Optimal Shell and Tube Heat Exchangers Design

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1. Introduction

Due to their resistant manufacturing features and design flexibility, shell and tube heat exchangers are the most used heat transfer equipment in industrial processes. They are also easy adaptable to operational conditions. In this way, the design of shell and tube heat exchangers is a very important subject in industrial processes. Nevertheless, some difficulties are found, especially in the shell-side design, because of the complex characteristics of heat transfer and pressure drop. Figure 1 shows an example of this kind of equipment.

In designing shell and tube heat exchangers, to calculate the heat exchange area, some methods were proposed in the literature. Bell-Delaware is the most complete shell and tube heat exchanger design method. It is based on mechanical shell side details and presents more realistic and accurate results for the shell side film heat transfer coefficient and pressure drop. Figure 2 presents the method flow model, that considers different streams: leakages between tubes and baffles, bypass of the tube bundle without cross flow, leakages between shell and baffles, leakages due to more than one tube passes and the main stream, and tube bundle cross flow. These streams do not occur in so well defined regions, but interacts ones to others, needing a complex mathematical treatment to represent the real shell side flow.

In the majority of published papers as well as in industrial applications, heat transfer coefficients are estimated, based, generally on literature tables. These values have always a large degree of uncertainty. So, more realistic values can be obtained if these coefficients are not estimated, but calculated during the design task. A few number of papers present shell and tube heat exchanger design including overall heat transfer coefficient calculations (Polley et al., 1990, Polley and Panjeh Shah, 1991, Jegede and Polley, 1992, and Panjeh Shah, 1992, Ravagnani, 1994, Ravagnani et al. (2003), Mizutani et al., 2003, Serna and Jimenez, 2004, Ravagnani and Caballero, 2007a, and Ravagnani et al., 2009).

In this chapter, the work of Ravagnani (1994) will be used as a base to the design of the shell and tube heat exchangers. A systematic procedure was developed using the Bell-Delaware method. Overall and individual heat transfer coefficients are calculated based on a TEMA (TEMA, 1998) tube counting table, as proposed in Ravagnani et al. (2009), beginning with the smallest heat exchanger with the biggest number of tube passes, to use all the pressure drop
and fouling limits, fixed before the design and that must be satisfied. If pressure drops or fouling factor are not satisfied, a new heat exchanger is tested, with lower tube passes number or larger shell diameter, until the pressure drops and fouling are under the fixed limits. Using a trial and error systematic, the final equipment is the one that presents the minimum heat exchanger area for fixed tube length and baffle cut, for a counting tube TEMA table including 21 types of shell and tube bundle diameter, 2 types of external tube diameter, 3 types of tube pitch, 2 types of tube arrangement and 5 types of number of tube passes.

Fig. 1. Heat exchanger with one pass at the tube side

Fig. 2. Bell-Delaware streams considerations in the heat exchanger shell side

Two optimisation models will be considered to solve the problem of designing shell and tube heat exchangers. The first one is based on a General Disjunctive Programming Problem (GDP) and reformulated to a Mixed Integer Nonlinear Programming (MINLP) problem and solved using Mathematical Programming and GAMS software. The second one is based on the Meta-Heuristic optimization technique known as Particle Swarm Optimization (PSO). The differences between both models are presented and commented, as well as its applications in Literature problems.
2. Ravagnani and Caballero (2007a) model formulation

The model for the design of the optimum shell and tube equipment considers the objective function as the minimum cost including exchange area cost and pumping cost, rigorously following the Standards of TEMA and respecting the pressure drop and fouling limits. Parameters are: \(T_{in}\) (inlet temperature), \(T_{out}\) (outlet temperature), \(m\) (mass flowrate), \(\rho\) (density), \(C_p\) (heat capacity), \(\mu\) (viscosity), \(k\) (thermal conductivity), \(\Delta P\) (pressure drop), \(rd\) (fouling factor) and area cost data. The variables are tube inside diameter \((d_{in})\), tube outside diameter \((d_{ex})\), tube arrangement \((arr)\), tube pitch \((pt)\), tube length \((L)\), number of tube passes \((N_{tp})\) and number of tubes \((N_t)\), the external shell diameter \((D_{s})\), the tube bundle diameter \((D_{ot})\), number of baffles \((N_{b})\), baffles cut \((l_{c})\) and baffles spacing \((l_{s})\), heat exchange area \((A)\), tube-side and shell-side film coefficients \((h_t\) and \(h_s)\), dirty and clean global heat transfer coefficient \((U_d\) and \(U_c)\), pressure drops \((\Delta P_t\) and \(\Delta P_s)\), fouling factor \((rd)\) and the fluids location inside the heat exchanger. The model is formulated as a General Disjunctive Programming Problem (GDP) and reformulated to a Mixed Integer Nonlinear Programming problem and is presented below.

Heat exchanger fluids location:
Using the GDP formulation of Mizutani et al. (2003), there are two possibilities, either the cold fluid is in the shell side or in the tube side. So, two binary variables must be defined, \(y_{1f}\) and \(y_{2f}\). If the cold fluid is flowing in the shell side, or if the hot fluid is on the tube side, \(y_{1f} = 1\). It implies that the physical properties and hot fluid mass flowrate will be in the tube side, and the cold fluid physical properties and mass flowrate will be directed to the shell side. If \(y_{1f} = 0\), the reverse occurs. This is formulated as:

\[
y_{1f} + y_{2f} = 1
\]

\[
m^h = m_1^h + m_2^h
\]

\[
m^c = m_1^c + m_2^c
\]

\[
m' = m_1^h + m_1^c
\]

\[
m' = m_2^h + m_2^c
\]

\[
m_1^h \leq m_{upper} y_{1f}
\]

\[
m_1^c \leq m_{upper} y_{2f}
\]

\[
m_2^h \leq m_{upper} y_{1f}
\]

\[
m_2^c \leq m_{upper} y_{2f}
\]

\[
\mu' = y_{1f} \mu^h + y_{2f} \mu^c
\]

\[
\mu' = y_{1f} \mu^h + y_{2f} \mu^c
\]
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\[ C_p' = y_1' C_p^h + y_2' C_p^f \]  \hspace{1cm} (12)

\[ C_p' = y_1' C_p^h + y_2' C_p^f \]  \hspace{1cm} (13)

\[ k' = y_1' k^h + y_2' k^f \]  \hspace{1cm} (14)

\[ k' = y_1' k^h + y_2' k^f \]  \hspace{1cm} (15)

\[ \rho' = y_1' \rho^h + y_2' \rho^f \]  \hspace{1cm} (16)

\[ \rho' = y_1' \rho^h + y_2' \rho^f \]  \hspace{1cm} (17)

For the definition of the shell diameter \((D_s)\), tube bundle diameter \((D_{otl})\), tube external diameter \((d_{ex})\), tube arrangement \((arr)\), tube pitch \((pt)\), number of tube passes \((N_{tp})\) and the number of tubes \((N_t)\), a table containing these values according to TEMA Standards is constructed, as presented in Table 1. It contains 2 types of tube external diameter, 19.05 and 25.4 mm, 2 types of arrangement, triangular and square, 3 types of tube pitch, 23.79, 25.4 and 31.75 mm, 5 types of number of tube passes, 1, 2, 4, 6 and 8, and 21 different types of shell and tube bundle diameter, beginning on 205 mm and 173.25 mm, respectively, and finishing in 1,524 mm and 1,473 mm, respectively, with 565 rows. Obviously, other values can be aggregated to the table, if necessary.

| \(D_s\) | \(D_{otl}\) | \(d_{ex}\) | \(arr\) | \(pt\) | \(N_{tp}\) | \(N_t\) |
|-------|--------|---------|--------|------|--------|--------|
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02379 | 1 | 38 |
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02379 | 2 | 32 |
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02379 | 4 | 26 |
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02379 | 6 | 24 |
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02379 | 8 | 18 |
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02540 | 1 | 37 |
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02540 | 2 | 30 |
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02540 | 4 | 24 |
| 0.20500 | 0.17325 | 0.01905 | 1 | 0.02540 | 6 | 16 |
| 1.52400 | 1.47300 | 0.02540 | 1 | 0.03175 | 6 | 1761 |
| 1.52400 | 1.47300 | 0.02540 | 1 | 0.03175 | 8 | 1726 |
| 1.52400 | 1.47300 | 0.02540 | 2 | 0.03175 | 1 | 1639 |
| 1.52400 | 1.47300 | 0.02540 | 2 | 0.03175 | 2 | 1615 |
| 1.52400 | 1.47300 | 0.02540 | 2 | 0.03175 | 6 | 1553 |
| 1.52400 | 1.47300 | 0.02540 | 2 | 0.03175 | 8 | 1522 |

Table 1. Tube counting table proposed

To find \(D_s, D_{otl, d_{ex}}, arr, pt, ntp\) and \(N_t\), the following equations are proposed:
\[ D_s = \sum_{i=1}^{565} d_{s,i}.ynt(i) \]  
\[ D_{od} = \sum_{i=1}^{565} d_{od,i}.ynt(i) \]  
\[ d_{ex} = \sum_{i=1}^{565} d_{ex,i}.ynt(i) \]  
\[ arr = \sum_{i=1}^{565} arr_i.ynt(i) \]  
\[ pt = \sum_{i=1}^{565} pti.ynt(i) \]  
\[ np = \sum_{i=1}^{565} np_i.ynt(i) \]  
\[ nt = \sum_{i=1}^{565} nti.ynt(i) \]  
\[ \sum_{i=1}^{565} ynt(i) = 1 \]  

Definition of the tube arrangement \((arr)\) and the arrangement \((pn\) and \(pp\)) variables:

\[pn = pn^1 + pn^2\]  
\[pp = pp^1 + pp^2\]  
\[pt = pt^1 + pt^2\]  
\[pn^1 = 0.5.pt^1\]  
\[pn^2 = pt^2\]  
\[pp^1 = 0.866.pt^1\]  
\[pp^2 = pt^2\]  
\[pt^1 \geq 0.02379 y_{arr}^{tri}\]  
\[pt^2 \geq 0.02379 y_{arr}^{cuay}\]  
\[pt^1 \leq 0.03175 y_{arr}^{tri}\]  
\[pt^2 \leq 0.03175 y_{arr}^{cuay}\]  
\[y_{arr}^{tri} + y_{arr}^{cuay} = 1\]
Definition of tube internal diameter ($d_{in}$):

This value, according to TEMA (1988) can be found for different values of $d_{ex}$ and BWG. In this case, just two tube external diameters will be considered, which implies just two set of possibilities of $d_{in}$, as can be seen on Tables 2 and 3. However, other values can be aggregated.

BWG determination can be formulated as:

for $d_{ex}=0.01905$, $BWG = \{10,11,12,\ldots,18\}$

for $d_{ex}=0.0254$, $BWG = \{8,9,10,11,12,\ldots,18\}$

\[
BWG_1 = \sum_{j=1}^{9} y_{1j}^{bg} BWG_j^1 \quad (39)
\]

\[
\sum_{j=1}^{9} y_{1j}^{bg} \leq 1 \quad (40)
\]

\[
BWG_2 = \sum_{j=1}^{11} y_{2j}^{bg} BWG_j^2 \quad (41)
\]

\[
\sum_{j=1}^{11} y_{2j}^{bg} \leq 1 \quad (42)
\]

\[
BWG = BWG_1 + BWG_2 \quad (43)
\]

d_{in} can be found by the following equations:

\[
d_{in_1} = \sum_{j=1}^{9} y_{1j}^{bg} d_{in}^1 \quad (44)
\]

\[
d_{in_2} = \sum_{j=1}^{11} y_{2j}^{bg} d_{in}^2 \quad (45)
\]

\[
d_{in} = d_{in_1} + d_{in_2} \quad (46)
\]

| BWG | $d_{in}$(m) |
|-----|-------------|
| 10  | 0.0122      |
| 11  | 0.0129      |
| 12  | 0.0135      |
| 13  | 0.0142      |
| 14  | 0.0148      |
| 15  | 0.0154      |
| 16  | 0.0157      |
| 17  | 0.0161      |
| 18  | 0.0166      |

Table 2. Determination of $d_{in}$ for $d_{ex} = 0.01905$ m
Table 3. Determination of $d_{in}$ for $d_{ex} = 0.0254$ m

| BWG | $d_{in}$(m) |
|-----|-------------|
| 8   | 0.0170      |
| 9   | 0.0179      |
| 10  | 0.0186      |
| 11  | 0.0193      |
| 12  | 0.0199      |
| 13  | 0.0206      |
| 14  | 0.0212      |
| 15  | 0.0217      |
| 16  | 0.0221      |
| 17  | 0.0225      |
| 18  | 0.0229      |

Definition of baffle spacing ($l_s$):
According to TEMA (1988), baffle spacing must be between $D_s$ and $D_s/5$. In this case, the following values will be considered:

$$l_s \leq D_s$$

$$l_s \geq D_s/5$$

Cross-flow at or near centerline for one cross-flow section ($S_m$):

$$S_m \leq l_s \left( D_s - D_{ol} + \frac{(pt - d_{ex})(D_{ol} - d_{ex})}{pt} \right) + M(1 - y_{arr})$$

$$S_m \geq l_s \left( D_s - D_{ol} + \frac{(pt - d_{ex})(D_{ol} - d_{ex})}{pt} \right) - M(1 - y_{arr})$$

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\[ S_m \leq \text{ls} \left( D_s - D_{ol} + \frac{(pt - d_a)(D_{ol} - d_a)}{pn} \right) + M(1 - y^{arr}) \]  
(57)

\[ S_m \geq \text{ls} \left( D_s - D_{ol} + \frac{(pt - d_a)(D_{ol} - d_a)}{pn} \right) - M(1 - y^{arr}) \]  
(58)

Definition of the flow regimen in the shell side:
Reynolds number \((Re_s)\) is given by:

\[ Re_s = \frac{m_s d_s}{\mu_s S_m} \]  
(59)

The shell side fluid velocity \((v_s)\) is given by:

\[ v_s = \frac{m_s}{\rho_s (D_s/pt)(pt - d_a)y_s} \]  
(60)

According to Smith (2005), the velocity limits must be:

\[ 0.5 \leq v_s \leq 2, \text{ } v_s \text{ in m/s} \]  
(61)

The flow regimen is defined as a function of Reynolds number. Considering that in real heat exchangers the Reynolds number are generally high, laminar flow can be neglected, and Reynolds number, in this work, will be considered just for values greater than 100.

\[ Re_{s_1} \geq 10^4, y_i^{arr} \]  
(62)

\[ Re_{s_1} \leq 10^6, y_i^{arr} \]  
(63)

\[ Re_{s_2} \geq 10^4, y_i^{arr} \]  
(64)

\[ Re_{s_2} \leq 10^6, y_i^{arr} \]  
(65)

\[ Re_{s_3} \geq 10^7, y_i^{arr} \]  
(66)

\[ \sum_r y_i^{arr} = 1 \]  
(67)

\[ Re_s = \sum_r Re_{sr} \]  
(68)

Colburn factor \((ji)\) and Fanning factor \((fl)\) determination:
Both, Colburn and Fanning factor are functions of Reynolds number and the tube arrangement, as shown on Table 4, extracted from Mizutani et al. (2003).

According to Mizutani et al. (2003), the DGP formulation is:

\[ \sum_r \sum_s y_{r,s}^{rear} A_{r,s}^{ji} = a_i \]  
(69)
\[ \sum \sum y_{r,s}^{rarr} A_{r,s}^a = a_2 \] (70)

\[ \sum y_{r,s}^{arr} A_{r,s}^a = a_3 \] (71)

\[ \sum y_{r,s}^{arr} A_{r,s}^b = a_4 \] (72)

\[ \sum \sum y_{r,s}^{rarr} A_{r,s}^b = b_1 \] (73)

\[ \sum \sum y_{r,s}^{rarr} A_{r,s}^{b_2} = b_2 \] (74)

\[ \sum y_{r,s}^{arr} A_{r,s}^{b_3} = b_3 \] (75)

\[ \sum y_{r,s}^{arr} A_{r,s}^{b_4} = b_4 \] (76)

| arr | Re_s | a_1 | a_2 | a_3 | a_4 | b_1 | b_2 | b_3 | b_4 |
|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|
| tri | 10^5-10^4 | 0.321 | -0.388 | 1.450 | 0.519 | 0.372 | -0.123 | 7.00 | 0.500 |
| tri | 10^4-10^3 | 0.321 | -0.388 | 1.450 | 0.519 | 0.486 | -0.152 | 7.00 | 0.500 |
| tri | 10^3-10^2 | 0.593 | -0.477 | 1.450 | 0.519 | 4.570 | -0.476 | 7.00 | 0.500 |
| tri | 10^2-10 | 1.360 | -0.657 | 1.450 | 0.519 | 45.100 | -0.973 | 7.00 | 0.500 |
| tri | < 10 | 1.400 | -0.657 | 1.450 | 0.519 | 48.000 | -1.000 | 7.00 | 0.500 |
| sq | 10^5-10^4 | 0.370 | -0.395 | 1.187 | 0.370 | 0.391 | -0.148 | 6.30 | 0.378 |
| sq | 10^4-10^3 | 0.107 | -0.266 | 1.187 | 0.370 | 0.082 | 0.022 | 6.30 | 0.378 |
| sq | 10^3-10^2 | 0.408 | -0.460 | 1.187 | 0.370 | 6.090 | -0.602 | 6.30 | 0.378 |
| sq | 10^2-10 | 0.900 | -0.631 | 1.187 | 0.370 | 32.100 | -0.963 | 6.30 | 0.378 |
| sq | < 10 | 0.970 | -0.667 | 1.187 | 0.370 | 35.000 | -1.000 | 6.30 | 0.378 |

Table 4. Empirical coefficients for equations (69) to (80) as function of Reynolds number and tube arrangement

\[ a = \frac{a_1}{1 + 0.14 (\text{Re}_s)^{0.4}} \] (77)

\[ ji = a_1,1064^a (\text{Re}_s)^{0.2} \] (78)

\[ b = \frac{b_3}{1 + 0.14 (\text{Re}_s)^{0.4}} \] (79)

\[ fl = b_4,1064^b (\text{Re}_s)^{0.2} \] (80)

\[ 1 - y_{res}^{rarr} + y_{arr}^{rarr} \geq 1 \] (81)
\[
\sum_s \sum_{r_s} y_{r,s} = 1 \quad (82)
\]

Number of baffles \((Nb)\):

\[
Nb = \frac{L}{ls} - 1 \quad (83)
\]

Number of tube rows crossed by the ideal cross flow \((Nc)\):

\[
Nc = \frac{D_l \left[1 - 2\left(\frac{l_c}{D_c}\right)\right]}{pp} \quad (84)
\]

\(l_c\) is the baffle cut. The most used value is

\[
l_c = 0.25.D_c \quad (85)
\]

Fraction of total tubes in cross flow \((Fc)\):

\[
Fc = \frac{1}{\pi} \left[\pi + 2.\lambda.\sin(arccos(\lambda)) - 2.arccos(\lambda)\right] \quad (86)
\]

where:

\[
\lambda = \frac{D_c - 2.l_c}{D_{ot}} \quad (87)
\]

Number of effective cross-flow tube rows in each windows \((Ncw)\):

\[
Ncw = \frac{0.8.l_c}{pp} \quad (88)
\]

Fraction of cross-flow area available for bypass flow \((Fsbp)\):

\[
Fsbp = \frac{ls.D_c - D_{ot}}{Sm} \quad (89)
\]

Shell-to-baffle leakage area for one baffle \((Ssb)\):

\[
Ssb = \frac{D_c.\delta_{sb}}{2} \left[\pi - \arccos\left(1 - \frac{2.l_c}{D_c}\right)\right] \quad (90)
\]

where

\[
\delta_{sb} = \left(\frac{3.1 + 0.004(D_c.1000)}{1000}\right)
\]

Angle values are in radians.

Tube-to-baffle leakage area for one baffle \((Stb)\):

\[
Stb = 0.0006223.dex.N.(1 + Fc), \text{ m}^2 \quad (91)
\]
Area for flow through window (Sw):
It is given by the difference between the gross window area (Swg) and the window area occupied by tubes (Swt):

\[ Sw = Swg - Swt \]  \hspace{1cm} (92)

where:

\[ Swg = \frac{(D_l)^2}{4} \left[ \arccos \left( 1 - 2 \frac{l_t}{D_l} \right) - \left( 1 - 2 \frac{l_t}{D_l} \right) \sqrt{1 - \left( 1 - 2 \frac{l_t}{D_l} \right)^2} \right] \]  \hspace{1cm} (93)

and:

\[ Swt = \left( \frac{N_t}{8} \right) (1 - Fc) \pi (D_l)^2 \]  \hspace{1cm} (94)

Shell-side heat transfer coefficient for an ideal tube bank (hoi):

\[ ho_i = \frac{j_i \cdot C_p \cdot m^2}{Sm} \left( \frac{k_i}{C_p \cdot \mu_i} \right)^{2/3} \]  \hspace{1cm} (95)

Correction factor for baffle configuration effects (Jc):

\[ Jc = Fc + 0.54 (1 - Fc)^{0.345} \]  \hspace{1cm} (96)

Correction factor for baffle-leakage effects (Jl):

\[ Jl = \alpha + (1 - \alpha) \exp \left( -2.2 \cdot \frac{Ssb + Stb}{Sm} \right) \]  \hspace{1cm} (97)

where:

\[ \alpha = 0.44 \left( 1 - \frac{Ssb}{Ssb + Stb} \right) \]  \hspace{1cm} (98)

Correction factor for bundle-bypassing effects (Jb):

\[ Jb = \exp (-0.3833 \cdot FsBP) \]  \hspace{1cm} (99)

Assuming that very laminar flow is neglected (Re_s < 100), it is not necessary to use the correction factor for adverse temperature gradient buildup at low Reynolds number.

Shell-side heat transfer coefficient (hsi):

\[ h_s = ho_i \cdot Jc \cdot Jl \cdot Jb \]  \hspace{1cm} (100)

Pressure drop for an ideal cross-flow section (\( \Delta P_{bi} \)):

\[ \Delta P_{bi} = \frac{2 \cdot Jl \cdot Nc \cdot (m_i)^3}{\rho \cdot Sm^2} \]  \hspace{1cm} (101)
Pressure drop for an ideal window section ($\Delta P_{wi}$):

$$\Delta P_{wi} = (2 + 0.6 \cdot N_{cw}) \cdot \frac{(m_{w})}{S_{t} \cdot \rho_{w} \cdot S_{m}}$$  \hspace{1cm} (102)

Correction factor for the effect of baffle leakage on pressure drop ($R_{l}$):

$$R_{l} = \exp \left[ -1.33 \left( 1 + \frac{S_{sb}}{S_{sb} + S_{tb}} \right)^{k} \right]$$  \hspace{1cm} (103)

where:

$$k = -0.15 \left( 1 + \frac{S_{sb}}{S_{sb} + S_{tb}} \right) + 0.8$$  \hspace{1cm} (104)

Correction factor for bundle bypass ($R_{b}$):

$$R_{b} = \exp \left[ -1.3456 \cdot F_{sbp} \right]$$  \hspace{1cm} (105)

Pressure drop across the Shell-side ($\Delta P_{s}$):

$$\Delta P_{s} = 2 \cdot \Delta P_{s_{h}} \left( 1 + \frac{N_{cw}}{N_{c}} \right) R_{b} + (N_{b} + 1) \cdot \Delta P_{s_{h}} \cdot R_{b} \cdot R_{l} + N_{b} \cdot \Delta P_{w_{i}} \cdot R_{l}$$  \hspace{1cm} (106)

This value must respect the pressure drop limit, fixed before the design:

$$\Delta P_{s} \leq \Delta P_{design}$$  \hspace{1cm} (107)

Tube-side Reynolds number ($Re_{t}$):

$$Re_{t} = \frac{4 \cdot m_{t} \cdot N_{o}}{\pi \cdot d_{m} \cdot \mu_{t} \cdot N}$$  \hspace{1cm} (108)

Friction factor for the tube-side ($f_{t}$):

$$\frac{1}{\sqrt{f_{t}}} = 0.27 \varepsilon + \left( \frac{7}{Re_{t}} \right)^{0.8}$$  \hspace{1cm} (109)

where $\varepsilon$ is the roughness in mm.

Prandtl number for the tube-side ($Pr_{t}$):

$$Pr_{t} = \frac{\mu_{t} \cdot C_{p_{t}}}{k_{t}}$$  \hspace{1cm} (110)

Nusselt number for tube-side ($Nu_{t}$):

$$Nu_{t} = 0.027 \cdot (Re_{t})^{0.8} \cdot (Pr_{t})^{1/3}$$  \hspace{1cm} (111)

Tube-side heat transfer coefficient ($h_{t}$):
$$h_t = \frac{Nu_t k_t d_{in}}{d_{ex}}$$

(112)

Tube-side velocity ($v_t$):

$$v_t = \frac{Re_t \mu_t}{\rho_t d_{in}}$$

(113)

The velocity limits are:

$$1 \leq v_t \leq 3, \quad v_t \text{ in m/s}$$

(114)

Tube-side pressure drop (including head pressure drop) ($\Delta P_t$):

$$\Delta P_t = \rho_t \left( \frac{2 fl N_s L (v_t)^2}{d_{in}} + 1.25 N_s (v_t)^2 \right)$$

(115)

This value must respect the pressure drop limit, fixed before the design:

$$\Delta P_t \leq \Delta P_{\text{design}}$$

(116)

Heat exchanged:

$$Q = m \cdot C_p \cdot (T_{in} - T_{out}), \quad \text{or: } Q = m \cdot C_p \cdot (T_{out} - T_{in})$$

(117.a)

$$Q = m \cdot C_p \cdot (T_{in} - T_{out}), \quad \text{or: } Q = m \cdot C_p \cdot (T_{out} - T_{in})$$

(117.b)

Heat exchange area:

$$Area = N \cdot \pi d_{ex} \cdot L$$

(118)

LMTD:

$$t_1 = T_{out} - T_{in}$$

(119)

$$t_2 = T_{in} - T_{out}$$

(120)

Chen (1987) LMDT approximation is used:

$$\text{LMDT} = \left[ t_1 t_2 (t_1 + t_2)/2 \right]^{1/3}$$

(121)

Correction factor for the LMDT ($F_t$):

For the $F_t$ determination, the Blackwell and Haydu (1981) is used:

$$R = \frac{T_{in} - T_{out}}{T_{out} - T_{in}}$$

(122)

$$S = \frac{T_{out} - T_{in}}{T_{in} - T_{out}}$$

(123)
\[ F_r = f_i(R,S) = \left( \frac{\sqrt{R^2 + 1}}{R - 1} \right) \log \left( \frac{1 - P_{i1}}{1 - R.P_{i1}} \right) \]  
\[ \log \left( \frac{2/ P_{i1} - 1 - R + \sqrt{R^2 + 1}}{2/ P_{i1} - 1 - R - \sqrt{R^2 + 1}} \right) \]  

(124)

where

\[ P_{i1} = 1 - \left( \frac{R.S - 1}{S - 1} \right)^{1/NS} \]  
\[ R - \left( \frac{R.S - 1}{S - 1} \right)^{1/NS} \]  

(125)

\( NS \) is the number of shells.

or, if \( R = 1 \),

\[ F_i = f_i(R,S) = \frac{P_{i2} - \sqrt{R^2 + 1}}{(1 - P_{i2})} \]  
\[ \log \left( \frac{2/ P_{i1} - 1 - R + \sqrt{R^2 + 1}}{2/ P_{i1} - 1 - R - \sqrt{R^2 + 1}} \right) \]  

(126)

where

\[ P_{i2} = P_1(NS - NS.S + P) \]  

(127)

\[ R_i \leq R + M(1 - y^i) \]  

(128)

\[ R_i \geq R - M(1 - y^i) \]  

(129)

\[ R \leq 0.99 + M(1 - y^i) \]  

(130)

\[ F_i \leq f_i(R,S) + M(1 - y^i) \]  

(131)

\[ F_i \geq f_i(R,S) - M(1 - y^i) \]  

(132)

\[ R \geq 0.99 - M(1 - y^i) \]  

(133)

\[ R \leq 1.01 + M(1 - y^i) \]  

(134)

\[ F_i \leq f_i(R,S) + M(1 - y^i) \]  

(135)

\[ F_i \geq f_i(R,S) - M(1 - y^i) \]  

(136)

\[ R \geq 1.01 - M(1 - y^i) \]  

(137)

\[ R_2 \leq R + M(1 - y^i) \]  

(138)
\[ R_2 \geq R - M (1 - y_M^2) \]  
\[ F_i \leq f_i(R, S) + M (1 - y_P^2) \]  
\[ F_i \geq f_i(R, S) - M (1 - y_P^2) \]  
\[ y_M^1 + y_P^1 + y_P^2 = 1 \]

According to Kern (1950), practical values of \( F_i \) must be greater than 0.75. This constraint must be aggregated to the model:

\[ F_i \geq 0.75 \]

Dirty overall heat transfer coefficient (\( U_d \)):

\[ U_d = \frac{Q}{\text{Area} \cdot \text{LMTD}} \]  

Clean overall heat transfer coefficient (\( U_c \)):

\[ U_c = \frac{1}{\left( \frac{d_{ex} \cdot r_m \cdot d_{ex} + d_{in} \cdot \log(d_{ex} / d_{in})}{d_{in} \cdot h_c} + \frac{r_{out} + 1}{h_c} \right)} \]  

Fouling factor calculation (\( r_d \)):

\[ r_d = \frac{U_c - U_d}{U_c \cdot U_d} \]

This value must respect the fouling heat exchanger limit, fixed before the design:

\[ r_d \geq r_{d,\text{design}} \]

For fluids with high viscosity, like the petroleum fractions, the wall viscosity corrections could be included in the model, both on the tube and the shell sides, for heat transfer coefficients as well as friction factors and pressure drops calculations, since the viscosity as temperature dependence is available. If available, the tubes temperature could be calculated and the viscosity estimated in this temperature value. For non-viscous fluids, however, this correction factors can be neglected.

Two examples were chosen to apply the Ravagnani and Caballero (2007a) model.

**2.1 Example 1**

The first example was extracted from Shenoy (1995). In this case, there is no available area and pumping cost data, and the objective function will consist in the heat exchange area minimization. Temperature and flow rate data as well as fluids physical properties and limits for pressure drop and fouling are in Table 5. It is assumed also that the tube thermal conductivity is 50 W/mK and the roughness factor is 0.0000457. Pressure drop limits are 42
kPa for the tube-side and 7 kPa for the shell-side. A dirt resistance factor of 0.00015 $m^{2}K/W$ should be provided on each side.

| Stream       | $T_{in}$ (K) | $T_{out}$ (K) | $m$ (kg/s) | $\mu$ (kg/ms) | $\rho$ (kg/m$^3$) | $C_p$ (J/kgK) | $K$ (W/mK) | $r_d$ (W/mK) |
|--------------|--------------|---------------|------------|---------------|-----------------|--------------|------------|------------|
| Kerosene     | 371.15       | 338.15        | 14.9       | .00023        | 777             | 2684         | 0.11       | 1.5e-4     |
| Crude oil    | 288.15       | 298.15        | 31.58      | .00100        | 998             | 4180         | 0.60       | 1.5e-4     |

Table 5. Example 1 data

With these fluids temperatures the LMTD correction factor will be greater than 0.75 and one shell is necessary to satisfy the thermal balance.

Table 6 presents the heat exchanger configuration of Shenoy (1995) and the designed equipment, by using the proposed MINLP model. In Shenoy (1995) the author uses three different methods for the heat exchanger design; the method of Kern (1950), the method of Bell Delaware (Taborek, 1983) and the rapid design algorithm developed in the papers of Polley et al. (1990), Polley and Panjeh Shah (1991), Jegede and Polley (1992) and Panjeh Shah (1992) that fixes the pressure drop in both, tube-side and shell-side before the design. The author fixed the cold fluid allocation on the tube-side because of its fouling tendency, greater than the hot fluid. Also some mechanical parameters as the tube outlet and inlet diameters and the tube pitch are fixed. The heat transfer area obtained is 28.4 $m^2$.

The other heat exchanger parameters are presented in Table 6 as well as the results obtained in present paper with the proposed MINLP model, where two situations were studied, fixing and not fixing the fluids allocation. It is necessary to say that Shenoy (1995) does not take in account the standards of TEMA. According to Smith (2005), this type of approach provides just a preliminary specification for the equipment. The final heat exchanger will be constrained to standard parameters, as tube lengths, tube layouts and shell size. This preliminary design must be adjusted to meet the standard specifications. For example, the tube length used is 1.286 m and the minimum tube length recommended by TEMA is 8 ft or 2.438 m. If the TEMA recommended value were used, the heat transfer area would be at least 53 $m^2$.

If the fluids allocation is not previously defined, as commented before, the MINLP formulation will find an optimum for the area value in 28.31 $m^2$, with the hot fluid in the tube side and in a triangular arrangement. The shell diameter would be 0.438 m and the number of tubes 194. Although with a higher tube length, the heat exchanger would have a smaller diameter. Fouling and shell side pressure drops are very close to the fixed limits.

If the hot fluid is previously allocated on the shell side, because of the cold fluid fouling tendency, the MINLP formulation following the TEMA standards will find the minimum area equal to 38.52 $m^2$. It must be taken into account that when compared with the Shenoy (1995) value that would be obtained with the same tube length of 2.438 m (approximately 53 $m^2$), the area would be smaller, as well as the shell diameter and the number of tubes.

### 2.2 Example 2

As previously commented, the objective function in the model can be the area minimization or a cost function. Some rigorous parameters (usually constants) can be aggregated to the cost equation, considering mixed materials of construction, pressure ratings and different types of exchangers, as proposed in Hall et al. (1990).
The second example studied in this chapter was extracted from Mizutani et al. (2003). In this case, the authors proposed an objective function composed by the sum of area and pumping cost. The pumping cost is given by the equation:

$$P_{cost} = c_{cost} \left( \frac{\Delta P_{m_s}}{\rho_s} + \frac{\Delta P_{m_t}}{\rho_t} \right)$$

(148)

The objective function to be minimized is the total annual cost, given by the equation:

$$\text{Min} \quad \text{total annual cost} = a_{cost} (\text{Area})^{b_{cost}} + P_{cost}$$

(149)

Table 7 presents costs, temperature and flowrate data as well as fluids physical properties. Also known is the tube thermal conductivity, 50 W/mK. As both fluids are in the liquid phase, pressure drop limits are fixed to 68.95 kPa, as suggested by Kern (1950). As in Example 1, a dirt resistance factor of 0.00015 m²K/W should be provided on each side.

Table 8 presents a comparison between the problem solved with the Mizutani et al. (2003) model and the model of Ravagnani and Caballero (2007a). Again, two situations were studied, fixing and not fixing the fluids allocation. In both cases, the annual cost is smaller than the value obtained in Mizutani et al. (2003), even with greater heat transfer area. It is because of the use of non-standard parameters, as the tube external diameter and number of tubes. If the final results were adjusted to the TEMA standards (the number of tubes would be 902, with \(d_{ex} = 19.05 \text{ mm}\) and \(Ntp = 2\) for square arrangement) the area should be approximately 264 m². However, the pressure drops would increase the annual cost. Using the MINLP proposed in the present paper, even fixing the hot fluid in the shell side, the value of the objective function is smaller.

Analysing the cost function sensibility for the objective function studied, two significant aspects must be considered, the area cost and the pumping cost. In the case studied the proposed MINLP model presents an area value greater (264.15 and 286.15 m² vs. 202.00 m²) but the global cost is lower than the value obtained by the Mizutani et al. (2003) model (5250.00 $/year vs. 5028.29 $/year and 5191.49 $/year, respectively). It is because of the pumping costs (2424.00 $/year vs. 1532.93 $/year and 1528.24 $/year, respectively). Obviously, if the results obtained by Mizutani et al. (2003) for the heat exchanger configuration (number of tubes, tube length, outlet and inlet tube diameters, shell diameter, tube bundle diameter, number of tube passes, number of shells and baffle spacing) are fixed the model will find the same values for the annual cost (area and pumping costs), area, individual and overall heat transfer coefficients and pressure drops as the authors found. It means that it represents a local optimum because of the other better solutions, even when the fluids allocation is previously fixed.

The two examples were solved with GAMS, using the solver SBB, and Table 9 shows a summary of the solver results. As can be seen, CPU time is not high. As pointed in the Computational Aspects section, firstly it is necessary to choose the correct tool to solve the problem. For this type of problem studied in the present paper, the solver SBB under GAMS was the better tool to solve the problem. To set a good starting point it is necessary to give all the possible flexibility in the lower and upper variables limits, prior to solve the model, i.e., it is important to fix very lower low bounds and very higher upper limits to the most influenced variables, as the Reynolds number, for example.
Table 6. Results for example 1

| Stream | \( T_{in} \) (K) | \( T_{out} \) (K) | \( m \) (kg/s) | \( \mu \) (kg/ms) | \( \rho \) (kg/m³) | \( Cp \) (J/kgK) | \( k \) (W/mK) | \( \Delta P_r \) (kPa) | \( r_d \) (W/mK) |
|--------|-----------------|-----------------|---------------|-----------------|-----------------|-----------------|----------------|-------------------|-----------------|
| 1      | 368.15          | 313.75          | 27.78         | 3.4e-4          | 750             | 2840            | 0.19           | 68.95             | 1.7e-4          |
| 2      | 298.15          | 313.15          | 68.88         | 8.0e-4          | 995             | 4200            | 0.59           | 68.95             | 1.7e-4          |

\( \alpha_{cost} = 123, \beta_{cost} = 0.59, \gamma_{cost} = 1.31 \)

Table 7. Example 2 data

3. The model of Ravagnani et al. (2009) PSO algorithm

Alternatively, in this chapter, a Particle Swarm Optimization (PSO) algorithm is proposed to solve the shell and tube heat exchangers design optimization problem. Three cases extracted from the literature were also studied and the results shown that the PSO algorithm for this...
type of problems, with a very large number of non linear equations. Being a global optimum heuristic method, it can avoid local minima and works very well with highly nonlinear problems and present better results than Mathematical Programming MINLP models.

|                          | Mizutani et al. (2003) | Ravagnani and Caballero (2007a) (Not fixing fluids allocation) | Ravagnani and Caballero (2007a) (fixing hot fluid on the shell side) |
|--------------------------|------------------------|---------------------------------------------------------------|---------------------------------------------------------------|
| Total annual cost ($/year) | 5250.00                | 5028.29                                                      | 5191.47                                                      |
| Area cost ($/year)       | 2826.00                | 3495.36                                                      | 3663.23                                                      |
| Pumping cost ($/year)    | 2424.00                | 1532.93                                                      | 1528.24                                                      |
| Area (m²)                | 202.00                 | 264.634                                                      | 286.15                                                       |
| Q (kW)                   | 4339                   | 4339                                                         | 4339                                                         |
| D₁ (m)                   | 0.687                  | 1.067                                                        | 0.838                                                        |
| D₁₉ (m)                  | 0.672                  | 1.022                                                        | 0.796                                                        |
| Nᵣ                       | 832                    | 680                                                          | 713                                                          |
| Nₙ                       | 8                      | 7                                                            | 18                                                           |
| lₛ (m)                   | 0.542                  | 0.610                                                        | 0.353                                                        |
| dₛₙ (mm)                 | 15.90                  | 25.04                                                        | 19.05                                                        |
| dₛₐ (mm)                 | 12.60                  | 23.00                                                        | 16.00                                                        |
| L (m)                    | 4.88                   | 4.88                                                         | 6.71                                                         |
| hₗ (W/m²°C)              | 6,480.00               | 1,986.49                                                     | 4,186.21                                                     |
| hₛ (W/m²°C)              | 1,829.00               | 3,240.48                                                     | 1,516.52                                                     |
| Uₗ (W/m°C)               | 655.298                | 606.019                                                      | 606.019                                                      |
| Uₛ (W/m°C)               | 860                    | 826.687                                                      | 758.664                                                      |
| ΔPᵢ (kPa)                | 22,676                 | 23.312                                                       | 13.404                                                       |
| ΔPₛ (kPa)                | 7,494                  | 4.431                                                        | 6.445                                                        |
| rₛ (m²°C/W)              | -----                  | 3.16e-4                                                      | 3.32e-4                                                      |
| vₛ (m/s)                 | -----                  | 1.058                                                        | 1.003                                                        |
| vₛ (m/s)                 | -----                  | 0.500                                                        | 0.500                                                        |
| NS                       | ----                   | 1                                                            | 1                                                            |
| Hot fluid allocation     | shell                  | tube                                                         | shell                                                         |

Table 8. Results for example 2

|                          | Example 1 | Example 2 |
|--------------------------|-----------|-----------|
| Equations                | 166       | 157       |
| Continuous variables     | 713       | 706       |
| Discrete variables       | 53        | 602       |
| CPU time *Pentium IV 1 GHz (s) | .251     | .561      |

Table 9. Summary of Solver Results

Kennedy and Elberhart (2001), based on some animal groups social behavior, introduced the Particle Swarm Optimization (PSO) algorithm. In the last years, PSO has been successfully applied in many research and application areas. One of the reasons that PSO is attractive is that there are few parameters to adjust. An interesting characteristic is its global search

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character in the beginning of the procedure. In some iteration it becomes to a local search method when the final particles convergence occur. This characteristic, besides of increase the possibility of finding the global optimum, assures a very good precision in the obtained value and a good exploration of the region near to the optimum. It also assures a good representation of the parameters by using the method evaluations of the objective function during the optimization procedure.

In the PSO each candidate to the solution of the problem corresponds to one point in the search space. These solutions are called particles. Each particle have also associated a velocity that defines the direction of its movement. At each iteration, each one of the particles change its velocity and direction taking into account its best position and the group best position, bringing the group to achieve the final objective.

In the present chapter, it was used a PSO proposed by Vieira and Biscaia Jr. (2002). The particles and the velocity that defines the direction of the movement of each particle are actualised according to Equations (153) and (154):

\[ v_{i,k+1} = w \cdot v_{i,k} + c_1 \cdot r_1 \cdot (p_{i,k}^{p} - x_{i,k}) + c_2 \cdot r_2 \cdot (p_{k,GLOBAL}^{p} - x_{i,k}) \]  
\[ x_{i,k+1} = x_{i,k} + v_{i,k+1} \]  

Where \( x_{i,k} \) and \( v_{i,k} \) are vectors that represent, respectively, position and velocity of the particle \( i \), \( w \) is the inertia weight, \( c_1 \) and \( c_2 \) are constants, \( r_1 \) and \( r_2 \) are two random vectors with uniform distribution in the interval \([0, 1]\), \( p_{i,k}^{p} \) is the position with the best result of particle \( i \) and \( p_{k,GLOBAL}^{p} \) is the position with the best result of the group. In above equations subscript \( k \) refers to the iteration number.

In this problem, the variables considered independents are randomly generated in the beginning of the optimization process and are modified in each iteration by the Equations (153) and (154). Each particle is formed by the follow variables: tube length, hot fluid allocation, position in the TEMA table (that automatically defines the shell diameter, tube bundle diameter, internal and external tube diameter, tube arrangement, tube pitch, number of tube passes and number of tubes).

After the particle generation, the heat exchanger parameters and area are calculated, considering the Equations from the Ravagnani and Caballero (2007a) as well as Equations (155) to (160). This is done to all particles even they are not a problem solution. The objective function value is obtained, if the particle is not a solution of the problem (any constraint is violated), the objective function is penalized. Being a heuristic global optimisation method, there are no problems with non linearities and local minima. Because of this, some different equations were used, like the MLTD, avoiding the Chen (1987) approximation.

The equations of the model are the following:

**Tube Side:**
- Number of Reynolds \( (Re_t) \): Equation (108);
- Number of Prandl \( (Pr_t) \): Equation (110);
- Number of Nusselt \( (Nu_t) \): Equation (111);
- Individual heat transfer coefficient \( (h_t) \): Equation (112);
- Fanning friction factor \( (f_t) \): Equation (109);
- Velocity \( (v_t) \): Equation (113);
- Pressure drop \( (\Delta P_t) \): Equation (115);
Shell Side:
Cross-flow area at or near centerline for one cross-flow section ($S_m$):

\[
\begin{align*}
\text{triangular} & \Rightarrow S_m = l_s \cdot \left[ D^t - D_f + \left( \frac{pt - d_{ex}}{pt} \right) \left( D_f - d_{ex} \right) \right] \\
\text{square} & \Rightarrow S_m = l_s \cdot \left[ D^t - D_f + \left( \frac{pt - d_{ex}}{pn} \right) \left( D_f - d_{ex} \right) \right] \\
\end{align*}
\]

(152)

Number of Reynolds ($Re_s$): Equation (59);
Velocity ($v_s$): Equation (60);
Colburn factor ($j_i$): Equations (77) and (78);
Fanning friction factor ($f_l$): Equations (79 and 80);
Number of tube rows crossed by the ideal cross flow ($N_c$): Equation (84);
Number of effective cross-flow tube rows in each window ($N_{cw}$): Equation (88);
Fraction of total tubes in cross flow ($F_c$): Equations (86) and (87);
Fraction of cross-flow area available for bypass flow ($F_{sbp}$): Equation (89);
Shell-to-baffle leakage area for one baffle ($S_{sb}$): Equation (90);
Tube-to-baffle leakage area for one baffle ($S_{tb}$): Equation (91);
Area for flow through the windows ($S_{w}$): Equation (92);
Shell-side heat transfer coefficient for an ideal tube bank ($h_{oi}$): Equation (94);
Correction factor for baffle configuration effects ($J_c$): Equation (95);
Correction factor for baffle-leakage effects ($J_l$): Equations (96) and (97);
Correction factor for bundle-bypassing effects ($J_b$): Equation (98);
Shell-side heat transfer coefficient ($h_s$): Equation (99);
Pressure drop for an ideal cross-flow section ($\Delta P_{bi}$): Equation (100);
Pressure drop for an ideal window section ($\Delta P_{wi}$): Equation (101);
Correction factor for the effect of baffle leakage on pressure drop ($R_l$): Equations (102) and (103);
Correction factor for bundle bypass ($R_b$): Equation (104);
Pressure drop across the Shell-side ($\Delta P_i$): Equation (105);
General aspects of the heat exchanger:
Heat exchanged ($Q$): Equations (117a) and (117b);
LMTD:

\[
\begin{align*}
\Delta T_1 &= T_{in}^k - T_{out}^c \\
\Delta T_2 &= T_{out}^k - T_{in}^c \\
\text{LMTD} &= \frac{\Delta T_1 - \Delta T_2}{\ln \left( \frac{\Delta T_1}{\Delta T_2} \right)} \\
\end{align*}
\]

(153)

Correction factor for the LMTD: Equations (122) to (127);
Tube Pitch ($pt$):

\[
pt = 1.25 \cdot d_{ex}'
\]

(154)

Baffles spacing ($l_s$):
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\[ l_s = \frac{L'}{(Nb + 1)} \]  \hspace{1cm} (155)

Definition of the tube arrangement \((pn \text{ and } pp)\) variables:

\[
\begin{align*}
\text{triangular} & \Rightarrow \begin{bmatrix} pn = 0.5 \cdot pt \\ pp = 0.866 \cdot pt \end{bmatrix} \\
\text{square} & \Rightarrow \begin{bmatrix} pn = pt \\ pp = pt \end{bmatrix}
\end{align*}
\]  \hspace{1cm} (156)

Heat exchange area \((Area)\):

\[ Area = n^1 \cdot \pi \cdot d_{ex}^1 \cdot L^1 \]  \hspace{1cm} (157)

Clean overall heat transfer coefficient \((Uc)\): Equation (145);
Dirty overall heat transfer coefficient \((Ud)\): Equation (144);
Fouling factor \((rd)\): Equation (146).

The Particle Swarm Optimization (PSO) algorithm proposed to solve the optimization problem is presented below. The algorithm is based on the following steps:

i. Input Data
- Maximum number of iterations
- Number of particles of the population \((Npt)\)
- \(c1, c2\) and \(w\)
- Maximum and minimum values of the variables (lines in TEMA table)
- Streams, area and cost data (if available)

ii. Random generation of the initial particles
There are no criteria to generate the particles. The generation is totally randomly done.
- Tube length (just the values recommended by TEMA)
- Hot fluid allocation (shell or tube)
- Position in the TEMA table (that automatically defines the shell diameter, the tube bundle diameter, the internal and the external tube diameter, the tube arrangement, the tube pitch, the number of tube passes and the number of tubes)

iii. Objective function evaluation in a subroutine with the design mathematical model
With the variables generated at the previous step, it is possible to calculate:
- Parameters for the tube side
- Parameters for the shell side
- Heat exchanger general aspects
- Objective Function
All the initial particles must be checked. If any constraint is not in accordance with the fixed limits, the particle is penalized.

iv. Begin the PSO
Actualize the particle variables with the PSO Equations (150) and (151), re-evaluate the objective function value for the actualized particles (step iii) and verify which is the particle with the optimum value;

v. Repeat step iv until the stop criteria (the number of iterations) is satisfied.
During this PSO algorithm implementation is important to note that all the constraints are activated and they are always tested. When a constraint is not satisfied, the objective
function is weighted and the particle is automatically discharged. This proceeding is very usual in treating constraints in the deterministic optimization methods. When discrete variables are considered if the variable can be an integer it is automatically rounded to closest integer number at the level of objective function calculation, but maintained at its original value at the level of PSO, in that way we keep the capacity of changing from one integer value to another.

Two examples from the literature are studied, considering different situations. In both cases the computational time in a Pentium(R) 2.8 GHz computer was about 18 min for 100 iterations. For each case studied the program was executed 10 times and the optima values reported are the average optima between the 10 program executions. The same occurs with the PSO success rate (how many times the minimum value of the objective function is achieved in 100 iterations).

The examples used in this case were tested with various sets of different parameters and it was evaluated the influence of each case in the algorithm performance. The final parameters set was the set that was better adapted to this kind of problem. The parameters used in all the cases studied in the present paper are shown in Table 10.

| c1   | c2   | w    | Npt |
|------|------|------|-----|
| 1.3  | 1.3  | 0.75 | 30  |

Table 10. PSO Parameters

3.1 Example 3

This example was extracted from Shenoy (1995). The problem can be described as to design a shell and tube heat exchanger to cool kerosene by heating crude oil. Temperature and flow rate data as well as fluids physical properties and limits for pressure drop and fouling are in Table 11. In Shenoy (1995) there is no available area and pumping cost data, and in this case the objective function will consist in the heat exchange area minimization, assuming the cost parameters presented in Equation (04). It is assumed that the tube wall thermal conductivity is 50 WmK⁻¹. Pressure drop limits are 42 kPa for the tube-side and 7 kPa for the shell-side. A fouling factor of 0.00015 m²KW⁻¹ should be provided on each side.

In Shenoy (1995) the author uses three different methods for the heat exchanger design; the method of Kern (1950), the method of Bell Delaware (Taborek, 1983) and the rapid design algorithm developed in the papers of Polley et al. (1990), Polley and Panjeh Shah (1991), Jegede and Polley (1992) and Panjeh Shah (1992) that fixes the pressure drop in both, tube-side and shell-side before the design. Because of the fouling tendency the author fixed the cold fluid allocation on the tube-side. The tube outlet and inlet diameters and the tube pitch are fixed.

Table 12 presents the heat exchanger configuration of Shenoy (1995) and the designed equipment, by using the best solution obtained with the proposed MINLP model of Ravagnani and Caballero (2007a) and the PSO algorithm proposed by Ravagnani et al. (2009). In Shenoy (1995) the standards of TEMA are not taken into account. This type of approach provides just a preliminary specification for the equipment. The final heat exchanger will be constrained by standard parameters, as tube lengths, tube layouts and shell size. This preliminary design must be adjusted to meet the standard specifications. For example, the tube length used is 1.286 m and the minimum tube length recommended by TEMA is 8 ft or 2.438 m. As can be seen in Table 12, the proposed methodology with
the PSO algorithm in the present paper provides the best results. Area is 19.83 m², smaller than 28.40 m² and 28.31 m², the values obtained by Shenoy (1995) and Ravagnani and Caballero (2007a), respectively, as well as the number of tubes (102 vs. 194 and 368). The shell diameter is the same as presented in Ravagnani and Caballero (2007a), i.e., 0.438 m, as well as the tube length. Although with a higher tube length, the heat exchanger would have a smaller diameter. Fouling and shell side pressure drops are in accordance with the fixed limits.

The PSO success rate (how many times the minimum value of the objective function is achieved in 100 executions) for this example was 78%.

| Stream          | \( T_{in} \) (K) | \( T_{out} \) (K) | \( m \) (kg/s) | \( \mu \) (kg/ms) | \( \rho \) (kg/m³) | \( C_p \) (J/kgK) | \( K \) (W/mK) | \( r_d \) (W/mK) |
|-----------------|------------------|------------------|----------------|------------------|-----------------|----------------|----------------|---------------|
| Kerosene        | 371.15           | 338.15           | 14.9           | 0.0023           | 777             | 2684           | 0.11           | 1.5e-4        |
| Crude oil       | 288.15           | 298.15           | 31.58          | 0.0100           | 998             | 4180           | 0.60           | 1.5e-4        |

Table 11. Example 3 data

|                                | Shenoy (1995) | Ravagnani and Caballero (2007a) best solution | Ravagnani et al. (2009) |
|--------------------------------|---------------|---------------------------------------------|-------------------------|
| Area (m²)                      | 28.40         | 28.31                                       | 19.83                   |
| D_s (m)                        | 0.549         | 0.438                                       | 0.438                   |
| Tube length (mm)               | 1286          | 2438                                        | 2438                    |
| \( d_{out} \) (mm)             | 19.10         | 19.10                                       | 25.40                   |
| \( d_{in} \) (mm)              | 15.40         | 17.00                                       | 21.2                    |
| Tubes arrangement              | Square        | Triangular                                  | Square                  |
| Baffle spacing (mm)            | 0.192         | 0.105                                       | 0.263                   |
| Number of baffles              | 6             | 6                                           | 8                       |
| Number of tubes                | 368           | 194                                         | 102                     |
| tube passes                    | 6             | 4                                           | 4                       |
| shell passes                   | 1             | 1                                           | 1                       |
| \( \Delta P^s \) (kPa)         | 3.60          | 7.00                                        | 4.24                    |
| \( \Delta P^t \) (kPa)         | 42.00         | 26.92                                       | 23.11                   |
| \( h_s \) (kW/m²°C)            | 8649.6        | 3831.38                                     | 5799.43                 |
| \( h_t \) (kW/m²°C)            | 1364.5        | 2759.84                                     | 1965.13                 |
| U (W/m²°C)                     | 1000.7        | 1017.88                                     | 865.06                  |
| \( r_d \) (m²°C/W)             | 0.00041       | 0.00030                                     | 0.00032                 |
| Ft factor                      | 0.9           | 0.9                                         | 0.9                     |
| Hot fluid allocation           | Shell         | Tube                                        | Tube                    |
| \( v_s \) (m/s)                | **            | 1.827                                       | 2.034                   |
| \( v_t \) (m/s)                | **            | 0.935                                       | 0.949                   |

Table 12. Results for the Example 2
3.2 Example 4

The next example was first used for Mizutani et al. (2003) and is divided in three different situations.

**Part A:** In this case, the authors proposed an objective function composed by the sum of area and pumping cost. Table 13 presents the fluids properties, the inlet and outlet temperatures and pressure drop and fouling limits as well as area and pumping costs. The objective function to be minimized is the global cost function. As all the temperatures and flow rates are specified, the heat load is also a known parameter.

**Part B:** In this case it is desired to design a heat exchanger for the same two fluids as those used in Part A, but it is assumed that the cold fluid target temperature and its mass flow rate are both unknown. Also, it is considered a refrigerant to achieve the hot fluid target temperature. The refrigerant has a cost of $7.93/1000 tons, and this cost is added to the objective function.

**Part C:** In this case it is supposed that the cold fluid target temperature and its mass flow rate are unknowns and the same refrigerant used in Part B is used. Besides, the hot fluid target temperature is also unknown and the exchanger heat load may vary, assuming a cost of $20/kW.yr to the hot fluid energy not exchanged in the designed heat exchanged, in order to achieve the same heat duty achieved in Parts A and B.

| Fluid | $T_{in}$ (K) | $T_{out}$ (K) | $m$ (kg/s) | $\mu$ (kg/ms) | $\rho$ (kg/m$^3$) | $C_p$ (J/kgK) | $k$ (W/mK) | $\Delta P_{max}$ (kPa) | $rd$ (W/mK) |
|-------|--------------|--------------|------------|---------------|------------------|---------------|-------------|-----------------------|-------------|
| A     | 368.15       | 313.75       | 27.78      | 3.4e-4        | 750              | 2,840         | 0.19        | 68.95                 | 1.7e-4      |
| B     | 298.15       | 313.15       | 68.88      | 8.0e-4        | 995              | 4,200         | 0.59        | 68.95                 | 1.7e-4      |

$$A_{cost} = 123 \cdot A^{0.59}$$

$$Pump_{cost} = 1.31 \left( \frac{\Delta P^1 \cdot m^1}{\rho^1} + \frac{\Delta P^2 \cdot m^2}{\rho^2} \right)$$

$/ year, A = m^2 \Delta P = Pa \ m = kg/s \ \rho = kg/m^3$

Table 13. Data for Example 6

All of the three situations were solved with the PSO algorithm proposed by Ravagnani et al. (2009) and the results are presented in Table 14. It is also presented in this table the results of Mizutani et al. (2003) and the result obtained by the MINLP proposition presented in Ravagnani and Caballero (2007a) for the Part A. It can be observed that in all cases the PSO algorithm presented better results for the global annual cost. In Part A the area cost is higher than the presented by Mizutani et al. (2003) but inferior to the presented by Ravagnani and Caballero (2007a). Pumping costs, however, is always lower. Combining both, area and pumping costs, the global cost is lower. In Part B the area cost is higher than the presented by Mizutani et al. (2003) but the pumping and the cold fluid cost are lower. So, the global cost is lower (11,572.56 vs. 19,641). The outlet temperature of the cold fluid is 335.73 K, higher than 316 K, the value obtained by Mizutani et al. (2003).

In Part C, the area cost is higher but pumping, cold fluid and auxiliary cooling service cost are lower and because of this combination, the global annual cost is lower than the
presented by Mizutani et al. (2003). The outlet cold fluid temperature is 338.66 K, higher than the value obtained by the authors and the outlet hot fluid temperature is 316 K, lower than the value obtained by Mizutani et al. (2003).

The PSO success rates 74%, 69% and 65% for Parts A, B and C, respectively.

4. Conclusions

In the present chapter two models for the optimal design of heat exchangers were presented, one based on Mathematical Programming and other one based on the PSO algorithm. The first one (Ravagnani and Caballero, 2007a) is based on GDP and the optimisation model is a MINLP, following rigorously the Standards of TEMA. Bell-Delaware method was used to calculate the shell-side variables. The model was developed for turbulent flow on the shell side using a baffle cut of 25% but the model can consider other values of baffle cuts.

The model calculates the best shell and tube heat exchanger to a given set of temperatures, flow rates and fluids physical properties. The major contribution of this model is that all the calculated heat exchanger variables are in accordance with TEMA standards, shell diameter, outlet tube bundle diameter, tube arrangement, tube length, tube pitch, internal and external tube diameters, number of baffles, baffle spacing, number of tube passes, number of shells and number of tubes. It avoids heat exchanger parameters adjustment after the design task. The tube counting table proposed and the use of DGP makes the optimisation task not too hard, avoiding non linearities in the model. The problem was solved with GAMS, using the solver SBB. During the solution of the model, the major problems were found in the variables limits initialisation. Two examples were solved to test the model applicability. The objective function was the heat exchange area minimization and in area and pumping expenses in the annual cost minimization. In the studied examples comparisons were done to Shenoy (1995) and Mizutani et al. (2003). Having a larger field of TEMA heat exchanger possibilities, the present model achieved more realistic results than the results obtained in the literature. Besides, the task of heat exchanger parameters adjustment to the standard TEMA values is avoided with the proposed MINLP formulation proposition. The main objective of the model is to design the heat exchanger with the minimum cost including heat exchange area cost and pumping cost or just heat exchange area minimization, depending on data availability, rigorously following the Standards of TEMA and respecting shell and tube sides pressure drops and fouling limits. Given a set of fluids data (physical properties, pressure drop and fouling limits and flow rate and inlet and outlet temperatures) and area and pumping cost data the proposed methodology allows to design the shell and tube heat exchanger and calculates the mechanical variables for the tube and shell sides, tube inside diameter \(d_{in}\), tube outside diameter \(d_{ox}\), tube arrangement, tube pitch \(pt\), tube length \(L\), number of tube passes \(np_t\) and number of tubes \(N_t\), the external shell diameter \(D_s\), the tube bundle diameter \(Dotl\), the number of baffles \(Nb\), the baffles cut \(lc\) and the baffle spacing \(ls\). Also the thermal-hydraulic variables are calculated, heat duty \(Q\), heat exchange area \(A\), tube-side and shell-side film coefficients \(h_t\) and \(h_s\), dirty and clean overall heat transfer coefficients \(U_d\) and \(U_c\), pressure drops \(\Delta P_t\) and \(\Delta P_s\),
|                      | Part A | Part B | Part C |
|----------------------|--------|--------|--------|
| Mizutani et al. (2003) | 5,250  | 19,641 | 21,180 |
| Ravagnani et al. (2003) | 5,028.29 | 4,563.18 | 4,000.38 |
| Ravagnani et al. (2009) | 3,944.32 | 13,556.1 | 1,103.176 |
| Ravagnani et al. (2009) | 11,572.56 | 5,653.77 | 6,095.52 |
| Ravagnani et al. (2009) | 19,641 | 11,409 | 6,095.52 |
| Total Cost ($/year) | 5,250  | 19,641 | 21,180 |
| Area Cost ($/year) | 2,826  | 3,200.46 | 2,943 |
| Pumping ($/year) | 2,424  | 1,638 | 2,868 |
| Cold Fluid ($/year) | --     | 1,355.61 | 1,103.176 |
| Aux. Cool. ($/year) | --     | -- | 3,960 |
| m_c (kg/s) | --     | 58 | 46 |
| T_c (K) | --     | 316 | 319 |
| T_h (K) | --     | -- | 316 |
| Area (m²) | 202    | 250.51 | 217 |
| D_s (mm) | 0.687  | 0.8382 | 0.754 |
| length (mm) | 4.88  | 4.88 | 4.88 |
| d_out (mm) | 15.19 | 19.05 | 19.05 |
| d_in (mm) | 12.6   | 14.83 | 18.60 |
| Tubes arrangement | Square | Square | Square |
| Baffle Cut | ** | 25% | ** |
| Baffle spacing (mm) | 0.542 | 0.610 | 0.610 |
| Baffles | 8 | 7 | 5 |
| No. of tubes | 832 | 687 | 940 |
| Tube passes | 2 | 4 | 4 |
| ΔP_s (kPa) | 7,494 | 5,097.04 | 5,814 |
| ΔP_t (kPa) | 4,431 | 1,219 | 1,219 |
| h_s (kW/m²K) | 1,829 | 3,102.73 | 3,173.352 |
| h_t (kW/m²K) | 3,240.48 | 3,400.49 | 3,400.49 |
| r_d (m²K/W) | ** | 3.400.49 | 3.400.49 |
| F factor | 0.812 | 0.750 | 0.801 |
| Hot Fluid Allocation | Shell | Tube | Shell |
| v_l (m/s) | ** | 1.058 | ** |
| v_s (m/s) | ** | 1.951 | ** |

* Not applicable
** Not available

Table 13. Results for Example 6
fouling factor \( (rd) \), log mean temperature difference \( (LMTD) \), the correction factor of LMTD \( (F_t) \) and the fluids location inside the heat exchanger.

The second model is based on the Particle Swarm Optimization (PSO) algorithm. The Bell-Delaware method is also used for the shell-side calculations as well as the counting table presented earlier for mechanical parameters is used in the model. Three cases from the literature cases were also studied. The objective function was composed by the area or by the sum of the area and pumping costs. In this case, three different situations were studied. In the first one all the fluids temperatures are known and, because of this, the heat load is also a known parameter. In the second situation, the outlet hot and cold fluids are unknown. In this way, the optimization model considers these new variables. All of the cases are complex non-linear programming problems. Results shown that in all cases the values obtained for the objective function using the proposed PSO algorithm are better than the values presented in the literature. It can be explained because all the optimization models used in the literature that presented the best solutions in the cases studied are based on MINLP and they were solved using mathematical programming. When used for the detailed design of heat exchangers, MINLP (or disjunctive approaches) is fast, assures at least a local minimum and presents all the theoretical advantages of deterministic problems. The major drawback is that the resulting problems are highly nonlinear and non-convex and therefore only a local solution is guaranteed and a good initialization technique is mandatory which is not always possible. PSO have the great advantage that do not need any special structure in the model and tend to produce near global optimal solutions, although only in an ‘infinite large’ number of iterations. Using PSO it is possible to initially favor the global search (using an l-best strategy or using a low velocity to avoid premature convergence) and later the local search, so it is possible to account for the tradeoff local vs. global search.

Finely, considering the cases studied in the present chapter, it can be observed that all of the solutions obtained with MINLP were possibly trapped in local minima. By using the PSO algorithm, a meta-heuristic method, because of its random nature, the possibility of finding the global optima in this kind of non-linear problems is higher. The percentage of success is also higher, depending on the complexity of the problem. Computational time (about 18 minutes for all cases) is another problem and the user must work with the possibility of a trade off between the computational effort and the optimum value of the objective function. But for small-scale problems the PSO algorithm proposed in the present paper presents the best results without excessive computational effort.

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