Supersonic mixing and combustion: advance in LES modeling

A Ingenito, C. Bruno**
University of Rome "La Sapienza",
Via Eudossiana 18, 00184 Rome, Italy.

Abstract

Mixing and combustion of supersonic reacting flows are currently under investigation for new generation launchers and trans-atmospheric vehicles. Experimental results with hydrogen injected at Mach 2.5 in a Mach 2 airstreams showed combustion taking place just in ~0.6 m: this indicates that supersonic combustion is feasible within short combustors. Large eddy numerical simulations including the subgrid scale model, ISCM, developed specifically for supersonic combustion have been done. This model takes into account the effect of compressibility on reaction rates and on mixing. Numerical simulations have pointed out that the flame is unsteady: it anchors at about 15 cm from the injector, develops downstream and lifts off. Periodical ignition and quenching have been investigated. Also the combustion regime in supersonic flows has been investigated and is reported.

1. Introduction

LES simulations can be of support in designing supersonic combustor if a subgrid scale model suitable to supersonic flows is implemented. In fact, numerical simulations with the Smagorinsky-Lilly SGS model often predict neither mixing nor combustion whilst experiments show both occurring over short lengths. Past evidence [1] shows that the physics of mixing and combustion is very different in subsonic and supersonic regimes. From a previous theoretical analysis[2] of the effects of high Mach number on turbulence and combustion it has been observed that high Mach number flows experience mainly streamwise vorticity and consequently maximum helicity. Both affect mixing and improve it at large scales. It has also been found that mixing can be improved by forcing transversal pressure gradients, e.g., by means of particular geometries (generating shocks) and devices (injectors).
In this test case, the bow shock due to the transversal injection induces the vorticity Furthermore, it has been shown that supersonic combustion takes place locally at approximately constant volume, and that collisional frequency increases due to local dilatation[3], resulting in faster kinetics. Based on the previous observations, a novel subgrid scale model, ISCM, has been developed. The ISCM model accounts for compressibility effects on mixing and on combustion. In particular, micro-scale physics has been included by means of a subgrid kinetic energy equation that is algebraically modelled to provide the velocity fluctuation needed by the eddy viscosity SGS closure. The subgrid scale model, (ISCM) accounts convincingly for key physics of supersonic combustion and can be used to suggest how to improve the supersonic combustor design.

2. Large Eddy Simulations of Supersonic Combustion with the ISCM model

2.1 NASA-Langley Test Case Geometry and Experimental Results

The geometry of the SCRJ combustor configuration is shown in Figure 1. A direct-connect supersonic combustor model, known by its acronym SCHOLAR has been developed at NASA- Langley Research Center. This configuration is that used during the NATO ATV-10 RTO project a few years ago[4]. This experiment has been designed to provide optical access to a reacting supersonic flowfield typical of the flow present in a scramjet engine. The model shown in Figure 1 consists of a section 546 mm in length constructed of copper for thermal control followed by a 914 mm long section of carbon steel attached to the aft end of the copper section. The copper section contains a single fuel injector that introduces gaseous hydrogen into the vitiated air stream flowing through the model.

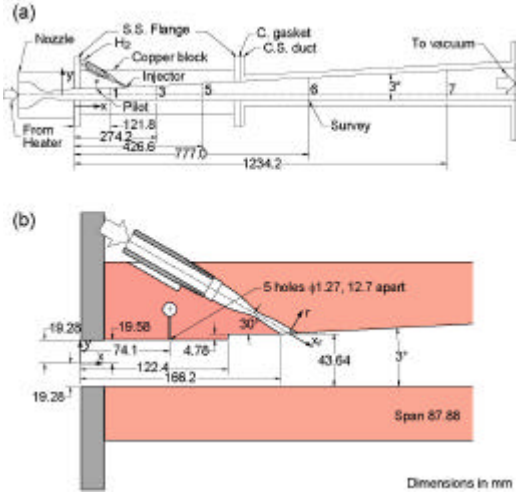

Figure 1 : Test model:
(a) nozzle and combustion chamber,
(b) detail in vicinity of fuel injector.

The injector region of the combustor model is shown in Figure 1b. The model consists of a constant area channel initially 38.6 mm high and 87.9 mm wide followed by a 4.8 mm rearward-facing step and a 43.8 mm long constant area section. Combustion heated vitiated air is introduced into the channel at Mach 2, 1184 K, and 100405 Pa.

The vitiated air contains 20.35 percent water by mass introduced by the facility heater. The injector lies on the duct centreline. The fuel injector is inclined at 30 degrees to the horizontal and has a circular cross-section 7.6 mm in diameter. It is located just downstream of the 3° divergence (~ 43.8 mm from the step) section. A 3 degree expansion of the upper wall begins immediately at the primary fuel injector. This 3 degree expansion continues along the upper wall of the carbon steel section that is attached to the copper combustor model.

Five measurement locations for optical access are provided in the copper part of the cobustor model. Two additional measurement stations are provided in the carbon steel section. From these single-shot measurements, averages and RMS values are derived. In additional to optical measurements, wall pressures are measured using an array of orifices.

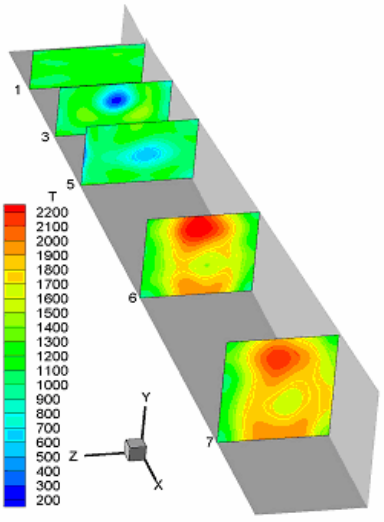

Figure 2 3D view of the experimental average temperature field

In Figure 2 a 3D view of the experimental average temperature field is shown. Experimental results predict the flame anchoring between cross sections 5 and 6. As this last section is at 77 cm from the combustor inlet plane, and at about 60 cm from the H_2 injector, mixing times can be estimated to be ~ 5×10^{-4}s (see

Table 1): this means that this supersonic flow mixes and burns in a very reasonably short time. Figure 2 shows that the flame is developed both at the bottom and upper wall. Maximum (averaged) temperature are about 2200 to 2300 K.

2.2 Numerical Scheme

Three-dimensional Large eddy simulations were performed with FLUENT 6.3 ™ code[5] commercial code to simulate the flowfield in the NASA Langley combustor model. Double precision has been used.

The LES solver is a coupled, upwind, explicit, third-order MUSCL, accurate both in space and time. This scheme was conceived from the original by blending a central differencing scheme and second-order upwind scheme. In FLUENT, compared to the second-order upwind scheme, the third-order MUSCL has the potential to improve spatial accuracy for all types of meshes by reducing numerical diffusion, most significantly for complex three-dimensional flows.

2.3 Computational Domain

The SCRJ combustor geometry of Figure 1 has been mapped by a 3-D grid.
This domain was discretized with a grid of 700 points in the streamwise direction, 46 points in the cross-stream direction, and 60 points in the spanwise direction. The grid was made finer near the step and the fuel injector. The number of hexahedral cells of the computational domain is 1,563,994, for a total of 1,626,578 nodes. Only the first 800 mm of the whole length of the combustor (1234.2 mm) have been simulated. With this grid, a very small wall Y^+, of order of 4-8 has been obtained near the step and the H2 injector, where the NASA experiment predicts bow shock formation. At the inlet, instead, the grid should be further refined to allow a better prediction of the boundary layer.
However, both the shock departing from the step and that just upstream the fuel injection are predicted by simulations, this leading the two counter-rotating vortices generation along the stream direction. Also shocks reflection between the upper and the bottom walls is predicted.

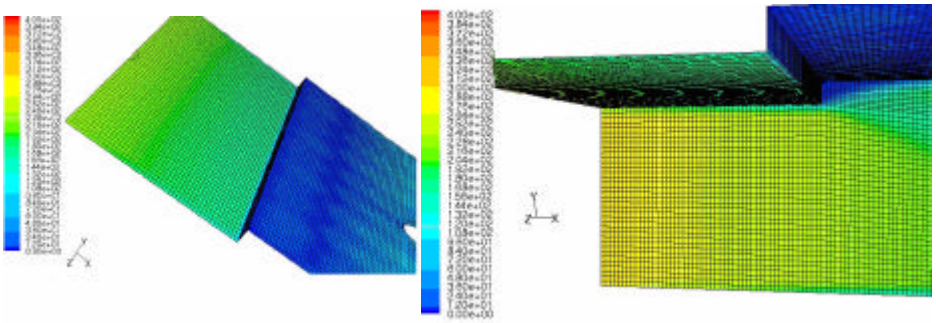

Figure 3 Instantaneous Contour of Wall Y^+ at the combustor inlet upper wall

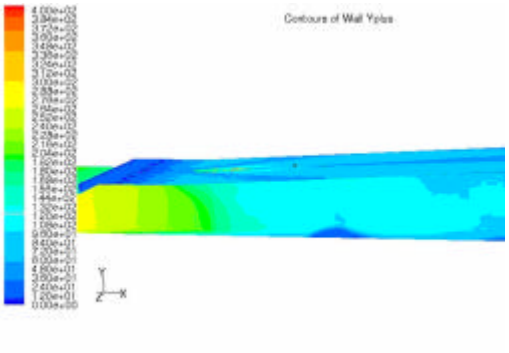

Figure 4 Instantaneous Contour of Wall Y^+ in the second part of the combustor

2.4 Inlet Boundary Conditions

Calculations begin at the x = 0 station of the SCHOLAR model, where vitiated air from the facility enters the duct. The initial channel cross-section is 38.6 mm high and 87.9 mm wide. Vitiated air entered the model at Mach 2.0 yielding a velocity of 1395.7 m/s, a static temperature of 1204 K, and a static pressure of 101325 Pa. Air inlet temperature is sufficiently high to produce self-ignition of the air-hydrogen mixture.
The mole fractions of the species present in the vitiated air are given in Table 1:

H2 mole fraction	1.3×10^{-5}
OH mole fraction	0.00071
O2 mole fraction	0.21
H2O mole fraction	0.217
N2 mole fractions	0.5722

Table 1 Vitiated air mole fractions at the inlet

The hydrogen fuel injector introduces hydrogen at Mach 2.5, a static temperature of 1343 K, and a static pressure of 202650 Pa. Air/H_2 equivalence ratio is ~ 1.

Combustor walls are non-adiabatic; in fact, the measured heat flux varies linearly from 0.7 MW/m^2 to 1.8 MW/m^2 along the x direction, corresponding to about 10% of the combustion heat release. The heat flux function has been implemented as BC for the energy equation by means of a user defined function in the FLUENT CFD code used in these simulations.
No-slip conditions were specified along the channel walls.

2.5 Turbulence and chemistry modelling

The subgrid scale model used for the turbulent closure of the filtered Navier Stokes equations is the ISCM model[6]. In brief, in the ISCM model:

1. micro-scale physics has been included by means of a subgrid kinetic energy equation that is algebraically modelled to provide the velocity fluctuation to be used in an eddy viscosity SGS closure;
2. reacting turbulent structures have been modelled by means of a reactor burning at constant volume;
3. the reaction rate depends on the local Mach number.

Hydrogen/air chemical kinetics has been modelled by means of a global 1-step reaction and 3 reacting species[7]:

$$H_2 + \tfrac{1}{2} O_2 = H_2O \qquad k_{global} = 1.8\times10^{13} \exp(-17614/T) [H_2]^{1.0}[O_2]^{0.5}$$

This scheme does not consider the effects of the small quantities of radicals species present in the vitiated air. However, the assumption of 1-step mechanism instead of a more detailed mechanism can be justified considering that anchoring at this air temperature and pressure is not controlled by kinetics. In fact, results obtained by CHEMKIN 3.7 code, concerning hydrogen/air combustion performed with a detailed mechanism consisting of 9 species and 20 reactions, have shown (for the same NASA-Langley test case conditions) very short ignition delay times, of order of 0.05 ms, ten times lower than the mixing time, as estimated from the experiments.

2.6 Simulations

Simulations performed with the ISCM subgrid model show the H_2 jet penetrating up to 0.5 diameters, and then bending down towards the bottom wall. A bow shock is located immediately in front of the injector.

Shock reflections between upper and bottom walls are predicted. Figure 5 shows vorticity is mainly streamwise. Figure 6 shows *averaged* temperature fields at sections 5 and 6. Two counter-rotating vortices move along the stream direction, spread the H_2 jet enhancing fuel-air mixing and reaction. The vortices also convect fluid toward the lower wall. Experimental data indicate a maximum temperature of between 2030K and 2300K, while simulations predict a maximum (averaged) temperature 2400 K. A “cold" core of unreacted hydrogen persists in both the data and the calculation at the end of combustor.

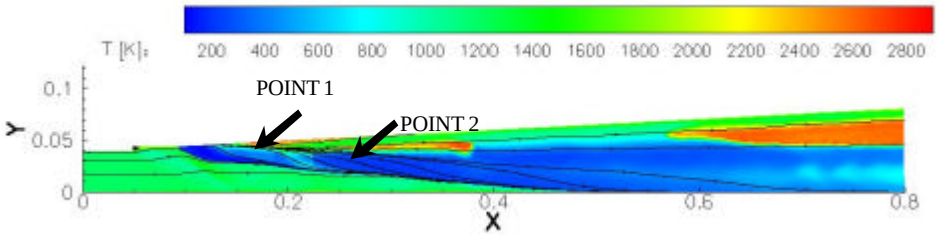

Figure 5 Instantaneous Temperature field and streamlines in the middle XY plane

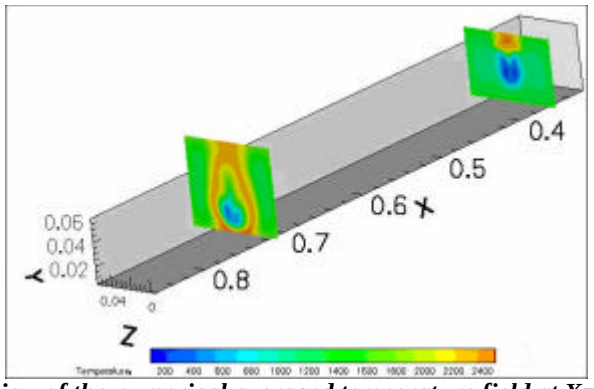

Figure 6 3D view of the numerical averaged temperature field at X=0.3 cm and X = 0.7 cm

Numerical simulations show also unsteady flame behaviour similarly to what reported in reference [8]. Numerical simulations show that combustion starts on the upper side of the hydrogen-air shear layer, at about 5 cm from the H_2 injector (Point 1). Here the mixture ignites periodically at about 2500 Hz. Mixture ignites also at about 15 cm from the H_2 injector (Point 2). From this point, the flame develops downstream, lifts off and is convected towards the exit. This phenomenon is periodical and forced by the ignition of reactants at point 1. After 4×10^{-4} s, the flame starts again to develop downstream and the whole phenomenon repeats. This means that the local temperature and equivalence ratio are such to allow the mixture re-ignition. Figures above show that *instantaneous* maximum temperatures are higher than temperatures measured in the experiments (by 15-20%). This is likely due to having imposed a single-step oxidation reactions (thus no radicals in the products). The two counter-rotating vortices shown on all planes promote mixing, thereby favouring flame propagation, albeit unsteady.

Combustion at the bottom of the combustor starts between section 5 and 6. The flame length, in good agreement with the experimental results, reaches the end of combustor and continues out.

Figure 5 shows flame anchoring on the upper wall, at 5 cm from injector, occurring in correspondence to the shock wave, where the density gradient is higher. This means that shocks play an important role in flame anchoring, possibly caused by increased mixing rates due the coupled effect of the density and pressure gradients on vorticity transport (baroclinic effect), and also due to the influence of the dilatational term on the reaction rate. Numerical results show that shock waves are steady; therefore the pulsating behaviour of the flame is not due to shock oscillation.

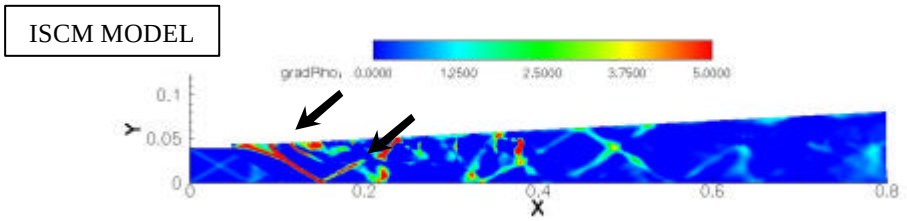

Figure 7 Shocks Waves Visualization

Numerical results point out that peaks of subgrid velocity fluctuations, defined here as $\sqrt{k_{SGS}}$, are less than 20 m/s and that turbulent viscosity predicted by the ISCM model is smaller than 0.001 kg/m·s. Maximum values are shown

at the hydrogen/air interface and where combustion occurs. Mixing and “instabilities” are analyzed in the following Sections.

3 Mixing and Combustion for Supersonic Flows

Flame-holding and mixing are critical issues in the design of supersonic/hypersonic combustors. In fact, in supersonic flows the residence time of the air stream within the combustion chamber is very short: for an airstream entering at Ma=2 in a combustor 1 meter long, it is about a millisecond. In this short time fuel and air must mix, ignite and burn. Incomplete or non-uniform mixing leads to unburned reactants with resulting loss in efficiency and may lead to production of pollutants. In principle, supersonic combustion is so fast that NO_x production may be considerably less than in conventional subsonic combustion. The ideal case of complete mixing is extremely difficult to achieve in practice. Increasing combustor length is not advisable due to skin friction losses: in fact, in a SCRJ vehicle, the combustor is responsible for about 60% of the total skin friction drag[9]. To improve mixing without increasing combustor length, several solutions have been investigated: transversal injection, lobe mixers[10], vortex generators and by devices exploiting the interaction with shock waves. The major drawback is in terms of thrust penalty: in fact, thrust losses scale with increasing jet Mach number[11].
Transverse injection, as in the NASA Langley test case, offer relatively rapid mixing and good fuel penetration. In fact, penetration of the fuel stream into the cross-flow is governed by the jet-to-freestream momentum flux ratio. The fuel jet interacts strongly with the cross-flow, producing a bow shock and a localized highly three-dimensional flow field. Vorticity addition to the air stream provides more significant mixing enhancement of fuel and air.

In order to estimate ignition times, the NASA-Langley test case initial conditions have been assumed, in particular: V = 1200 m/s, P=1atm, Φ=1. The averaged mixture temperature (between air at 1204 and fuel at 103 K) is therefore about 1180 K. The chemical time, τ_{chem}, for a well mixed reactor, is about ~ 50 μs.

The distance at which spontaneous ignition occurs in a medium flowing at a velocity U is of order $L_{chem} = U \times t_i = \sim 6$ cm. This distance is in good agreement with that predicted by numerical simulations (~ 5 cm).

Because of these small ignition delay times, the Damkoehler number, defined as the ratio between convective and chemical time, is:

$$Da_I = \frac{t_{conv}}{t_{chem}} \cong \frac{833ms}{50ms} \cong 16 > 1 \qquad (1)$$

This means that *if fuel and air are well mixed*, ignition occurs within the combustor, and as a consequence *chemistry does not control combustion*.

Once established that flame anchors, a study on the reasons for flame unsteadiness has been done. In fact, supersonic flows where large temperature changes occur across the shocks, at the hydrogen-air interface and across the flame, the reaction rate $\omega_r = \exp(-E/RT_i)$ (E is the activation energy and T_i is the initial reactant temperature) may change by orders of magnitude. Since the activation energy is generally large (here is of order 35 kcal/mol), the reaction rate is very temperature-sensitive. Thus, any fluctuation in the flame temperature will result in a large change in the reaction rate, leading to ’instability’ of the flame front. Furthermore, rapid density changes across the flame can drive acoustic wave generation that can couple with the increase of the burning rate to induce acoustic-driven instability. Combustion unsteadiness is likely due to this interaction between heat release, acoustics and kinetics mechanisms.
In order to understand this periodical behaviour, an analysis of the characteristic times has been performed. In fact, because of the S-curve of the hydrogen/air autoignition, if the temperature of the reactants mixture is below a threshold temperature about 900-1000 K, kinetics becomes slower. For a scramjet combustor, where reactants are not premixed but, for instance, cold hydrogen is injected into hot air, temperature varies significantly with equivalence ratio throughout the mixing layer around the jet. At lower temperature ignition delay times decrease and combustion become eventually controlled by kinetics[12]. As shown in the previous Section, the ignition delay time ($\sim 5\times10^{-5}$ s) is smaller than residence time ($\tau_{conv} \sim L/U = 8.3\times10^{-4}$ s), so kinetics is fast enough to let the flame ignite during a convective time.

An analysis of mixing at small scales has been conducted by looking at the local value of the Da, Ma and Re number. By looking at the instantaneous field of the chemical times, it turns out that in the part of combustor downstream of the injector these times are shorter than 1 ms. In particular, the chemical times, calculated by:

$$t_{chem} = \left(\frac{\dot{w}}{r} \right)^{-1} \qquad (3)$$

goes from 10^{-5} s to 10^{-3} in the zone where combustion takes place. Turbulent convective times in the flow field, calculated as ratio between the cell dimension and the subgrid scale velocity fluctuations:

$$t_{conv} = \frac{\Delta}{\sqrt{k_{sgs}}} \qquad (4)$$

range from about 8×10^{-4}s to 10^{-3}s.

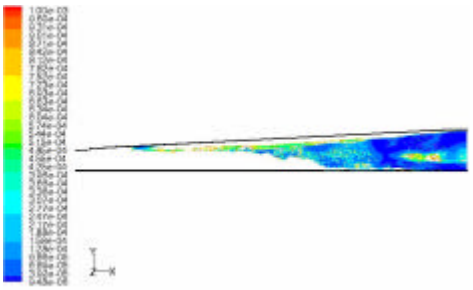

Figure 8 Instantaneous Contour of the chemical times

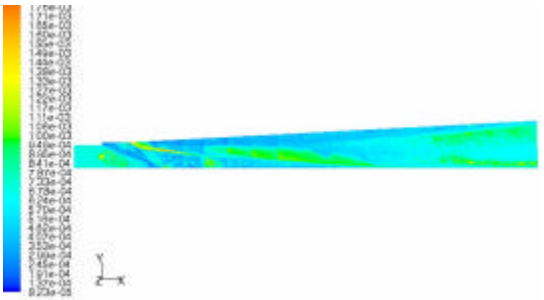

Figure 9 Instantaneous Contour of the Turbulence convective times

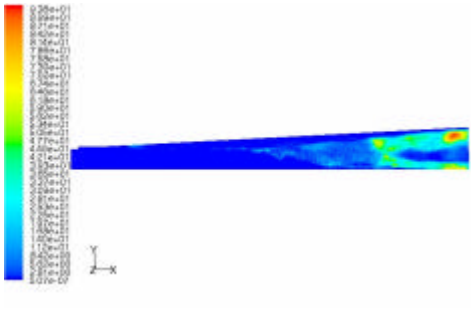

Figure 10 Instantaneous Contour of the Da number

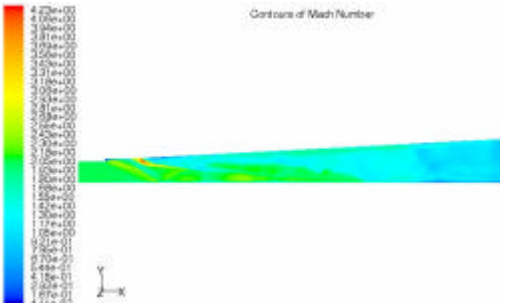

Figure 11 Instantaneous Contour of the Ma number

The local turbulent Da_t number, i.e., the ratio between the turbulent convective and the chemical times, calculated in each computational cell is shown in Figure 10. Where $Da_t<1$, combustion does not occur. Values of $Da_t>1$ are present only in the second part of the combustor, downstream of the injector. Maximum Da_t values are of order of 90, even if the Da_t number assumes generally values of about 20-40. Figure 11 shows that where combustion occurs, the Mach number decreases. This is due to the effect of the heat addition to a supersonic flow in a constant area combustor, as predicted by Rayleigh. In this case, due to the fact that the chamber is slightly divergent the flow stays supersonic and does not choke.

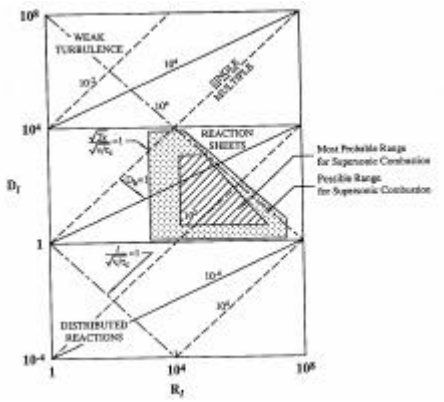

Figure 12 Williams-Klimov diagram

Da_t and Re_t numbers predicted by numerical simulations are in the same regime of that predicted by the Williams-Klimov diagram for subsonic flames. The combustion regime for these characteristic numbers corresponds to the

reaction sheet regime: this means that the flame is corrugated.

4. CONCLUSIONS

In this work, numerical simulations of the NASA-Langley test case have been performed. These simulations have pointed out that the flame is unsteady: it anchors and quenches periodically. This may be explained as due to the effect of the high temperature gradients due to the shock waves and to the local compressions on the reaction rate. In fact, below a threshold temperature of about 900-1000 K, ignition delay times may become longer than the mixing times. By a comparison with the large-scale characteristic times in a supersonic combustor it can be shown that the chemical time is shorter than the residence time and the flame anchors within the combustor. By comparing small-scale characteristic times, one may tentatively conclude that combustion occurs in the reaction sheet regime.

Acknowledgments

This work was performed within the 'Long-Term Advanced Propulsion Concepts and Technologies' (LAPCAT) project investigating high-speed airbreathing propulsion. LAPCAT, coordinated by ESA-ESTEC, is supported by the EU within the 6th Framework Programme Priority 1.4, Aeronautic and Space, Contract no.: AST4-CT-2005-012282. Further info on LAPCAT can be found on http://www.estec.esa.int/techresources/lapcat.

1 Ingenito, A., De Flora, M. G., Giacomazzi, E., Bruno, C. and Steelant, J., "LES Modeling of Scramjet Combustion", 44th AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, 9-12 January 2006;

2 Ingenito, A., "Supersonic Combustion Modeling", Ph.D. Dissertation, Mechanics and Aeronautics Department, University of Rome "La Sapienza", Rome, October 2005, (in Italian);

3 Giordano, D., "The Influence of Medium Comprimibility on Chemical-Reaction Rates", Part I: Theoretical Considerations, 36th AIAA Thermophysics Conference, AIAA paper 2003-4057, Orlando, Florida, 23 - 26 June 2003;

4 Drummond, J. P., Diskin, G. S., Cutler, A. D., "Fuel-Air Mixing and Combustion in Scramjets", Technologies for Propelled Hypersonic Flight, NATO Research and Technology Organization, Working Group AVT 10, Final Report, January 2001;

5 http://www.fluent.com;

6 Ingenito, A., De Flora, M. G., Giacomazzi, E., Bruno, C. and Steelant, J., "A novel Model of Turbulent Supersonic Combustion: Development and Validation", 42nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Sacramento, California, July 9-12, 2006;

7 Marinov, N.M., Westbrook, C.K., Pitz, W.J., "Detailed and Global Chemical Kinetics Model for Hydrogen", Transport Phenomena in Combustion, Vol. 1, Taylor and Francis, Washington, DC, 1996, pp. 118-129.

8 Choi, J., Yang, V., "Flow Oscillations in Hydrogen-Fueled Scramjet Combustors", International Colloquium on Hypersonic Propulsion, September, 2003, Beijing, China;

9 Paull, A., Stalker, R. J., and Mee, D. J., "Experiments on supersonic combustion ramjet propulsion in a shock tunnel," Journal of Fluid Mechanics, Vol. 296, Aug. 1995, pp. 159–183.

10 Campuzano, M. F., Dang, T. Q., "Numerical study of lobed-mixer fuel-injection strut in scramjet engine", ASME, SAE, and ASEE, Joint Propulsion Conference and Exhibit, 31st, San Diego, CA, July 10-12, 1995;

11 Stalker, R. J., Paull, A., Mee, D. J., Morgan, R. G., and Jacobs, P. A., "Scramjets and shock Tunnels - The Queensland experience", Progress in Aerospace Science, Vol. 41 2005, pp. 471-513;

12 A. Ingenito, E. Giacomazzi, C. Bruno and Johan Steelant, "LES Modeling of Scramjet Combustion", 14th AIAA/AHI Space Planes and Hypersonic Systems and Technologies Conference, Canberra, Australia, 6-9 November 2006.

A revised version of this article is availabe here.