LARGE EDDY SIMULATION OF A SUPERSONIC HYDROGEN-AIR DIFFUSION FLAME

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Abstract. *The application of LES to supersonic reactive flows is still a technical and scientific challenge. A Large Eddy Simulation (LES) has been performed to simulate the NASA supersonic hydrogen flame of Cheng and Wehrmeyer [1, 2]. The combustion model is a two-step Arrhenius law fitted to capture the flame stabilization. The results show a good agreement with experimental data, and help to understand the influence of injected turbulence. It is then demonstrated that LES is an efficient tool for supersonic reactive configurations, giving new insights for engineering design purposes.*

1 INTRODUCTION

Supersonic combustion is a promising field of investigation. It is involved in supersonic ramjets (scramjets) or in rocket engine devices. The extreme operating conditions of these applications, such as Mach 7 airflow for scramjets or ambiant vacuum for rocket engine ignition, induce expensive and non-realistic ground based experiments. The use of CFD may help to fill the gap between affordable test devices and the final design.
The work of Cheng and Wehrmeyer with the supersonic burner (SSB) at the NASA Langley Research Center (LaRC) provided accurate experimental data about the dynamics, the mixing and the combustion conditions at various locations downstream the injector. Reynolds Averaged Navier-Stokes (RANS) simulations already successfully predicted the mean flow properties, using a turbulent combustion model based on Probability Density Function (Toone *et al.* [7]) or on reduced chemical kinetics mechanisms and *in situ* adaptive tabulation algorithm speeding up the detailed chemistry (Montgomery *et al.* [5]). The present work is a first attempt to apply Large Eddy Simulation (LES) to this configuration, in order to predict fluctuation levels and investigate the unsteady behavior of the flame.

2 EXPERIMENT DESCRIPTION

The SSB sketched in Fig. 1 produces an axy-symmetric flame from a sonic pure hydrogen cold jet surrounded by a largely supersonic (Mach 2) jet of hot products generated by a lean combustor. The SSB global equivalence ratio is close to 0.1. The Reynolds number is 100 000 and the convective mach number is 0.12.

Cheng and Wehrmeyer measured temperature, oxygen and nitrogen concentrations and velocity with coherent anti-Stokes Raman spectroscopy and laser Doppler velocimetry. They obtained simultaneous measurements of temperature and concentration of major species (H_2,O_2,N_2,H_2O) and OH radicals with ultraviolet spontaneous vibrational Raman scaterring combined with laser induced predissociative fluorescence. Measurements were made in the radial direction at the downstream locations $x/D = 0.85, 10.8, 21.5, 32.3$ and 43.1, x being the downstream distance and $D = 2.36mm$ the inside diameter of the fuel jet. A long exposure visual photograph enhances the lifted flame aspect located ignition close to $x/D = 25$.

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Dimensions	
Nozzle exit inner diameter	$17.78\,mm$
Fuel injector inner diameter	$2.36\,mm$
Fuel injector outer diameter	$3.81\,mm$
Vitiated Air Exit Conditions	
Pressure	$107\,kPa$
Temperature	$1250\,K$
Mach number	2.0
Velocity	$1420\,m/s$
O_2 mole fraction	0.201
N_2 mole fraction	0.544
H_2O mole fraction	0.255
Fuel Exit Conditions	
Pressure	$112\,kPa$
Temperature	$540\,K$
Mach number	1.0
Velocity	$1780\,m/s$
H_2 mole fraction	1.0

Table 1: Experimental parameters.

3 COMPUTATIONAL DOMAIN

The computed domain is a half sphere of radius $70D$ shown in Fig. 2. The plane boundary is set as a tri coaxial inlet. At the center, a supersonic fuel inlet is specified with a turbulence injection. It is surrounded by an oxidizer inlet with a second turbulence injection. The turbulence injected in the fuel has an integral scale of $0.8mm$ and a RMS velocity of $180m/s$, while in the oxidizer the integral scale is $6mm$ and the RMS velocity is $125m/s$. A co-flow of $20m/s$ is finally imposed on th.e outer ring. The convex boundary on the sphere is a freestream outlet for subsonic zones. All boundary conditions are set with the NSCBC method [6].

The mesh contains $807\,520$ tetrahedras for $139\,560$ nodes, allowing a resolution of 25 to 30 nodes in the diameter of both fuel an oxidizer jets. It is designed to resolve the main structures occuring around the cylindrical mixing layer between oxidizer and fuel in the first ten diameters.

4 MODELS

Simulations were performed with the code AVBP developed at CERFACS. The multi-species fluid dynamics solver involves a Third order Taylor Galerkin Compact (TTGC) scheme for space direction, and a third order Runge-Kutta scheme for explicit time advancement. A specificity of the present flow is the necessity of handling chemistry and turbulence but also shocks: LES is not well established for non-reacting flows with shocks and is still exploratory when combustion bust also be taken into account as it is the case here. For the present computation, the following strategy was used:

1. a penalty method on Euler fluxes based on the Von-Neumann Richtmyer viscosity [8] was employed to capture the shocks.

2. local sensors were used to add artificial viscosity in strong gradient zones (typically near the inlet conditions).

3. chemistry was modeled explicitly by using Arrhenius rates because flamelet approaches for example are very difficult to implement in a flow with varying pressure, ignition mechanisms and shocks.

In a very first approach, the chemistry model is a two-step scheme (Table 2). The produced species pool **P** results from the equilibrium mixture reached after a stoechiometric combustion between Oxydant and Fuel. The induction step is mimicked through the non-exothermic formation of an intermediate species pool **I** .

Chemical kinetics are fitted on autoignition. According to the work of R. Knikker *et al.* [4], the ignition time of a mixing layer between hot oxidizer and cold fuel can be estimated from the homogeneous mixing ignition time. Simulation performed with the CHEMKIN package and the 9 species - 19 reactions scheme of Yetter *et al.* [9] predict the minimum ignition time $t_{ign}^{HMI} = 5.6\ 10^{-5}s$. The simplified chemistry model detailed in Table 2 is designed to give the same minimal ignition time for a one-dimensional auto-igniting mixing layer.

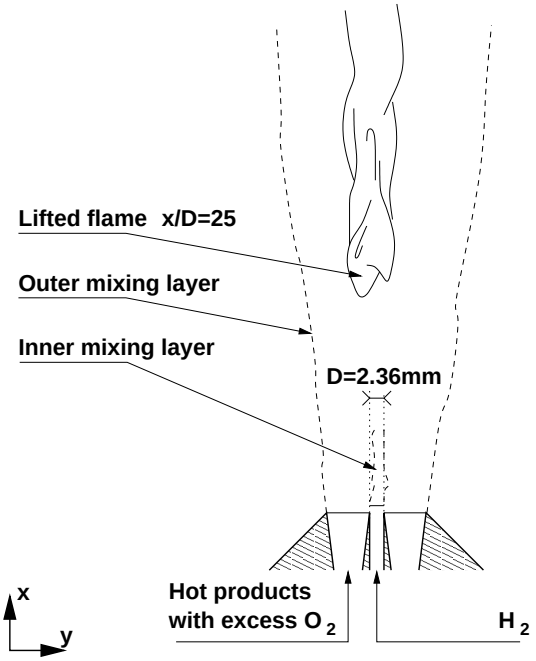


Figure 1: Sketch of Supersonic Burner installed at NASA Langley Research Center

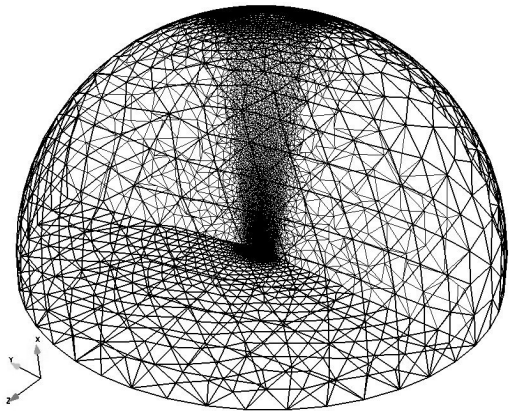


Figure 2: Skin and middle plane of the unstructured mesh

Step	**reaction**	A	β	E_0
Induction	$0.68H_2 + 0.34O_2 \Rightarrow I$	$1.0\,10^{15}$	0	20000
Run off	$I \Rightarrow 0.73P$	$1.0\,10^{9}$	0	27000

Table 2: The two-steps auto-ignition scheme based upon the ignition time

5 RESULTS

The simulation leads to a lifted flame as in experiement. Fig. 3.a shows the brutal rise of temperature of $1500K$ around $x/D = 15$ on the intantaneous image. This rise is smoothed downstream over $5D$ on the time averaged image. The lift-off length is then around $x/D = 17$, to be compared with the experimental value of $x/D = 25$. The fluctuating nature of the reactive mixing layer is illustrated on Fig. 3.b where the production of **P** is plotted. Strong large structures comparable to Kelvin-Helmoltz eddies can be seen in the lift-off region $0 < x/D < 15$. The pressure field in Fig. 3.c presents two diamond-shock patterns relative to Oxidizer and Fuel injection. The shock pattern relative to the fuel moves in response to the turbulence injected so it vanishes quickly on the average field before $x/D = 2.5$ but stay visible in the instantaneous flow down to $x/D = 7$. The shock pattern relative to the Oxidizer gets stronger from the injected static pressure ratio of 1.05 up to 1.3. The pressure oscillation, which reaches $0.6Bars$, is strongly coupled with the reaction zones (See Driscoll *et al.* [3]).

5.1 Longitudinal evolution

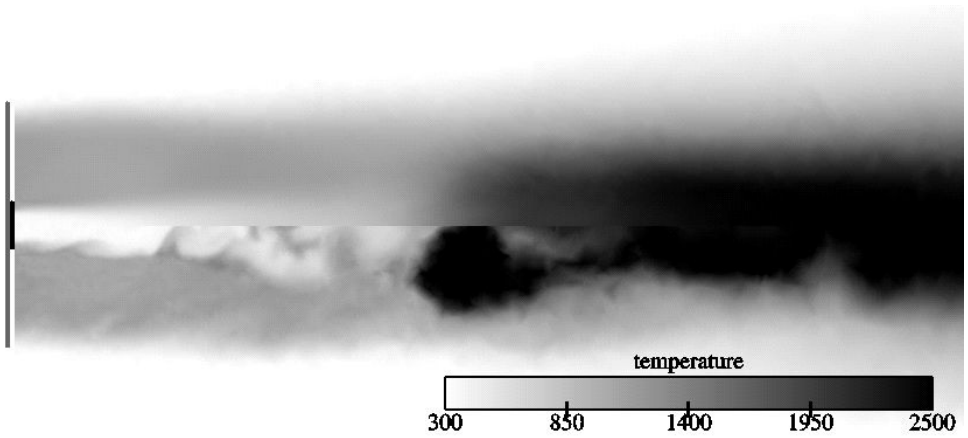
Along the longitudinal axis, the mean velocity, temperature, water concentration and mixture fractions are compared to experiment data. In Fig. 4.a, the axial velocity decreases from hydrogen to hot products bulk velocity (1780 to 1420 m/s) in the first ten diameters. Small accelerations about $200m/s$ occur in the diamond-shock pattern. The mean inlet velocity is slightly higher than the experimental one because of mesh requirements, to keep the correct mass flow rate

The mean temperature and water concentration show similar behaviors (Figs. 4.b and 4.c), reaching their maximum around $x/D = 17$, then decreasing slowly to 50% of the maximum value at $x/D \sim 60$. An induction zone is visible up to $x/D \sim 10$ then the equilibrium is reached as fast as the experiment. This too fast combustion is due to thesimplified kinetic model of Table 2. Finally, the slow decrease is the result of diffusion that is too fast in the range $20 < x/D < 70$, where the Smagorinsky model is active on an underresolved grid. This effect is also visible on the mixture fraction longitudinal (Fig. 4.d) and transversal profiles (Fig. 5.d).

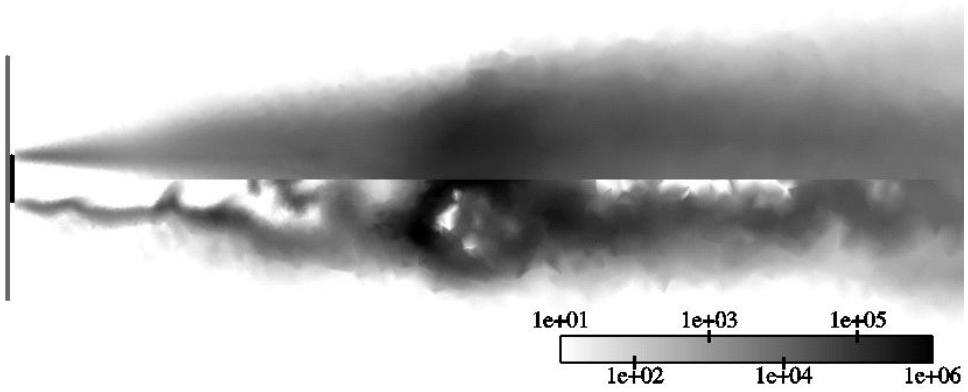
5.2 Transverse evolution

The mean profiles of velocity, temperature and water concentration on Fig. 5 show a fair agreement with experimental data. Fig. 5.a shows that the simulated jet spreads radially over $10D$, as in the the experimental evolution. Temperature and water concentration profiles of Figs. 5.b and 5.c present the correct evolution but the main ignition occurs before $x/D = 21.5$, much closer to the injector than in the experiment.

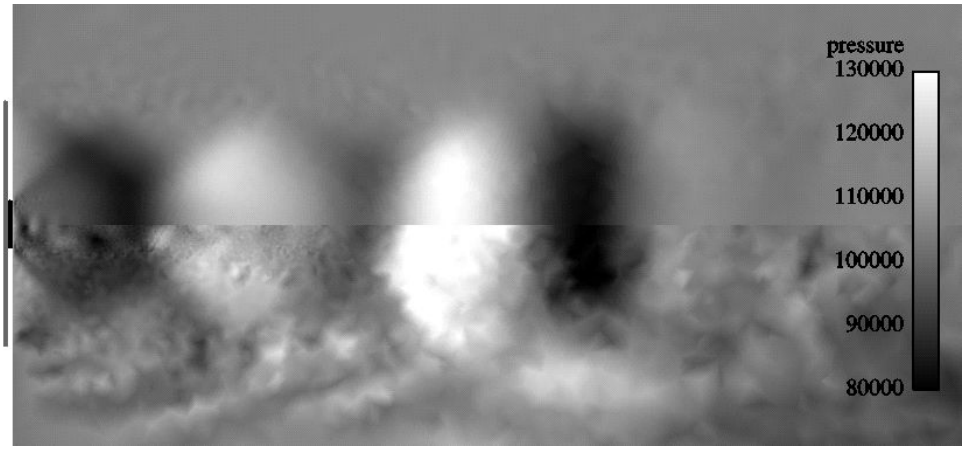
The RMS profiles of velocity, temperature and water concentration are plotted on Fig. 6. The injected coherent structures give strong velocity fluctuations (Fig. 6.a). The first profile at $x/D = 0.85$ shows clearly the difference between fluctuations of the fuel and the oxidizer jets. These fluctuations are weakly damped during their convection downstream in spite of the diffusion by the Smagorinsky subgrid scale model on the coarse mesh. Temperature and water concentration fluctuation levels are similar to the experimental measurements, with the same discrepancy already observed on the mean profiles due to the advanced ignition.



a) Mean (top) and instantaneous (bottom) temperature in K.



b) Mean (top) and instantaneous (bottom) production of products **P** in $mol.m^{-3}.s^{-1}$.



c) Mean (top) and instantaneous (bottom) pressure in Pa.

Figure 3:

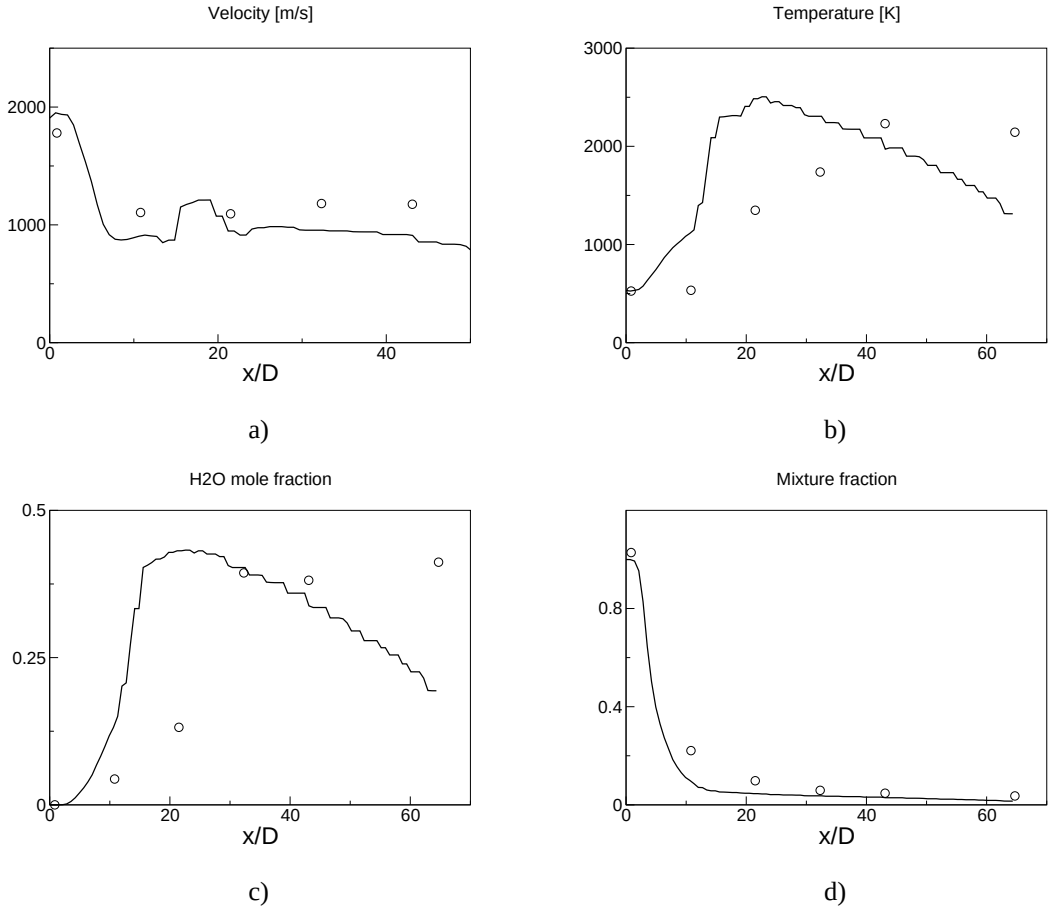


Figure 4: Mean profiles on the longitudinal axis. Symbols: expt, line: LES.

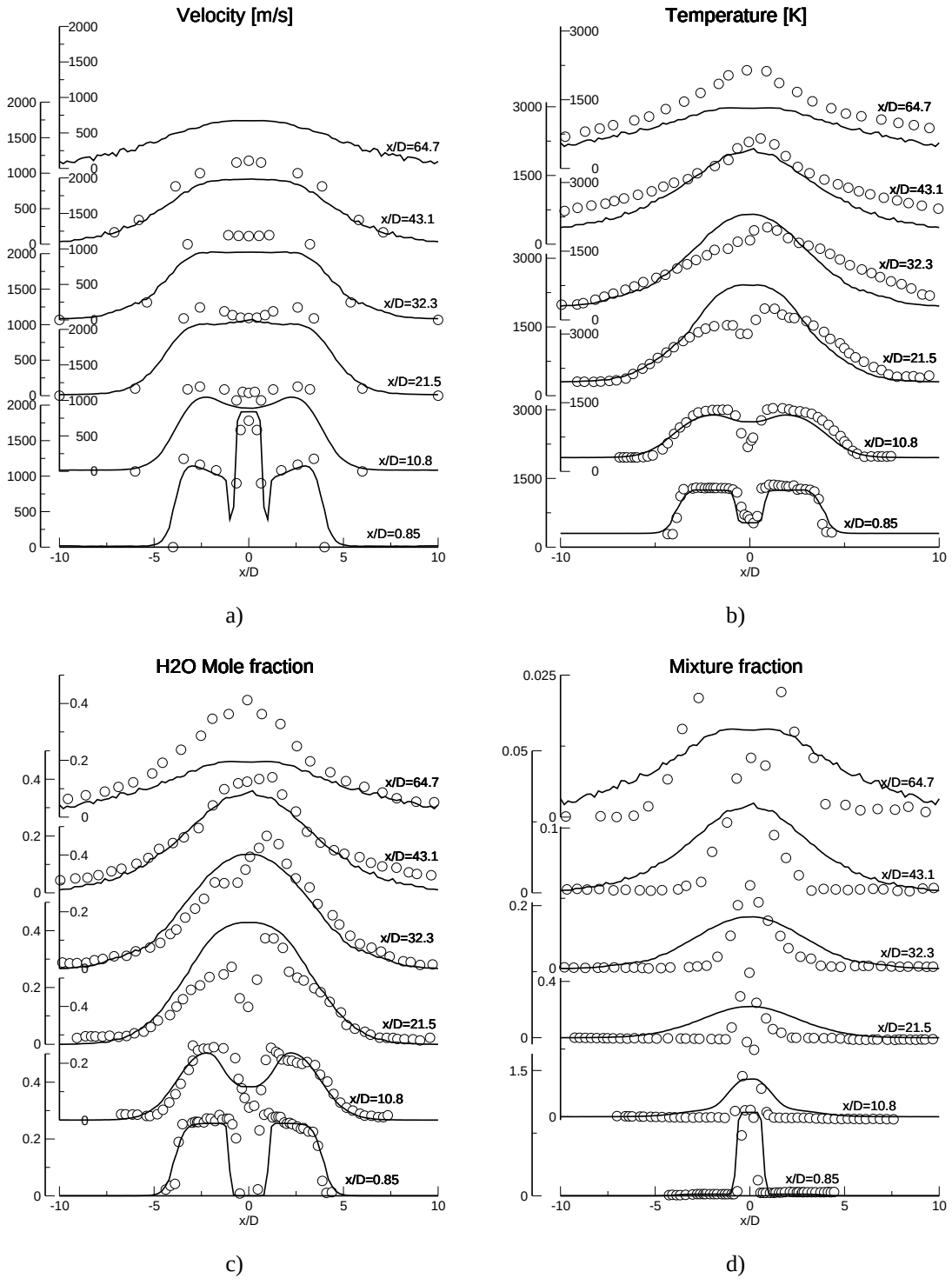


Figure 5: Mean profiles for six transversal planes. Symbols: expt, line: LES.

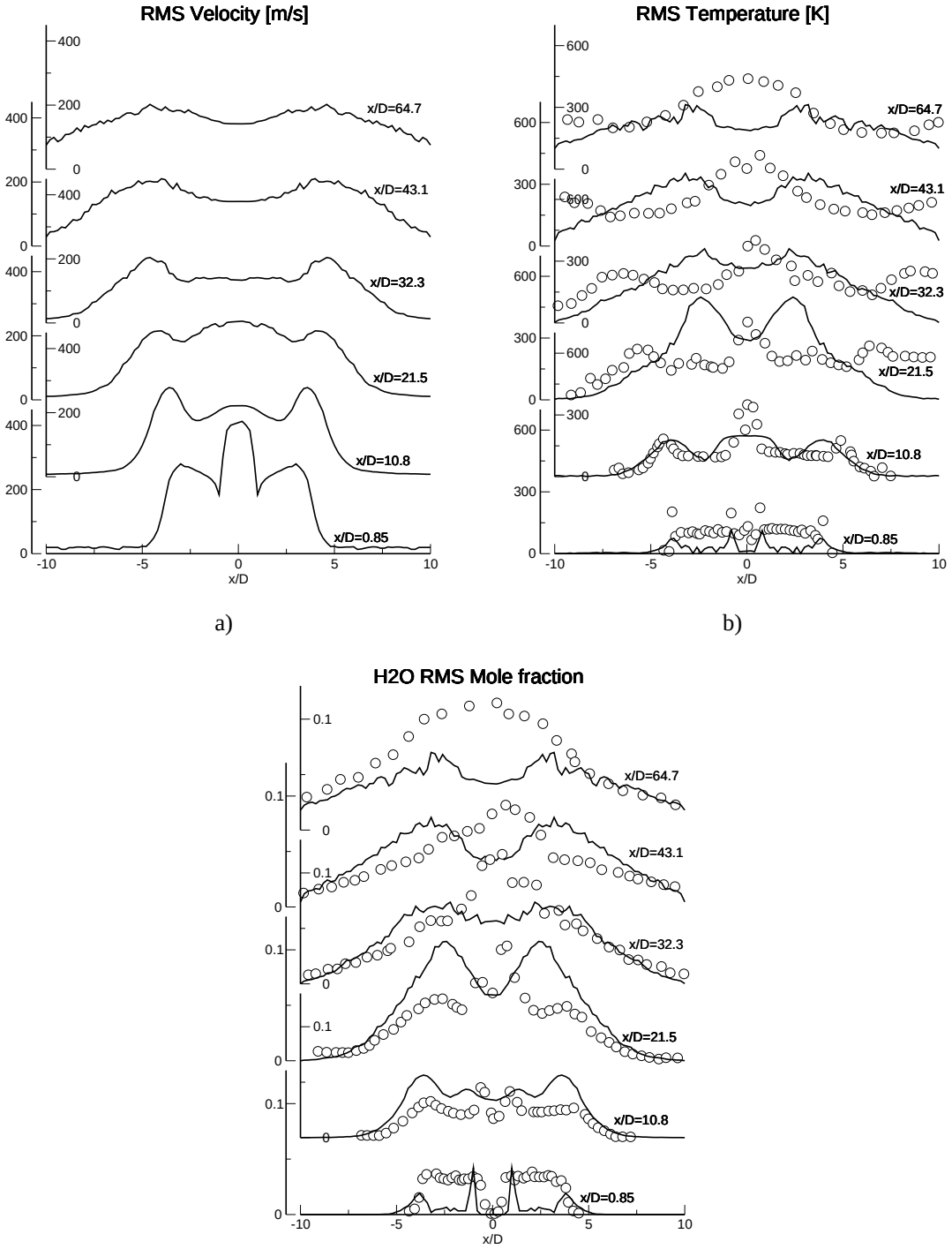


Figure 6: Root Mean Square profiles for six transversal planes. Symbols: expt, line: LES.

6 CONCLUSION

A first attempt to simulate the supersonic flame experiment of Cheng and Wehrmeyer [1, 2] with a Large Eddy Simulation approach has been performed and obtained a good agreement with the experiment. The lifted flame is clearly captured with a two-step chemistry. The simulation reproduced the fluctuating mixing layer between oxidizer and fuel developed 15 diameter downstream to the injection, and the complex diamond-shock pattern coupled with combustion as observed by Driscoll *et al.* [3]. Despite a very coarse mesh leading to over-diffusion by the Smagorinski subgrid-scale model, not only the mean quantities of the flows are well predicted in terms of shape, amplitude, and evolution, but even the level of fluctuations predicted is close to the experimental values. These first results are very encouraging and prove that LES is an efficient tool to study supersonic reactive flows. For much high speed flames, however, more complex chemical schemes will be needed in the future.

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