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Investigations CFD Numerical of the Combustion of Methane or Propane: Aero-Thermo-Chemical Study

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Abstract: In this paper, we simulated numerically the non-premixed combustion provided by two coaxial methane-propane/air jets in a cylindrical combustion chamber. Using CFD Fluent commercial calculation software. In order to find the aero-thermo-chemical characteristics in the burner: temperature, axial velocity and mass fraction of carbon monoxide CO. To study this kind of phenomenon we used a special treatment of the mathematical model and we chose two models of computation large eddy simulation (LES) and the probability density function (PDF). The objective of this work is to reduce the emission of carbon monoxide CO, and what is considered a gas toxic to the environment. The results obtained give the fuel of methane reduces the carbon monoxide in the products of combustion.

Key words: Models LES and PDF; Combustion Chamber; Methane; Propane; Numerical Simulation CFD**.**

1. Introduction

In 2002, fossil fuels accounted for almost 80% of the world's commercial primary energy consumption, a little over 10 Gtep, split between oil (3.7), gas (2.2) and coal (2.4) [1]. Because of their flexibility of use and their high energy density, these energy sources are assured of a long-term preponderance for the production of electricity and supremacy in transport. Despite controversies over the estimation of fuel reserves and their extraction costs, the trend seems to be for a steady, even irreversible, price increase. At the same time, preserving the environment becomes an important argument in the face of economic interests alone, for the direction of an energy policy. Legislation to reduce polluting emissions is becoming increasingly restrictive. Electricity generation and transport are the first two sectors responsible for carbon dioxide emissions (41% and 21% respectively). Over the last century, these activities have become the driving force behind economic growth and the essential components of the western way of life. Fossil fuel consumption forecasts for the coming decades all agree to growth, due to the explosion of demand in the emerging market. Therefore, the economic competitiveness of these clusters is a strategic issue. In the long term, the capture and sequestration of carbon dioxide, often considered for power plants, is not applicable to the transport vehicle without the synthesis of a carbon-free fuel such as hydrogen [2].

In this work, a simulation study of the combustion of methane and propane in a combustion chamber. Then, we used FLUENT-CFD in the numerical calculation based on aero-thermo-chemical equations for the control. In addition, we used for these objective mathematical models, especially large eddy simulation (LES) for dynamic parameters and probability density function (PDF) for thermo-chemical parameters in order to reduce the number of equations. Consequently, we studied the numerical validation of the LES/PDF models with the experimental data to study the

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behavior of non-premixed combustion fueled by CH4 and C3H8 fuels. Considering that, the study consists of three parameters: average temperature, average axial velocity and the average mass fraction of carbon monoxide CO. The main objective of this work is to reduce the emission of carbon monoxide CO, and what is considered a gas toxic to the environment. The results obtained give the fuel of methane reduces the carbon monoxide in the products of combustion.

2. Experimental Configuration

The configuration is a combustion chamber is given in figure 1. Where it has been the subject of many experimental researches because of its relatively simple geometry and its similarity with the gas turbine burner [3-7]. The cylindrical combustion chamber of radius R4=61.15 mm and length L=1 m provided by two coaxial jets CH4-C3H8/air, the central jet having an internal radius equal to R1=31.57 mm and an external radius R2=31.75 mm , which injects the fuel with a speed V1=92.78 cm/s and the temperature T1=300 K. and the annular jet has an internal radius equal to R3≡ R=46.85 mm, which injects the air with a speed V2=20.63 m/s and preheated to a temperature T2=750 K. The combustion chamber is pressurized to p=3.8 bar and has a wall at constant temperature equal to T=500 K [3-7].

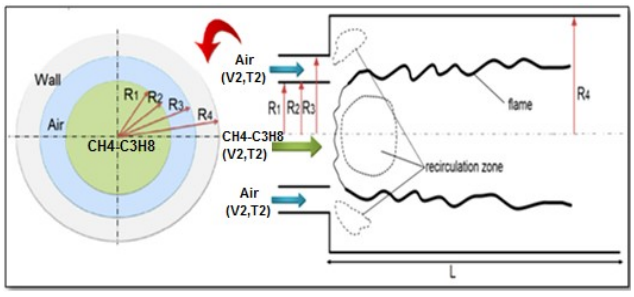


Fig. 1 Schematic of the burner.

3. Governing Equations

In this paper, we study the behavior of non-premixed turbulent combustion in three dimensions using numerical simulation. We can write the control equations for the compressible flow in Cartesian coordinates as follows [3-7]:

Continuity:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i) = 0 \quad (1)$$

Momentum:

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) = -\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i u_j} - \widetilde{u}_i\widetilde{u}_j)] - \frac{\partial \overline{p}}{\partial x_j} + \frac{\partial \overline{\tau_{ij}}}{\partial x_i} \quad (2)$$

Energy:

$$\frac{\partial}{\partial t}\overline{\rho}\widetilde{h} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{h}) = -\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i h} - \widetilde{u}_i\widetilde{h})] + \frac{\partial \overline{p}}{\partial t} + \frac{\partial}{\partial x_i}\overline{u_j \tau_{ij}} \quad (3)$$

Species:

$$\frac{\partial}{\partial t}\overline{\rho}\widetilde{Y}_f + \frac{\partial}{\partial x_i}(\overline{\rho}u_i\widetilde{Y}_f) = -\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i Y_f} - \widetilde{u}_i\widetilde{Y}_f)] + \overline{\dot{\omega}}_f \quad (4)$$

Where:

i = 1, 2, 3 and j = 1, 2, 3.

Thermodynamic state:

$$\overline{p} = \overline{\rho} R_m \widetilde{T} \quad (5)$$

- Unresolved Reynolds stresses, $(\overline{u_i u_j} - \widetilde{u}_i\widetilde{u}_j)$ requiring a subgrid scale turbulence model.
- Unresolved species fluxes $(\overline{u_i Y_f} - \widetilde{u}_i\widetilde{Y}_f)$ and enthalpy fluxes $(\overline{u_i h} - \widetilde{u}_i\widetilde{h})$ requiring a probability density function (PDF) approach.
- Filtered chemical reaction rate by $\overline{\dot{\omega}}_f$.

The LES models and the PDF approach explained and detailed in previous work [8-12].

4. Results and Discussion

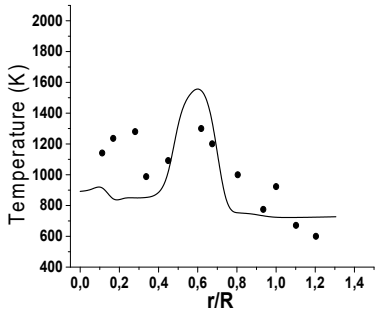
We begin with the validation of the coupled models with the experimental data [7]. After that, the same parameters used for the validation are used also to control the flame behavior supplied by the CH_4 or C_3H_8. Moreover, the presentation and comparison of results are based on normalizing length and velocity by using,

respectively, the injector radius (R≡R3) and the inlet bulk velocity of the air (U≡V2).

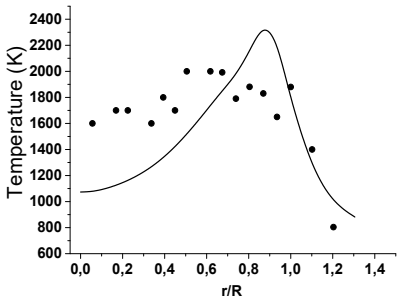
4.1 Validation of Numerical Models

4.1.1 Temperature

For the experimental part of this study [7] temperature measurements are made via thermocouple probes. The comparison of our temperature profile with others obtained by some simulation models using the experimental data is presented in figure 2. The station x/R=0.89 is situated in the region of the combustion chamber, d close to the mixing zone of the fuel and oxidizer. So close to the shear layer (flame zone). Therefore, at station x/R=4.52, the temperature takes maximum values at the center of the combustion chamber. This is called the hot zone where chemical reactions, which means a considerable increase in temperature in this area. The numerical and experimental temperature profiles have almost the same tendency, it begins to decrease when moving away from this zone until reaching the temperature of the wall. It is found that the agreement of the profiles is verified, with an average relative uncertainty between the simulation and the experiment of 10%. The temperature range which favors the generation of soot is between T=900 K and T=1600 K for the station x/R= 0.89, is between T=1050 K and T=2300 K for the second station. The discrepancy between the experimental data and the numerical results may be justified by the uncertainty regarding the condition of the isothermal walls. Since to the experiment, the walls are cooled by water until reaching T=500 K, to experimentally insure walls is permanently impossible. The anomalies between the experimental results and the results obtained by the simulation can be justified by the errors or the uncertainty of the experimental equipment of temperature measurement.



a) x/R=0.89



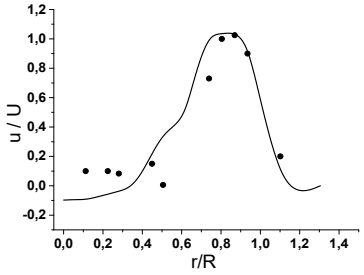
b) x/R=4.52

Fig.2 Radial profiles of average temperature, ___ Simulation (LES/PDF), • Experiment [7].

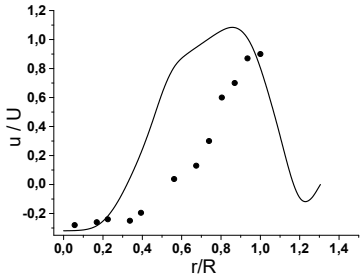
4.1.2 Axial velocity:

Figure 3 show the results of the radial variation of the axial velocity of coupled LES/PDF models compared with the experimental data [7] in the same axial stations. In fact, the two results, experimental and numerical, are in good agreement in the measurement stations: x/R=0.14 and x/R=1.27. Thus, on average there is a relative lag between the experimental data and the numerical results which does not exceed 7%. The important values of the velocity are in the region of the flame as presented in the peaks. Consequently, the negative values of the axial velocity at the shear zones where the two flows meet. Therefore, the air flow (high speed) is delayed by the flow of methane (low speed). The range of the variation of the mean axial velocity is -0.35 to 1.05, where the maximum is located at the level of the shear layer on which the flame is found. Where, the formation of two recirculation zones is observed. The first located in the center of the burner at the level of the methane jet, generated by the delayed flow of methane. The second is that the velocity of the methane flow is relatively low relative to that of the air, which gives a negative gradient towards the center of the burner, identified experimentally in this central recirculation zone. The divergence may be due to the fact that fully developed fuel and air intake conditions were assumed in the simulations. But in the experiment the input flows of the devices were located only short distance upstream of the burner. The existence of the flame in this zone interpreted by the meeting of

methane and air, which creates a mixing zone where the two gases mix intimately due to the turbulence which gives a richer mixture.



a) x/R=0.14

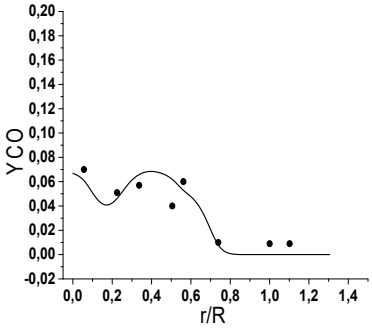


b) x/R=1.27

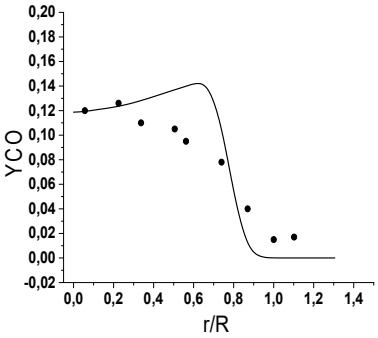
Fig.3 Radial profiles of average axial velocity, ___ Simulation (LES/PDF), • Experiment [7].

4.1.3 Mass fraction of carbon monoxide:

Figure 4 shows the comparison of the mass fraction of carbon monoxide CO obtained by the numerical simulation for the "LES/PDF" model and the experimental data [7]. The values of the mass fraction of carbon monoxide are high in the center of the combustion chamber because it is the reaction zones where the production of chemical species, which decreases from the center of the burner. The agreement between the experiment and the calculation is satisfactory the relative difference between the two on average is 5%. In fact, the CO mass fraction profiles have the same tendency with the temperature profiles that explain the high values of CO in the flame zone, reaction zone and CO production. The tuning is satisfactory further downstream in the first station. In the station x/R=0.21, the CO values are low relative to the other station x/R=3.16. However, the mixture of methane and air is caused by the effect of turbulence, which allows their mixing and combustion in order to produce CO with high values. It is noted that the mass fraction of CO increases what proves that occur in combustion.



a) x/R=0.21



b) x/R=3.16

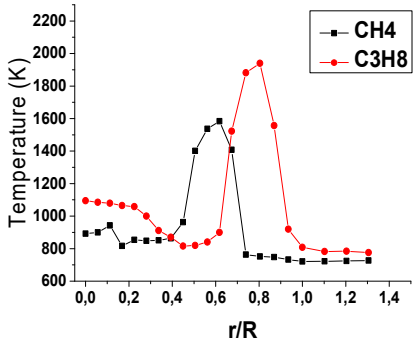
Fig.4 Radial profiles of the average mass fraction of carbon monoxide, ___ Simulation (LES/PDF), • Experiment [7].

4.2 Validation of Numerical Models

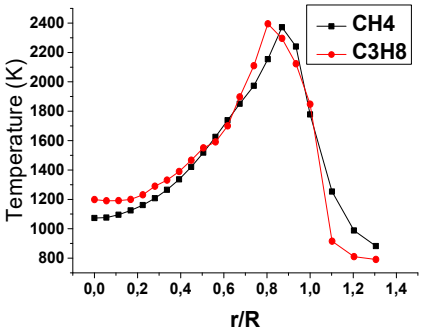
4.2.1 Temperature:

Comparison is made at the same stations x/R=0.89 and x/R=4.52 of measurements considered by methane and propane for the temperature present in figure 5. In the flame zone the temperature profiles show peaks in the stations, and then decrease to equal the temperature of the walls equal to T=500 K. The radial temperature profiles have the same tendency for the two fuels especially in the last station, with the difference of 7%. In the station x/R=0.89, the temperature range which favors soot generation is between T=800 K and T=2000 K for the combustion of C3H8, is between T=1100 K and T=2400 K for the second station x/R=4.52.The high temperature values are located in the flame zone, because this zone is the same

zone of chemical reactions, and these reactions are considered as exothermic reactions. It should be noted that the profile of the propane temperature shifted at the level of the jet of air in the first station. The difference in temperature of CH4 and C3H8 can be interpreted by the adiabatic temperature difference as each smoke characteristic.



a) x/R=089

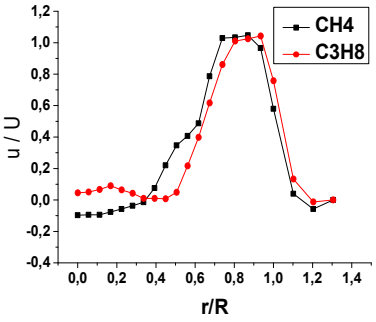


b) x/R=4.52

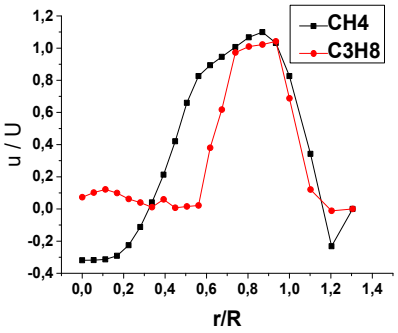
Fig.5 Comparison of the temperature between CH_4 and C_3H_8

4.2.2 Axial velocity

The radial profiles of the axial velocity illustrated in figure 6 are given the comparison between the methane fuel and the propane in the various stations x/R=0.14 and x/R=1.27 inside the burner. The range of the mean axial velocity variation is between -0.05 and 1.02 for propane fuel, where the maximum is located at the level of the shear layer on which the flame is found. The high axial velocity values are those in the flame zone. Station x/R=0.14 we observe that we have the same profile of the velocity profiles between the two CH4-C3H8 fuels in all zones with an average relative uncertainty of≈2%. On the other hand, the average relative uncertainty shows that we have the same profile of the speed between the two fuels is equal to 7% in the station x/R=1.27. The high air velocity axial velocity values presented by the peaks in stations x/R=0.14 and x/R=1.27, where it is in the flame area. There are also negative values in the velocity profiles which show the recirculation regions: in the center of the burner and close to the walls. It is observed that the velocity of the methane is greater than the propane velocity caused by the molar mass of methane below the mass of propane.



a) x/R=0.14



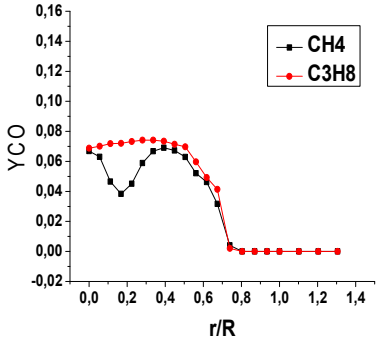
b) x/R=1.27

Fig. 6 Comparison of the axial velocity between CH_4 and C_3H_8

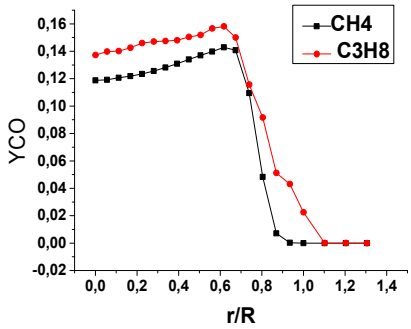
4.2.3 Mass fraction of carbon monoxide

Figure 7 shows the comparison between the mass fraction of carbon monoxide CO resulting from the combustion of methane and propane. The radial profiles of the mass fraction of carbon monoxide present through the x/R=0.21 and x/R=3.16 stations. The difference between the two curves resulting from CH4 and C3H8 is about 4%. The profiles of these stations show that the mass fraction of CO takes high values in the middle of the combustion chamber where the hot zone is located, so the combustion efficiency is high ie we have a good mix which implies a high mass fraction of CO. At the inlet of the combustion chamber, the value of CO is considerable, especially in the first station x/R=0.21, and the product of carbon monoxide CO by the combustion of CH4 is monk relative to

C3H8. The second station x/R=3.16, the mass fraction of the CO have the same tendency at the preview station, the values of the CO produced by the CH4 and the C3H8 higher compared to the CO values produced by the previous station. The mass fraction values of CO are always high at the flame region. In general, the results clearly show that the carbon monoxide CO value of propane is high than methane.



a) **x/R=0.21**



b) x/R=3.16

Fig. 7 Comparison of the mass fraction of CO between CH_4 and C_3H_8

6. Conclusions

In this paper, we performed a 3D numerical simulation based on the LES model coupled to the PDF approach, using the Fluent calculation. Non-premixed turbulent combustion fueled by methane-propane/air. In addition, the following conclusions can be drawn from this study:

- The LES model is applied to give the ability to detect the morphology of the flow. This model makes it possible to calculate the speed directly in the zone close to the walls.
- The PDF approach is used to assist in the evaluation of the mean of the scalar parameters without the need to calculate the source terms of the species.
- The emission of carbon monoxide less existing for the combustion of methane relative to that of propane since the methane has a carbon element but the propane has three elimination.
- Higher temperature for propane fuel versus methane fuel, in different stations.
- The methane velocity is faster than that of propane since the molar mass of methane is smaller than propane.

With these results, we conclude that methane fuel is better than propane, which is cleaner and less harmful to the environment compared to propane.

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