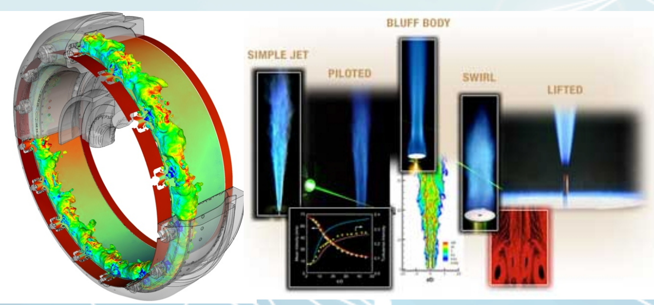
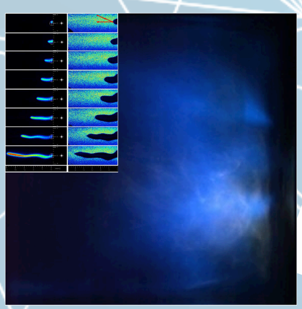
3rd Int. Workshop on Laminar Burning Velocity, Lisbon April 14, 2019

CERFACS

CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

LES of industrial turbulent reacting flows: modeling effects and challenges





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[1] CERFACS - CFD combustion team, Toulouse
[2] CNRS - IMFT, Toulouse
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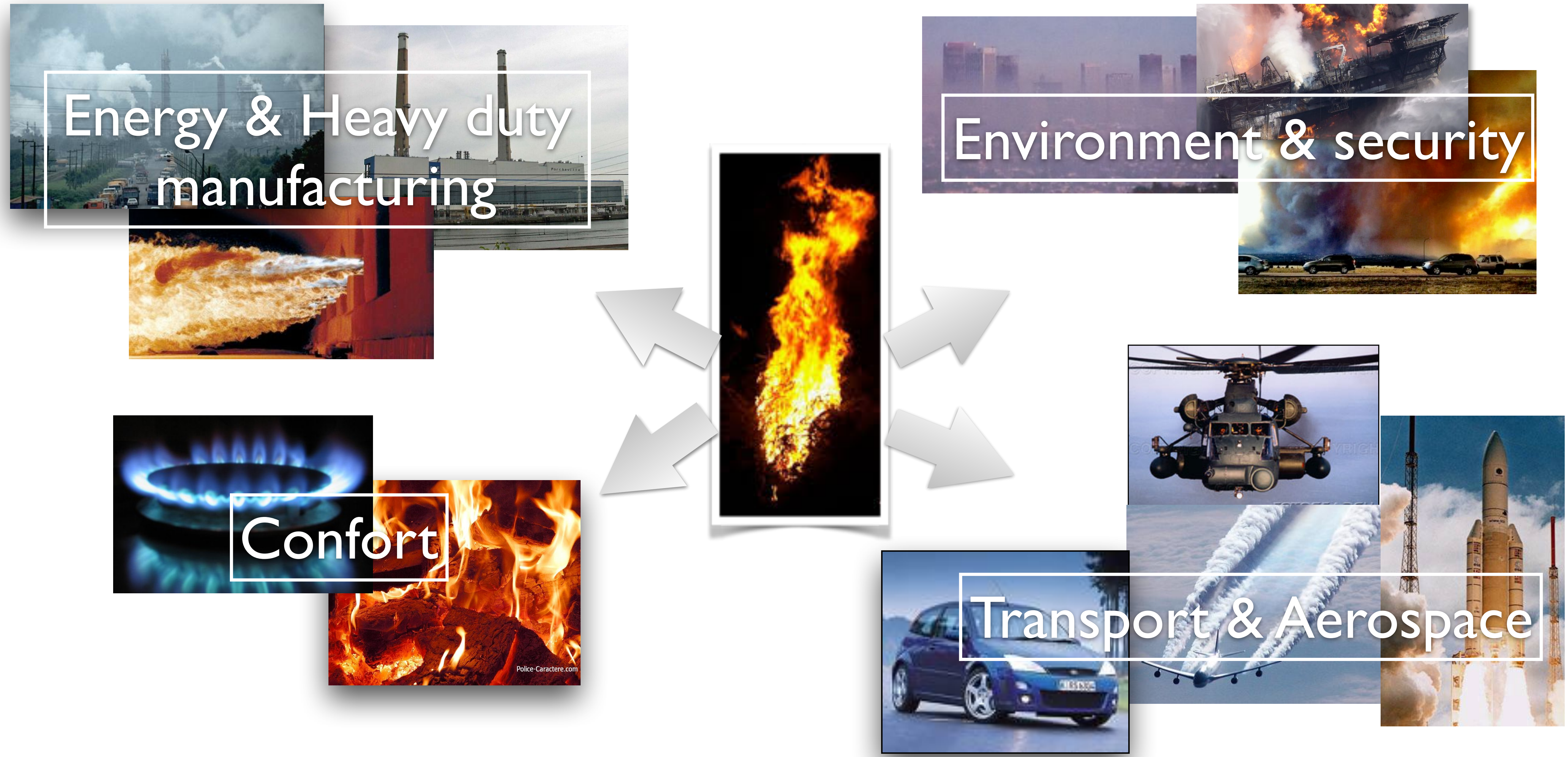
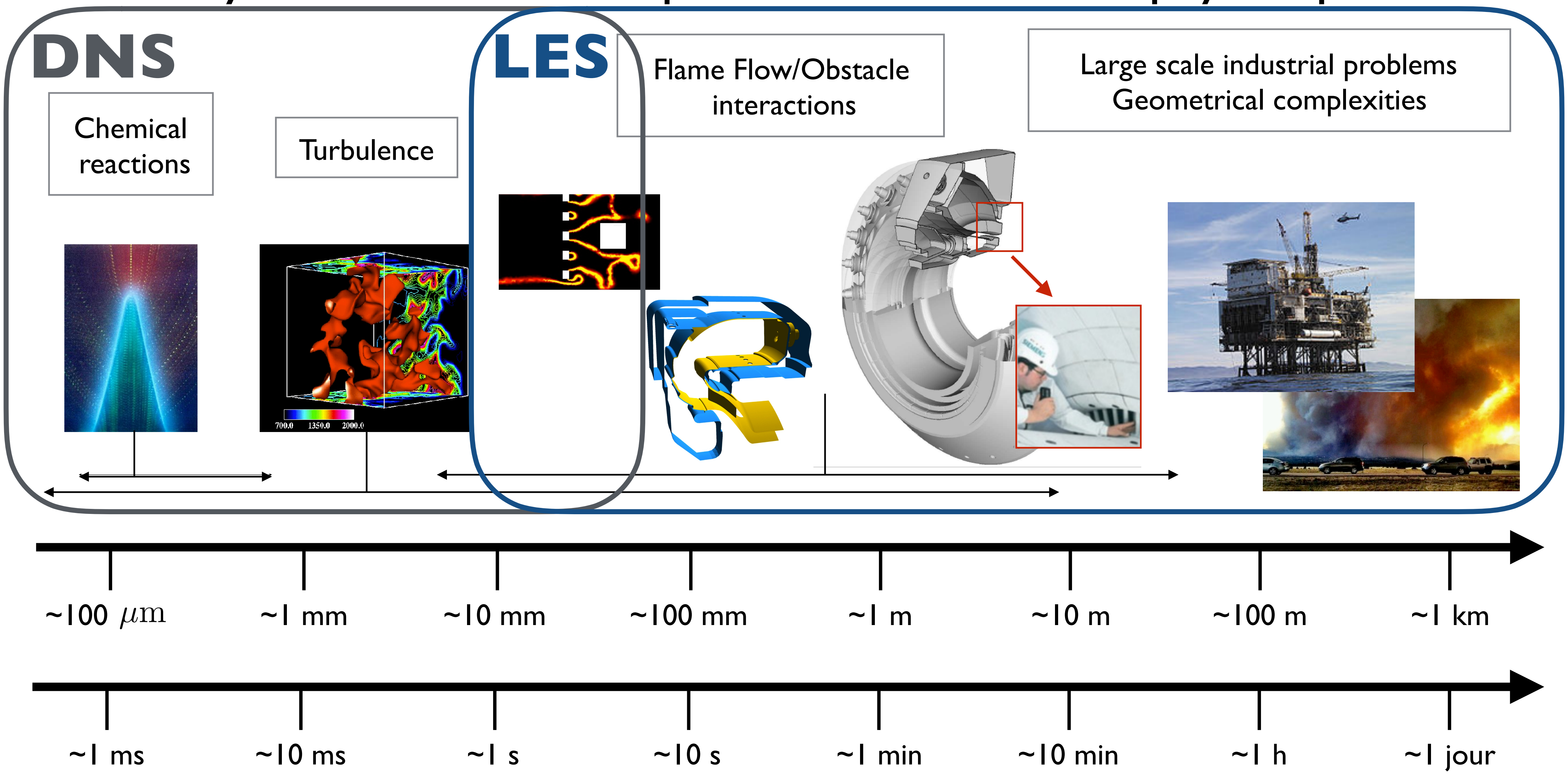
Context and Objectives of the CFD combustion team @ CERFACS

Combustion: An engineering science at the cross-road between *chemistry & fluid mechanics* with strong *technological / industrial and societal* implications



I] HPC & turbulent reacting flow CFD

Turbulent reacting flows have been from the beginning studied and theoretically addressed as true/pure multi-scale multi-physics problems:

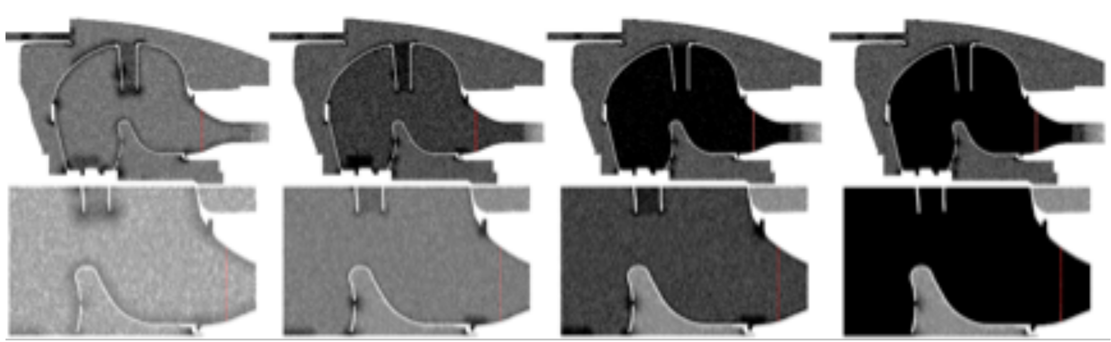


Recent industrial achievement by SAFRAN SHE

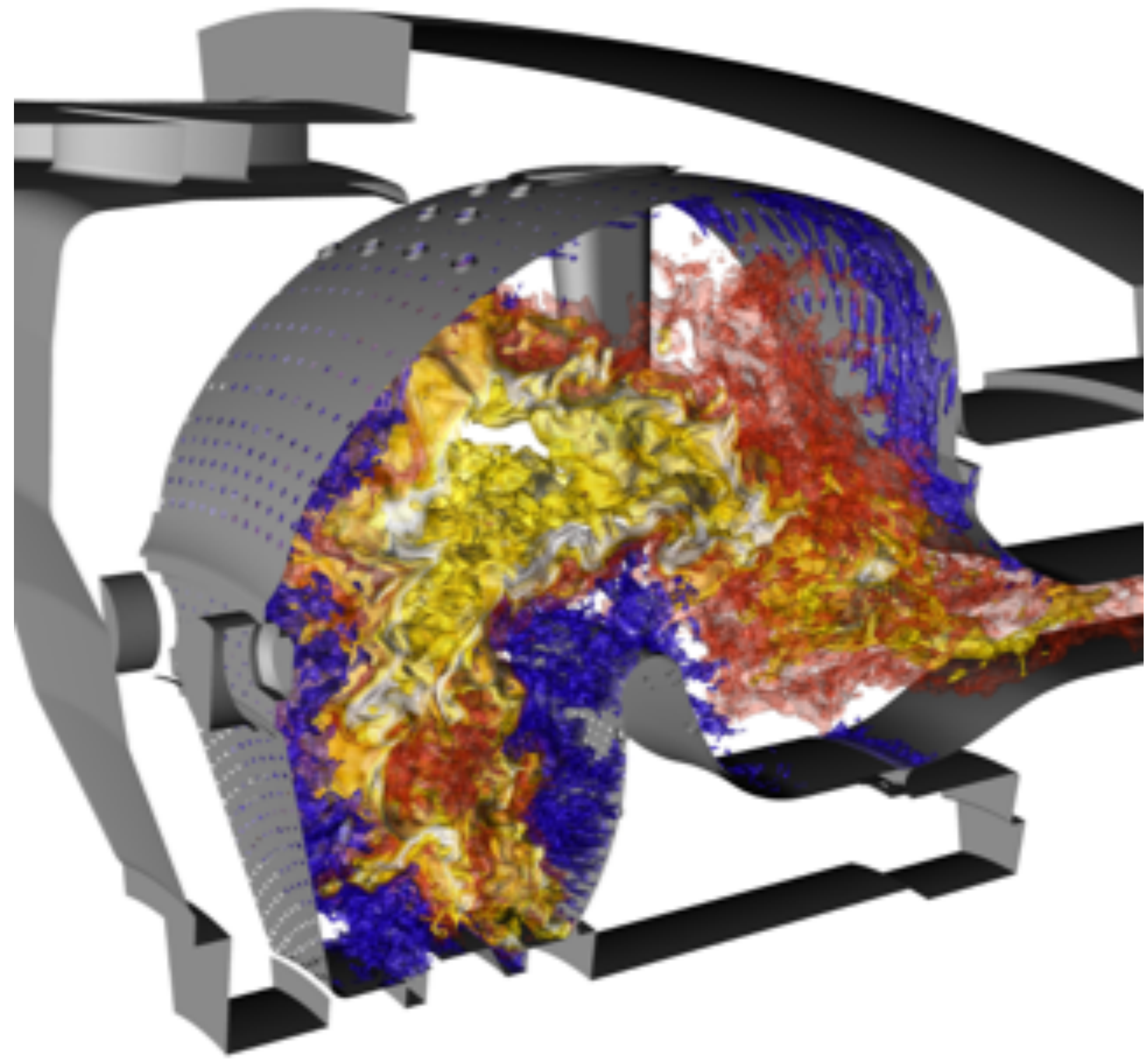
J. Lamouroux et al (SAFRAN HE) - presented at the ASME TurboExpo conference, Charlotte june 2017.

- Industrial burner with **1.1B** elements for the geometry
- Turbulent compressible, gaseous reacting LES

Selective refinement (chamber only) based on the ***Pampa*** Library using MMG3D (collaboration with *C. Lachat & C. Dobrzynski, A. Froelhy* from INRIA*)*

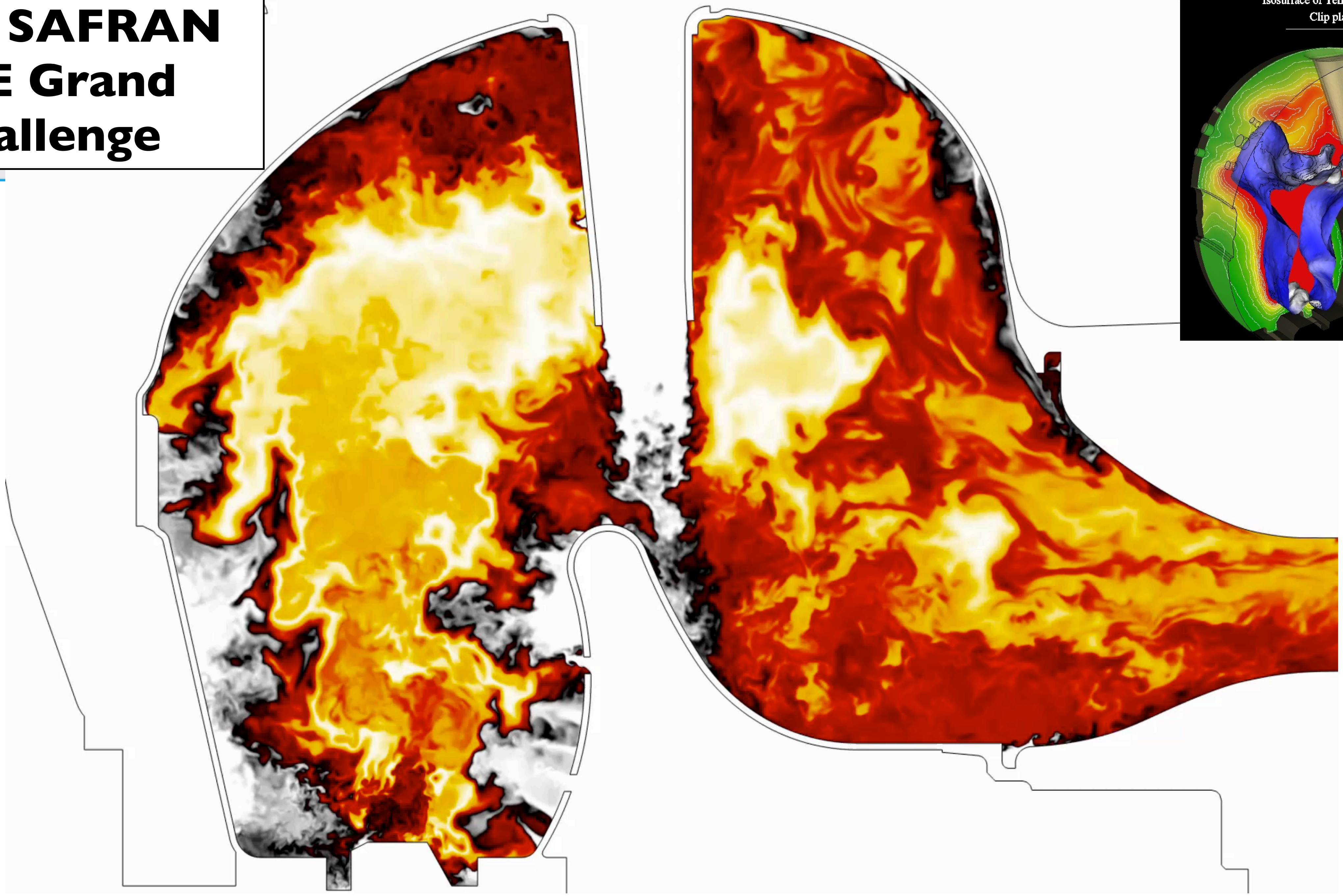


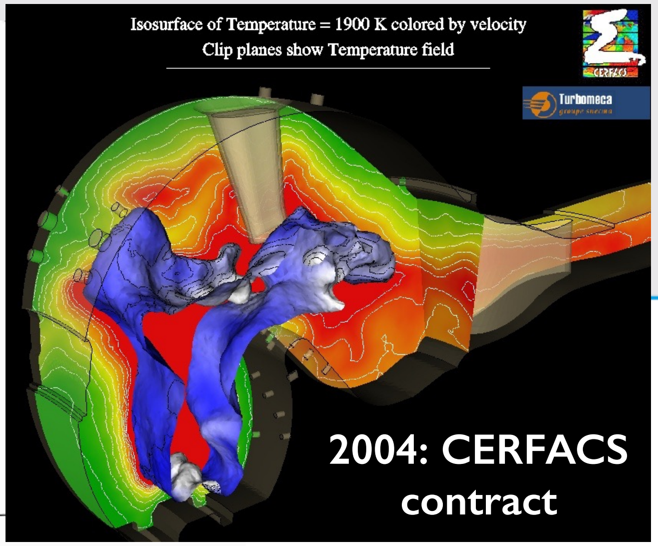
Case	# of cells	360 equiv # of cells	Δ_{cell}	$\mathscr{F}_{max}$
mesh 1	11M	220M	Δ_0	100
mesh 2	33M	660M	$\Delta_0/2$	50
mesh 3	220M	4400M	$\Delta_0/4$	25
mesh 4	1030M	20600M	$\Delta_0/7$	14



CCRT supercomputing center: COBALT grand challenges

2016: SAFRAN SHE Grand Challenge

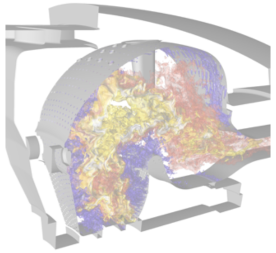




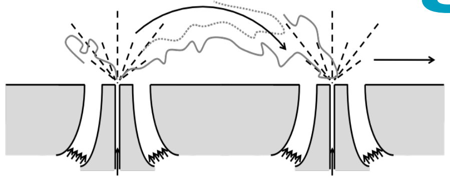
Twelve years to do:

- ~1 500 times on the number of cells and ~250 times on the number of procs
- improved reduced chemistry model *PLUS* NOx and CO (crude models)
- homogeneous vs heterogeneous multi perforated plate model
- full transfer to the industry

I] HPC & turbulent reacting flow CFD

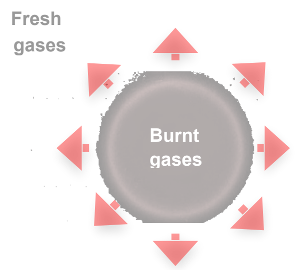


II] Ignition / transient turbulent reacting flows



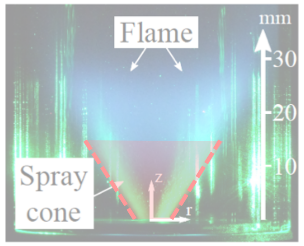
2.1 GT context: engine ignition prediction
2.2 Explosion: deflagrating fronts


Buncefield, 2005



III] Difficulty of the initial phase

IV] GT applications: emission predictions & multi phase flows



Conclusions and perspectives

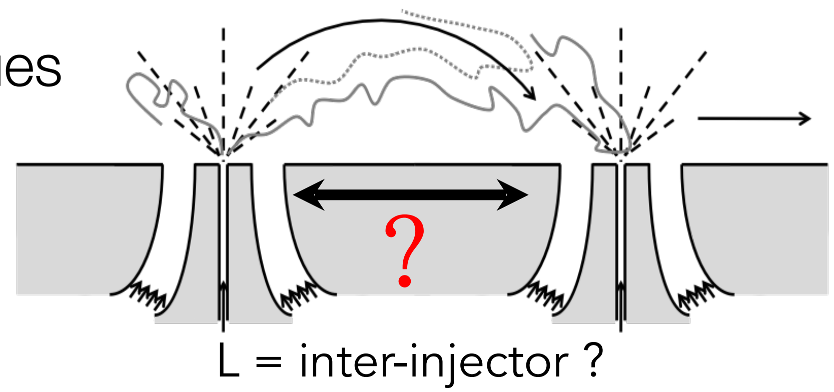
II] Ignition / transient turbulent reacting flows

Ignition = fully transient laminar/turbulent reacting flow

Aeronautical GT's:

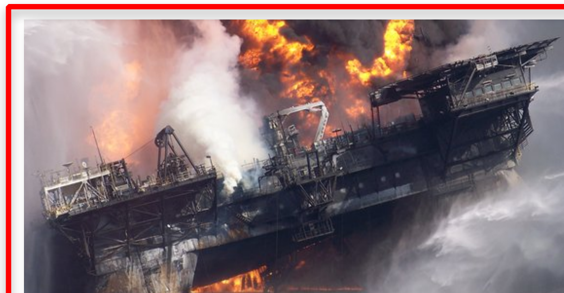
- Ignition = first design phase

  => light around time: fctt of the burner size…
- Safety issues

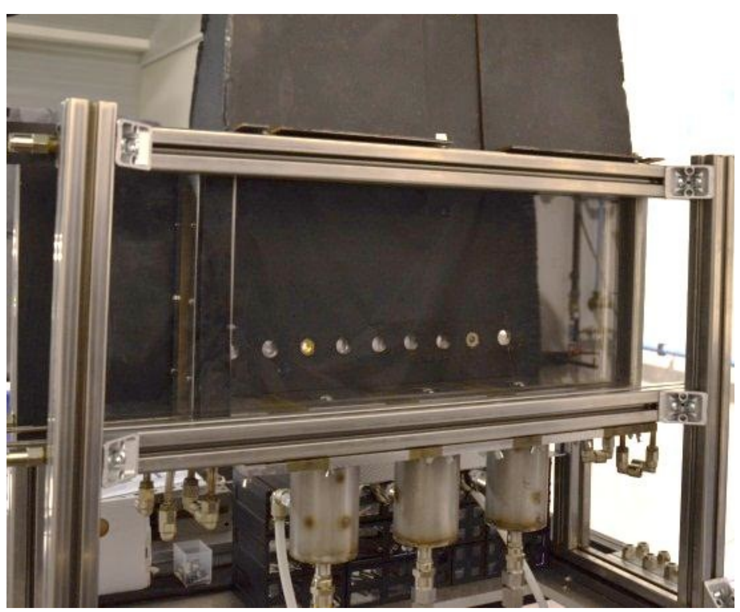


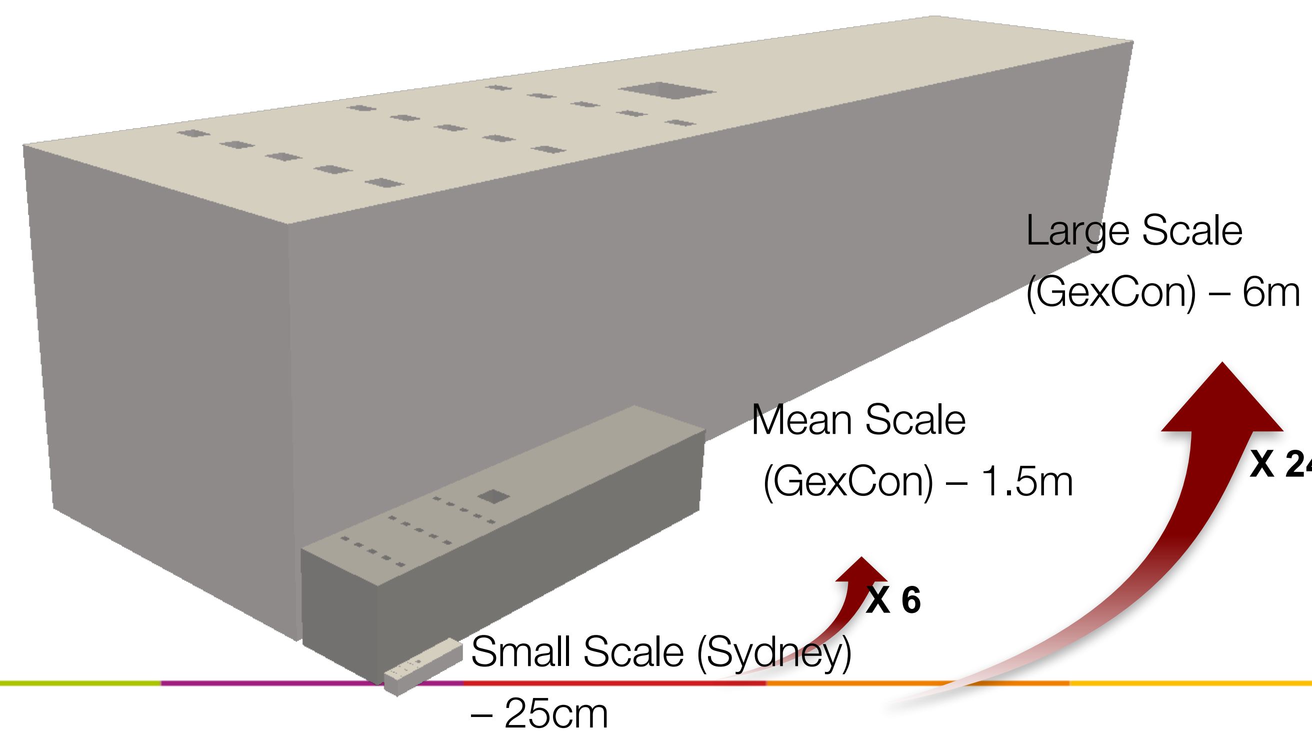
Fuel plants:

- Security issue / risk management


Deepwater horizon, 2010


Buncefield, 2005



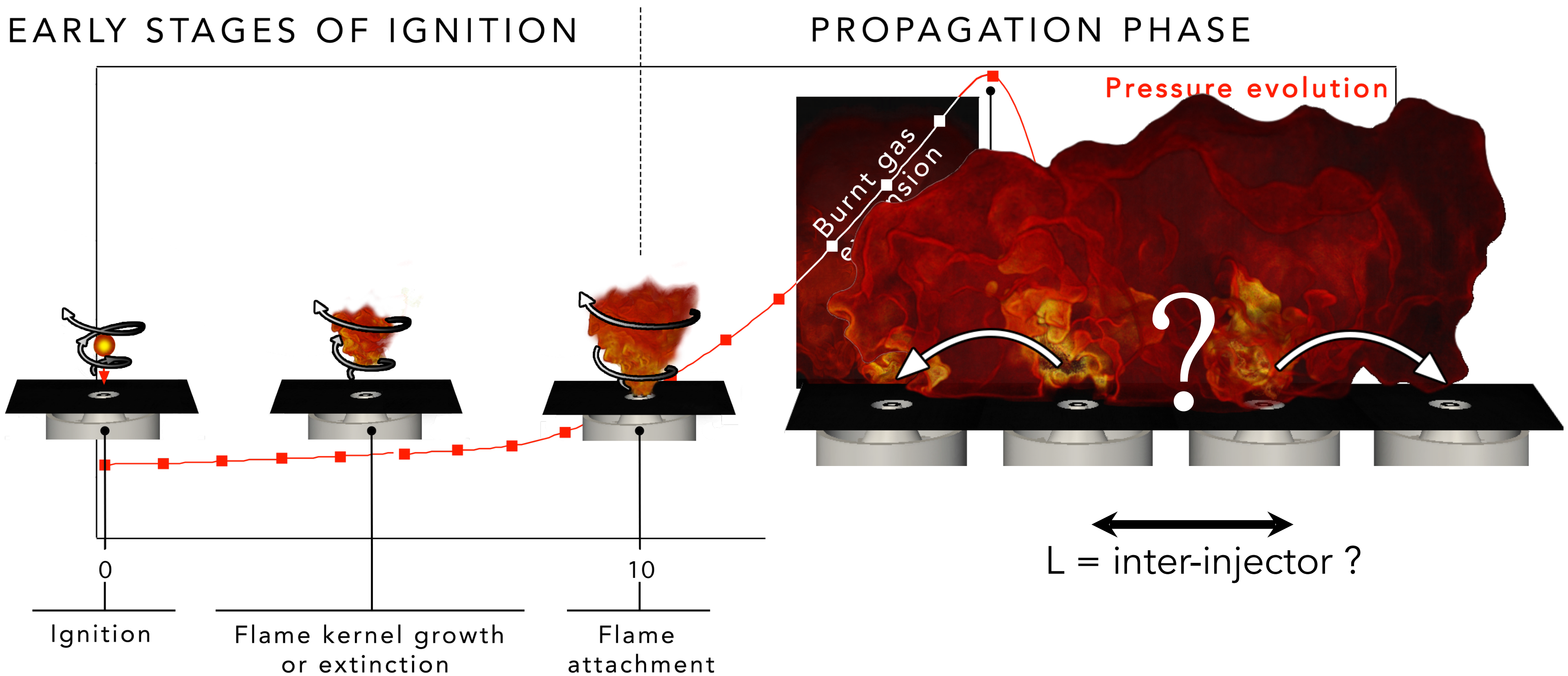


Common features & differences

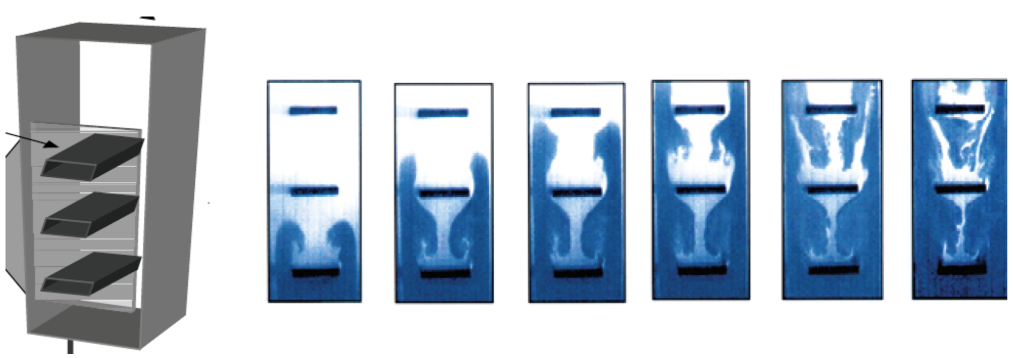
GT context

Single sector configuration

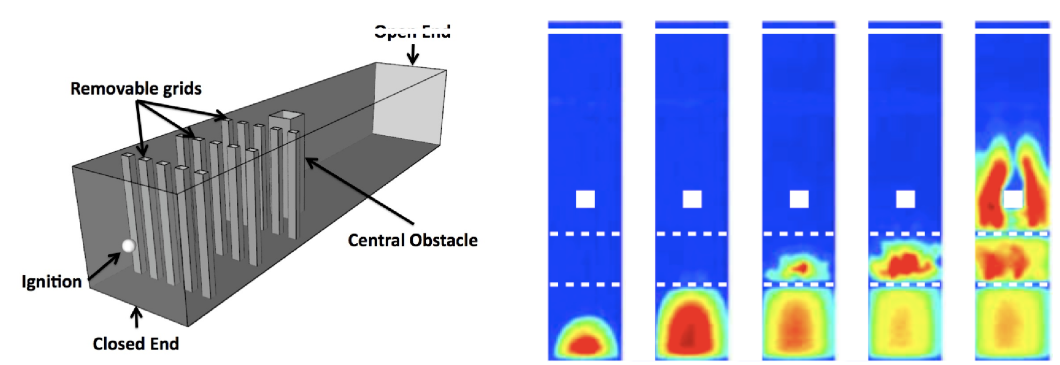
Multi sector configuration



Security



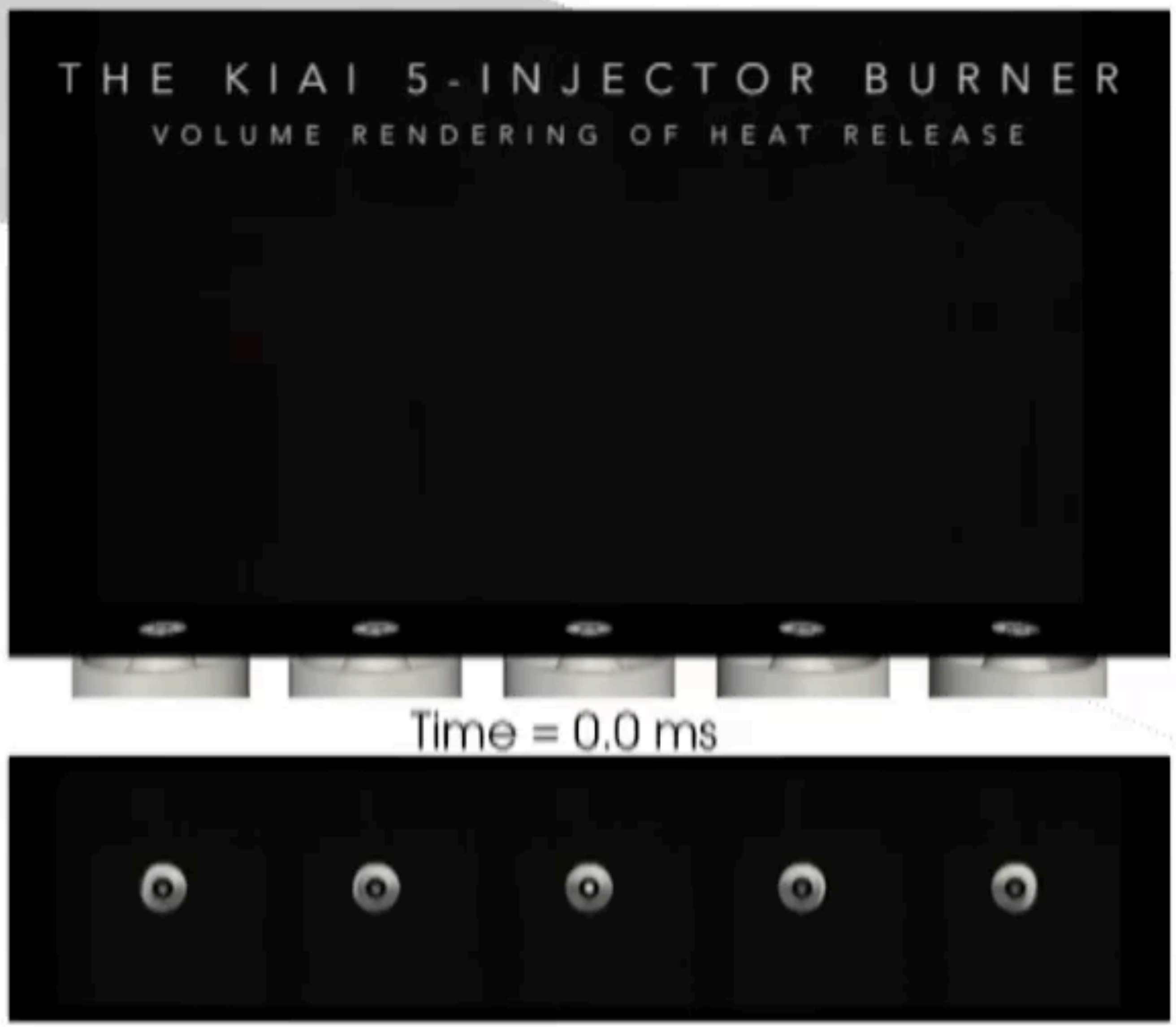
Patel, S. *et al.* *Proc. Combust. Inst. (2002)*

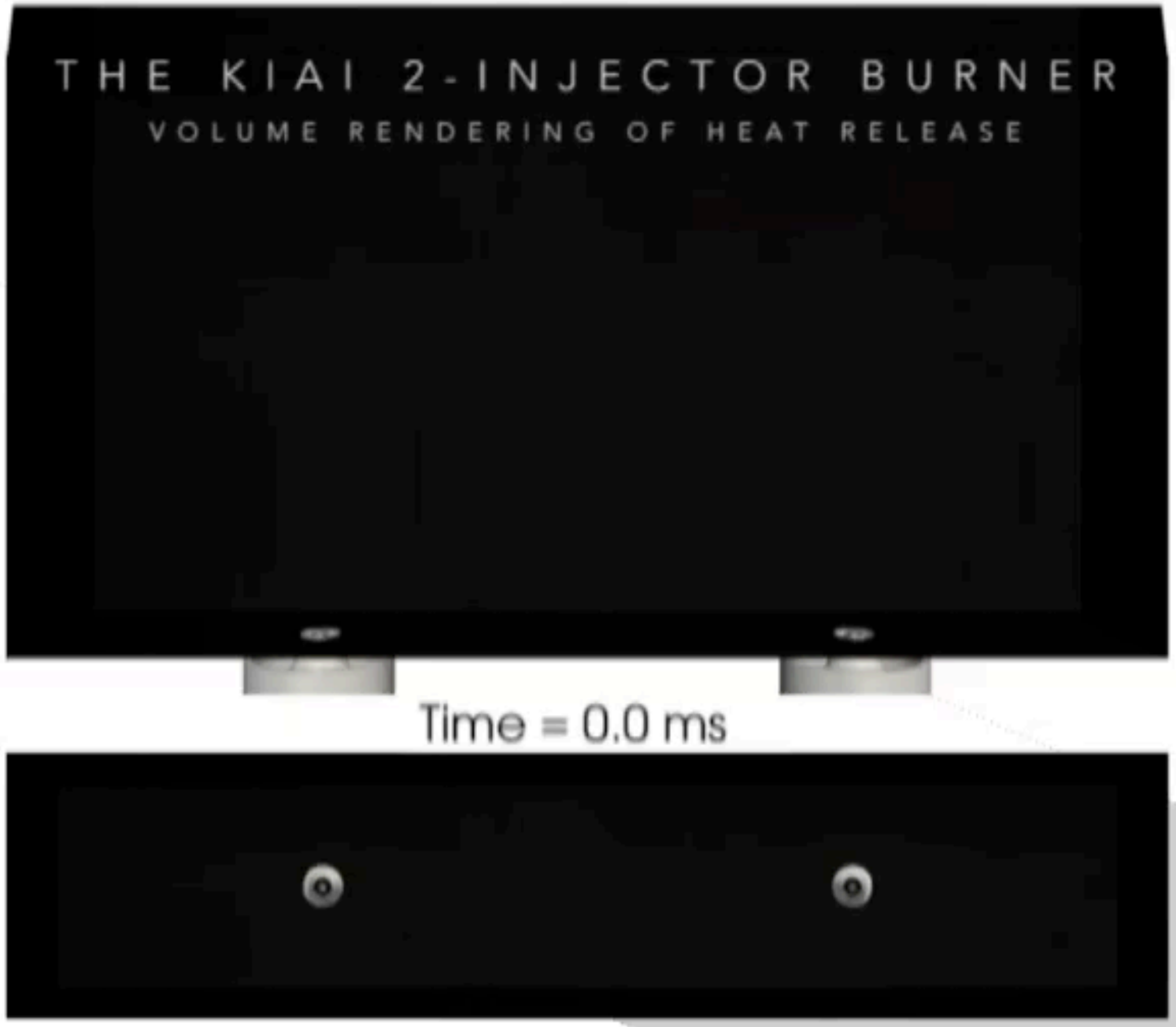


Kent, *J. et al. 5th Asia-Pacific Conf. Combust. , Adelaide, Australia (2005)*

II.1] Light-around phase - turbulent combustion dominated problem

- Low injector spacing (SP9)
- High injector spacing (SP26)

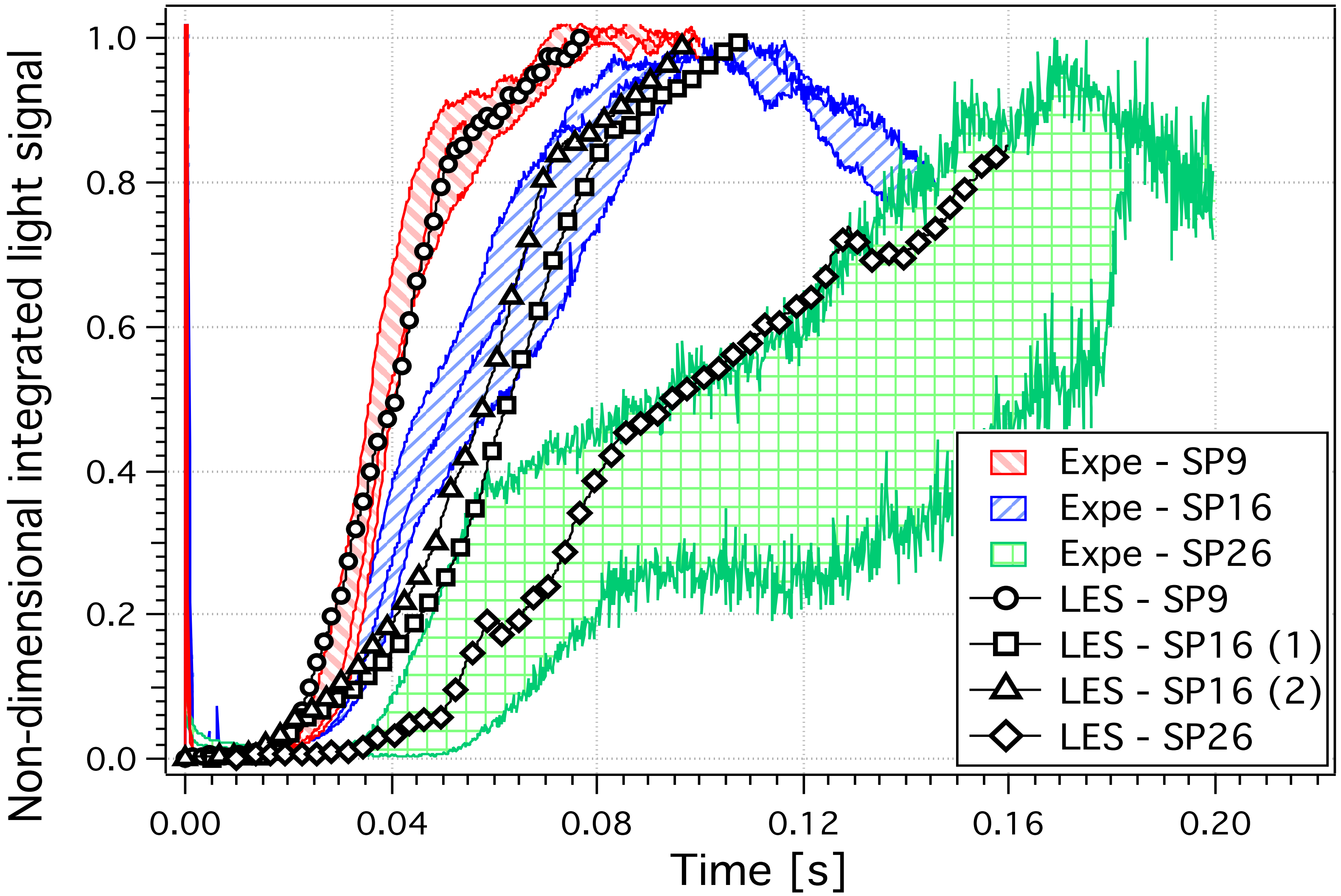




➡ Radial flame propagation

➡ Axial flame propagation

- Evolution of the luminous signal (CH emissions vs. Heat release images):

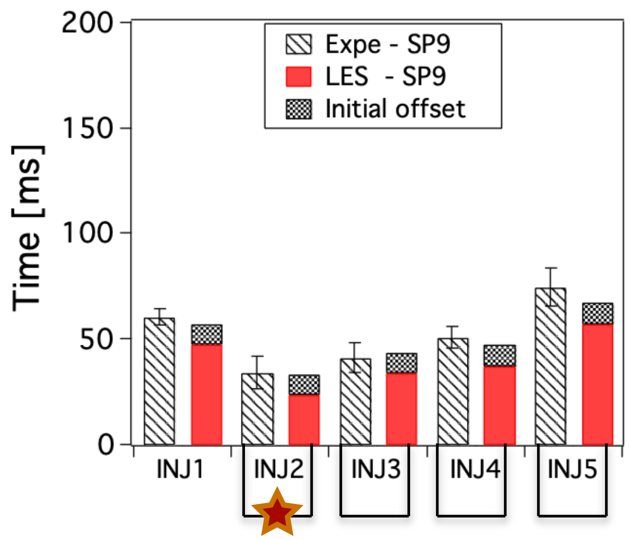


Large spacing:
- Experimental variability
- Large overall ignition time

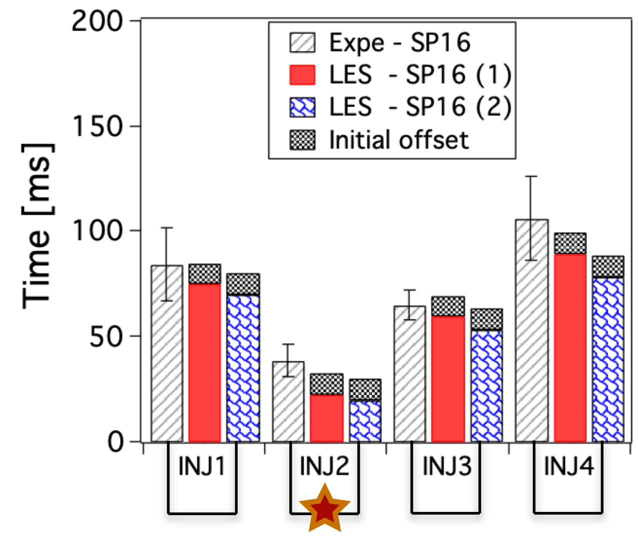
Low spacing:
- High repeatability
- Rapid ignition process

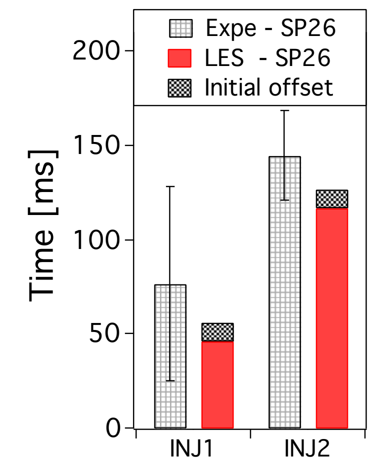
- Ignition times for each injector

SP9

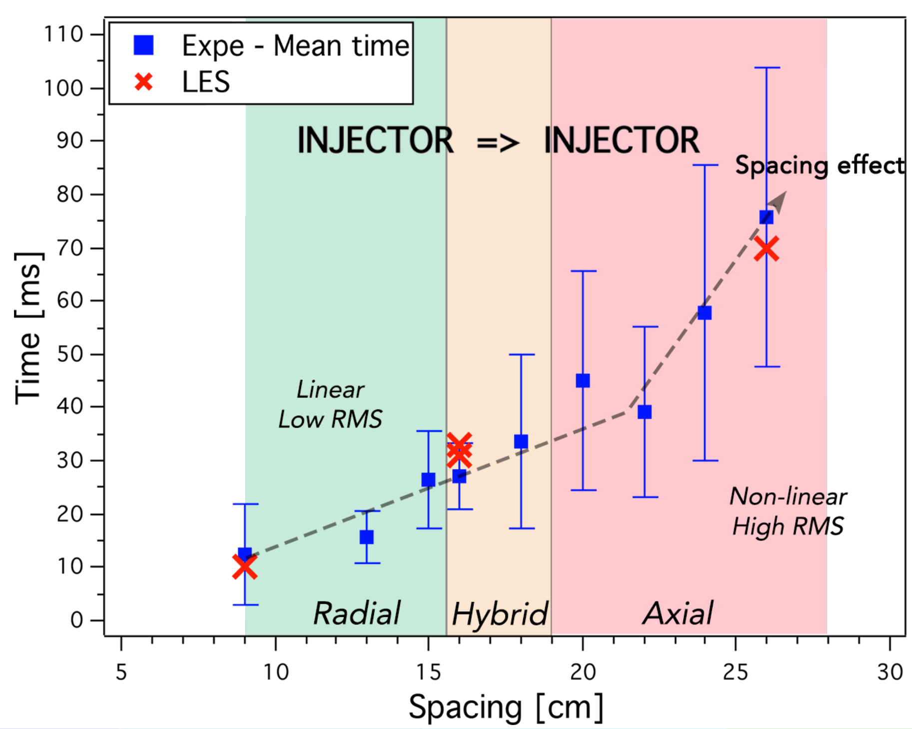


SP16





- Ignition time between two consecutive injectors



- Good estimation of the ignition times for each injectors
- 2 distinct propagation modes (inj/inj propagation times)

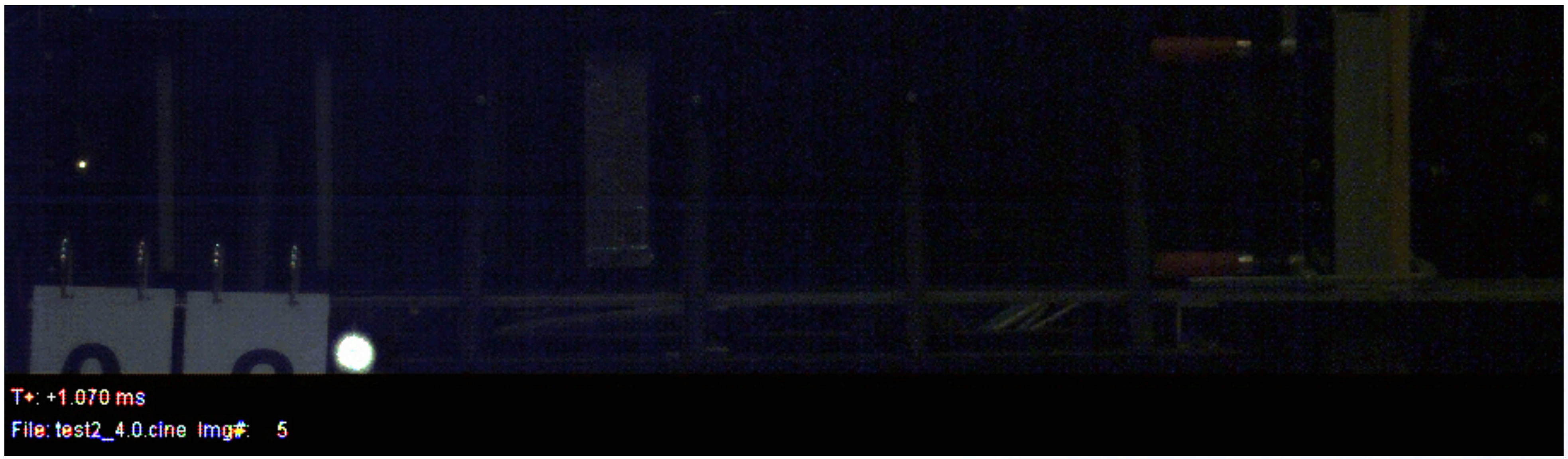
II.2] Deflagration problem - fully transient and transitioning problem

Experiments

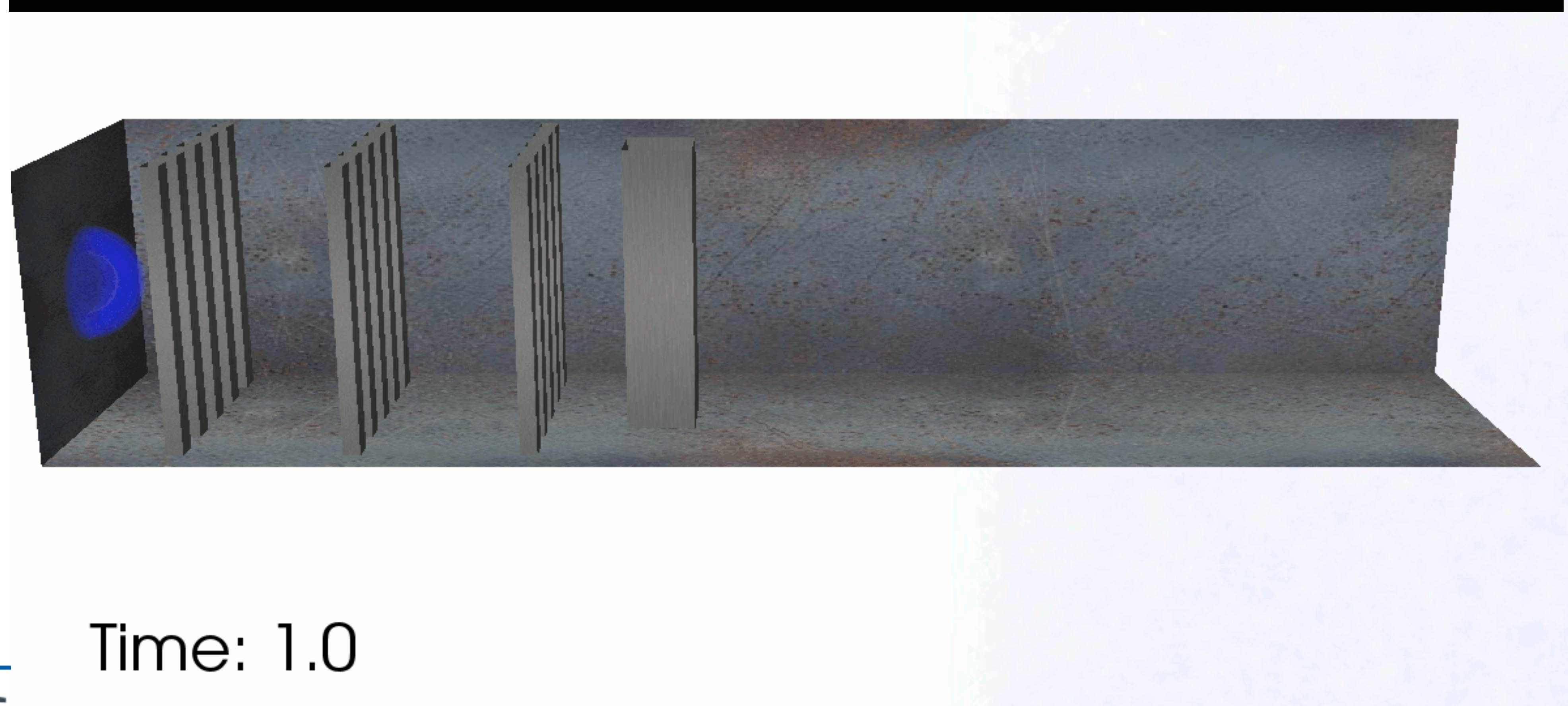
Conducted by

cmr Gexcon

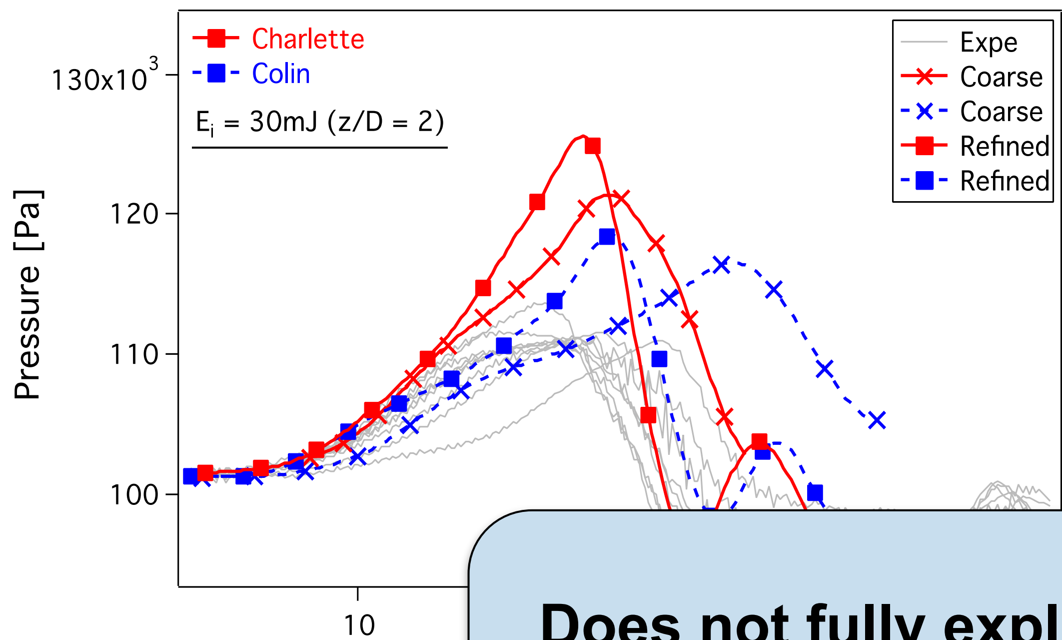
Medium scale problem: i.e L ~1.5 m



LES



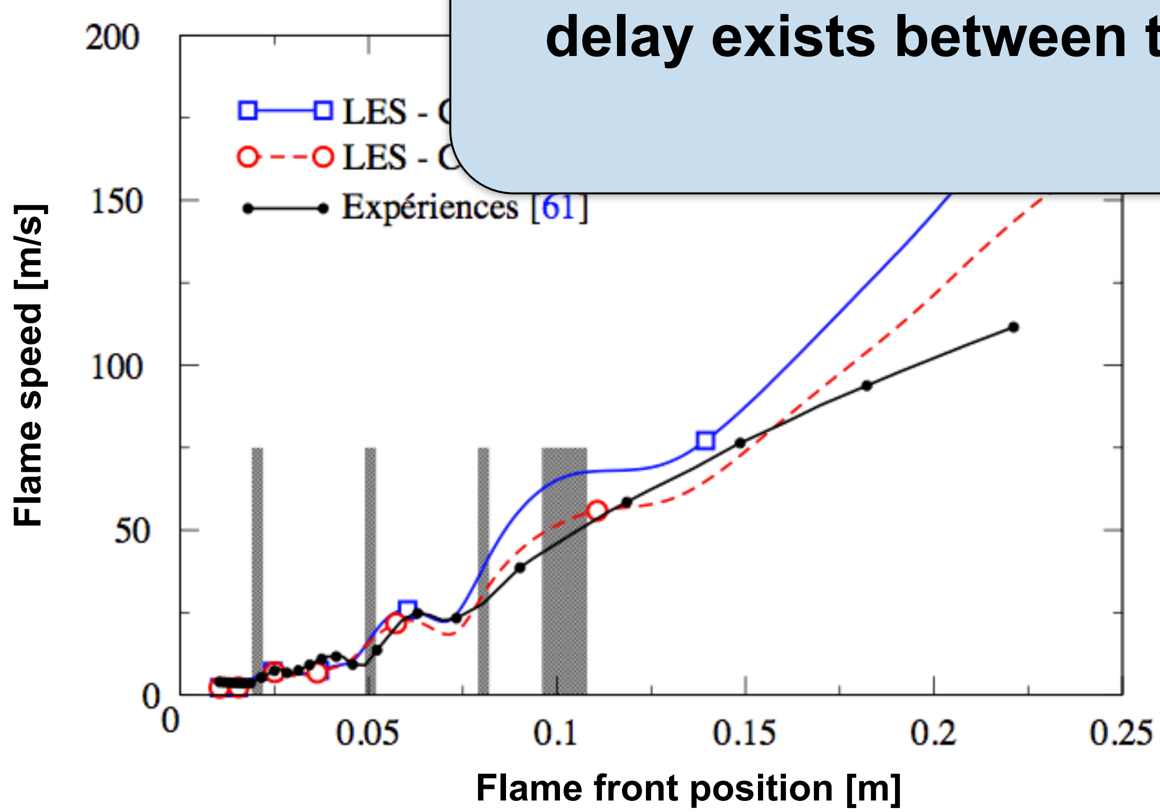
SGS modeling impact on the predictions

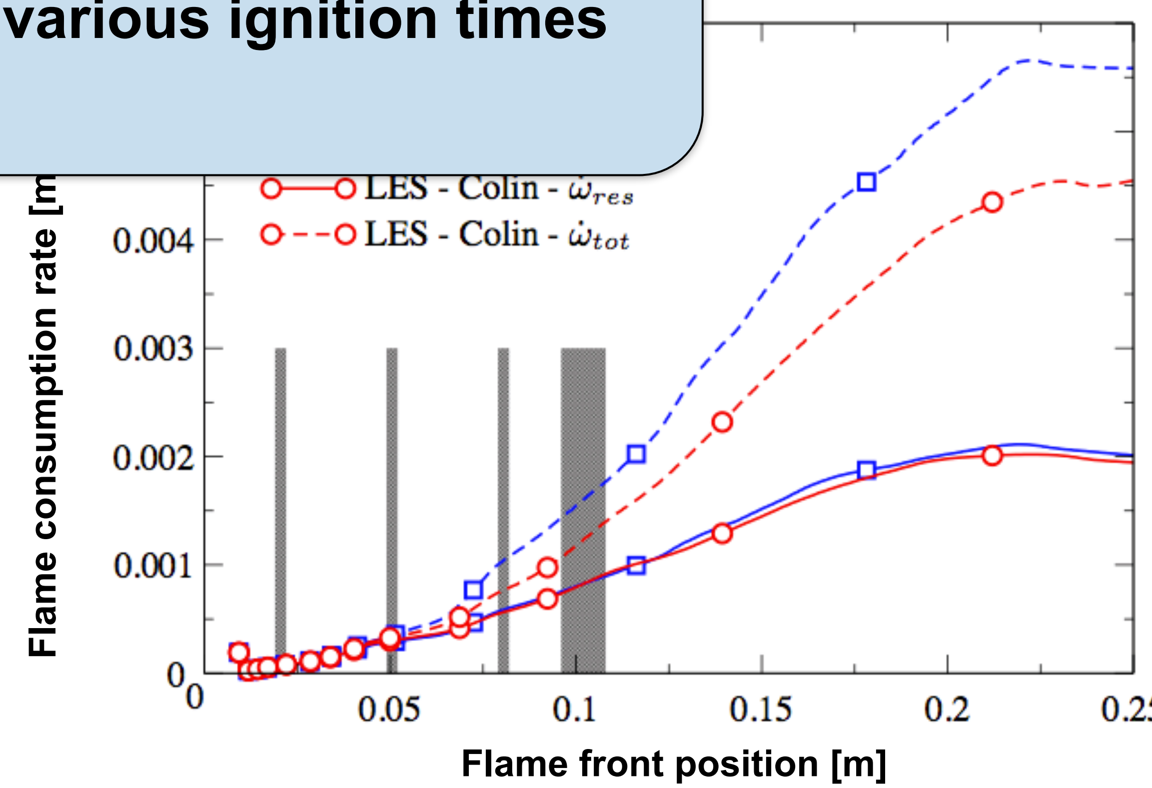


- **Reaction rate**:
  - Fixed resolved contribution regardless of the modeling
  - Modeling effectively scales the SGS contribution and thereof the net consumption rate (=> shift in time)
- Different modeling = different turbulent combustion flame speeds
- Faster combustion = higher peak pressure

⇒ High sensitivity to SGS model !!

Does not fully explain the reason why a constant delay exists between the various ignition times





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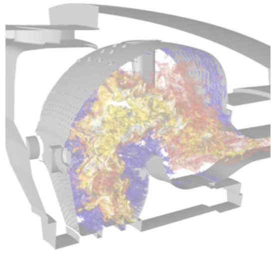

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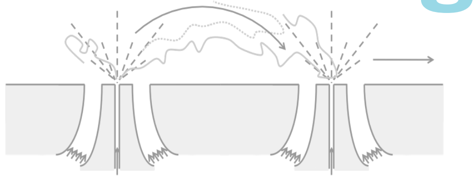

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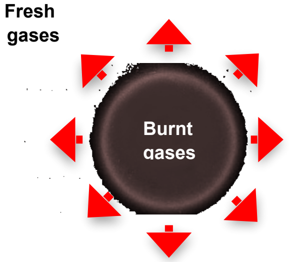
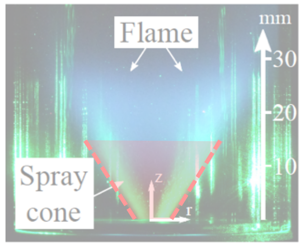


IV] GT applications: emission predictions & multi phase flows



Conclusions and perspectives

III] Initial phase issues

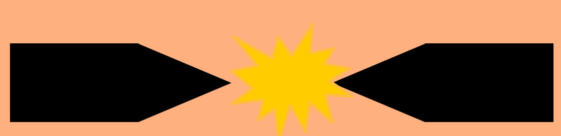
Major issues:

- it is not clear what is the initial state of these flow problems
- we do not know what and how much energy is deposited…
  - => pseudo deterministic / stochastic description
  - => difficult to know what really counts…

Very few data is available on the experimental side and most of the time it is time or spatially integrated….

IGNITION SYSTEM STUDIES

Small scale / lab-scale configuration
<1ms



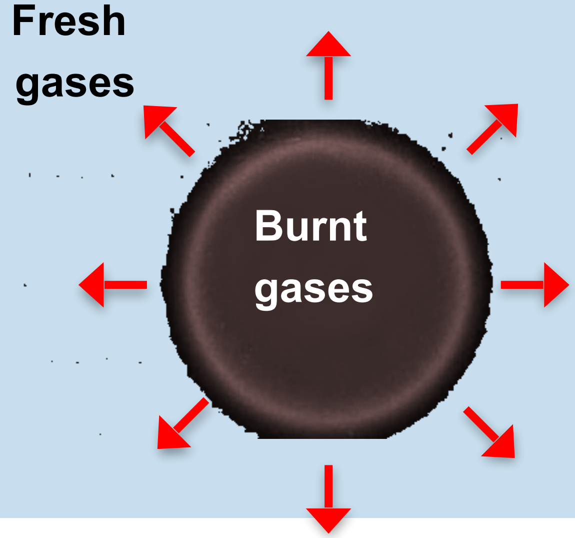
- Plasma physics
- Ignition chemistry
- Heat transfer

Input for a model initial state

IGNITION TRANSIENT STUDIES (NUMERICS / LES)

Effect of stretch on the fuel consumption speed

$$S_c = S_L^0 - \mathcal{L}_a^c \kappa$$ with $$\kappa = \frac{1}{S}\frac{\partial S}{\partial t}$$ (stretch)

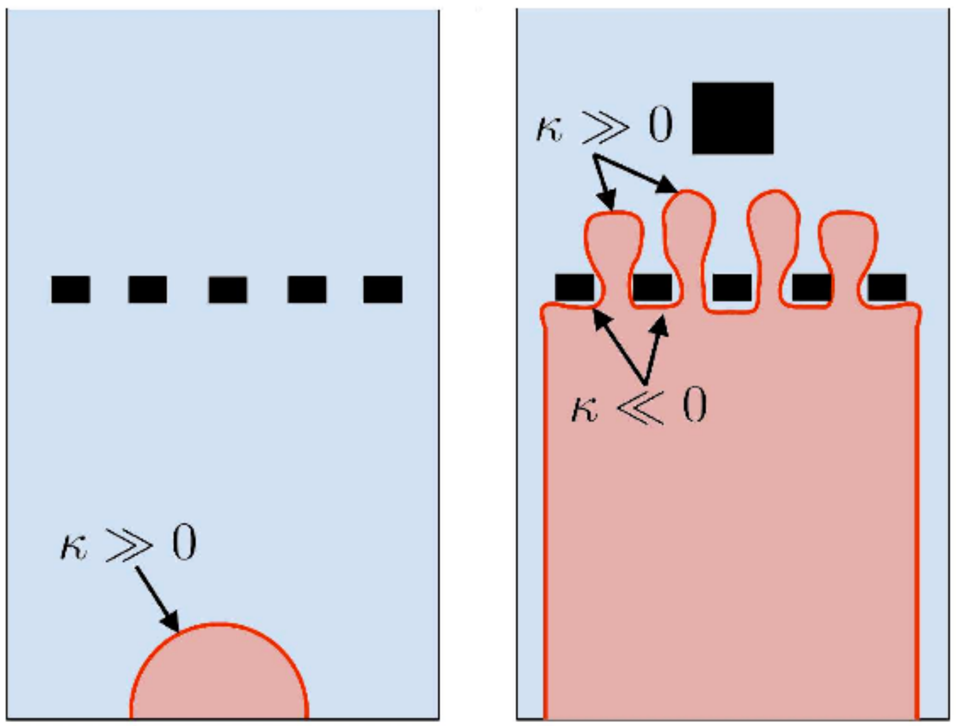


$$\mathcal{L}_a^c = \frac{1}{2}\beta\,(Le_{\text{fuel}} - 1)\,\delta_L^0$$

$$\left(\frac{T_{FG}}{T_{BG} - T_{FG}}\right)$$

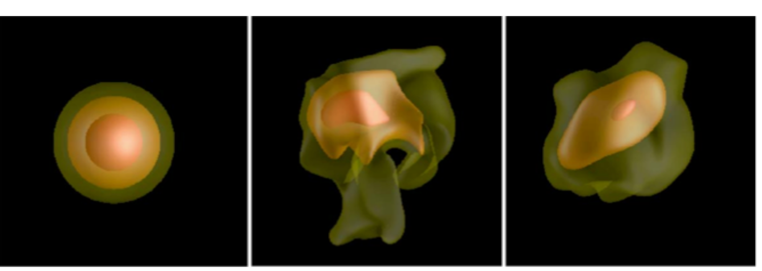
$$\int_0^{\frac{T_{BG}-T_{FG}}{T_{FG}}} \frac{ln(1+x)}{x}\,dx$$

1/ Potential importance in deflagration simulations:

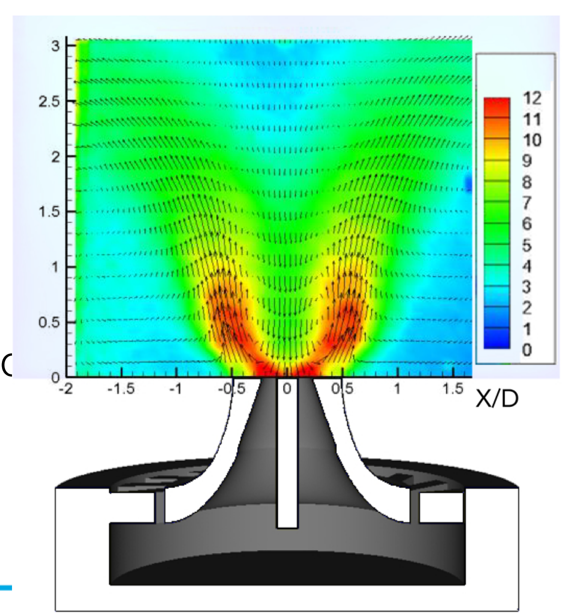


- Stretch definitely can play a role in the early Instants (always spheric and laminar)
- Thermo diffusive instabilities can appear here !!
  - $\Rightarrow$ Impact on the local transition to turbulence (?)
- Stretch is also present when the flame front reaches obstacles…

2/ Potential importance in GT simulations:



Darmstadt (Klein et al., Flow Turbulenc Combust, 2008)



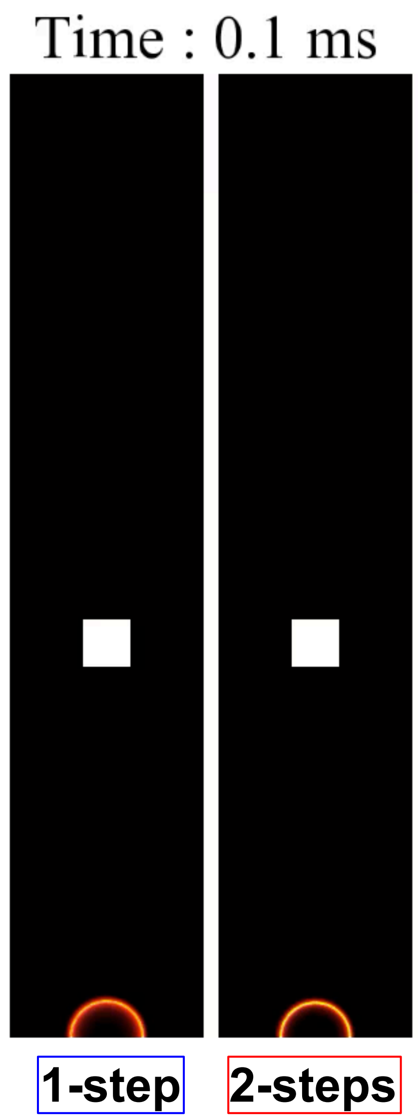
- Stretch is rapidly present and strongly impact the initial kernel behavior (quenching…)
- As the flame propagates in the turbulent flow, it faces very different turbulent flow states…

Thermo-chemical model and its impact

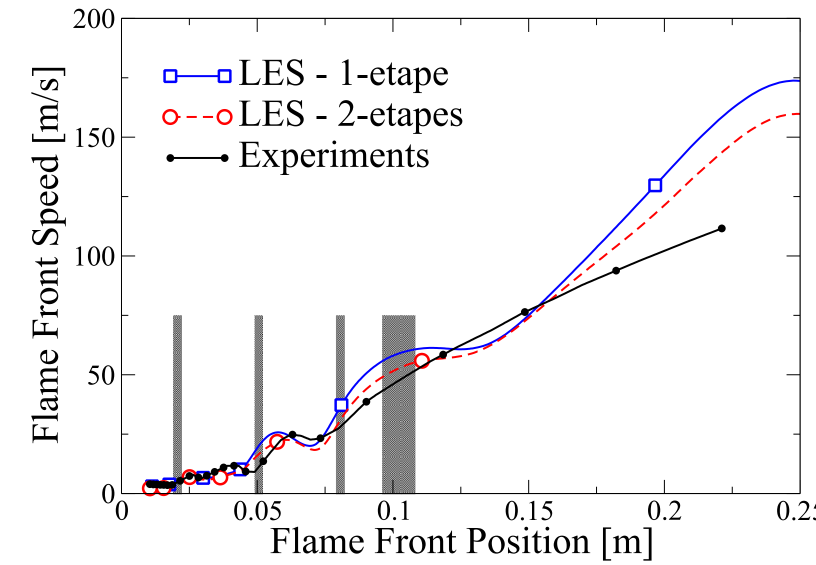
Flame propagation: C3H8, 0 array

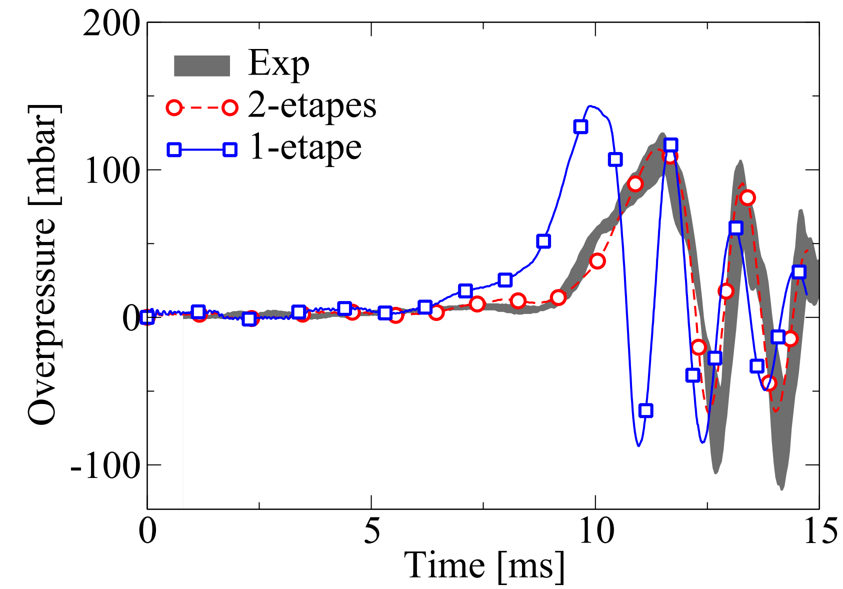
φ =1	S_L^0	T_{ad}
GRI-MECH	38.4 cm/s	2275 K
2-steps	38.4 cm/s	2289 K
1-step	38.4 cm/s	2400 K

- ϕ =1 : same laminar flame speed
- 1-step adiab. Temp. overestimated by 5%
  $\Rightarrow$ $S_d = \rho_{GF}/\rho_{GB} * S_L^0$ overshot



Characteristic diag.: C3H8, 3-arrays





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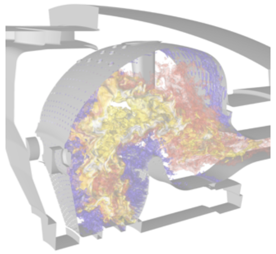

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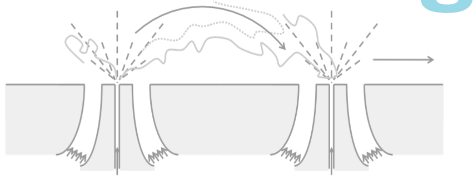

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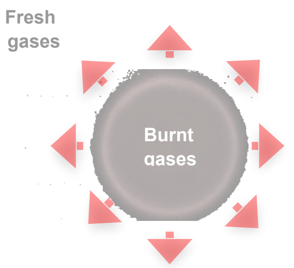

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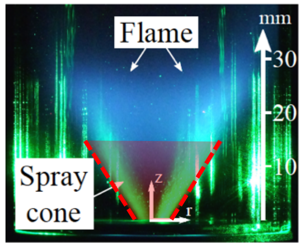


Conclusions and perspectives

IV] Application to a GT: pollutant emissions & multi-phase flows

Today reduced chemistry schemes are accessible in terms of tools and CPU[4-6]

Analytically Reduced Chemistry (ARC) for C3H8 / air combustion

***Pepiot-Desjardins / Jerzembeck* skeletal scheme[1]:**

Derived from the LLNL comprehensive mechanisms
99 transported species
669 reactions

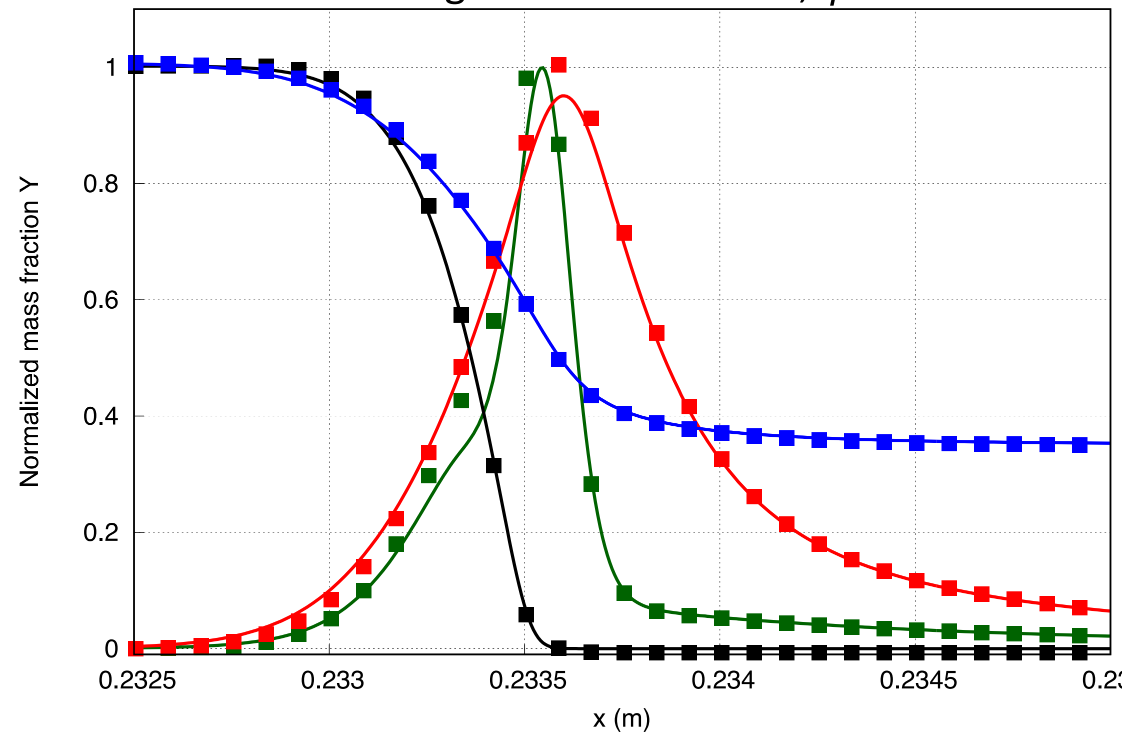
reference mechanism => skeletal mechanism:
DRGEP[2]

skeletal mechanism => reduced scheme:
QSSA using the LOI[3] criterion

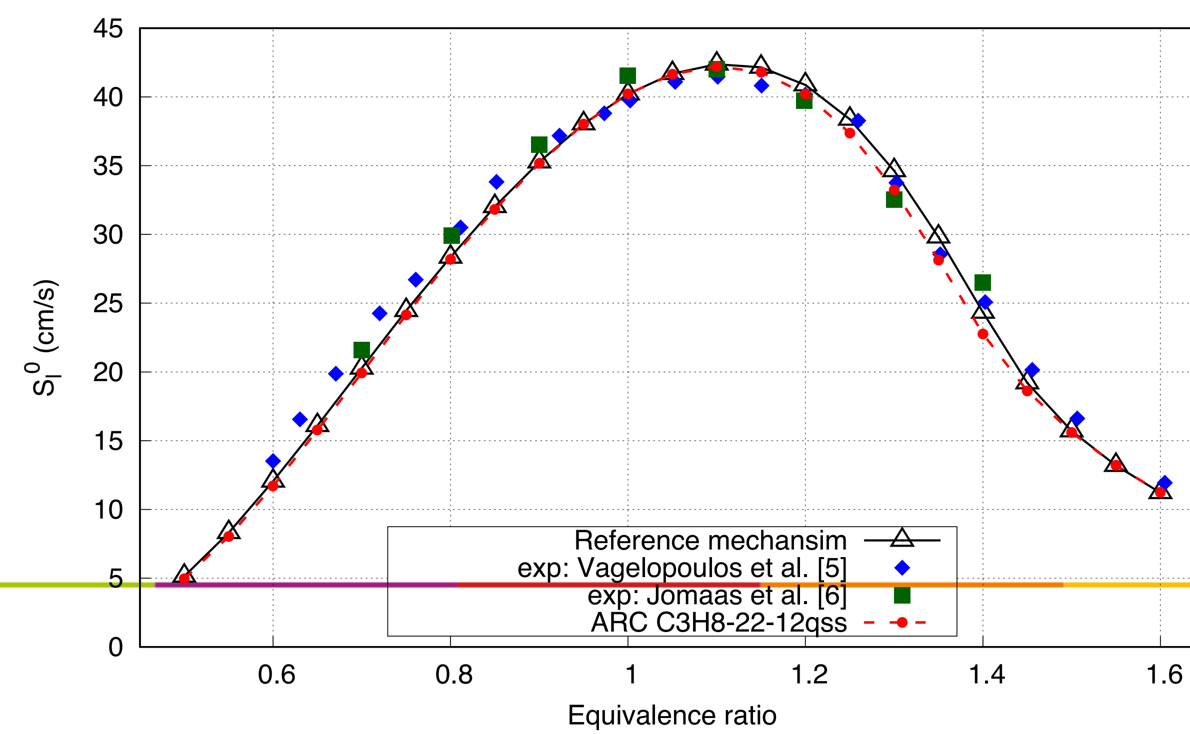
ARC C3H8-22-12qss:

22 transported species
173 reactions
12 QSS species

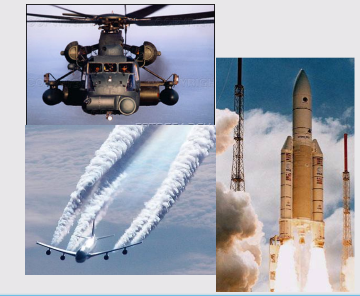
1D flame using AVBP at T = 288 K, ϕ = 0.65



S_l^0 for T= 288 K as function of the equivalence ratio



1 Jerzembeck, S., et al (2009). *Combustion and Flame*, *156*(2), 292-301.
2 Pepiot-Desjardins, P., et al (2008). Combustion and Flame, 154(1), 67-81.
3 Løvås, T., et al (2002). *Proceedings of the Combustion Institute*, *29*(1), 1387-1393.
4 Jaravel, T. et al (2016), *Proceedings of the Combustion Institute*, 36.
5 Schulz, O. et al (2016), *Proceedings of the Combustion Institute*, 36.
6 Felden, A. et al (2016), *Proceedings of the Combustion Institute*, 36.

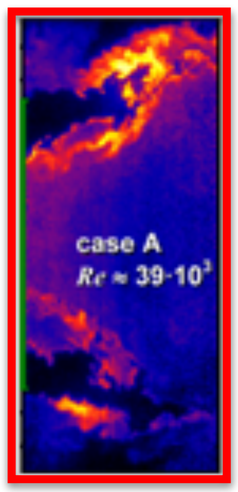


OH PLIF [1]

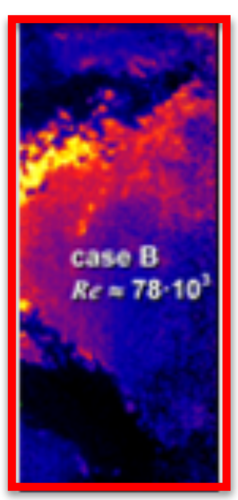
LES
OH Concentration

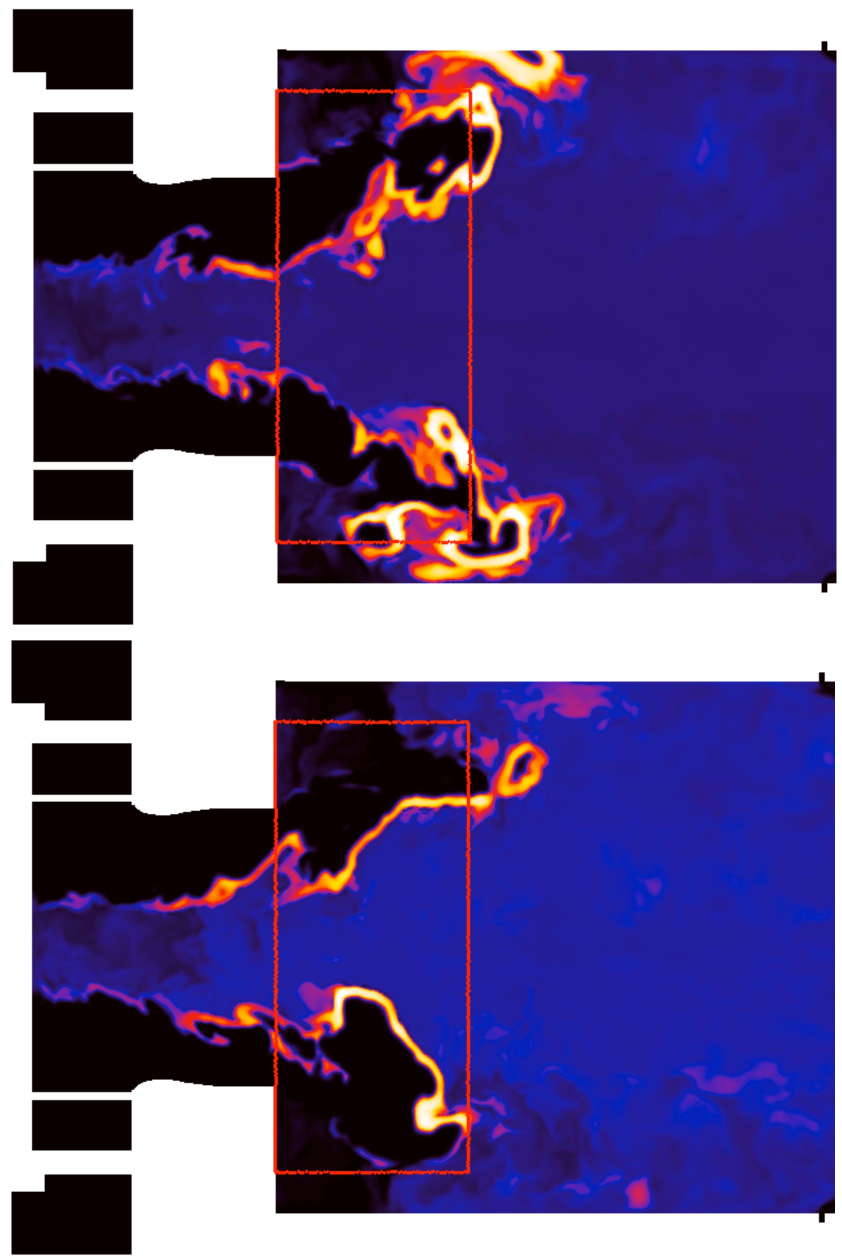
Heat release rate

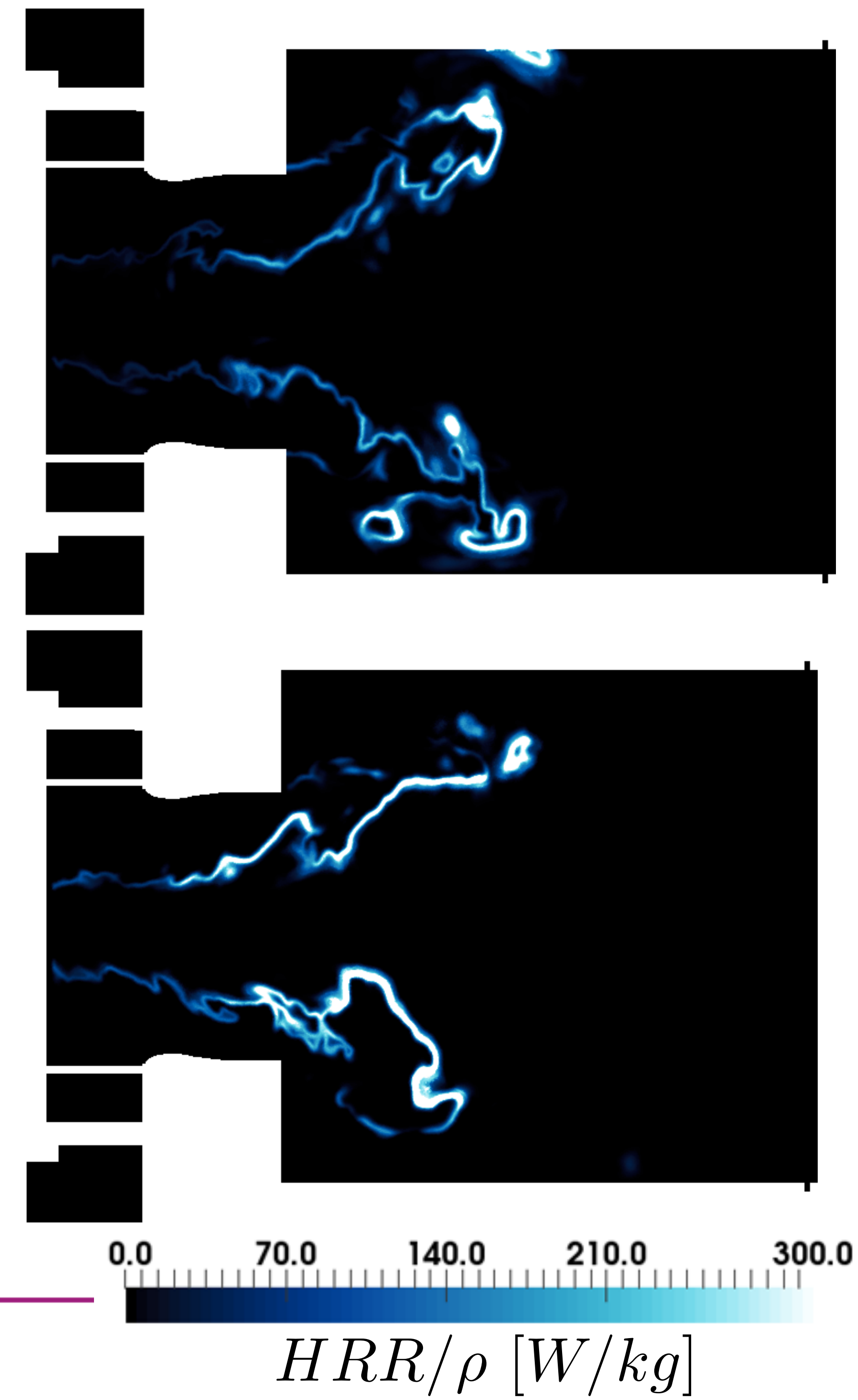
3 Bars



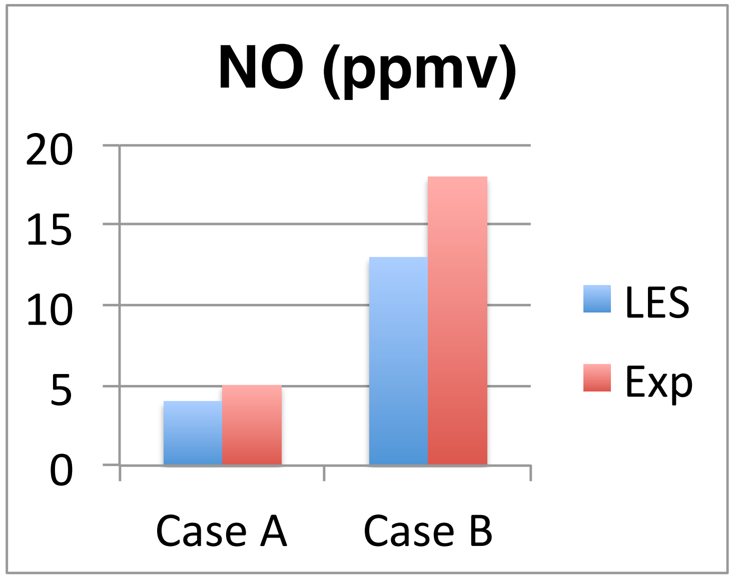
6 Bars

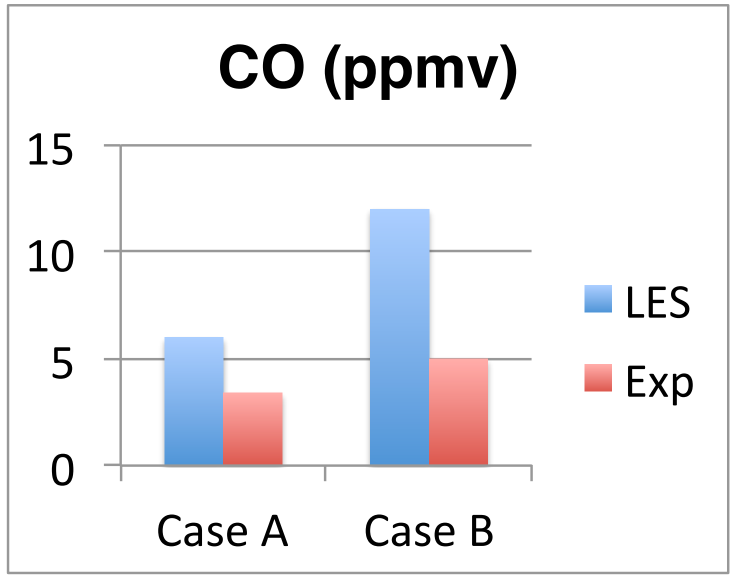




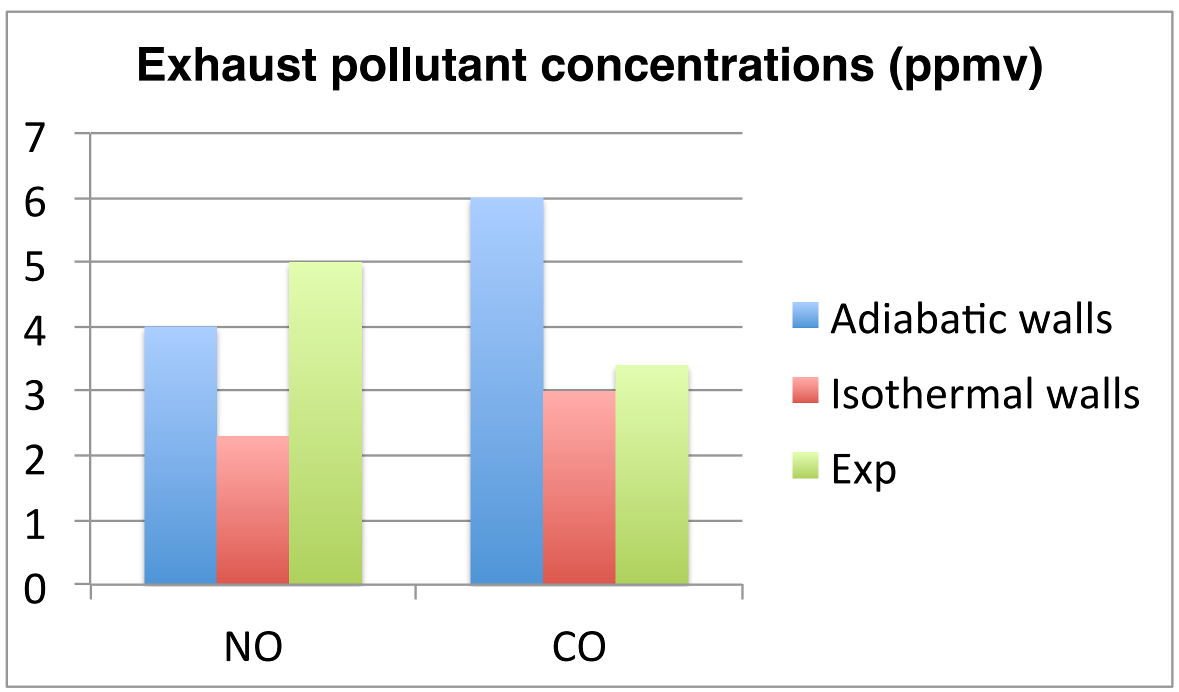


Exhaust pollutant concentrations





- NO
  - Satisfactory prediction
    - Slight under-prediction
  - Trend correctly recovered
- CO
  - Significant over-prediction



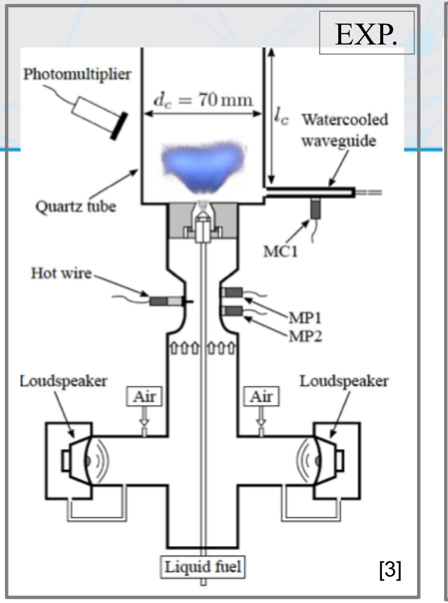
Deterioration of **NO prediction**

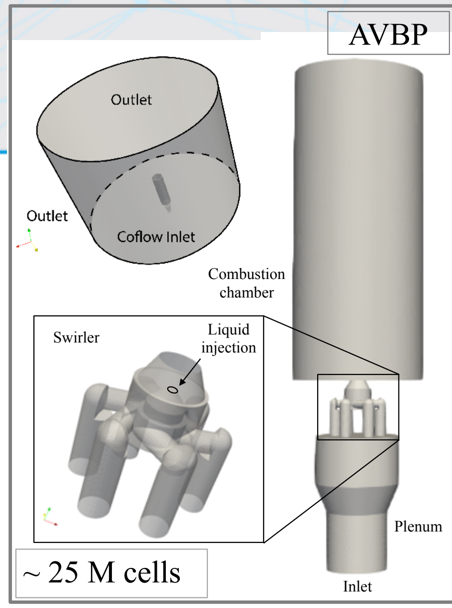
➡ Improvement of **temperature prediction**

➡ Significant improvement of **CO prediction** at the exit: driven by **equilibrium**

Multi-phase reacting flows

Single burner setup: SICCA-Spray

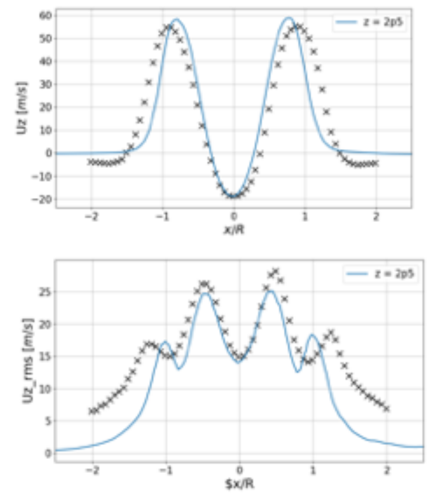


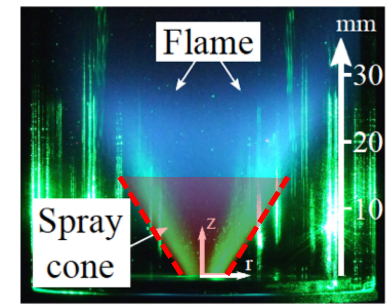


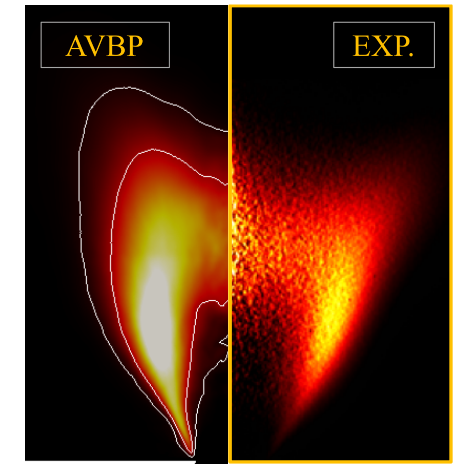
EM2C laboratory (Paris)

Steady operating conditions

- cold non-reacting
- reacting spray flame

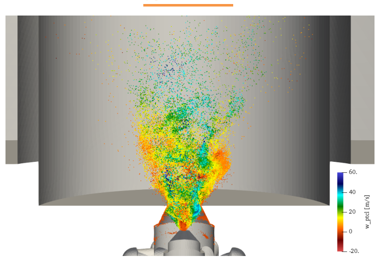


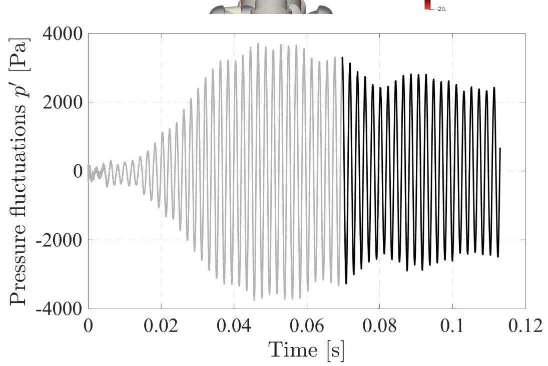




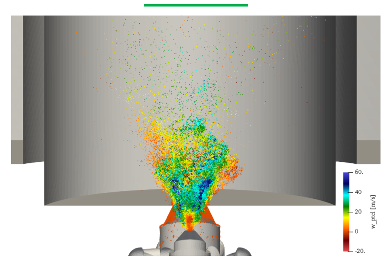
Thermo acoustically unstable configuration

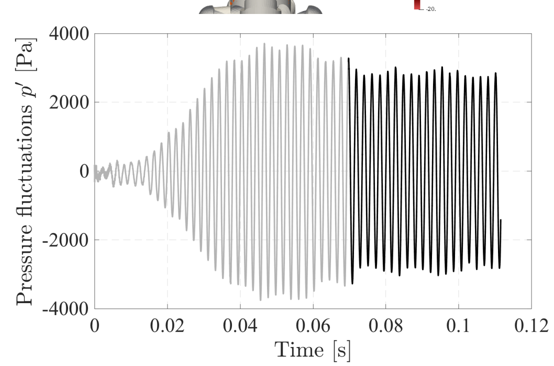
Wall interaction model:
SLIP

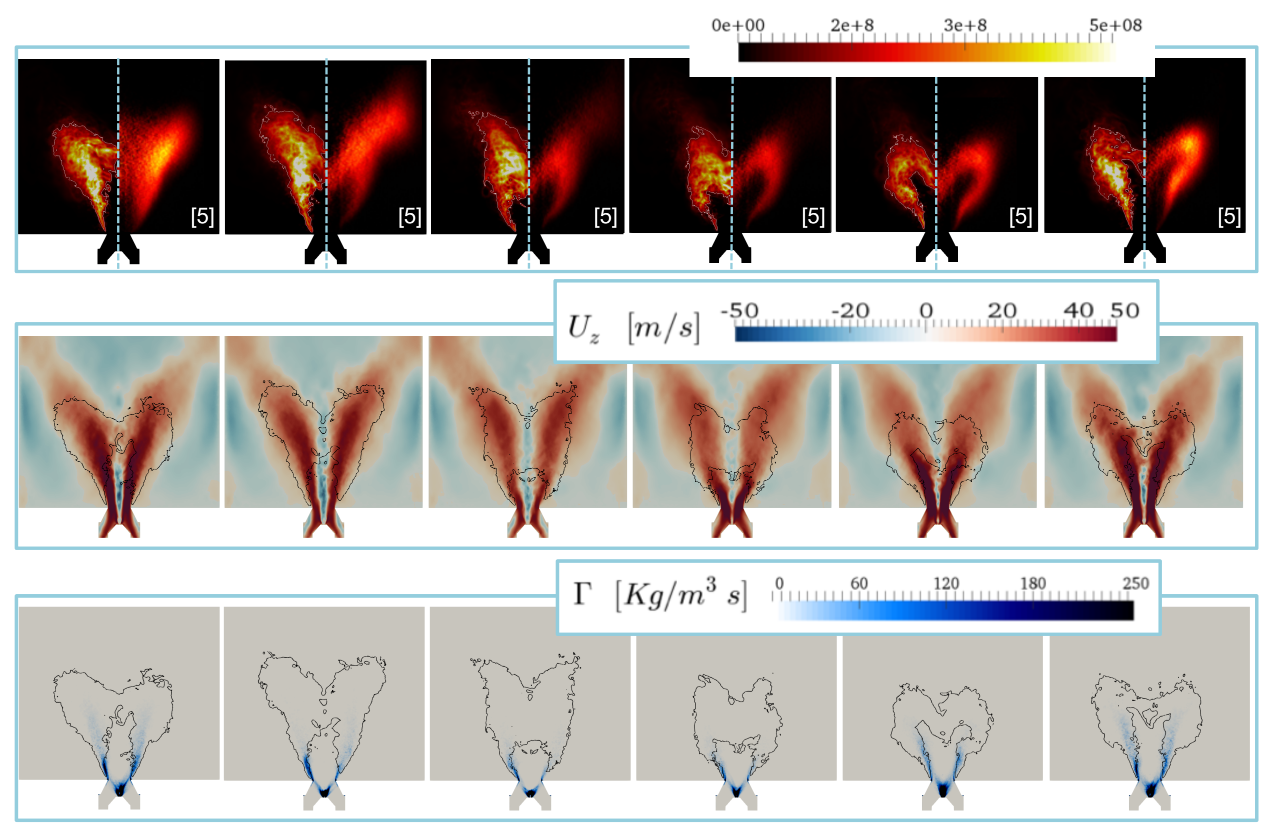




Wall interaction model:
FILM







Conclusions & perspectives

Current progresses in LES @ CERFACS include more and more complexity

=> In terms of chemistry: ARC schemes needed to predict pollutants will improve the quality of the laminar flame speed predictions for simple flames provided that these schemes are properly constructed from adequate reference schemes.

=> ARC will however not alleviate the dependency of the turbulent combustion closure to the laminar flame speed (and thickness) for non-planar flames… i.e. how to properly incorporate stretch and strain effects

=> Multi-phase flames clearly add complexity: depending on the droplets, different regimes of combustion appear and their effect on the flame thickness and speed are not fully understood…