LES of Laser ignition in a H2-O2 micro-combustor

G. Lacaze[1], **B. Cuenot**[1], **T. Poinsot**[2]

[1]Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique,
31057 Toulouse, France

[2]Institut de Mécanique des Fluides de Toulouse,
31400 Toulouse, France

1 Introduction

Large Eddy Simulation (LES) is a powerfull tool to study unsteady complex flows. The concept of explicitely solving for the large geometry-dependent turbulent scales while modelling the dissipative behavior of the smaller scales, combined with high order numerical schemes and optimized unstructured meshes, has already shown its accuracy for gaseous turbulent flows [1, 2, 3, 4]. Its recent extension to reacting flows confirmed this potential [5, 6, 7]. Application of LES to the highly compressible and reacting flows that appear in rocket engines is therefore a natural evolution of this method [8].
In the last years CERFACS in collaboration with IFP has developed a numerical tool (AVBP) devoted to the LES of reacting flows in gas turbines and piston engines geometries. It is used here to compute the laser ignition of gaseous O2/H2 in the M3 micro-combustor installed at DLR [9]. The test case is a good candidate for LES application as ignition and flame stabilisation are transient phenomena that require accurate discretisation and modelling. It corresponds to the experimental case "GGA 24"[11], which is a 140 mm long chamber with a single H2-O2 coaxial injector and a 4 mm diameter exhaust nozzle. Initially, the chamber is full of nitrogen to define a reference state and then it is purged by the propellants during the purge phase before ignition by a laser. The filling phase lasts 370 ms. Oxygen and hydrogen are injected as gas through a coaxial injector: the oxygen inlet flow is sonic with a mass flow rate of 1.135g/s whereas hydrogen stays subsonic (M=0.28) and flows into the chamber at 0.592 g/s in addition, the exhaust nozzle becomes chocked during the filling phase.

2 Numerical configuration and simulation

The LES code AVBP solves the filtered Navier-Stokes conservation equations on unstructured meshes, using a finite volume formulation and explicit integration schemes. Realistic thermochemistry is used, allowing multi-step kinetics for the oxidation of hydrocarbons or hydrogen. Boundary conditions are set with the NSCBC method [13] based on characteristic variables. All simulations presented in this paper are run with the second-order Lax-Wendroff scheme.

The numerical configuration reproduces the 3D combustion chamber with the H2 and O2 inlet tubes and the exit throat (Fig.1). The injection systems with the domes are not included in the simulation. To minimize the impact of the exit boundary condition, the ambiant atmosphere around the chamber outlet is also calculated on a coarse mesh added to the chamber exit. The mesh is refined around the jets at inlet and downwards where the jets mix, develop and are ignited by the laser beam. The configuration and a zoom of the mesh near the injection are represented in Fig. 1. The final mesh is fully unstructured and uses tetrahedral cells. It counts around 630000 nodes, with the smallest cell volume being of the order of 10^{-13} m^3.

Correspondence to : guilhem.lacaze@cerfacs.fr

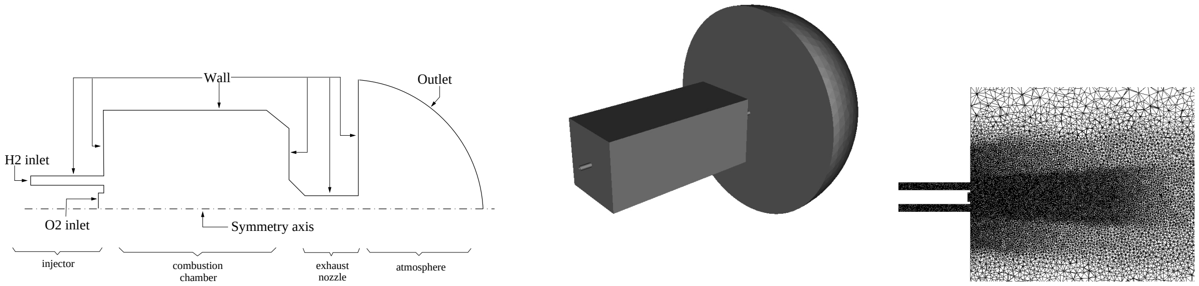

Figure 1: Sketch and view of the computing domain and zoom of the mesh of the M3 micro-combustor.

At inlets the momentum, temperature and mass fractions are imposed (as well as the pressure in the case of the O2 sonic inlet condition), whereas the exit surface (which is located outside the chamber, in the free atmosphere) is relaxed to the ambiant pressure using NSCBC [13]. All solid boundaries are isothermal slip walls, at the temperature 300K. The seven-step kinetic scheme including six species used in this study has been developed from the scheme proposed by Baurle [10]. The main objectives of this kinetic system are to accurately reproduce laminar flame speed and adiabatic temperature over a large equivalence ratio spectrum and to take pressure effects into account. Turbulent combustion interactions are modeled with the dynamic Thickened Flame model [12] which has been slightly modified during the ignition phase. Laser ignition is reproduced through an energy deposition at the location of the laser beam impact. The complex physical and chemical phenomena that are induced by the laser beam are not simulated (breakdown and plasma). The computation only takes into account the resulting effective energy input to the gas, estimated at 40 mJ for 500 ns, spread over a 6mm diameter sphere.

3 Results

3.1 The filling phase

To capture the flame ignition and stabilisation mechanisms, it is necessary to establish the correct flow structure and reactants distribution at ignition time. To compute this initial condition, a preliminary 3D LES of the purge phase of the chamber (initially filled with N2) was performed. The instantaneous axial velocity field obtained at the end of the purge phase shows recirculation zones starting at the corners of the chamber and developing downwards around the jets. Results show that nearly all the nitrogen has been purged: the remaining N2, mostly trapped in the recirculation zones, has a maximum mass fraction of the order of 0.17. The reactants are well mixed in most of the chamber and segregation appears only in the vicinity of the inlet jets.

3.2 Ignition

The solution obtained at the end of the purge phase at 370 ms is ignited and Fig. 2 shows series of snapshots of the fields of density gradient at three different times ($t = 37, 247, 683\ \mu s$ after ignition). Schlieren photographs taken from experimental results at $35, 250$ and $680 \mu s$ after ignition are also shown on Fig. 2. The comparison shows that the simulation captures the correct flame behavior as well as the global flame shapes although at t=$683 \mu s$, a little delay is observed.

The laser beam impact is located in a segregated zone where the local stoichiometric ratio is around 2 and where the turbulence intensity of the axial fluctuation is about 20% which leads to $u'/S_l \approx 3$ (with u' the root mean square of the velocity fluctuation and S_l the laminar flame speed). In the early time after ignition, the hot gas kernel is convected down stream by the jet without being stretched. Then chemical reactions start and as the kernel grows its surface is increasingly wrinkled by turbulence. As the flame expands in all directions, it encounters mixtures with different equivalence ratios: the front propagating towards the walls and the exit burns a mixture at $\Phi = 4$ but the front propagating towards the injection jets sees more and more segregated reactants. At $t \approx 200\mu s$ part of the upward propagating flame front encounters a mixture close to stoichiometry and accelerates. At the same time the pressure starts rising, until the flame reaches the walls and burns the fuel trapped between the flame front and the wall. The pressure rise makes the flame propagate even faster which enable it to come further upstream into the injection jet. At $t = 683\mu s$ the chamber is almost completely filled with burnt gas and at about 1 ms, a lifted flame settles into the mixing layer near the injection. After complete combustion of the fuel trapped near the walls, the premixed flame extinguishes in this zone and only the flame stabilised at the injectors remains. The pressure chamber evolution is presented in Fig. 3 and compared with experiment.

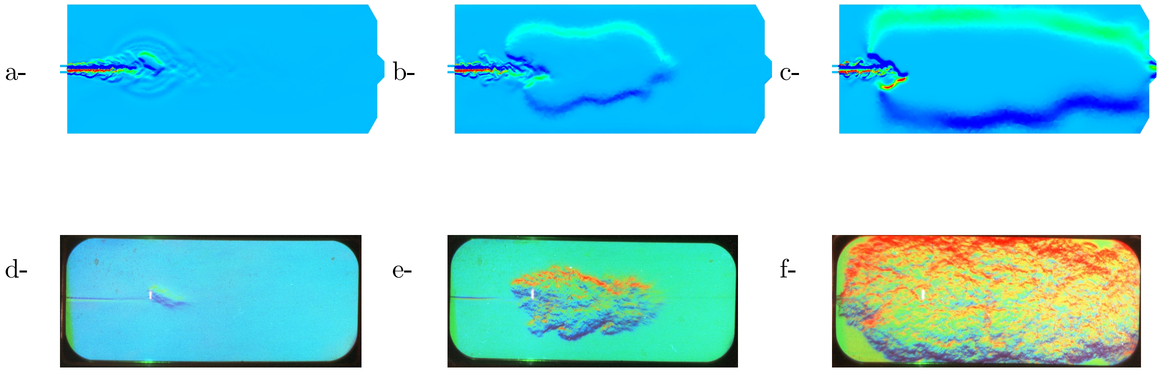

Figure 2: Snapshots of the density gradient field at three different times after ignition (a: $t = 37\mu s$, b: $t = 247\mu s$, c: $t = 683\mu s$) and Schlieren photographs at three different times after ignition (d: $t = 35\mu s$, e: $t = 250\mu s$, f: $t = 680\mu s$).

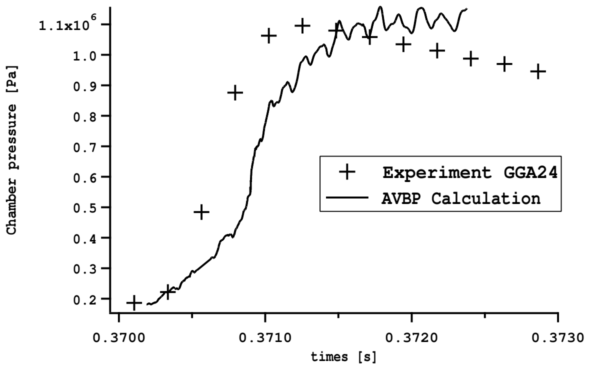

Figure 3: Temporal evolution of the chamber pressure compared with experiment (pressure taken at the real probe location).

4 Conclusion

A first attempt to apply Large eddy simulation to the laser ignition of the M3 burner of DLR has been presented. Results are qualitatively in good agreement with experimental observations, showing that the simulation captures the right mechanisms for flame propagation and stabilisation. It may be concluded that the flow and flame structure are now better understood and that complex chemistry simulations can be started to allow a full and quantitative validation.

Acknowledgments

The authors gratefully acknowledge the support of Snecma (Safran group) and of the computing center CINES, as well as DLR for fruitful discussions.

References

[1] P. Moin, K. Squires, W. Cabot, and S. Lee, *A dynamic subgrid-scale model for compressible turbulence and scalar transport*, Physics of Fluids, **3**, 11, pp.2746-2757, 1991.

[2] M. Lesieur and O. Metais, *New Trends in Large-Eddy Simulations of Turbulence*, Annual Review of Fluid Mechanics, **28**, pp. 45-82, 1996.

[3] M. Lesieur and P. Comte, *Large-Eddy Simulations of Compressible Turbulent Flows*, Turbulence in Compressible Flows, pp. 4.1-4.39, 1997.

[4] Garnier E., Sagaut P. and Deville M., *Large Eddy simulation of shock/homogeneous turbulence interaction*, Computers and Fluids, **31**, 2, pp. 245-268, 2002.

[5] L. Selle *et al.*, *Compressible Large-Eddy Simulation of turbulent combustion in complex geometry on unstructured meshes*, Combustion and Flame, **137**, 4, pp.489–505, 2004.

[6] H. Pitsch *et al.*, *Flamelet modeling of non-premixed turbulent combustion with local extinction and re-ignition*, Comb. Theory Modelling, 2002.

[7] C. Prière *et al.*, *Experimental and numerical studies of dilution systems for low emission combustors.* AIAA Journal, 43(8):1753-1766, 2005.

[8] A. Dauptain, *Allumage des moteurs fusée cryotechniques*, PhD thesis, INPT, CERFACS, 2006.

[9] V. Schmidt, U. Wepler, O. Haidn and M. Oschwald, *Characterization of the Primary Ignition Process of a Coaxial GH2/LOX Spray*, AIAA-2004-1167, 42nd AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, 2004.

[10] R.A. Baurle, S.S. Girimaji, *Assumed PDF turbulence-chemistry closure with temperature-composition correlations*, Combustion and Flame, Vol. 134, p. 131-148, 2003.

[11] V. Schmidt, D. Klimenko, M. Oschwald, *Preliminary Results of Test Case "A" Laser Ignition Tests for Coaxial GH2/GO2-Injection*, DLR, Lampoldshausen, 2003.

[12] O. Colin, F. Ducros, D. Veynant and T. Poinsot, *A thickened flame model for Large Eddy Simulations of turbulent premixed combustion*, Physics of Fluids 12, 7, 2000.

[13] T. Poinsot and S. Lele, *Boundary conditions for direct simulations of compressible viscous flows*, Journal of Computational Physics, **101**, 1, pp.104-129, 1992.