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Global optimization of the design of horizontal shell and tube condensers

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HIGHLIGHTS

- Design optimization of shell and tube condensers.
- The design procedure always identify the global optimum.
- The solution is obtained through an integer linear programming.
- Comparison with textbook examples show reduction of the heat transfer area.

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ABSTRACT

The literature about heat exchanger design optimization encompasses a large number of papers, but only a small fraction is dedicated to phase change systems. This article presents for the first time a linear design optimization approach for horizontal shell and tube condensers that guarantees global optimality. Area is minimized using an integer linear model. This model is obtained from a mathematical reformulation of the original nonlinear thermofluid dynamic equations and it is solved using integer linear programming (ILP). Because of the linear nature of the proposed model, the global optimum is always attained, without the need of using specialized global solvers, selection of good initial estimates or drawbacks related to convergence issues. Numerical results indicate that the proposed approach can present solutions with lower heat transfer areas than two design procedures presented in chemical process design textbooks.

1. Introduction

Condensers are equipment widely employed in chemical process industries. For example, a condenser is a fundamental equipment in a distillation column system, providing reflux to promote the separation. Condensers may also be found in certain reaction units, where they are employed to recover a desired product from the outlet stream of a reactor from gaseous components. Condensers are also present in power stations based on Rankine cycle, where they are responsible for the condensation of the turbine exhaust steam. Refrigeration cycles also involve the presence of a condenser, which promotes the heat rejection to the environment. While other kinds of heat exchangers may be employed in some of the aforementioned applications (e.g. gasketed plate, air coolers, etc.), the shell-and-tube heat exchanger is still the main option.

Textbooks present several worked examples of the design of condensers, such as Kakaç and Liu (2002), Smith (2005), Serth (2007), Towler and Sinnot (2008), Cao (2010), and Smith (2016) using heuristics based on choices made by the designer. The main concept is to find one viable exchanger, not necessarily the optimal one; in other words, optimality is not a goal of these heuristics-based procedures. Soltan et al. (2004) investigated finding the optimal value of the baffle spacing of shell and tube condensers for the minimization of the total annualized cost using the Simplex method (Nelder and Mead, 1965). Allen and Gosselin (2008) employed genetic algorithms for the determination of the minimum total annualized cost of condensers, including the possibility of condensation in the shell-side or tube-side. Hajabdollahi et al. (2011) compared the utilization of genetic and particle swarm algorithms for the design of shell and tube condensers, showing that genetic algorithms presented a better computational performance. Chandrakanth et al. (2018) investigated the design optimization of a condenser for a desalination plant through an approach based on design of experiments. Finally, Xiao et al.

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Nomenclature

Parameters

$\widehat{Aexc}$	excess area (%)
$\widehat{C}$	correlation parameter
$\widehat{Cpt}$	tube-side stream heat capacity (J/(kg·K))
$\widehat{F_{SC}}$	heat exchanger structure factor
$\widehat{g}$	gravitational acceleration (m/s^2)
$\widehat{ks}$	shell-side condensate thermal conductivity (W/(m·K))
$\widehat{kt}$	tube-side stream thermal conductivity (W/(m·K))
$\widehat{k}_{tube}$	tube wall thermal conductivity (W/(m·K))
$\widehat{ms}$	shell-side stream mass flow rate (kg/s)
$\widehat{mt}$	tube-side stream mass flow rate (kg/s)
$\widehat{pDeq}_{srow}$	equivalent diameter parameter (m)
$\widehat{pDs}_{srow}$	discrete values of shell diameter (m)
$\widehat{pdte}_{sd}$	discrete values of outer tube diameter (m)
$\widehat{pdte}_{srow}$	discrete values of outer tube diameter related to a combinatorial representation (m)
$\widehat{pdti}_{srow}$	discrete values of inner tube diameter (m)
$\widehat{pFAR}_{srow}$	free area ratio parameter
$\widehat{phs}_{srow}$	shell-side convective heat transfer coefficient parameter (W/(m^2.K))
$\widehat{pht}_{srow}$	tube-side convective heat transfer coefficient parameter (W/(m^{2}K))
$\widehat{pL}_{srow}$	discrete values of tube length (m)
$\widehat{pNb}_{srow}$	discrete values of number of baffles
$\widehat{pNpt}_{srow}$	discrete values of number of tube passes
$\widehat{pNtt}_{srow}$	discrete values of the total number of tubes
$\widehat{Prt}$	tube-side stream Prandlt number (dimensionless)
$\widehat{p\Delta Ps}_{srow}$	shell-side pressure drop parameter (Pa)
$\widehat{p\Delta Ptcab}_{srow}$	pressure drop in the exchanger heads parameter (Pa)
$\widehat{p\Delta Ptturb1}_{srow}$	pressure drop constraint parameter (Pa)
$\widehat{pP\Delta Ptturb2}_{srow}$	pressure drop constraint parameter (Pa)
$\widehat{Q}$	heat load (W)
$\widehat{Rfs}$	shell-side fouling factor (m^{2}K/W)
$\widehat{Rft}$	tube-side fouling factor (m^{2}K/W)
$\widehat{Tci}$	inlet temperature of the cold stream (°C)
$\widehat{Tco}$	outlet temperature of the cold stream (°C)
$\widehat{Thi}$	inlet temperature of the hot stream (°C)
$\widehat{Tho}$	outlet temperature of the hot stream (°C)
$\widehat{Tsat}$	saturation temperature (°C)
$\widehat{vsmax}$	upper bound on shell-side velocity (m/s)
$\widehat{vsmin}$	lower bound on shell-side velocity (m/s)
$\widehat{vtmax}$	upper bound on tube-side velocity (m/s)
$\widehat{vtmin}$	lower bound on tube-side velocity (m/s)
$\widehat{\Delta H}_{vap}$	latent heat of vaporization (J/kg)
$\widehat{\Delta Psdisp}$	available shell-side pressure drop (Pa)
$\widehat{\Delta Ptdisp}$	available tube-side pressure drop (Pa)
$\widehat{\Delta Tlm}$	logarithmic mean temperature difference (°C)
$\widehat{\mu s}$	shell-side condensate dynamic viscosity (Pa·s)
$\widehat{\mu t}$	tube-side stream dynamic viscosity (Pa·s)
$\widehat{\mu vs}$	shell-side vapor dynamic viscosity (Pa·s)
$\widehat{\rho s}$	shell-side condensate density (kg/m^3)
$\widehat{\rho t}$	tube-side stream density (kg/m^3)
$\widehat{\rho vs}$	shell-side vapor density (kg/m^3)
ϕ_{VO}	average two-phase pressure-drop multiplier

Variables

A	heat transfer area (m^2)
Ar	flow area in shell-side (m^2)
$Areq$	required area (m^2)
Deq	equivalent diameter (m)
Ds	shell diameter (m)
dte	outer tube diameter (m)
dti	inner tube diameter (m)
FAR	free area ratio
fs	shell-side friction factor
ft	tube-side friction factor
F_{TC}	correction factor related to the tube bundle
hs	shell-side convective heat transfer coefficient (W/(m^{2}K))
ht	tube-side convective heat transfer coefficient (W/(m^{2}K))
$\widehat{K}$	pressure drop parameter
$\widehat{Klay}$	layout 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 pass
Ntt	total number of tubes
Nut	tube-side Nusselt number (dimensionless)
Res	shell-side Reynolds number (dimensionless)
Ret	tube-side Reynolds number (dimensionless)
$Tsurf$	tube surface temperature (°C)
U	overall heat transfer coefficient (W/(m^{2}K))
vs	shell-side flow velocity (m/s)
vt	tube-side flow velocity (m/s)
yd_{sd}	binary variable representing the tube diameter
$yrow_{srow}$	binary variable representing the set of variables
ΔPs	shell-side pressure-drop (Pa)
ΔPs_{VO}	shell-side pressure drop associated to the inlet conditions of the vapor flow (Pa)
ΔPt	tube-side pressure-drop (Pa)

(2019) employed a combined genetic algorithm/simulated annealing for the optimization of heaters using condensing stfeam in the investigation of heat exchanger network synthesis.

It is important to observe that no method employed in the aforementioned previous references can guarantee global optimality. Stochastic optimization methods can avoid be trapped in local optimum, and there is evidence that they often attain the global optimum, but this is never known unless a proven global optimization method is used. Finally, these methods require a lot of parameter tuning that is many times specialized to the problem in question, and is a result of several trial and error steps and authors seldom publish these details. This makes the results reported many times irreproducible. The possible utilization of mathematical programming through mixed integer nonlinear programming using local solvers would also render optima that do not guarantee globality. While global mathematical programming solvers are available, they are known to fail sometimes or they need initial data to reduce computational time, or to function at all.

As far as we know, we could not find in the literature an optimization methodology to obtain global optimal designs for condensers. We offer one in this paper by solving an integer linear programming (ILP) problem. The corresponding linear model is based on a mathematical reformulation of the nonlinear thermofluid dynamic equations using the techniques originally presented in Gonçalves et al. (2017a, 2017b). This mathematical reformulation is rigorous, without involving any kind of approximation in relation to the original equations (that is, no truncated Taylor expansions or similar techniques). In other words the math-

ematical reformulation is rigorous that the solution of the original nonlinear model is a solution of the reformulated model and vice versa. The mathematical reformulation also presents several advantages: it always identify the global optimum, does not depend of initial estimates, is robust in the sense that it always arrives at a solution and does not present convergence problems.

The current article is organized as follows. We start presenting the thermal and hydraulic model equations employed in the design in its original form, together with additional optimization constraints and the objective function. We consider pure component condensation on the shell-side of horizontal condensers. We then discuss the mathematical reformulation of the original equations using binary variables in a linear form. Numerical results are presented comparing the optimal solution obtained through the proposed approach with design procedures presented in textbooks. Finally, conclusions are presented.

2. Condenser optimization model

There are different arrangements of shell-and-tube condensers and the spatial orientation of these configurations, vertical or horizontal, has a strong impact in the heat transfer coefficient. Additionally, the allocation of the condensing streams, shell-side or tube-side, is also important. Thus, four alternatives of shell-and-tube heat exchanger systems are applied as condensers:

(i) horizontal exchanger with condensation in the shell-side,
(ii) horizontal exchanger with condensation in the tube-side,
(iii) vertical exchanger with condensation in the shell-side, and
(iv) vertical exchanger with condensation in the tube-side.

The selection of the best alternative depends on several factors, such as, operation pressure and temperature, available pressure drop, corrosion, fouling, etc. (Mueller, 2008). In general, the most common alternatives are the shell-side condensation in horizontal heat exchangers and the tube-side condensation in vertical heat exchangers (Smith, 2016).

Therefore, the current paper is focused on shell-and-tube condensers with an E-type shell, horizontally oriented, where the condensation occurs in the shell-side. The shell-side inlet stream is assumed to be pure component saturated vapor and the outlet stream is saturated condensate; consequently, there is no temperature variation in the shell-side. The tube-side coolant is assumed to be a no phase change stream in turbulent flow, as it is common in industrial equipment. The physical properties are assumed constant, based on average values. The heat transfer equations are based on Smith (2016) and the hydraulic equations are based on Kern (1950), Saunders (1988), and Serth (2007).

The structure of the condenser optimization model is illustrated in Fig. 1 and the details of the set of equations are shown below. In the description of the optimization model, the problem parameters, which are fixed prior to the optimization, are represented with the symbol "^" on top.

2.1. Tube-side thermal and hydraulic equations

The heat transfer coefficient for the tube-side in turbulent flow is calculated by (Smith, 2016):

$$Nut = \widehat{C} Ret^{0.8} \widehat{Prt}^{0.4} \tag{1}$$

where *Nut*, *Ret* and *Prt* are the Nusselt, Reynolds and Prandtl numbers, and $\widehat{C}$ is a correlation parameter that is equal to 0.024 for heating and 0.023 for cooling. The expressions of the dimensionless groups present in Eq. (1) are:

$$Nut = \frac{ht\ dti}{\widehat{kt}} \tag{2}$$

$$Ret = \frac{dti\ vt\ \widehat{\rho t}}{\widehat{\mu t}} \tag{3}$$

$$\widehat{Prt} = \frac{\widehat{Cpt}\ \widehat{\mu t}}{\widehat{kt}} \tag{4}$$

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 *dti* is the inner tube diameter. The flow velocity can be calculated by:

$$vt = \frac{4\ \widehat{mt}}{Ntp\ \pi\ \widehat{\rho t}\ dti^2} \tag{5}$$

where $\widehat{mt}$ is the mass flow rate and *Ntp* is the number of tubes per pass, which is related to the total number of tubes (*Ntt*) and the number of passes in the tube-side (*Npt*):

$$Ntp = \frac{Ntt}{Npt} \tag{6}$$

Min Heat transfer area

Subject to:

- Tube-side heat transfer coefficient evaluation
- Tube-side pressure drop evaluation
- Shell-side heat transfer coefficient evaluation
- Shell-side pressure drop evaluation
- Evaluation of the overall heat transfer coefficient
- Heat transfer rate equation
- Bounds on pressure drops, flow velocities and Reynolds numbers
- Geometric constraints

Fig. 1. General structure of the condenser optimization model.

The total number of tubes that fits in a certain shell diameter can be calculated according to a relation, equivalent to a tube count table, presented in Smith (2016):

$$Ntt = \text{round}\left(\frac{\pi Ds^2}{4ltp^2 Klay F_{TC}\widehat{F_{SC}}}\right) \tag{7}$$

where Ds is the shell diameter, ltp is the tube pitch, $Klay$ is a constant equal to 0.866 for triangular layout and 1 for square layout, F_{TC} is a correction factor that considers the clearance shell-tube bundle and tube omissions due to the presence of multiple passes, and $\widehat{F_{SC}}$ is a factor that depends on the heat exchanger structure. For shell diameters higher than 0.337 m, the factor F_{TC} is equal to 1.08 for Npt = 1, 1.11 for Npt = 2, 1.45 for Npt = 4 or 6 and $Ds \leq 0.635$ m, and 1.18 for Npt = 4 or 6 and Ds > 0.635 m. The factor $\widehat{F_{SC}}$ is equal to 1.0 for fixed tubesheet, 1.15 for floating head, 1.05 for U-tube, and 1.09 for U-tube with pitch ratio 1.25 and outer tube diameter 0.025 m.

The head loss in the tube-side can be evaluated by the Darcy-Weisbach equation summed with a term that accounts the head loss in the exchanger heads (the pressure drop in the nozzles is dismissed) (Saunders, 1988):

$$\frac{\Delta Pt}{\widehat{\rho t}\,\hat{g}} = \frac{ft\ Npt\ L\ vt^2}{2\ \hat{g}\ dti} + \frac{K\ Npt\ vt^2}{2\,\hat{g}} \tag{8}$$

where ΔPt is the tube-side pressure drop, L is the tube length, $\hat{g}$ is the gravitational acceleration, ft is the Darcy friction factor, and the parameter K 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 can be calculated by:

$$ft = 0.014 + \frac{1.056}{Ret^{0.42}} \tag{9}$$

2.2. Shell-side thermal and hydraulic equations

The condensation in the shell-side is considered as a film condensation, the most common pattern observed in industrial operations. According to the Nusselt model, the convective heat transfer coefficient (hs) associated to the film condensation over the outer surface of a single tube is given by (Smith, 2016):

$$hs = 0.725\left[\frac{\widehat{\rho s}\left(\widehat{\rho s} - \widehat{\rho vs}\right)\ \hat{g}\ \widehat{ks}^3\ \widehat{\Delta H}_{vap}}{dte\ \widehat{\mu s}\ \left(\widehat{Tsat} - Tsurf\right)}\right]^{\frac{1}{4}} \tag{10}$$

where dte is the outer tube diameter, $\widehat{\rho s}$, $\widehat{\mu s}$, and $\widehat{ks}$ are the density, viscosity and thermal conductivity of the condensate, $\widehat{\rho vs}$ is the vapor density, $\hat{g}$ is the gravity acceleration, $\widehat{\Delta H}_{vap}$ is the phase change enthalpy, $\widehat{Tsat}$ is the saturation temperature, and $Tsurf$ is the heat transfer surface temperature. This model assumes laminar flow and the absence of shear stress in the vapour-liquid interface. The exclusion of possible turbulence effects and vapor flow influence in the liquid film are conservative hypothesis because these aspects intensify the heat transfer, therefore these assumptions become an additional design margin (safe side design).

In order to avoid the need to evaluate the surface temperature in the model, the following relation is considered:

$$hs\ Ntt\ \pi\ dte\ L\left(\widehat{Tsat} - Tsurf\right) = \widehat{ms}\ \widehat{\Delta H}_{vap} \tag{11}$$

where $\widehat{ms}$ is the total mass flow rate that is condensated and L is the tube length. Therefore, the substitution of $\left(\widehat{Tsat} - Tsurf\right)$ from Eq. (11) into Eq. (10) and the insertion of a correction factor to include the effect of the dripping of condensate over successive tubes along each vertical row in a circular tube bundle yields the final form of the heat transfer coefficient expression (Smith, 2016):

$$hs = 0.954\left[\frac{\widehat{\rho s}\left(\widehat{\rho s} - \widehat{\rho vs}\right)\ \hat{g}\ \widehat{ks}^3\ L}{\widehat{ms}\ \widehat{\mu s}}\right]^{\frac{1}{3}} Ntt^{2/9} \tag{12}$$

The shell-side pressure drop can be calculated by the equivalent pressure drop associated to the total mass flow rate as vapor at the inlet conditions (ΔPs_{VO}) corrected by an average two-phase multipliers ($\bar{\phi}^2_{VO}$) (Serth, 2007):

$$\Delta Ps = \bar{\phi}^2_{VO}\Delta Ps_{VO} \tag{13}$$

A conservative value of 0.5 is employed to describe the two-phase multiplier in total condensation.

The pressure drop of the total mass flow rate as vapor at the inlet condition can be calculated using the Kern model (Kern, 1950):

$$\frac{\Delta Ps_{VO}}{\widehat{\rho vs}\ \hat{g}} = fs\frac{Ds(Nb+1)}{Deq}\left(\frac{vs^2}{2\,\hat{g}}\right) \tag{14}$$

where fs is the shell-side friction factor, Nb is the number of baffles, Deq is the equivalent diameter, and vs is the vapor velocity at the inlet. The equivalent diameter and the flow velocity are given by:

$$Deq = \frac{4ltp^2}{\pi dte} - dte\ \ (\text{Square pattern}) \tag{15}$$

$$Deq = \frac{3.46ltp^2}{\pi dte} - dte\ \ (\text{Triangular pattern}) \tag{16}$$

$$vs = \frac{\widehat{ms}}{\widehat{\rho vs}\ Ar} \tag{17}$$

where Ar is the free area between adjacent baffles. The expression for evaluation of Ar is:

$$Ar = Ds\ FAR\ lbc \tag{18}$$

where lbc is the baffle spacing and FAR is the free area ratio. The free area ratio is calculated by:

$$FAR = \frac{(ltp - dte)}{ltp} = 1 - \frac{dte}{ltp} = 1 - \frac{1}{rp} \tag{19}$$

where rp is the tube pitch ratio. The baffle spacing is determined by the number of baffles and the tube length:

$$Nb = \frac{L}{lbc} - 1 \tag{20}$$

The friction factor is given by:

$$fs = 1.728Res^{-0.188} \tag{21}$$

where Res is the Reynolds number. The expression for evaluation of the Reynolds number is:

$$Res = \frac{Deq\ \ vs\ \ \widehat{\rho vs}}{\widehat{\mu vs}} \tag{22}$$

where $\widehat{\mu vs}$ is the vapor viscosity.

2.3. Overall heat transfer coefficient

The overall heat transfer coefficient (U) is given by:

$$U = \frac{1}{\frac{dte}{dti\ ht} + \frac{\widehat{Rft}\ dte}{dti} + \frac{dte\ln\left(\frac{dte}{dti}\right)}{2\ \widehat{ktube}} + \widehat{Rfs} + \frac{1}{hs}} \tag{23}$$

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

2.4. Heat transfer rate equation

The heat transfer rate is represented by the LMTD method:

$$\widehat{Q} = UAreq\widehat{\Delta Tlm} \tag{24}$$

where $\widehat{Q}$ is the heat load, $Areq$ is the required area, $\widehat{\Delta Tlm}$ is the logarithmic mean temperature difference (LMTD). No correction factor for the LMTD is needed, because there is no temperature variation of the condensing stream (assumed composed of a pure component).

The LMTD is given by:

$$\widehat{\Delta Tlm} = \frac{\left(\widehat{Thi} - \widehat{Tco}\right) - \left(\widehat{Tho} - \widehat{Tci}\right)}{\ln\left(\frac{\left(\widehat{Thi}-\widehat{Tco}\right)}{\left(\widehat{Tho}-\widehat{Tci}\right)}\right)} \tag{25}$$

where $\widehat{Thi}$ and $\widehat{Tho}$ are the inlet and outlet temperatures of the hot stream, and $\widehat{Tci}$ and $\widehat{Tco}$ are the inlet and outlet temperatures of the cold stream (according to the hypothesis of the condensation of a pure stream: $\widehat{Thi} = \widehat{Tho}$).

The heat transfer area (A) is represented by the sum of the surface area of all tubes:

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

The exchanger area must be higher than the required area according to a certain “excess area” ($\widehat{Aexc}$), specified to provide a design margin in relation to the uncertainties in the parameters and in the modelling:

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

Finally, Eqs. (24) and (27) can be reorganized together, thus yielding:

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

2.5. Bounds on pressure drops, flow velocities and Reynolds numbers

The pressure drop in the tube and shell sides must be limited to the available pressure drop:

$$\Delta Pt \leq \widehat{\Delta Ptdisp} \tag{29}$$

$$\Delta Ps \leq \widehat{\Delta Psdisp} \tag{30}$$

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

$$vt \geq \widehat{vtmin} \tag{31}$$

$$vt \leq \widehat{vtmax} \tag{32}$$

$$vs \geq \widehat{vsmin} \tag{33}$$

$$vs \leq \widehat{vsmax} \tag{34}$$

The flow velocity bounds in the shell-side are imposed considering the inlet flow rate of the vapor stream.

According to the validity range of the correlations for evaluation of the convective heat transfer coefficient for the tube-side and the friction factor for the shell-side, the following bounds are applied:

$$Ret \geq 10^4 \tag{35}$$

$$Res \geq 500 \tag{36}$$

2.6. Geometric constraints

The baffle spacing must be bounded by (Taborek, 2008a):

$$lbc \geq 0.2Ds \tag{37}$$

$$lbc \leq 1.0Ds \tag{38}$$

The ratio between tube length and shell diameter is limited (Taborek, 2008b):

$$L \geq 3Ds \tag{39}$$

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

2.7. Objective function

The objective function corresponds to the minimization of the heat transfer area:

$$\min A \tag{41}$$

3. Integer linear model

The set of design variables that represents the degrees of freedom of the search space is depicted in Table 1. Due to commercial standards or its physical nature, the design variables are available only in discrete values. The tube thickness is assumed constant, according to the mechanical design, then the inner and outer tube diameters correspond to only one degree of freedom.

The formulation of the optimization problem using the original equations of the thermofluid dynamic model is a nonconvex mixed-integer nonlinear programming (MINLP). The solution of this problem in this form presents some drawbacks: convergence may not be attained and the solution may be trapped in a poor local optimum, if local solvers are employed. Aiming at circumventing these limitations, we apply a mathematical reformulation technique that yields an equivalent linear formulation. This mathematical reformulation does not involve any approximation, i.e. the solution of the reformulated problem is rigorously the same of the original MINLP and vice versa. The new linear formulation corresponds to an integer linear model (ILM) and is generated using the techniques presented in Gonçalves et al. (2017a) and Gonçalves et al. (2017b). We show in the next paragraphs the techniques employed in the mathematical reformulation, the objective function, and the constraints of the resultant ILM, which we later solve using integer linear programming (ILP).

Table 1
List of design variables.

Variable	Symbol
Inner and outer tube diameter	dti and dte
Tube length	L
Tube pitch ratio	rp
Tube layout (square or triangular)	lay
Shell diameter	Ds
Number of passes in the tube-side	Npt
Number of baffles	Nb

3.1. Representation of the search space

The search space can be represented in two forms, a simple discrete representation and a combinatorial representation. We discuss both next.

The typical representation of discrete variables in mathematical programming associates each discrete value to a binary variable. We call it here a discrete representation of the search space. For example, the outer tube diameter, *dte*, can be represented by a set of binaries yd_{sd}, that are related to the corresponding discrete values, $\widehat{pdte}_{sd}$:

$$dte = \sum_{sd=1}^{sdmax} \widehat{pdte}_{sd} yd_{sd} \tag{42}$$

Additionally, it must be imposed that only one diameter option is selected at the solution, i.e. only one of the binaries is nonzero:

$$\sum_{sd=1}^{sdmax} yd_{sd} = 1 \tag{43}$$

In turn, a combinatorial representation of the search space combines all variables to represent each potential solution. Indeed, instead of using binaries to represent each separate discrete variable, as shown in Eq. (42), a unique set of binaries is employed to represent combination of values of the design variables, i.e. each binary variable represents a solution candidate associated to a set of discrete values of the design variables. These binaries are indexed by a multi-index *srow*, such that, *srow* = (*sd*, *sL*, *srp*, *slay*, *sDs*, *sNpt*, *sNb*), where *sd*, *sL*, *srp*, *slay*, *sDs*, *sNpt*, and *sNb* are the individual indices related to the tube diameter, tube length, tube pitch ratio, tube layout, shell diameter, number of tube passes, and number of baffles, respectively. In this new form, the outer tube diameter becomes represented by:

$$dte = \sum_{srow} \widehat{pdte}_{srow} yrow_{srow} \tag{44}$$

where $\widehat{pdte}_{srow}$ is the outer tube diameter of the solution candidate associated to the binary variable $yrow_{srow}$. A constraint equivalent to Eq. (43) must also be added:

$$\sum_{srow} yrow_{srow} = 1 \tag{45}$$

Relations equivalent to Eq. (44) can be established for all design variables. According to Gonçalves et al. (2017b) in relation to the design of shell and tube heat exchangers without phase change and Souza et al. (2018) in relation to air coolers, the mathematical reformulation based on this combinatorial representation of the search space is associated to smaller computational times than an equivalent mathematical reformulation employing different sets of binaries.

3.2. Substitution of the binaries in the model

The nonlinearities present in the original model presented above can be eliminated through the substitution of all design variables by their representation using binary variables, as illustrated in Eq. (44). After subsequent rigorous mathematical reformulation, the final equations containing only the binary variables are in linear form.

The procedure is illustrated through the lower bound on the Reynolds number, Eqs. (35), which is, together with Eqs. (3), (5), (6), equivalent to:

$$Ret = \frac{dti\ \widehat{\rho t}}{\widehat{\mu t}} \left[\frac{4\ \widehat{mt}}{\pi\ \widehat{\rho t}\ dti^2} \left(\frac{Npt}{Ntt} \right) \right] \geq 10^4 \tag{46}$$

The design variables *dti* and *Npt* correspond to:

$$dti = \sum_{srow} \widehat{Pdti}_{srow} yrow_{srow} \tag{47}$$

$$Npt = \sum_{srow} \widehat{PNpt}_{srow} yrow_{srow} \tag{48}$$

The substitution of Eqs. (47)–(48) into Eq. (46) yields:

$$\frac{4\widehat{mt}}{\pi\widehat{\mu t}} \sum_{srow} \frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow}\widehat{Pdti}_{srow}} yrow_{srow} \geq 10^4 \tag{49}$$

where $\widehat{pNtt}_{srow}$ is the total number of tubes of the candidate solution *srow*, as calculated by Eq. (7), prior to the optimization. It must be noted that Eq. (49) is linear and contains only our unique kind of binary variable. An important aspect that allowed the elimination of the nonlinearities originally present in Eq. (46) is the relation described in Eq. (45), which imposes that, at the solution, only one term in the summation will remain. The application of this procedure to all equations of the model generates the linear model represented below.

3.3. Constraints

The set of constraints is composed of Eq. (45) and Eq. (49) together with the equations described below.

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

$$\hat{Q} \left(\sum_{srow} \frac{\widehat{Pdte}_{srow}}{\widehat{Pht}_{srow}\widehat{Pdti}_{srow}} yrow_{srow} + \widehat{Rft} \sum_{srow} \frac{\widehat{Pdte}_{srow}}{\widehat{Pdti}_{srow}} yrow_{srow} + \frac{\sum_{srow} \widehat{Pdte}_{srow} \ln\left(\frac{\widehat{Pdte}_{srow}}{\widehat{Pdti}_{srow}} \right) yrow_{srow}}{2\ ktube} + \widehat{Rfs} + \sum_{srow} \frac{1}{\widehat{Phs}_{srow}} yrow_{srow} \right) \leq \left(\pi \sum_{srow} \widehat{PNtt}_{srow}\widehat{Pdte}_{srow}\widehat{PL}_{srow} yrow_{srow} \right) \left(\frac{100}{100 + \widehat{Aexc}} \right) \widehat{\Delta Tlm} \tag{50}$$

The parameters associated to the heat transfer coefficients are given by the equations listed below:

$$\widehat{Phs}_{srow} = 0.994 \left[\frac{\widehat{\rho s}\left(\widehat{\rho s} - \widehat{\rho v s}\right)\widehat{g}\,\widehat{ks}^3\widehat{PL}_{srow}}{\widehat{ms}\,\widehat{\mu s}} \right]^{\frac{1}{3}} \times \widehat{PNtt}_{srow}^{\ 2/9} \tag{51}$$

$$\widehat{Pht}_{srow} = \frac{\widehat{kt}\,\widehat{C}\left(\frac{4\widehat{mt}}{\pi\widehat{\mu t}}\right)^{0.8} \widehat{Prt}^{0.4}}{\widehat{Pdti}_{srow}^{1.8}} \left(\frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow}} \right)^{0.8} \tag{52}$$

The bound on the tube-side pressure drop is represented by:

$$\sum_{srow} \left(\widehat{P\Delta Ptturb1}_{srow} + \widehat{P\Delta Ptturb\,2}_{srow} + \widehat{P\Delta Ptcab}_{srow}\widehat{K}_{srow} \right) yrow_{srow} \leq \widehat{\Delta Ptdisp} \tag{53}$$

where:

$$\widehat{P\Delta Ptturb\,1}_{srow} = \left(\frac{0.112\widehat{mt}^2}{\pi^2 \rho t} \right) \left(\frac{\widehat{PNpt}_{srow}^{\ 3}\widehat{PL}_{srow}}{\widehat{PNtt}_{srow}^{\ 2}\widehat{Pdti}_{srow}^{\ 5}} \right) \tag{54}$$

$$P\Delta \widehat{Ptturb2}_{srow} = 0.528\left(\frac{4^{1.58}\widehat{mt}^{1.58}\widehat{\mu t}^{0.42}}{\pi^{1.58}\widehat{\rho t}}\right)\frac{\widehat{PNpt}_{srow}^{2.58}\widehat{PL}_{srow}}{\widehat{PNtt}_{srow}^{1.58}\widehat{Pdti}_{srow}^{4.58}} \tag{55}$$

$$p\Delta \widehat{Ptcab}_{srow} = \left(\frac{8\widehat{mt}^2}{\pi^2\widehat{\rho t}}\right)\frac{\widehat{PNpt}_{srow}^{3}}{\widehat{PNtt}_{srow}^{2}\widehat{Pdti}_{srow}^{4}} \tag{56}$$

The shell-side pressure drop bounds is given by:

$$\sum_{srow}\widehat{P\Delta Ps}_{srow}yrow_{srow} \le \Delta \widehat{Psdisp} \tag{57}$$

$$\widehat{P\Delta Ps}_{srow} = \bar{\phi}_{VO}^{-2}0.864 \times \frac{\widehat{ms}^{1.812}\widehat{\mu vs}^{0.188}}{\widehat{\rho vs}}\left(\frac{(\widehat{PNb}_{srow}+1)^{2.812}}{\widehat{PDs}_{srow}^{0.812}\left(\widehat{PFAR}_{srow}\widehat{PL}_{srow}\right)^{1.812}\left(\widehat{PDeq}_{srow}\right)^{1.188}}\right) \tag{58}$$

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

$$\widehat{vsmin} \le \frac{\widehat{ms}}{\widehat{\rho s}}\sum_{srow}\frac{\left(\widehat{PNb}_{srow}+1\right)}{\widehat{PDs}_{srow}\widehat{PFAR}_{srow}\widehat{PL}_{srow}}yrow_{srow} \tag{59}$$

$$\widehat{vsmax} \ge \frac{\widehat{ms}}{\widehat{\rho s}}\sum_{srow}\frac{\left(\widehat{PNb}_{srow}+1\right)}{\widehat{PDs}_{srow}\widehat{PFAR}_{srow}\widehat{PL}_{srow}}yrow_{srow} \tag{60}$$

$$\widehat{vtmin} \le \frac{4\widehat{mt}}{\pi\widehat{\rho t}}\sum_{srow}\frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow}\widehat{Pdti}_{srow}^{2}}yrow_{srow} \tag{61}$$

$$\widehat{vtmax} \ge \frac{4\widehat{mt}}{\pi\widehat{\rho t}}\sum_{srow}\frac{\widehat{PNpt}_{srow}}{\widehat{PNtt}_{srow}\widehat{Pdti}_{srow}^{2}}yrow_{srow} \tag{62}$$

The lower bound on the shell-side Reynolds number is given by:

$$\frac{\widehat{ms}}{\widehat{\mu s}}\left(\sum_{srow}\frac{\widehat{pDeq}_{srow}(\widehat{pNb}_{srow}+1)}{\widehat{pDs}_{srow}\widehat{pFAR}_{srow}\widehat{pL}_{srow}}yrow_{srow}\right) \ge 500 \tag{63}$$

The linear form of the geometric constraints become:

$$\sum_{srow}\frac{\widehat{PL}_{srow}}{\left(\widehat{PNb}_{srow}+1\right)}yrow_{srow} \le 1.0\sum_{srow}\widehat{PDs}_{srow}yrow_{srow} \tag{64}$$

$$\sum_{srow}\frac{\widehat{PL}_{srow}}{\left(\widehat{PNb}_{srow}+1\right)}yrow_{srow} \ge 0.2\sum_{srow}\widehat{PDs}_{srow}yrow_{srow} \tag{65}$$

$$\sum_{srow}\widehat{PL}_{srow}yrow_{srow} \le 15\sum_{srow}\widehat{PDs}_{srow}yrow_{srow} \tag{66}$$

$$\sum_{srow}\widehat{PL}_{srow}yrow_{srow} \ge 3\sum_{srow}\widehat{PDs}_{srow}yrow_{srow} \tag{67}$$

3.4. Objective function The linear representation of the objective function is:

$$\mathrm{Min}\,\pi\sum_{srow}\widehat{PNtt}_{srow}\widehat{Pdte}_{srow}\widehat{PL}_{srow}yrow_{srow} \tag{68}$$

The above model is linear and does not contain continuous variables. It is, therefore, an Integer Linear Model (ILM). We solve it using Integer Linear Programming (ILP).

4. Results

We discuss two examples: the design of an overhead condenser and the design of a heater, where the condensation corresponds to utility saturated steam. The application of the design optimization through mathematical programming to these examples was compared with the results obtained using the design procedures described in Smith (2005) and Smith (2016), called here S1 and S2, respectively. The mathematical programming solutions were obtained through the software GAMS using the CPLEX solver.

The design procedure S1 starts through the designer's selection of the number of passes in the tube-side, tube diameter, tube pitch, and tube layout. Additionally, the designer must also choose the tube length to shell diameter ratio. Using these values, the required area is determined. The design procedure S2 is similar, but, instead of fixing the ratio tube length / shell diameter, it is based on the selection of the tube-side flow velocity (or, alternatively, the tube-side pressure drop). Considering that in practice the design variables are usually based on commercial/standard values, after the finalization of the design procedures S1 and S2, a last step is included to round the tube length and shell diameter towards the next larger values in the available set of options.

The model equations presented in Smith (2005) and Smith (2016) are slightly different, then, in order to allow a direct comparison among the results, we solved the design problems using the procedure S1 employing the same condenser model equations originally employed in S2. It is important to observe that these design procedures do not consider additional important constraints to yield a practical design, which are included in the mathematical programming approach (e.g. flow velocity bounds). Consequently, nonrealistic solutions may be obtained in some problems using these approaches.

4.1. Example 1

This example corresponds to the design of a heat exchanger to condensate an overhead distillation vapor stream of pure acetone. This problem was initially proposed by Smith (2005) and addressed later by Smith (2016). Table 2 displays the problem data and Table 3 reports the physical properties of the streams. The flow velocity bounds and maximum pressure drops present in Table 2 are not present in the original references and were inserted here considering the practical aspects of heat exchanger design. The values adopted for the corresponding bounds were based on Smith (2016) even though the procedures S1 and S2 do not consider

Table 2
Example 1: Design problem data.

	Hot stream Acetone	Cold stream Cooling water
Mass flow rate (kg/s)	5.8	68.55
Inlet temperature (°C)	67	25
Outlet temperature (°C)	67	35
Fouling factor (m^2K/W)	9.0×10^{-5}	2.0×10^{-4}
Flow velocity bounds (m/s)	10–30	1–3
Available pressure drop (Pa)	20,000	70,000

Table 3
Example 1: Physical properties.

	Hot stream Acetone	Cold stream Cooling water
Liquid density (kg/m^3)	736	996
Vapor density (kg/m^3)	3.12	–
Liquid heat capacity (J/(kg·K))	2320	4180
Liquid viscosity (Pa·s)	0.213×10^{-3}	0.797×10^{-3}
Vapor viscosity (Pa·s)	1.4×10^{-6}	–
Liquid thermal conductivity (W/(m·K))	0.137	0.618
Vaporization enthalpy (J/kg)	494×10^3	–

Table 4
Example 1: Design variables alternatives.

Variable	Values
Outer tube diameter (m)	0.016, 0.018, 0.020, 0.022, 0.025, 0.030, 0.032, 0.038, 0.040, 0.070
Tube length (m)	1.219, 1.829, 2.439, 3.049, 3.659, 4.877, 6.098
Tube pitch ratio	1.25, 1.33, 1.50
Tube layout	1 = Square, 2 = Triangular
Number of tube passes	1, 2, 4, 6
Number of baffles	1, 2, …, 20
Shell diameter (m)	0.438, 0.489, 0.540, 0.591, 0.635, 0.686, 0.737, 0.787, 0.838, 0.889, 0.940, 0.991

Table 5
Example 1: Design solutions.

	Proposed procedure	Procedure S1	Procedure S2
Heat transfer area (m^2)	100.6	122.8	105.1
Total number of tubes	547	534	343
Tube diameter (m)	0.016	0.020	0.020
Tube length (m)	3.659	3.659	4.877
Tube pitch ratio	1.33	1.25	1.25
Tube layout	Triangular	Square	Square
Number of tube passes	2	2	2
Shell diameter (m)	0.590	0.737	0.590
Number of baffles	6	4	8

Table 6
Example 1: Thermofluid dynamic results of the design solutions.

	Proposed procedure	Procedure S1	Procedure S2
Tube-side velocity (m/s)	2.2	1.3	2.0
Shell-side velocity (m/s)	24.3	17.2	29.0
Tube-side heat transfer coefficient (W/(m^2·K))	10077.1	6120.7	8701.4
Shell-side heat transfer coefficient (W/(m^2·K))	1334.6	1327.4	1324.1
Overall heat transfer coefficient (W/(m^2·K))	775.5	742.3	776.1
Tube-side pressure drop (Pa)	48,932	13,422	37,998
Shell-side pressure drop (Pa)	16,727	5850	21,711

them. In order to provide an equivalent comparison of the mathematical programming approach with S1 and S2, no excess area was adopted in the problem resolution.

The condenser to be designed is a floating head heat exchanger with tubes of thickness 2 mm with wall thermal conductivity equal to 45 W/(m·K). The available options of the design variables are displayed in Table 4. These data are consistent with the available commercial options and standard values (Mukherjee, 1998; Jones, 2002; Smith, 2016).

The results obtained using the procedures S1 and S2, together with the optimal solution obtained through the proposed approach, are displayed in Tables 5 and 6. S1 and S2 results were obtained adopting a tube length/shell diameter ratio equal to 5 and a tube-side velocity equal to 2 m/s, respectively. The number of baffles reported in Table 5 for S1 and S2 solutions were evaluated after the determination of the heat transfer area for comparison purposes and corresponds to the lowest possible value (i.e. the maximum baffle spacing) in order to reduce the pressure drop.

The results in Table 5 indicate that the proposed optimization approach attained a solution with a smaller heat transfer area than the design procedures S1 and S2. The higher difference of the heat transfer area occurs in relation to S1, where the heat transfer area is 22.1% higher than the optimal solution attained by the proposed procedure. The analysis of the pressure drops in Table 6 indicates that the shell-side pressure drop associated to the procedure S2 is higher than the adopted upper bound, because this constraint is not included in this design procedure. Differently, because the pressure drop bounds are constraints inserted into the optimization formulation, the optimal solution obeys the corresponding maximum limits. The higher value of the tube-side pressure drop in the optimal solution when compared with S1 and S2 results is associated to the higher flow velocity and the lower tube diameter. These choices increase the pressure drop, but are also directly associated to the higher value of the tube-side heat transfer coefficient.

4.2. Example 2

This example corresponds to the design of a heater of a methanol stream using saturated steam. The streams data and their physical properties are shown in Tables 7 and 8.

The alternatives for the design variables are identical of the values employed in Example 1, described in Table 4. The tube thickness and thermal conductivity of the wall are also the same. The design procedures S1 and S2 are applied using the same premises reported in Example 1. All results are presented in Tables 9 and 10.

The heat transfer area attained by the mathematical programming approach for the design presented in Example 2 is also smaller than the solutions obtained through the procedures S1 and S2. The higher difference corresponds to the result obtained using the procedure S2, which presents a heat transfer area 25.4% higher than the solution obtained through the proposed optimization. Additionally, it should be observed that the solution obtained using the procedure S1 presents a tube-side flow velocity higher than

Table 7
Example 2: Design problem data.

	Hot stream Saturated steam	Cold stream Methanol
Mass flow rate (kg/s)	9.35	133.3
Inlet temperature (°C)	177	30
Outlet temperature (°C)	177	80
Fouling factor (m^2K/W)	2.0×10^{-4}	1.0×10^{-4}
Flow velocity bounds (m/s)	10–30	1–3
Available pressure drop (kPa)	20	70

Table 8
Example 2: Physical properties.

	Hot stream Saturated steam	Cold stream Methanol
Liquid density (kg/m^3)	890	750
Vapor density (kg/m^3)	4.83	–
Liquid heat capacity (J/(kg·K))	4393	2840
Liquid viscosity (Pa·s)	0.153×10^{-3}	0.340×10^{-3}
Liquid thermal conductivity (W/(m·K))	0.674	0.19
Vaporization enthalpy (J/kg)	2025×10^3	–

Table 9
Example 2: Design solutions.

	Proposed procedure	Procedure S1	Procedure S2
Heat transfer area (m^2)	118.2	122.7	148.2
Total number of tubes	617	534	967
Tube diameter (m)	0.020	0.020	0.020
Tube length (m)	3.049	3.659	2.439
Tube pitch ratio	1.25	1.25	1.25
Tube layout	Triangular	Square	Square
Number of tube passes	2	2	2
Shell diameter (m)	0.737	0.737	0.991
Number of baffles	4	4	2

Table 10
Example 2: Thermofluid dynamic results of the design solutions.

	Proposed procedure	Procedure S1	Procedure S2
Tube-side velocity (m/s)	2.9	3.3	1.8
Shell-side velocity (m/s)	21.6	18.0	12.0
Tube-side heat transfer coefficient (W/(m^2·K))	5510.3	6185.4	3843.3
Shell-side heat transfer coefficient (W/(m^2·K))	6866.4	7066.0	7043.4
Overall heat transfer coefficient (W/(m^2·K))	1338.6	1392.4	1187.9
Tube-side pressure drop (Pa)	36,076	54,239	13,189
Shell-side pressure drop (Pa)	18,413	14,004	5456

3 m/s, which can cause erosion, and the solution obtained through the procedure S2 is associated to a tube length/shell diameter ratio equal to 2.46, which is lower than the recommended range (Taborek, 2008b). The proposed minimization of the heat transfer area is associated to higher pressure drops when compared with the solution procedure S2, but without violating the limits established in the design problem.

5. Conclusions

This paper presented a mathematical programming approach for the determination of the global optimum solutions for the design of horizontal shell-and-tube condensers. The original representation of the design optimization problem corresponds to a mixed-integer nonlinear programming (MINLP). The application of a set of proper algebraic techniques allowed a mathematical reformulation of the problem, then represented as an integer linear programming (ILP). This new representation of the problem presents two main advantages: it does not depend of initial estimates and always converge to the global optimum solution, thus avoiding drawbacks associated to nonlinear formulations.

A comparison with results obtained through procedures reported in the literature for the design of an overhead condenser and a heater using saturated steam indicated that the proposed approach can provide solutions with lower values of heat transfer area in all cases. The solutions obtained using the procedures proposed by Smith (2005) and Smith (2016) are associated to heat transfer areas up to 22.1% and 25.4% higher, respectively. Additionally, some solutions obtained using these methods do not obey all necessary design constraints. The pressure drops obtained using the proposed optimization procedure are usually higher, but always obeying the limits established in the problem, which is acceptable according to the design problem formulation.

The thermofluid dynamic model employed in the proposed optimization is based on the assumption of uniform physical properties evaluated at their average values. In certain situations, this assumption may compromise the solution accuracy. Therefore, future advances in the design optimization must include discretization techniques to describe the energy balance along the heat transfer surface for each point of the grid domain, thus allowing the evaluation of the heat transfer coefficients using local values of the physical properties, as pointed by Costa and Bagajewicz (2019).

Additional new developments in future works may also consider a more realistic objective function. Instead to use the heat exchanger area, the optimization can be formulated to minimize the heat exchanger cost, evaluated by a mathematical function involving the mechanical design of all exchanger components. This function may be also associated to the evaluation of the operational costs, related to the pressure drops, thus exploring the corresponding tradeoff, represented through the minimization of the total annualized cost.

CRediT authorship contribution statement

Igor P.S. Pereira: Software, Validation, Writing - review & editing. **Miguel J. Bagajewicz:** Conceptualization, Methodology, Writing - original draft, Writing - review & editing. **André L.H. Costa:** Conceptualization, Methodology, Writing - original draft, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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