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Syngas Combustion Characteristics in Counter-Flow Configuration

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Abstract— **Hydrogen-rich alternative fuels such as syngas are expected to serve as a clean energy in power generation systems. Fuels containing large amounts of hydrogen have combustion properties highly depending on composition, in particular hydrogen concentration, and operating conditions such as pressure. A thorough understanding of strained laminar flames is a prerequisite to achieve improved knowledge of more complex system.**

A numerical study of a syngas opposed-jet diffusion flame is carried out in order to analyse the impact of fuel composition (H_2/CO molar fraction = 0.4 to 2.4), operating pressure (1-10 atm) and strain rate ($1\text{-}10^3$ s^{-1}) on the flame structure and emissions including NO. The combustion model applied is the laminar flamelet approach and the chemical mechanism used is the GRI-Mech 3.

The computational predictions showed that flame structure and emissions are impacted by syngas composition and ambient pressure. Maximum flame temperature exhibits a peak at intermediate scalar dissipation rate for a given value of H_2/CO ratio. For values of strain rate lower than the intermediate value, flame temperature changed due to the combined effects of adiabatic temperature and radiation heat loss, whereas only adiabatic temperature effect prevails at higher values of strain rate. Hydrogen-rich syngas flames produce more NO at lower strain rates while NO levels increase towards hydrogen-lean syngas flames at higher strain rates. Besides, flame thickness decreased with H_2 enrichment and ambient pressure rise.
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Keywords— **Syngas composition – Non-premixed flames – Pressure – Strain rate – Pollutant emissions - NO – Carbon monoxide – carbon dioxide.**

I. INTRODUCTION

Syngas is mainly a mixture of hydrogen and carbon monoxide and can be obtained from natural gas, coal, petroleum, biomass and organic waste. The use of gasified fuels for electricity production is of increasing interest as an alternative to traditional fuels especially in regions with abundant biomass or coal resources. Nevertheless, its use in current power generation systems like gas turbine is challenging due to the differences in fuel composition with respect to conventional fuels. The actual defy is to design syngas combustors with reduced NOx emissions in agreement with the actual environment regulation.

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The numerical studies about syngas flames are recent in literature. Reference [1] studied experimentally and numerically a counterflow syngas flames at different ambient pressures. They found that flame temperature increases with increasing hydrogen contain and pressure. Reference [2] conducted a numerical study to understand the impact of fuel composition on flame structure in H_2/CO synthetic gas diffusion flame with and without CO2 dilution at atmospheric pressure. Effects of radiative heat loss to flame characteristics are also examined. They noticed that fractional flame temperature loss by flame radiation increased as CO and CO_2 mole fractions increased. It is also seen from the inspection of flame structure of major chemical species that the oxidation process of H_2 and CO can be modified through fuel composition and added CO_2 mole fraction. Reference [3] performed a computational study of combustion and extinction in opposed-jet syngas diffusion flames. They showed that the flame structures and extinction are impacted by the composition of syngas significantly. Flame temperature increases with increasing hydrogen while flame thickness decreases with pressure.

In this context, this study is conducted where the aim is to analyse the effects of syngas composition, operating pressure and strain rate on the flame structure and CO_2 and NO emissions in counter-flow configuration. Flame structure is characterized by solving flamelet equations in mixture fraction space with the consideration of radiation which is accounted for by optically thin assumption. A non-premixed configuration is chosen because syngas premixed flames are responsible of many problems (flashback) as the fuel contains important amounts of hydrogen.

This article consists of three parts. First, the laminar flamelet model is presented, followed by some simulation details. Simulation results are presented in the 2nd section with a discussion and comments. Finally, a conclusion summarizes the findings of this work.

II. NUMERICAL MODELS AND SIMULATION DETAILS

The combustion model adopted in this study is the laminar flamelet approach. This model has been introduced as an alternative to the equilibrium chemistry models [4]. The flamelet equations are written in mixture fraction space. Species mass fraction Y_n and temperature T transport equations are as follows:

$$\rho \frac{\partial Y_n}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 Y_n}{\partial z^2} + \qquad (1)$$

$$\rho \frac{\partial T}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 T}{\partial z^2} - \frac{1}{c_p} \sum_n H_n \, \dot{\omega}_n + \frac{1}{2 c_p} \rho \chi \left[\frac{\partial c_p}{\partial z} + \sum_n c_{p,n} \frac{\partial Y_n}{\partial z} \right] \frac{\partial T}{\partial z}$$

$$(2)$$

where ρ is the nth density, c_p,n is the specific heat

coefficient of species n at constant pressure, $\dot{\omega}_n$ is the nth species reaction rate and χ the instantaneous scalar dissipation rate defined by :

$$\chi = 2 \, D_z \, |\nabla Z|^2 \qquad (3)$$

χ is modeled using the stoichiometric scalar dissipation rate χst [5] :

$$\chi = \chi_{st} \frac{\phi}{\phi_{st}} \frac{g(Z)}{g(Z_{st})} \qquad (4)$$

where ϕ is a factor introduced in order to consider the effect of density variation [5] :

$$\phi = \frac{1}{4} \frac{3 \left(\sqrt{\rho_\infty/\rho} + 1 \right)^2}{2 \sqrt{\rho_\infty/\rho} + 1} \qquad (5)$$

The subscript ∞ means the oxidizer stream. The function g(Z) is given as follows [5] :

$$g(Z) = exp \left[-2 \left(erfc^{-1} (2Z) \right)^2 \right] \quad (6)$$

where $erfc^{-1}$ is the inverse of the complementary error function.

The syngas oxidation chemistry is modelled by using the detailed GRI Mech-3.0 [6] mechanism that involves 53 species and 325 reactions. The inlet temperatures are taken 300 K for both the fuel and the oxidiser. The laminar flamelets libraries are generated for different values of the scalar dissipation and ambient pressure.

III. RESULTS AND DISCUSSION

A. *The effect of strain rate on maximum flame temperature and NO emissions*

The first part of this work concerns the study of the influence of the strain rate on maximum flame temperature and NO emissions. Figure 1 shows the maximal temperature as a function of H_2/CO for different strain rates. Strain rate χ is an indicator of the flame stretch. For strain rates lower than

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10 s-1, maximum temperature increases with H_2/CO ratio and while for decreases for higher scalar dissipation rate values. Temperature behavior is due to the combined effects of adiabatic temperature and radiation heat loss. Temperature peak increased with pressure, the increase being rapid in the initial ranges up to 5 atm. Figure 2 represents the maximum NO mass fraction as a function of strain rates for different values of H_2/CO ratio. The evolution of NO is similar to that of maximum temperature (figure above). NO increases continuously with H2 enrichment and until 10 s^{-1}. Beyond this value, an opposite behaviour is noticed.
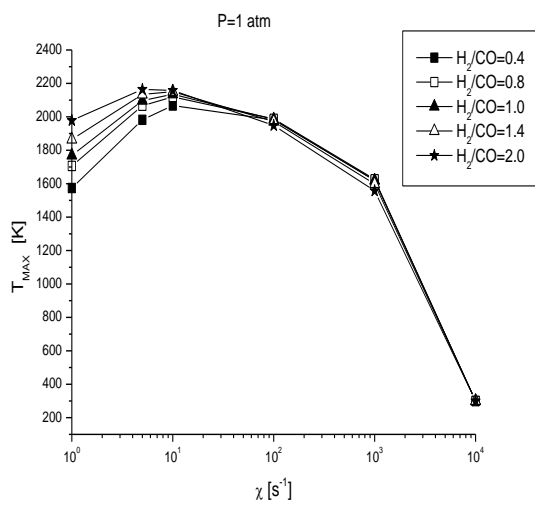
Fig. 1 Maximum flame temperature as a function of scalar dissipation   rate at different values of H_2/CO ratio (1 atm, 300 K)
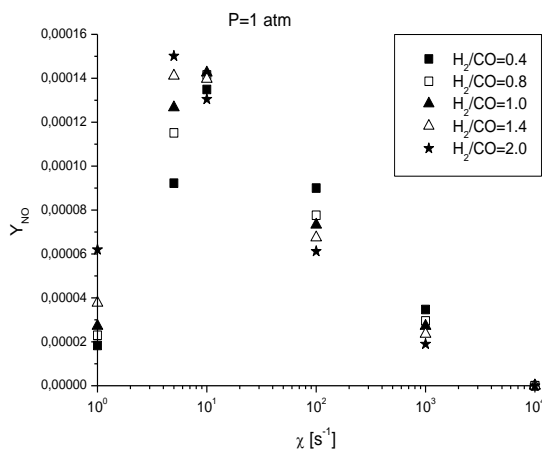

Fig.2 Maximum NO mole fraction as a function of scalar dissipation rate at different values of H_2/CO ratio (1 atm, 300 K)

B. The effect of syngas composition and pressure on flame structure and emission

The influence of the syngas composition on the flame temperature and pollutant emissions is analyzed at $\chi = 1$ s-1 in the second part of this work. First, the results at P = 1 atm are presented followed by those corresponding to higher pressure.

Figures 3,4,5 and 6 depicts the flame structures including the distribution of flame temperature and mass fraction of CO, CO2 and NO at $\chi = 1$ s^{-1}. Ambient temperature and pressure are 300 K and 1 atm, respectively. According to this figure, hydrogen addition induces a shift of the radial spreading profiles of the involved temperature and species towards the air side. The flame is thinner when H_2 increases in the syngas. This is due to high diffusivity and lightness of hydrogen. Temperature (figure 3) exhibits the same shape for the H_2/CO molar ratios considered: it increases to reach a peak then decreases. The maximal value of temperature increases with H_2 enrichment. An increase in hydrogen concentration results in a lower carbon input to the flame, and thereby reduces CO (figure 4) and CO2 formation (figure 5). NO profiles (figure 6) have the same tendency as temperature. A major observation is that H_2 rich syngas produces more NO than CO rich syngas. It is important to notice that syngas do not contain nitrogen and that prevents the formation of fuel bound NO.
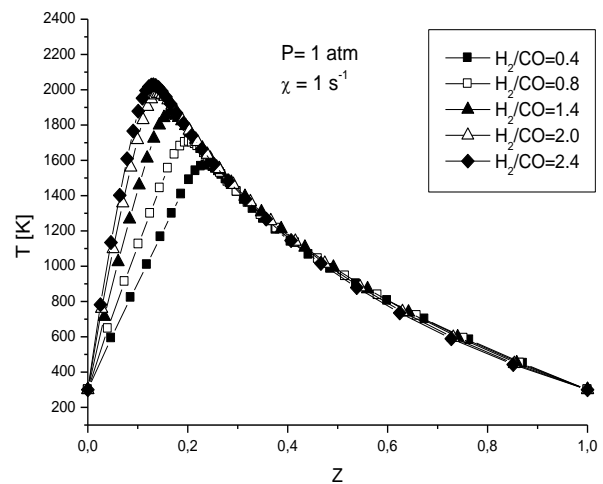

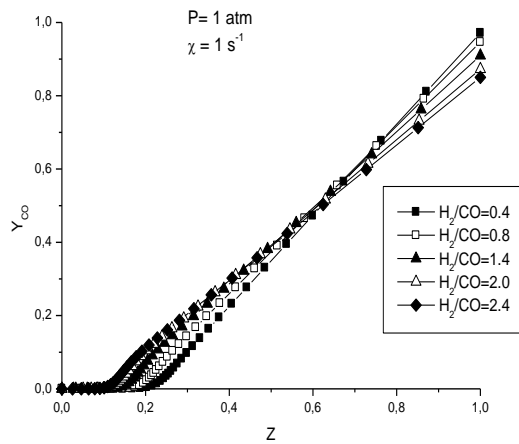Fig. 3   Effect of H_2/CO molar rate on Temperature profiles ($\chi = 1$ s-1, 1 atm,

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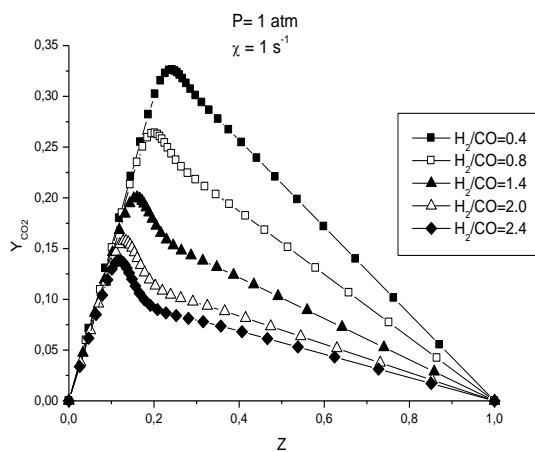Ghardaïa – Algérie 15, 16 et 17 Octobre 2012

Fig. 4   Effect of H$_2$/CO molar rate on CO profiles (χ = 1s^{-1}, 1atm, 300K)

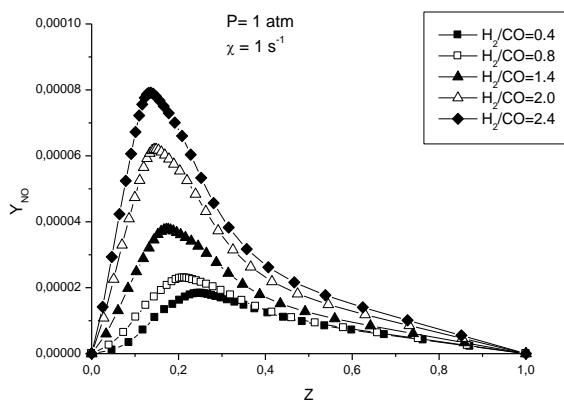Fig. 5   Effect of H$_2$/CO molar rate on CO$_2$ profiles (χ = 1s^{-1}, 1atm, 300K)

Fig. 6   Effect of H2/CO molar rate on NO profiles (χ = 1s-1, 1atm, 300K)

The pressure effects on syngas flames are presented in figure 4 for H$_2$/CO=1.0 at χ = 1s-1. One may see that temperature, CO2 and NO mass fractions increase with pressure. According to the principle of Le Châtelier, a pressure increase in a combustion system reduces the amount of dissociation, and the maximum flame temperature increases (figure 7). Although temperature is higher as pressure increases, thermal radiation becomes progressively less important since it is inherently a volumetric phenomenon. A fast increase of the peak of temperature, NO and CO2 (figures 7, 9 and 10) is noticed from 1 to 5 atm, whereas slower increase can be seen from 5 to 10 atm. The active O and OH radical concentrations in the flame keep decreasing with pressure. The significant

effects of pressure on these concentrations is attributed to the recombination reactions involving a third body which are more favoured at high pressure. NO increases at high pressures for both H$_2$- lean and H$_2$- rich syngas. Fig.8 shows that pressure variations don not really affect CO except in the flame front where CO slightly decreases with pressure. This is due to the fact that CO is one of syngas components and is renewed during the combustion.
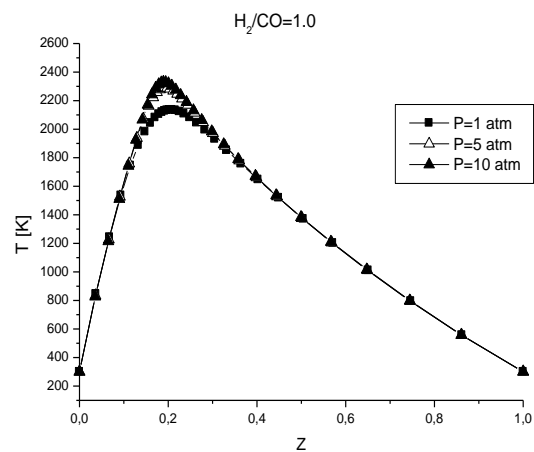

Fig. 7   Effect of pressure on temperature profiles (χ = 1s-1, 1atm, 300K)

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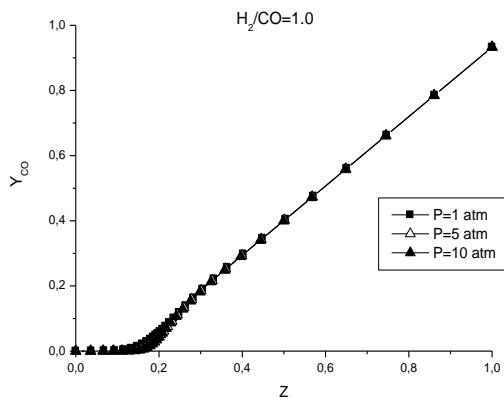Ghardaïa – Algérie 15, 16 et 17 Octobre 2012

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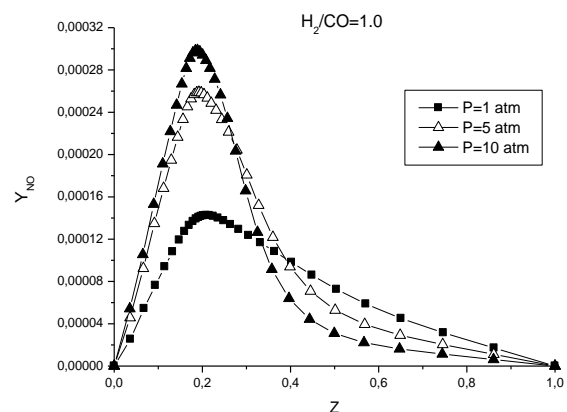Fig. 8   Effect of pressure on CO profiles ($\chi = 1s^{-1}$, 1atm, 300K)

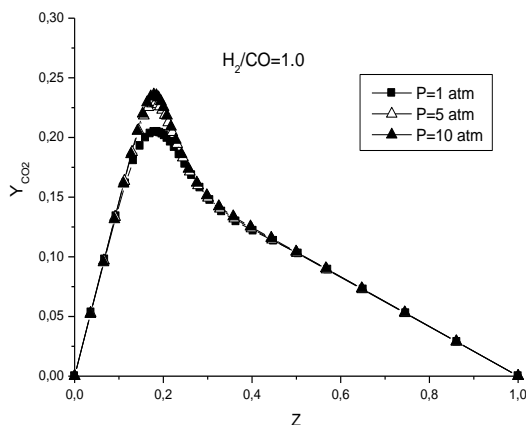Fig. 10   Effect of pressure on NO profiles ($\chi = 1s^{-1}$, 1atm, 300K)

Fig. 9   Effect of pressure on CO profiles ($\chi = 1s^{-1}$, 1atm, 300K)

IV. CONCLUSIONS

A numerical simulation of a non-premixed syngas flame is conducted using flamelet model with the full GRI 3 mechanism. The investigation has been done in a wide range of operating. It is found that:

The flame temperature increases more the syngas is H_2-rich.

The flame is thinner for H_2-rich syngas.

CO and CO_2 are significantly reduced for H_2-rich syngas.

NO emissions depends strongly on temperature, that means that thermal NO is more important than prompt NO in syngas flames and fuel NO does not exist because syngas does not contain nitrogen.

Strain rate variations affect flame structure and pollutant emissions. There is a limit beyond which temperature and NO mass fraction decreases.

NO and CO_2 mass fractions are affected by pressure rise.

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