

DIRECT NUMERICAL SIMULATION OF $CO - H_2$ PREMIXED TURBULENT FLAME

F. Battista¹, F. Picano², G. Troiani³, C.M. Casciola¹

francesco.battista@uniroma1.it

¹ Department of Mechanical and Aerospace Engineering,
Sapienza University, via Eudossiana 18, 00184 Rome, Italy

² Linné FLOW centre, KTH Mechanics, Stockholm, Sweden

³ C.R. ENEA Cascaccia, Italy

Abstract

The use of syngas is becoming more and more frequent in power generation. Syngas is a mixture of hydrogen and carbon monoxide CO in different relative concentration. The effects of the different syngas composition have to be studied in order to design new efficient combustion chambers. Aim of this work is to address the dynamics of turbulent hydrogen/air and hydrogen/carbon-monoxide/air Bunsen flames by means of Direct Numerical Simulation. The main issue is to characterize thermo-diffusive instabilities in H_2 /air flame that leads to local quenching and temperature peaks in the flame that may increase pollutant formation (e.g. NO_x). The presence of carbon monoxide in the fuel mixture has significant effects in flame dynamics where we observe a damping of the H_2 /air flame instabilities with less apparent quenching and high temperature peaks.

1 Introduction

Modern internal combustion engines and power generators have to take particular care to environment safeguard, so in the recent years more attention was deserved to the development of alternative fuels e.g. hydrogen and syngas.

The gaseous hydrogen was considered both for its chemical enthalpy and the absence of carbon atoms preventing CO and soot formation. On the other hand some critical phenomena concerning the hydrogen air combustion should be prevented like e.g. the flame instability due to the extreme diffusivity of the gaseous and atomic hydrogen. It produces local quenching and high temperature peaks, above the adiabatic one, which promote the production of pollutants as NO_x . An alternative combustible is the so-called syngas. It consists on the mixture of hydrogen carbon-monoxide and in some cases also methane.

The aim of this works is to analyze combustion instabilities in hydrogen flames and understand how they are affected by the presence of CO in syngas mixtures. The purpose is pursued by means of the Direct Numerical Simulation (DNS) of two

Bunsen premixed flames: the first with pure hydrogen in air, the second consist of a mixture of CO/H_2 (50% – 50%) in air.

We will show that the additional presence of CO reduces both the local quenching and the local temperature peaks which control the pollutant production.

2 Methodology

Turbulent combustion of H_2 - CO /Air premixed flame is studied by means of a Direct Numerical Simulation (DNS) of a turbulent Bunsen burner.

The algorithm discretizes the Low-Mach number formulation of the Navier-Stokes equations in a cylindrical domain which describes a reactive flow at low Mach number with arbitrary density variations, neglecting acoustics effects.

Spatial discretization is based on central second order finite differences in conservative form on a staggered grid. Concerning scalars, the convective terms of the relevant reaction-advection-diffusion equations are discretized by a bounded central difference scheme designed to avoid spurious oscillations. Low-storage third order Runge-Kutta scheme is employed for temporal integration.

Turbulent velocity profile is enforced at the inflow section (Dirichelet condition) and is provided by a cross-sectional plane of a periodic turbulent pipe flow evolving simultaneously with the jet flow. A convective outflow condition is adopted together with a traction-free condition at the side boundary to mimic the open environment surrounding the flame, see [1, 2] for additional details on the code and the validation.

In order to address the effects of carbon-monoxide on hydrogen combustion two chemical kinetics are employed: the GRIMech 2.1 chemical kinetics [3] with 9 species and 5 steps and the chemical kinetics provided in [4] with 10 species and 24 reaction. The first one (S1) purely concerns the hydrogen/air combustion, the second one (S2) concerns the hydrogen carbon-monoxide combustion.

The DNS simulations reproduce the flame in a premixed Bunsen burner with diameter-based Reynolds number $Re_D = U_0 D / \nu_\infty = 6000$, with U_0 the bulk velocity and diameter D .

The parameters of the simulation correspond to a lean premixed Bunsen flame with the mixture composition summarized in table 1. The heat capacity ratio is $\gamma = c_p / c_v = 1.33$, while temperature dependent viscosity according to a sort of Sutherland's law, $\mu \propto \sqrt{T}$. The diffusion coefficients of the several species are computed taking into account that the gaseous nitrogen is significantly abundant.

The computational domain, $[\theta_{max} \times R_{max} \times Z_{max}] = [2\pi \times 6.2D \times 7D]$, is discretized by $N_\theta \times N_r \times N_z = 128 \times 201 \times 560$ nodes with radial mesh stretching for accurate resolution of the shear layer and of the instantaneous flame front (4 – 5 points within the instantaneous flame thickness), see [1, 2] for details and tests.

The simulation run for more than $30 D / U_0$ to achieve the statistical steady state before collecting one hundred sample uncorrelated fields, separated by $0.125 D / U_0$, for statistical analysis.

	n_{fuel}/n_{tot}	n_{CO}/n_{H_2}
S1	0.5	–
S2	0.4	0.5

Table 1: Reactive mixture composition for the two analyzed flames. In the first row n denotes the moles of a species, in particular n_{fuel} denotes the hydrogen moles for the first flame and the mole of the $CO - H_2$ mixture for the second flame, which composition is reported in the third column.

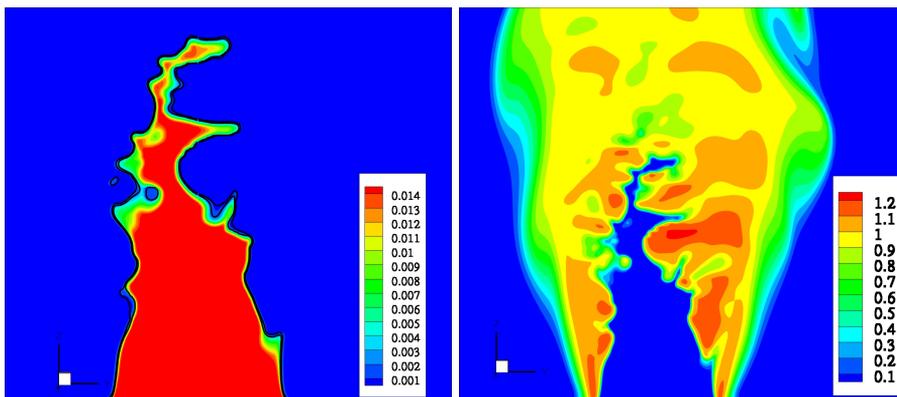


Figure 1: Snapshots of the hydrogen concentration Y_{H_2} , left panel, and of the progress variable based on the temperature $c_T = T - T_u / (T_{ad} - T_u)$ (T temperature, T_{ad} adiabatic flame temperature, T_u unburned mixture temperature), right panel.

3 Results

The first topic that is worth to be discussed is a qualitative description of the main instantaneous fields, which provide interesting hints about the interaction between turbulence and chemistry, as well as the presence of the thermo-diffusive instabilities (typical effects consequent of the non-unity fuel Lewis number Le); see also the experimental [5] and numerical [6] studies concerning similar flames.

Figure 1 (left panel) shows the contours of the molecular hydrogen’s concentration Y_{H_2} field which presents well-delineated features. The front, here marked by the thin region where Y_{H_2} displays large variations, has been severely wrinkled by turbulence even to the extent of tearing off pockets of fresh gas, which are carried into the product side where are eventually consumed. Actually, the flame front exhibits an interesting peculiar behavior: it is indeed constituted essentially by areas convex towards the burnt gases, which will be from now on referred as “gullies”, presenting extensive curvatures and “bulges”, region convex towards the fresh gases which are characterized, on the contrary, by smoother profiles with lower curvatures, see also [5]. The temperature-based progress variable $c_T = T - T_u / (T_{ad} - T_u)$ (T temperature, T_{ad} adiabatic flame temperature, T_u unburned mixture temperature), is presented in the right panel of figure 1 for the same instant of the Y_{H_2} snapshot.

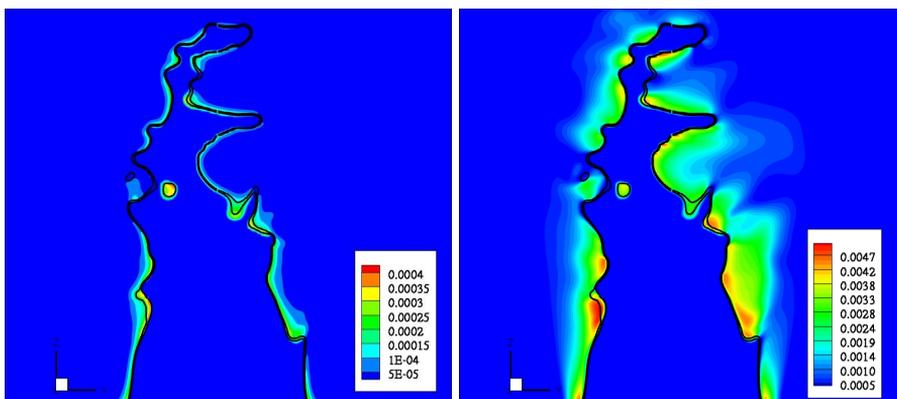


Figure 2: Snapshots of the radical concentrations Y_H and Y_{OH} , left and right panels, respectively.

Bulges appear characterized by c_T significantly larger than unity, assuming values up to 1.2 (super-adiabaticity), while sub-adiabatic conditions, $c_T < 1$ occur in gullies even where the hydrogen concentration Y_{H_2} is almost null.

Further considerations concerning these areas can be deduced observing radical concentrations Y_H , Y_{OH} , figure 2, whose profiles follow quite closely the flame zone, meaning, therefore, they can be rightfully considered good markers of the combustion proceeding, in accordance with general combustion literature [5, 7, 8]. Actually, the Y_H field appears more “sharp” compared to Y_{OH} that seems more elongated through the burnt region, nevertheless both these radicals display their maxima concentration in the flame front confirming their ability to mark regions with high chemical activity. The bulges are characterized by high level of radical concentration denoting an intense chemical activity, while radicals lack in the gullies suggesting an almost quenched region [5].

The intense activities associated to the high concentration of radicals and super-adiabaticity characterizing the bulges can be related to the local equivalence ratio ϕ_L [6, 9], that causes, due to a local mixture enrichment, higher temperatures and chemical activity in respect to the corresponding laminar adiabatic and unstretched flames. The opposite behavior, connected to gullies, may be justified by small local equivalence ratio ϕ_L with analogous considerations.

Actually these phenomena are a direct consequence of the high diffusion coefficient of molecular hydrogen H_2 compared to thermal conduction so that Lewis number is smaller than unity $Le < 1$. In bulges, in fact, reactants diffuse towards burnt gases faster than heat diffuse towards fresh gases, so they are heated and burn faster, increasing the local flame speed S_L , which is higher than the speed of the laminar flame front. On the other hand, in gullies reactants diffuse in a large zone and the flame velocity is decreased, causing an unstable situation [10].

Dealing with the carbon-monoxide hydrogen combustion figure 3 reports the temperature instantaneous field (left panel) the OH concentration (middle panel) and the

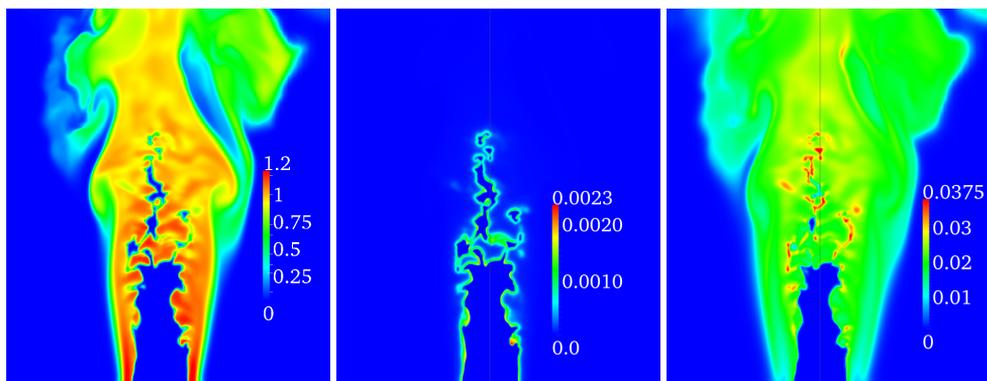


Figure 3: Instantaneous fields of Hydrogen/carbon-monoxide/air flame S2: progress variable c_T (left panel), OH concentration (middle panel) and CO_2 concentration (right panel).

CO_2 concentrations. Despite the slightly different equivalent ratio ϕ respect the pure hydrogen flame some common features can be observed. In particular the remarkable corrugation of the flame front is apparent also in this one where a large unburned gas pockets are present well inside in the burned gas region. Similarly the first case the OH is mainly concentrated just beyond the flame front and its maximum values in the bulgies, i.e. areas convex towards the products. On the other hand in this flame (S2) the local quenching are not apparent in the gullies regions as in the pure hydrogen flame. In this region the reaction is sustained by the oxidation of the carbon monoxide and the temperature is large enough to support the OH production. The evidence of this phenomenon is given by the right panel of figure 3 representing the CO concentration which are found to peak in the gullies.

Hence the presence of carbon monoxide reduces the occurrence of quenching regions and tend to make more uniform the temperature fields.

References

- [1] F. Picano, F. Battista, G. Troiani, and CM Casciola. Dynamics of PIV seeding particles in turbulent premixed flames. *Experiments in Fluids*, pages 1–14, 2010.
- [2] F. Battista, F. Picano, G. Troiani, and CM Casciola. Intermittent features of inertial particle distributions in turbulent premixed flames. *Physics of Fluids*, 23(12):123304–123304, 2011.
- [3] C.T. Bowman, R.K. Hanson, W.C. Gardiner, V. Lissianski, M. Frenklach, M. Goldenberg, and G.P. Smith. Gri-mech 2. 11: An optimized detailed chemical reaction mechanism for methane combustion and no formation and reburning. NASA, (19980005146), 1997.

- [4] P. Saxena and F.A. Williams. Testing a small detailed chemical-kinetic mechanism for the combustion of hydrogen and carbon monoxide. *Combustion and Flame*, 145(1):316–323, 2006.
- [5] Y.C. Chen and R.W. Bilger. Experimental investigation of three-dimensional flame-front structure in premixed turbulent combustion: Ii. lean hydrogen/air bunsen flames. *Combustion and flame*, 138(1):155–174, 2004.
- [6] J.B. Bell, R.K. Cheng, M.S. Day, and I.G. Shepherd. Numerical simulation of lewis number effects on lean premixed turbulent flames. *Proceedings of the Combustion Institute*, 31(1):1309–1317, 2007.
- [7] P. Ewart and S.V. O’Leary. Detection of oh in a flame by degenerate four-wave mixing. *Optics letters*, 11(5):279–281, 1986.
- [8] Q.V. Nguyen and R.W. Dibble. Raman-lif measurements of temperature, major species, oh, and no in a methane-air bunsen flame. *Combustion and flame*, 105(4):499–510, 1996.
- [9] H.G. Im and J.H. Chen. Preferential diffusion effects on the burning rate of interacting turbulent premixed hydrogen-air flames. *Combustion and flame*, 131(3):246–258, 2002.
- [10] M. Baum, T.J. Poinso, D.C. Haworth, and N. Darabiha. Direct numerical simulation of h₂/o₂/n₂ flames with complex chemistry in two-dimensional turbulent flows. *Journal of Fluid Mechanics*, 281:1–32, 1994.