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NUMERICAL STUDIES OF FUEL-RICH MICRO COMBUSTION: EFFECT OF N_2 DILUTION ON NO_x EMISSIONS

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Abstract.
The characteristics of micro-combustion have been studied as an alternative power supply in micro-device systems, because of the high energy density when compared with the typical batteries. It is known that heat release at micro scales results in different flame behavior as compared to conventional scales, leading to several practical limitations in both design and performance. For this reason the study of geometry, mixture stoichiometry, flow rates, wall temperatures are widely covered in literature to better understand the limits of a stable flame. Due to the important role on controlling the flame behavior and subsequent pollutants emissions at micro scales, the dilution effects still need further study. In this work the effects of the dilution levels on the combustion characteristics of premixed hydrogen/air, for different equivalence ratios in the fuel-rich regime of flammability limits ($\phi = 1.6$ and $\phi = 6.4$) were numerically studied. The simulations were performed in a axis-symmetric micro channel (with diameter $D = 0.8\,mm$ and length $L = 10\,mm$), using very detailed chemical kinetics (32 species and 173 reactions), and for the heat transfer control it was imposed a hyperbolic temperature profile on the wall, which increases from 300 K at the inlet to 1300 K at the outlet. More specifically, detailed results obtained for the ignition process, for the flame dynamics and stabilization, and NO_x emissions are reported for the different operating conditions.

Keywords: *Numerical simulation, Micro-combustion, NO_x emissions*

1. INTRODUCTION

The advances in the fabrication of devices at micro scales and the multifunctionalization of mechanical and electronic systems, allowed the development of Micro-Electro-Mechanical Systems (MEMS) devices. This type of devices are the integration of microelectronic and micro-mechanical systems on a single chip, which can be used in several applications. However, their dependence on batteries for power supply limits their applicability. As an alternative, studies of micro combustion had been performed as a stable power source, with the advantage of being more compact due to the high energy density of the fuels. For this reason, combustion characteristics at small scales have been continuously studied, but it is known that heat release at micro scales results in different flame behavior as compared to meso and macro scales, leading to limitations in establishing a stable flame.

Several numerical studies have been performed to better understand the combustion characteristics at micro scales, specially the stable flame limits for different parameters, such as geometry, mixture stoichiometry, flow rates and wall temperatures, (Li *et al.*, 2008; Aikun *et al.*, 2011; Xu *et al.*, 2013; Hossain and Nakamura, 2015; Xu *et al.*, 2016; Cova *et al.*, 2017; Ayoobi and Schoegl, 2017). Li *et al.* (2008) conducted numerical simulations for premixed hydrogen/air flames, in small scaled cylindrical and parallel plates, to study the effect of geometry and inlet velocity, and referenced the

importance of axial heat conduction to preheat the unburned mixture. To analyze the 3D effect in the flame temperature and length, Aikun *et al.* (2011) simulated the combustion of a hydrogen/air mixture in a 3D rectangular micro-channel, varying the wall material, channel height and the inlet velocity, and concluded that the flame remained stable and persisted for a wide velocity range. More recently, Xu *et al.* (2016) studied an experimental and numerical diffusion microflame of liquid biobutanol under electric field, and reported that the quenching flow rate decreased and increased after it reached its minimum, as the electric field intensity increased. They also verified that the traditional gas jet diffusion flame theory was not suitable to simulate the micro scale flame for the smaller tube, with 0.4mm of diameter. Moreover, increasing the electric field intensity the flame height had an opposite behaviour on the quenching flow rate, increasing at first and then decreasing. Also the maximum flame height is reach more faster for the smaller tube.

The dilution effect on combustion emissions and burning velocities of premixed combustion were the subject of several studies at macro and meso scales, for example Miao *et al.* (2009), Li *et al.* (2016) or Duan and Liu (2017). Miao *et al.* (2009) studied the impact of the dilution with N_2 of the initial pressure on the flame propagation for premixed H_2/air and natural gas/air mixtures, and reported that the laminar burning velocities decreased with dilution and pressure. The study of Li *et al.* (2016) consisted in the analysis of the impacts of N_2 and CO_2 dilutions on premixed syngas spherical flames at conventional scales. They concluded that laminar burning velocities are more susceptible to the thermal effects than the chemical effects, specially with the CO_2 dilution. Recently, Duan and Liu (2017) obtained a similar behaviour to that found by Miao *et al.* (2009), a reduction of the laminar burning velocities with the increase of diluents concentrations of N_2 and H_2O.

The impact of dilution effects on combustion at micro scales needs further studies, Resende *et al.* (2017), since at such scales the importance of controlling the flame and pollutant emissions is crucial. Therefore, in this work we investigate the impact of dilution levels in fuel-rich micro-combustion regime, for premixed air-hydrogen flames. Detailed results for flame dynamics, flame stabilization, NO_x emissions and ignition process were obtained for several operation conditions.

2. METHODOLOGY

The simulations had been performed in OpenFoam, using a detailed kinetic mechanism of 32 species and 173 reactions for the chemical reaction of premixed hydrogen combustion, devepoled by CRECK Modelling Group from the Polytechnic University of Milan, (Ranzi *et al.*, 2012). The governing equations used for the combustion simulation are the conservation equations for a continuous, compressible, multi-component, and thermally-perfect gas mixture for Newtonian fluids in laminar regime, and were implemented in the laminarSMOKE code by Cuoci *et al.* (2013). The conservation equations of total mass, momentum, species mass fractions and energy are the following

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \tag{1}$$

$$\rho \left[\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{uu} \right] = -\nabla p + \nabla \cdot \vec{\tau} + \eta_s \nabla^2 \mathbf{u} + \rho \mathbf{g} \tag{2}$$

$$\frac{\partial}{\partial t}(\rho Y_k) + \nabla(\rho Y_k \mathbf{u}) = -\nabla(\rho Y_k \mathbf{V_k}) + \dot{R}_k \qquad k = 1, \ldots, N_C \tag{3}$$

$$\rho C_P \frac{\partial T}{\partial t} + \rho C_P \mathbf{u} \nabla T = -\nabla \mathbf{q} - \rho \sum_{k=1}^{N_C} C_{P,k} Y_k V_k - \sum_{k=1}^{N_C} h_k \dot{\Omega}_k \tag{4}$$

where, ρ, t, τ, $\mathbf{u}$, $\mathbf{g}$, and p represent the mixture density, time, the fluid stress tensor, the mixture velocity vector, the acceleration vector due to gravity and the pressure, respectively. N_C is the total number of species, T is the temperature, and Y_k , $\mathbf{V_k}$, $\dot{R}_k$, h_k and $\dot{\Omega}_k$ are the mass fraction, the diffusion velocity, the formation rate, the enthalpy and the net production rate of the k^{th} species, respectively. C_p represents the specific heats. The gas mixture is assumed to be an ideal gas and its density is calculated through the equation of state. The heat flux vector, $\mathbf{q}$, is defined as:

$$\mathbf{q} = -\lambda \nabla T + \mathbf{q}_{rad} \tag{5}$$

where λ is the mixture thermal conductivity and $\mathbf{q}_{rad}$ is the radiative heat transfer, which is calculated by Eq. (6).

$$\nabla \vec{q}_{rad} = -4\sigma a_P (T^4 - T_{env}^4) \tag{6}$$

where, σ is the Stefan-Boltzmann constant, a_P is the Planck mean absorption coefficient and T_{env} is the environment temperature. The diffusion velocities of species k are calculated from Fick's law and the thermal diffusion effect:

$$\mathbf{V_k} = -\frac{D_k}{Y_k} \nabla Y_k - \frac{D_k \Theta_k}{X_k} \frac{1}{T} \nabla T \tag{7}$$

where, X_k, Θ_k, and D_k are the mole fraction, the thermal diffusion and the mixture-averaged diffusion coefficient of species k. D_k is related to the binary diffusion coefficients $\Gamma_{jk}$by the following expression.

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k}^{NC} \frac{X_k}{\Gamma_{jk}}} \tag{8}$$

The boundary conditions (BC) and the used geometry configuration are described in the next section.

3. NUMERICAL SIMULATION

In the present work, a combustion of a premixed hydrogen/oxygen diluted with N_2 is simulated, using detailed chemical kinetics (32 species and 173 reactions). The combustor chamber is an axis-symmetric micro channel (diameter $D = 0.8$ mm and length $L = 10$ mm), where the heat transfer at the wall is considered by imposing a hyperbolic temperature profile, with the wall temperature increasing from 300 K at the inlet to 1300 K at 3/8 of channel length, a typical boundary condition used in both experiments and simulations, Maruta *et al.* (2005) and Pizza *et al.* (2008). For all simulations, the inlet mean velocity was 4 m/s, assuming fully developed profile, and a mesh resolution for the computational domain with 30x200 cells. The schematic illustration of the computational domain and the temperature profile can be observed in Fig. 1.

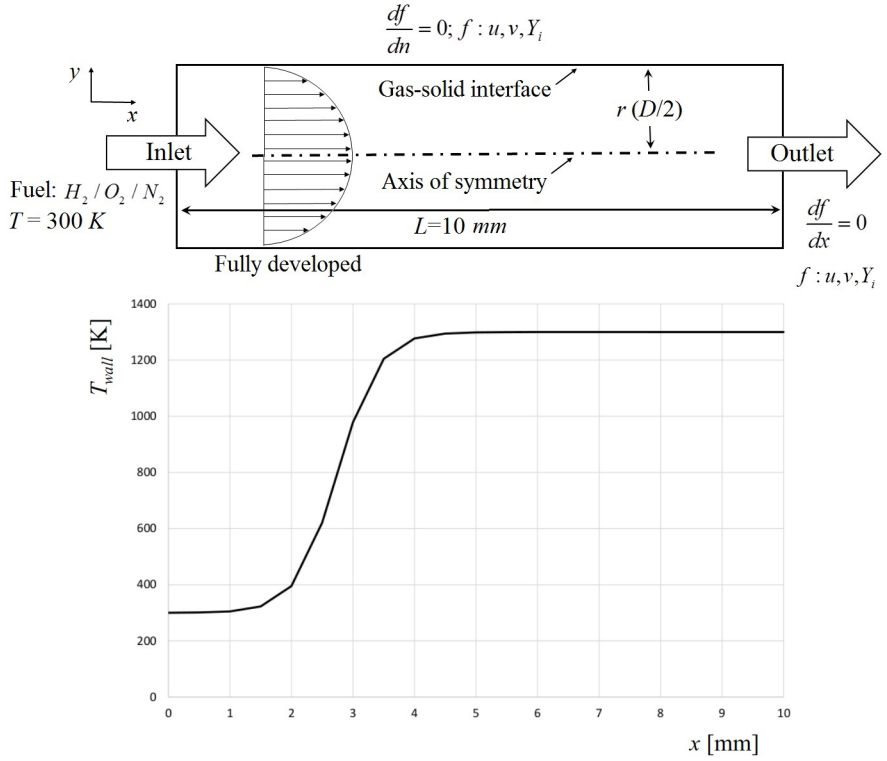

Figure 1. Schematic illustration of the computational domain and the temperature profile at the wall

With this setup, a range of equivalence ratios from lower to high flammability limit of hydrogen ($\phi = 1.6$ and $\phi = 6.4$) was investigated. The stoichiometry reaction for a typical hydrogen/air mixture combustion is given by the Eq. (9), but in the present study for each equivalence ratio, the excess dilution (using N2) is gradually increased, according with reaction Eq. (10), where the reactants mixture with equivalence ratio, ϕ, and excess dilution is represented by n. The dilution impact is analyzed by comparison with the other cases.

$$\mathrm{H_2} + \frac{1}{2}\left[\mathrm{O_2} + 3.76\,\mathrm{N_2}\right] \tag{9}$$

$$\phi\mathrm{H_2} + \frac{1}{2}\left[\mathrm{O_2} + 3.76\,\mathrm{n\,N_2}\right] \rightarrow \text{products} \tag{10}$$

4. RESULTS

The dilution effect on premixed hydrogen-rich flames inside of the burner for different equivalent ratios at micro scale, and the emission of pollutant gases, are investigated numerically. The flame shape for different equivalence ratios, at 1.6

and 6.4, with N_2 dilution, followed by the relation $n = x1.14$, where x=1, 2, 3, 4, 5 and 6, can be accessed by the heat release distribution, Figure 1. As expected for lower ϕ and higher dilution the heat release decreases, and the flame adopts a V shape as the dilution increases. However, for richer hydrogen mixtures the V-shaped flame tends to an oval shaped, smaller and less intense. This can be observed in Figure 2, where it is presented the total heat release for all tested cases, and as the mixture becomes richer, the total heat release decreases. The reduction of the total heat release (%) for the different equivalence ratios and N_2 dilution cases is presented in Tab. 1, where the reference case is n=1x1.14, without excess of N_2 dilution.

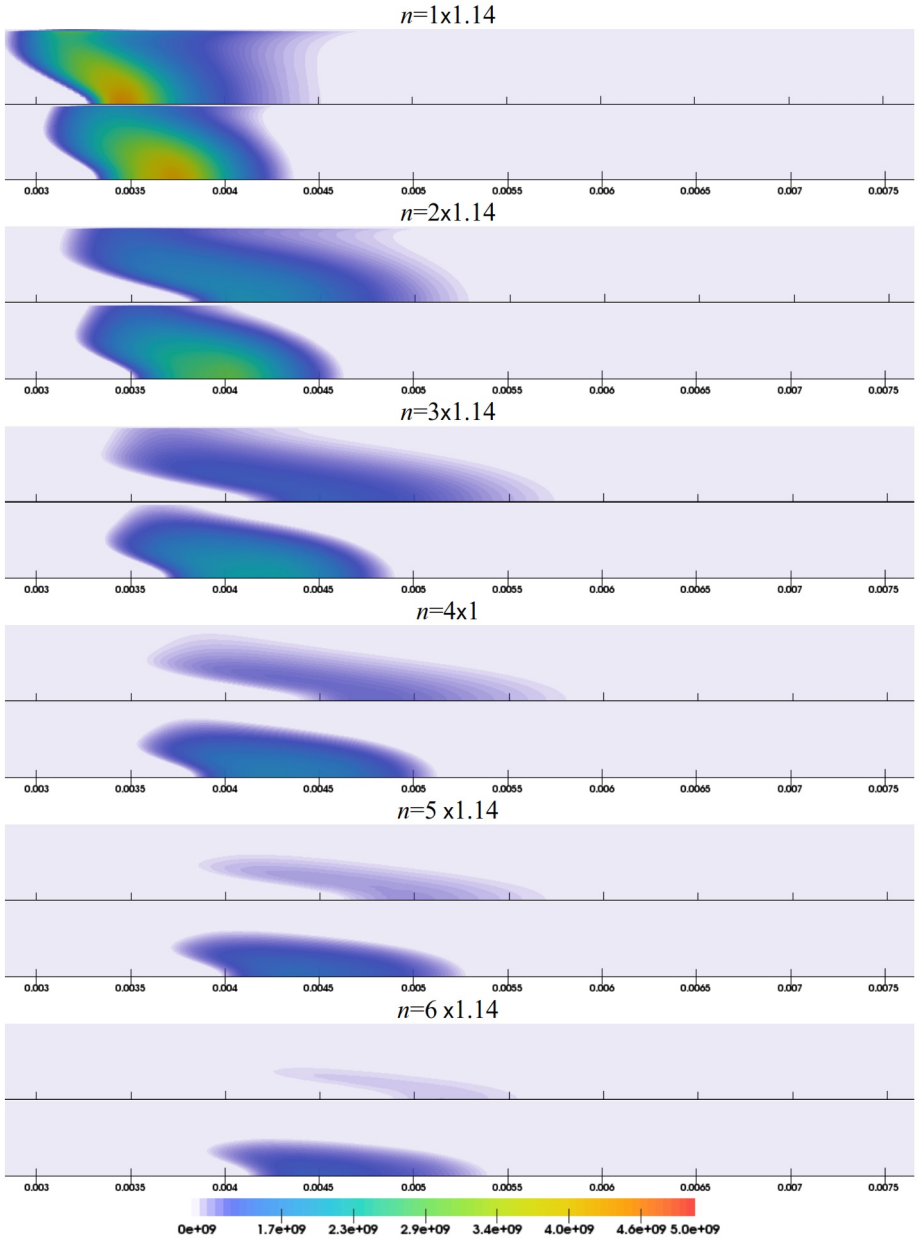

Figure 2. Heat release distribution for different equivalence ratios: 1.6 (top) and 6.4 (bottom), with N_2 dilution (n=1x1.14, 2x1.14, 3x1.14, 4x1.14, 5x1.14 and 6x1.14)

Figure 2 presents the mass flow rates of NO_x release for the same equivalence ratios and dilute mixtures presented before. As expected, there is a reduction of the NO_x, emissions with the increase of dilution, being more intense at $\phi = 1.6$, with a relative reduction of approximately 73%. For higher equivalence ratios the NO_x reduction becomes less intense with the increase of the N_2 dilution, achieving a maximum relative reduction of 45%. It is also possible to observe different behaviours, for $\phi = 1.6$; the maximum NO_x emission occurred to n=1x1.14 and decreased exponentially with the dilution increase, but for higher equivalence ratios values, $\phi = 6.4$, there is initially a small increase of the NO_x emission achieving a maximum value at n=2x1.14 and then reducing with low intensity.

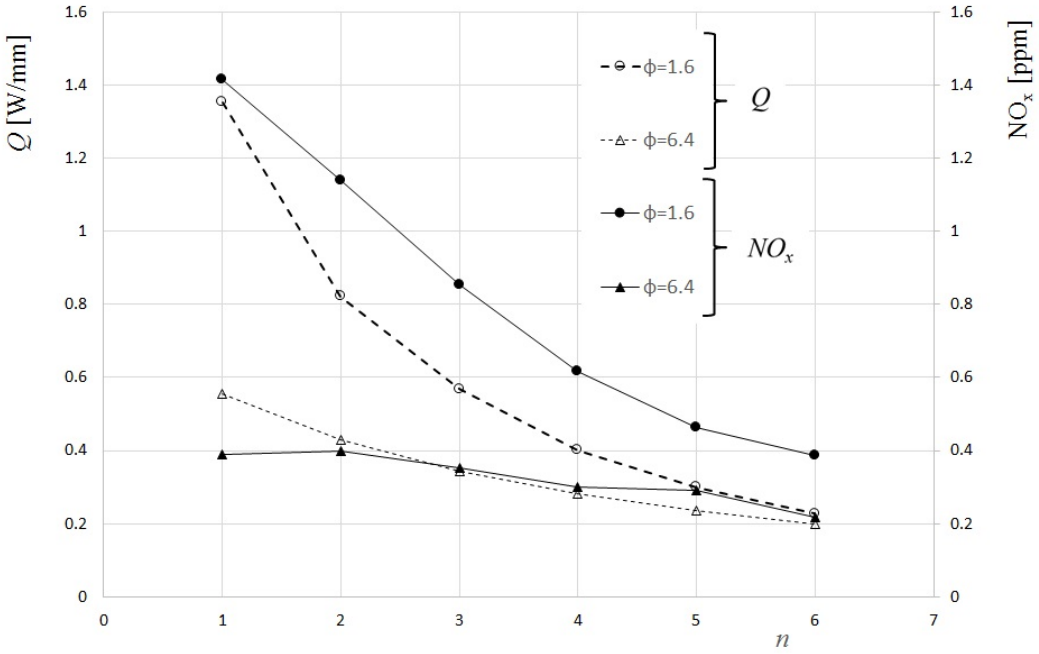

Figure 3. Total heat release, Q, and mass flow rate of NO_x for different equivalence ratios: 1.6 and 6.4, with N_2 dilution (n=1x1.14, 2x1.14, 3x1.14, 4x1.14, 5x1.14 and 6x1.14)

Table 1. Total heat release reduction (%)

	n=1x1.14	n=2x1.14	n=3x1.14	n=4x1.14	n=5x1.14	n=6x1.14
$\phi = 1.6$	-	39	58	70	78	83
$\phi = 6.4$	-	23	38	49	58	64

5. CONCLUSIONS

A numerical study was performed in order to study the flame characteristics and the NO_x emission, in the premixed hydrogen-rich combustion for different degree of N_2 dilution at micro scale. The results obtained by the present work may be summarized as follows:

1. The flame presented a V-shaped form as the dilution increases at lower equivalence ratios, however in the limits of higher dilution and equivalence ratios, the flame tends to into an oval shaped form.

2. A reduction of the total heat release occurs in both situations of higher equivalence ratios and N_2 dilute cases, as expected, being more intense at $\phi = 1.6$.

3. The NO_x emissions from hydrogen combustion are reduced at rich combustion and higher values of N_2 dilution. For lower equivalence ratio, $\phi = 1.6$, there is a significant NO_x reduction as the dilution increases. However, for higher equivalence ratios, the dilution has small impact on NO_x reduction.

6. ACKNOWLEDGEMENTS

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