SELF-IGNITION IN SUPERSONIC CONFINED FLOWS: HYDROGEN VERSUS HYDROCARBONS/HYDROGEN MIXTURES - CHEMISTRY/MIXING INTERPLAY

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Content

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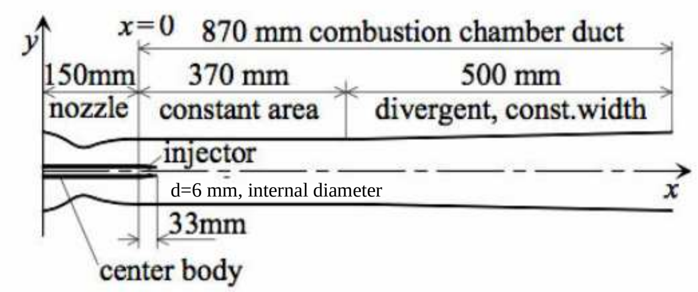
- Operating conditions
- Pressure distribution: a) weak and b) abrupt self-ignition modes
- Instantaneous OH-PLIF images
- Two types of self-ignition : a) weak self-ignition mode, b) abrupt self-ignition mode

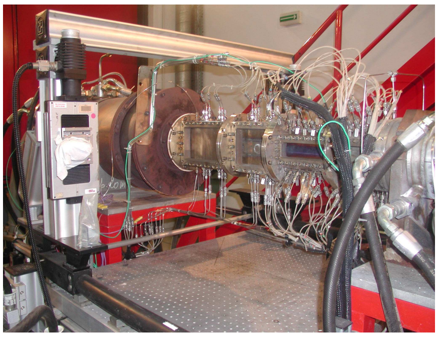
II. **LES simulation of weak self-ignition mode. Comparison with experiment**

III. **Unsteady RANS simulation of abrupt self-ignition mode. Comparison with experiment**

Conclusions

LAERTE test facility (1/3)



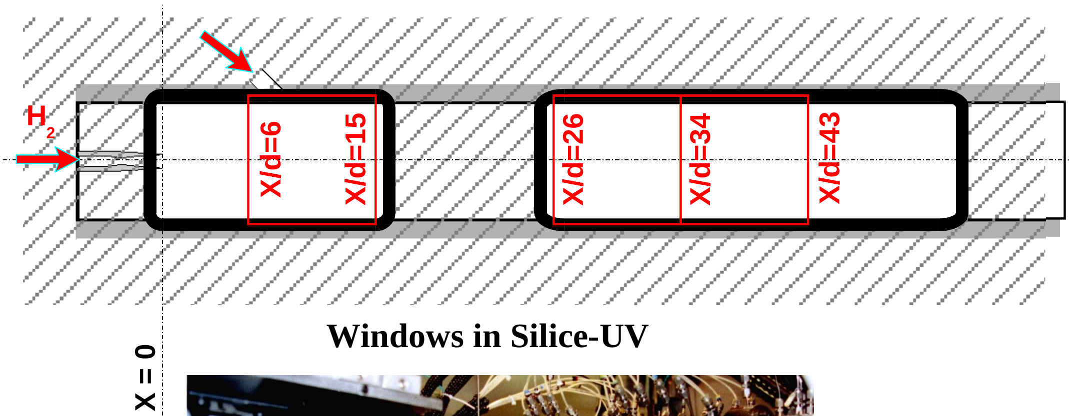


- Coaxial fuel injection: adapted static pressures injection
- Constant section during the first 370 mm of the duct, after diverges with a half-angle of 1.15°

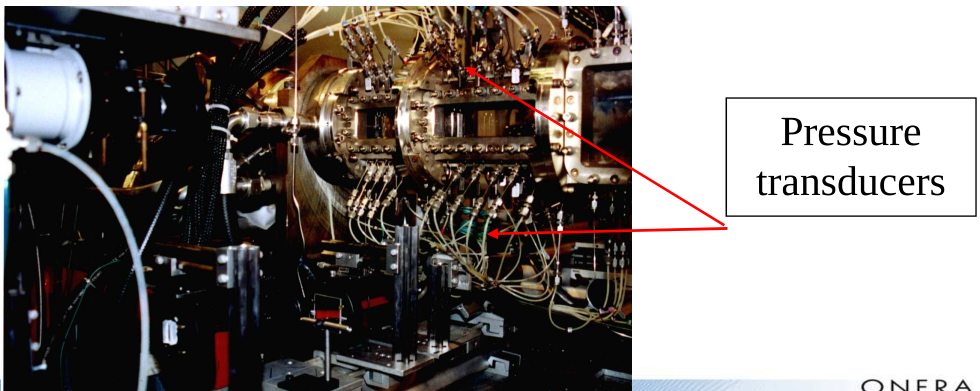
Operating conditions	Air	H_2	26% C_2H_4 / 74% H_2 (molar fractions)	50% C_2H_4 / 50% H_2 (molar fractions)
Mach number	**2**	**2**	**2**	**2**
Static Pressure (MPa)	**0.08**	**0.08**	**0.08**	**0.08**
Total Temperature (K)	**1850**	**300**	**300**	**300**
Static Temperature (K)	**1200**	**160**	**160**	**160**
Mass flow rate (g/s)	**650**	**6.2**	**12.8(C_2H_4) + 2.6(H_2)**	**16.2(C_2H_4)+ 1.2(H_2)**
velocity (m/s)	**1336**	**1970**	**950**	**730**

LAERTE test facility (2/3)

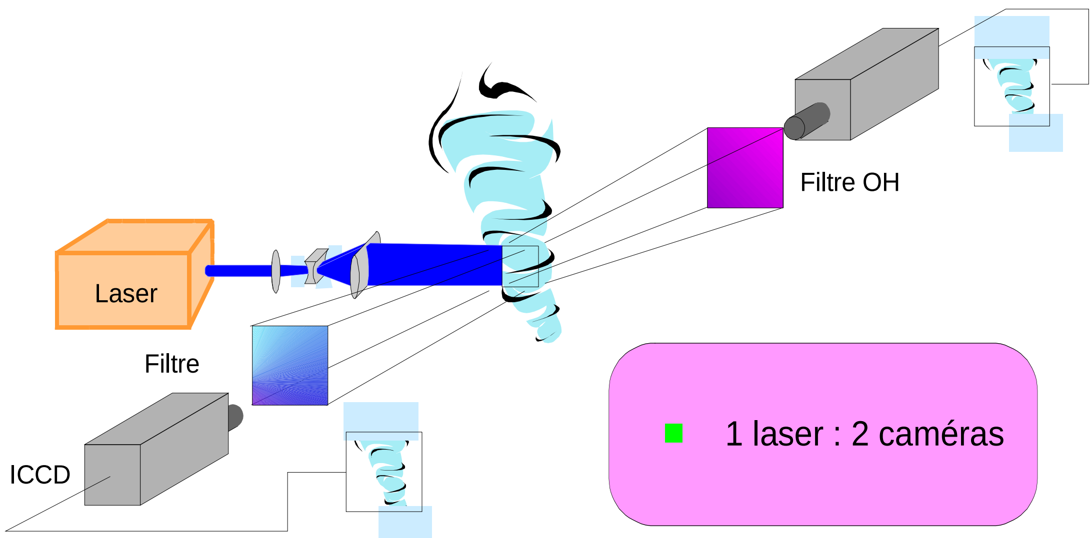
Optical access through the test section



Windows in Silice-UV



Experimental optical facility (OH-Ac PLIF)

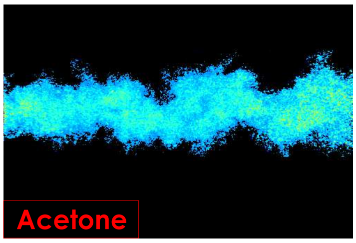


- 1 laser : 2 caméras

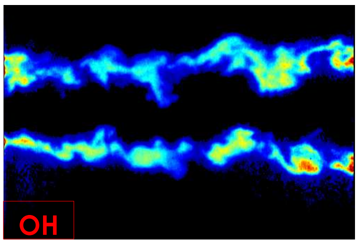
Results : joint OH and Acetone PLIF

- LIF OH et Ac. 1 λ → N_{OH} et $N_{ac.}$

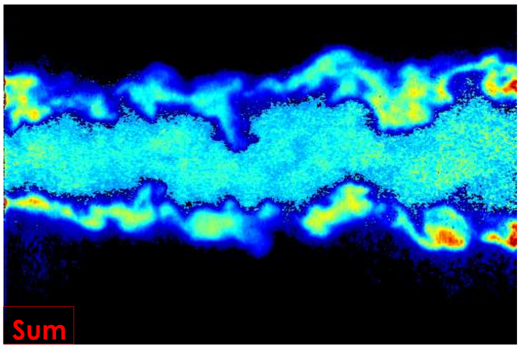
Acetone + H_2 →



Acetone + H_2 →



Acetone + H_2 →

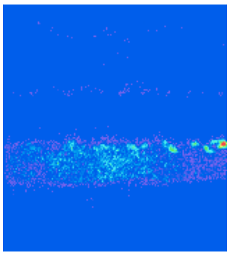


λ=282 nm

Structure of supersonic mixing layer – OH-PLIF

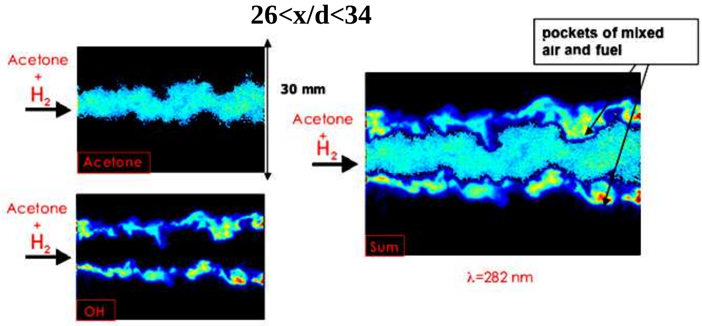
2 different regions in the flow

$6<x/d<14$



close from the injector

$26<x/d<34$

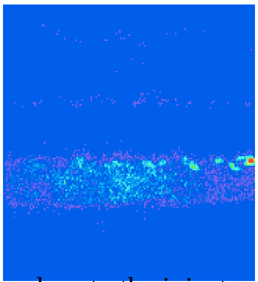


far from the injector

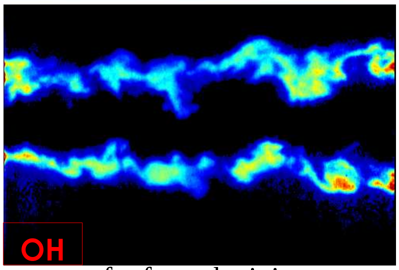
pockets with size less 1 mm in intermittent combustion. Pockets composed of fuel and air coming from the external boundary layer of the injector. Temperature of this air: 1600K (close from stagnation temperature de la temperature of 1850 K)

« large » pockets with a characteristic size of 5 mm in combustion, composed of hot air, fresh fuel and burnt gases.

Instantaneous OH-PLIF images (pure H_2 jet)



close to the injector
$6<(x-x_{inj})/d<15$



far from the injector
$26<(x-x_{inj})/d<34$

(The flow is from left to right)

Main characteristics of the self-ignition process:

- **self-ignition has a spotty character and appears in the form of random pockets**
- **self-ignition involves the intricate interplay between the mixing and the chemistry**
- **each pocket has its unique history, as a consequence mixing and self-ignition chemistry cannot be decoupled**
- **flamelet models are not adequate for LES modeling self-ignition of supersonic fuel jet in hot supersonic air stream**

LAERTE test facility (3/3)

Wall pressure measurements

- **Pressure transducers**
  - *80 channels distributed on the top and on the bottom of the combustion chamber*

- **Locations:**
  - *step of 10 mm on the first 150 mm of the duct*
  - *step of 15 mm between 150 mm < x < 370 mm*
  - *step of 30 mm between 370 mm < x < 870 mm*

- **Pressure rise characterizes the amount of heat release**
  - *evaluation of auto-ignition by comparing reacting and non-reacting cases*

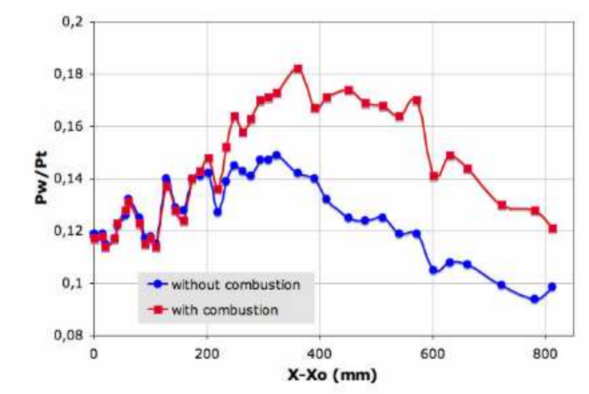
Two types of autoignition

- **weak ("smooth") mode:**
  - *progressive and moderate heat release*
  - *wall pressure profile with a low rise of pressure due to combustion*

- **"abrupt " mode:**
  - *sudden and brutal heat release*
  - *wall pressure profile with a large rise of pressure due to combustion*

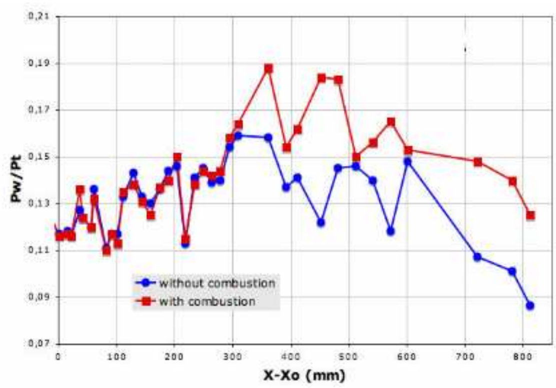
Experimental data (1/2)

Weak (smooth) mode of self-ignition. Pressure distributions along the combustor



Pure hydrogen fuel jet: mass rate 6.2 g/s, x_0=33mm

Self-ignition length – 15 cm



26% C_2H_4 / 74% H_2 mixture fuel jet:

mass rate 12.8 (C_2H_4) g/s+ 2.6 (H_2) g/s

Self-ignition length – 25 cm

- **The flow is supersonic throughout the combustor**

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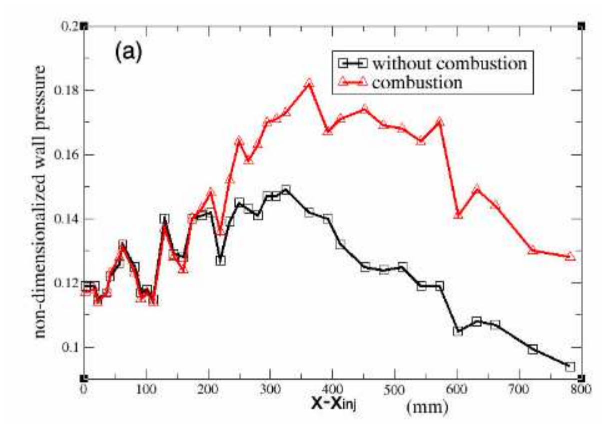
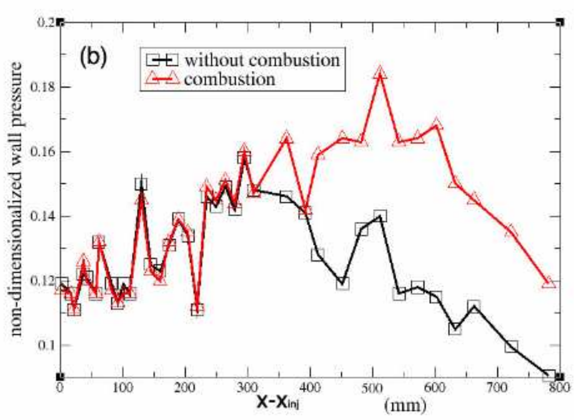
Experimental data (1/2)



Pure hydrogen jet (1998), mass rate: 6.2 g/s



73% methane/27% hydrogen jet (mass fractions) mixture (2004),

mass rate: 7.4 g/s CH_4+2.8 g/s H_2

Self-ignition lengths are:

- 15 cm for H_2,
- 33 cm for CH_4- H_2 mixture

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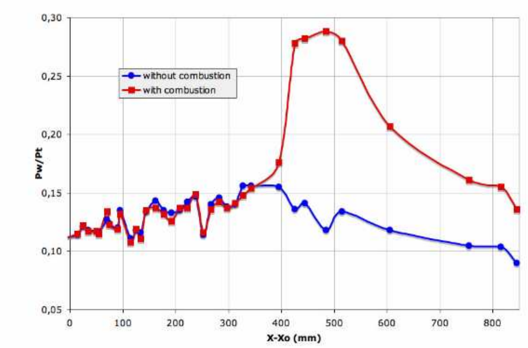
Experimental data (2/2)

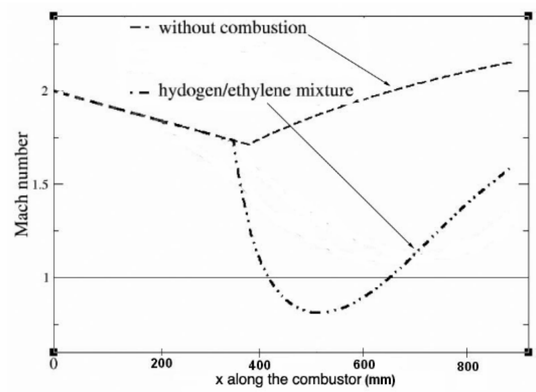
Abrupt mode of self-ignition. Pressure distribution along the combustor



50% C_2H_4 / 50% H_2 mixture fuel jet
mass rate: 16.2 (C_2H_4) g/s + 1.2 (H_2) g/s

Self-ignition length is about 35 cm

- **Abrupt mode arises if content C_2H_4 exceeds 29% (molar fraction)**



1D calculation. Mach number distribution for 50% C_2H_4 / 50% H_2 mixture fuel jet

- thermal chocking takes place
- subsonic region appears between 0.4 m < $x-x_o$ < 0.63 m

Synthesis of experimental results

- **2 scenarios based on observations**

  Smooth mode

  • at the stagnation temperature 1850K and entrance Mach numberM=2, the self-ignition of pure hydrogen starts smoothly

  • with the increase of the ethylene concentration in the ethylene/hydrogen mixture and for CH_4/H_2 mixture the delay length of self-ignition increases

  Abrupt mode

  •at some critical value of ethylene concentration self-ignition starts suddenly and strongly.

- **Importance of mixing time**

  • with increasing of an air/fuel premixing (i.e. after fuel injection), self-ignition can be brutal such as for premixed mixtures

  • interaction between chemistry an mixing (turbulence) controls the self-ignition regime

LES simulations of weak self-ignition mode

LES subgrid flow model – Smagorinski model
LES combustion model – PaSR-Vulis model
Chemical mechanisms:

- H_2 : Jachimowski - 7 species / 9 reactions
- CH_4/H_2 : Davidenko – 21 species / 79 reactions
- C_2H_4/H_2: Singh - 9 species /10 reactions

LES Combustion Model: PaSR – Vulis model

Multi-scale model based on the assumption that reactions take place on the smallest *fine structures* (*) embedded in the *surroundings* (^{0})

Subgrid balance equations

$$\begin{cases} \bar{\rho}(Y_i^* - \tilde{Y}_i) = \tau_m \dot{w}_i(\bar{\rho}, Y_i^*, T^*) \\ \bar{\rho}\sum_{i=1}^{N}(Y_i^* h_i^* - \tilde{Y}_i \tilde{h}_i) = \tau_m \sum_{i=1}^{N} h_{i,f}^{\theta} \dot{w}_i(\bar{\rho}, Y_i^*, T^*) \end{cases}$$

$$\bar{\dot{w}}_i = \dot{w}_i(\bar{\rho}, Y_i^*, T^*)$$

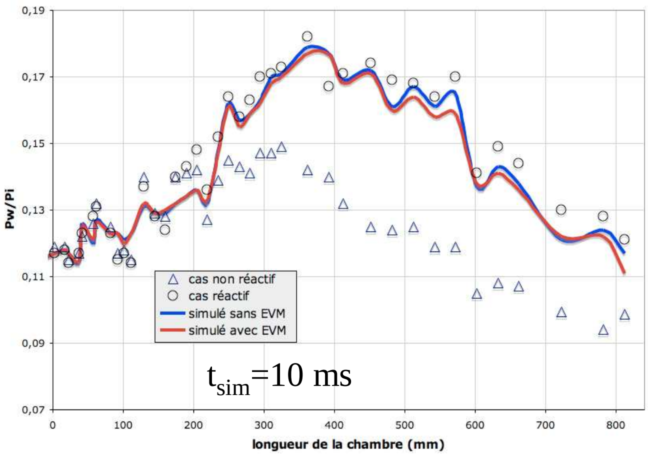
$$\tau_m^{-1} = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}} \qquad \tilde{S}_{ik} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_k} + \frac{\partial \tilde{u}_k}{\partial x_i} - \frac{2}{3}\frac{\partial \tilde{u}_l}{\partial x_l}\delta_{ik}\right)$$

$$\partial_t(\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\tilde{Y}_i) = \nabla\cdot((D_i + \mu_k / Sc_k)\nabla Y_i) + M_i P_{ij}\dot{w}_j(Y_i^*, T^*)$$

LES simulations: pure H2 jet

pure hydrogen reacting case (experiment 1998):

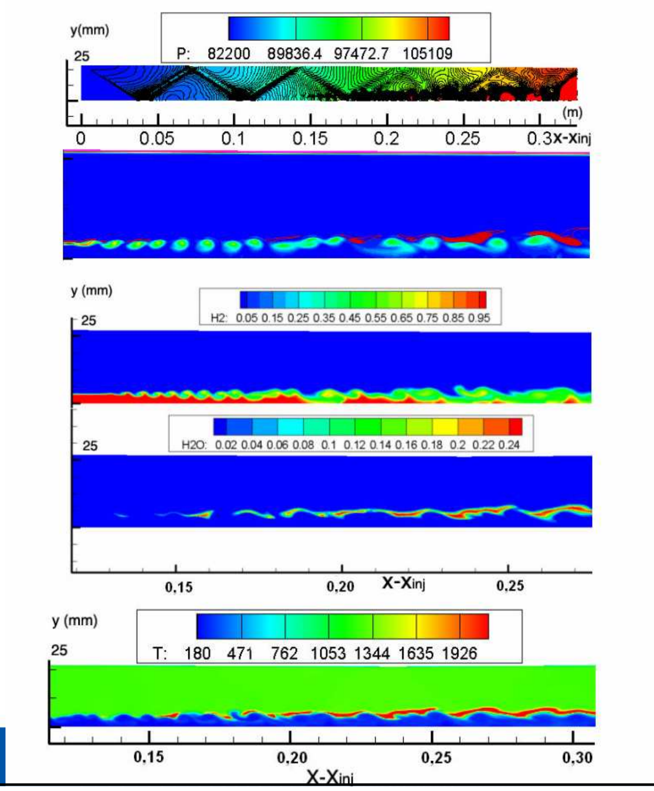
wall-pressure profiles



- good estimation of ignition delay and pressure level for pure hydrogen (same behaviour for 2004 case)
- no influence of PaSR-VM: hydrogen is highly reactive - no need to been well mixed to air for burning

LES simulations: pure H2 jet

instantaneous snapshots



Static pressure

OH radical (red) and vorticity field

H_2 field

H_2O field

Static temperature

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LES simulations: pure H2 jet

combustion η_c and mixing η_m efficiencies

$$\eta_m(x) = \frac{\dot{m_{mix}}}{\dot{m_Z}}$$

$$\dot{m_{mix}} = \int\int \frac{Z}{max(\phi,1)}\overline{\rho}\widetilde{u}dS_x$$

$$\dot{m_Z} = \int\int Z\overline{\rho}\widetilde{u}dS_x$$

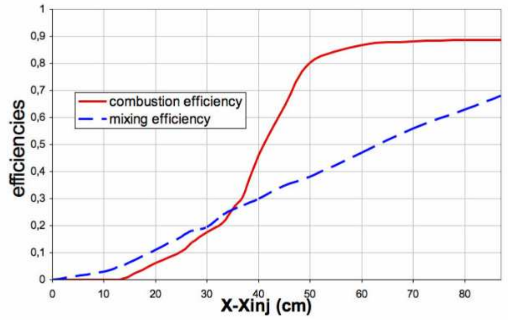
$$\phi = \frac{Z}{1-Z}\frac{1-Z_{st}}{Z_{st}}$$

$$Z_{st} = \frac{1}{1+r}$$

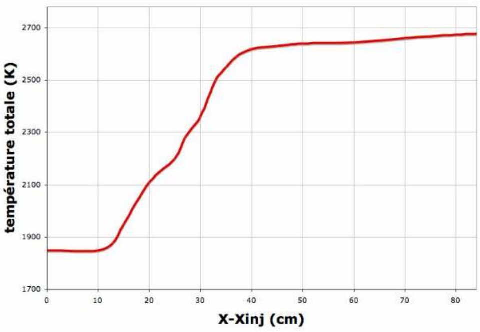
$$Z = \frac{Y_{N_2}^{air} - Y_{N_2}}{Y_{N_2}^{air}}$$

$$\eta_c(x) = 1 - \frac{\dot{m_f}}{\dot{m_{mix}}}$$

$$\dot{m_f} = \int\int \widetilde{Y}_{fuel}\overline{\rho}\widetilde{u}dS_x$$

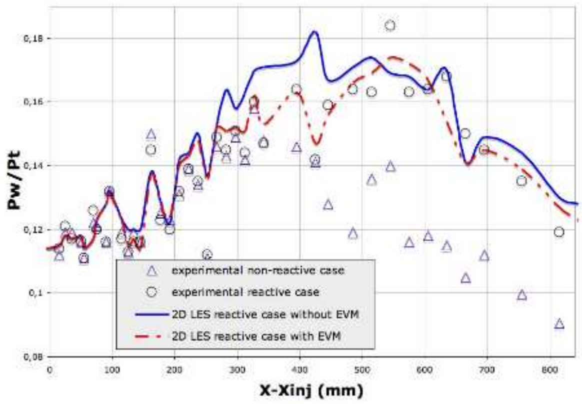


: Mixing and combustion efficiencies. Axial distributions for pure hydrogen



Maximal total temperature, axial distribution along the combustor for the pure hydrogen

LES simulations: CH_4/H_2 mixture jet



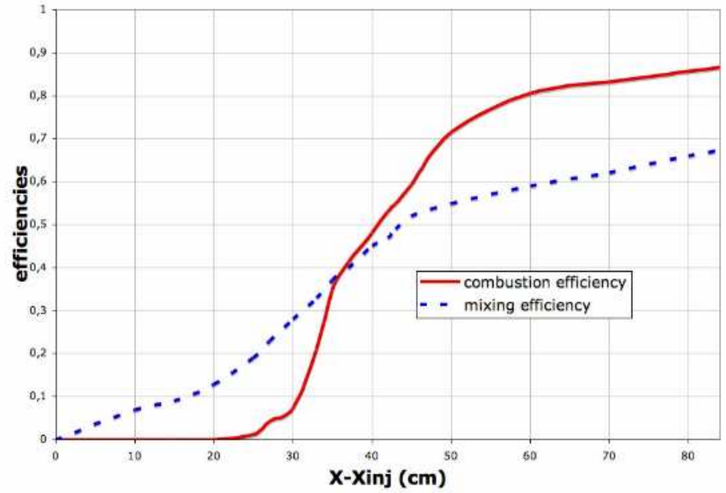
Normalized mean wall pressure distributions along the combustor for methane-hydrogen mixture injection

Self-ignition lengths:

- 33 cm in the experiment
- 33 cm with EVM
- 25 cm without EVM

LES without EVM overestimates the pressure rise due to heat release in the region 25 cm <$(x-x_{inj})/d$< 50 cm

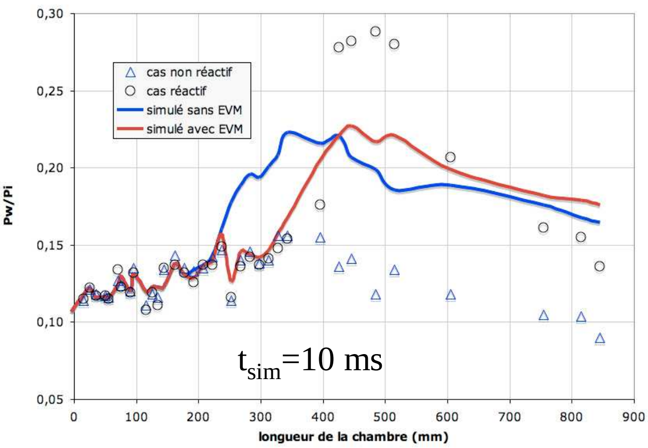
LES simulations: CH_4/H_2 mixture jet



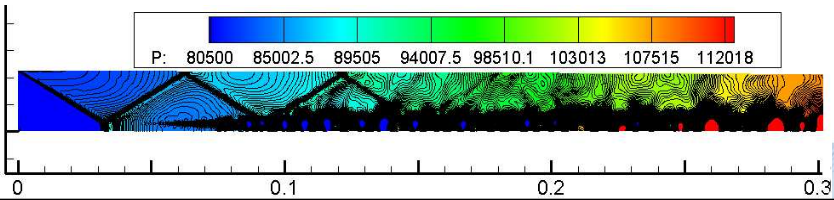
Mixing and combustion efficiencies. Axial distributions for methane-hydrogen mixture

LES simulations: C_2H_4/H_2 mixture jet

wall-pressure profiles



- Pressure levels are in both cases under-estimated
- EVM gives better self-ignition delay
- Simulation time might be too short
- 1D analysis shows to possibility of thermal shocking (heat release greater than the critical value)
- LES is too expensive, RANS will be used to study the thermal shocking regime



URANS simulations of abrupt self-ignition mode: C_2H_4/H_2 mixture

50% C2H4 / 50% H2 mixture fuel jet
mass rate: 16.2 (C2H4) g/s + 1.2 (H2) g/s

One-dimensional analysis of the flow Thermal shocking investigation (1/2)

• Advantage to be “easy”, cheap & gives good information on crucial parameters of the flow. Takes into account the skin friction & heat losses of

$$\frac{dP}{P} = \frac{-\gamma M^2}{1-M^2}\left(\frac{-dS}{S} + 2\xi\frac{dx}{D_h} + \frac{1}{C_pT}(dQ + h.dS(T_w - T))\right) \quad (1)$$

$$\frac{dT}{T} = \frac{1}{1-M^2}\left((\gamma-1)M^2\frac{dS}{S} + 2\xi(1-\gamma)M^2\frac{dx}{D_h} + \frac{1-\gamma M^2}{C_pT}(dQ + h.dS(T_w - T))\right) \quad (2)$$

$$\frac{dM}{M} = \frac{1}{1-M^2}\left((-1+\frac{1-\gamma}{2})M^2\frac{dS}{S} + \xi(1+\gamma)M^2\frac{dx}{D_h} + \frac{1+\gamma M^2}{2C_pT}(dQ + h.dS(T_w - T))\right) \quad (3)$$

where P is the static pressure, T the static temperature, T_w the wall temperature, M the Mach number, D_h the hydraulic diameter , ξ the skin friction coefficient, h the heat transfer coefficient, and Q the integral heat release from the injection point to the position x.

$\tilde{Q}_{cr} = 0.50$

• Critical value for heat release in the test tube

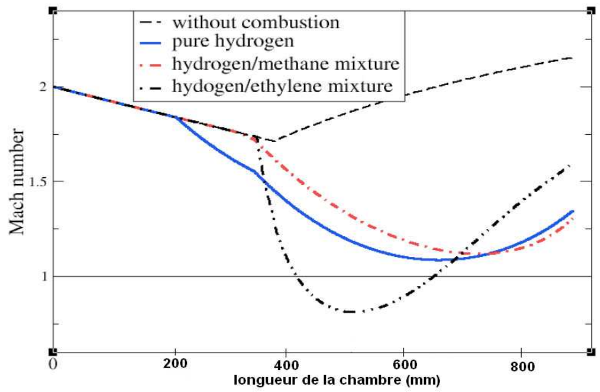
$$\tilde{Q} = \left(1 - \frac{1}{{M_{a0}}^2}\right)^2 \frac{{M_{a0}}^2}{2(1+\gamma)}$$

• pure hydrogen = 0.47

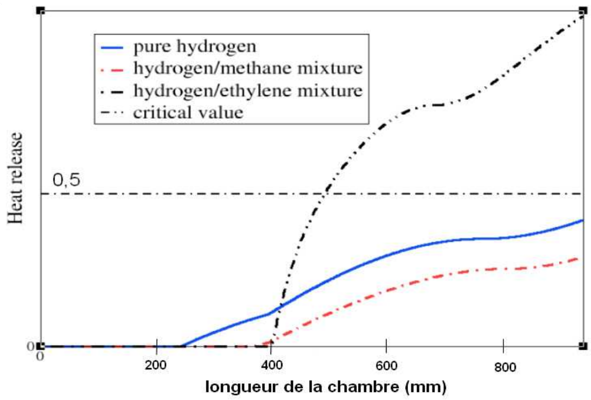
• methane/hydrogen mixture = 0.43

• ethylene/hydrogen = 0.58

One-dimensional analysis of the flow
Thermal shocking investigation (2/2)



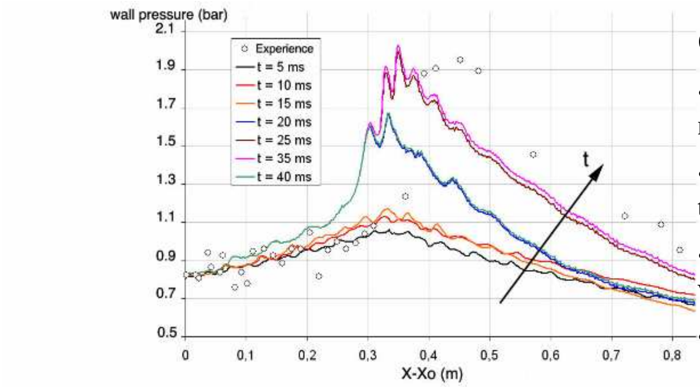
Mach number distribution



Heat release distribution

- **The ethylene/hydrogen mixture is able to be "thermal shocked"**
- **Thermal choking could explain the different modes of combustion**
- **RANS approach is chosen for this study of thermal shocking regime**

URANS simulation results (1/4)



Observations:

• Self-ignition is premature that explained by neglecting turbulence-chemistry interaction

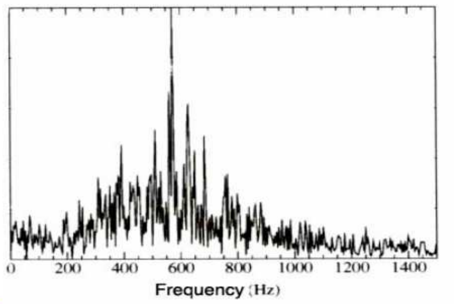
• Transient period from initial state lasts a long time –35 ms (35 residence time)

• Maximum pressure rise is in good agreement with experiments

• Pressure is essentially non-steady

Mean wall pressure distributions for different instants, arrow points in the direction of the time evolution

Pressure FFT



Power spectral density of pressure for thermal choking

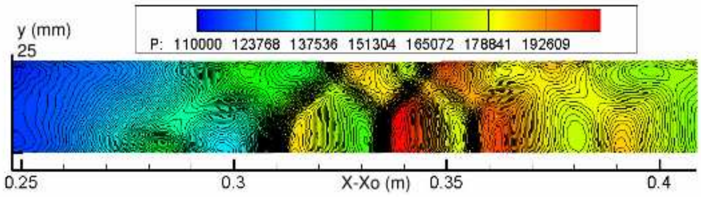
• Pressure waves moves upstream and downstream with amplitude about 3 cm, and 4.2 bar amplitude

• Power pressure spectrum has the peak of 580 Hz (1.72 ms oscillation period)

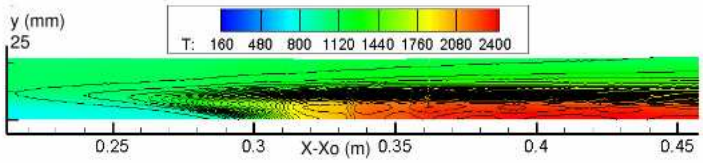
URANS simulation results (2/4)

Instantaneous pressure ant static temperature snapshots

Unsteady behaviour of self-ignition (heat release in the duct). Mach structures are observed



Instantaneous snapshot of mean pressure field in the combustor



Instantaneous snapshot of static temperature field with *OH* radical field (black lines)

Observations:

•Unsteady behaviour of self-ignition (heat release in the duct)

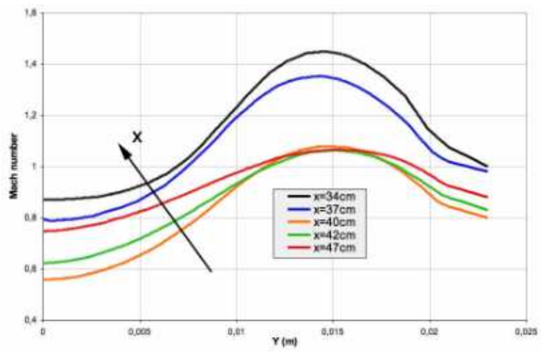
•Bifurcated shocks (Mach structure)

• Shock train region is formed in which pressure build-up develops

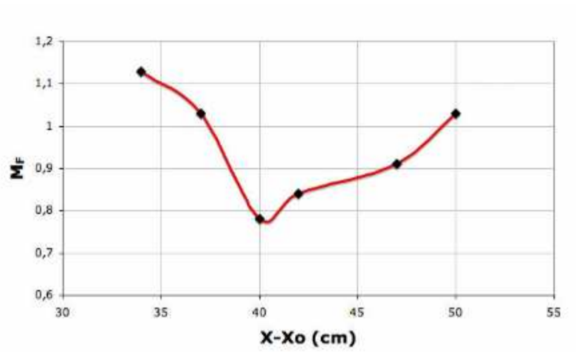
• The formation of OH starts at $(x\text{-}x_o) \approx 21$ cm

URANS simulation results (3/4)

Axial evolution of velocity profiles in transonic zone



Transversal Mach number profiles in the transonic zone, arrow points in the direction of *x* rise



Cross-area mean Mach number axial distribution

$$M_F^{-2}(x) = \frac{1}{S(x)} \int M^{-2}(y)dS$$

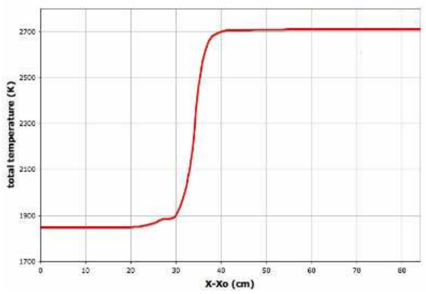
where $S(x)$ cross-area section at location x.

Observations:

• Mean Mach number M_F is less than one in the domain 37.5 cm < (x-x$_o$) < 49 cm

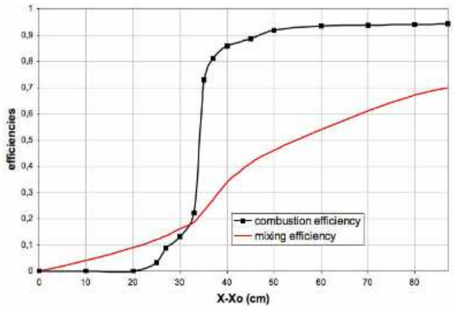
URANS simulation results (4/4)

Combustion η_c and mixing η_m efficiencies



Maximal total temperature

along the combsutor



Combustion and mixing efficiencies

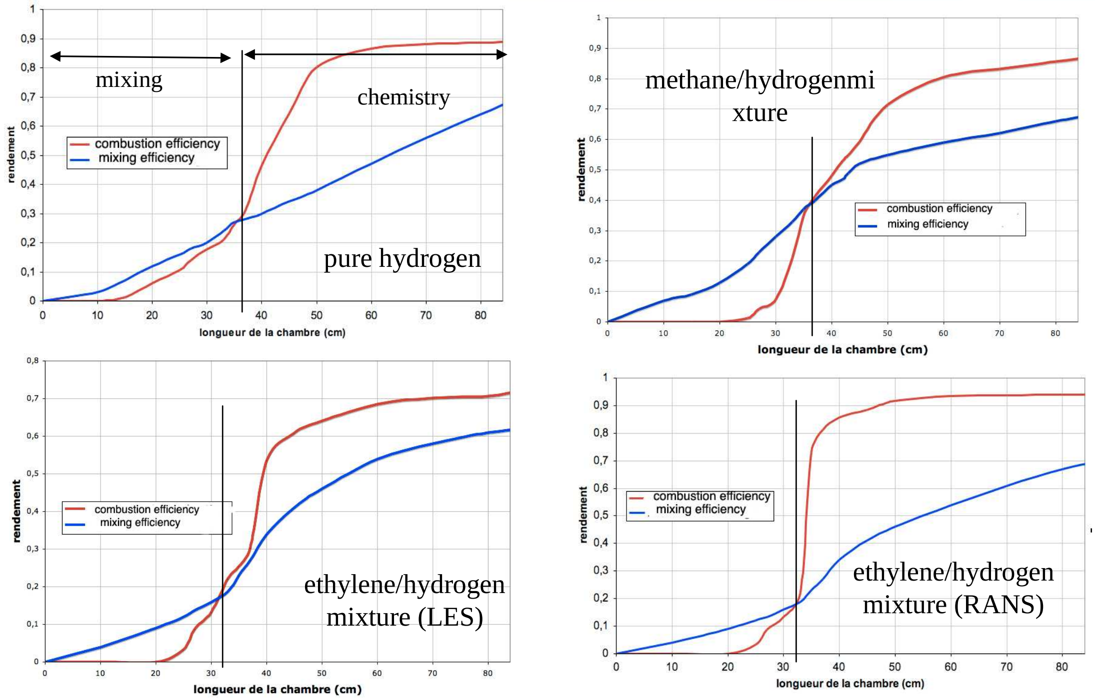
along the combustor

Observations:

• The combustion is mixing controlled

• Practically overall heat release occurs on 5 cm length

Mixing/Combustion Efficiencies



The more hydrocarbon we have, the more mixing is important for premixing followed by burning 20 cm for H_2, 10 cm for CH_4/H_2 and 6 cm for C_2H_4/H_2

Conclusions

• Self-ignition of H_2, C_2H_4/H_2 and CH_4/H_2 jets in a supersonic vitiated confined flow is studied. Two modes are found

- weak mode – thermal chocking is absent
- abrupt mode – with following thermal chocking

• Weak mode was simulated with LES

• Abrupt mode was simulated with URANS

- abrupt mode is essentially non-steady
- the flow oscillations are driven by interaction between thermal choking and upstream fuel-air mixing

• Additional study is needed to establish which mechanism between two :

- acoustic, through local subsonic zone
- pure gas dynamic, by impact of heat release fluctuations on the thermal chocking position

is in the origin of flow oscillations