Étude numérique de mélange H2-air de jets turbulents coaxiaux

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Numerical Study of Hydrogen-Air Mixing in Turbulent Compressible Jets

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Résumé :

Des simulations numériques sont réalisées pour étudier le développement spatial du mélange de jets hydrogène-air déchargeant dans un environnement confiné. Les équations de Navier-Stokes sont résolues avec un schéma d'ordre élevé de type Godounov (PPM) combiné à un solveur de Roe. Le cas considéré dans cette étude est basé sur les travaux expérimentaux de Eggers (1971). Une grande attention a été accordée au calcul des champs dynamique et scalaire. Nous nous limitons au mélange sans réaction chimique, afin de se concentrer sur l'effet des structures turbulentes sur le processus de mélange d'hydrogène et d'air. Sur la base des statistiques et de la visualisation de l'écoulement, on observe que l'échange de matière entre les deux flux se caractérise principalement par diffusion moléculaire dans la première zone du développement des jets. En aval, une grande partie du mélange turbulent est contrôlée par les tourbillons cohérents. Un fort contraste est observé entre le champ de du mélange H2-air et la vorticité. L'approximation bidimensionnelle a permis de reproduire d'une manière approchante les statistiques essentielles (valeurs moyennes et turbulentes) basées sur des informations temporelles et spatiales, comparativement aux mesures expérimentales.

Abstract :

Numerical simulations are carried out to study the space development of hydrogen-Air mixing jets discharging in to confined environment. The full Navier-Stokes equations are solved with a high order Godunov's scheme piecewise parabolic method (PPM) with the approximate Riemann solver of Roe. The case considered in this study is based on the experimental work of Eggers (1971). A great attention has been paid to the computation of the dynamic and concentrations fields. We restrict ourselves to mixing without chemical reaction, in order to concentrate on the effect of the turbulent structures on the mixing process of hydrogen and air. On the basis of flow visualization and statistics, the mass exchange between the two jets is due to molecular diffusion in the upstream. Downstream, a large part of the turbulent mixing is controlled by the coherent vortices. A great contrast between the mixing and the vorticity fields is observed. The two-dimensional approximation has reproduced roughly the essential statistics based on temporal and spatial information comparatively to experimental measurements.

1 Introduction

The increased interest in hydrogen utilization as principal or addition fuel has known a great importance from the point view of research studies as well as industrial applications. The present investigation is focused on H2-air mixing process in compressible jets. Gas jets are widely used in chemical engineering process, the comprehension of the turbulent mixing included hydrogen helps for the new design and performance improvement of devices.

Numerical simulations offer a cost-effective alternative to the comprehension of the turbulent mixing in jets. A better hydrogen and air turbulent mixing is of crucial importance to lead to higher combustion efficiency, and performance improvement of such devices.

In this framework, the present work is focused on the study and analysis of compressible turbulent H2-air mixing in confined coaxial jets. Confined coaxial jets are made when the streams meet and mix in confined environment. Coaxial jets have been expensively studied numerically and experimentally [2][3][7][8], however a few investigations [4] have deeply analysed the mixing of H2-air in compressible situation.

The aim of the present work is to investigate the mixing of jets by using numerical simulations in two-dimensional approximation as a tool of investigation. Chemical reaction is avoided in this step, in order to concentrate on the effect of the turbulent structures on the mixing process of hydrogen and air. In this context,

a great attention has been paid to detailed evolution of the spatial and temporal evolution of the mixing fraction, while benefiting from the advantage of the spatially developing approach. Numerical description is strengthen by means of visualization of snapshots of the flow and statistics based on temporal and spatial information of the compressible flows.
The numerical simulations are complex because of supersonic/subsonic flows transition, mixing mechanism between hydrogen and air, reflexion of Mach waves, convection of species. We are interested in the far-off mixing jets (figure 1) without in quest of to represent the mechanisms of generation of shearing associated to the nozzle exit.

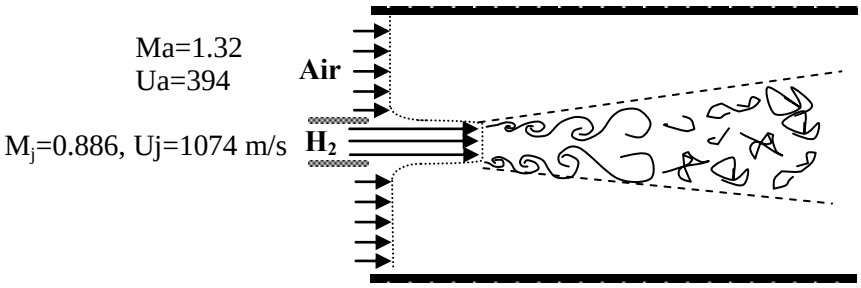

Figure. 1 – Sketch of the spatial developing jets .

2 Governing Equations and the numerical method

Numerical simulations are performed here, by solving the complete compressible Navier-Stockes equations (the equations for conservation of mass, momentum, energy and detailed mass of each species i are written in conservative form).The fourth order accurate piecewise parabolic method (PPM) together with the approximate Riemann Solver of Roe solve the inviscid equations. The overall scheme is second order accurate in time. An optimal value of the time step Δt is selected at each time t. A diffusion-reaction operator is added as source term in Navier-Stockes equations, and switched on or off depending on the problem under consideration, especially with regard to the character, direct or large eddy, of numerical simulation.
Computations of high speed jets are performed using a code specifically developed to numerically simulate gas flows whose composition may evolve with location $\vec{X}$ and time t. It is based on the usual set of gas flow equations, with the vector of the conserved variables is :

$$U(\vec{X},t)=\{\rho,\rho U_1,\rho U_2,\rho U_3,\rho e,\rho Y_i\}^T \tag{1}$$

ρ is the density, (u1,u2,u3) the three velocity components, e the total energy per unit mass, Y_i is the mass fraction of the species i. The total energy of the flow is defined by:

$$e=\frac{1}{2}(U_1^2+U_2^2+U_3^2)+\overline{C_v}T \tag{2}$$

Where the average heat capacity per unit mass $\overline{C_v}$ is $\overline{C_v}=\sum_{i=1}^{n_s}C_{vi}Y_i$ (n_s is the number of involved species).
Thermo-dynamics of the gas mixture is modeled with an ideal gas equation. The pressure P and the temperature T are related by:

$$\frac{P}{\rho}=\frac{RT}{\overline{M}} \tag{3}$$

where R is the universal gas constant and $\overline{M}$ is the average molar mass calculated from the molar mass M_i

of each species i : $\overline{M}^{-1} = \sum_{i=1}^{n_s} Y_i / M_i$

Each component of $U(\vec{X},t)$ corresponds to a conserved quantity like mass, momentum or energy. The total energy e is the sum of the mechanical and internal energies of gas mixture.
The equations for conservation of mass, momentum, energy and detailed mass of species i are written in conservative form.

$$\frac{\partial U(\vec{X},t)}{\partial t} + \sum_{j=1}^{2} \frac{\partial F_j(U(\vec{X},t))}{\partial X_j} = S(U(\vec{X},t)) \tag{4}$$

$$F_j(U(\vec{X},t)) = \begin{Bmatrix} \rho U_j \\ \rho U_j U_1 + \delta_{j1} P \\ \rho U_j U_2 + \delta_{j2} P \\ \rho U_j U_3 + \delta_{j3} P \\ (\rho e + p) U_j \\ \rho \mathrm{Y_i} U_j \\ \dots \end{Bmatrix}$$

Where:
The right-hand side term of equation (4) contains terms for viscous stress, scalar diffusivity.

$$S(U) = \begin{Bmatrix} 0 \\ \sum_{j=1}^{j=3} \frac{\partial (\frac{\rho}{\mathrm{Re}}) \tau_{1j}}{\partial X_j} \\ \sum_{j=1}^{j=3} \frac{\partial (\frac{\rho}{\mathrm{Re}}) \tau_{2j}}{\partial X_j} \\ \sum_{j=1}^{j=3} \frac{\partial (\frac{\rho}{\mathrm{Re}}) \tau_{3j}}{\partial X_j} \\ \nabla \cdot (\frac{\overline{Cp}\rho}{\mathrm{Pr}.\mathrm{Re}} \nabla T) + \nabla \cdot (\frac{\rho}{\mathrm{Re}} \vec{U}.\bar{\bar{\tau}}) \\ \nabla \cdot (\frac{\rho}{Sc.\mathrm{Re}} \nabla Y_i) \\ \dots \end{Bmatrix}$$

$$\tau_{ij} = \frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i} - \frac{2}{3} \delta_{ij} \sum_{K=1}^{K=3} \frac{\partial U_K}{\partial X_K}$$

δ is the Dirac delta. Re, Pr and Sc are the Reynolds number, Prandtl and Schmidt numbers respectively. $\overline{Cp}$ is the heat capacity at constant pressure of the mixture per unit mass. The values of $\overline{Cp}$, $\overline{Cv}$ and $\overline{M}$ evolve and have to be calculated at each $(\vec{X},t)$.
The full compressible Navier-Stokes equations (4) are split up in two one-dimensional inviscid operators

L_j (j=1,2) :

$$L_j : \quad \frac{\partial U(\vec{X},t)}{\partial t} + \frac{\partial F_j(U(\vec{X},t))}{\partial X_j} = 0 \tag{5}$$

and three-dimensional viscous-diffusive operator :

$$\psi : \quad \frac{\partial U(\vec{X},t)}{\partial t} = S(U(\vec{X},t)) \tag{6}$$

The fourth order accurate piecewise parabolic method (PPM)[5] together with the approximate Riemann solver of Roe[6] solve the equations (5).
All simulation are carried out on the same grid which consists in 1072×656 points with a domain size of along the streamwise $37D_j$ and the transverse direction $13D_j$.
The experiment carried out by Eggers (1971) gives us an opportunity for comparing numerical simulations results and laboratory real flow scales. Computation parameters were designed to fit the real jets configuration. The jet at the injector exit is made of a Hydrogen at Mach number $M_j = 0.886$, the adjacent jet is made of air at Mach number $M_a = 1.32$. All gases are assumed to be ideal. Velocity, density and pressure are made non-dimensional by using the values at the injector exit. Lengths are scaled on the diameter D_j of the hydrogen injector exit. Table 1 summarizes the flow parameters.

Flow	Mach	Speed (m/s)	Total Temperature (°K)
H2 jet	0.886	1074	300
Air co-flow	1.32	394	300

Table 1 – Physical parameters for the Air-Hydrogen jet

3 Main Results

To qualitatively point up mixing with a set of pictures once the flow becomes statistically quasi- stationary and the effect of the initial condition has decayed, the instantaneous planar flow visualization is shown in figure 2a. We can observe the natural quasi-linear region until $x/D \approx 7$ where the instabilities grow freely as the inlet perturbation is based on white noise. The introduction of white noise perturbation avoids difficulties in specifying random perturbation with a given spectrum. For $x/D>7$, one can observe the interaction of the two distinct mixing layers in the transition region and merge into an inflate enclosure with a big spot of hydrogen. This enclosure deflates forthwith in the next nearer spatial positions which an indicative of constriction and relaxation process. In the zone of turbulence, one can see mixing over the entire thickness of the overall jet development. The hydrogen is sometimes dispersed top down, following the dynamics of the pulse enclosure. Spatially, the intermittent extent of the mixing is evident. The induction of the enclosure is also visible on the vorticity field (figure 2b) for $10<x/D<15$. Beyond, eddies remain well organized and keep a high level of turbulence energy as it is evident on figure 4a. The contrast between the vorticity field and mixing field is visible; the animations indicate different mechanisms. The penetration of air in the H2 jet is absolutely dominated by molecular diffusion in nearfield. This observation is also buttressed by statistics, especially the mean mixing fraction profiles. For $x/D<10$, the mass fraction of H2

remain constant (figure 4c). Whereas, the radial profiles at various downstream positions indicate clearly for $x / D<10$, a mixing activity at the interface between the two species H2 and air; the rms of the mixing fraction is very low in this region (figure 4b). The comparison between the experimental measurements of Eggers(1971) and the present numerical computations (figures 3 and 4) shows some difference, but the results are qualitatively oncoming. The difference between the numerical and experimental is due to the linear region which induces a delay in the transition process. The turbulent mixing activity is confined in narrow thickness |r/D|<1 in transition region, however it extends downstream over twice, as it is visible on figure 4b.

Conclusion

These numerical simulations are a first step of our research on mixing H2-air in compressible jets. Further investigations based on 3D Monotone Large Eddy Simulations are under consideration and will be presented in the future paper. Although 2D approach is limited to represent all the features of the turbulent mixing H2-air physics, the statistics indicate roughly quantitative estimations. Results are encouraging for further calculations in 3 D configuration. Especially as previous studies have shown that MILES is adequate to track the mixing. The numerical scheme used in this study "PPM advection scheme" by approximating the variable evolution along each mesh with a monotonous parabola (monotonicity is guaranteed by the overall conservation laws of the whole system including large and subgrid scales) , behaves as a subgrid scale filter for scales smaller than several grid sizes.

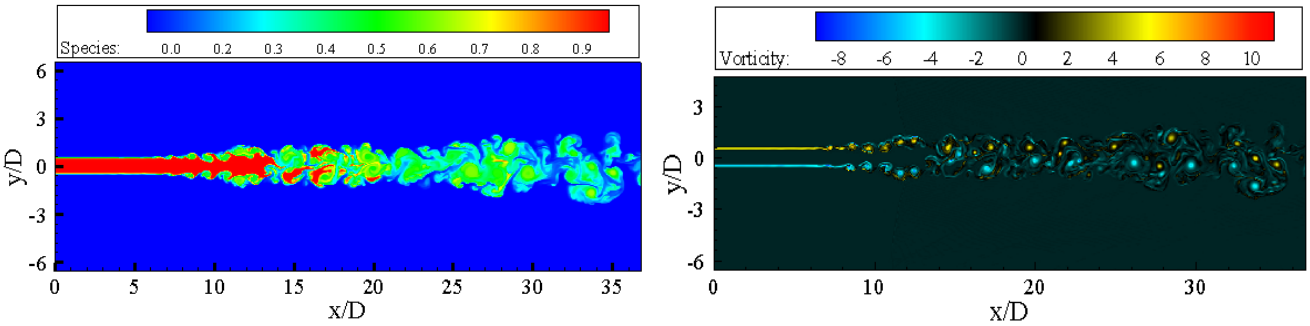

Figure. 2 – Instantaneous contours: a) mixture fraction of Hydrogen-Air: 0 (blue) to 1 (red)
b) vorticity field .

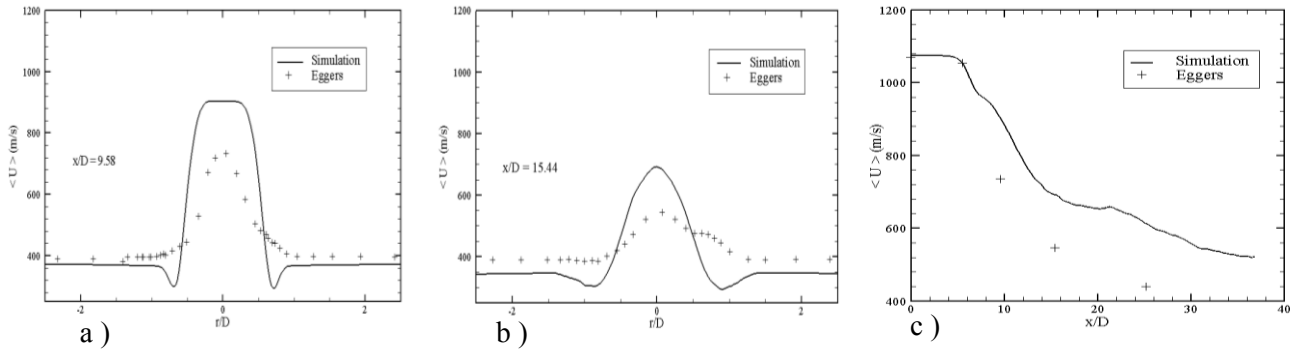

Figure. 3 – a ,b) Mean radiale velocity profiles at two downstream locations, c) downstream evolution of the axial mean velocity at the jet centerline).

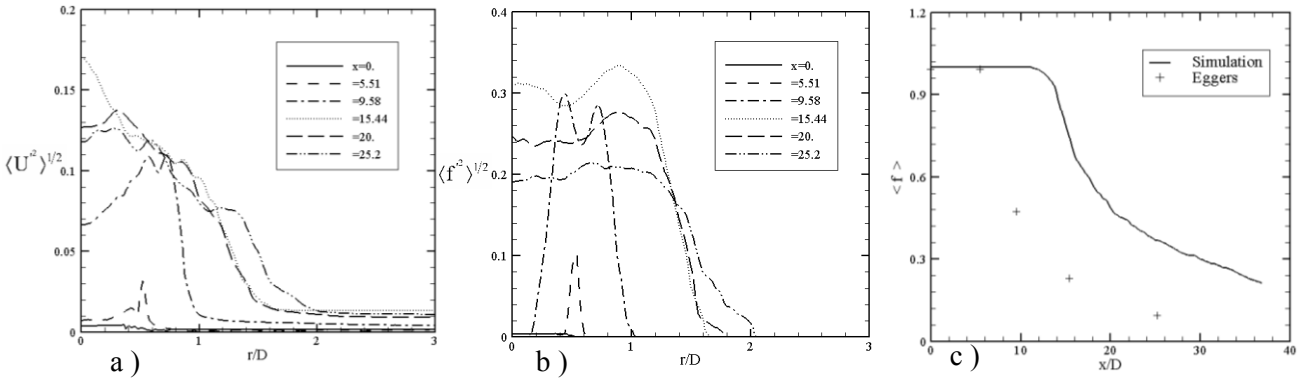

Figure. 4 – a) Radial evolution rms velocity at several downstream locations; b) Radial evolution of the mixing fraction rms at several downstream locations; c) Downstream evolution of the axial mean mixing fraction at the jet centerline

REFERENCES

[1] Eggers J.M. Turbulent mixing of coaxial compressible hydrogen-air jets. Tech. Rep. NASA-TN D-6487, 1971.

[2] Balarac, G., Si-Ameur, M., Métais, O., Lesieur, M. Direct numerical simulations of high velocity ratio coaxial jets : Mixing properties and upstream conditions influence » Journal of turbulence, Volume 8, N22, 2007.

[3] Balarac, G., Si-Ameur, M., Métais, O., Lesieur, M.. Large Eddy Simulation of Coaxial jets : Coherent structures and mixing properties, Direct and Large-Eddy Simulation VI , Volume 10, pp 277-284 , 2006

[4]Mehmet K, Fedioun I, Lardjane N, High-speed turbulent mixing and combustion : Miles vs physical LES, Seventh International Symposium on Turbulence and Shear-Flow Phenomena, TSFP-7,July 28-31, 2011, Ottawa, Canada.

[5]Colella, P. and Woodward, P.R.The piecewise parabolic method (PPM) for gas-dynamical simulations.J.Comput.Phys.54:174-201, 1984

[6] Roe, P.L.Approximate Riemann Solvers, parameter vectors and difference schemes. J.Comput.Phys. 43:357-372,1981.

[7]H. Rehab, E. Villermaux, and E. J. Hopfinger. Flow regimes of large-velocity-ratio coaxialjets. J. Fluid Mech., 345, 357-381, 1997.

[8] Villermaux, E., and H. Rehab. Mixing in coaxial jets. J. Fluid Mech., 425 ,161-185, 2000.