve any numerical approximation, i.e., the solution of the resultant formulation rigorously guarantees the global optimum of the design problem.

The product of binary variables in an expression like the one shown in Eq. 60 can be grouped in a continuous nonnegative variable  $w_{i,j,...,k}$  as follows:

$$w_{i,j,\ldots, k} = y p_j \ y q_j \ldots \ y z_k \tag{97}$$

Then (60) can be rewritten as follows

$$p^{n1}q^{n2}\cdots z^{nm} = \sum_{i,j,k} \widehat{pd_i}^{n1} \widehat{qd_j}^{n2} \cdots \widehat{qd_k}^{nm} w_{i,j,\dots,k}$$
(98)

However (97) can be substituted by

$$w_{i,j,\ldots, k} \le y p_i \tag{99}$$

$$w_{i,j,\ldots, k} \le yq_j \tag{100}$$

$$w_{i,j,\ldots, k} \leq y z_k \tag{101}$$

$$w_{i,j,...,k} \ge yp_i + yq_j + \ldots + yz_k - (m-1)$$
 (102)

where m is the number of binary variables in the product. Consequently, the original nonlinear term related to the product of binaries is substituted by linear constraints.

## **Final MILP Problem**

After the application of the technique described above, the problem becomes a MILP. Aiming to decrease the computational effort, additional constraints are included to reduce the search space, as described at the end of this section.

The MILP equations of the heat exchanger design problem are shown below.

#### **Binary variables equality constraints**

The following constraints guarantee that in the solution only one of the integer values will be selected:

$$\sum_{sd=1}^{sd\max} yd_{sd} = 1 \tag{103}$$

$$\sum_{sL=1}^{sL\max} yL_{sL} = 1 \tag{104}$$

$$\sum_{sNb=1}^{sNbmax} yNb_{sNb} = 1$$
(105)

$$\sum_{sNpt=1}^{sNpt} yNpt_{sNpt} = 1$$
(106)

$$\sum_{srp=1}^{t} yrp_{srp} = 1$$
(107)

$$\sum_{sDs=1}^{sDsmax} yDs_{sDs} = 1$$
(108)

$$\sum_{slay=1}^{slay=1} ylay_{slay} = 1$$
(109)

## Heat transfer rate equation

The heat transfer rate equation in the MILP formulation contains all the expressions related to the heat transfer coefficients and heat transfer area:

$$\begin{split} \widehat{Q}\left(\sum_{sDs=1}^{sDsmax}\sum_{sd=1}^{sdmax}\sum_{sNpt=1}^{sNptmax}\sum_{srp=1}^{srpmax}\sum_{slay=1}^{slaymax}\frac{\widehat{pdte}_{sd}}{\widehat{pht}_{sDs,sd,sNpt,srp,slay}\widehat{pdti}_{sd}}^{WVt_{sDs,sd,sNpt,srp,slay}} Wt_{sDs,sd,sNpt,srp,slay}\right) \\ &+ \widehat{Rft}\sum_{sd=1}^{sdmax}\widehat{pdte}_{sd}}{pdti}_{sd} yd_{sd} + \frac{\sum_{sd=1}^{sdmax}\widehat{pdte}_{sd}\ln\left(\frac{\widehat{pdte}_{sd}}{pdti}\right)yd_{sd}}{2 ktube} + \widehat{Rfs} + \sum_{srp=1}^{srpmax}\sum_{sd=1}^{sdmax}\sum_{slay=1}^{slaymax}\sum_{sDs=1}^{sDsmax}\sum_{sDs=1}^{sDsmax}\sum_{sDs=1}^{sDsmax}\sum_{sDs=1}^{sDsmax}\frac{1}{phs}\frac{1}{phs}\frac{1}{srp,sd,slay,sDs,sL,sNb}} Whs_{sDs,srp,sL,sNb,sd,slay} \\ &= \left(\pi \sum_{sDs=1}^{sDsmax}\sum_{sNb=1}^{sdmax}\sum_{sNpt=1}^{sNptmax}\sum_{srp=1}^{srpmax}\sum_{slay=1}^{slaymax}\sum_{sL=1}^{sLmax}\widehat{pNtt}s_{Ds,sd,sNpt,srp,slay}\widehat{pdte}_{sd}\widehat{pL}sL \cdot WA1P_{sDs,sd,sNpt,srp,slay,sL}\right) \\ &= \left(\frac{100}{100+\widehat{Aexc}}\Delta\widehat{Tlm} + \left(\pi \ \widehat{FMP}\sum_{sDs=1}^{sDsmax}\sum_{slay=1}^{sdmax}\sum_{sNpt=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\widehat{pMtt}s_{Ds,sd,sNpt,srp,slay}\widehat{pdte}_{sd}\widehat{pL}sL \cdot WA1P_{sDs,sd,sNpt,srp,slay,sL}\right) \\ &= \left(\pi \ \widehat{FMP}\sum_{sDs=1}^{sDsmax}\sum_{slay=1}^{slaymax}\widehat{pRtt}s_{Slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\widehat{pNtt}s_{Ds,sd,sNpt,srp,slay}\widehat{pdte}_{sd}\widehat{pL}sL \cdot WA1P_{sDs,sd,sNpt,srp,slay,sL}\right) \\ &= \left(\frac{100}{100+\widehat{Aexc}}\Delta\widehat{Tlm}\right) d\widehat{Tlm} \right) \left(\frac{100}{100+\widehat{Aexc}}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\widehat{pNtt}s_{Ds,sd,sNpt,srp,slay}\widehat{pdte}_{sd}\widehat{pL}sL \cdot WA1P_{sDs,sd,sNpt,srp,slay,sL}\right) \right) \\ &= \left(\frac{100}{100+\widehat{Aexc}}\Delta\widehat{Tlm}\right) d\widehat{Tlm} \right) \left(\frac{100}{100+\widehat{Aexc}}\sum_{slay=1}^{slaymax}\sum_{slay=1}^{slaymax}\widehat{pNtt}s_{Slay,slay,slay,slay,slay,sL}\right) d\widehat{Tlm} \right) d\widehat{Tlm}$$

(110)

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The constraint in Eq. 111 has continuous variables:  $wvt_{sDs,sd,sNpt,srp,slay}$ ,  $whs_{sDs,srp,sL,sNb,sd,slay}$ ,  $wAIP_{sDs,sd,sNpt,srp,-slay,sL}$ , and  $wA_{sDs,sd,sNpt,srp,slay,sL}$ . The relations of these variables and the corresponding binary variables are:

$$wvt_{sDs,sd,sNpt,srp,slay} \le yDs_{sDs}$$
 (111)

$$wvt_{sDs,sd,sNpt,srp,slay} \le yd_{sd} \tag{112}$$

$$wvt_{sDs,sd,sNpt,srp,slay} \le yNpt_{sNpt}$$
 (113)

$$wvt_{sDs,sd,sNpt,srp,slay} \le yrp_{srp}$$
 (114)

$$wvt_{sDs,sd,sNpt,srp,slav} \le ylay_{slav}$$
 (115)

$$wvt_{sDs,sd,sNpt,srp,slay} \ge yDs_{sDs} + yd_{sd} + yNpt_{sNpt} + yrp_{srp} + ylay_{slay} - 4$$
(116)

$$whs_{sDs,srp,sL,sNb,sd,slay} \le yrp_{srp}$$
 (117)

$$whs_{sDs,srp,sL,sNb,sd,slay} \le yd_{sd}$$
 (118)

$$whs_{sDs,srp,sL,sNb,sd,slay} \le ylay_{slay}$$
 (119)

$$whs_{sDs,srp,sL,sNb,sd,slay} \le yDs_{sDs}$$
 (120)

$$whs_{sDs,srp,sL,sNb,sd,slay} \le yL_{sL}$$
 (121)

$$whs_{sDs,srp,sL,sNb,sd,slay} \leq yNb_{sNb}$$
 (122)

$$whs_{sDs,srp,sL,sNb,sd,slay} \ge yrp_{srp} + yd_{sd} + ylay_{slay} +yDs_{sDs} + yL_{sL} + yNb_{sNb} - 5$$
(123)

 $wA1P_{sDs,sd,sNpt,srp,slay,sL} \le wA_{sDs,sd,sNpt,srp,slay,sL}$ (124)

$$wA1P_{sDs,sd,sNpt,srp,slay,sL} \le yNpt_{sNpt1}$$
(125)

$$wA1P_{sDs,sd,sNpt,srp,slay,sL} \ge wA_{sDs,sd,sNpt,srp,slay,sL} + yNpt_{sNpt1} - 1$$
(126)

$$wA_{sDs,sd,sNpt,srp,slay,sL} \le yDs_{sDs}$$
(127)

$$wA_{sDs,sd,sNpt,srp,slay,sL} \le yd_{sd}$$
(128)

$$wA_{sDs,sd,sNpt,srp,slay,sL} \le yNpt_{sNpt}$$
(129)

$$wA_{sDs,sd,sNpt,srp,slay,sL} \le yrp_{srp}$$
(130)  
$$wA_{sDs,sd,sNpt,srp,slay,sL} \le ylay$$
(131)

$$wA_{sDs,sd,sNpt,srp,slay,sL} \le ylay_{slay}$$
(131)  
$$wA_{sDs,sd,sNpt,srp,slay,sL} \le ylay_{slay}$$
(132)

$$wA_{sDs,sd,sNpt,srp,slay,sL} \le yL_{sL}$$
(132)

$$\frac{WA_{sDs,sd,sNpt,srp,slay,sL} \ge yDs_{sDs} + ya_{sd} + yNpt_{sNpt}}{+ yrp_{srp} + ylay_{slay} + yL_{sL} - 5}$$
(133)

# Bounds on pressure drops, flow velocities, and Reynolds numbers

The linear form of the bound on the shell-side pressure drop is:

$$\sum_{sDs=1}^{sDsmax} \sum_{sNb=1}^{sNbmax} \sum_{srp=1}^{srpmax} \sum_{sL=1}^{sLmax} \sum_{sd=1}^{srpmax} \sum_{slay=1}^{slaymax} p\widehat{\Delta Ps}_{sDs,sNb,srp,sL,sd,slay} \cdot wDPs_{sDs,sNb,srp,sL,sd,slay} \leq \Delta \widehat{Psdisp}$$
(134)

The constraints relating the *wDPs<sub>sDs,sNb,srp,sL,sd,slay* continuous variable and the respective binary variables are:</sub>

$$wDPs_{sDs,sNb,srp,sL,sd,slay} \le yDs_{sDs}$$
(135)

$$wDPs_{sDs,sNb,srp,sL,sd,slay} \le yNb_{sNb}$$
(136)

$$wDPs_{sDs,sNb,srp,sL,sd,slay} \le yrp_{srp}$$
(137)

$$wDPs_{sDs,sNb,srp,sL,sd,slay} \le yL_{sL}$$
(138)

$$wDPs_{sDs,sNb,srp,sL,sd,slay} \le yd_{sd} \tag{139}$$

$$wDPs_{sDs,sNb,srp,sL,sd,slay} \le ylay_{slay} \tag{140}$$

$$wDPs_{sDs,sNb,srp,sL,sd,slay} \ge yDs_{sDs} + yNb_{sNb} + yrp_{srp} + yL_{sL} + yd_{sd} + ylay_{slay} -5$$
(141)

The tube-side pressure drop constraint is:

$$\sum_{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slaymax} \sum_{slaymax} \sum_{sL=1}^{slaymax} p\Delta P \widehat{tturb1}_{sNpt:sL,sDs,sd,srp,slay} \\ \cdot wvtturb_{sDs,sd,sNpt,srp,slay,sL} + \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNptmax} \sum_{srp=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{sL=1}^{slaymax} p\Delta P \widehat{tturb2}_{sNpt,sL,sDs,sd,srp,slay} \cdot wvtturb_{sDs,sd,sNpt,srp,slay,sL} \\ + \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNptmax} \sum_{sNptmax} \sum_{srp=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{sDs=1}^{slaymax} \sum_{slay=1}^{slaymax} \sum_{sNptmax} \sum_{slay=1}^{slaymax} \sum_{slay=1}^{slay=1} p\Delta \widehat{Ptclab}_{slb} \sum_{slay=1}^{slay=1} \sum_{s$$

The constraints relating the  $wvtturb_{sDs,sd,sNpt,srp,slay,sL}$  and  $wvt1P_{sDs,sd,sNpt,srp,slay}$  continuous variables and the respective binary variables are:

$$wvtturb_{sDs,sd,sNpt,srp,slay,sL} \le wvt_{sDs,sd,sNpt,srp,slay}$$
(143)

$$wvtturb_{sDs,sd,sNpt,srp,slay,sL} \le yNpt_{sNpt}$$
(144)

$$wvtturb_{sDs,sd,sNpt,srp,slay,sL} \le yL_{sL}$$
(145)

$$wvtturb_{sDs,sd,sNpt,srp,slay,sL} \le yd_{sd} \tag{146}$$

$$wvtturb_{sDs,sd,sNpt,srp,slay,sL} \ge wvt_{sDs,sd,sNpt,srp,slay} + yNpt_{sNpt} + yL_{sL} + yd_{sd} - 3$$
(147)

$$wvt1P_{sDs,sd,sNpt,srp,slay} \le wvt_{sDs,sd,sNpt,srp,slay}$$
 (148)

$$wvt1P_{sDs,sd,sNpt,srp,slay} \le yNpt_{sNpt1}$$
(149)

$$wvt1P_{sDs,sd,sNpt,srp,slay} \ge wvt_{sDs,sd,sNpt,srp,slay} + yNpt_{sNpt1} - 1$$
(150)

The linear form of the bounds on the shell-side flow velocity are:

$$\widehat{vsmin} \leq \frac{\widehat{ms}}{\widehat{\rho s}} \sum_{sDs=1}^{sDsmax} \sum_{srp=1}^{srpmax} \sum_{sL=1}^{sLmax} \sum_{sNb=1}^{sNbmax} \frac{(pN\widehat{b_{sNb}}+1)}{\widehat{pDs}_{sDs}p\widehat{FAR}_{srp}\widehat{pL}_{sL}} WVS_{sDs,srp,sL,sNb}$$
(151)

$$v\widehat{smax} \ge \frac{\widehat{ms}}{\widehat{\rho s}} \sum_{sDs=1}^{sDsmax} \sum_{srp=1}^{srpmax} \sum_{sL=1}^{sLmax} \sum_{sNb=1}^{sNbmax} \frac{(pNb_{sNb}+1)}{\widehat{pDs}_{sDs}p\widehat{FAR}_{srp}\widehat{pL}_{sL}} wvs_{sDs,srp,sL,sNb}$$
(152)

The constraints relating the *wvs<sub>sDs,srp,sL,sNb</sub>* continuous variable and the corresponding binary variables are:

$$wvs_{sDs,srp,sL,sNb} \le yDs_{sDs}$$
 (153)

$$wvs_{sDs,srp,sL,sNb} \le yrp_{srp}$$
 (154)

$$wvs_{sDs,srp,sL,sNb} \le yL_{sL} \tag{155}$$

$$wvs_{sDs,srp,sL,sNb} \leq yNb_{sNb}$$
 (156)

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 $wvs_{sDs,srp,sL,sNb} \ge yDs_{sDs} + yrp_{srp} + yL_{sL} + yNb_{sNb} - 3$ (157)

The bounds on the tube-side flow velocity are:

$$\widehat{vtmin} \leq \frac{4 \ \widetilde{mt}}{\pi \ \widehat{\rho t}} \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNptmax} \sum_{srp=1}^{srpmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay}\widehat{pdti}_{sd}^2} Wvt_{sDs,sd,sNpt,srp,slay}$$
(158)

$$v\widehat{tmax} \geq \frac{4 \ \widehat{mt}}{\pi \ \widehat{\rho t}} \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{srpmax} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay}\widehat{pdti}_{sd}^{2}} wvt_{sDs,sd,sNpt,srp,slay}$$
(159)

The bounds on the Reynolds numbers are:

$$\frac{\widehat{ms}}{\widehat{\mu s}} \sum_{srp=1}^{srpmax} \sum_{sd=1}^{sdmax} \sum_{slay=1}^{slaymax} \sum_{sDs=1}^{sDsmax} \sum_{sL=1}^{sLmax} \sum_{sNb=1}^{sNbmax} \frac{\widehat{pDeq}_{srp,sd,slay} \left(\widehat{pNb}_{sNb} + 1\right)}{\widehat{pDs}_{sDs} \widehat{pFAR}_{srp} \widehat{pL}_{sL}} \cdot whs_{sDs,srp,sL,sNb,sd,slay} \\ \ge 2 \cdot 10^3$$

$$\frac{4 \ \widehat{mt}}{\pi \ \widehat{\mu t}} \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} \frac{\widehat{pNpt}_{sNpt}}{\widehat{pNtt}_{sDs,sd,sNpt,srp,slay}\widehat{pdti}_{sd}} \cdot wvt_{sDs,sd,sNpt,srp,slay} \ge 10^4$$
(161)

### Geometric constraints

The constraints related to the maximum and minimum baffle spacing are:

$$\sum_{sL=1}^{sL\max} \sum_{sNb=1}^{sNb\max} \frac{p\widehat{L}_{sL}}{(pN\widehat{b}_{sNb}+1)} webc_{sL,sNb} \leq 1.0 \sum_{sDs=1}^{sDs\max} \widehat{pDs}_{sDs} yDs_{sDs}$$
(162)

$$\frac{\sum_{sL=1}^{sLmax} \sum_{sNb=1}^{sNbmax}}{\left(\frac{pL_{sL}}{(pNb_{sNb}+1)}webc_{sL,sNb}} \ge 0.2 \sum_{sDs=1}^{sDsmax} \widehat{pDs}_{sDs} yDs_{sDs}$$
(163)

The constraints relating the  $webc_{sL,sNb}$  continuous variable and the corresponding binary variables are:

$$webc_{sL,sNb} \le yL_{sL}$$
 (164)

$$webc_{sL,sNb} \leq yNb_{sNb}$$
 (165)

$$webc_{sL,sNb} \ge yL_{sL} + yNb_{sNb} - 1 \tag{166}$$

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

$$\sum_{sL=1}^{sL\max} \widehat{pL}_{sL} \ yL_{sL} \ge 3 \sum_{sDs=1}^{sD\max} \widehat{pDs}_{sDs} \ yDs_{sDs}$$
(167)

$$\sum_{sL=1}^{sLmax} \widehat{pL}_{sL} \ yL_{sL} \le 15 \ \sum_{sDs=1}^{sDsmax} \widehat{pDs}_{sDs} \ yDs_{sDs}$$
(168)

## **Objective function**

The objective function is:

$$\operatorname{Min} \pi \sum_{sDs=1}^{sDsmax} \sum_{sd=1}^{sdmax} \sum_{sNpt=1}^{sNptmax} \sum_{srp=1}^{srpmax} \sum_{slay=1}^{slaymax} \sum_{sL=1}^{slaymax} \widehat{pMtt}_{sDs,sd,sNpt,srp,slay} \ \widehat{pdte}_{sd} \widehat{pL}_{sL}$$

$$\cdot wA_{sDs,sd,sNpt,srp,slay,sL}$$
(169)

## **Feasible Set Reduction**

## Velocity bounds

The analysis of the feasible set allows the introduction of additional constraints, which can accelerate the solution algorithm. Bounds on flow velocities are imposed by the constraints in the Eqs. 158 and 159, but the analysis of these conditions indicates that an extra set of constraints can also be added to the problem formulation:

$$wvs_{sDs,srp,sL,sNb} = 0 \text{ for } (sDs, srp, sL, sNb) \in (Svsminout \cup Svsmaxout)$$
(170)

$$wvt_{sDs,sd,sNpt,srp,slay} = 0 \text{ for } (sDs, srp, sL, sNb) \in (Svtminout \cup Svtmaxout)$$
(171)

The sets *Svsminout*, *Svsmaxout*, *Svtminout*, and *Svtmaxout* are established prior to the optimization, based on the values of the set of problem parameters, as follows:

$$Svsminout = \left\{ (sDs, srp, sL, sNb) / \widehat{pvs}_{sDs, srp, sL, sNb} \le v\widehat{smin} - \varepsilon \right\}$$
(172)

$$Svsmaxout = \{(sDs, srp, sL, sNb) / \widehat{pvs}_{sDs, srp, sL, sNb} \ge vsmax + \varepsilon\}$$
(173)

Svtminout=

(160)

$$\left\{ (sDs, sd, sNpt, srp, slay) / \widehat{pvt}_{sDs, sd, sNpt, srp, slay} \le v \widehat{tmin} - \varepsilon \right\}$$
(174)

Svtmaxout=

$$\left\{ (sDs, sd, sNpt, srp, slay) / \widehat{pvt}_{sDs, sd, sNpt, srp, slay} \ge v \widehat{smax} + \varepsilon \right\}$$
(175)

where  $\varepsilon$  is a small positive number.

#### Shell-side pressure upper bound

The same logic can be employed in relation to the upper bound on the shell-side pressure drop in Eq. 134, thus yielding:

$$wDPs_{sDs,sNb,srp,sL,sd,slay} = 0 \text{ for } (sDs, sNb, srp, sL, sd, slay) \\ \in SDPsmaxout$$
(176)

$$SDPsmaxout = \{(sDs, sNb, srp, sL, sd, slay) / p\widehat{\Delta Ps}_{sDs, sNb, srp, sL, sd, slay} \ge \Delta \widehat{Psdisp} + \varepsilon\}$$
(177)

## **Baffle** spacing

The baffle spacing constraints in Eqs. 162 and 163 yield the following additional constraints:

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 $yL_{sL} + yNb_{sNb} + yDs_{sDs} \leq 2 \text{ for } (sL, sNb, sDs) \\ \in (SLNbminout \cup SLNbmaxout)$ 

$$SLNbminout = \left\{ (sL, sNb, sDs) / \frac{\widehat{pL}_{sL}}{\widehat{pNb}_{sNb} + 1} \le 0.2\widehat{PDs}_{sDs} - \varepsilon \right\}$$
(179)

$$SLNbmaxout = \left\{ (sL, sNb, sDs) / \frac{\widehat{pL}_{sL}}{\widehat{pNb}_{sNb} + 1} \ge 1.0\widehat{PDs}_{sDs} + \varepsilon \right\}$$
(180)

## Tube length/shell diameter

The ratio between the tube length and shell diameter yields in Eqs. 167 and 168 yield the following additional constraints:

$$yL_{sL} + yDs_{sDs} \leq 1 \text{ for } (sL, sDs) \\ \in (SLDminout \cup SLDmaxout)$$
(181)

$$SLDminout = \left\{ (sL, sDs) / \widehat{pL}_{sL} \le 3\widehat{PDs}_{sDs} - \varepsilon \right\}$$
(182)

$$SLD\max out = \left\{ (sL, sDs) / \widehat{pL}_{sL} \ge 15\widehat{PDs}_{sDs} + \varepsilon \right\}$$
(183)

## Heat transfer area

The heat transfer area is the objective function and, a priori, does not have a bound constraint. However, based on maximum velocity limits, it is possible to determine maximum values for the convective heat transfer coefficients and, therefore, to evaluate a maximum value for the overall heat transfer coefficients. Finally, based on this parameter, it is possible to establish a minimum value for the heat transfer. The expression of the additional constraint is:

$$wA_{sDs,sd,sNpt,srp,slay,sL} = 0 \text{ for } (sDs, sd, sNpt, srp, slay, sL) \\ \in SAminout$$

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

$$SAminout = \{(sDs, sd, sNpt, srp, slay, sL)/\pi \widehat{pNtt}_{sDs, sd, sNpt, srp, slay} \widehat{pdte}_{sd} \widehat{pL}_{sL} \le \widehat{Amin} - \varepsilon\}$$
(185)

The lower bound on the heat transfer area can be determined through the following set of equations:

$$A\min = \frac{\widehat{Q}}{\widehat{U\max \Delta Tlm}}$$
(186)

 $U \max =$ 

$$\frac{1}{h\overline{max}}d\overline{r\min} + \widehat{Rft} \cdot d\overline{r\min} + \frac{\widehat{pdte}_{sd1}\ln\left(\widehat{dr\min}\right)}{2\ k\overline{tube}} + \widehat{Rfs} + \frac{1}{h\overline{max}}$$
(187)

1

$$\widehat{htmax} = \max\left(\widehat{pht}_{sDs,sd,sNpt,srp,slay}\right)$$
(188)

$$\widehat{hsmax} = \max\left(\widehat{phs}_{srp,sd,slay,sDs,sL,sNb}\right)$$
(189)

$$\widehat{dr\min} = \min\left(\widehat{pdte}_{sd}/\widehat{pdti}_{sd}\right) \tag{190}$$

Table 1. Design Data

Hot stream	Cold stream
Crude oil	Cooling water
Shell side	Tube side
110	228.8
90	30
50	40
0.0002	0.0004
100	100
[1.0 3.0]	[0.5 2.0]
	Crude oil Shell side 110 90 50 0.0002 100

#### Results

(178)

(184)

The application of the proposed MILP approach is illustrated by its utilization in the solution of a typical design task described in Table 1. The physical properties of the streams are shown in Table 2. The standard values of the design variables are displayed in Table 3, related to a fixed tubesheet type exchanger with E-shell, single segmental baffles, 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 is based on Kakaç et al.<sup>28</sup>

The design task was solved using the MILP formulation implemented in the optimization software GAMS using the solver CPLEX. The objective function, and the design and thermo-fluid dynamic variables in the solution obtained are shown in Tables 4 and 5.

The analysis of the results indicates that the optimal solution is coherent with general optimization trends employed in heat exchanger design. The pressure drops in the shell and tube sides are close to the allowable values, i.e., the optimal solution promotes a good exploration of the available pressure drop aiming to increase the overall heat transfer coefficient and, consequently, to diminish the heat transfer area.

#### Performance analysis

Aiming to provide a clearer assessment of the performance of the proposed approach when compared to conventional nonlinear alternatives (MINLP), a set of 10 different design tasks were tested (the problem discussed above is the first example of the sample). These tasks involve streams typically found in heat exchanger design problems: methanol, ethanol, acetone, sucrose solution, crude oil, cooling water, and hot water.<sup>28,29</sup> The standard values of the design variables are equal to the data displayed in Table 3 and the properties and flows of the fluids for each example are shown in the Appendix.

The problem sample was solved using the MILP formulation and compared to the original nonlinear model (Eqs. 1–41, 44–58) using an MINLP approach with two different solvers: DICOPT and SBB. The DICOPT algorithm is the outer approximation with equality relaxation and augmented penalty algorithm (OA/ER/AP) and the SBB is a branch-and-bound algorithm (BB). The MINLP formulation employed for the performance analysis is composed of the constraints in Eqs. 1– 40, objective function in Eq. 41, and the description of the

Table 2. Physical Properties of the Streams

	Hot stream	Cold stream
Density (kg/m <sup>3</sup> )	786.4	995
Heat capacity (J/(kg·K))	2177	4187
Viscosity (Pa·s)	$1.89 \cdot 10^{-3}$	$0.72 \cdot 10^{-3}$
Thermal conductivity (W/(m·K))	0.122	0.59

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Table 3. 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, $pDs_{sDs}$ (m)	0.787, 0.838, 0.889, 0.940,0.
Shell diameter, $p \ge \sigma_{SDS}$ (iii)	991, 1.067, 1.143,
	1.219, 1.372, 1.524
Tube layout, $\hat{play}_{slay}$	1 = Square, $2 =$ triangular

 Table 4. Heat Exchanger Design Results

	MILP
Area (m <sup>2</sup> )	624
Outer tube diameter (m)	0.019
Tube length (m)	4.9
Number of baffles	7
Number of tube passes	4
Tube pitch ratio	1.25
Shell diameter (m)	1.219
Tube layout	Triangular
Total number of tubes	2139
Baffle spacing (m)	0.610
Tube pitch (m)	0.024

**Table 5. Thermo-Fluid Dynamic Results** 

	MILP
Shell-side flow velocity (m/s)	0.94
Tube-side flow velocity (m/s)	2.2
Shell-side heat transfer coefficient (W/m <sup>2</sup> K)	1163
Tube-side heat transfer coefficient (W/m <sup>2</sup> K)	9206
Overall heat transfer coefficient (W/m <sup>2</sup> K)	584
Shell-side pressure drop (kPa)	84.9
Tube-side pressure drop (kPa)	91.9

discrete variables in Eqs. 44–58. An initialization procedure was provided for initial estimates of the thermal variables based on the flow velocity bounds in the MINLP algorithms. No initial estimates were employed in the MILP runs.

The description of all design tasks and the corresponding solutions can be found in the Supporting Information online provided with this article. The heat transfer area of the solutions and the computational time employed are displayed in Table 6. The computational times were measured using a computer with a processor Intel Core i7 3.40 GHz with 12.0 GB RAM memory.

The results displayed in Table 6 indicate a considerable number of occasions where the MINLP algorithms failed to converge. This problem has occurred in 40% of the problems when using the solvers DICOPT and SBB. The analysis of the converged results also indicates that the MINLP algorithms may be trapped in local optima. This problem has occurred in 33% of the converged runs of the DICOPT solver and 17% of the solutions when using the SBB solver. The comparison of the solution time (evaluated using the elapsed time command in GAMS) indicates that the MILP approach is usually much slower than the MINLP algorithms. However, the observed solution times of the MILP approach do not compromise its use in practical applications, varying between about 3 to 45 min.

## Effect of pressure drop

As mentioned above the objective function can be formulated differently. One of the issues is the pressure drop as it is associated to pumping costs. In this case one could construct an objective function that is a linear combination of the amortized cost of area, and the pressure drops. Because the coefficients of such cost function depend a lot on the context, that is, whether the exchanger is alone needing (or not) pumping for a source pressure to a delivery pressure, or is part of a network, we believe that it is best to study the effect of the pressure drop on the final design. To do this we prepared three runs related to the design task described in Table 1, one limiting the pressure drop on tubes to an 80% smaller value. We do the same for the shell and finally, for completeness we add both. The results of these runs, together with the original design are shown in Table 7.

The analysis of the results indicates that the reduction of the allowable pressure drop determined a reduction in the flow velocity, which causes a decrease of the corresponding heat transfer coefficient. Consequently, the smaller value of the overall heat transfer coefficient implies an increase of the area necessary to fulfill the design task. Because the heat transfer coefficient in the shell-side is lower than in the tube-side, the area increase is more pronounced when the allowable shell-side pressure drop is reduced. The allowable tube-side pressure drop reduction determines an area increase of 10% and the equivalent shell-side pressure drop reduction determines an increase when both parameters are reduced.

Heat transfer area (m <sup>2</sup> )					Solution time (s)	
Example	MILP	MINLP DICOPT	MINLP SBB	MILP	MINLP DICOPT	MINLP SBE
1	624	NC	NC	1772	NC	NC
2	319	319	319	1606	8.8	1.3
3	199	NC	NC	211	NC	NC
4	872	872	872	153	87	0.4
5	144	NC	NC	931	NC	NC
6	332	355	341	2824	5061	1.8
7	207	225	207	2529	1.5	0.9
8	914	914	914	171	19	0.7
9	287	287	287	2058	9.3	0.9
10	327	NC	NC	2329	NC	NC

Table 6. Performance Comparison

Note: NC, non-convergence.

Table 7. Effect of the Allowable Pressure Drop in the Optimal Design
--

	MILP without changes	Lower pressure drop on tubes	Lower pressure drop on shell	Lower pressure drop on tubes and shell
Area (m <sup>2</sup> )	624	684	855	855
Tube length (m)	4.9	4.9	6.1	6.1
Number of baffles	7	8	5	5
Number of tube passes	4	2	4	2
Shell diameter (m)	1.219	1.372	1.372	1.372
Tube layout	Triangular	Square	Square	Square
Total number of tubes	2139	2344	2344	2344
Baffle spacing (m)	0.610	0.542	1.016	1.016
Shell-side flow velocity (m/s)	0.94	0.94	0.50	0.50
Tube-side flow velocity (m/s)	2.2	1.0	2.0	1.0
Shell-side heat transfer coefficient (W/m <sup>2</sup> K)	1163	1009	714	714
Tube-side heat transfer coefficient $(W/m^2K)$	9206	4914	8556	4914
Overall heat transfer coefficient (W/m <sup>2</sup> K)	584	511	442	422
Shell-side pressure drop (kPa)	84.9	73.7	15.7	15.7
Tube-side pressure drop (kPa)	91.9	10.9	93.8	13.3

#### Conclusions

An MILP model for the design of shell and tube heat exchangers was presented. The model is linear, thanks to the fact that several geometric design variables are discrete and therefore amenable to be expressed in terms of binary variables. When these expressions are substituted in the model, the resulting equations are nonlinear expressions containing binary variables. We therefore reformulate the problem as a linear one without losing any rigor.

The comparison of the MILP model with an MINLP formulation through the solution of the same sample of heat exchanger design problems shows drawbacks in the MINLP approach in relation to non-convergence and local optima. Due to its linear nature, the MILP model proposed here is immune to these obstacles, always reaching the global optimum.

The computational time for the MILP model is remarkable higher than the required by others, but it is still satisfactory for its use in practice. Further research will be devoted to identify algorithmic options to reduce the computational effort. An important aspect that must also be noted is that the linear nature of the proposed model makes it amenable to be easier to add to other broader models (i.e., HEN synthesis with simultaneous heat exchanger design).

#### Notatio

## Sets

sd = tusDs = shsL = tuslav = tulsNb = nusNpt = nusrp = tulParame

pDe

 $\widehat{pdti}_{sd}$  = inlet tube diameter, m  $\widehat{pL}_{sL}$  = tube length, m  $play_{slay}$  = tube layout  $\widehat{pNb}_{sNb}$  = number of baffles  $\widehat{pNpt}_{sNpt}$  = number of tube passes  $\widehat{pNtt}_{sDs,sd,sNpt,srp,slay}$  = total number of tubes  $\widehat{prp}_{srp}$  = tube pitch ratio  $\hat{Pr} = \text{Prandtl number}$  $\widehat{Q}$  = heat duty, W  $\widehat{R}$  = for calculating the correction factor F  $\widehat{Rf}$  = fouling factor, m<sup>2</sup> K/W  $\widehat{T}$  = temperature, °C  $\hat{\rho} = \text{density, kg/m}^2$ 

- $\hat{\mu}$  = viscosity, Pa·s
- $\Delta P disp$  = pressure drop available, Pa
- $\Delta T lm = \log$ -mean temperature difference

#### **Binary** variables

 $vd_{sd}$  = variable representing the tube diameter

- $yDs_{sDs}$  = variable representing the shell diameter
- $yL_{sL}$  = variable representing the tube length
- $y lay_{slay}$  = 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

#### Continuous variables

	$A = area, m^2$
	Ar = flow area in the shell side, m <sup>2</sup>
ion	d = tube diameter, m
	Deq = equivalent diameter, m
ube diameter, 1sdmax shell diameter, 1sDsmax ube length, 1sLmax ube layout, 1sNpmax number of baffles, 1sNbmax number of tube passes, 1sNptmax ube pitch ratio, 1srpmax ube pitch ratio, 1srpmax <b>reters</b> $\widehat{Aexc} = \text{excess area}, \%$ $\widehat{cp} = \text{heat capacity, J/kg K}$ $\widehat{FMP} = \text{correction factor of the LMTD for a configuration}$	
with a single shell pass and an even number of tube passes $\hat{g} = \text{gravity acceleration, m/s}^2$ $\hat{k} = \text{thermal conductivity, W/m K}$ $\hat{m} = \text{mass flow rate, kg/s}$ $\hat{n} = 0.4$ for heating services; 0.3 for cooling services $\hat{P} = \text{for calculating the correction factor F}$ $\widehat{Peq}_{srp,sd,slay} = \text{equivalent diameter, m}$ $\widehat{pDs}_{sDs} = \text{shell diameter, m}$ $pdte_{sd} = \text{outer tube diameter, m}$	$Ntp = \text{number of tubes per passes}$ $Ntt = \text{total number of tubes}$ $Nu = \text{Nusselt number}$ $Re = \text{Reynolds number}$ $rp = \text{tube pitch ratio}$ $U = \text{overall heat transfer coefficient, W/m^2 K}$ $v = \text{velocity, m/s}$ $\Delta P = \text{pressure drop, Pa}$ $wA_{sDs,sd,sNpt,srp,slay,sL} = \text{variable representing the area}$ $wA1P_{sDs,sd,sNpt,srp,slay,sL} = \text{variable representing the area and one pass in the tube}$

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- $wDPs_{sDs,sNb,srp,sL,sd,slay} =$  variable representing the pressure drop in the shell
- $webc_{sL,sNb} = \text{variable representing the baffle spacing}$   $whs_{sDs,srp,sL,sNb,sd,slay} = \text{variable representing the heat transfer coefficient in the shell side}$   $wvs_{sDs,srp,sL,sNb} = \text{variable representing the shell side velocity}$   $wvt_{sDs,sd,sNpt,srp,slay} = \text{variable representing the tube side velocity}$   $wvt1P_{sDs,sd,sNpt,srp,slay} = \text{variable representing the tube side velocity}$ and one pass in the tube
- $wvtturb_{sDs,sd,sNpt,srp,slay,sL}$  = variable representing the tube side velocity and turbulent flow

#### **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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## APPENDIX A

Example	1	2	3	4	5
Service	Crude oil cooler	Crude oil cooler	Methanol cooler	Methanol cooler	Methanol heater
Hot stream	Crude oil	Crude oil	Methanol	Methanol	Hot water
Cold stream	Cooling water	Cooling water	Cooling water	Cooling water	Methanol
Tube-side stream	Cold	Cold	Hot	Hot	Hot
Example	6	7	8	9	10
Service	Ethanol cooler	Sucrose solution heater	Sucrose solution cooler	Acetone ethanol exchanger	Acetone ethanol exchanger
Hot stream	Ethanol	Hot water	Sucrose solution	Ethanol	Ethanol
Cold stream	Cooling water	Sucrose solution	Cooling water	Acetone	Acetone
Tube-side stream	Cold	Hot	Cold	Cold	Hot

Table A2. Hot Stream Data

Example	1	2	3	4	5	6	7	8	9	10
$\widehat{m}$ (kg/s)	110.0	50.0	27.8	69.4	40.0	55.6	40.0	83.3	111.1	111.1
Inlet $\widehat{T}$ (°C)	90.0	100.0	70.0	100.0	220.0	150.0	220.0	90.0	190.0	190.0
Outlet $\widehat{T}$ (°C)	50.0	50.0	40.0	40.0	110.2	60.0	80.8	40.0	120.0	120.0
max $\Delta P$ (kPa)	100	60	70	70	70	70	70	100	100	100
$\rho (\text{kg/m}^3)$	786	786	750	750	888	789	888	1080	789	789
$\hat{\mu}$ (mPa·s)	1.89	1.89	0.34	0.34	0.15	0.67	0.15	1.30	0.67	0.67
$c\hat{p}$ (J/kg·K)	2177	2177	2840	2840	4312	2470	4312	3601	2470	2470
$\hat{k}$ (W/m·K)	0.12	0.12	0.19	0.19	0.70	0.17	0.70	0.58	0.17	0.17
$\widehat{Rf}$ (m <sup>2</sup> K/W)	0.0002	0.0002	0.0002	0.0002	0.0001	0.0002	0.0001	0.0001	0.0002	0.0002

Table A3. Cold Stream Data

Example	1	2	3	4	5	6	7	8	9	10
$\widehat{m}$ (kg/s)	228.8	130.0	56.6	353.3	133.3	295.0	133.3	358.3	166.7	166.7
Inlet $\hat{T}$ (°C)	30.0	30.0	30.0	32.0	30.0	30.0	30.0	30.0	30.0	30.0
Outlet $\widehat{T}$ (°C)	40.0	40.0	40.0	40.0	80.0	40.0	80.0	40.0	79.7	79.7
max $\Delta P$ (kPa)	100	50	100	70	70	70	70	100	100	100
$\rho (\text{kg/m}^3)$	995	995	995	995	750	995	1080	995	736	736
$\hat{\mu}$ (mPa·s)	0.72	0.72	0.72	0.72	0.34	0.72	1.30	0.80	0.21	0.21
$\widehat{cp}$ (J/kg·K)	4187	4187	4187	4187	2840	4187	3601	4187	2320	2320
$\hat{k}$ (W/m·K)	0.59	0.59	0.59	0.59	0.19	0.59	0.58	0.59	0.14	0.14
$\widehat{Rf}$ (m <sup>2</sup> K/W)	0.0004	0.0003	0.0002	0.0004	0.0001	0.0004	0.0001	0.0004	0.0002	0.0002

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