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METAHEURISTIC OPTIMIZATION AND SIMULATION OF SHELL AND TUBE HEAT EXCHANGERS

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Abstract. *The heat exchanger is the main industrial equipment used for heat transfer between two fluids. Due to its wide use and importance, the present work aims at the modelling and optimization of a shell and tube heat exchanger by the Gray Wolf Optimization (GWO) method. Three cases were analyzed: 1) methanol-water, 2) kerosene-crude oil and 3) distillated water-raw water. The optimized variables were the shell's internal diameter, the tube's external diameter and the baffle's spacing, in order to reduce the exchanger's initial investment and operational cost. The classic GWO and a modified version were used, in which parameters within the code varied by exponential, gaussian and beta functions. Case 3 exchanger was also simulated in software Chemcad® in order to compare with some of the modelling's values and fully design the equipment. The results obtained by the classic GWO were superior than the modified code, with costs reduction of 13.4 and 46.34% for the first and third cases, respectively. The second exchanger had its total cost increased. The simulation in Chemcad® was performed successfully, with great agreement between the thermal and hydraulic coefficients. The equipment was fully designed, having the remaining physical parameters and its type defined.*

Keywords: *Heat Exchanger; Shell and Tube; Optimization; Gray Wolf Optimization; Chemcad simulation.*

1. INTRODUCTION

Heat exchangers are the mainly used equipment for the transfer of heat between fluids. The existing types are: shell and tube (STHE), plate (PHE), compact, finned, among others. The first is one of the most commonly used, often found in chemical processing industries. It is composed of several tubes that are specifically arranged inside a shell, equipped with supporting baffles. One fluid flows into the tubes and the other runs along the shell, being deflected by the baffles, in order to promote turbulence and improve the transfer of energy. Also, the STHEs can have multiple passes on the shell, tube or both sides. One pass refers to when the fluid crosses the exchanger's length once. The objective of using passes is to increase the contact of the fluids and, therefore, increase the equipment's efficiency (Çengel & Ghajar, 2012 & Lavine *et al.*, 2014).

The flow of the process fluids may be co-current (in which they enter and leave the exchanger at the same end), countercurrent (enter/leave at opposite ends) or crossed. These different types of flow grant variations on the outlet temperatures, as well as their profiles. When flowing parallelly, the temperature difference in the equipment will gradually decrease and the hot fluid will always leave the exchanger still hotter than the cold one. When it is countercurrent, the temperature difference remains approximately constant and the outlet cold stream can leave the exchanger hotter than the outlet hot one (Çengel & Ghajar, 2012). The tubes' configuration (pitch) inside the shell can be squared, triangular, rotated square or triangular with cleaning lanes. Such spacing between each tube directly interferes with the pressure drop and transfer coefficients of the equipment (Kern, 1987).

The process of transferring energy that occurs in a heat exchanger is due to the temperature difference between the fluids, the driving potential for the phenomenon. For a fixed transfer rate, the lower the magnitude of the temperature difference, the greater the required heat transfer area. Larger areas mean a higher cost, which is a limiting design factor. Thus, means to optimize the process and reduce investment and operating costs are very attractive. The cost of operating a heat exchanger is not only due to the construction and maintenance of the equipment itself, but also comes from the power of pumps and fans required for the flow of the fluids, that which is directly linked to the pressure drop (Kreith & Bohn, 2003).

According to Kuppan (2013), the main components of STHEs are the shell, tubes, baffles, inlet head, outlet head and nozzles. The shell diameter can reach up to 2 meters, with temperature ranges between -20 ºC and 500 ºC. The maximum operating pressure is approximately 600 atmospheres. It is advantageous for its flexible design, easy maintenance and repair. In Fig. (1), from Walas (1990), it is possible to visualize a schematic of the equipment, denoting its constructive parts.

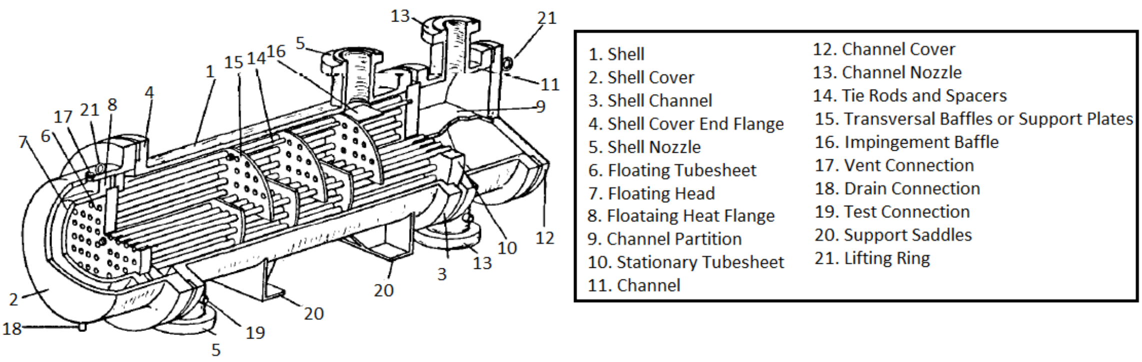

Figure 1 - Shell and Tube Heat Exchanger scheme with its main parts.

With the focus on cost minimization, some meta-heuristic optimization studies have emerged in the study of heat exchangers, including the Genetic Algorithm (GA), which was used by Caputo *et al.* (2008) and Particle Swarm Optimization (PSO) applied by Rao & Patel (2010). In the present work, the Gray Wolf method (GWO, Gray Wolf Optimizer), proposed by Mirjalili *et al.* (2014), was implemented in order to optimize the cost of three different STHEs. The GWO is bio-inspired in the gray wolf, which is considered an elite predator and usually walks in packs of 5 to 12 wolves, possessing well-defined social positions. The method was inspired in these hierarchies to obtain the optimization of the variables (Mirjalili *et al.*, 2014).

Therefore, the general objective of this study is to perform the mathematical modeling and optimization of a shell and tube heat exchanger and compare the performance of the meta-heuristic optimization method Gray Wolf Optimizer (GWO) with the original designs from Sinnott *et al.* (1996) and Kern (1987). The variables submitted to optimization were the internal diameter of the shell, D_s, the external diameter of the tubes, d_o, and the spacing between the baffles, B. After optimization, the third heat exchanger was submitted to simulation in software Chemcad® in order to fully design it. Comparison between thermal and hydraulic parameters from simulation and modelling was also fulfilled.

2. METHODOLOGY

Before implementing the GWO, it was necessary to perform the mathematical modeling of the exchanger; acquire the relevant thermophysical properties (specific mass, specific heat, dynamic viscosity, thermal conductivity) and determine the required correlations for the calculation of the convective heat transfer coefficients.

The results obtained by the optimization of the GWO were compared, mainly, to the study of Sinnott *et al.* (1996) and Kern (1987), which provided the original design of the exchangers. Additionally, the work of Caputo *et al.* (2008) and Rao & Patel (2010) also serves as comparative data, in which the GA and PSO were used, respectively. The dimensions of the shell, tubes, the coefficients, the flow parameters and, mainly, the initial investment and operating costs were compared. From the results obtained it was possible to analyze the effects of the exchanger's variables on their final cost.

Three cases were studied, varying the fluids, their inlet conditions and with different rates of heat transfer (fixed for each case). The first (methanol-water) and third (water-water) cases were proposed by Sinnott *et al.* (1996) and the second (kerosene-crude oil) by Kern (1987). The flow in the exchanger in the three cases is countercurrent and the logarithmic mean temperature difference method (referred to as LMTD) was used for mathematical modeling, as all temperature values were known. The fluid's thermophysical properties were estimated at the mean temperature between the inlet and outlet ones. Both the modelling and the optimization were performed in Matlab®.

2.1 Mathematical Modelling of the Exchanger

The main equation that governs heat exchangers, which relates its four major variables (total heat transfer rate, the global transfer coefficient, the total transfer area and the mean temperature difference), is the generalized Newton's Cooling Law, Eq. (1).

$$\dot{q} = U.A_{ht}.(F.\Delta T_{ML}). \quad (1)$$

The knowledge of transfer rate, global coefficient and mean temperature difference allows to explicit and determine the required thermal exchange area, and the tube's length, in Eq. (1). The term ΔT_{ML} refers to the mean logarithmic temperature difference, which must take into account the temperature profile along the interior of a tube. This profile varies according to what the fluid is subjected to: constant thermal flow or constant surface temperature. When the second case is considered, an energy balance shows that the temperature inside the tube varies exponentially. The type of flow also interferes with ΔT_{ML}. For the present work, countercurrent exchangers were used, so that Eq. (2) is the appropriate form.

$$\Delta T_{ML} = \left[\left(T_{i,s} - T_{o,t}\right) - \left(T_{o,s} - T_{i,t}\right)\right]/ln\left[\frac{(T_{i,s}-T_{o,t})}{(T_{o,s}-T_{i,t})}\right], \quad (2)$$

where $T_{i,s}$ and $T_{o,s}$ are the inlet and outlet temperatures in the shell, respectively. The inlet and outlet tube temperatures are $T_{i,t}$ e $T_{o,t}$, respectively. The variable F in Eq. (1) refers to the LMTD correction factor, required when there are multiple passes (more than one in the shell and/or in the tube). Its value can be acquired from graphs available in Çengel & Ghajar (2012) or calculated analytically. This factor is function of two ratios of temperatures, R and P. They are calculated by Eq. (3) and Eq. (4) respectively. The factor F was, then, calculated by Eq. (5), according to Selbas *et al.* (2006).

$$R = \frac{T_{i,s}-T_{o,s}}{T_{o,t}-T_{i,t}}, \quad (3)$$

$$P = \frac{T_{o,t}-T_{i,t}}{T_{i,s}-T_{i,t}}, \quad (4)$$

$$F = \frac{\sqrt{R^2+1}}{R-1}.\ln\left\{\frac{\left[\frac{(1-P)}{(1-P.R)}\right]}{ln\left[\frac{\left(2-P.R+1-\sqrt{R^2+1}\right)}{\left(2-P.R+1+\sqrt{R^2+1}\right)}\right]}\right\}. \quad (5)$$

The term U in Eq. (1) is the global heat transfer coefficient, which is calculated as the sum of the inverse of the system's thermal resistances. These are: the internal convection in the tube, the internal fouling, the conduction along the thickness of the tube, the external fouling and external convection (in the shell). Neglecting the heat conduction in the tube's thickness, Eq. (6) was used, encompassing all these terms (Lavine *et al.*, 2014).

$$U = \left[\frac{1}{h_s + R_{f,s} + \left(\frac{d_o}{d_i}\right).\left(\frac{R_{f,t}+1}{h_t}\right)}\right]^{-1}. \quad (6)$$

Where $R_{f,s}$ is the shell's fouling factor (a thermal resistance consequence of material deposition) and $R_{f,t}$ is the tube's. Their values were acquired from Rao & Patel (2010). The inner diameter of the tube is d_i and the outside is d_o. The terms h_s and h_t are the convective heat transfer coefficients on the shell and tube sides, respectively. The coefficient of the tube, for turbulent ($Re > 10{,}000$) and fully developed flow, was calculated by the correlation of Sieder & Tate (1936), represented by Eq. (7). It is written in its dimensionless form, in terms of the average Nusselt number of the tube, that which is calculated by Eq. (8).

$$\overline{Nu_t} = 0.027.Re_t^{0.8}.Pr_t^{1/3}.\left(\frac{\mu_t}{\mu_{wt,t}}\right)^{0.14}, \quad (7)$$

$$\overline{Nu_t} = \frac{h_t.d_i}{k_i}. \quad (8)$$

The average signal will be omitted from the convective coefficient. It can be seen in Eq. (7) that the tube's Nusselt number is a function of the Reynolds number, Eq. (9), and the Prandtl number, Eq. (10), of that side. The first is used for the characterization of the flow between laminar, transition and turbulent. The second is a ratio between the diffusion of moment and heat. This dimensionless parameter also expresses the relation between the velocity and thermal boundary layers' thickness.

$$Re_t = \frac{\rho_t.d_t.v_t}{\mu_t}, \quad (9)$$

$$Pr_t = \frac{\mu_t . c_{p,t}}{k_t}. \quad (10)$$

The Nusselt number of the shell, for segmented baffles and $2{,}000 < Re < 1{,}000{,}000$, was calculated by the correlation presented by Kern (1987), which is Eq. (11). The dimensionless number for this side is expressed as in Eq. (12), from which the convective coefficient is determined. Again, the average signal will be omitted from the convective coefficient.

$$\overline{Nu_s} = 0.36 . Re_s^{0.55} . Pr_s^{1/3} . \left(\frac{\mu_s}{\mu_{wt,s}}\right)^{0.14}, \quad (11)$$

$$\overline{Nu_s} = \frac{h_s . D_e}{k_s}. \quad (12)$$

The shell's Reynolds number is written in terms of the external mass flow ($G = \dot{m}_s / A_s$), as indicated in Eq. (13). The Prandtl number is calculated the same way as previously shown, but naturally using the shell's fluid properties, Eq. (14).

$$Re_s = \frac{G . D_e}{\mu_s} = \frac{\dot{m}_s . D_e}{A_s . \mu_s}, \quad (13)$$

$$Pr_s = \frac{\mu_s . c_{p,s}}{k_s}. \quad (14)$$

The viscosity ratio in Eq. (7) and Eq. (11) serves for processes with large temperature variations where the numerator property is evaluated at the mean temperature of the fluid and the denominator term is evaluated at the wall temperature. Since case 2 has a non-specified fluid (crude oil) and case 3 has very small temperature variation, the ratio of viscosity was neglected. The internal diameter of the tube was calculated by means of Eq. (15), as 80% of the external diameter.

$$d_i = 0.8 . d_o. \quad (15)$$

According to Kern (1987), the calculation of the shell's external hydraulic diameter, D_e, depends on the type of arrangement of the tubes. Of the several forms that this arrangement can be made, the square and triangular ones are emphasized. They can be seen in Fig. (2).

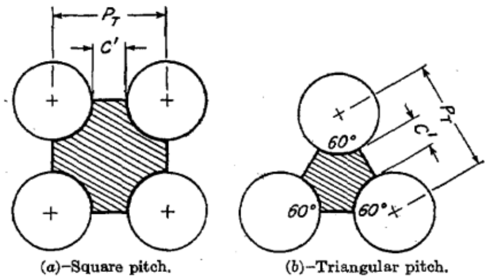

Figure 2 - Tube arrangement or pitch type: square (left) and triangular (right).

The calculation for the square arrangement is described in Eq. (16) and for the triangular in Eq. (17), respectively,

$$D_e = 4 . \left[P_t^{\,2} - \left(\frac{\pi . d_o^{\,2}}{4}\right)\right] / (\pi . d_0), \quad (16)$$

$$D_e = 4 . \left[0.43 . P_t^{\,2} - \left(\frac{0.5 . \pi . d_o^{\,2}}{4}\right)\right] / (0.5 . \pi . d_0). \quad (17)$$

Where P_t is the distance between the center of adjacent tubes (as can be seen in Fig. 2) and d_o is the outside diameter of the tube (in inches). The calculation of P_t and C', from Fig. 2, is done by Eqs. (18) and (19), respectively.

$$P_t = 1.25 . d_o, \quad (18)$$

$$C' = P_t - d_o. \quad (19)$$

The term A_s in Eq. (13) is the flow area, which is given by Eq. (20). Where D_s is the inside diameter of the shell, B is the distance between the baffles, d_o is the outer tube diameter and P_t comes from Eq. (18),

$$A_s = D_s.B.\left[1 - \left(\frac{d_o}{P_t}\right)\right]. \tag{20}$$

The fluids' velocities in the shell and tube are calculated by Eqs. (21) and Eq. (22), respectively, as,

$$v_s = \frac{\dot{m}_s}{A_s.\rho_s}, \tag{21}$$

$$v_t = \frac{\dot{m}_t}{(\pi/4).d_i^2\rho_t}\left(\frac{n}{N_t}\right). \tag{22}$$

Where $\dot{m}_i$ is the mass flow rate of the respective fluid, ρ_i is the specific mass and A_s is the flow area determined by Eq. (20). The variable n in Eq. (22) is the number of passages on the tube side, N_t the total number of tubes and d_i is the internal diameter. The number of tubes of the heat exchanger was calculated by Eq. (23) (Rosenow & Hartnett, 1973) as,

$$N_t = C.\left(\frac{D_s}{d_o}\right)^{n_1}. \tag{23}$$

This variable depends on the internal diameter of the shell, the outer diameter of the tube and the two constants, C and n_1. Their values vary according to the number of tube passes and their pitch. The values assumed for these constants, acquired from Sinnott *et al.* (1996), can be verified in Table 1.

Table 1 - Constants for the number of tubes calculation.

Number of passes	Triangular arrange		Squared Arrange	
	$P_t = 1.25.d_o$		$P_t = 1.25.d_o$	
	C	n_1	C	n_1
1	0.319	2.142	0.215	2.207
2	0.249	2.207	0.156	2.291
4	0.175	2.285	0.158	2.263
6	0.0743	2.499	0.0402	2.617
8	0.0365	2.675	0.0331	2.643

The total cost of the heat exchanger, the objective function, given by Caputo *et al.* (2008), is calculated by,

$$C_{tot} = C_i + C_{oD}. \tag{24}$$

The total cost is the sum of invested capital, C_i, and the discounted operation cost of the equipment, C_{oD}. Taking the correlation provided by Sinnott *et al.* (1996), the cost of investment is calculated to follow as a function of the heat exchange area and three constants.

$$C_i = a_1 + a_2.A^{a_3}, \tag{25}$$

where the constants are $a_1 = 8{,}000$ €, $a_2 = 259.2$ €/m^2 and $a_3 = 0.93$ for a heat exchanger made with stainless steel in both shell and tubes (Rao & Patel, 2010). The discounted operation cost (C_{oD} in €) is determined as,

$$C_{oD} = \sum_{k=1}^{ny} \frac{C_o}{(1+i)^k}. \tag{26}$$

The period of operation is $ny = 10$ years and the discount rate is $i = 0.1$ (10%), the parameter C_o is the annual operating cost, measured in (€/year), calculated by Eq. (27), where P is the pumping power (W), C_e is the energy cost (€/kWh) and H is the number of hours of annual operation. It was considered an energy cost of 0.12 €/kWh and an annual operation time lapse of 7,000 hours (Sinnott *et al*, 1996),

$$C_o = P.C_e.H. \tag{27}$$

The pumping power of the exchanger is calculated by,

$$P = \frac{1}{\eta}.\left(\frac{\dot{m}_t}{\rho_t}.\Delta P_t + \frac{\dot{m}_s}{\rho_s}.\Delta P_s\right). \tag{28}$$

It is related to the pressure losses in the tube and shell, indicated by ΔP_t and ΔP_s, respectively. The term η refers to the efficiency of the pump, which was assumed to be 80% (Segundo *et al.*, 2017). The pressure drop in the tube side was calculated with Eq. (29) (Sinnott *et al*, 1996 and Rao & Patel, 2010). With n being the number of passes of the tube, f_t is the tube's friction factor and p is an empirical constant. Its value was assumed as 2.5 based on Sinnott *et al.* (1996) for cases 1 and 3. For case 2 it was taken as 4 (Kern, 1987),

$$\Delta P_t = \left(\frac{\rho_t . v_t^2}{2}\right) . \left(\frac{L}{d_i} . f_t + p\right) . n. \tag{29}$$

The Darcy friction factor for the tube, f_t, was determined according to Rao & Patel (2010) as,

$$f_t = [1.82(\log_{10} Re_t) - 1.64]^{-2}. \tag{30}$$

This is an empirical correlation dependent on the Reynolds number. As for the shell's pressure loss, the following equation was used,

$$\Delta P_s = f_s . \left(\frac{\rho_s . v_s^2}{2}\right) . \left(\frac{L}{B}\right) . \left(\frac{D_S}{D_e}\right), \tag{31}$$

where f_s is the Darcy friction factor on this side of the exchanger, calculated with,

$$f_s = 2. b_o . {Re_s}^{-0.15}, \tag{32}$$

where the parameter b_o is a constant dependent on the value of the Reynolds number. For $Re_s < 40{,}000$ it assumes the value of 0.72, according to Peters & Timmerhaus (1991). The input parameters of the exchanger and the thermophysical properties of the fluids for cases 1, 2 and 3 can be visualized in Table 2.

Table 2 - Fluid's thermophysical properties and initial parameters for all 3 cases.

Fluid's Properties	Unit	Case 1		Case 2		Case 3	
		Methanol	Brackish Water	Kerosene	Crude Oil	Distillated Water	Raw Water
Location	-	Shell	Tube	Shell	Tube	Shell	Tube
Nº of passes	-	1	2	1	4	1	2
$\dot{m}$	kg/s	27.8	68.9	5.52	18.8	22.07	35.31
T_{in}	ºC	95*	25	199	37.8	33.9	23.9
T_{out}	ºC	40	40	93.3	76.7	29.4	26.7
ρ	kg/m³	750	995	850	995	995	999
c_p	J/kg.K	2,840	4,200	2,470	2,050	4,180	4,180
μ	Pa.s	0.00034	0.0008	0.0004	0.00358	0,0008	0.00092
μ_{wt}**	Pa.s	0.00038	0.00052	-	-	-	-
k	W/m.K	0.19	0.59	0.13	0.13	0.62	0.62
R_f	m².K/W	0.00033	0.00020	0.00061	0.00061	0.00017	0.00017
Tube Arrange	-	Triangular		Square		Triangular	
$\dot{q}$	MW	4.34		1.44		0.46	

*Methanol's inlet pressure is 4 bar, so that its saturation temperature is approximately 103 ºC.
**Values acquired from Segundo *et al.* (2017).

The previous equations for calculating the tube's heat transfer coefficient consider a fully developed flow. Such evaluation (for turbulent flow) in both hydrodynamic and thermal cases can be done by Eq. (33) (Çengel & Ghajar, 2012). The length in which the flow becomes developed is the value of x_{fd},

$$\left(x_{fd,i}\right)_{turb} \approx d_i . 10. \tag{33}$$

For a laminar condition, the fully developed velocity and thermal lengths are determined with Eqs. (34) and (35), respectively, (Çengel & Ghajar, 2012).

$$\left(x_{fd,h}\right)_{lam} \approx d_i . 0.05. Re_t, \tag{34}$$

$$\left(x_{fd,t}\right)_{lam} \approx d_i . 0.05 . Re_t . Pr_t . \quad (35)$$

When the flow is not fully developed in the thermal case (or in both thermal and hydraulic for $Pr_t > 5$), the average Nusselt number for laminar regime (and constant wall temperature) is determined by

$$\overline{Nu_t} = 3.66 + \frac{0.0668 . Gz_t}{1+0.04 . Gz_t^{2/3}}, \quad (36)$$

with Gz being the Graetz Number,

$$Gz_t = \frac{d_i}{L} . Re_t . Pr_t , \quad (37)$$

a dimensionless parameter for the non-developed (entry region) flow.

2.2 Optimization via GWO

The algorithm proposed by Mirjalili *et al.* (2014) is modeled using the hierarchy of gray wolves as its basis. In the mathematical model, the optimization (hunting) process is guided by three main wolves: alpha (α), the solution most suited to the problem, followed by other two possible candidates, beta (β), as the second option, and delta (δ), the third option. There is also the omega (ω) wolves, which represents the rest of the solution candidates, who follow the leading of the first three.

The initial wolf pack is randomly generated, from which the hunt (optimization) begins. While hunting, the gray wolves track (chase), encircle and, finally, attack their prey. At each iteration the search agent positions are updated as they search for the solution. The alpha, beta and delta wolves estimate the actual position of the prey and the other wolves position themselves randomly around it. The functions that reflect the encircling process are the following,

$$\vec{D} = |\vec{C} \cdot \overrightarrow{X_p}(t) - \vec{X}(t)|, \quad (38)$$

$$\vec{X}(t+1) = \overrightarrow{X_p}(t) - \vec{A} \cdot \vec{D}, \quad (39)$$

where t corresponds to the current iteration, $\vec{A}$ and $\vec{C}$ are specific coefficients vectors, $\vec{X}$ is the position of the wolf and $\overrightarrow{X_p}$ is the position of the prey. Vector $\vec{A}$ is determined by

$$\vec{A} = 2\vec{a} \cdot \vec{r_1} - \vec{a} \quad (40)$$

This vector is responsible for making the search agent attack the best solution, which occurs when the value of $\vec{a}$ decreases. Its value varies between 2 and 0 and has a linear decrease. When the value of $|\vec{A}|$ is less than 1, the search agent attacks the prey. Otherwise, it is forced to seek a more refined solution and withdraw from the current prey. The parameter $\vec{r_1}$ is a random vector, whose value ranges between [0,1]. The vector $\vec{C}$ is calculated by,

$$\vec{C} = 2 \cdot \vec{r_2}. \quad (41)$$

This variable helps the method to create a more random behavior for the optimization, in order to favor exploration and avoid local optimums. It can be considered a vector that creates the effects of obstacles that occur while the wolves are hunting in the wild. Unlike vector $\vec{A}$, it does not decrease linearly, always having random values (between the interval [0, 2]) both at the beginning and at the end of the iterations, to emphasize the exploration during the whole search. The parameter $\vec{r_2}$ is also a random vector between 0 and 1.

In addition to the classic GWO, some variations were inserted into the code to check for possible improvements in the overall solution. The variables r_1 and r_2 were varied according to the exponential, Gaussian and beta functions, respectively,

$$r_i = 1/[1 + exp(-iter/maxiter)] \quad (42)$$
$$r_i = 0.5 + 0.5 * randn \quad (43)$$
$$r_1 = betarnd(0.1 * rand, rand) \quad (44)$$
$$r_2 = betarnd(rand, 0.1 * rand) \quad (45)$$

Where *iter* is current iteration number from the iterative process and *maxiter* was used as 5,000 in this study. A total of 30 runs were performed. In the previous equations, "rand" and "randn" differs from each other within Matlab's functions. The first grants uniformly distributed random numbers and the latter grants normally distributed random numbers. The optimized design variables are presented in Table 3, as in accordance to the TEMA standard (Tubular Exchanger Manufactures Association)

Table 3 - Variable's Constraints.

Variable	Range	Unit
D_s (Shell's internal diameter)	$0.1 \leq D_s \leq 1.5$	m
d_o (Tube's outer diameter)	$0.015 \leq d_o \leq 0.051$	m
B (Baffle spacing)	$0.05 \leq B \leq 0.50$	m

2.3 Chemcad Simulation

After the mathematical modelling and optimization via GWO, the case study 3 was simulated in the software Chemcad®. The objective of the simulation was to define the remaining design variables of the exchanger (baffle type, nozzle dimensions, type of head, shell thickness), by the insertion of the cases' input parameters and GWO's results in the program. As the mathematical modelling was performed assuming ideal behavior of the species the same option was selected in the initialization of the simulation. In the software, the ideal consideration of the fluids is accounted by choosing the Raoult's Law (Ideal) Thermodynamic Model. Figure 3 shows the equipment scheme window.

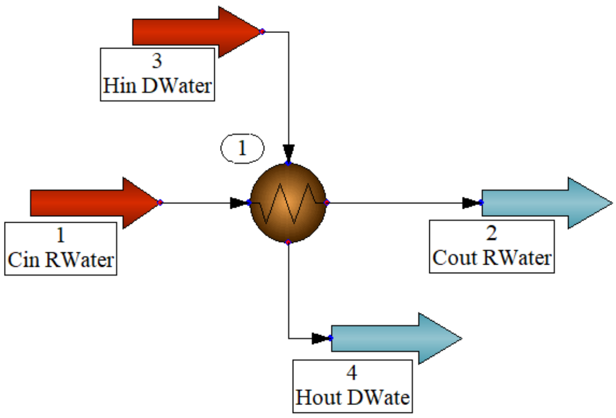

Figure 3 - Chemcad® equipment window.

In Chemcad®, there are two ways to simulate a heat exchanger: rating or design. In the first, the user must input several dimensions and values, and the program calculates the resulting exchanger, no matter how high the pressure losses are or if any dimension extrapolates the TEMA rules for design. In the latter, the program requires the user to specify upper and lower limits of some variables and will try to converge using the granted range. The design mode will only grant the sizing and coefficient's values once convergence has been achieved.

Since three physical dimensions of the program were already optimized by the GWO, and the objective of the simulation is to continue the sizing (and eventually compare any differences), only the rating mode was required. The values of number of tubes, arrange, diameters and spacing were all taken from the input parameters and modelling results and inserted in Chemcad®.

The program initialization requires the selection of the Thermodynamic Model that will calculate the various parameters from the present species. Since the streams' temperatures and pressures are moderate, the consideration of ideal behavior is safe, with little sacrifice of precision (Van Ness, 2007). Thus, the selected model was the "Ideal Vapor Pressure (Raoult's Law)". Great divergence in the behavior of solution or gas phase is seen in more extreme systems, with temperatures close to the critical (or above) ones and either vacuum or high-pressure conditions.

Then, once all the physical parameters, fluid's conditions and modelling settings (such as the used correlations and the thermodynamic model) were defined, the program was set to run. The TEMA sheet was generated, along with the individual results for shell, tube, baffles and nozzles' dimensions.

3. RESULTS AND DISCUSSION

In regards to the variations inserted to the GWO's Matlab® code, the exponential and beta functions for variables r_1 and r_2 promoted changes on the physical variables (and they were very subtle). The Gaussian function granted the same values that the classic GWO. As the different physical parameters resulted in a higher cost for the exchangers, which is not desired, it is believed, therefore, that the global optimum has already been found by the classic code. For that reason, the results of the altered GWO are omitted from this section. Classic GWO, Exponential and Gaussian functions took no more than 4 minutes to complete the 30 runs. Beta function took approximately 1 hour and 20 minutes.

The obtained results were compared with the values from Sinnott *et al.* (1996) and Kern (1987), the original designs. The results for the optimization of the three cases are presented in Table 4.

Table 4 - Results for GWO optimization (all 3 cases).

Parameters	Case 1		Case 2		Case 3	
	Sinnot *et al.* (1996)	GWO	Kern (1987)	GWO	Sinnot *et al.* (1996)	GWO
D_S (m)	0.894	0.775	0.539	1.2847	0.387	0.541
B (m)	0.356	0.434	0.127	0.05	0.305	0.500
d_o (m)	0.020	0.0150	0.025	0.0150	0.013	0.0150
d_i (m)	0.016	0.0120	0.020	0.012	0.0104	0.0120
L (m)	4.830	3.327	4.88	1.412	4.88	2.148
$x_{fd,h}$ (m)	-	0.120	-	0.357	-	0.120
$x_{fd,t}$ (m)	-	0.120	-	20.207	-	0.120
N_t	918	1,502	158	2,080	160	680
A_{ht} (m²)	278.6	235.393	61.5	248.55	46.6	68.837
v_t (m/s)	0.75	0.815	1.44	0.179	1.76	0.919
Re_t	14,925	12,169.1	8,227	596.564	36,400	11,948.823
Pr_t	5.7	5.695	55.2	56.454	6.2	6.203
h_t (W/m² K)	3,812	4,642.5	619	115.327	6,558	4,665.03
f_t	0.028	0.0298	0.033	0.0859	0.023	0.0299
ΔP_t (Pa)	6,251	7,115.4	49,249	898.204	62,812	6,630.3
v_s (m/s)	0.58	0.551	0.47	0.505	0.94	0.409
Re_s	18,381	12,975.2	25,281	15,942.5	16,200	5,443.945
Pr_s	5.1	5.082	7.5	7.60	5.4	5.3935
D_e (m)	0.014	0.0107	0.025	0.0148	0.013	0.0107
h_s (W/m² K)	1,573	1,972.7	920	1,191.278	5,735	4,135.484
f_s	0.33	0.3479	0.315	0.343	0.337	0.396
ΔP_s (Pa)	35,789	15,833.4	24,909	69,224.648	67,684	7,213.6
U (W/m² K)	615	737.372	317	76.9307	1,471.0	1,120.749
C_i (€)	51,507	49,630.8	19,007	51,789.6	16,549	21,268.1
C_o (€/yr)	2,111	1,010.3	1,304	506.2	4,466	380.5
C_{od} (€)	12,973	6,208.1	8,012	3,110.1	27,440	2,337.8
C_{tot} (€)	64,480	55,838.0	27,020	54,899.7	43,989	23,605.9

In regards to the simulation in Chemcad®, only case 3 was simulated, as it has granted the best cost reduction and there is great similarity between the software's thermophysical properties data base and the admitted values for the mathematical modelling. For case 1, methanol's thermophysical properties diverge considerably and case 2 fluids are not within the Chemcad's data base.

3.1 Methanol and Brackish Water (GWO Optimization)

In the first case, an exchanger with two passages in the tube and one in the shell was used, with a triangular tube pitch. The results showed a significant increase in the number of tubes and decrease in all diameters (internal and external from both shell and tube). This provided a reduction of 15.6% in the heat transfer area and slightly increased the velocity of the fluid inside the tube. As the Reynolds number is a function of both velocity and internal diameter, it suffers both reduction (from d_i) and raise (from v_t), resulting in its decrease. However, as the convective coefficient itself is function of Nu_t and d_i, and both decrease, the global effect is its increase in approximately 22%.

Increasing the baffle spacing generates less turbulence (lower Reynolds), increase the shell's flow area and consequently decreases the velocity of the fluid therein. This effect alone would lower the shell's convective coefficient. However, as the hydraulic diameter (D_e) drops, the global effect on h_s is an enhancement of 25%. The pressure drop in both shell and tube has decreased, with emphasis on the shell's, whose reduction was that of 55.8%. That was a result of the combined effects of higher baffle spacing, smaller shell diameter and lower velocity for methanol.

GWO was able to reduce the total cost by 13.4% in comparison with the literature's design. Figure 4 compares the results for the 4 calculated costs.

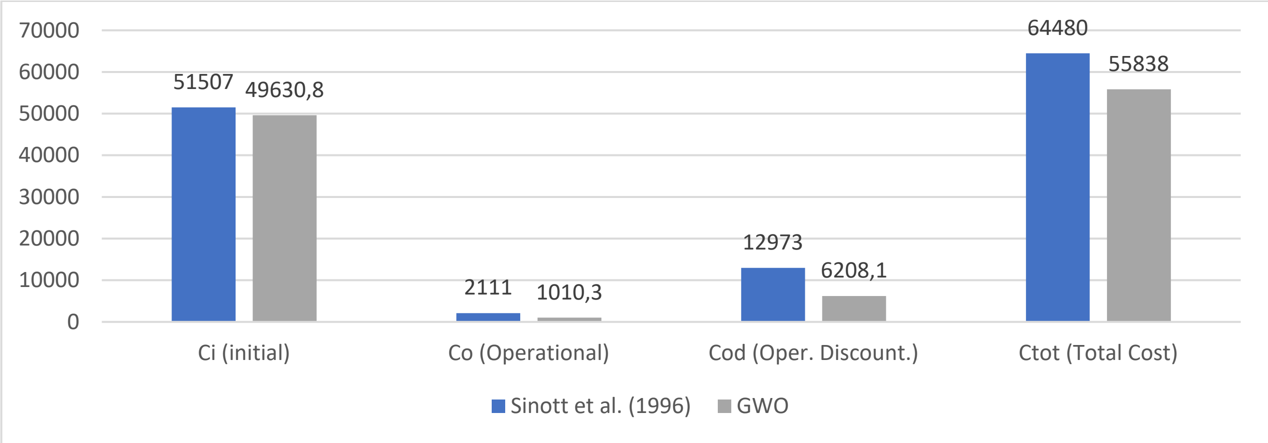

Figure 4 - Costs comparison for the shell-and-tube exchanger – case 1.

3.2 Kerosene and crude oil (GWO Optimization)

As it is shown in Table 4, the fully developed length for velocity and thermal conditions are 0.357 m and 20.207 m, respectively. As the exchanger's length is 1.412 m, the present equipment has the "combined entry length problem". This means that both velocity and temperature profiles develop simultaneously in a far part of the tube, and are not readily developed in the beginning, as it happens in "fully developed" flows. This complicates the determination of the convective coefficient, as it ceases to be independent of the position. The resolution of these cases requires the use of a different dimensionless parameter called the Graetz number, Eq. (35), and the Nusselt correlations become substantially more complicated, as Eq. (34). Also, the tube's Reynolds number reduces so much that it goes from transition to laminar condition (Re < 2,300), meaning that its convective coefficient is vastly overestimated when turbulent-flow expressions are used.

As the Graetz Number (required for h_t) is dependent on the exchanger's length, that which is calculated after the knowledge of the global coefficient in the modelling, an iterative process is required, where Gz, Nu_t, h_t, U, A_{ht} and L are continuously calculated. They all converge on the values shown in Table 4.

The second case counts with an exchanger with four passages in the tube and one in the shell, with a square tube pitch. The number of tubes increased by approximately 13 times, while their diameters decreased. Although the latter effect rises the fluid's speed, Eq. (22) shows that N_t is inversely proportional to v_t. Ultimately, the crude oil's velocity diminishes by almost 10 times. That, along with the fact that the flow regime is laminar instead of transition, results in a way lower value for the tube's convective coefficient. It can be seen by Eq. (20) that the effect of the smaller baffle spacing is a lower flow area for kerosene, which ultimately increase its velocity. The reduction in the hydraulic diameter grants a lower Reynolds number, which also lowers the Nusselt number. However, as D_e also interferes directly with h_s, the global effect is an increase by 29.5%.

The comparison of the process' costs can be observed in Fig. (5).

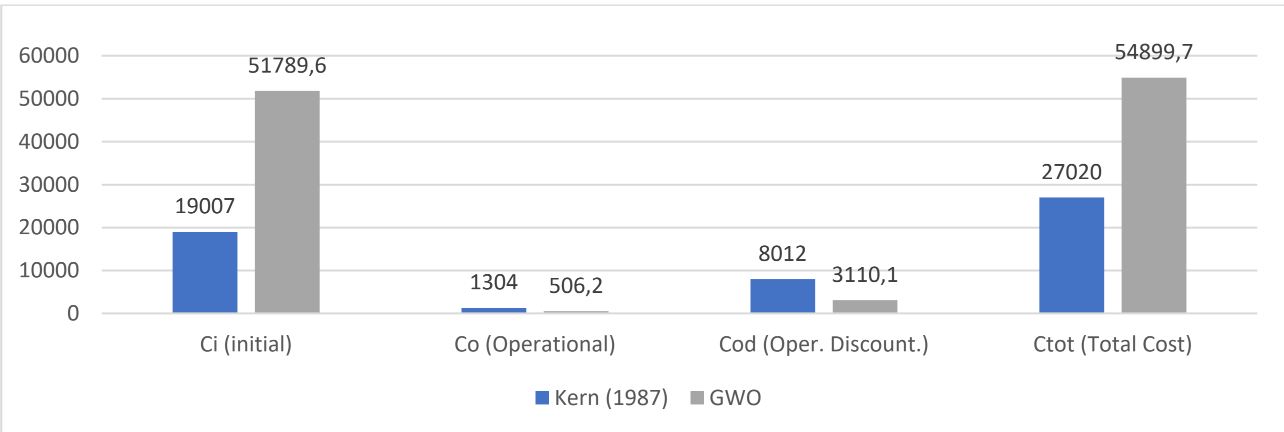

Figure 5 – Costs comparison for the shell-and-tube exchanger – case 2.

The pressure loss on the tube side is immensely reduced (around 50 times) as the crude oil's velocity and the tube's length are vastly diminished. On the other hand, the shell's pressure drop is increased by a series of combined effects (D_s, v_s, f_s, D_e and B). The final effect is an increase of ΔP_s by approximately 2.8 times. As for the GWO optimization, the initial and total costs ended up surpassing the literature. Even with the lower values for the operational and discounted operational costs, the total expense with the equipment heightened considerably. That was expected, seeing how much the heat transfer area increased. As the laminar condition is less effective in transferring heat (in comparison to turbulent flow), in order to grant the same service (same heat transfer rate and temperature difference), the exchanger requires more area, as the global coefficient U (which has greatly decreased) is inversely proportional to the heat transfer area A_{ht}, as can be seen in Eq. (1).

3.3 Water-water

3.3.1 GWO Optimization

Case study 3 is an exchanger with two passes on the tubes (triangular pitch) and one pass on the shell. The large increase in the number of tubes and the slight increase of the internal diameter (which is squared in Eq. (22)) of the tube, together, provided a severe reduction in the tube's fluid velocity. Consequently, there was a reduction of approximately 28.9% on the tube's convective coefficient.

As the shell's internal diameter and baffle spacing both increased considerably, the flow area increased and the velocity reduced around 56.5%. Not only that, but the hydraulic diameter also decreased considerably, making it so that the convective coefficient of the shell diminished. The result was a smaller value for U.

In terms of pressure drop, the exchanger had excellent results, as both shell and tube's values decreased by almost 10 times. With higher baffle spacing and lower length and velocity, ΔP_s ended up 89.3% smaller. Similarly, as the length of the equipment has significantly decreased, so has the raw water's velocity, resulting in a reduction of 89.4% for ΔP_t.

As the total heat transfer rate is constant and previously defined, the reduction of the overall transfer coefficient and, because it is the case with the lowest value for the ΔT_{ML} (6.312 ºC), the thermal exchange area (A_{ht}), by Eq. (1), has undergone a considerable increase. This justifies a higher initial cost of capital (C_i). The annual cost, C_0, however, reduced so much (91.5%) that it has provided a large reduction in the total cost of the equipment. Among the three cases, this was the one that obtained the better results, with a reduction of almost 47% in relation to the original design.

It should be noted that the shell's Reynolds number decreased so much that the flow regime changed from turbulent to transition (value bellow 10,000). Lavine *et al.* (2014) comments that when turbulent correlations are used for a transition region, the resulting convective coefficient is overpredicted. Specific correlations for that flow should be applied for more precise results. A discussion of the transition region is available in Ghajar and Tam (1994). The comparison of the results of the investment, operational and total costs can be observed in Fig. (6).

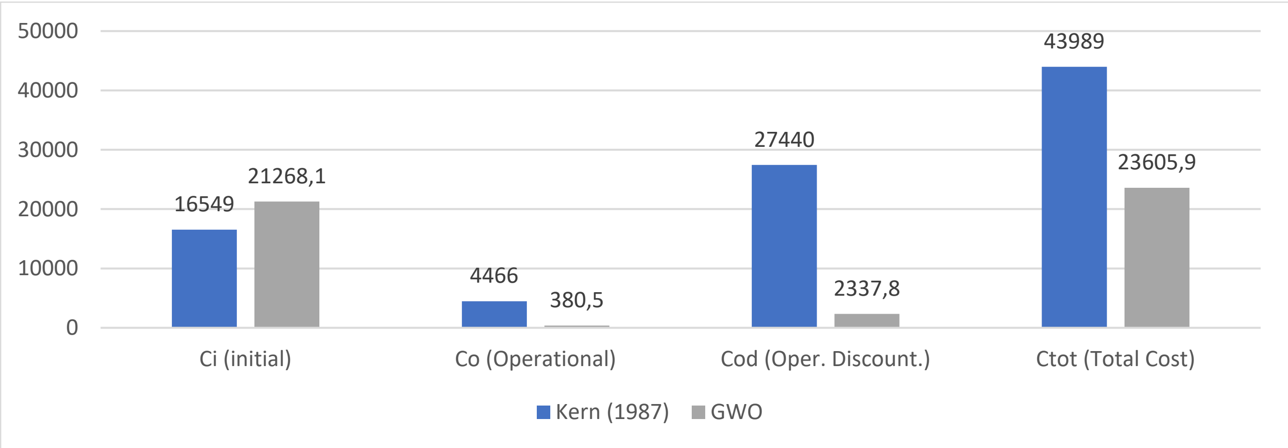

Figure 6 - Costs comparison for the shell-and-tube exchanger – case 3.

3.4 Chemcad Simulation

The simulation in the exchanger was performed successfully, with a small divergence in the mass flow rate of the distilled water stream (21.982 kg/s). This divergence was a consequence of the software using slightly different values for the transport properties. The "rating mode" was applied to the equipment in order to define the remaining physical parameters (not calculated by the GWO) and compare some of the thermal and hydraulic variables. These results are shown in Tables 5 and 6, respectively.

Table 5 - Case 3 Exchanger's Simulation Results (physical and operational parameters).

Tubes		Shell		Other Specifications	
Variable	Value	Variable	Value	Variable	Value
Int. Diam. (m)	0.0117	Internal Diam.	0.54	Nozzle Diam. (m) (tube/shell)	0.154
Ext. Diam. (m)	0.015	External Diam.	0.57		
BWG	16	Front Head	A	N. of Baffles	3
Thickness (m)	0.0015	Shell	E	Baffle Type	Single-Segm.
Pitch (m)	0.01875	End Head	S	Baffle Cut (%)	25
Material	Stainless Steel	Material	Stainless Steel	Baffle Center-Center Spacing (m)	0.5
Pressure (bar)	1.4	Pressure (bar)	1.4		

Table 6 - Case 3 Exchanger's Simulation Results (thermal and hydraulic parameters).

Tube		Shell		General	
Variable	Value	Variable	Value	Variable	Value
h_t (W/m² K)	4,462.08	h_s (W/m² K)	4,126.86	U_{dirty}	1,067
Re_t	12,012	Re_s	5,461	U_{clean}	1,802.8
ΔP_t (Pa)	8,400	ΔP_s (Pa)	2,000	A_{ht} (m²)	68.8
v_t (m/s)	0.92	v_s (m/s)	0.41	$\dot{q}$ (MW)	0.4143

The type of exchanger was chosen as AES because of the need to access the exterior of the pipes for cleaning and maintenance. Continuous operation of the exchanger (even with distilled water on the shell) causes continuous deposition of salts, which increases the fouling resistance and reduces the efficiency of the exchanger. The considerable elevated difference between the overall heat transfer coefficients of clean and dirty service (Table 6) makes it clear that deposition impairs the operation of the equipment.

The software allowed the exchanger's calculation but issued an alert for the number of tubes (680) inserted. The respective shell diameter, arrangement and tube pitch comprises, according to the calculation carried out by the program, 642 tubes. There is a considerable amount in excess from that determined by Eq. (23). It is necessary to evaluate if this quantity of tubes effectively fits inside the respective shell and also allows the good flow of the fluid. This is something that is difficult to predict by the optimization program and it becomes necessary to evaluate for the case of adaptation in a real exchanger.

The maximum limit for the number of baffles was 3 because larger quantities would result in a spacing between them smaller than the diameter of the nozzles, which is not possible, since the baffle would be in the same position as the inlet nozzle. Therefore, three were used, with fixed center-center spacing of 0.5 m. The "single-segmented" type was provided by the program as the default. The 25% baffle cut was chosen based on Kern (1987).

The calculation of the convective coefficients by the software can be done by different correlations that are available in its database. The value presented in Table 6 is the result of applying the Dittus-Boelter correlation, which is similar to Sieder and Tate's correlation (used in the modeling). When tested for the Sieder and Tate correlation, Chemcad's value was 5,269.45 W/m².K, which is surprisingly higher than what calculated by the code. In section 2 it was commented that the ratio of viscosities in Eq (7) was neglected for case 3 as the temperature difference is so small that the ratio itself would be practically equal as unity. As the Reynolds, Prandtl and thermal conductivity from Chemcad and Matlab are of very similar values, the only difference would come from the viscosity ratio in the simulation.

For the shell's coefficient, the method of Kern (1987) was chosen, whose resulting value was 4,126.99 W/m².K, which is almost exactly the same as calculated. The Reynolds number was also very close, showing great agreement in the parameters defined in the simulation and in the considerations and correlations used in the mathematical modeling.

Chemcad's pressure loss of the tube side presented better agreement with the modeling's value. Both fluid's velocities in the simulation were equal as the ones from the code. Therefore, with the thermal and hydraulic parameters reaching a sufficient degree of similarity correlations, some remaining dimensions of the equipment were defined, in order to complete the heat exchanger's dimensioning.

4. CONCLUSIONS

The present work had as objective the modeling, optimization and simulation of a countercurrent shell and tube heat exchanger applied to three distinct cases, varying, among them, fluids, operating conditions and transfer rates. The aim was to reduce the cost by optimizing three design variables: the internal diameter of the shell, the tube's external diameter and the spacing between the baffles. The method of optimization applied was the Gray Wolf Optimizer (GWO), the Gray Wolf method. Posterior simulation of case 3 in software Chemcad® was performed for comparison and analysis.

The results obtained by the classical GWO were mostly better than the compared literature, with a reduction in total cost by 13.4% for the first case, 46.34% for the third case and a considerable increase in cost for the second case. The results of the modified GWO were identical to those of the classical method, with the exception of exponential function. Having generated worse results for the cost, there are strong indications that the classical GWO has achieved the overall optimum by itself. Optimizations aimed at reducing costs have generated a great interest for the industry, because with the correct design the effectiveness of the exchanger is slightly (or none) affected and large cost reductions are possible, depending on the case. It was possible to observe during the study that the GWO has guaranteed convergence, presenting very satisfactory results. The method has low complexity, with few parameters and is easy to implement.

The simulation of case 3 in Chemcad® was successfully performed, showing good agreement with the calculated values in the Matlab® code of the modelling. As not all the exchanger's dimensions were calculated, the simulation aimed determining the remaining physical parameters, as the nozzles, baffle specifications, exchanger type and shell and tube's thickness. The equipment was fully designed and selected as AES type.

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