encit 2020

ABCM
Associação Brasileira de Engenharia e Ciências Mecânicas

18th Brazilian Congress of Thermal Sciences and Engineering
November 16–20, 2020 (Online)

ENC-2020-0449
Case study of the metamodels of a shell-and-tube heat exchanger

Wagner Henrique Saldanha
Felipe Raul Ponce Arrieta
Pontifícia Universidade Católica de Minas Gerais - PUC-MG, Department of Mechanical Engineering
wagnerh.saldanha@yahoo.com.br; felipe.ponce@pucminas.br

Gustavo Luís Soares
Pontifícia Universidade Católica de Minas Gerais - PUC-MG, Department of Electrical Engineering
gsoares@pucminas.br

Abstract. *This paper is aimed at a case study in which a shell-and-tube heat exchanger (STHE) metamodel is developed from its analytical functions. The techniques for generating the STHE metamodel were Multivariate Adaptive Regression Splines (MARS) and the Multilayer Perceptrons (MLP) neural network, being implemented in the toolbox MATLAB ARESLab and nnstart, respectively. The results obtained by the two techniques had suitable Mean Square Error (MSE), thus, it is concluded that these techniques can be used for the development of the STHE metamodel, and should continue to be explored in other engineering problems.*

Keywords: *Metamodel, Shell-and-tube heat exchanger, Multivariate Adaptive Regression Spline, Neural network*

1. INTRODUCTION

Heat exchangers are used to conserving and utilizing thermal energy. Heat exchanger equipment is tailor-made for process industry applications according to specified characteristics, such as the inlet and outlet temperatures of fluids, flow rates, and heat duty. Examples of such equipment include shell-and-tube heat exchangers (STHEs) and plate heat exchangers. Usually, the mathematical model of a heat exchanger may be analytical with empirical or semi-empirical relationships, or numerical.

It is known that one of the problems in engineering is the approximation of functions, given only their values for a dependent set of points in the variable space. According to Friedman (1991), research in this area occurs in applied mathematics, statistics, and computer science, in the respective fields of multivariate approximation function, multiple nonparametric regression, and neural networks. Still according to Friedman (1991) the objective is to model the response of a value $\mathbf{y}$ for variables $x_1, ..., x_n$, for data $\{y_n i, x_{1i}, ..., x_{ni}\}_1^N$, where N is the number of samples. So the data generate the following system:

$$\mathbf{y} = \mathbf{f}(x_1, ..., x_n) + \epsilon \tag{1}$$

where ϵ is a stochastic value or also called a value attributed to the error generated in the model.

Data is used to build functions $\widehat{\mathbf{f}}(x_1, ..., x_n)$ that serve as a reasonable approximation of $\mathbf{f}(x_1, ..., x_n)$. The symbol $\widehat{\mathbf{f}}$ represents a metamodel. According to Pina (2010) metamodels are used to: assist in the calculating sensitivity of simulation models, replacing simulations that require a lot of computational resources, improve the performance of iterative optimization algorithms keeping the computational cost fixed. Some of the main metamodeling techniques are Response Surface, Taguchi models, Kriging, Multivariate Adaptive Regression Spline (MARS), and Artificial Neural Networks.

Zhang and Goh (2016) used Multivariate Adaptive Regression Spline (MARS) and Artificial Neural Networks for assessing pile drivability in relation to the prediction of the Maximum compressive stresses (MCS), Maximum tensile stresses (MTS), and Blow per foot (BPF).

Crino and Brown (2007) presented a procedure for approximating the global optimum in structural design by combining multivariate adaptive regression splines (MARS) with a response surface methodology (RSM). The MARS function approximation results was compared to Neural Networks.

Krzywanski (2019) developed a neural network and validated against the desired data on a large falling film evaporator. The authors considered this approach to be a complementary technique to the heat exchanger design procedures. Becoming an alternative to existing approaches such as analytical and numerical methods.

Friedman (1991) used the MARS technique to perform function simulations. Yang and Tseng (1996) applied the single-layer orthogonal neural network developed to approximate functions. Frisso *et al.* (2011) also performed the meta-modeling of deterministic functions, however, using the Response Surface technique.

Thus, motivated by the works listed in the paragraphs above, the main contribution of this work is to apply Multivariate Adaptive Regression Splines (MARS) (Friedman, 1991) and the Multilayer Perceptrons (MLP) neural network (Haykin, 2007) to generate metamodels of the shell-and tube-heat exchangers (STHE) from its analytical model. The goal is to generate a supplementary approach to the problem of design and optimization of this equipment.

2. ANALYTICAL MODEL STHE

This section presents the analytical model used to calculate the heat exchange area A and pumping power $P_{s,t}$ of an STHE with the geometry shown in Fig. 1 (Saldanha *et al.*, 2020):

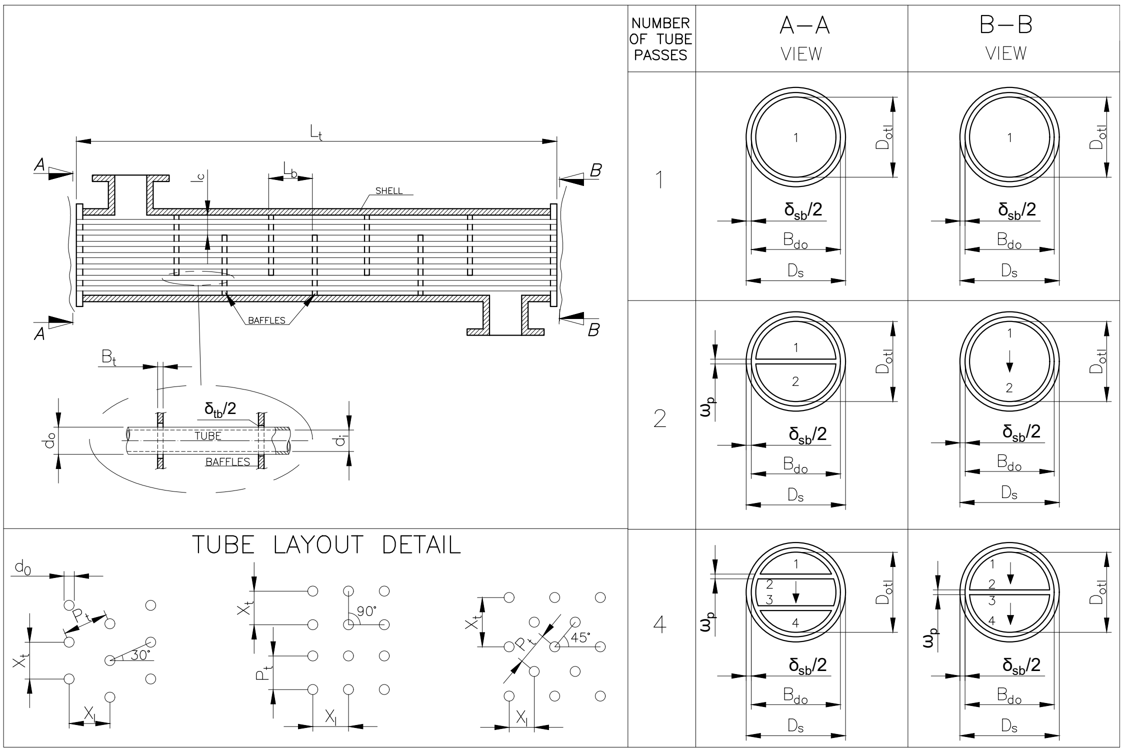


Figure 1: Shell-and-tube heat exchanger

The equations for the geometric characteristics of the STHE (Shah and Sekulic, 2003; Kakac and Liu, 2012) are:

$$P_t = 1.25 \times d_o \ , \tag{2}$$

where P_t is the tube pitch.

For tube layout (ap) triangular 30^o,

$$X_t = P_t \ , \tag{3}$$

$$X_l = \sqrt{\frac{3}{2}} \times P_t . \tag{4}$$

For tube layout (ap) square 45^o,

$$X_t = \sqrt{2} \times P_t \ , \tag{5}$$

$$X_l = \frac{P_t}{\sqrt{2}} . \tag{6}$$

For tube layout (ap) square 90^o,

$$X_t = P_t \ , \tag{7}$$

$$X_l = P_t \ , \tag{8}$$

where X_t is the transverse pitch of the tube and X_l is the longitudinal pitch of the tube.

The inner diameter of each tube is:

$$d_i = d_o - 2 \times esp \ , \tag{9}$$

where esp is the thickness of each tube. Tab. 1 shows the tube thickness values in relation to the outer diameter of the tubes used in this study. The minimum thickness of the tubes is calculated as a function of pressure, and in this case, the lowest allowed thickness value according to (TEMA, 2007) is applied.

Table 1: Outer diameter and thickness of the STHE tubes

Symbol	Values	Symbol	Values
d_o	0.015875 m	esp	1.2446×10^{-3} m
	0.019050 m		1.6510×10^{-3} m
	0.025400 m		2.1082×10^{-3} m
	0.031750 m		2.1082×10^{-3} m
	0.038100 m		2.1082×10^{-3} m
	0.050800 m		2.1082×10^{-3} m

The number of dividing lanes N_p in this work is 0, 1, and 2, for the number of tubes passes n_p equal to 1, 2, and 4, respectively, as done in (Fettaka *et al.*, 2013; Saldanha *et al.*, 2017).

The number of STHE tubes is:

$$N_t = \frac{A_D}{\pi \times d_o \times L_t} \ , \tag{10}$$

where L_t is the tube length, and A_D is the design heat exchanger area. It is considered a percentage for A_D above the required heat exchange area A, which is known as *overdesign* (Mukherjee, 2008).

The outer diameter of tube bundle (Towler and Sinnott, 2008; Thakore and Bhatt, 2007) is:

$$D_{otl} = d_o \times \left(\frac{N_t}{K_1}\right)^{\frac{1}{n_1}} \ , \tag{11}$$

and the parameters K_1 and n_1 are obtained in (Towler and Sinnott, 2008), considering $P_t = 1.25 \times d_o$.

The outer diameter of the baffle is:

$$B_{do} = \frac{D_{otl}}{0.95} \ . \tag{12}$$

The diameter of the shell (Fettaka *et al.*, 2013) is:

$$D_s = B_{do} + \delta_{sb} \ . \tag{13}$$

where δ_{sb} is clearance between the shell and the baffle. The Tab. 2 shows the values of δ_{sb} in relation to the outer diameter of the baffle B_{do}.

The specified diameter of the circle through the centres of the outermost tubes D_{ctl} (Shah and Sekulic, 2003) is:

$$D_{ctl} = D_{otl} - d_o \ . \tag{14}$$

Table 2: Values of the clearances between the baffles and the shell

B_{do} (m)	δ_{sb} (mm)
$0 \leq B_{do} < 0.4522$	3.2
$0.4522 \leq B_{do} < 1.0096$	4.8
$1.0096 \leq B_{do} < 1.3891$	6.4
$1.3891 \leq B_{do} < 1.7685$	7.9
$1.7685 \leq B_{do} < 2.1479$	9.5
$B_{do} \geq 2.1479$	11.1

The assumed thickness for the pass partition plate w_p is shown in Tab. 3.

Table 3: Pass partition plate thickness

D_s (m)	w_p (mm)
$0 \leq D_s < 0.61$	9.5
$0.61 \leq D_s < 1.549$	12.7
$D_s \geq 1.549$	15.9

The cut size of the baffles is:

$$l_c = D_s \times bc \,. \tag{15}$$

where bc is the baffle cut. In this study, the baffle cut was equal to 25%.

According to TEMA (2007), the tube-to-baffle diametrical clearance δ_{tb} was 0.3 mm.

The required heat exchange area A (Shah and Sekulic, 2003) for STHE is:

$$A = \frac{Q}{U \times \Delta T_{lm} \times F} \,. \tag{16}$$

The heat duty Q is:

$$Q = \dot{m}_h \times c_{p,h} \times (T_{h,i} - T_{h,o}) = \dot{m}_c \times c_{p,c} \times (T_{c,o} - T_{c,i}) \,, \tag{17}$$

where $c_{p,h}$ is the specific heat at constant pressure of the fluid that flows on the hot side; $c_{p,c}$ is the specific heat at constant pressure of the fluid that flows on the cold side, $T_{h,i}$ is the inlet temperature of the hot side's fluid; $T_{h,o}$ is the outlet temperature of the hot side's fluid; $T_{c,i}$ is the inlet temperature of the cold side's fluid; $T_{c,o}$ o is the outlet temperature of the cold side's fluid; and $\dot{m}_h$ is the mass flow rate of the hot side. For the case study, the mass flow rate and specific heat of the hot side will be the same as of those of the shell ($\dot{m}_h = \dot{m}_s$, $c_{p,h} = c_{p,s}$). As $\dot{m}_c$ is the mass flow on the cold side, the cooling flow occurs in the tubes ($\dot{m}_c = \dot{m}_t$, $c_{p,c} = c_{p,t}$).

Thus, the mass flow rate of the fluid that circulates in the tubes can be calculated similarly to the way discussed in (Kakac and Liu, 2012; Thakore and Bhatt, 2007; Serth and Lestina, 2014):

$$\dot{m}_t = \frac{Q}{c_{p,t} \times (T_{c,o} - T_{c,i})} \,. \tag{18}$$

The logarithmic mean temperature difference ΔT_{lm} is:

$$\Delta T_{lm} = \frac{(T_{h,i} - T_{c,o}) - (T_{h,o} - T_{c,i})}{ln\left(\frac{T_{h,i} - T_{c,o}}{T_{h,o} - T_{c,i}}\right)} \,. \tag{19}$$

The factor correction F is:

$$F = \frac{\sqrt{(R^2+1)} \times ln\left(\frac{1-SS}{1-R \times SS}\right)}{(R-1) \times ln\left[\frac{2-SS\times\left(R+1-\sqrt{(R^2+1)}\right)}{2-SS\times\left(R+1+\sqrt{(R^2+1)}\right)}\right]} . \tag{20}$$

The parameter equation correction factors R and SS are:

$$R = \frac{T_{h,i} - T_{h,o}}{T_{c,o} - T_{c,i}} \,, \tag{21}$$

$$SS = \frac{T_{c,o} - T_{c,i}}{T_{h,i} - T_{c,i}}. \tag{22}$$

If the number of tube passes is equal to 1, the correction Factor F is also 1.
The overall coefficient of heat transfer U is:

$$U = \frac{1}{\left(\frac{1}{h_o} + R_s + \frac{d_o \times ln\left(\frac{d_o}{d_i}\right)}{2 \times K_w} + \left(R_t \times \frac{d_o}{d_i}\right) + \frac{d_o}{h_i \times d_i}\right)} \,, \tag{23}$$

where h_o is the heat transfer coefficient of the fluid that flows in the shell, h_i is the heat transfer coefficient of the fluid that flows in the tubes, R_s is the fouling factor of the shell, R_t is the fouling factor of the tube, and K_w is the thermal conductivity of the tube wall.

As presented in (Shah and Sekulic, 2003; Kakac and Liu, 2012) the shell heat transfer coefficient h_o obtained by the Bell Delaware method is:

$$h_o = h_{id} \times J_c \times J_l \times J_b \times J_s \times J_r \,, \tag{24}$$

where h_{id} is the ideal heat transfer coefficient of the fluid that flows on the shell side; J_c is the correction factor for the baffle cut and spacing, J_l is the correction factor for tube-to-baffle and baffle-to-shell leakage, J_b is correction factor for bundle and pass partition bypass stream, J_s is the correction factor for large baffle spacing at the inlet and outlet sections compared to the central baffle spacing and J_r is the correction factor for adverse temperature gradient build-up in laminar flows.

The heat transfer coefficient inside the tubes according to Shah and Sekulic (2003) is:

$$h_i = \frac{Nu_t \times k_t}{d_i} \,, \tag{25}$$

where k_t is the thermal conductivity of the fluid that flows into tubes, and Nu_t is the Nusselt number for the flow inside the tubes. The Petukhov – Popov correlation was applied to turbulent flow, and the Taborek correlation was applied to transition flow; they are presented in (Shah and Sekulic, 2003).

According to Shah and Sekulic (2003), for laminar flow ($Re_t \leq 2100$), the Nusselt number for the flow inside the tubes is:

$$Nu_t = 4.364 \,. \tag{26}$$

The nomenclature $Nu_{t,laminar}$ is adopted when this correlation is employed in Eq. 28.

According to Shah and Sekulic (2003), if $4000 \leq Re_t \leq 5 \times 10^6$ and $0.5 \leq Pr_t \leq 10^6$ Petukhov-Popov correlation is:

$$Nu_t = \frac{\frac{f_t}{2} \times Re_t \times Pr_t}{1.07 + \frac{900}{Re_t} - \frac{0.63}{1+10 \times Pr_t} + 12.7 \times \left(\frac{f_t}{2}\right)^{\frac{1}{2}} \times \left(Pr_t^{\frac{2}{3}} - 1\right)} \,. \tag{27}$$

The nomenclature $Nu_{t,turbulento}$ is adopted when this correlation is employed in Eq 28.

According to Shah and Sekulic (2003), if $2000 < Re_t < 8000$:

$$Nu_t = Nu_{t,laminar} \times \left(1.33 - \frac{Re_t}{6000}\right) + \left[1 - \left(1.33 - \frac{Re_t}{6000}\right)\right] \times Nu_{t,turbulento} \,. \tag{28}$$

In this study, Eq. 28 is used to implement the calculation of the transition regime when $2100 < Re_t \leq 4000$.

The Fanning friction factor (Kakac and Liu, 2012; Shah and Sekulic, 2003), which is valid for $Re_t \leq 2100$, is:

$$f_t = \frac{16}{Re_t} \,. \tag{29}$$

The friction factor for the flow inside the tubes according to the correlation of Bhatti and Shah (Shah and Sekulic, 2003) is:

$$f_t = AA + BB \times Re_t^{-1/m} \,, \tag{30}$$

for 2100 $\leq Re_t \leq$ 4000 the parameter values are listed as follows: AA equals 0.0054, BB equals 2.3x10^{-8}, and m equals -2/3. For 4000 $\leq Re_t \leq 10^7$; AA equals 0.00128, BB equals 0.1143 and m equals 3.2154.

The pumping power $P_{s,t}$ is:

$$P_{s,t} = \frac{\Delta P_t \times \dot{m}_t}{\rho_t \times \eta} + \frac{\Delta P_s \times \dot{m}_s}{\rho_s \times \eta} \,, \tag{31}$$

where ΔP_t is the pressure drop to the tube side, ΔP_s is the shell pressure drop, ρ_s is the shell fluid density and η is the pumping efficiency, which is 0.85 in this study. The pressure drop ΔP_s by the Bell Delaware method (Shah and Sekulic, 2003) is:

$$\begin{aligned} \Delta P_s \; &= [(N_b - 1) \times \Delta P_{bid} \times \zeta_b + N_b \times \Delta P_{wid}] \\ &\times \zeta_l + 2 \times \Delta P_{bid} \times \left(1 + \frac{N_{rcw}}{N_{rcc}}\right) \times \zeta_b \times \zeta_s \end{aligned} \,, \tag{32}$$

where ΔP_{bid} is the pressure drop for liquid flow in an ideal cross-flow between two baffles; ΔP_{wid} is the pressure drop associated with an ideal one-window section; ζ_b is the correction factor for bypass flow; ζ_l is the correction factor for tube-to-baffle and baffle-to-shell leakage streams; ζ_s is the correction factor for inlet and outlet sections that have different baffle spacings than the central section; N_{rcw} is the number of effective tube rows in cross-flow in each window; N_{rcc} is the number of tube rows crossed during the flow through one cross-flow section between baffle tips, N_b is the number of baffles.

The pressure drop to the tube side, as shown in (Fettaka *et al.*, 2013), is:

$$\Delta P_t = n_p \times \left(\frac{4 f_t \times L_t}{d_i} + FQPT\right) \times \frac{\rho_t \times v_t^2}{2} \,, \tag{33}$$

where $FQPT$ is the pressure drop factor in the tubes. As explained in Towler and Sinnott (2008), this factor is a factor for the tube pressure drop due to tube inlet contraction, tube outlet expansion and reverse flow. The assumed value for $FQPT$ is 2.5.

2.1 Parameters used in the thermal and hydrodynamic calculation of STHE

The parameters used in the thermal and hydrodynamic calculation of STHE with single-phase flow in the shell and tubes used specifically in this case study are presented in the Tab. 4.

Table 4: Parameters used in the STHE analytical model

	Tube	**Shell**
Fluid	**Seawater**	**Oil**
Flow rate (kg/s)	Eq. 18	36.3
Inlet temperature (ºC)	32.2	65.6
Outlet temperature (ºC)	37.42	60.4
Density (kg/m^3)	993.816	849.000
Specific heat at constant pressure (J/ kg K)	4178.204	2094.000
Viscosity (Pa s)	0.00072764	0.06460000
Thermal conductivity (W/m K)	0.62494	0.14000
Fouling resistance (m^2 K/W)	0.000175	0.000150
Wall thermal conductivity	111	
Number of sealing strip pairs	2	

3. MULTIVARIATE ADAPTIVE REGRESSION SPLINES (MARS)

Multivariate adaptive regression splines (MARS) is a nonparametric regression technique, which was proposed by Friedman (1991). MARS study the nonlinear relationship between a response variable and the set of predictor variables using splines and fits a model in the form of an expansion in product spline basis functions of predictors chosen during a forward and backward recursive partitioning strategy. MARS uses piecewise linear or cubic splines for local fit.

According to Friedman (1991) the model produced by the MARS technique, with cubic splines, involves a sum of products of function of the form:

$$b(x|s,t) = [s(x-t)]_+ \tag{34}$$

In continuous derivatives produced, each function is replaced by a corresponding truncated cubic function:

$$C(x|s=+1,t_-,t,t_+) = \begin{cases} 0 \text{ if } x \leq t_- \\ p_+(x-t_-)^2 + r_+(x-t_-)^3 \text{ if } t_- < x < t_+ \\ x-t \text{ if } x \geq t_+ \end{cases} \tag{35}$$

$$C(x|s=-1,t_-,t,t_+) = \begin{cases} -(x-t) \text{ if } x \leq t_- \\ p_-(x-t_+)^2 + r_-(x-t_+)^3 \text{ if } t_- < x < t_+ \\ 0 \text{ if } x \geq t_+ \end{cases} \tag{36}$$

When $t_- < t < t_+$:

$$\begin{cases} p_+ = (2t_+ + t_- - 3t)/(t_+ - t_-)^2 \\ r_+ = (2t - t_+ - t_-)/(t_+ - t_-)^3 \\ p_- = (3t - 2t_- - t_+)/(t_- - t_+)^2 \\ r_- = (t_- + t_+ - 2t)/(t_- - t_+)^3 \end{cases} \tag{37}$$

where t is the knot location.

According to Koc and Bozdogan (2015), the form of the MARS model defined to approximate the function Eq 34 is defined as:

$$\widehat{f}(\mathbf{x}) = \beta_0 + \sum_{m=1}^{M} \beta_m B_m(\mathbf{x}) \tag{38}$$

where $B_m(\mathbf{x})$ represents the base function (BF) in m, M is the total number of base functions (BF). The term β is constant coefficients estimated using the least-squares method.

4. ARTIFICIAL NEURAL NETWORKS

Artificial neural networks are computational models, which through a set of very simple processing elements (artificial neurons) highly connected and processing in parallel, inspired by the neural structure of intelligent organisms, acquire knowledge through experience.

Each artificial neuron has a number n of entries whose sum weighted by the w weights passes through the activation function, some of which are the sigmoid and hyperbolic tangent to simulate the natural neuron. The w weights are variable only in the training phase. After this phase, the neuron becomes a non-linear function of $R^n \to R$. So, all the knowledge of a neural network is in the weights attributed to the connections between neurons.

According to Haykin (2007), a Multilayer Perceptrons (MLP) neural network has three characteristics that distinguish it from other types of networks:

- For each neuron in the network there is a nonlinear activation function, whose curvature is soft.
- The network contains one or more hidden layers, which are different from the input and output. The neurons in these hidden layers are responsible for ability to learn complex problems.
- There is a high degree of connectivity between neurons. This means that a neuron any layer of the network is connected to all neurons.

The training of the MLP network is of the supervised type, being known as learning by experience and occurs by iterations. Generally, a popular algorithm called error backpropagation is used. This algorithm is based on a learning rule that "corrects" the error during training. The error back-propagation process consists of two phases: a signal propagation phase (feedforward) and an error backpropagation phase (backpropagation). Weights are adjusted so that the distance between the network response and the desired response is reduced.

The Levenberg-Marquardt algorithm is a supervised training algorithm. It uses the Jacobian Matrix J of the derivatives of the error e about the weights. Its formula is given by:

$$\Delta w_j^{(k)} = (J^T J + \mu I)^{-1} J^T e \tag{39}$$

where $\Delta w_j^{(k)}$ is the j-th adjustment of the weights in a given layer k, μ is the learning rate, I is the identity matrix.

5. CASE STUDY AND RESULTS

The MATLAB toolbox *nnstart* was used to generate approximations of the STHE model functions. The neural network used was the Multilayer Perceptrons (MLP) (Haykin, 2007), 10 hidden layers were used, which has the sigmodal function. And the output neuron is linear. The network was trained with the Levenberg-Marquardt backpropagation algorithm. The training was performed with 629 samples (70 % of the data), the validation with 135 samples (15 % of the data), and the test with 135 samples (15 % of the data).

The metamodels generated by MARS (Friedman, 1991) were implemented in the MATLAB toolbox *ARESLab* (Jekabsons, 2016), and in this case only cubic splines were used.

The input data used to generate the STHE metamodels are shown in Tab. 5:

Table 5: STHE inputs

Inputs	Symbol	Description	Values
x_1	d_o	Tube outer diameter (m)	0.015875; 0.01905; 0.0254; 0.03175
x_2	L_t	Tube length (m)	2.438; 3.048; 3.658; 4.877; 6.096
x_3	L_b	Baffle spacing (m)	0.3245 to 1.5240
x_4	A_D	Design heat exchanger area (m^2)	30.0055 to 59.6715
x_5	n_p	Number of tube passes	1; 2; 4
x_6	a_p	Tube layout pattern	triangular (30^o); square (45^o)

The output data used are required heat exchange area A and pumping power $P_{s,t}$. In this study, the values are:
- A: 25.0865 to 59.2119 m^2,
- $P_{s,t}$: 243.9 to 4736.0 W.

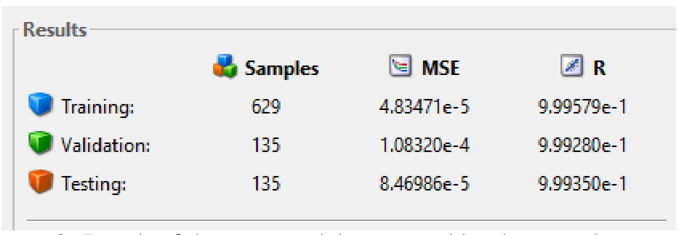
All data has been normalized to minimize problems arising from the use of different units and dispersions between the different inputs.

According to Roitman (2001), the precision calculation of the metamodel is done by the difference between the real value and the value adjusted by the model. One of the ways to calculate this precision is to evaluate the mean square error (Mean Square Error or MSE), this is used for statistical models and network models neural. Its formulation is:

$$MSE = \frac{1}{n} \sum_{t=1}^{n} (f_t - \widehat{f}_t)^2, \tag{40}$$

where n is the number of observations, f_t is the actual value in t, $\widehat{f}_t$ is the predicted value in t.

The first experiment with the Neural Network used the 6 classes of defined input data, for the two outputs A and $P_{s,t}$, respectively. The results are shown in the Fig. 2:


Results

	Samples	MSE	R
Training:	629	4.83471e-5	9.99579e-1
Validation:	135	1.08320e-4	9.99280e-1
Testing:	135	8.46986e-5	9.99350e-1

Figure 2: Result of the metamodel generated by the neural network.

Given the MSE values presented in Fig. 2, it was found that Levenberg-Marquardt training was effective for this case study, since the weights were adjusted in such a way as to reduce the distance between the network response and the output from the STHE analytical model.

In the toolbox *ARESLab* the outputs A and $P_{s,t}$ were used separately, because the toolbox, despite generating the metamodel when using more than one output, does not allow visualizing the approximation functions in that case. Thus, the results are presented by groups of categorical inputs. The complete data had 899 samples, from this set, the groups of categorical inputs were separated, with the respective quantitative variables belonging to the group. The Tab. 6 shows the MSE values of the metamodel generated using the toolbox *ARESLab*:

Table 6: Results of the metamodel generated by MARS

Categorical inputs	MSE for output A	MSE for output $P_{s,t}$
x_5 = 1, x_6 = 30º	3.55x10^{-6}	2.98x10^{-6}
x_5 = 1, x_6 = 45º	1.36x10^{-5}	1.41x10^{-4}
x_5 = 2, x_6 = 30º	1.33x10^{-5}	8.52x10^{-7}
x_5 = 2, x_6 = 45º	1.55x10^{-5}	7.21x10^{-5}
x_5 = 4, x_6 = 45º	2.57x10^{-7}	2.28x10^{-4}

As an example, given the categorical inputs x_5 = 1, x_6 = 30º the metamodel is in linear format (Koc and Bozdogan, 2015) generated by the toolbox *ARESLab* for the required thermal exchange area A is shown in Fig. 3. It is observed that the coefficients were obtained by cubic splines, only the format of the metamodel that is linear.

```
A:
'BF1 = max(0, x4 -0.73325)'
'BF2 = max(0,0.73325 -x4)'
'BF3 = max(0, x2 -0.66676)'
'BF4 = max(0,0.66676 -x2)'
'BF5 = max(0, x1 -0.2)'
'BF6 = max(0,0.2 -x1)'
'BF7 = max(0, x3 -0.60402)'
'BF8 = max(0,0.60402 -x3)'
'BF9 = BF3 * max(0, x1 -0.2)'
'BF10 = BF3 * max(0,0.2 -x1)'
'BF11 = BF4 * max(0, x3 -0.83077)'
'BF12 = BF4 * max(0,0.83077 -x3)'
y = 0.43038 +0.30021*BF1 -0.25773*BF2 -0.31334*BF3 +0.2937*BF4 +0.70141*BF5 -
0.65872*BF6 +0.44375*BF7 -0.63013*BF8 -0.22834*BF9 +2.0184*BF10 -0.54418*BF11
+0.31621*BF12
```

Figure 3: MARS metamodel for output A

Analyzing Fig. 3, it was found that the metamodel of the required heat exchange area (A) produced by the MARS technique (Eq 38) had 12 base function (BF).

The result of the neural network has an appropriate MSE value and a correlation coefficient R very close to 1. The interpretation is that the neural network was able to reproduce the STHE model properly with the data that was provided. The MARS technique also enabled adequate MSE values. Therefore, this approach achieved the objective of generating a consistent metamodel for the SHTE model.

6. CONCLUSION

Comparing the neural network and MARS techniques to generate the metamodel was relevant. It was seen that both are suitable to approximate the functions of this problem. And that the use of two different techniques enables reliability since the range of MSE values of both techniques are close.

The two toolboxes are easy to use. It is noticed that the neural network toolbox (nnstart) has the advantage of generating a metamodel code, thus, only changing the inputs allows new outputs. The MARS technique toolbox (ARESLab) does not generate output in code format, however, it is possible to view the terms that constitute the generated metamodel.

An advantage of the STHE metamodel generated by the MARS technique is obtaining continuous functions. And the advantage of the neural network compared to the MARS technique was to enable the use of both categorical and quantitative inputs.

In general, this study was important, it was possible to generate adequate metamodels of an analytical model that has a non-linear behavior. However, as a suggestion for future work, it is necessary to obtain adequate metamodels with fewer expressions, so it is easier to interpret. It was concluded that the objective of the study was achieved, a different approach to a known model was obtained. It was intended to complement existing ideas, and other possibilities of study may occur as other comparisons between STHE metamodels, development of metamodels from numerical STHE models, and apply the gradient optimization method to metamodels formed by cubic splines.

7. ACKNOWLEDGEMENTS

This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001; the Pontifical Catholic University of Minas Gerais (PUC MINAS); and FAPEMIG [research project PPM-00381-16].

8. REFERENCES

Crino, S. and Brown, D.E., 2007. "Global optimization with multivariate adaptive regression splines". *IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics)*, Vol. 37, No. 2, pp. 333–340.

Fettaka, S., Thibault, J. and Gupta, Y., 2013. "Design of shell-and-tube heat exchangers using multiobjective optimization". *International Journal of Heat and Mass Transfer*, Vol. 60, No. 1, pp. 343–354. ISSN 00179310.

Friedman, J.H., 1991. "Multivariate adaptive regression splines". *The annals of statistics*, pp. 1–67.

Frisso, C., Scarpel, R.A. and Ferrari, D., 2011. "Metamodelagem de funções determinísticas por composição integrada de especialistas locais". *XLIII Simpósio Brasileiro de Pesquisa Operacional*.

Haykin, S., 2007. *Redes neurais: princípios e prática*. Bookman Editora.

Jekabsons, G., 2016. "Areslab: Adaptive regression splines toolbox for matlab/octave". URL `https://www.cs.rtu.lv/jekabsons`.

Kakac, S. and Liu, H., 2012. *Heat exchangers: selection, rating, and thermal design*. CRC press.

Koc, E.K. and Bozdogan, H., 2015. "Model selection in multivariate adaptive regression splines (mars) using information complexity as the fitness function". *Machine Learning*, Vol. 101, No. 1-3, pp. 35–58.

Krzywanski, J., 2019. "A general approach in optimization of heat exchangers by bio-inspired artificial intelligence methods". *Energies*, Vol. 12, No. 23, p. 4441.

Mukherjee, R., 2008. "Practical thermal design of shell-and-tube heat exchangers". *High Temperature Material Processes*, Vol. 12, No. 1-2.

Pina, A., 2010. *A; Metodologias de Análise, Síntese e Otimização de Sistemas para Produção de Petróleo Offshore Através de Metamodelos e Enxame de Partículas*. Ph.D. thesis, Dissertação de M. Sc., COPPE/UFRJ, Rio de Janeiro, RJ, Brasil.

Roitman, V.d.L., 2001. *Um Modelo Computacional de Redes Neurais para Predição do Índice de Desemprego Aberto*. Ph.D. thesis, PhD thesis, Programa de Pós-Graduação de Engenharia Civil da Universidade . . . .

Saldanha, W.H., Soares, G.L., Machado-Coelho, T.M., dos Santos, E.D. and Ekel, P.I., 2017. "Choosing the best evolutionary algorithm to optimize the multiobjective shell-and-tube heat exchanger design problem using promethee". *Applied Thermal Engineering*, Vol. 127, pp. 1049–1061. doi:10.1016/j.applthermaleng.2017.08.052.

Saldanha, W.H., Arrieta, F.R.P., Ekel, P.I., Machado-Coelho, T.M. and Soares, G.L., 2020. "Multi-criteria decision-making under uncertainty conditions of a shell-and-tube heat exchanger". *International Journal of Heat and Mass Transfer*, Vol. 155, pp. 1–13.

Serth, R.W. and Lestina, T., 2014. *Process heat transfer: Principles, applications and rules of thumb*. Academic Press.

Shah, R.K. and Sekulic, D.P., 2003. *Fundamentals of heat exchanger design*. John Wiley & Sons.

TEMA, 2007. *Standards of the Tubular Exchanger Manufacturers Association and others*. Tubular Exchanger Manufacturers Association, Inc., Tarrytown, New York.

Thakore, S.B. and Bhatt, B.I., 2007. *Introduction to process engineering and design*. McGraw-Hill Education.

Towler, G. and Sinnott, R., 2008. *Chemical engineering design: principles, practice and economics of plant and process design*. Amsterdam, Netherlands: Elsevier.

Yang, S.S. and Tseng, C.S., 1996. "An orthogonal neural network for function approximation". *IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics)*, Vol. 26, No. 5, pp. 779–785.

Zhang, W. and Goh, A.T., 2016. "Multivariate adaptive regression splines and neural network models for prediction of pile drivability". *Geoscience Frontiers*, Vol. 7, No. 1, pp. 45–52.

9. RESPONSIBILITY NOTICE

The authors are solely responsible for the printed material included in this paper.