

# CFD Study of Methane-Hydrogen Behavior in a Non-Premixed Combustion Chamber

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**Abstract**—In this paper, the numerical results of the study of a turbulent flame of methane-hydrogen/air generated by a cylindrical burner are presented. The numerical simulations are carried out using the CFD code "FLUENT" and "Gambit" for the meshing process. The finite volume method was used to solve the Navier-Stokes equations governing the flow. The coupling of the LES/PDF models is used to model the turbulence/chemistry interaction in the system's transport equations. The results of the calculations are expressed and analyzed in terms of axial velocity, temperature and mass fraction of carbon monoxide CO. The results of the numerical calculations are compared and validated against experimental data. In addition, the same parameters considered above are used in the study of the combustion behavior of CH<sub>4</sub>/H<sub>2</sub> fuels. The obtained results confirm the fact of considering hydrogen as a clean non-polluting fuel compared to methane, since it has no carbon monoxide emissions in combustion products. Besides this fact, the hydrogen gas velocity in the flame is significantly higher by comparing it to the methane gas velocity.

**Key words**— Non-Premixed Combustion; Turbulence; Hydrogen; Methane; CFD Simulation.

## I. INTRODUCTION

Today, with increasing concerns about the reduction of energy production and protection of the environment, research on alternative fuels has been widely studied in recent years by a large number of researchers. In addition, the increasingly rigorous regulation of CO<sub>2</sub> emissions on the one hand and the depletion of fossil fuel reserves on the other have prompted the scientific community to find alternatives to these fuels. Indeed, the increase in the car fleet has led to an increase in the consumption of conventional fuels, which are responsible for the continuous increase in emissions of pollutants. Research in the fields of fuel quality and combustion will lead to a gradual reduction of pollutant emissions, increased environmental protection and improved living conditions. The addition of hydrogen to methane has an effect on reducing the ignition time of the mixture and increasing the ignition advance and reducing pollution [1].

In this context, natural gas offers many economic and environmental benefits. It is mainly made up of methane, natural gas at lower levels of pollutant emissions compared to other fossil fuels. With regard to carbon dioxide, the combustion of natural gas generates respectively 30 to 40% less than oil and coal with the same amount of energy consumed. However, emissions of

pollutants from natural gas combustion can be reduced. An interesting alternative is to substitute hydrogen for part of the natural gas, creating a less polluting hybrid fuel. This solution is a first step towards a hydrogen economy in order to gradually adapt infrastructures, standards and regulations as well as inform and prepare the public [2]. Evatt et al. [3] used the Direct Numerical Simulation to study the effects of H<sub>2</sub> enrichment on lean premixed methane-air flames. They found that lower CO emissions per unit fuel consumption are observed for the enriched flame, consistently with experimental data [3]. In their experimental work, Akansu et al. [4] considered to control the effect of a spark ignition engine of mixtures of hydrogen and methane. Although, they obtained the test results for a four-cylinder engine with mixtures of hydrogen in methane of 0, 10, 20 and 30% by volume. Showing that NO emissions increase, HC, CO and CO<sub>2</sub> emission amounts decrease with increasing hydrogen percentage.

The main objective was the numerical simulation of non-premixed turbulent combustion in a cylindrical combustion chamber supplied by methane-hydrogen/air. We used the commercial CFD code FLUENT. Three parameters are considered: the average axial velocity, the temperature and the mass fraction of the carbon monoxide CO. In the first step, we validate the coupling of the large eddy simulation (LES) models and the probability density function (PDF) approach [5,6] with the experimental data in the same stations and the same conditions. The results show that the select models give a satisfactory agreement with all the regions considered. In the second step, the same parameters considered previously are used in the study of the combustion behavior of methane-hydrogen fuels. The two CH<sub>4</sub>-H<sub>2</sub> fuels are compared to choose the least carried out on the environment.

## II. BURNER CONFIGURATION

The configuration which confines the combustion chamber is given in figure 1. The cylindrical combustion chamber, presenting a radius R<sub>4</sub>=61.15 mm and a length L=1 m, is supplied by two coaxial jets CH<sub>4</sub> or H<sub>2</sub>/air. The central jet presents an internal radius equal to R<sub>1</sub>=31.57 mm and an outer radius R<sub>2</sub>=31.75 mm, in order to inject methane or hydrogen with an inlet mass flow rate Q<sub>1</sub>=7.2 g/s at a temperature T<sub>1</sub>=300 K. The annular jet has an internal radius equal to R<sub>3</sub>=46.85 mm, which injects air with an inlet mass flow equal to Q<sub>2</sub>=137

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g/s and a preheated temperature  $T_2=750$  K. The chamber of combustion is pressurized by a value equal to  $p=3.8$  atm and to a constant temperature wall equal to  $T=500$  K [5,6]. In the aim to present and compare our results we have carried out the simulations based on the normalization of length (x-position) and velocity using characteristic values, i.e. injector radius ( $R \equiv R_3$ ) and inlet air velocity ( $U \equiv V_2$ ).

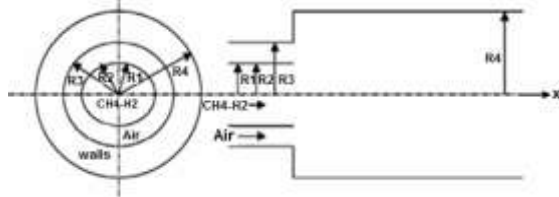


Fig. 1 Schematic presentation of the burner

### III. GOVERNING EQUATIONS

In this paper, we studied the behavior of non-premixed turbulent combustion in three dimensions using numerical simulation. The governing equations for the compressible flow can be written in Cartesian coordinates as summarized in Table 1.

Table 1: Governing equations.

Description	Equation
Continuity	$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i) = 0$
Momentum	$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{u}_j) = -\frac{\partial}{\partial x_i} [\bar{\rho} (\overline{u_i u_j} - \tilde{u}_i \tilde{u}_j)] - \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \bar{\tau}_{ij}}{\partial x_i}$
Energy	$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{h}) = -\frac{\partial}{\partial x_i} [\bar{\rho} (\overline{u_i h} - \tilde{u}_i \tilde{h})] + \frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_i} \overline{u_j \tau_{ij}}$
Species	$\frac{\partial \bar{\rho} \tilde{Y}_f}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{Y}_f) = -\frac{\partial}{\partial x_i} [\bar{\rho} (\overline{u_i Y_f} - \tilde{u}_i \tilde{Y}_f)] + \bar{\omega}_f$
Thermodynamic state	$\bar{p} = \bar{\rho} R_m \bar{T}$

In these equations, the unresolved Reynolds stresses  $(\overline{u_i u_j} - \tilde{u}_i \tilde{u}_j)$  require a subgrid scale turbulence model. The unresolved species fluxes  $(\overline{u_i Y_f} - \tilde{u}_i \tilde{Y}_f)$  and the enthalpy fluxes  $(\overline{u_i h} - \tilde{u}_i \tilde{h})$  require a probability density function (PDF) approach. The filtered chemical reaction rate is characterized by  $\bar{\omega}_f$ .

The LES models and the PDF approach explained and detailed in previous work [5,6].

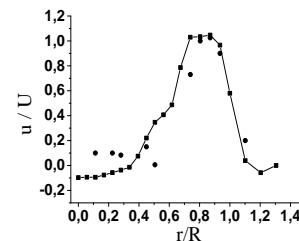
### IV. RESULTS AND DISCUSSION

Firstly, we have validated our trend to couple the LES models and the PDF approaches against the experimental data [6] at same stations and for same conditions. Secondly, we have exploited the same parameters considered previously to study the combustion behaviour of methane-hydrogen fuels.

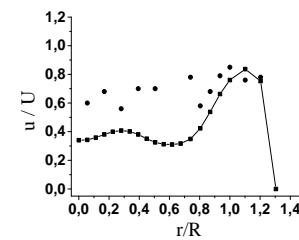
## 1. Numerical Validation

### 1.1 Axial Velocity

Comparison of the predicted radial profiles of the mean axial velocity with the experimental data in the stations  $x/R=0.14$  and  $x/R=4.67$  are presented in figure 2. In fact, the numerical and experimental profiles have almost the same tendency. Thus, the mean relative gap between the numerical calculations and the experimental reference data [6] is about 7%, which is almost acceptable in combustion applications. The high values of the axial velocity are located in the center of the burner presented by the peaks in the  $x/R=0.14$  and  $x/R=4.67$  stations. In the last station  $x/R=4.67$ , the difference between the numerical profile and the experimental profile may be due to the fact that the fully developed methane and air intake conditions were assumed in the simulations. However, in the experiment, the inlet flow devices were located only a short distance upstream of the burner. In the two recirculation regions shown in schematic presentation of the burner (figure 1), the negative axial velocity values are observed due to turbulence. The first region located at the fuel jet is due to the delay of the generated flow. However, for the second region it is caused by the sudden change between the conditions of entry of coaxial jets ( $\text{CH}_4/\text{Air}$ ).



(a)  $x/R=0.14$



(b)  $x/R=4.67$

Fig. 2 Radial profiles of average axial velocity,   
 — Simulation, • Experiment [6]

### 1.2 Temperature

Figure 3 shows the comparison of the radial profiles of the mean temperature obtained by the numerical simulation of the coupled LES/PDF models and the experimental data considered in reference [6], for the same stations defined by  $x/R=1.57$  and  $x/R=4.52$ . Numerical and experimental profiles have almost the same tendency. The mean relative gap between the numerical calculations and the experimental data is about 10% which concedes satisfactory agreement between

simulations and experiments. The high temperature values are located around the flame zone and begin to decrease with the radial distance to reach the temperature of the cooling isothermal wall at  $T=500$  K. The shear layers which are in the same zone where fuel and air meet. The shear zone is created to improve the mixing of the two coaxial jet streams ( $\text{CH}_4/\text{Air}$ ) to supply the combustion chamber with a rich mixture. Furthermore, the apex based on the temperature profiles is attenuated downstream of the burner. As a result, this disagreement is due to regions with high temperature fluctuations and to the difficulty of perfectly ensuring the conditions of experience of the walls.

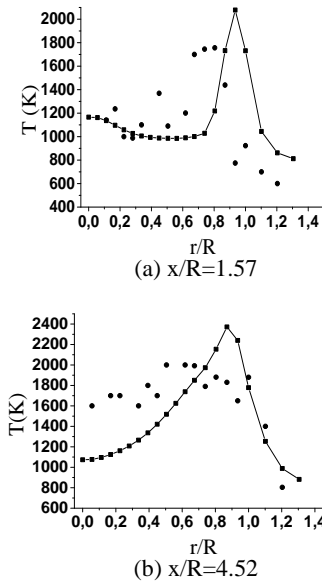


Fig. 3 Radial profiles of average temperature, — Simulation, • Experiment [6]

### 1.3 Mass Fraction of Carbon Monoxide CO

Figure 4 illustrates the comparison of the numerical and experimental radial profiles of the mass fraction of carbon monoxide CO for different stations of the burner defined by  $x/R=0.21$  and  $x/R=3.84$ . In fact, the numerical calculations of the CO mass fraction significantly present a good agreement with the experimental data [6]. The gap between the numerical results and the experimental data is about 5%. The high values of the CO mass fraction located in the center of the combustion chamber decrease as they move away from the burner center. The radial profiles of the mass fraction of CO have the same tendency with the radial temperature profiles which explain the high CO values in the reaction zone (the flame zone). This zone is rich and reactive and produces monoxide of carbon CO. In the first station  $x/R=0.21$ , the CO values are low compared to the second station  $x/R=3.84$ . Turbulence is caused by the mixing effect of fuel and air, which allows their mixing and combustion to produce CO with high values.

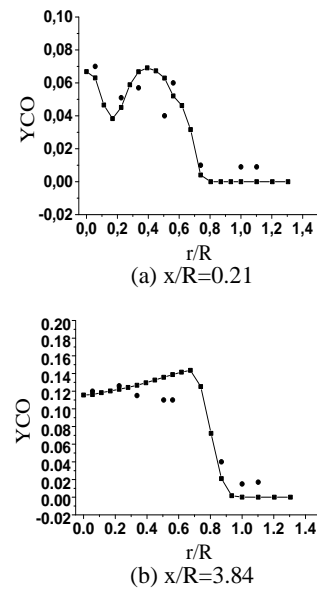
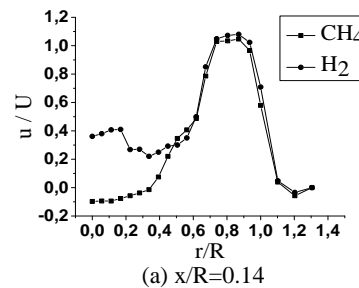


Fig. 4 Radial profiles of average CO mass fraction, — Simulation, • Experiment [6]

## 2. Comparison of $\text{H}_2$ and $\text{CH}_4$ Fuels

### 2.1 Axial Velocity

Figure 5 illustrates the comparison between the mean axial velocity of  $\text{H}_2$  and  $\text{CH}_4$  in different stations, defined by  $x/R=0.14$  and  $x/R=4.67$ , in a three-dimensional combustion chamber. These profiles are characterized by peaks in the stations. The numerical profiles of  $\text{H}_2$  and  $\text{CH}_4$  have almost the same tendency especially in the first station, and the values of axial velocity of hydrogen elevated with respect to the methane velocity especially in the last station. The values of rate of hydrogen velocity are greater than 1. In these conditions, the values of the velocity of the  $\text{H}_2$  are high in the middle of the combustion chamber compared with the speed of  $\text{CH}_4$ . Thus, we can also see the  $\text{H}_2$  speed profiles completely applicable on the profiles of the  $\text{CH}_4$  near the burner walls in both stations. Indeed, it has been observed that the velocity of hydrogen is greater than the speed of methane almost the molar mass of hydrogen is less than the molar mass of methane.



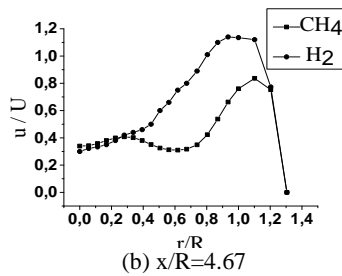


Fig. 5 Profiles of the axial velocities considered for hydrogen and methane

## 2.2 Temperature

Figure 6 shows the distribution of the average temperature of hydrogen and methane. The radial temperature profiles for the two fuels have the same tendency, are presented by the peaks in the stations defined by  $x/R=1.57$  and  $x/R=4.52$ . The temperature high values are in the flame zone for both  $H_2$  and  $CH_4$  fuels, as this area is the same area of chemical reactions. The positions of the peaks in all stations move at the jet of air for the case of hydrogen, with a slight increase compared to the values of the temperature of the methane. In the middle of the combustion chamber, the values of the temperature of the methane is equal to  $T=1200$  K and decreases at the value of the hydrogen temperature until  $T=600$  K, in both stations. The observed shift of  $CH_4$  and  $H_2$  temperatures obtained by calculations is owed to the molar masses difference between these fuels, since the chemical composition is the key parameter in rising combustion temperatures.

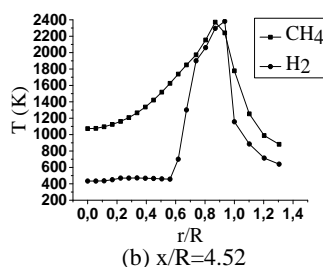
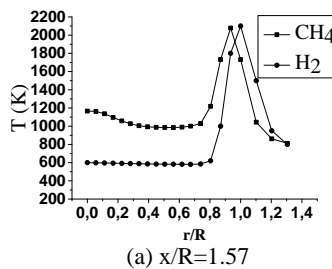


Fig. 6 Profiles of the temperatures considered for hydrogen and methane

## 2.3 Mass Fraction of Carbon Monoxide CO

The curve of the numerical calculation of the CO mass fraction of methane is presented in figure 4. The curve of the hydrogen profiles is a straight line of the form  $y_{co}=0$  applicable to the x-axis. The results clearly illustrate that the fuel CO values of hydrogen are zero and are quite

important for methane fuel. Whereas in the center of the combustion chamber, the values of the mass fraction of CO are high for the fuel  $CH_4$ , equal to  $y_{co}=0.06$  for the first station  $x/R=0.21$ . Indeed, it is observed that the quantity of carbon monoxide is double for the second station  $x/R=3.84$  and is characterized by  $y_{co}=0.12$ . The CO mass fraction values decrease with the radial distance.

## V. CONCLUSION

In this paper, we have presented the results obtained by numerical simulations using CFD code FLUENT tools in non-premixed turbulent combustion fueled by two methane-hydrogen/air fuels. The main results obtained in this study:

- The results give a satisfactory agreement between the numerical calculations of the coupled LES/PDF models and the experimental data.
- The emission of carbon monoxide is non-existent for combustion of hydrogen in the combustion chamber at all monitoring stations but exists for methane.
- Generally, a certain temperature discrepancy between the studied fuels was observed in different stations, which can be owed to the molar mass role played in combustion flame temperatures.
- The hydrogen velocity is faster than that of methane since the molar mass of hydrogen is smaller than methane.

With these results, we can confirm the fact that hydrogen is better than methane when used as fuel, because it is cleaner and less harmful to the environment.

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