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REACTIVE FLOW SIMULATION USING LIQUID BIOFUEL

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Abstract. *The present study describes the analysis of axisymmetric reactive flows using free jet liquid fuel injection with the goal of verifying the influence of fuel injection type and to estimate temperature, velocity and species concentration fields. The combustion reaction analysis is carried out for ethanol, having as oxidant the air under ambient conditions. The combustion regime considered is non-premixed. Two types of reaction mechanism were used, the mechanism of chemical kinetics considering a global, irreversible and infinite rate reaction, and the detailed chemical kinetic mechanism imported from the CHEMKIN program file. The reactive flow is solved numerically by the Finite Volume Method in a structured mesh using the ANSYS Fluent computational code. The velocity and temperature results are compared with experimental data from the literature and show the general behavior of the adopted simulation conditions. The effect of the variation of the fuel injection type and the kinetic reaction mechanism was analyzed from the results of the concentration fields of the chemical species CO, CO_2 and H_2O, as well as the temperature field, respectively.*

Keywords: *Reactive flow, Ethanol, Non-premixed combustion.*

1. INTRODUCTION

Currently, combustion processes are responsible for a large part of world energy production, including Brazil, in transportation (cars, airplanes, trains, ships, etc.), thermoelectric plants, industrial processes, domestic heating, generators, food cooking and others. Due to great part of fuels being fossil fuels, there is a growing concern with pollutant emissions, which makes biomass derivatives a potential alternative, such as ethane which is a liquid biofuel widely used mainly in the transportation industry. Therefore, the analysis of these biofuels is a relevant issue to be studied aiming to improve combustion efficiency and to avoid a higher production of pollutants, including the emissions of unburned hydrocarbons and secondary products.

Spray turbulent flames are relevant to many practical combustion devices, such as internal combustion engines, gas turbine combustion chambers, rockets and missiles burners, as well as burners for boilers, furnaces and process heaters (Turns, 2000). Consequently, the analysis of pulverized fuel is of great importance for the investigation of the combustion efficiency of biofuel derivatives.

Despite the increase in research using biofuels, there is still a need for further exploration of the combustion process for this type of fuel, mainly from the point of view of numerical simulation, since in the literature most of the works are experimental. This highlights the importance of many works such as de Rochaya (2007), Duwel et al (2007) and Hu and Kurose (2018) that have attempted to find or propose models in the study of these phenomena. The objective of this work is to simulate pulverized fuel combustion, ethanol, for the analysis of reactive flow behavior and flame formation, with the purpose of estimating the temperature, velocity and concentration fields of species in the products of combustion reaction, verify the combustion efficiency and the behavior of the chemical species under different boundary conditions. The results will be compared to those obtained by Rodrigues et al. (2015) and Masri and Gounder (2010).

2. METHODOLOGY

The simulated nozzle consists of an air-free circular jet which carries fuel droplets, with a high temperature condition at the inlet of the nozzle, to provide the heat that would be supplied by a pilot flame. The turbulence model adopted was the κ-epsilon because it is the most widespread among these types of simulation, also it represents the reality with certain precision and a relatively low computational time. The flames were simulated with the Marinov (1999) reaction mechanism composed of 56 species and 351 reversible reactions, and imported from the CHEMKIN program. Due to the presence of droplets in the flow, it was used in the simulation the continuous phase, which represents the gas phase modeled by Eulerian equations, and the discrete phase, representing the dispersion of the droplets by Lagrangian equations, these phases were coupled.

2.1 Turbulence Model

In the approach of Reynolds-averaged Navier-Stokes equations (RANS), the variables are calculated to their mean values. The RANS equations are obtained by the mean of the instantaneous equations. Due to the necessity of a closing rule for the transport equations, turbulence models are used according to the flow dynamics. For the combustion study, the reaction in turbulent flow requires a turbulent viscosity model that captures the effects of the chemical species modification and the release of heat from the process in the flow. The widely used turbulent viscosity models are the κ-ε models, because they have robustness, shorter computational time and are consolidated models.

Turbulence models of two equations allow the determination of both mixing length and time scale by solving two different transport equations. In the derivation of the model, it is assumed that the flow is totally turbulent, and the effects of molecular viscosity are insignificant. The κ-ε models are valid for completely turbulent flows.

The realizable κ-ε model differs from the standard model in two respects, the first because it has an alternative formulation for turbulent viscosity, in which G_μ is no longer a constant but calculated by (Fluent, 2011):

$$G_\mu = \frac{1}{A_0 + A_s \frac{kU^*}{\varepsilon}} \tag{1}$$

And secondly, its transport equation has been modified to the dissipation rate ε, which has been derived from an equation for the medium-quadratic transport of vorticity fluctuation.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_j) = \frac{\partial}{\partial x_j}\left[(\mu + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\epsilon - Y_M + S_k \tag{2}$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_i}(\rho \epsilon u_j) = \frac{\partial}{\partial x_j}\left[(\mu + \frac{\mu_t}{\sigma_k})\frac{\partial \epsilon}{\partial x_j}\right] + \rho C_1 S_\epsilon - \rho C_2 \frac{\epsilon^2}{k + \sqrt{\nu\epsilon}} + C_{1\epsilon}\frac{\epsilon}{k} C_{3\epsilon} G_b + S_\epsilon \tag{3}$$

In which G_k represents the kinetic energy generation due to the average velocity gradients, G_b is the generation of turbulent kinetic energy due to fluctuations. Y_M represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, C_2, and $C_{1\varepsilon}$ are constants σ_k and σ_ε are the turbulent Prandtl numbers for k and ε, respectively S_k and S_ε are user-defined source terms (Fluent, 2011).

2.2 Combustion Model

For the combustion treatment, the non-premixed combustion regime was considered. In non-premixed combustion the reactants enter the computational domain without being mixed, and two regions are observed; one where the fuel and oxidant are separated and another is the reaction zone where the heat of combustion is generated. That reaction zone is between the fuel and the oxidant.

This option was made due to the fact that the configuration of the physical problem studied here is adequate, as well as advantages such as greater safety in the storage and transportation of the fuel avoiding the risk of autoignition because the reactants are only in the combustion chamber. Although the configuration studied here considers the fuel and oxidant entering together through the same nozzle in the computational domain, the fact that the fuel is in the form of droplets being carried by the air still allows to maintain the non-premixture characteristic since the mixture does not occur with the liquid but occurs only after fuel evaporation and then vapor mixes with the air surrounding the droplets.

In ANSYS Fluent, non-premixed combustion modeling involves the solution of transport equations for conserved scalars. The concentrations of the species are derived from the predicted mix fraction fields. The thermochemical calculations are pre-processed and stored to be required whenever required by the program through the chemical interaction with the turbulence given by the PDF Method (Probability Density Function) with pre-assumed form.

2.3 Probabilty Density Function Method

The combustion in turbulent flows considers that the flow is governed by the equations of conservation of momentum, but the solutions of these equations demand a high computational time for the calculations. The species are described by the RANS equations, however unknown terms for rate of dissipation and reaction arise. The program treats the turbulent flow in non-premixed combustion from the diffusion gradient and convection through the turbulent flow as a reinforcement of the diffusion effect. These equations, even if they can be modeled by models such as Eddy-Dissipation, or EDC Finite Rate, the reaction speed generally has significant non-linear behavior so the chances of calculation errors are too high.

Assuming this, the Probability Density Function derives the equations of Reynolds, species and energy averages for a single-point transport equation. Where this function considers the fraction of time of each state of species, temperature and pressure in the flow. From the PDF, any thermochemical state at the single point (e.g., the mean temperature, the average reaction rate) can be calculated (Fluent, 2011). Written mathematically:

$$p(f)\Delta \mathrm{f} = \lim_{T\to\infty} \frac{1}{T} \sum_{i} \tau_i \tag{4}$$

The PDF method is described by the instantaneous relations between mixing fraction and species fractions, density and temperature. In this case, ANSYS Fluent predicts the reactive turbulent flow, taking into account the prediction of the average values of the floating scalar. Like these mean values of the turbulent flow, the instantaneous values that depend on the chemical - turbulence interaction model are treated by the code using the PDF - shape approach - assumed as the closure model when using the non - premixed combustion model.

2.4 Flamelet Model

The flamelet approach models consider a turbulent flame as a set of discrete laminar flames. Individual diffusion flamelets with the same laminar flame structure are considered as in simple configurations, and are obtained through experiments or calculations (Fluent, 2011). Using this approach, ANSYS Fluent allows you to import CHEMKIN files from mechanisms with detailed chemistry allowing results that report data closer to reality. The probability density function method incorporates these diffusion flamelets into the turbulent flame.

This possibility of treating the turbulent flame with effect of the actual chemical kinetics, is a great advantage of this approach. The computational computation time reduction is obtained since the chemical kinetics calculations are preprocessed and stored for later reference, whenever necessary. However, the flame diffusion model of permanent diffusion is limited to the combustion modeling with relatively fast chemistry. The flame is treated to respond instantaneously to aerodynamic stress; therefore, the model may not capture deep non-equilibrium effects, such as ignition, extinction, and slow chemistry as NOx (Fluent, 2011).

In the laminar flamelet model, it is assumed that the structure of the turbulent diffusion flame is locally that of a laminar diffusion flame at the same instantaneous value of the mixture fraction Z and scalar dissipation, χ (Tsuji and Yamaoka, 1966, Peters, 1984). The scalar dissipation rate is defined by (Rochaya, 2007):

$$\chi = 2\delta \left[\left(\frac{\partial z}{\partial x}\right)^2 + \left(\frac{\partial z}{\partial y}\right)^2 + \left(\frac{\partial z}{\partial z}\right)^2 \right] \tag{5}$$

2.5 Continuous and Discrete Phase Coupling

ANSYS Fluent allows the coupling between the discrete phase and the continuous phase, so that the continuous phase is constantly influenced by the effects of the discrete phase and vice-versa. The dispersed phase can exchange momentum, mass and energy with the fluid phase.

The program calculates the particles trajectory by storing the input and output results of heat, mass and momentum in the particle flow, these values are required and included in the continuous phase calculations. In this way, not only the influence of the gas phase in the liquid are taken into account, but also the effects of the discrete phase in the continuous phase.

2.6 Atomization

Considering that in sprays the atomization happens soon after the exit of the nozzle, it is presumed that there is no liquid nucleus; all liquid is transformed into droplets, that is, primary breakage of droplets. The program provides some modeling options for dispersion of droplets through atomizer models. The atomizer creates initial conditions for later calculation of the trajectory of the particles from the definition of the initial diameter of the drops, the speed and cone angle of the spray. These values can be obtained in empirical relations based on experimental data. Since the state of the internal flow through the nozzle is known, calculation of the initial droplet diameter and velocity were performed.

The atomizer models use stochastic trajectory and scaling to achieve a random distribution. Stochastic trajectory selection is the initial random dispersion of the droplet direction. Every atomizer model provides an initial dispersion angle and the stochastic trajectory selection takes an initial direction within this angle. This approach improves the accuracy of results for fuel spraying. The droplets will be more evenly distributed between the computational cells near the atomizer, which improves coupling with the gas phase by propagating the drag more smoothly on the cells next to the injection. The source terms in the conservation equations of energy and species are also distributed more evenly between neighboring cells, improving the convergence of the solution.

The flat orifice atomizer model is one of the most common and easy to apply models, although the physical characteristics of its internal flow are not simple. This model accelerates the liquid through a nozzle, forming a jet of liquid and then breaks down to form droplets (Fluent, 2011). In order to accurately predict the characteristics of the spray, the model aims to identify the correct state of the flow in the internal nozzle since this aspect has a huge effect on spray formation.

The second type of injection that will be presented is the surface injection. In this type of injection, a particle flow will be released from each face of the surface. The number of faces is intrinsically related to the number of divisions adopted in the mesh of this surface. Even without atomizer, the initial injection conditions can be specified in the same way in the computational domain.

2.7 Simulation Modeling (Computational domain, initial, and boundary conditions)

The geometry to be studied was based on simple nozzles studied in the literature, in which the free jet of air and fuel in non-premixed regime. The spray configuration was constructed with a single entry, as to resemble the geometry of the experimental apparatus of Masri and Gounder (2010) and as can be observed in Figure 1.

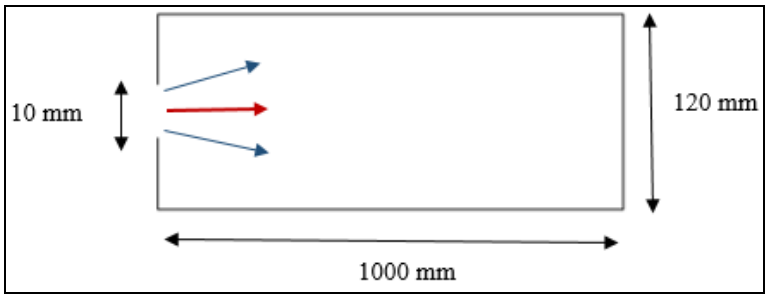


Figure 1. Geometry Scheme Illustration.

The geometry was simplified as two-dimensional and axisymmetric, in order to reduce computational cost. After the construction of the geometry, a structured and refined mesh was made for the computational domain, composed by 8,400 elements and 8,643 nodes. The regions near the nozzle exit and along the center line, where there is a greater interest in the precision of the results, only the number of elements were increased due to the possibility of recirculation flow and the mass fraction concentration of the chemical species. The mesh is shown in Figure 2.

The parameters used for the first simulation, SIMULATION I, in Fluent were made using the standard κ-ε turbulence model, since this is widely used, as in the work of Sacomano (2011). In spite of the existence of a pre-mixture region near the injection nozzle (Gounder et al., 2005), combustion in the non-premixed regime, using the reaction mechanisms of the CHEMKIN software for ethanol, was considered, allowing the results to be closer to the real one. This first simulation has a qualitatively objective of comparing the results and verifying if the project that includes geometry, mesh and model arrangement shows the same tendency of the experimental results.

After the simulation, modifications in the viscosity model were made in the fuel injection type, as well as in the mechanism of kinetics considering chemical equilibrium and steady diffusion flamelet using detailed chemical kinetic data imported from the CHEMKIN software. These modifications allowed visualizing and understanding the degree of importance and effects of the models and parameters on the simulation of the spray combustion process.

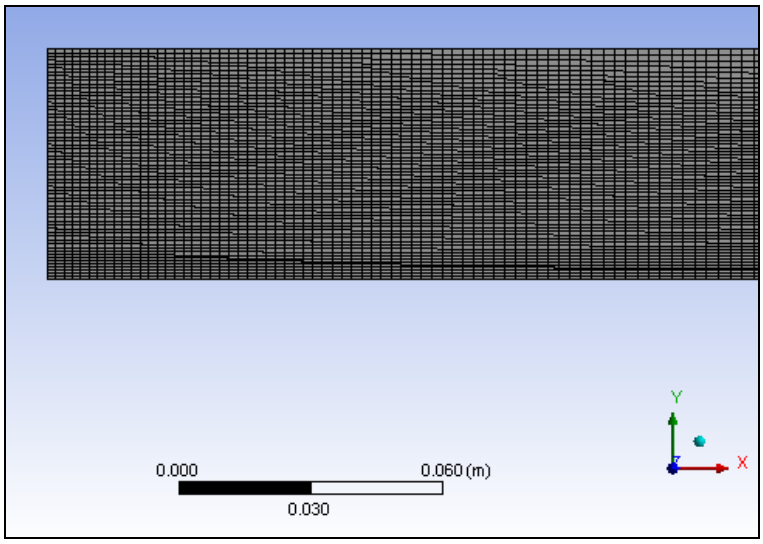


Figure 2. View of mesh generated in ANSYS Meshing.

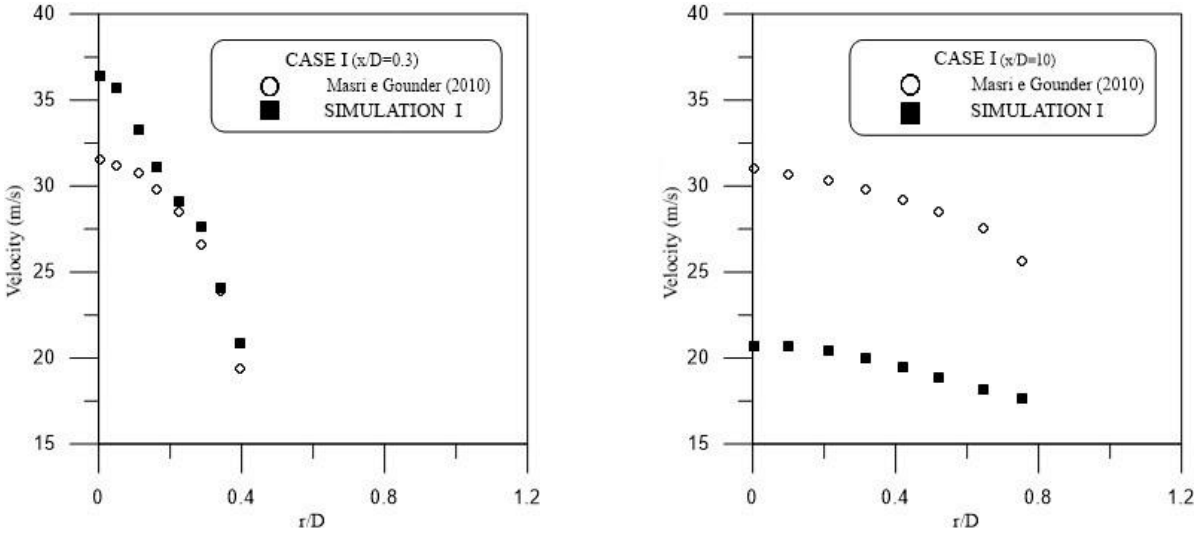
3. RESULTS AND DISCUSSION

The velocity profile results of the simulations are shown together with the experimental data collected by Masri and Gounder (2010) without drop diameter limitation. Figure 3 shows the comparison between the numerical and experimental results of the velocity profiles without drop restriction considering the axial positions of the outlet nozzle equal to x/D = 0.3 and x/D = 10. It was observed that the results presented in Figure 3 show that the model used in the present study captures qualitatively the behavior of the experimental results. The obtained solutions had a considerable precision with discrepancy of the numerical values of the compared profiles between 12.5% and 28%.

For the analysis of SIMULATION I, the following input data were used:

Table 1. Experimental data from the article by Masri and Gounder (2010).

Ethanol Spray Flame	Air Velocity (m/s)	Fuel mass flow (kg/s)	Equivalent ratio at nozzle outlet ($\Phi_{s,j}$)
CASE I	24	5.118E-04	0.85



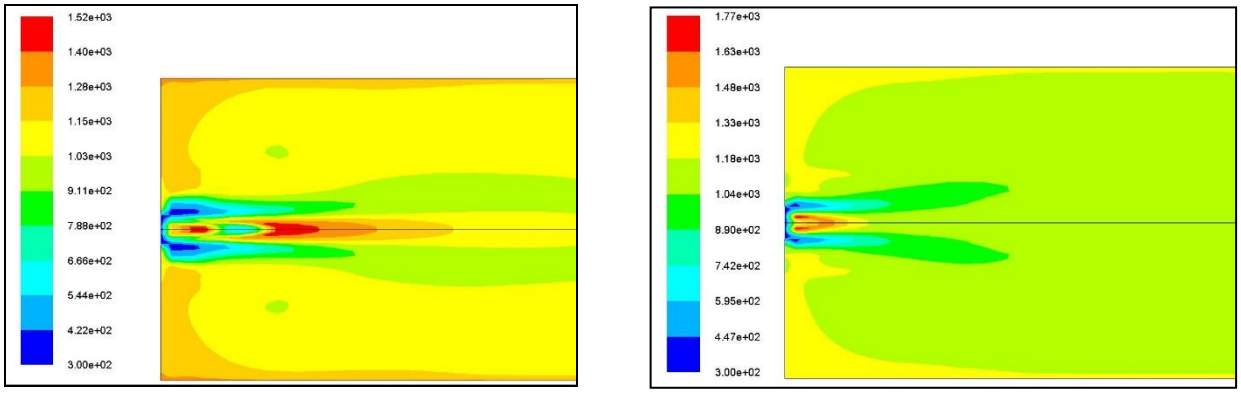
(a) **(b)**

Figure 3. Comparison between the radial velocity profiles of CASE I. (a) x/D = 0.3; (b) x/D = 10.

For the reaction mechanism analysis, two simulations were performed with a chemical mechanism with a global reaction equation and the detailed mechanism described by Marinov (1999). Figure 4 presents the generated temperature profile for CASE I at positions x/D = 10 and x/D = 20.

From the results, a uniform behavior of the flame was observed, by visualizing the temperature gradients generated using the imported CHEMKIN mechanism. Also, it was able to capture the higher temperature values and less pronounced flame lengths. Even though there were differences, the temperature distribution generated by the simulation when using the global reaction presents reasonable results that would be considered adequate depending on the focus of the research, in addition to the fact that it requires less computational effort, since it has a reduced number of reactions. However, the focus of this work is on flame formation and reactive flow behavior, which makes the detailed kinetic mechanism more suitable due to the amount of information.

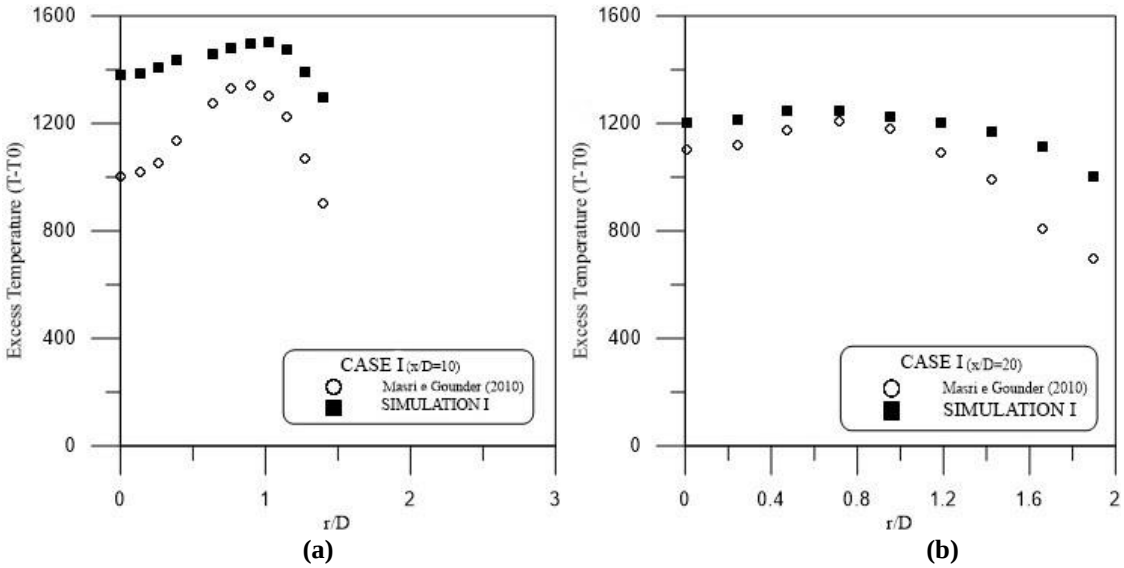
It is possible to verify that the profiles presented in Figure 4 show the same behavior trend as the experimental data, with discrepancies of 44% and 44.5%, showing that SIMULATION I was able to qualitatively predict the temperature behavior along the domain. The investigation for the other cases and the temperature, velocity and concentration of species in products of the combustion reaction will be evaluated later in this work, as well as its relation with the combustion efficiency.



(a) **(b)**

Figure 4. Temperature distribution using: a) global reaction, b) detailed mechanism described by Marinov (1999).

The excess temperature profiles (T-T_0) were also compared with the profiles provided by Masri and Gounder (2010), where T_0 is the initial temperature. In consistent experimental work such as Masri and Gounder (2010) and Rodrigues et al. (2015) it is shown that the peak temperature of the flame lies along the axis line of the spray. The flamelet model usually has some deficiency in predicting the formation of fine flames, however for this simulation a good temperature prediction was observed, as shown in Figure 5.



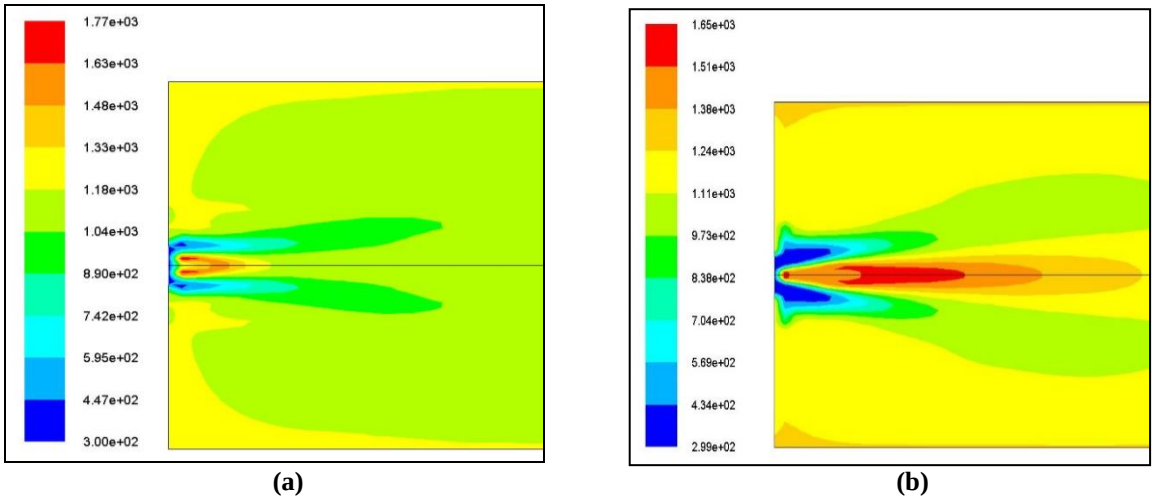
(a) **(b)**

Figure 5. Comparison between the excess temperature profiles (T-To) at position (a) x/D = 10; (b) x/D = 20.

In order to verify the influence of the injection type, this study analyzed two types of liquid fuel injection offered by the software to observe the behavior and formation of the flame. For this, a comparison of the temperature and mass fraction fields of species resulting from the combustion product was made.

The types of injection studied here are surface injection with momentum equal to zero, causing the droplets of liquid fuel to be diluted in the air flow and to be inserted in the computational domain only by the air that accelerates and drags them; and plane orifice injection, which sprays the fuel into the computational domain.

Based on the distribution of the temperature field, it is possible to state that the temperature range predicted in the simulation using injection with diluted droplets in the flow is higher for CASE I than the temperature range resulting from the simulation using the sprayer. In addition to observing that the best distribution of the temperature gradient is presented in Figure 6a. The temperature profile using surface injection showed a much shorter flame, characterizing a smaller reaction zone, resulting from a faster and more efficient mixing rate. This type of analysis is very useful for the design of more compact equipment.

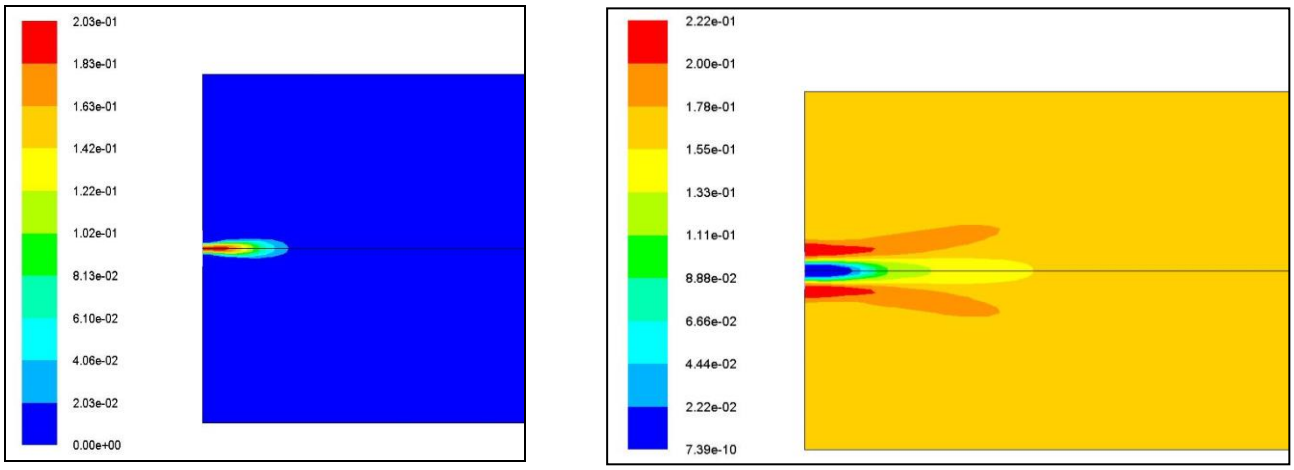


(a) **(b)**

Figure 6. Temperature distribution using injection type: a) Surface, b) Flat orifice

The effect of the injection type on the flame formation can also be analyzed by the fuel and oxygen mass fraction distribution, as well as by the effects on the combustion process by analyzing the concentration distribution of CO, CO_2 and H_2O as combustion products.

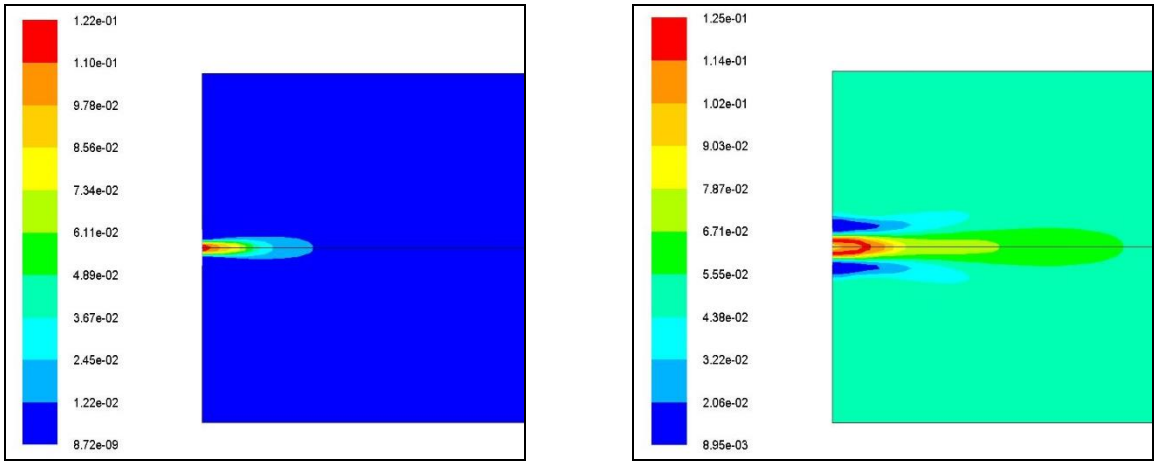
The fuel mass distribution, shown in Figure 7a, only confirms that the higher fuel concentration is in the vicinity of the outlet nozzle and the amount of fuel decreases as it moves away from the nozzle due the evaporation and burning of the droplets. Comparing Figures 7a and 7b, it is possible to observe a opposite behavior to the distribution of higher concentration of each reagent. This behavior indicates the diffusion of the reactants, confirming the non-premixed combustion regime even though the fuel droplets are diluted in the flow and their distribution is more homogeneous in the computational domain.



(a) **(b)**

Figure 7. Mass fraction distribution of a) fuel and b) oxygen using surface type injection

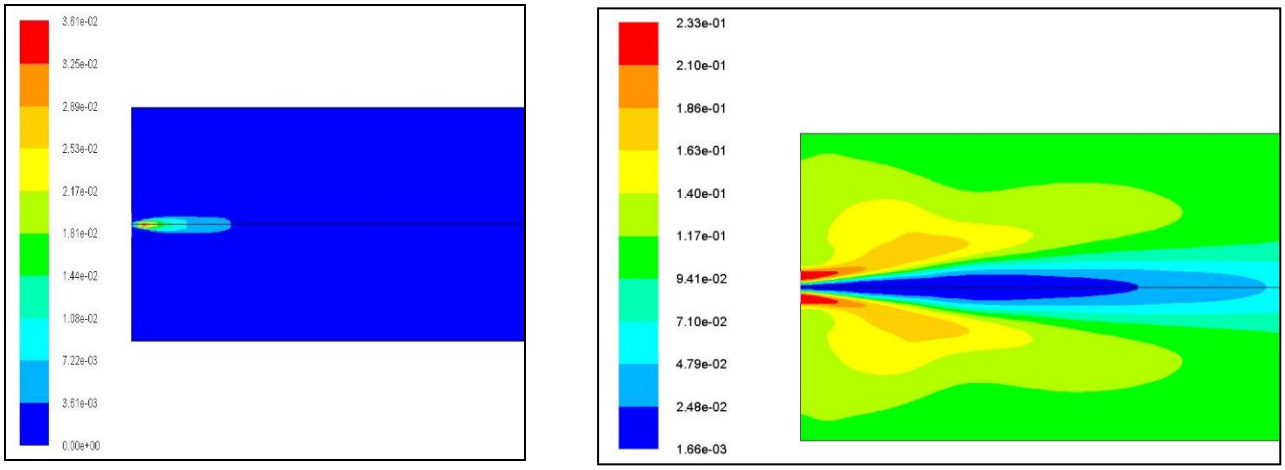
It is observed in Figure 8 that the region with the highest concentration of the mass fraction of CO is near the injection nozzle. Since the combustion reactions start in the vicinity of the nozzle and this chemical species is an intermediate compound in the combustion process, this explains the higher concentration in this region. Figure 8b shows the distribution of the mass fraction field of the chemical species CO_2, and this species indicates that the combustion reactions were complete because it is a final chemical compound. Since the CO-species is an intermediate compound of CO_2 formation, the concentration of CO is distributed in the vicinity of where CO concentrations are observed in Figure 8a. Figure 8b also shows that a high amount of CO_2 is distributed throughout the reactor, this can be explained by considering that the recirculation zones of the flow present in the surface injection caused the concentration of CO_2 to be distributed throughout the reactor to the two cases.



(a) **(b)**

Figure 8. Mass fraction distribution of a) CO and b) CO_2 using surface type injection

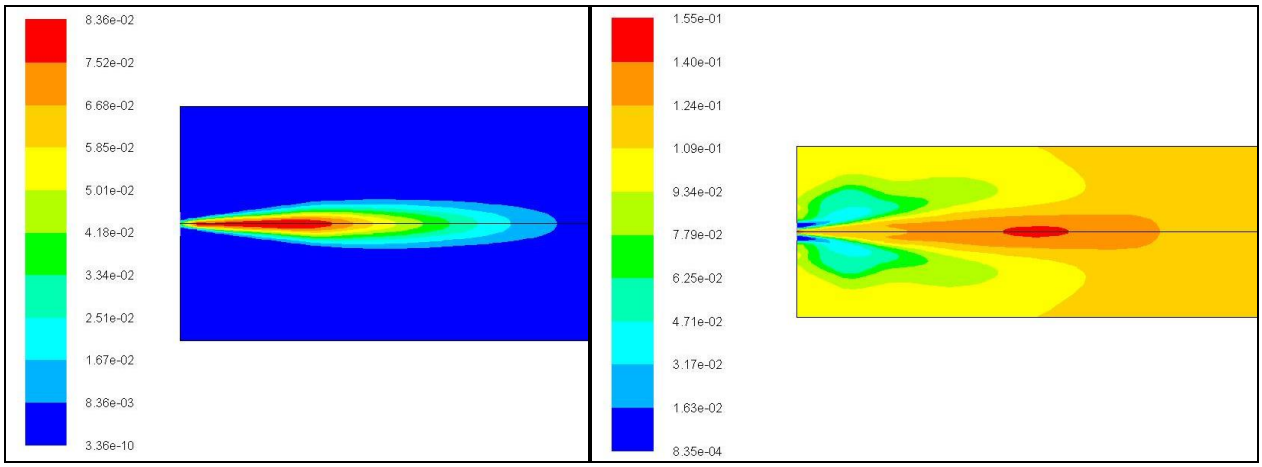
Analyzing the distribution of the C_2H_5OH fuel mass concentration range, shown in Figure 9a, it is evident that the concentration area is smaller in relation to the areas shown in Figure 7a. The radial diffusion of the fuel droplets is small, concentrating on the axis line, as well as the penetration in the computational domain is smaller, leading to believe that the inertia to be overcome by the droplets is larger, therefore the evaporation is slower as well as the mixing ratio. This is characteristic of fuel spraying over the previous injection contributes to a slower combustion reaction rate, i.e., the droplet distribution and the evaporation time, thereof, were reduced by using flat orifice injection.



(a) **(b)**

Figure 9. Mass fraction concentration distribution of a) fuel and b) oxygen using flat orifice injection type.

When analyzing Figure 10, which shows the mass fraction distribution of carbon monoxide and carbon dioxide, it is observed that, when using this injector, the amount of CO in the combustion process is much smaller than using surface injection, besides the concentration is better distributed over of the region neighboring the flame. By increasing the amount of air mass and decreasing the amount of fuel, a more pronounced reduction in CO concentration occurs.



(a) **(b)**

Figure 10. Mass fraction distribution of de a) CO and b) CO_2 using flat orifice injection type.

4. CONCLUSIONS

From the generated results of temperature and velocity profile, it was possible to validate the simulation with the comparison with the experimental data of Masri and Gounder (2010). In order to verify the influence of the reaction mechanism in the analysis of the results, two were made, one referring to the reaction mechanism containing only one global equation, and another with a detailed mechanism imported from CHEMKIN. It was observed that, in general, good results were achieved, and when the intention of the study is the analysis of the final products and the amount of heat generated as a general result of the combustion process, it is presented as an excellent option both to offer the necessary results and to reduce the computational cost involved in this type of analysis, along with the advantaged of easy implementation in computational fluid dynamics codes.

In the analysis of injection by flat orifice, it is noticed that, in general, the reaction zone moved downstream of the nozzle in comparison to the surface injection type. Besides, the resulting temperature range was smaller. In the analysis of the reaction products it can be seen that the use of injection by flat orifice allows for a greater distribution of droplets in the reactive flow, in order to provide smaller distributions of mass fraction of CO and CO_2.

5. ACKNOWLEDGEMENTS

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