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Large Eddy Simulation of Transient Flame-Vortex Interactions during Explosions of Hydrogen-Enriched Methane/Air Mixtures

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Large Eddy Simulation (LES) was used to study transient interactions between hydrogen-enriched methane/air premixed flames and toroidal vortex structures at the wake of a circular orifice. Computations were run for stoichiometric mixtures with hydrogen mole fraction in the fuel (hydrogen plus methane), x_{H2}, varying in the range of 0-0.5.
LES predictions reproduce well previously obtained experimental data, confirming that the intensity of the flame-vortex interaction increases with increasing x_{H2}. This is a direct result of the higher reactivity (i.e., higher laminar burning velocity) of the hydrogen-enriched mixtures that produces faster flame propagation upstream of the orifice and, thus, higher rotational velocity for the toroidal vortex at the orifice wake, leading to further increase in the burning rate resulting from the interaction.

1. Introduction

Hydrogen-enrichment has been recognized as a useful method to overcome several drawbacks (local flame extinction, combustion instabilities, lower power output, etc.) encountered during turbulent premixed combustion of natural gas in both stationary (Schefer et al., 2002) and mobile (Bauer and Forest, 2001) systems.
Experimental and computational studies performed in simplified flow configurations have shown that the hydrogen addition to methane (the main constituent of natural gas) increases the laminar burning velocity (i.e., the flame reactivity) (Di Sarli and Di Benedetto, 2007; Halter et al., 2007; Boushaki et al., 2012), the resistance to extinction (Ren et al., 2001; Schefer et al., 2002; Jackson et al., 2003; Hawkes and Chen, 2004) and the flame front wrinkling (i.e., the flame surface area) (Hawkes and Chen, 2004; Halter et al., 2007), thus enhancing robustness and stability of the flame. These positive effects have been attributed to the increase in both flame temperature (thermal effects) and supply of active radicals (chemical effects). Also, non-equidiffusive effects (i.e., non-unity Lewis number and preferential diffusion) have been invoked, especially for lean flames (Ren et al., 2001; Jackson et al., 2003; Hawkes and Chen, 2004; Halter et al., 2007).
For the safe use of hydrogen-methane blends, it is essential to fully characterize and understand their explosion behavior.
In practical situations, when an explosion occurs, the premixed flame propagating away from an ignition source encounters obstacles (vessels, pipes, tanks, walls, flow cross-section variations, instrumentation, etc.) along its path. The unsteady coupling of the moving flame and the flow field induced by the presence of local blockage produces vortex structures of different length and velocity scales ahead of the flame front. The flame-vortex interaction leads the initially laminar flame to burn through various turbulent combustion regimes, which are dependent on both size and velocity of the vortices encountered (Di Sarli

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et al., 2009a; 2012a; 2012b). The flame acceleration associated with the regime transition increases the rate of pressure rise (Di Sarli et al., 2009a; 2009b).
In previous papers (Cammarota et al., 2009; 2010; Salzano et al., 2012), we ran explosion tests for stoichiometric hydrogen-methane/air mixtures in a closed cylindrical vessel. The effect of the hydrogen-enrichment has been quantified, for different initial pressures, in terms of increase in maximum pressure, maximum rate of pressure rise and laminar burning velocity.
In a more recent work (Di Sarli et al., 2012c), we used time-resolved Particle Image Velocimetry (PIV) to study transient interactions between hydrogen-methane/air premixed flames and simple toroidal vortex structures generated, in a controlled manner, at the wake of a circular orifice. Lean and stoichiometric mixtures with hydrogen mole fraction in the fuel (hydrogen plus methane), x_{H2}, varying in the range of 0-0.5 were investigated. Results have shown that, regardless of the mixture stoichiometry, the hydrogen-enrichment leads to a transition from a combustion regime in which the vortex only wrinkles the flame front ($x_{H2} < 0.2$) to a more vigorous regime in which the interaction almost results in the separation of small flame pockets from the main front ($x_{H2} > 0.2$).
In this work, we aimed to gain insights into how the hydrogen substitution to methane affects the mechanisms of transient flame-vortex interaction. In particular, we focused our attention on the effects of the hydrogen-enhanced reactivity. To this end, we used a Large Eddy Simulation (LES) model coupled to a combustion sub-model that takes into account the effects of the hydrogen-enrichment only in terms of increased laminar burning velocity. With this model, we ran computations for our recent experiments (Di Sarli et al., 2012c).

2. Experiments simulated in this work

Our recent experiments (Di Sarli et al., 2012c) were carried out by using a combustion bomb (schematized in Figure 1) that consisted of a small cylindrical pre-chamber (height = 35 mm; diameter = 70 mm) linked to a much larger main chamber (150 mm x 150 mm x 150 mm) via an orifice (height = 25 mm; diameter = 30 mm; 90° corners at both the inlet and exit faces). Premixed charges of fuel (hydrogen plus methane) and air were ignited (from rest) at the center of the bottom face of the pre-chamber. Experiments were run for lean and stoichiometric mixtures with hydrogen mole fraction in the fuel, x_{H2}, equal to 0, 0.2, 0.4 and 0.5. After ignition, the propagation of the flame front set in motion unburned gas ahead of it through the orifice. The interaction of this movement with the downstream static charge resulted in a shear layer at the orifice exit and, thus, shedding of a toroidal vortex into the main chamber. As the flame front progressed through the charge, it interacted with this vortex, distorting the flame and altering its burning velocity.

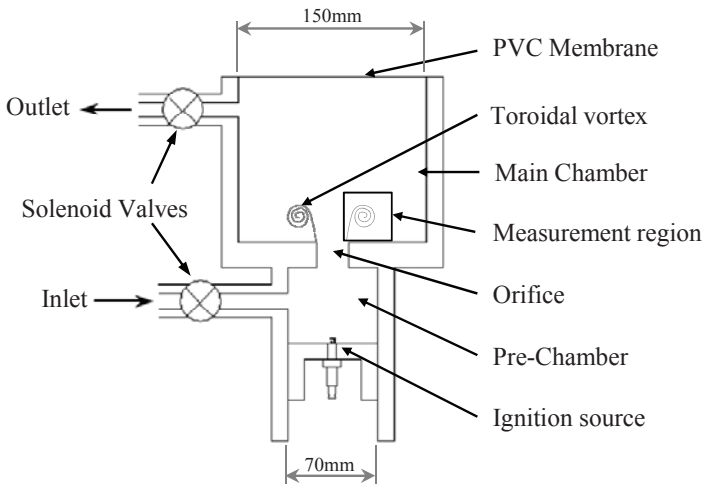

Figure 1: Schematic representation of the combustion bomb used in the experiments simulated in this work (not to scale) (from Di Sarli et al., 2012c).

In this work, large eddy simulations were performed for stoichiometric mixtures with different x_{H2} values.

3. The Large Eddy Simulation (LES) model

The Large Eddy Simulation (LES) model of unsteady premixed flame propagation used in this work has been described and validated previously for stoichiometric methane/air mixture (Di Sarli et al., 2009a; 2010; 2012d). Briefly, the model equations were obtained by filtering the governing equations for unsteady compressible flows with premixed combustion, i.e., the reactive Navier-Stokes equations for conservation of mass, momentum, energy and chemical species, joined to the constitutive and state equations. The species balance equations were recast in the form of a transport equation for the reaction progress variable, c (c = 0 within fresh reactants and c = 1 within burned products) (Libby and Williams, 1994). To filter the governing equations, a low-pass box filter in the physical space was used (Poinsot and Veynante, 2005). The filter width, Δ, was equal to the characteristic length of the grid cell.

The sub-grid scale (SGS) stress tensor was described using the dynamic Smagorinsky-Lilly eddy viscosity model (Lilly, 1992). The closure for the SGS fluxes of heat and reaction progress variable was achieved through the gradient hypothesis along with the SGS turbulent Prandtl and Schmidt numbers (Poinsot and Veynante, 2005).

To handle the flame-turbulence interaction, the Flame Surface Density (FSD) formalism was used (Poinsot and Veynante, 2005). The filtered term of molecular diffusion and the SGS reaction rate were included in a single flame front displacement term, $\overline{\rho w|\nabla c|}$, which was expressed as

$$\overline{\rho w|\nabla c|} = \overline{\nabla\cdot\left(\rho D\nabla c\right)} + \overline{\dot{\omega}}_c = \left\langle \rho w\right\rangle_S \Sigma \tag{1}$$

where Σ is the SGS flame surface density (i.e., the SGS flame surface per unit volume) and $\langle \rho w\rangle_s$ is the surface-averaged mass-weighted displacement speed, which was approximated by the product of the fresh gas density, ρ_0, and the laminar burning velocity, S_L (Trouvé and Poinsot, 1994). Σ was expressed as a function of the SGS flame wrinkling factor (i.e., the SGS flame surface divided by its projection in the propagating direction), Ξ_Δ, which takes into account the coupling of flame propagation and unresolved turbulence:

$$\overline{\rho w|\nabla c|} = \left\langle \rho w\right\rangle_S \Sigma = \rho_0 S_L \Xi_\Delta \left|\nabla \overline{c}\right| \tag{2}$$

Ξ_Δ in Eq. 2 was modeled according to the SGS combustion closure by Charlette et al. (2002). Such a closure is essentially a flame wrinkling model that, however, also works well beyond the wrinkled regime of combustion (Charlette et al., 2002; Di Sarli et al., 2009a; 2012a; 2012b).

The effects of the hydrogen-enhanced reactivity were taken into account assuming the laminar burning velocity (S_L in Eq. 2) of the stoichiometric hydrogen-methane/air flames simulated equal to 0.41 m/s at x_{H2} = 0 (pure methane), 0.45 m/s at x_{H2} = 0.2, 0.54 m/s at x_{H2} = 0.4 and 0.61 m/s at x_{H2} = 0.5. Such values were obtained from CHEMKIN computations (Di Sarli et al., 2012c).

The LES model equations were discretized using a finite-volume formulation on a grid with cell characteristic length, Δ, equal to 0.5 mm.

Bounded central differences were used to discretize convective terms and second-order central differences to calculate diffusion terms. Second-order implicit time integration was used to discretize temporal derivatives.

Adiabatic boundary conditions were applied at the walls (bottom, lateral and top faces of the pre-chamber; lateral face of the orifice; bottom and vertical faces of the main chamber). Outside the main chamber, the computational domain was extended to simulate the presence of a dump vessel. At the boundaries of this additional domain, the static pressure was imposed as equal to the atmospheric pressure (initial pressure). The initial conditions had energy and reaction progress variable set to zero everywhere. The initial velocity field was quiescent. Ignition was obtained by means of a hemispherical patch, with a radius equal to 1 mm, of hot combustion products at the center of the bottom end of the pre-chamber.

The specific heats of the unburned and burned mixtures were approximated as piecewise fifth-power polynomial functions of temperature. The molecular viscosity was calculated according to Sutherland's law for air viscosity.

Computations were run by means of the segregated pressure-based solver of the ANSYS Fluent (release 13.0) code (www.ansys.com).

4. Results and discussion

The behavior of a premixed flame propagating through a turbulent flow field is strictly dependent on both size and velocity of the vortex structures encountered. In agreement with the experiments (Di Sarli et al., 2012c), the LES results obtained in this work show that, as x_{H2} increases, the velocity of the toroidal vortex induced in the orifice wake increases, whereas its diameter remains near identical. The velocity trend can be attributed to the increase in the laminar burning velocity, S_L, with increasing x_{H2}. In Figure 2, the maximum rotational velocity of the vortex core, $u_{\theta,max}$, is plotted versus S_L as extracted from the LES predictions of the velocity vector field at the onset of the flame-vortex interaction. In the figure, the experimental curve (extracted from PIV measurements) is also shown.

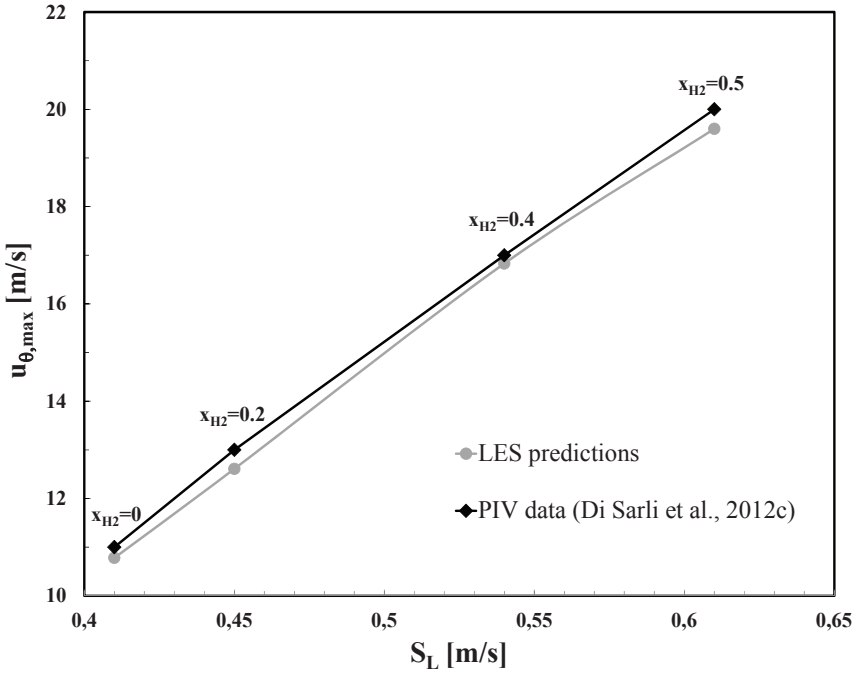

Figure 2: Maximum rotational velocity of the vortex core, $u_{\theta,max}$, versus the laminar burning velocity, S_L: LES predictions and experimental data obtained for stoichiometric fuel/air mixtures with different x_{H2} values.

There is good agreement between LES predictions and experimental data. The laminar burning velocity dictates the flame speed and, thus, the flow velocity exiting the orifice (upstream of the orifice, the flame propagation is substantially laminar). $u_{\theta,max}$ linearly increases with S_L. In particular, the value of $u_{\theta,max}$ almost doubles itself when S_L varies from 0.41 m/s (x_{H2} = 0, pure methane) to 0.61 m/s (x_{H2} = 0.5).

Figure 3 shows the time sequences of the instantaneous LES maps of the reaction progress variable, c, obtained during the flame-vortex interaction at the wake of the orifice for different x_{H2} values. The time interval between two consecutive maps is equal to 0.5 ms for all fuel compositions.

As the flame propagates through the charge, the burned gas area increases and the rate of its growth is enhanced by the presence of hydrogen. The flame exiting the orifice is substantially flat. During the interaction with the vortex, a progressive increase in flame front wrinkling can be observed. The intensity of the interaction increases with x_{H2}. For the case of pure methane, the interaction only wrinkles the flame front, leaving the front structure essentially unperturbed. On the contrary, in the presence of hydrogen (especially at x_{H2} = 0.4 and 0.5), in addition to wrinkling the flame, the interaction with faster vortices can be seen to locally break the continuity of the front. This break-up process leads to the formation of openings in the main front and almost results in the separation of small flame pockets.

When comparing the time sequences of Figure 3 with the experimental time sequences (Di Sarli et al., 2012c), it can be seen that, for all fuel compositions, the LES model reproduces well the flame-vortex interaction and the associated effects on the flame shape and structure.

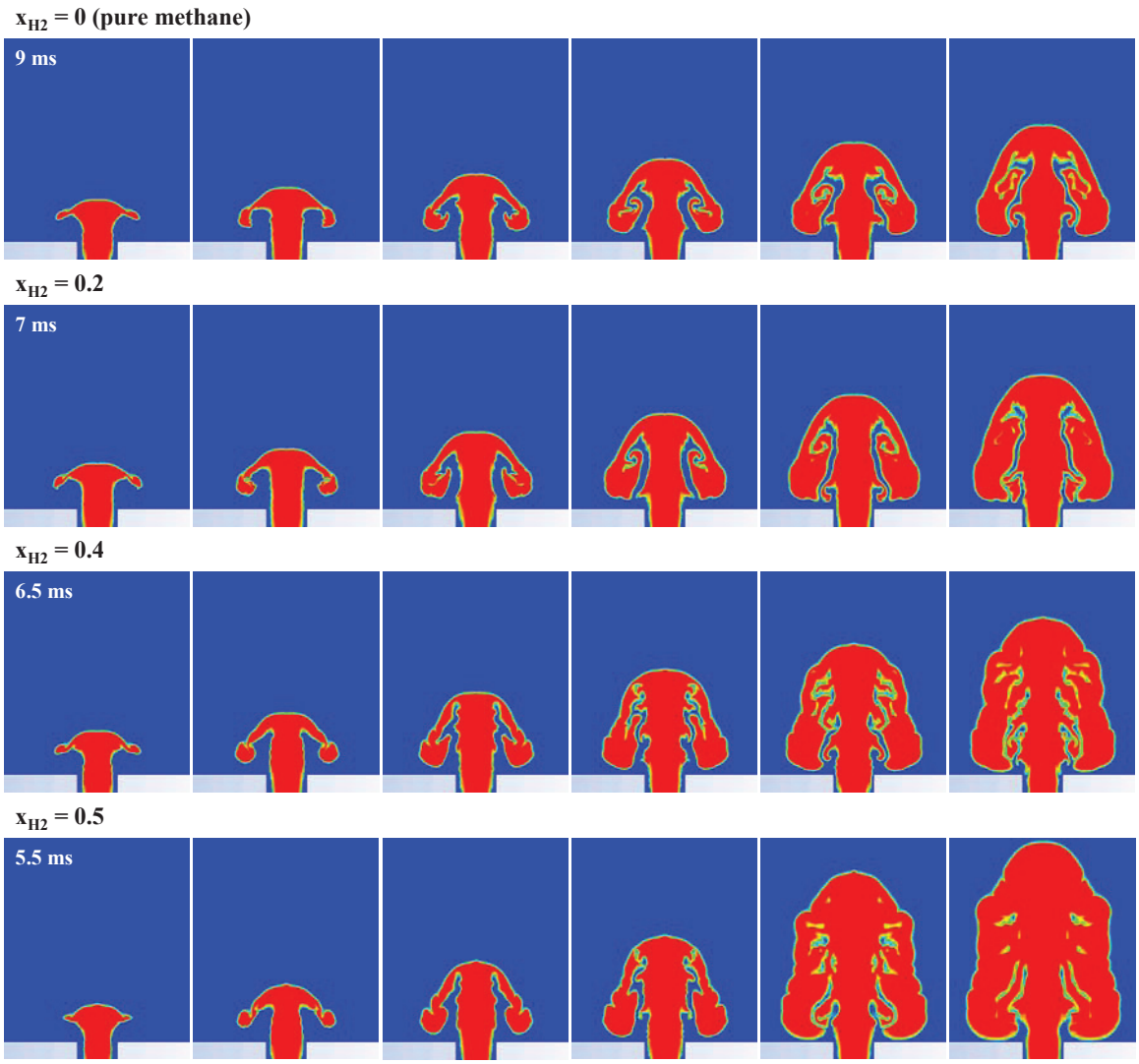

Figure 3: Time sequences of the instantaneous LES maps of the reaction progress variable, c, obtained during the flame-vortex interaction at the wake of the orifice for stoichiometric fuel/air mixtures with different x_{H2} values.

5. Conclusions

A Large Eddy Simulation (LES) model was developed to study transient interactions between hydrogen-enriched methane/air premixed flames and toroidal vortex structures at the wake of a circular orifice. The LES model was coupled to a combustion sub-model that takes into account the effects of the hydrogen-enrichment only in terms of increased laminar burning velocity. Computations were run for stoichiometric mixtures with hydrogen mole fraction in the fuel (hydrogen plus methane), x_{H2}, varying in the range of 0-0.5.

Numerical results agree well with previously obtained experimental data (Di Sarli et al., 2012c), confirming that the hydrogen substitution to methane leads to a transition from a regime in which the vortex only wrinkles the flame front ($x_{H2} < 0.2$) to a more vigorous regime in which the vortex almost disrupts the continuity of the front, causing the creation of reaction zones that are only narrowly linked together ($x_{H2} > 0.2$). This increase in intensity of the flame-vortex interaction is a direct result of a self-reinforcing mechanism established between flame propagation and combustion-induced flow field. That is, the higher reactivity (i.e., the higher laminar burning velocity) of the hydrogen-enriched mixtures produces faster flame propagation upstream of the orifice and, thus, higher rotational velocity for the toroidal vortex at the orifice wake. This, in turn, leads to further increase in the burning rate resulting from the interaction.

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