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COMBUSTION SIMULATION IN A GAS TURBINE COMBUSTION CHAMBER

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Abstract: *The use of gas turbines for electrical power generation represents an important fraction in the Brazilian energy matrix and shows a trend to grow in the next years. That justifies the importance of knowing how this equipment works, in order to increase the production efficiency, reduce operating costs and minimize the pollutant emissions. Therefore, this article proposes the use of CFD simulation to study the operation of a gas turbine combustion chamber, since this component is directly related to the efficiency of the fuel consumption process. In order to perform the simulation, the software STAR-CCM+® was applied, using models of combustion and emissions available in the software. During the simulation, the flow, temperature, pressure and mass flow profiles in the combustion chamber were evaluated, and the results were compared with the operating parameters of an actual gas turbine used for electric energy generation. From this comparison, it was observed that the flow, pressure and temperature profiles corresponded to reality, which allowed the validation of the used models.*

Keywords: *Gas Turbine, Combustion, Combustion Chamber, Computational Fluid Dynamics (CFD), STAR-CCM+®, Simulations*

1. INTRODUCTION

The use of natural gas in power generation has increased in the last decades and tends to grow in the next years, since this fuel generates less pollutant emission when compared to other sources of thermal energy, such as coal. Besides, the installation of gas power plants demands less time and fewer financial resources. (Tomalsquim, 2016).

Considering this growth, the knowledge of these machines is important to make sure that the power plant operates in an efficient way. In order to guarantee this efficiency, simulations were performed using Computational Fluid Dynamics (CFD) to study the working principles and to improve the design of gas turbines. The study was related to the combustion chamber, which is the component that has greater influence in the total efficiency. In addition, the use of CFD simulations reduce the costs in a project, since it decreases the need of studies in real physical models which would require more time and greater financial resources to perform.

Thus, the combustion chamber studied in this article was modeled using the software STAR-CCM+®, which allowed to determine the parameters of flow, temperature, pressure and mass flow rate profiles of the component, making it possible to evaluate the influence of those parameters in this system.

2. COMPUTATIONAL PROCEDURES

This section presents the definition of the case study, the resources used, the steps followed for the modeling and simulation of the combustion chamber in this article.

2.1 Problem Definition

The combustion chamber studied in this article is part of a heavy duty gas turbine used for power generation in a gas power plant. The gas turbine operates using natural gas in a combined cycle, meaning that the hot gases generated by the combustion in the gas turbine are used to move a steam turbine.

The gas turbine operation starts with an air intake system, consisting of a set of filters and an evaporative cooler. The purpose of this system is to provide clean and cooled atmospheric air to the compressor, in order to prevent the entrance of foreign bodies that could damage the turbine components. Moreover, the evaporative cooler increases the air mass flow rate that is conducted to the combustion chamber through the compressor, increasing the combustion efficiency.

The combustion system is composed by 16 combustion chambers, Figure 1, assembled in a circular arrangement. Each combustion chamber has a basket, where the combustion occurs, a transition piece, which directs the hot gases produced in the combustion to the turbine, and a set of injectors, which has a pilot injector surrounded by eight secondary injectors.

The injectors, Figure 2, conduct the fuel gas into the combustion chamber through calibrated holes that promote a strong turbulence, favoring the mixture between the compressed air that comes from the compressor, and the fuel. The secondary injectors are geometrically equal and they are called stages A and B, alternately arranged around the pilot injector. The pilot injector differs from the others by its size and presence of a complementary part used for air injection, which characterizes the low NO_x emission system.

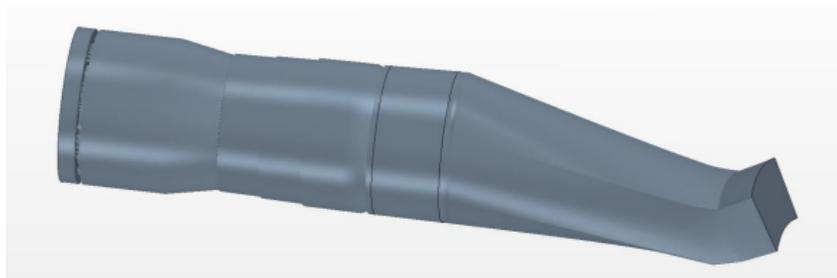


Figure 1. Combustion Chamber in present paper.

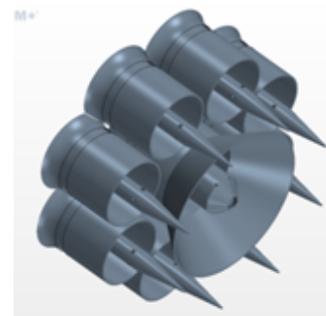


Figure 2. Injectors.

2.2 Resources

The geometry was modeled in the Computer Aided Design (CAD) software SolidWorks® and the simulations were executed using the Computer Aided Engineering (CAE) software STAR-CCM+® version 11.04.010. This software offers a greater number of combustion models when compared to other commercial CFD software, allowing a precise and detailed definition of the parameters that define the problem. It also provides the necessary tools to import and create geometries, to generate a mesh, and to solve the problem by governing equations given by the software.

2.3 Modeling

The mesh was generated after modeling the geometry and it is a non-structured polyhedral mesh with prism layers next to the combustor walls. The polyhedral elements were chosen since they are the most suitable for problems involving heat transfer, vortices and complex flows, which are characteristics that are presented in the studied problem.

The main parameters defined to generate the mesh are shown in Table 1. The low value of the Relative Minimum Size parameter is justified by the presence of very small regions in the fuel injectors, which are essential for the definition of the combustion process, and therefore must be represented with a high degree of precision. The mesh, represented in Figures 3 and 4, had a quality that was suitable to solve the simulation, with absence of negative cells or equal to zero.

Once the mesh has been created, the physical models, boundary conditions and initial parameters were defined. The models selection started by choosing the time, space and material of the analyzed problem. In the case of the combustion chamber studied, the space was three dimensional and the analysis was performed in steady state. As the fuel is natural gas, the material is composed by a gas with several different components. In order to determine the type of reaction that occurs between the gas components, it was necessary to indicate whether the combustion occurs with or without premixed combustion. By analyzing the problem in question and taking into consideration the manner of operation of the injectors, where the pilot operates with premix and the secondary injectors without premix, it was decided to use the

PARAMETER	ABSOLUTE VALUE
Base Size	0.1 m
Number of Prism Layers	5
Prism Layer Stretching	1.5
Prism Layer Thickness	1.5
Relative Minimum Size	1e-4 m
Relative Target Size	0.01 m

Table 1. Mesh generation - Parameters.



Figure 3. Volumetric Mesh.

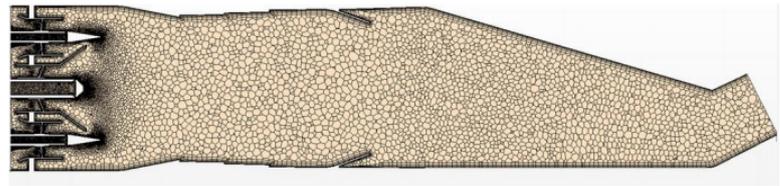


Figure 4. Mesh - Section View.

partially-premixed combustion model.

In order to represent the combustion that occurs in the combustion chamber, the steady partially premixed Eddy break-up combustion model was selected, which offers a general approach, but is still suitable for simulating the combustion process in a gas turbine. This model was also used by Wang Huang and Deng (2009), presenting good results, which validates the use of this model for this simulation. In addition, models of ideal gas and segregated flow were chosen to solve the equations of mass conservation, moment and flow energy, since these models are in accordance with the proposed problem and requires less computational cost.

After the selection of the models mentioned above, it was necessary to select a model that represented the turbulence of the process. It is known that the combustion efficiency depends directly on the turbulence present in the flow, so the Realizable K-Epsilon Two-Layer turbulence model was selected, which is a two-equation model that solves transport equations for the turbulent kinetic energy and the turbulent dissipation rate in order to determine the turbulent viscosity. This model was chosen since it requires less computational cost and provides good and precise results when combined with the Eddy Break-up Model.

The program provides specific models to predict the NO_x emissions in partially premixed combustion. It was selected the NO_x Prompt Model, which is recommended by the User Guide of STAR-CCM+® (2016), where is characterized by the formation of NO_x in a short period of time, occurring mainly in regions that are rich in fuel. It was also selected the NO_x Thermal Model by the Zeldovich method which is a model that presents a general approach and do not demands the definition of specific parameters.

Finally, with the defined models of flow, combustion, turbulence and emission of NO_x, it was decided to add a gravity model to approximate the simulation with the reality. It is important to emphasize that the simulations were performed in a commercial software, which justifies the lack of detailing in equations found in the theoretical basis.

2.4 Parameters Definition

2.4.1 Reference Values

After selecting the models, it was necessary to define the reference values, initial conditions and boundary conditions that influenced the final solution. The reference values, presented in Table 2, are associated with the solver used by the software, which means that not all of these values correspond to physical parameters of the problem.

2.4.2 Initial Conditions

The initial conditions correspond to conditions where the fluid is found when the simulation starts. In this problem, it was considered that at the beginning of the simulation, the combustion chamber was filled with only air under the conditions showed in Table 3.

In addition, the temperature was arbitrarily chosen, since the fuel and the air injection temperature are known and defined in the boundary conditions and during the interactions, the solver of the program calculates the equilibrium

PARAMETER	VALUE
Gravity	[0.0, -9.81, 0.0] m/s^2
Reference Altitude	[0.0, 0.0, 0.0] m
Reference Density	1.169 kg/m^3
Minimum Allowable Temperature	100 K
Maximum Allowable Temperature	5000 K
Reference Pressure	101325.0 Pa

Table 2. Reference Values.

temperature within the combustion chamber.

Pressure	1362675 Pa	
Mass Fraction of Species	CO_2	0.0
	CH_4	0.0
	H_2O	0.0
	C_4H_{10}	0.0
	C_3H_8	0.0
	CO	0.0
	O_2	0.219
	N_2	0.781
Temperature	400 K	
Velocity	1 m/s	

Table 3. Initial Conditions.

2.4.3 Boundary Conditions

In order to apply the boundary conditions, the geometry of the combustion chamber was divided into regions. The regions corresponding to fuel and air inlets were modeled as mass flow inlets, while the outlet was modeled as a flow region. The other regions of the combustor were defined as walls, due to their corresponding of solid surfaces.

The parameters of the boundary conditions such as mass flow, molar fraction of species, pressure and temperature, were known from the gas turbine operation conditions and varied according to the type of condition chosen for each region.

The secondary injectors A and B operate under the same conditions, so their boundary conditions are the same, while the pilot stage operates with a different mass flow. Those parameters are showed in table 4.

Boundary Conditions - Fuel Input (Pilot, A and B)		
Mass Flow - Pilot	0.031875 kg/s	
Mass Flow - A and B	0.271875 kg/s	
Molar Fraction of Species	CO_2	0.0156
	CH_4	0.8934
	H_2O	0.0
	C_4H_{10}	0.0085
	C_3H_8	0.0758
	CO	0.0
	O_2	0.0
	N_2	0.0067
Pressure	2998675 Pa	
Temperature	418.15 K	

Table 4. Boundary Conditions - Fuel Input (Pilot, A and B).

The boundary conditions of the air input were the same as the initial conditions and they are represented in table 5. Different from the boundary conditions of the fuel input, it was chosen to use the mass fraction of the species instead of the molar fraction.

The only parameter in the outlet region was the Split Ratio, which determines the fluid fraction that leaves in this region. In the case of the studied combustor, where there is only one output, the value of the Split Ratio was 1, meaning

Boundary Conditions - Air Input		
Mass Flow	25 kg/s	
Mass Fraction of Species	CO_2	0.0
	CH_4	0.0
	H_2O	0.0
	C_4H_{10}	0.0
	C_3H_8	0.0
	CO	0.0
	O_2	0.219
	N_2	0.781
Pressure	1362675 Pa	
Temperature	693.15 K	

Table 5. Boundary Conditions - Air Input.

that all the mass flow of the gases leaves by this boundary. Moreover, the solid surfaces of the combustor defined as walls regions, were modeled as adiabatic and impermeable, presenting low roughness.

2.4.4 Combustion

To use the Eddy Break-up combustion model it was necessary to define the reactions that occur between the oxidizer and the fuel. Since the fuel is natural gas and the main component of this fuel is methane, the Westbrook Dryer mechanism, indicated in (1) and (2), was used.



Since the molar fractions of the propane (C_3H_8) and butane (C_4H_{10}) are small when compared to the amount of methane present in the fuel, the reactions were considered stoichiometric.

2.4.5 Solvers

Solvers are mathematical models used by the software to solve the problem and they are automatically selected after choosing the models. For each solver it is possible to determine and change some parameters used to solve the problem. In the simulation studied in this article, the only parameter that was changed was the Under Relaxation Factor, which determines the influence of an iteration on the next one, determining the speed that the solver reaches the solution. The values of this factor can range from 0 to 1, where ideally all should be defined as 1. However, considering the complexity of the problems that are normally analyzed, the definition of high values for the Under Relaxation Factors can lead to instabilities in the solver and the non-convergence of the solution. (Ferziger and Peric, 2002; STAR-CCM+® User Guide, 2016).

Thus, at the beginning of the interactions, where only the flow of gases were being analyzed, the values of Under Relaxation Factor were kept standard, while in the combustion phase these values were manipulated to reduce the oscillation of the residuals.

2.4.6 Convergence of Solution

One of the most used methods to determine the convergence of a solution obtained through iterative methods is the analysis of the difference between the results of two consecutive iterations, which can be done through the residual analysis.

The residuals are calculated in each cell at each iteration and represent how the discrete equation is satisfied, in other words, the error in the solution of a variable. A simulation is considered converged when the values of the residuals are reduced by three or four orders of magnitude of its initial value. However, the results must be monitored to ensure the convergence, since the residuals are influenced by the initial conditions defined by the user, so that if the initial values are close to the final solution, the decay of the residuals may be very small (Ferziger J. and Peric M., 2002).

2.4.7 Running the Simulation

The residual graph obtained after the end of the simulation is presented in Figure 5. It is possible to notice that there are three peaks of residuals representing the flow of gases, the combustion and the activation of the NOx models.

The first region performed 1300 iterations until the flow reached a steady state. At this point, the combustion model was activated and the simulation executed another 2100 iterations until the convergence of the solution. It is possible to observe that even with some oscillations, the residuals were in an order of 10^{-3} or less, fulfilling the convergence criterion. Finally, with the convergence of the combustion simulation, the NOx emission models were activated and the simulation performed another 2600 iterations, until the convergence again.

Although the residuals of CO₂ presented values slightly higher than the recommended, after 6000 iterations the simulation was considered converged, due to the coherence of the results of the variables of interest and the small influence of the carbon dioxide in the combustion process.

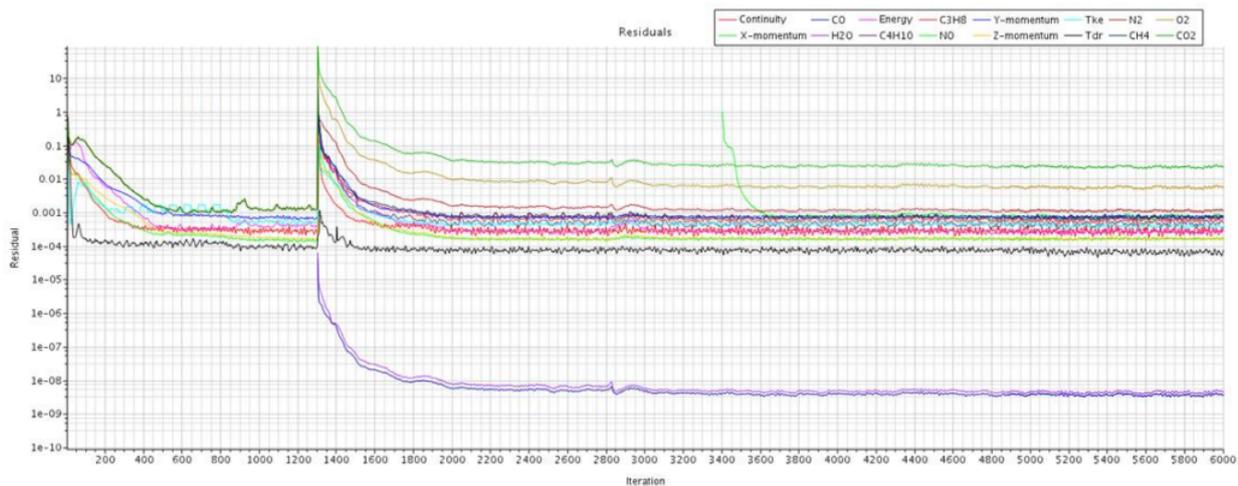


Figure 5. Residuals of the Simulation.

3. RESULTS AND DISCUSSIONS

After the convergence of the solution, scalar and vector scenes were created to visualize the solution graphically. The first one represents the streamlines, shown in Figure 6. In this scene, it is possible to visualize the strong turbulence generated by the combustion process as expected. Also, it is possible to observe the presence of vortices in the central area of the combustion chamber, starting intensely in the basket close to the injectors, Figure 7, and propagating until the end of the transition piece.

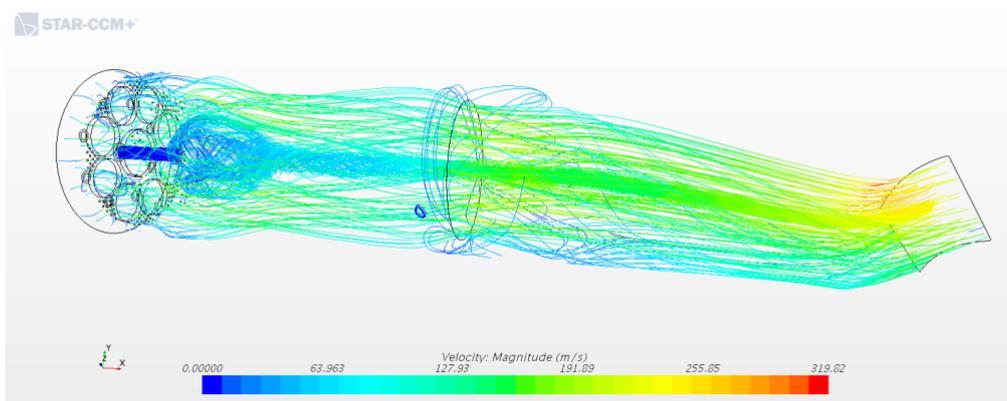


Figure 6. Flow Profile.

From the velocity vector scene, Figure 8, it can be seen that the maximum velocity reached by the gases within the combustion chamber is approximately 315 m/s with an average of 160m/s. Those results are consistent and the high speed is justified by the injection of fuel and air in high pressure by the combustion process itself.

The temperature was the main parameter analyzed in this simulation, since that with this result is possible to identify the flame region and evaluate the average temperature in the combustion chamber, allowing the validation of the results. In Figure 9, it is possible to notice that the flame region, which is the region where the natural gas burns, has temperatures around 2600K and it is located near the injectors. This is a parameter that is already known, allowing the validation of the simulation.

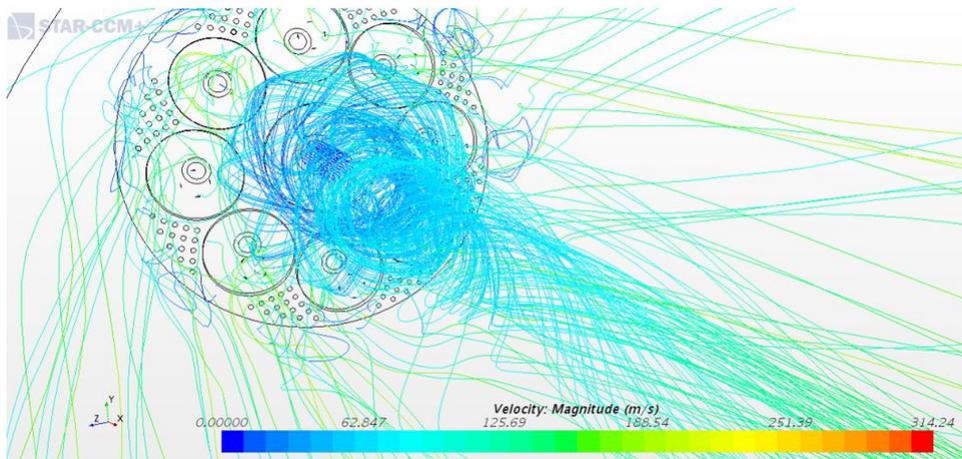


Figure 7. Internal Flow - Basket

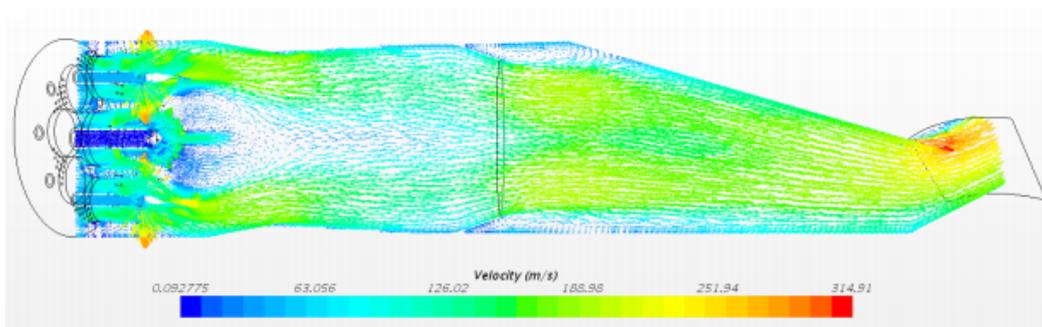


Figure 8. Velocity Vector Scene.

It can be seen that the largest flame area is close to the secondary injectors and not in the center of the basket as expected. This behavior can be justified by the presence of the air injection piece in the pilot injector, which causes a greater dilution of the fuel in the air. In addition, the flame zone should be located in a region further the injectors, since the actual reactions do not occur instantaneously after the injection of the fuel. This behavior is justified by the way the Eddy Break-up model works, assuming that all reactions occur quickly after blending the fuel with the oxidant.

By evaluating the flame temperature, it can be seen that its value is higher than predicted in the literature for the burning of methane, which would be approximately 2200 K under ideal conditions. This high temperature is justified by the Westbrook Dryer mechanism, adopted for the combustion of methane that overestimates the flame temperature.

The average temperature of the combustion chamber output is given by the turbine manufacturer, and this temperature is approximately 1561 K. Considering the errors associated by solving the problem through the simulation and the low complexity of the models, the average temperature found, which was approximately 1450 K, can be considered as an indication of convergence of the solution proposed, confirming the validity of the model.

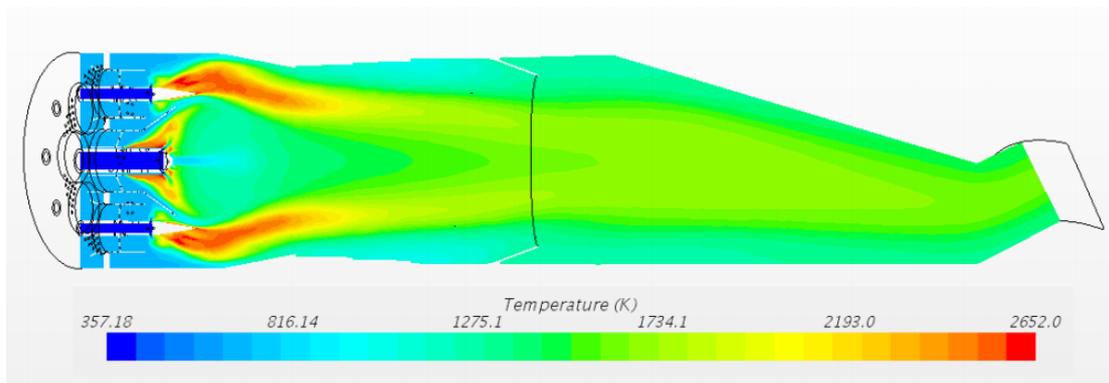


Figure 9. Temperature Profile.

The pressure profile, showed in Figure 10, is another important parameter in the combustion process. It can be seen that the pressure shows small variations along the combustion chamber. The largest value correspond to the fuel injection

pressure, considering the lost of pressure that occurs due to the presence of the injectors holes.

The pressure range from 1.1056 to approximately 1.3213 MPa. This behavior was expected, since the simulation was developed in a steady state condition. It is known that the actual operating pressure of the combustion chamber is approximately 1.46 MPa, and considering the simplifications used during the modeling of the problem, it can be said that the pressure profile found, which presents an average pressure of 1.21 MPa, is as expected, validating the simulation.

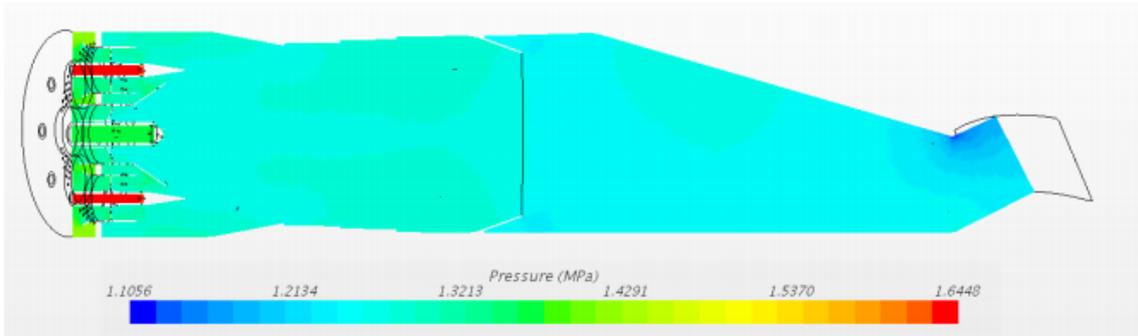


Figure 10. Pressure Profile.

The evaluation of the fuel mass fraction profile within the combustion chamber is important for the verification of the region in which the combustion occurs and for analyzing whether the combustion occurs completely or incompletely. Therefore, the mass fraction profiles of butane, methane and propane were analyzed.

The Figure 11 shows the mass fraction profile of CH_4 . It is possible to see that the combustion of this component occurs almost completely as soon as the fuel is injected into the combustion chamber. The same result occurs with the mass fraction profile of propane and butane.

The fast consumption of these fuel components can be justified by the Eddy Break-up combustion model, which assumes that all reactions occurs immediately after the mixture between the fuel and the oxidant in the combustion chamber.

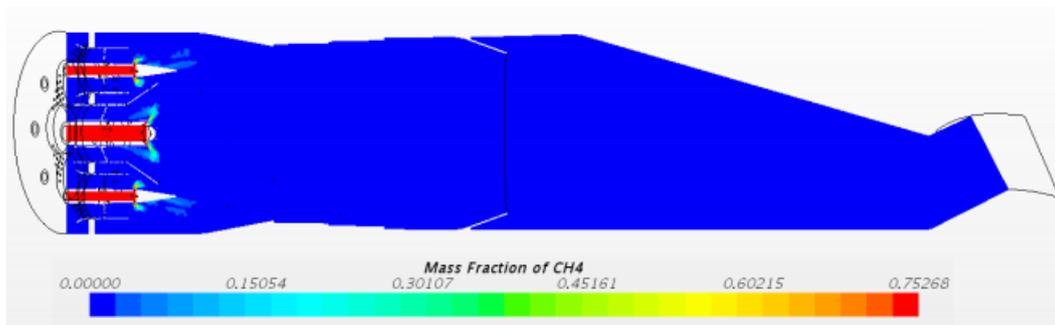


Figure 11. Mass Fraction - CH_4 .

It was also analyzed the mass fraction profile of CO, showed in Figure 12. By comparing this profile with the temperature profile, it can be seen that the regions with the highest concentration of carbon monoxide correspond to the regions where the temperatures are higher. This behavior is expected since the CO production increases with increasing temperature, validating the simulation.

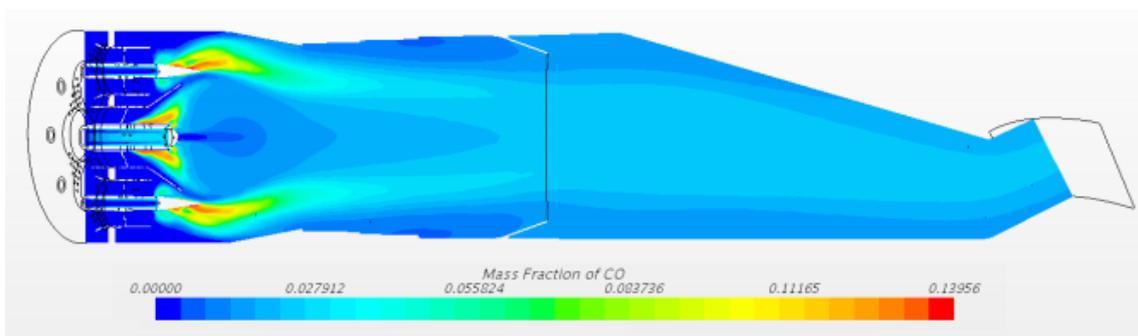


Figure 12. Mass Fraction - CO .

The same analysis was performed for the NO profile, showed in Figure 13. The behavior was the same observed in the CO analysis, where the highest concentration of NO correspond to the regions where the temperatures are higher.

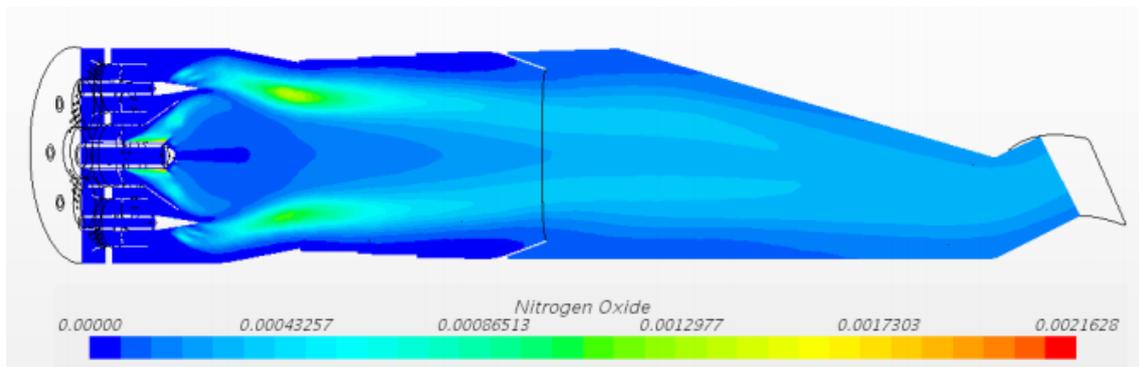


Figure 13. Mass Fraction - *NO*.

Although this behavior was expected, the values obtained for NO in the simulation especially at the exit of the combustion chamber, are very low. Moreover, these values are very low when compared to the values of the mass fractions of CO, since that in regions with higher flame temperatures, the production of nitric oxide must be higher than that of CO.

The reference values found in the literature for the amount of NO and CO produced in a combustion process are given in parts per million by volume (ppmv) based on a 15% oxygen condition. Since STAR-CCM+® does not offer the option of visualizing the results in this unit and to make the conversion of the mass fraction to the corrected ppmv it would be necessary to know the characteristics of the fuel that are unknown, it was not possible to validate the results of these parameters.

4. CONCLUSION

Simulations of natural gas combustion were run in a CFD commercial software in order to analyze the main characteristics of the combustion that occurs in a gas turbine combustion chamber. The problem was modelled based on real operation parameters found in the literature, in order to describe the problem as close as possible to the reality, considering the limitations found. The simulation results, when compared to a real gas turbine operation, allowed the validation of the models. The flow profile presented the turbulence that was expected due to the combustion process and showed formation of eddies next to the injectors. Although the temperature and pressure profiles presented results that do not correspond exactly to the known operation parameters due to simplifications applied in the modeling process, the results were consistent with the models, making possible to validate them.

In order to obtain better results for the profiles of temperature and pressure it will be necessary the utilization of complex models that would incorporate more details about the reaction mechanism. In addition, tests with different models of turbulence can be performed to analyze the influence of this phenomenon in the combustion process. In order to predict the mass flow profile of NO_x that are consistent with reality, it will be necessary a better study and evaluation of the available emission models for use in the simulations, including testing different parameters and analyzing the influence of combustion models and reaction mechanism.

Another important phenomenon that must be studied when the analysis of gas turbine operation is performed is the combustion dynamics, which consists the pressure pulsation generated by the combustion process. To study this phenomenon, it would be necessary to perform simulations in the transient state, aiming to monitor the pressure variations throughout the combustion process.

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