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HIERARCHIC MODELING FOR SIMULATION OF HEAT EXCHANGERS

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Abstract. The aim of this work is the development of hierarchical procedures for calculating the evaluation parameters of shell and tube heat exchangers with adequate accuracy and low computational cost, facilitating the process simulation and optimization, implemented in the EMSO simulator. The developed models allow the simulation of segmentally baffled heat exchangers of the E Shell, F Shell, and multipass types in agreement with the TEMA standards for this equipment. Several simulations had been carried out in a battery of heat exchangers of an atmospheric distillation unit of an oil refinery. The obtained results allow the user to have easy access to the parameters of the heat exchanger, or to incorporate new procedures for the calculation of these pieces of equipment.

***Key words**:* Heat Exchangers, Simulation, EMSO.

1. INTRODUCTION

Heat exchangers are largely employed equipment in industries in general, serving as a basic component for so many engineering processes. Among the many possibilities of this equipment, shell and tube heat exchangers are the most versatile due to its advantages that present, such as fabrication, costs, and mainly, thermal performance. With growing concern of industry to improve its processes, minimize costs, and make rational use of energy serves as motivation for the design optimization of these equipments. At a first glance, heat exchanger design is conceptually quite straightforward. However, there are some terms used in heat exchanger specification problems and their solutions, which are often confused (Bell, 1983). These are 'design' and 'rating'.

Design is the process of determining all essential constructional dimensions of an exchanger that must perform a given heat duty and respect limitations on shell side and tube side pressure drop. A number of other criteria are also specified, such as minimum or maximum flow velocities,

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ease of cleaning and maintenance, erosion, size and/or weight limitations, tube vibration, and thermal expansion. Each design problem has a number of potential solutions, but only one will have the best combination of characteristics and cost. 'Rating' is the computational process in which the inlet flow rates and temperatures, the fluid properties, and the heat exchanger parameters are taken as input and the outlet temperatures and thermal duty of the heat exchanger are calculated as output. In either case, the pressure drop of each stream will also be calculated.

Figure 1 shows the basic logical structure of the process heat exchanger design according to Bell (1983), showing clearly that a thermal and hydrodynamic analysis of the equipment (rating process) becomes an important part of the design effort.

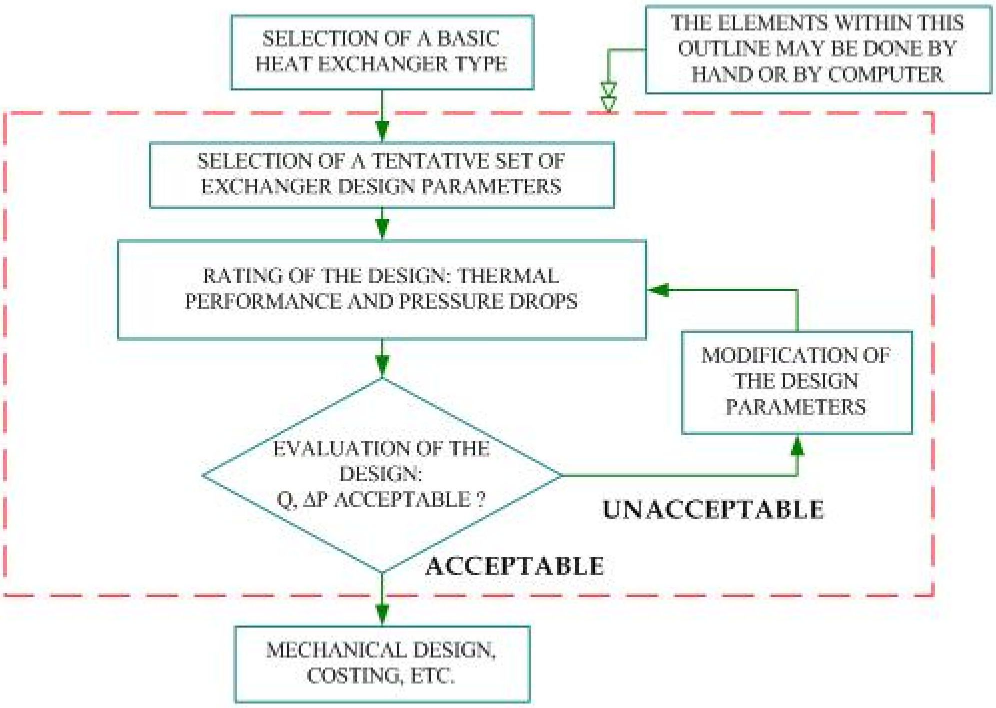

Figure 1 – Basic logical structure for process heat exchanger design (Bell, 1983).

This means if the exchanger configuration selected for rating gives acceptable thermal performance with pressure drops in both streams near but below the maximum allowable, this configuration may be considered a solution to the problem and the designer can move on to the mechanical design, cost estimation, etc. Otherwise, if the evaluation demonstrates to be deficient in some of the restrictions, a modification in the essential parameters of the design is made necessary.

This fact points out the importance to the process engineer a basic understanding in those parameters, as well as the correct selection of the analysis method to be used in the rating process.

In this paper, the procedure developed for the evaluation of parameters of segmentally baffled shell and tube heat exchangers with the adequate accuracy and low computational cost is presented, which can effectively predict the thermal and hydraulic behavior of such equipment. As additional results, the necessary information for further assessment and optimization of the process are also produced. The computational tool used for the implementation of the models was the EMSO processes simulator (Soares and Secchi, 2003). The aim of this implementation is to incorporate heat exchanger models to the model library of the simulator.

2. HIERARCHYC MODELING

Currently, there are many commercial heat exchangers softwares for rating and design, such as Aspen B-JAC, Hysys, HTFS, HTRI, among others. However, these softwares are expensive for obtaining license and the employed correlations are not entirely of public domain, which is also not appropriate for heat exchangers research and teaching. These softwares are easy to use, through friendly graphical drag-and-drop interfaces where the modeling system is simply realized through utilization, configuration and connection of pre-existing components. This causes a modeling flexibility detriment, because if the end user needs to develop a new equipment model or try to do any code alterations, this will imply in time allocation for carrying out such task.

With the EMSO process simulator, time spent on new models development is decreased significantly due to the modeling structure to be based on equation (equation-oriented modeling) and for having a high level of utilization of concepts derived from object-oriented programming (OOP), such as composition and inheritance.

The composition allows the equipment model construction to be comprised of one or more pre-existing models. For instance, a shell and tube heat exchanger shows a different behavior for the fluid which flows inside the tubes and for the fluid which flows on the shell side. New model can be created for the shell and another one for the tubes and combine them to the final model of the heat exchanger through their composition. On the other hand, the code re-utilization is a key word in the inheritance concept, allowing the different types of heat exchangers to be derived from a base model. When a new model needs to be created, it may inherit all the characteristics of the base model through inheritance, and there is no need to re-write the code. Figure 2 illustrates the hierarchy used in shell and tube heat exchangers mathematical modeling and the methods for calculation from the basic models.

The different types of shell and tube heat exchangers have common characteristics that may be described in one basic model. These characteristics (parameters, variables and equations) are described in separate models and that through composition and inheritance is added to the basic model. This causes modeling to be structured through hierarchies between the models, decreasing the equipment equationing complexity and with a greater capability of code reuse.

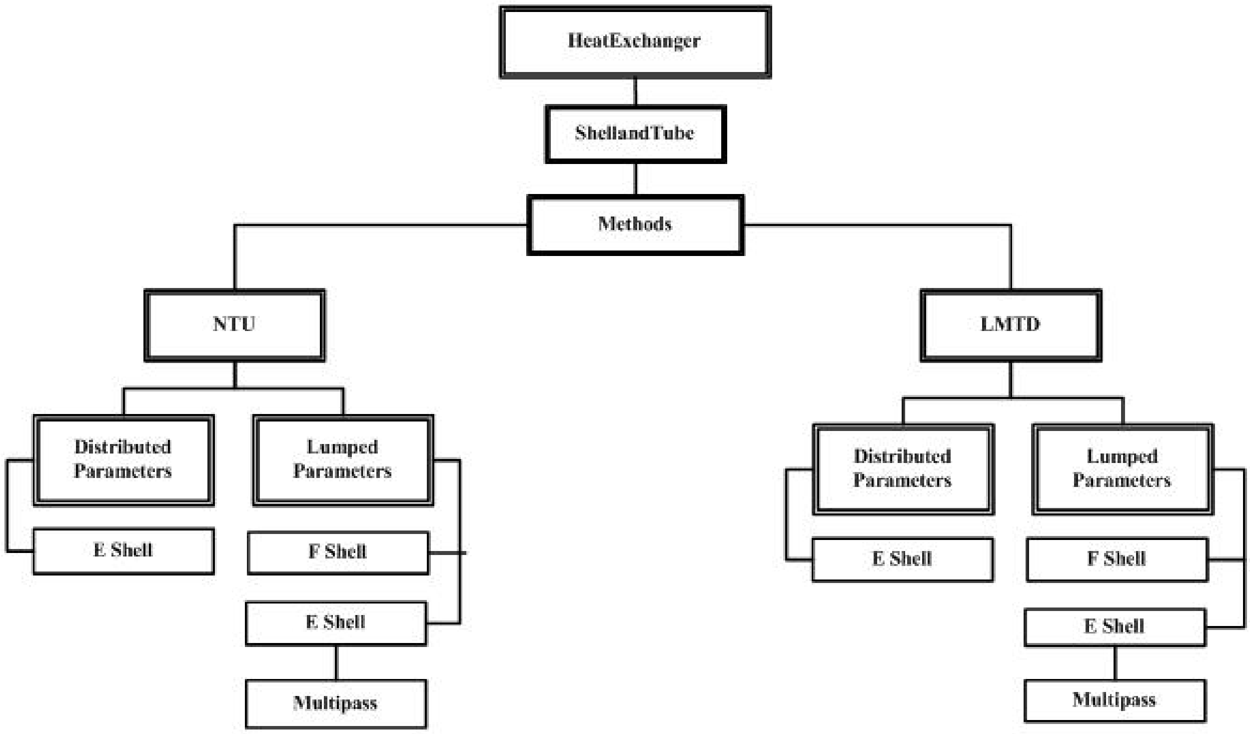

Figure 2 – Model hierarchy for modeling and simulation of heat exchangers.

The block, in Figure 2, named *HeatExchanger* is a basic model and the mathematical abstraction for a determined equipment behavior. This block is comprised in various sub-models and it contains the common equations for heat exchangers, such as mass and energy balances and fluid properties calculation. The basic model contains *ports* which are connection points of the information that gets in and out of the equipment and that is associated to the material streams model, which carries the process information (temperature, flow rates, composition, pressure, etc.). This way it is possible to connect the heat exchanger model to any other equipment through its ports.

The thermo-physical properties of the fluids are calculated through an external routine to the simulator, because EMSO contains interface mechanisms that allow the user to loading different physical properties packages or to recreate their own routines for such purpose. Each different type of heat exchanger may be included in the structure showed in the Figure 2, making it very flexible.

The block named *ShellandTube* is a particular class of heat exchangers. That class contains the peculiar characteristics of shell and tube heat exchangers besides those inherited of the *HeatExchanger* block. To differentiate in the calculation method and modeling type, the procedure consisted of creating models for the methods, named *LMTD* and *NTU*. The first one contains the heat transfer equations based on the Logarithmic Mean Temperature Difference (LMTD), while the second makes use of the Effectiveness-Number of Transfer Units (ε - NTU) method.

Through the composition of those blocks, two new blocks were created for each method of employed calculation. The *Lumped Parameters* block describes the macroscopic modeling of heat exchangers and the *Distributed Parameters* block describes the microscopic modeling of *E Shell* heat exchangers.

The developed models allow the simulation of the shell and tube heat exchangers types commonly used in the industry and designated by the TEMA standards (1988) as:

- *E Shell* – one pass-shell and an even number of tube passes;
- *F Shell* – two pass-shell and an even number of tube passes;
- *Multipasses* – a system of multiple-tube pass heat exchangers in series. Each unit in series has one shell pass and an even number of tube passes;

In the lumped parameters modeling, the physical properties of the streams are evaluated as average values, that is, the mean value between the entrance and exit temperatures of the equipment. The film coefficients are also average values and, consequently, it is obtained a mean value for the overall heat transfer coefficient. In the distributed parameters modeling, the heat exchanger shell is divided into a number of heat transfer zones where the heat transfer and pressure drop calculations are performed along each interval. The total number of zones in a heat exchanger shell is calculated by the Equation 1, as it is shown in Figure 3.

$$Zones = Total\ Number\ of\ Baffles\ +\ 1 \tag{1}$$

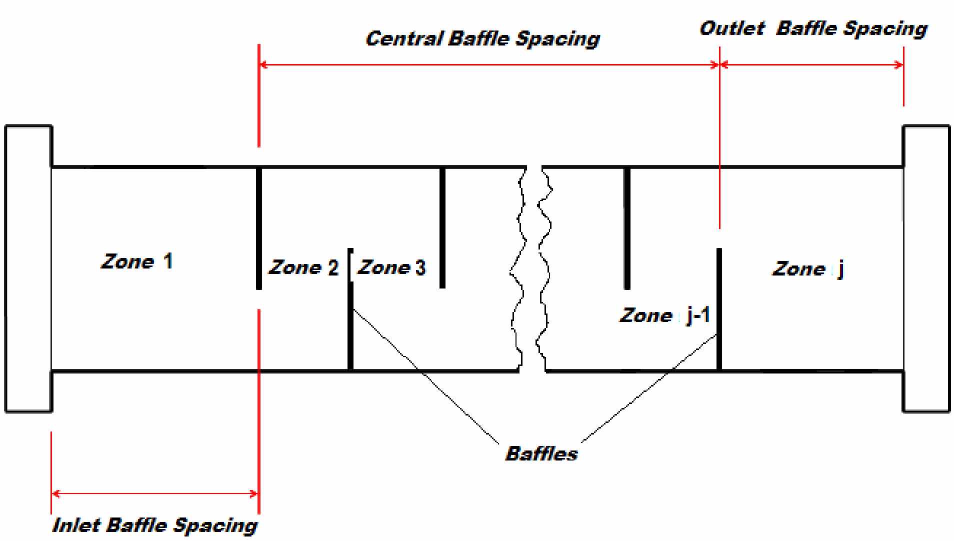

Figure 3 – Distributed parameter model.

3. TUBE SIDE ANALYSIS

3.1 Heat Transfer

The heat transfer coefficient in the tube side is evaluated according to the available correlations. For laminar flow the Hausen (Incropera and Dewitt, 1988) correlation is used in the range of Reynolds number (Re_D) less than 3000. For turbulent flow, Petukhov (Incropera and Dewitt, 1988) correlation is employed in the range of $10^4 < Re_D < 5.10^6$ and, Gnielinski (1976) equation is used for transition flow in the range of $3000 < Re_D < 5.10^6$.

For distributed parameters system, the heat transfer coefficient in laminar flow is evaluated from analytical expressions (Shah and London, 1978) while for the turbulent regime the Petukhov equation is used. Besides those, other correlations can be included easily in the model, due to the modular structure.

3.2 Pressure Drop

The pressure drop on the tube side of the heat exchanger is composed of several different terms: the pressure losses in the inlet and outlet nozzles, and the frictional losses of the flow in the tube.

The frictional pressure loss inside the tube is calculated using the Fanning equation below (Saunders, 1988):

$$\Delta P_{tube} = \frac{2 \cdot f \cdot L \cdot N_{pt} \cdot \rho \cdot V^2}{D_i \cdot \phi} \tag{2}$$

where N_{pt} is the number of tube passes, L is the tube length, ρ , D_i and V are respectively, the fluid density, the inner tube diameter and the average fluid velocity inside the tubes. The Fanning friction factor (f) is evaluated according to the flow regime. For turbulent and transition flow the friction factor is given by (Incropera and Dewitt, 1988):

$$f = (0{,}790 \cdot \ln \mathrm{Re}_D - 1{,}64)^{-2} \tag{3}$$

and for laminar flow (Incropera and Dewitt, 1988):

$$f = \frac{64}{\mathrm{Re}_D} \tag{4}$$

The viscosity correction factor is given by (Sieder and Tate, 1936):

$$\phi = \left(\frac{\mu}{\mu_w} \right)^{0{,}14} \tag{5}$$

where μ_w and μ are the dynamic viscosities at the wall and bulk fluid, respectively.

For the inlet and outlet nozzles, the losses are expressed in terms of K (dimensionless) velocity heads (Saunders, 1988):

$$\Delta P_{nozzles} = K \frac{\cdot \rho \cdot V_{nozzle}^{2}}{2} \tag{6}$$

$$K = 1.1 \quad \text{(Inlet nozzle)} \tag{7}$$

$$K = 0.7 \quad \text{(Outlet nozzle)} \tag{8}$$

The total tube side pressure drop is computed by:

$$\Delta P_{total} = \Delta P_{tube} + \Delta P_{nozzles} \tag{9}$$

4. SHELL SIDE ANALYSIS

In order to calculate shell side heat transfer coefficient and pressure drop, the method proposed by Bell (1963) is employed. The Bell method is considered by Palen and Taborek (1969) to be the best available in the open literature and the most suitable for shell side analysis. The Bell method (1963) uses the principles of Tinker's flow distribution model (Tinker, 1958). Tinker presented an elaborate model based on the concept of stream analysis in which the flow through the bundle was assumed to be divided into various flow paths (see Figure 4) as follows:

Stream A: is the leakage stream in the orifice formed by the clearance between the baffle tube hole and the tube wall;

Stream B: is the main effective cross-flow stream, which can be related to flow across ideal tube banks;

Stream C: is the tube bundle bypass stream in the gap between the bundle and the shell wall.

Stream E: is the leakage stream between the baffle edge and shell wall;

Stream F: is the bypass stream in flow channels due to omission of tubes in tube pass partitions. This stream has been added to the original Tinker model by Palen and Taborek (1969).

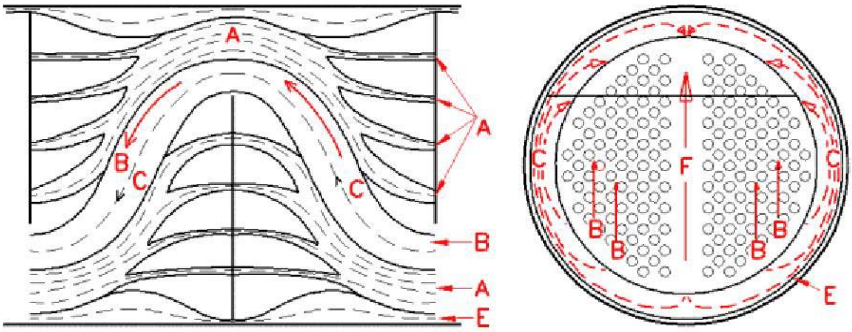

Figure 4 – Shell side flow streams (Tinker, 1958).

4.1 Heat Transfer

Each of the above streams introduces a correction factor to the heat transfer correlation for ideal cross flow across a bank of tubes. The basic equation for calculating the effective average shell side heat transfer coefficient is given as:

$$h_c = h_{ideal} \cdot J_c \cdot J_l \cdot J_b \cdot J_r \cdot J_s \tag{10}$$

where h_{ideal} is the heat transfer coefficient for pure cross flow in an ideal tube bank.

Jc – is the correction factor for baffle cut and spacing.

Jl - is the correction factor for baffle leakage effects.

Jb - is the correction factor for bundle bypass flow (C and F streams).

Js - is the correction factor for variable baffle spacing in the inlet and outlet sections.

Jr - is the correction factor for adverse temperature gradient build-up.

4.2 Pressure Drop

For a shell and tube heat exchanger with bypass and leakage streams, the total pressure drop is calculated as the sum of the following components (Figure 5):

ΔP_c – Pressure drop in the interior cross flow sections (Figure 5-a).

ΔP_w – Pressure drop in the window sections (Figure 5-b).

ΔP_e – Pressure drop in the entrance and the exit sections (Figure 5-c).

$\Delta P_{nozzles}$ – Pressure drop in the inlet and outlet nozzles (Figure 5-d).

Finally, the total shell side pressure drop is given as:

$$\Delta P_{total} = \Delta P_c + \Delta P_w + \Delta P_e + \Delta P_{nozzles} \tag{11}$$

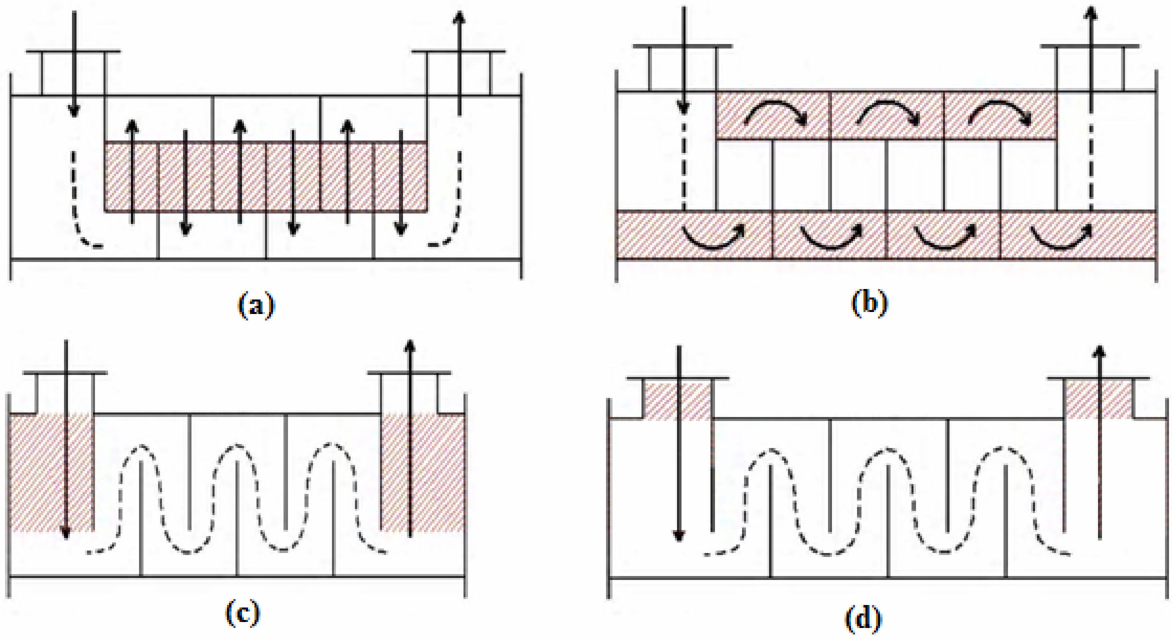

Figure 5 – Flow region considered for shell side pressure drop.

5. APPLICATIONS

For model validation, several simulations have been carried out in a series of heat exchangers of an atmospheric distillation unit of an oil refinery. The evaluated equipments were shell and tube heat exchangers of type E shell, and the streams process were characterized originally by pseudo-components and, starting from information of the database supplied by the refinery, the physical properties of those streams and their dependences with the temperature change were correlated by fit data and calculated by an external routine. For demonstration purposes, only the results of one of the simulations are shown.

The heat exchanger mechanical data are presented in Table 1 and stream data are presented in Table 2.

Two strategies of simulations were accomplished: the first with the lumped parameters model and the second with the distributed parameter model. In both simulations the user obtains information about the total heat rate, the film coefficients, shell side and tube side velocities, the overall heat transfer coefficient and the correction factors for heat transfer in the shell side estimated by the Bell-Delaware method. Figure 6 shows the hot and cold temperatures profiles along the equipment.

Table 1. Heat exchanger mechanical data.

Data	
Heat Exchanger Configuration	TEMA AES
Number of Tube Passes	2
Number of Tubes	775
Tube Pattern	90°
Tube Length (m)	5.970
Outer Tube Diameter (m)	0.01905
Inner Tube Diameter (m)	0.01483
Tube Pitch (m)	0.0254
Tube Side Nozzle Diameter (m)	0.15405
Shell Diameter (m)	0.914
Shell Side Nozzle Diameter (m)	0.38735
Baffle Cut	30%
Number of Baffles	8
Bundle to Shell Clearances (m)	0.0430898
Baffle to Shell Clearances (m)	0.0047625
Tube to Baffle Hole Clearances (m)	0.0003969
Inlet Baffle Spacing (m)	0.807813
Central Baffle Spacing (m)	0.622
Outlet Baffle Spacing (m)	0.807813

Table 2. Stream data.

Data	Tube Side	Shell Side
Fluid/Stream	Crude / Hot	Mixture / Cold
Inlet Temperature (K)	419.25	363.35
Inlet Pressure (atm)	7.23474	21.8136
Flow mol (mol/s)	40.476	121.698
Vapor Fraction	0	0

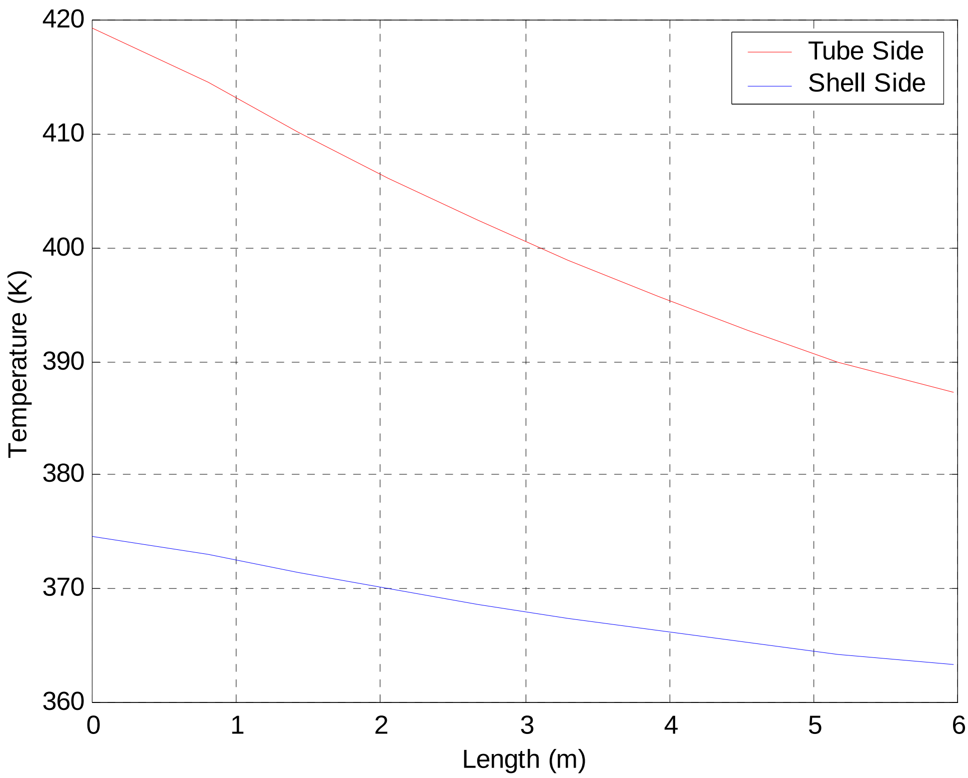

Figure 6 – Temperatures profiles.

Table 3 shows the distribution of the pressure drop in the several sections of the shell. Figure 7 illustrates the pressure profiles along the length of the heat exchanger.

Table 3. Shell side pressure drop.

Section	Pressure Drop (atm)
Window	0.1570
Cross Flow	0.0508
Entrance and the exit sections	0.0242
Nozzles	0.0972
Total Pressure Drop	**0.3292**

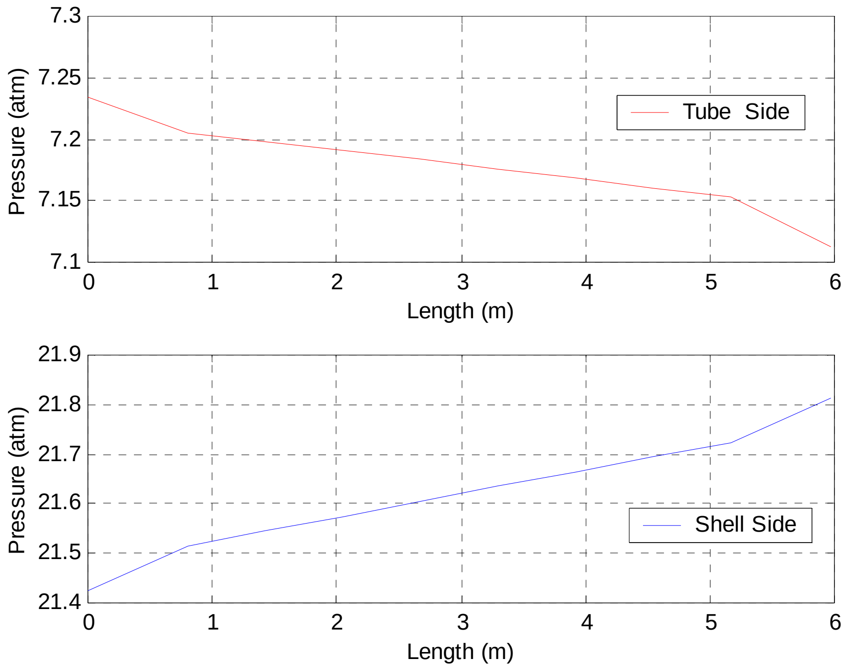

Figure 7 – Pressure profiles.

The simulation results were compared with plant data and with the simulation results from the software *Xist*, a program from Heat Transfer Research Institute (HTRI) used to design heat exchangers on a rigorous way. Table 4 shows a summary of the comparisons.

Table 4 – Results of simulation 1.

	Description	EMSO		XIST	
		Inlet	Outlet	Inlet	Outlet
Shell	Temperature (K)	363.35	374.68	363.35	374.69
	Pressure (atm)	21.8136	21.2564	21.8136	21.4685
	Total Pressure Drop (atm)	0.32914		0.34503	
	Film Coefficient (W/m^2 K)	713.95		1133.19	
	Vapor Fraction	0	0	0	0
	Prandtl Number	84.26		78.01	
	Reynolds Number	3180		4202	
	Viscosity Correction	1.026		1.025	
	Nozzles Velocities (m/s)	1.18	1.19	1.18	1.19
	Nozzles Pressure Drop (atm)	0.04951	0.04769	0.02813	0.02724
Tube	Temperature (K)	419.25	389.47	419.25	387.25
	Pressure (atm)	7.23474	7.10588	7.23474	7.10072
	Total Pressure Drop (atm)	0.12886		0.13402	
	Film Coefficient (W/m^2 K)	649.861		614.22	
	Vapor Fraction	0	0	0	0
	Prandtl Number	27.14		28.30	
	Reynolds Number	7053		6751	
	Viscosity Correction	0.965		0.973	
	Nozzles Velocities (m/s)	2.65	2.58	2.65	2.58
	Nozzles Pressure Drop (atm)	0.019859	0.030453	0.01934	0.03119
Heat Duty (MW)		2.889		2.886	
Overall Heat Transfer Coefficient (W/m^2 K)		292.513		330.66	

6. CONCLUSIONS

The obtained results were satisfactory with relative difference in streams temperatures less than 0.6%. With the object-oriented programming language resources available in the EMSO simulator, it was possible to structure the thermal exchange equipment modeling in a modular manner, making use of the composition and inheritance concepts. In that way, the user can include new correlations and methodologies of calculations or to develop new heat exchangers models without need to copy or to do significant modifications in the code.

Future advances in the models may involve the phase change and new types of heat exchangers.

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