



CFD Analysis and NO_x Prediction in H₂ and CH₄ Turbulent Non-premixed Flame Compared with Swirling Flame

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ABSTRACT

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This work is devoted to the comparative study for the formation and dissociation of nitrogen oxides by the numerical simulation of turbulent combustion without premix in a combustion chamber having a cylindrical shape with two coaxial jets, two flames using the ANSYS fluent software 16.0. The study focuses on the influence of the type of fuel on the composition of discharges in content with NO_x, that is to say two cases are treated and compared. Turbulence is modeled by the k-ε model and the chemical aspect of combustion is treated by the PDF model for each flame. The calculation results relate to the characteristics of dynamic fields, temperature, the mass fractions of different species involved in the combustion process and the NO_x prediction. The effect of the swirl is also tested in this study with a CFD prediction of non premixed swirling flame. These results are compared with measurements and confrontations is satisfactory.

1. INTRODUCTION

One of the most important processes in the production of energy is combustion. It converts chemical energy into mechanical energy. Thus, the control of combustion constitutes a vital capacity in the development of new industrial systems, such as propulsion systems. One of the challenges facing the industry today to support technological development is to reduce the impact of combustion on the environment. This impact manifests itself in the rejection of polluting chemical species, of which we find, in the first rank, nitrogen oxides (NO_x) and gases participating in the greenhouse effect such as carbon oxides, CO and CO₂. This challenge obliges engine manufacturers to offer ever more innovative solutions to achieve the objectives set [1].

The several studies aim to minimize these emissions by introducing techniques such as lean combustion, the combustion of fuels of renewable origin and which does not contain carbon.

Combustion is one of the main themes of energy. This is why this work aims to simulate turbulent reactive flows, in particular the numerical study of turbulent diffusion flames (not premixed). Indeed, the latter are found in various technological applications such as industrial burners, diesel engines, industrial ovens etc. This type of flame is studied mainly for ecological reasons and because it is often easier to control combustion when the oxidant is injected separately from the fuel.

Combustion is a very complex phenomenon and its experimental investigation poses many difficulties. So, the experimental approach remains expensive and limited to certain operating conditions. However, digital computing can be the most suitable solution, given the progress made in the

field of computer science and modeling. There are several simulation models, either to simulate only the flow, or to simulate it by associating other joint phenomena [2].

Hydrogen (H₂) and methane CH₄ are two important fuels from an energy point of view. The physico-chemical description of their oxidation is the basic element for the study of more complex fuels. In practice H₂ is mainly used as fuel in rocket engines used as space launchers. CH₄ has an important practical application in the energy sector since it is the major constituent of natural gas.

Hydrogen is a clean fuel with no carbon emissions: its combustion produces only water and a reduced amount of nitrogen oxides. Hydrogen is not a primary energy, but an energy carrier [3]. The combustion of these mixtures would allow an overall reduction in emissions pending the development of new technologies [4]. Some studies have shown that enriching the combustion process with H₂ has effects on the location of the reaction zone, on the concentration of OH radicals, on the maximum temperature and consequently on NO_x emissions [5].

2. MATHEMATICAL MODEL

2.1 Equations

The balance equations governing the reacting flow are: mass conservation momentum spaces and the energy equation [3, 4].

2.2 NO_x formation during the combustion process

Nitrogen oxides are considered the most relevant pollutants.

The principal nitrogen oxides found in the atmospheric are nitric oxide (NO), nitrogen dioxides (NO₂), which is normally referred to as NO_x, and nitrous oxide (N₂O) [6-8]. The NO_x and N₂O pollutant emissions in the atmosphere have increased since the middle of the last century. Researchers have recently conducted studies to reduce NO and general NO_x emissions in combustion systems. NO is mostly produced within the reaction zone. The eventual oxidation to NO₂ occurs in a post-burn process away from the combustion region [9-11]. N₂O is mostly emitted from combustion sources. Four main NO sources are produced in the combustion process: thermal NO or Zeldovich mechanism, prompt NO or Fennimore mechanism, fuel NO, and N₂O. The main features of each NO formation mechanism are discussed in the following section [12].

2.3 Thermal NO_x

The construction of thermal NO corresponds to the direct oxidation of nitrogen molecules. The three principal reactions of the thermal NO formation mechanism are indicated as follows:

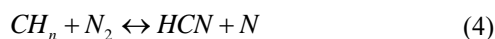


Thermal NO or Zeldovich mechanism is produced during the combustion process. Eqns. (1) and (2) show that N₂ and O₂ form the chain propagating steps known as the Zeldovich mechanism. The rate limiting reaction in NO formation is the N₂+O↔NO+N reaction. Thermal NO is strongly dependent on temperatures above 1500°C. The rate of formation rapidly increases with increasing temperature as a result of high activation energy (approximately Ea = 319 kJ/mol) [13, 14].

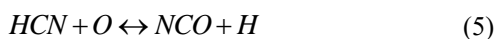
2.4 Prompt NO_x

Prompt NO formation, which occurs in fuel-rich systems, is a nitrogen oxide formation method described by Fennimore. Prompt NO can be found in the flame zone and involves a hydrocarbon species and the atmospheric nitrogen N₂. This NO formation mechanism is popularly termed 'prompt' because of the very early appearance of the flame at the flame front. The formation mechanism depends on the mixing rate of fuel and air. The formation of prompt NO follows the following reaction paths [15, 16]:

- (1) The reactions of N₂ with hydrocarbon fragments produce cyanide (HCN).



- (2) Ammonia radicals (NH, NH₂) are generated by HCN hydrogen abstraction reactions with oxy-cyanogens.



- (3) Ammonia radicals form NO.



2.5 Fuel NO_x

Fuel NO_x commonly originates from nitrogen-bearing fuels, such as certain solid and liquid fuels. Fuel NO_x is formed through the nitrogen oxidation contained in the fuel. Fuel NO_x is created once the nitrogen is chemically bound to the fuel by excess oxygen during combustion. During combustion, the nitrogen bound to the fuel is released as a free radical and ultimately forms free N₂ or NO. The production of fuel NO_x is dependent on the stoichiometric ratio between air and fuel. Fuel-rich mixtures generally result in high NO_x formation, implying that such process is independent of fuel type [17-19].

2.6 Turbulence model

The kinetic and the dissipation equation of the k-ε model are:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k u_j) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon = 0 \quad (9)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(\rho \varepsilon u_j) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \quad (10)$$

where:

$$C_{1\varepsilon}=1.44; C_{2\varepsilon}=1.92; C_{\mu}=0.09; \sigma_k=1.0; \sigma_\varepsilon=1.3$$

3. METHOD OF RESOLUTION

The resolution is made by the fluent code version 16 with an Upwind diagram of order 2. The pressure velocity coupling is ensured by the simple algorithm the convergence criterion 10-3. For the turbulence we chose the k-ε model, and for the combustion the Eddy dissipation model [20, 21].

4. GEOMETRICAL CONFIGURATION

A cylindrical geometry 450 mm in diameter and 1800 mm in length is used as a combustion chamber, a menu of a line for injecting fuel (methane or hydrogen) 10 mm in diameter and 50 mm in length (Figure 1).

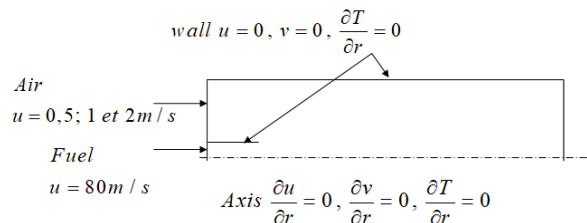


Figure 1. Geometrical configuration

The air enters at an ambient temperature of 300° K and with a speed of 0.5 m / s. The fuel (CH₄ or H₂) has the same temperature (300° K) and at a speed of 80m / s as shown in the following figure. A refinement of the areas in the vicinity of

the inlet and the axis of symmetry of the combustion chamber has been taken into account to capture the various phenomena that can occur in these areas, in particular the speed gradients.

5. RESULTS AND DISCUSSIONS

In order to compare the results of the two fuels (CH₄ and H₂) the temperature and some species are calculated in different sections.

Our comparison was carried out on the two fuels for the case of a flow rate corresponding to the air inlet speed of 0.5 m / s and 80m / s for the fuel inlet speed and in well-defined positions such that ((a): x = 300mm, (b): x = 400mm, (c): x = 500mm) for the profiles.

The temperature is raised in the center of the combustion chamber "the hot zone", and decreases until the wall temperature (300° k).

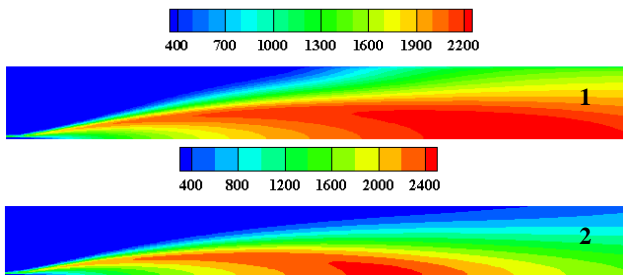


Figure 2. Temperature Contours of the two fuels: 1. (CH₄) et 2. (H₂)
(T_{max}(CH₄) = 2320°k et T_{max}(H₂) = 2490°k)

Note that the temperature is higher for the H₂ fuel in these stations than for the CH₄ fuel (Figure 2). This is for stations that are greater than x = 300cm (Figure 3: (a), (b) and (c)). The NO molar fractions for CH₄ fuel at these stations are higher than for those for H₂ fuel.

It is always observed that the fractions are high in the center of the combustion chamber (Figure 4, 5), it is the reaction zone.

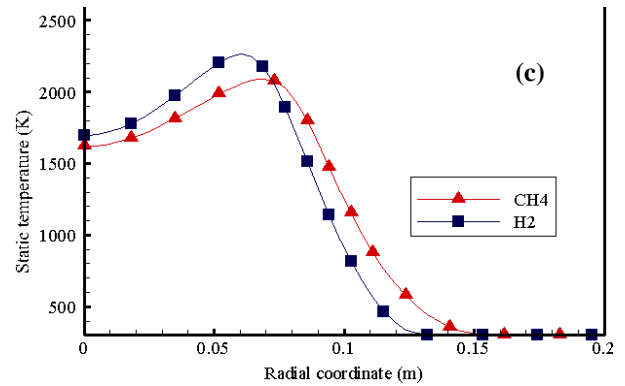
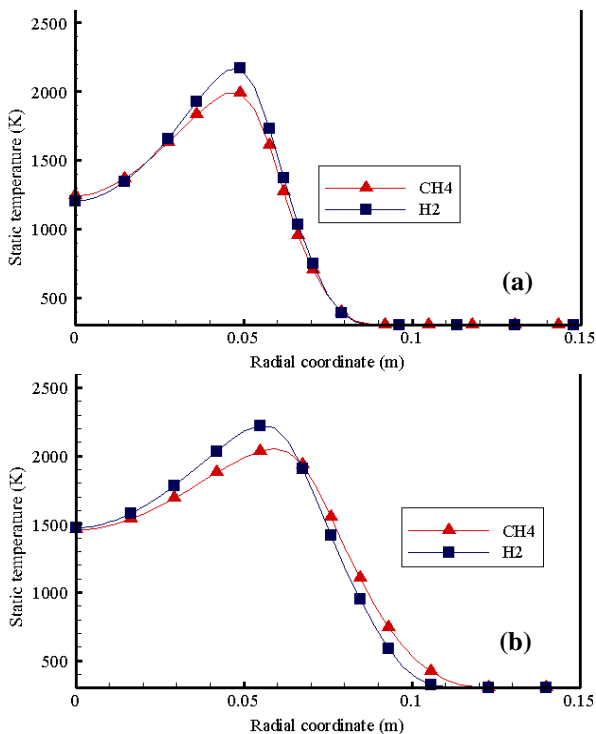


Figure 3. Temperature profiles of CH₄ and H₂

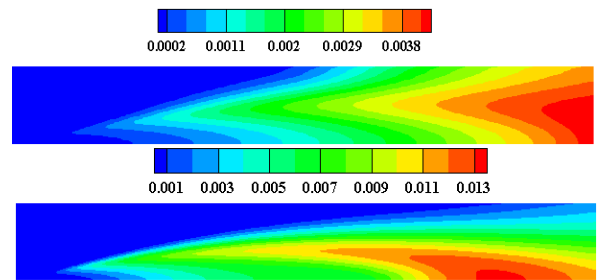
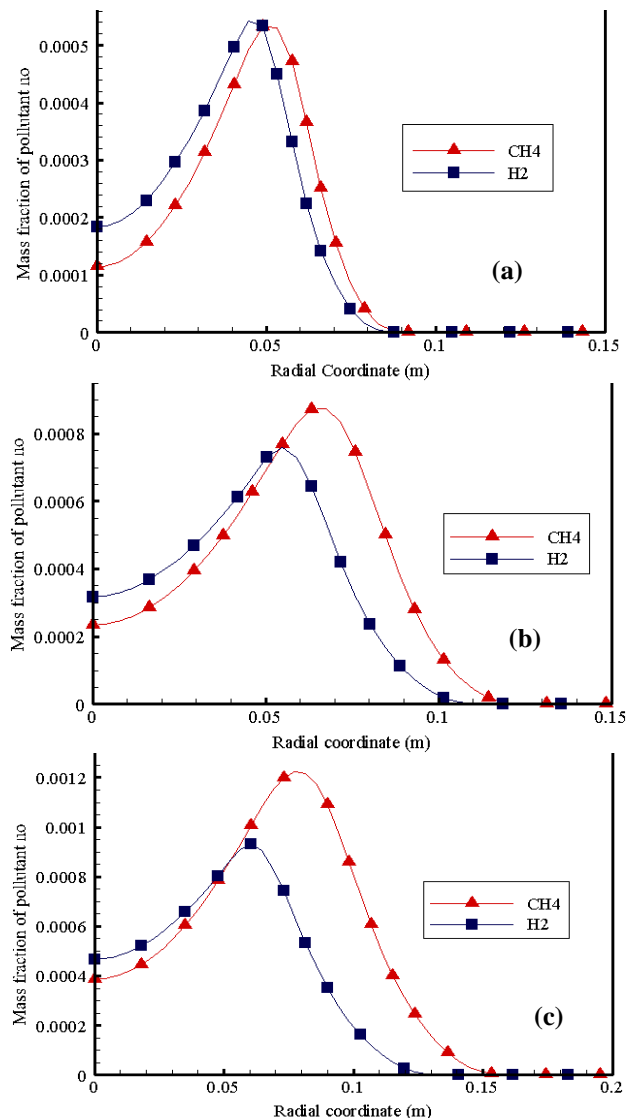


Figure 4. No Mass fraction contours of CH₄ and H₂



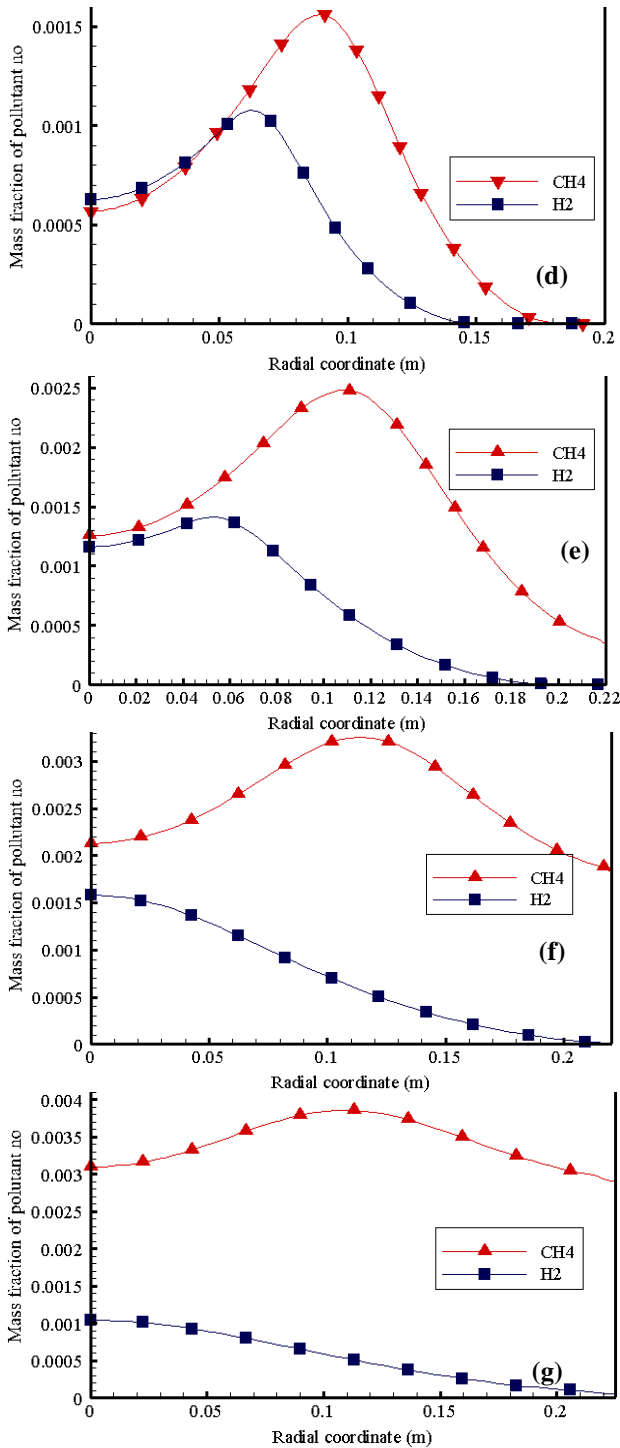


Figure 5. The molar fraction of pollutant NO for two fuels (CH₄ et H₂) at different position ((a): x = 300 mm, (b): x = 400 mm, (c): x = 500 mm, (d): x = 600mm, (e): x = 900 mm, (f): x = 1200 mm, (g): x =1500 mm)

The hydrogen fuel in the reaction mixture minus the nitrogen monoxide NO in the combustion products Figure 6.

In another study for swirling non premixed flame, we validate the obtained results by the experimental [16]. This validation is conducted by the axial velocity profiles, Figure 7.

In the first, we can be seen the existence of negative values, that explain the creation of the recirculation zone near the injection and the at the axis. It is the right prediction of the corner zone (CRZ) and the toroidal zone (CTRZ) [21].

The goal of this study is to predict the effect of the recirculation zone at the formation of the NO_x in the swirling flame. Figure 8 shows the temperature evolution profiles, it

can be seen that the profiles take two peak, the first peak in before the recirculation toroidal recirculation zone and the last after the recirculation zone.

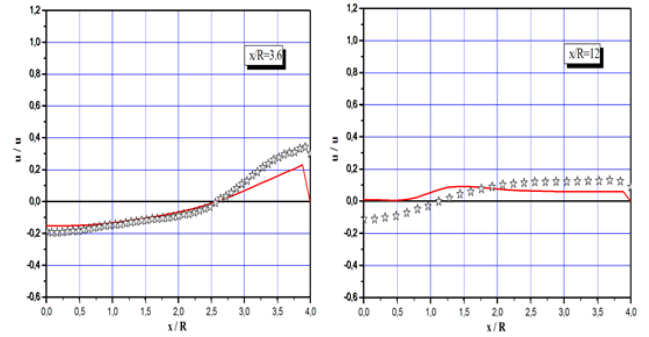


Figure 6. Validation with experiment of axial velocity at different section

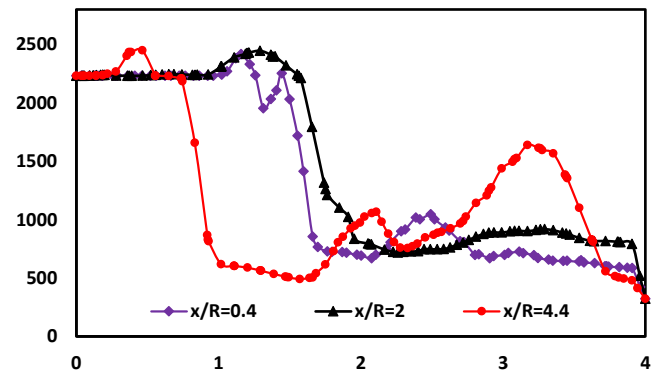


Figure 7. Profile of temperature in deferent section

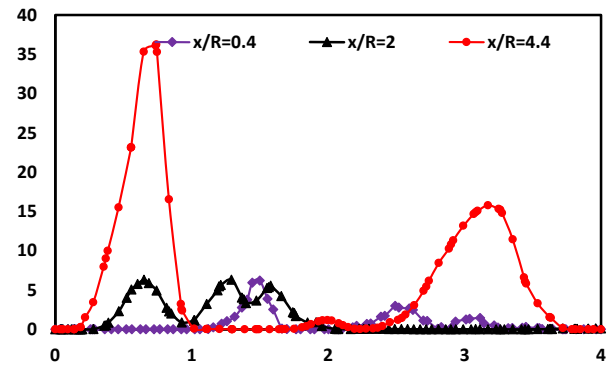


Figure 8. Profile of NO ppm: Prompt NO_x Formation

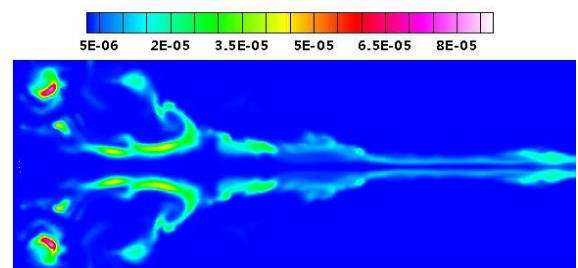


Figure 9. Contours of NO Mass Fraction: Thermal NO_x Formation

The NO_x formation in the swirling flame it is also described in the Figure 9. The NO_x profiles are plotted in deferent section, it can be concluded that the formation of NO_x is linked to the evolution of temperature. Where there are high

values the formation is greater, Figure 10. Formation of NOx is linked to the evolution of temperature. where there are high values the formation is greater, it is also important to give the description of the properties of this flame, where we have plotted the evolution curves of CH₄, O₂ and CO₂, these results confirm our prediction Figure 11. The last point in this study is a CFD prediction of all flame proprieties presented by the O₂, CO₂, H₂O and OH contours Figures 12, 13 and 14.

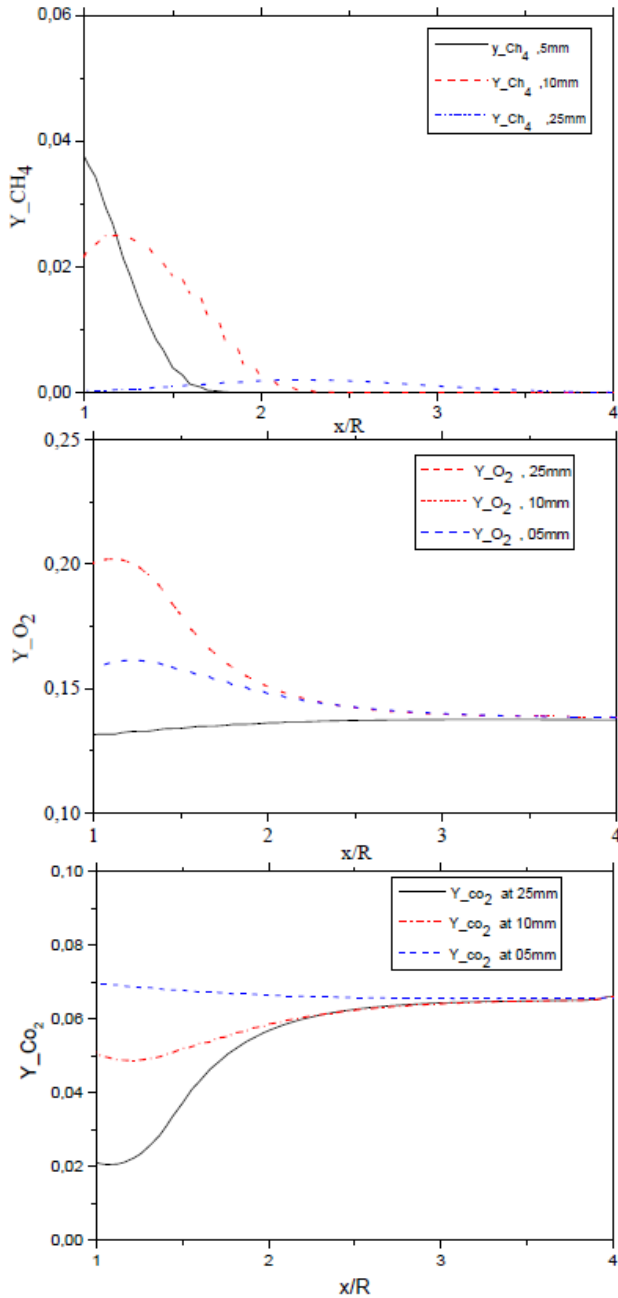


Figure 10. CH₄, O₂ and CO₂ evolution at different section

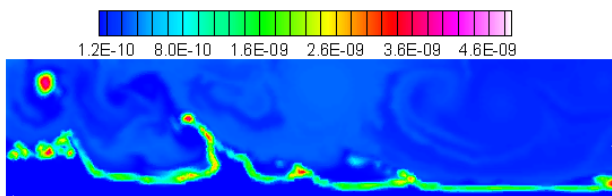


Figure 11. Contour of the O₂ consumption evolution in the combustion process

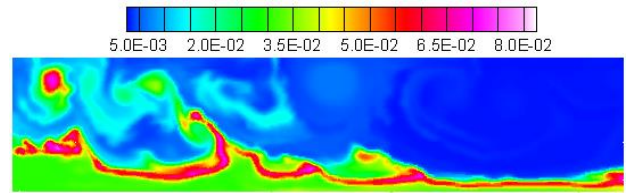


Figure 12. Contour of H₂O evolution formation in the combustion process

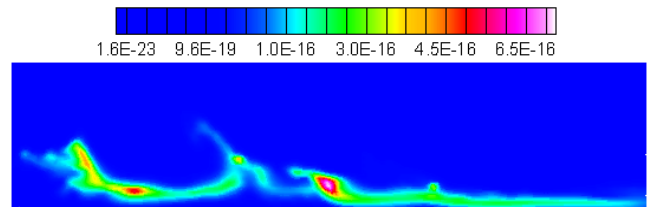


Figure 13. Contour of CO₂ in the combustion chamber

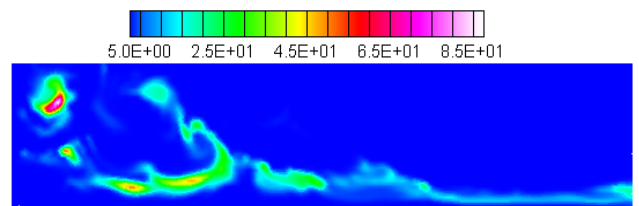


Figure 14. Contour of OH in the combustion process

6. CONCLUSION

In this work we studied numerically a flow with the reaction of chemical species in an enclosure similar to a combustion chamber. The flow being ax symmetric and turbulent, as can be encountered in diffusion flames (non-premixed), using the k-ε model and the Eddy Dissipation model. We used the Fluent CFD code. Our numerical simulations were presented for two different fuels (CH₄, H₂) in order to see their effects on the maximum temperature and the production of NO_x.

There are several different factors which directly influence the formation of NO_x but the most important is the high temperature. Another important factor is the nature of the fuel due to the fact that the formation of NO_x is dependent on the fuel used for combustion.

Oxides and oxides of nitrogen are the main pollutants emitted by combustion plants. NO_x has effects on the destruction of the ozone layer as well as on the ecosystem and human health. Pollutant releases can be controlled by regulations that encourage manufacturers to use combustion, to improve engines technologically or by reducing energy consumption by manufacturers.

Hydrogen is a clean fuel and can be obtained by renewable means (e.g. biomass or cracking of water by solar energy [14]). The replacement of a fuel by hydrogen is beneficial, because it is clean but remains dangerous and requires a lot of modifications in the installations, given its diffusion and its very high calorific value, Pci H₂ = 119,930 kJ / kg, PciCH₄ = 50020 kJ / kg [14]. To benefit in the short term from hydrogen, the solution is to replace part (10% by volume for example) of the fuel in a lean combustion, this makes it possible to keep the same installations with minimal modifications. This study it concluded by CFD prediction a swirling non premixed flame,

where the description of the NO_x formation is very clear and low than the other precedent flames.

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NOMENCLATURE

K	Turbulent Kinetic energy
M _f	Methane mass flow of kg/h
P	Pressure, Pas
V	Radial velocity, m/s
U	Axial velocity, m/s
W	Tangential velocity, m/s
Y _f	Methane and hydrogen mass fraction
Re	Reynolds number

Greek symbols

ν	Kinematic viscosity
ε	Dissipation rate
λ	Air equivalence ratio