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BEHAVIOR ANALYSIS OF OZONE ADDITION TO AN ETHANOL/O₂ REACTIVE FLOW SIMULATION.

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Abstract. Rocket engines powered by liquid propellant use combustion processes with sprays. The main advantages of this process are related to the increase of flame control, thus enabling the interruption and restart of the combustion process and higher safety in controlling the fuel. Based on the above, this paper presents an analysis of a reactive axisymmetric flow, using a free jet liquid fuel injection. Ethanol and Oxygen are used as fuel and oxidizer, respectively, and Ozone as an additive to increase combustion efficiency. The behavior of the reactive flow and flame formation are calculated by CFD, whereas the phenomenon is approached by the Finite Volumes Method in a mesh generated by Ansys®Fluent. The mechanism of chemical kinetics considers a global reaction, irreversible and the combustion regime considered is non-premixed. The results obtained for speed and temperature are compared to experimental results in the literature and show the general behavior of the adopted simulation conditions, showing that the arrangement of defined models managed to capture reasonable results for comparison purposes.

Keywords: : Ansys®Fluent, Reactive Flow, Ethanol, Ozone.

1. INTRODUCTION

Currently, aerospace technology is present in an extremely significant way. The media and global positioning systems rely on satellites that orbit the earth to obtain and repeat information. These satellites are launched into orbit by rockets, which can be used in various types of propulsion. For this application, sufficient force is required to overcome the escape velocity of the Earth's atmosphere. Therefore, the most appropriate propulsion is the direct combustion of a fuel, which may be liquid. The use of liquid rocket engines in space launchers offers advantages such as the possibility of re-ignition in flight and the control of the magnitude of the impulse vector. One of the ways to increase the performance of this type of propulsion is by using ozone as an additive, applied to obtain the highest yield for chemical reaction occurred. Therefore, it is extremely important to investigate the behavior of pulverized fuel combustion. Figure 1 below shows the air and fuel being sprayed, and a second inlet air, where ozone is injected as additive.

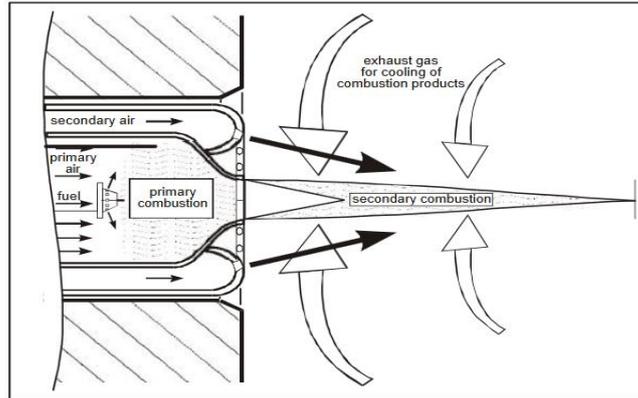


Figure 1: Nozzle of an air staged high velocity burner (Wüning, 2013).

The spray performed is essential in the analysis of the combustion, because it establishes in what form the combustion process will occur. This formation involves transport and fluid dynamics phenomena, which will be controlled by the combustion of a set of individual droplets or by the combustion of a cloud of fuel vapor. This internal combustion is affected by the interaction between the liquid and the gaseous phases, thus facilitating the greater interaction of the reaction.

2. EXPERIMENTAL PROCEDURE

Ansys®Fluent software was used in simulations and mesh generation. Thus, it has become necessary to create a geometry, which has been simplified in a two-dimensional view with an air-fuel inlet nozzle and an axisymmetric axis, thus allowing only half drawing geometry, reducing computational costs. This software allows interactions among the viscosity models, in which the used ones are the model *k-ε* standard and *k-ε* achievable. The first presents a semi-empirical model and it is assumed that the flow is completely turbulent and the effects of the turbulent viscosity are negligible; the second presents a better performance for flows involving rotation, layer under strong pressure gradient, separation and recirculation. The internal pressure is set to 60 bar and in this simulation was adopted the input temperature of the elements at 300K, in the combustion the permanent regime was considered not premixed since the reagents enter the computational domain without being mixed, therefore assumed that the equivalence ratio is 0.3. The configuration adopted to perform the simulation was spray, since it is considered a multiphase flow, where there is in the domain a dispersed liquid phase in the form of drops and a continuous gas phase. This in the computational field is a type of free jet, consisting of a single entrance for the three chemical elements proposed, so that they do not have any interference in the jet and the flow, as shown in the schematic drawing of the physical problem (Figure 2). An inlet nozzle with a 10 millimeters diameter was considered, where both air and fuel droplets flow. The blue arrow represents air, the red one represents the fuel and black represents the additive.

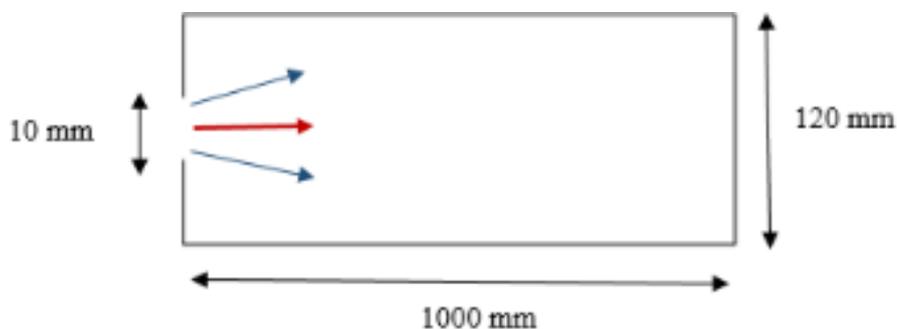


Figure 2: Geometry Scheme (Costa, 2016)

Ansys Meshing Software was used to generate a structured mesh based on the mentioned geometry, and as it is of a uniform two-dimensional geometry, quadrilateral elements were adopted. The mesh was composed of 8400 elements and 8643 nodes, shown in Figure 3.

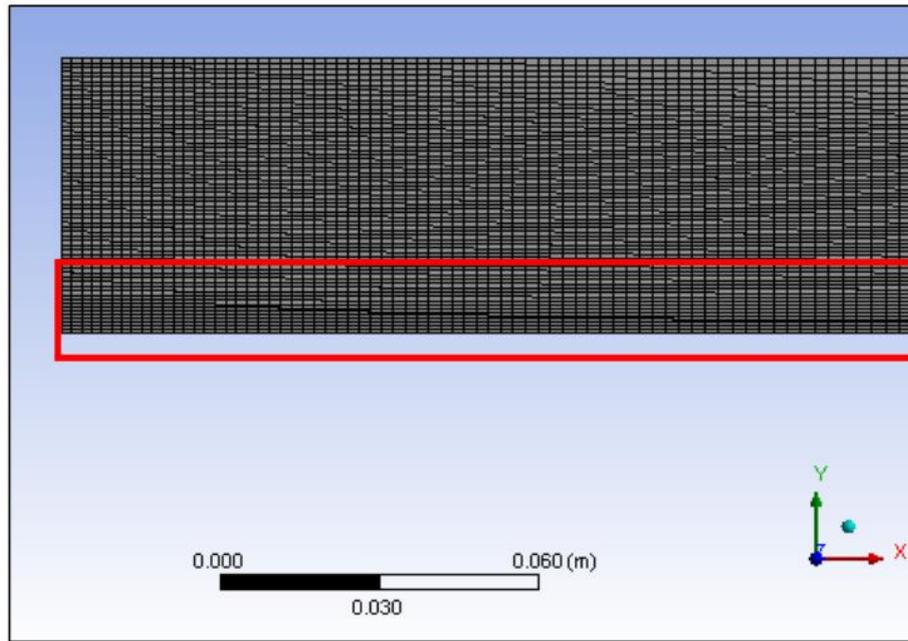


Figure 3: View of mesh generated in ANSYS Meshing.

3. COMPUTATIONAL STUDY

The spray combustion phenomena presented in this work consists of a flow that has turbulence, chemical reaction and interaction between the turbulent flow in the atomization of liquid ethanol fuel and with the additive ozone, the turbulence models chosen for the treatment of turbulent flow are widely diffused in the literature, and since it is satisfactory for the study, the chemical reactions that occur in this process are performed by the combustion models, according to the form of reagents that mixes well the premixed and partially premixed, as the fuel droplets are in liquid form the Discrete Phase-MFD model is implemented, so it is possible to detect change in droplet injection results until its evaporation.

The k - ε turbulence models adopted have two equations that allow the determination of mixing length and time scale through the resolution of two different transport equations, which are present in the ANSYS FLUENT model k - ε , on which it has a base in transport equations for the kinetic energy of turbulence k and its dissipation rate ε , these are presented below.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k V_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon V_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \quad (2)$$

In these equations G_k is presented the generation of turbulent kinetic energy due to the velocity gradients, G_b the generation of turbulent kinetic energy due to buoyancy, Y_M represents the contribution of the floating expansion in compressible turbulent flow to the overall dissipation rate. The realizable K - ε model is also adopted for the work, because it presents a better performance and thus can compare the obtained results, as well as mathematical modeling for transport equations for K and ε are next.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k V_j) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (3)$$

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_j}(\rho\varepsilon V_j) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 S_\varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{V\varepsilon}} + C_{1\varepsilon} \frac{\varepsilon}{\kappa} C_3 G_b + S_\varepsilon \quad (4)$$

At where

$$C_1 = \text{máx} \left[0.43, \frac{n}{n+5} \right] \quad (5)$$

$$n = S \frac{\kappa}{\varepsilon}, S = \sqrt{2S_{ij}S_{ij}} \quad (6)$$

4. NUMERICAL STUDY

In the numerical study of the combustion of liquid fuel, we consider that some mathematical equations that describe the movement of particles in the reactive flow are the transport equation, ANSYS FLUENT adopts the conservative form of the equations, considering that, within an infinitesimal control volume, the spatial variation.

$$\frac{\partial}{\partial t} \rho + \nabla \cdot \rho \vec{V} = 0 \quad (7)$$

Therefore, for the fluid system properties to be conveyed continuously through a volume can be described by the momentum equation, which was considered a Newtonian fluid, the exact solution variables of the Navier-Stokes equation are decomposed into the mean components and floating.

$$V_i = \overline{V_i} + V_i' \quad (8)$$

The quantity of motion for compressible fluid equation adopted in this work is presented as

$$\frac{\partial}{\partial t}(\rho V_i) + \frac{\partial}{\partial x_j}(\rho V_i V_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial V_l}{\partial x_l} \right) \right] + \frac{\partial}{\partial x_j} (-\rho \overline{V_i' V_j'}) \quad (9)$$

Thus, the left side of the equation represents the rate of change in the amount of movement that crosses the control surface per unit volume, the right side of the equation represents the external forces by volume units, which are the ones that act in the volume of control as the fluctuation generated by the turbulence.

5. RESULTS AND DISCUSSION

The results of the spray combustion simulations were analyzed considering the same computational domain. The different velocity and temperature profiles were analyzed, corresponding to a drop diameter range. In the region near the nozzle, defined by the section $x/D = 0.3$, the model captures results closer to the ones in the literature.

Considering the same geometry and computational domain, the amount of air mass, corresponding to an injection velocity of 24 m / s, was analyzed in the case of the reactive flow. The model k-ε standard was used to predict the flow range, pressure, temperature and molar fraction of each element.

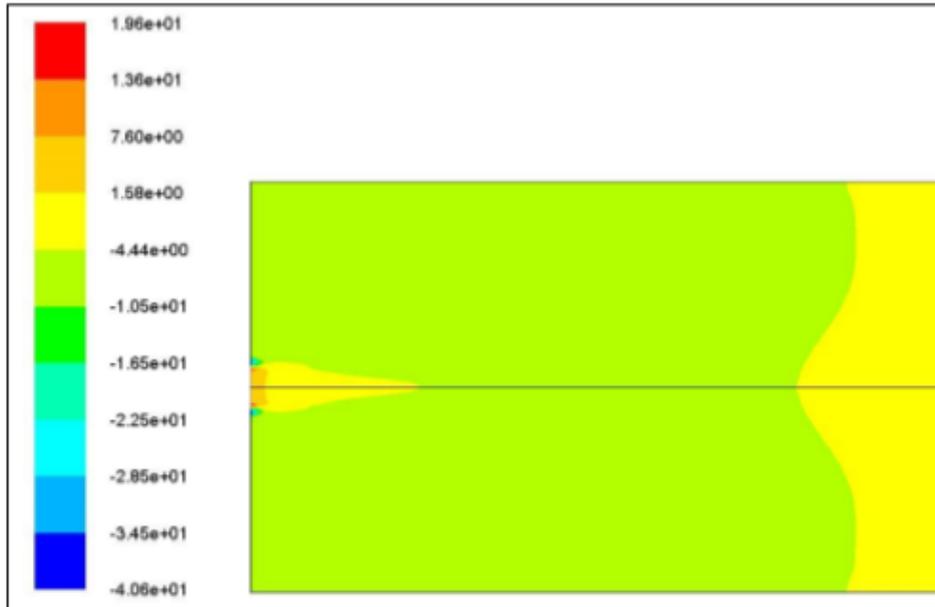


Figure 4: Pressure field (Pa).

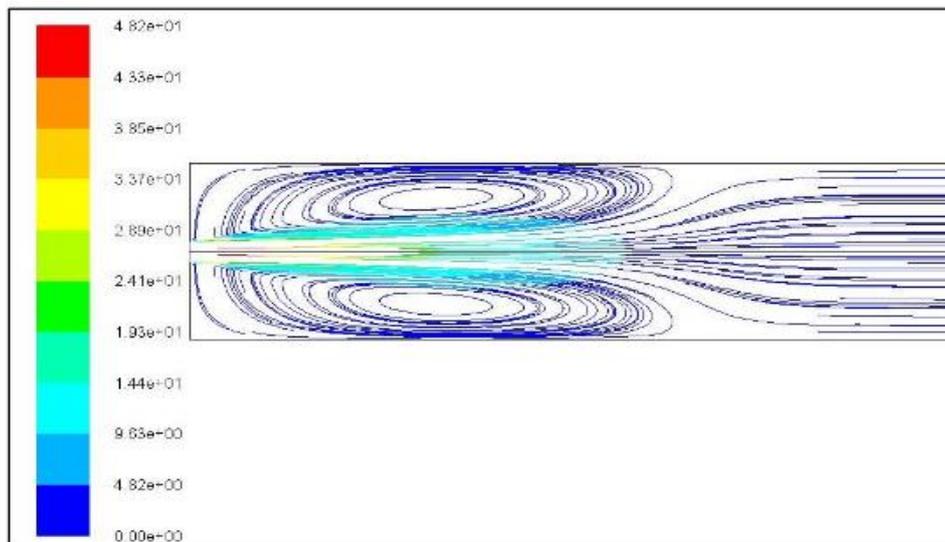


Figure 5: Lines of speed currents.

Thus, Figure 4 shows the pressure field indicating that in the region near the exit nozzle it presents areas of low pressure, where it characterizes a space of recirculation of the flow. Therefore, in the figure when analyzing the speed lines, observe areas of recirculation, indicated in the fields of pressure. Thus it is possible to perceive the point of stagnation, where the flow becomes critical and the velocity has its positive values, the position of this stagnation point defines the length of the recirculation zone and the flow after this region constitutes the main flow.

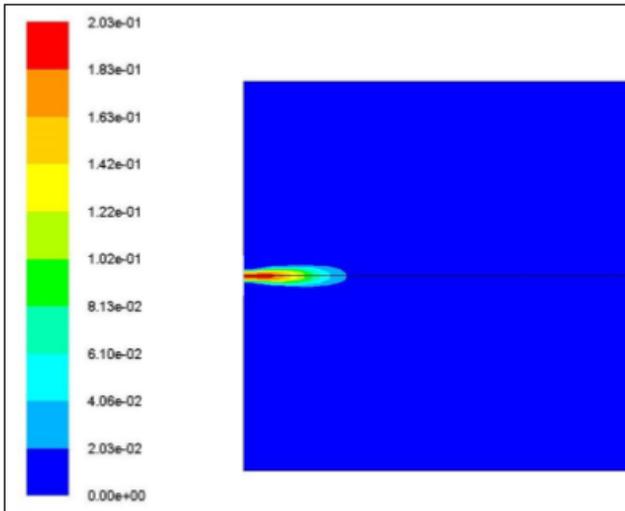


Figure 6: Molar fraction of the fuel

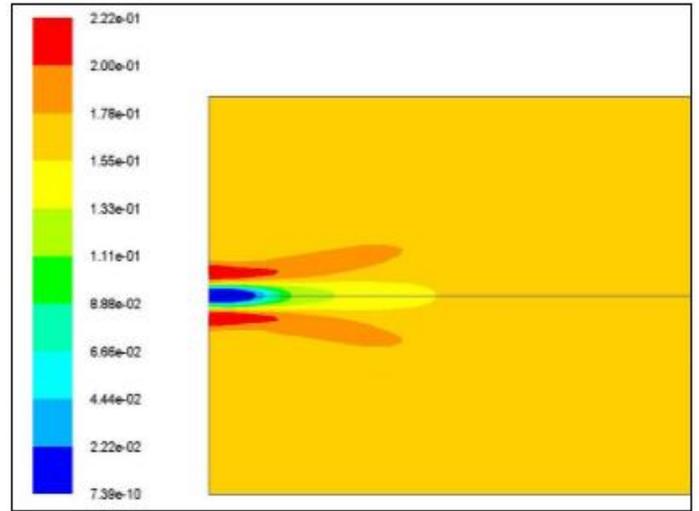


Figure 7: Molar fraction of Oxygen.

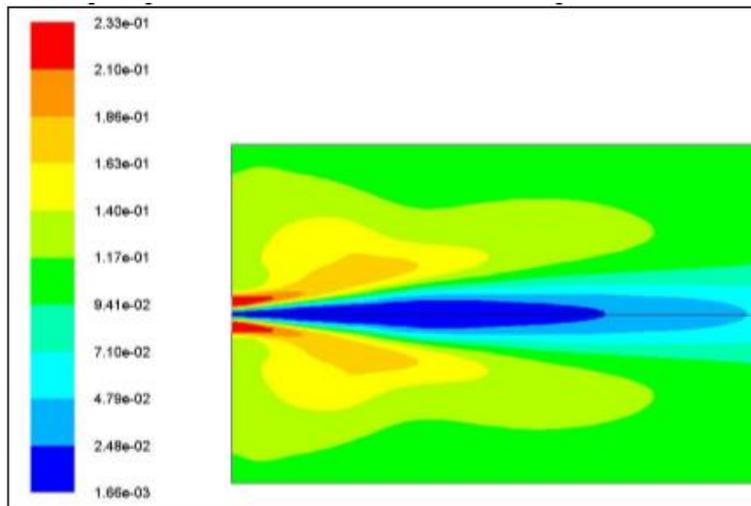


Figure 8: Molar fraction of ozone.

The above mass fraction of fuel only proves the fuel concentration around the outlet nozzle and that the amount of fuel is reducing as it moves away from the nozzle, thereby increasing the degree of flow turbulence, this confirms when analyzing and therefore it is possible to observe the dissipation of ozone when it is with oxygen and with the fuel.

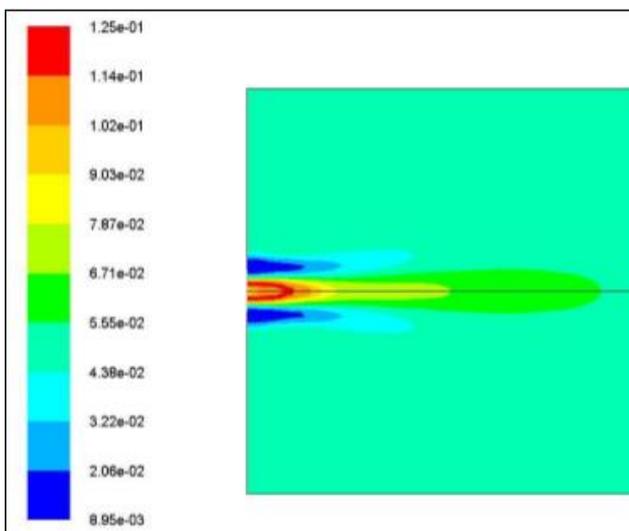


Figure 9: molar fraction of CO₂.

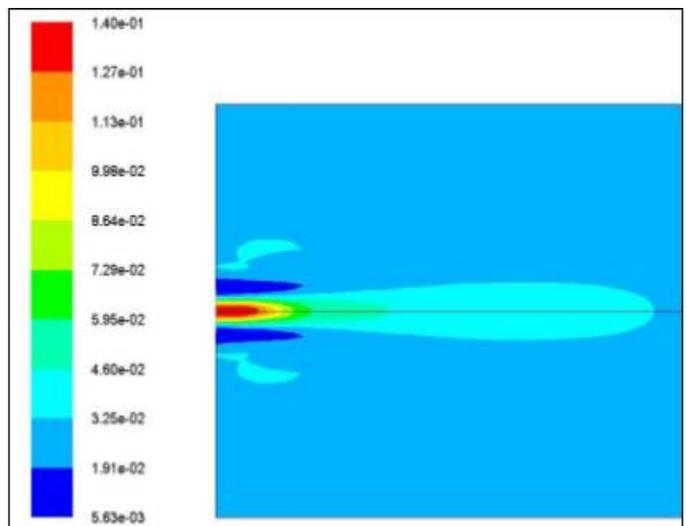


Figure 10: Molar fraction of H₂O.

The concentration fields of the CO₂ mole fraction are distributed around the flame region, where through the complete combustion is presented, being a chemical element presented at the end of combustion together with the water that is sampled as final compound so the distribution of the water vapor concentration field as it is installed near the nozzle and local flame region that occurs combustion, thus observing the behavior is similar to the CO₂ concentration field.

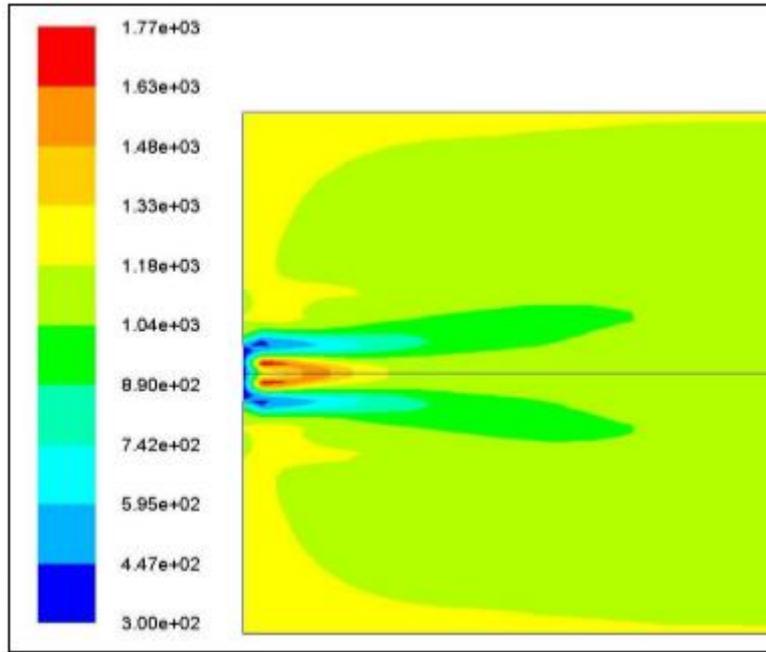


Figure 11: Temperature field.

In the figure 11 shows the distribution of the temperature field where it indicates the formation of the flame near the outlet nozzle, which is observed by the temperature gradient difference, since the maximum temperature recorded is 770K, so it is observed that at the outlet of the nozzle the temperature recorded is the highest because the region immediately next has a larger amount of fuel, this is due to the ethanol fuel conditions, because it is a volatile substance, combining this effect with the increase of temperature of the air provoked by the effect of convection and the addition of additive Ozone, causes the mixing fraction to rapidly increase close to the outlet nozzle, thus, consequently, the formation of the flame. Therefore, the effect of the ozone additive generates the increase of the combustion rate for pre-mixed flames of ethanol and air, where it was analyzed by the simulations. The rates of laminar combustion with O₃ additive obtained results in comparison with the literature. Therefore, the addition of O₃ as an additive allowed a comparison of the measurements. Burning velocity where the remarkable increase in firing speed was observed under stoichiometric conditions. The simulation data show an increase in the maximum firing rate of ~ 5.5%.

6. CONCLUSIONS

In this paper, a study was conducted in a reactive axisymmetric turbulent flow using ethanol as fuel, air as oxidizer and ozone as additive. The behavior of the velocity field was observed with the addition of ozone in the combustion reaction. The presence of O₃ in the combustion of ethanol increases the burning rate. Therefore, improvements in the flame velocity behavior were observed, so that it could be applied in an auxiliary method of swirling in the outlet nozzle as well as the use of other fuels.

7. REFERENCES

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