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SCIROCCO

ERC advanced grant: cerfacs.fr/scirocco

Can we simulate safety scenarios linked to combustion ?

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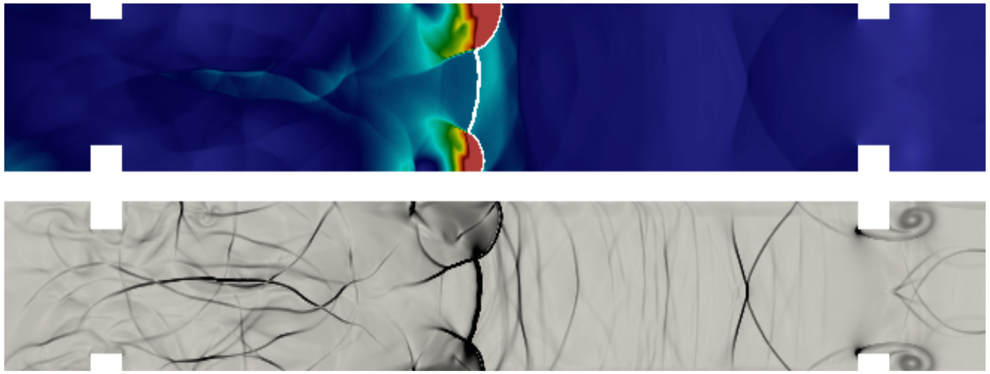
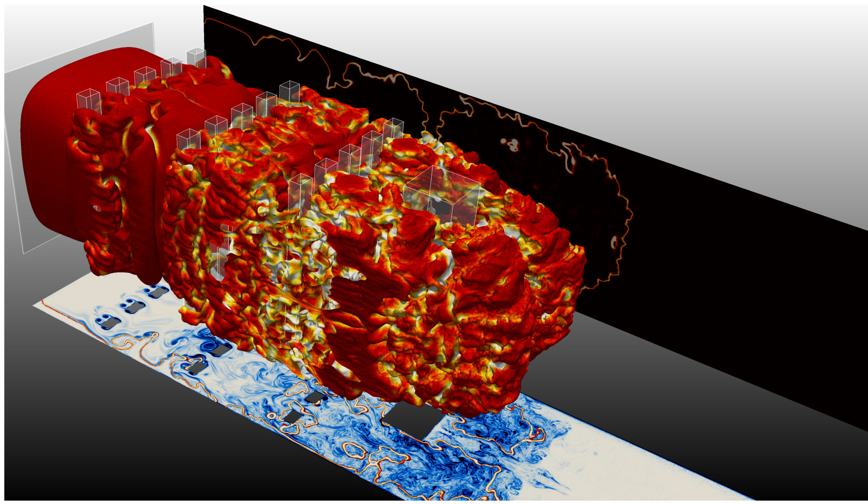




Thanks to: European Research Council, TOTALENERGIES, AIR LIQUIDE, GRTGAZ, EDF, AIRBUS, SAFRAN, ARIANEGROUP, SIEMENS, ALSTOM

CONTEXT:

- WE FOCUS TODAY ON ***ONE*** ASPECT OF SAFETY: WHAT HAPPENS IF A COMBUSTIBLE GAS MIXES WITH AIR AND IGNITES (right away or later)

OUTLINE

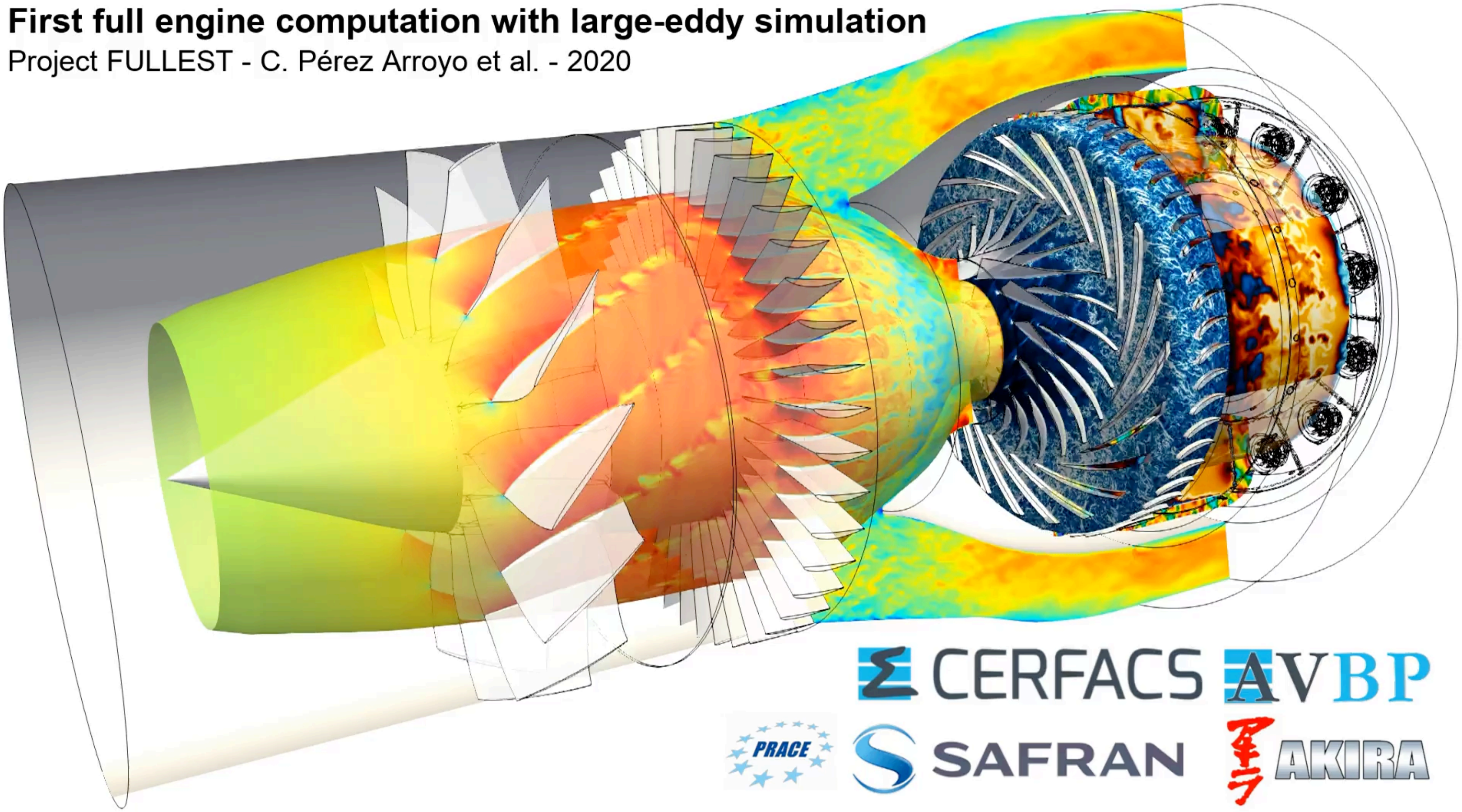
- SAFETY AND COMPUTATIONAL FLUID DYNAMICS: can we believe simulations (***Computational Fluid Dynamics: CFD***) for safety scenarios ?

- THE SPECIFIC CASE OF ***HYDROGEN***

INTRODUCTION: Computational Fluid Dynamics

In many fields, CFD has almost replaced tests:

- aerodynamics around an aircraft



INTRODUCTION: Computational Fluid Dynamics

- But CFD is not as present for safety

- Historical but also good technical reasons:
  - Very large domains to compute
  - Vague initial and boundary conditions (too many possible scenarios)
  - Unprecise CFD methods

Why would we want to use Computational Fluid Dynamics for SAFETY ?

- Simulating an incident linked to combustion is usually cheaper than doing an experiment
- Regulations might include simulations in the future
- **To understand the mechanisms and imagine the scenarios. Examples:**
  - « can this scenario lead to autoignition ? »
  - « can this autoignition lead to detonation ? »

INTRODUCTION: H_2

- Of course, H_2 has been here for a long time
- But the use of H_2 is growing fast now in areas where it was not used before: cars, planes, boilers, gas turbines, heating systems.

SIMULATIONS, H_2 and SAFETY ?

Why H2 now ? Back to energy: a useful concep to count it -> the « N » number (Jancovici: theshiftproject.org/en/home/)

N= number of human 'slaves' who should work for you full time (no sleep) to provide the energy you use on average ?

Counting energy: a useful concept by Jancovici

Today we have replaced animals by machines

Here N=2 ?

Do you know what this number N is today ?

N=200 in the world

600 in France/Japan

Unfortunately, fossil fuels and combustion

What makes these machines work ?

Combustion is amazingly efficient

=

But we should stop…

Hydrogen burns very well indeed…

And, for journalists at least, burning H2 does not produce CO2…

Two reasons we look at H2:

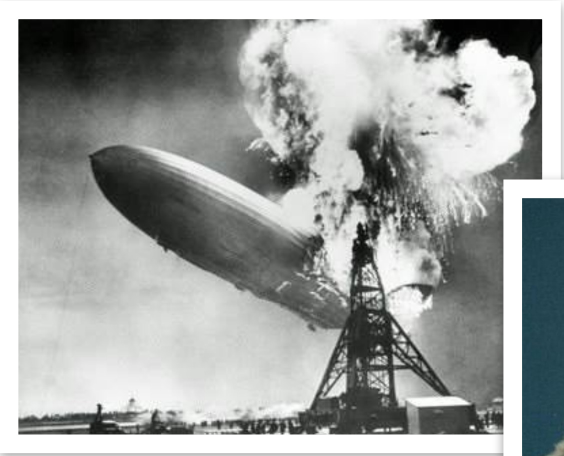
- Hydrogen to be used in more fields including transportation -> TRAIN, AIRCRAFT ?

- Safety of hydrogen solutions

We assume that H2 can/will be produced ‘green’

H_2 for transportation and safety: the Hindenburg syndrome

- Public perception of hydrogen is ambiguous:
  - hydrogen = energy of the future (energy vector, energy storage)
  - hydrogen = danger



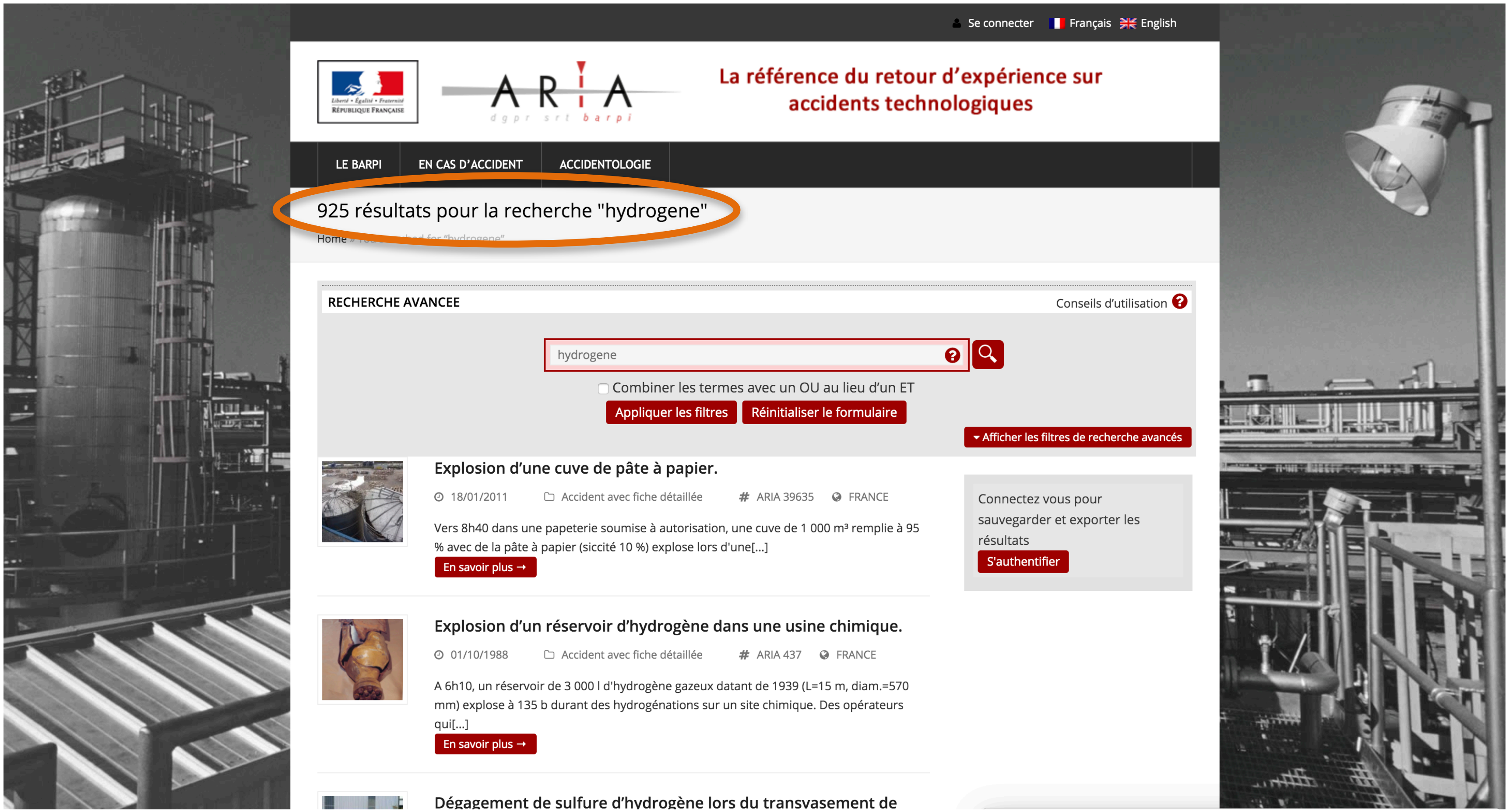
Hindenburg 1937

Challenger 1986

Fukushima 2011

Accidents involving H_2

- ARIA database (Analyse, Recherche et Information sur les Accidents)



CERFACS

- Seriousness of H2 accidents:

	Nb of cases	%
Deaths	25	12
Serious injuries	28	13
Injuries (including serious ones)	70	33
Internal material damage	183	86
External material damage	17	8
Internal operating losses	89	42
Evacuated population	8	3,8

- Many sectors of activity:
  - activities where hydrogen is either produced or used : chemical, refining, transport, packaging, nuclear industry,
  - activities where hydrogen is accidentally produced : metallurgy and metal works, sanitation, waste treatment and recycling, nuclear power plants.

	Nb of cases	%

AND NOW: ENERGY AND TRANSPORT

Energy storage (Power2gas)

Transportation: cars, aircraft, trains, ships

FOCUSING ON COMBUSTION: H2 IS VERY DIFFERENT FROM OTHER FUELS

- ★ Hydrogen ignites much more easily in a wider range of compositions

- ★ Hydrogen burns much faster than all other fuels

- ★Hydrogen detonates easily…

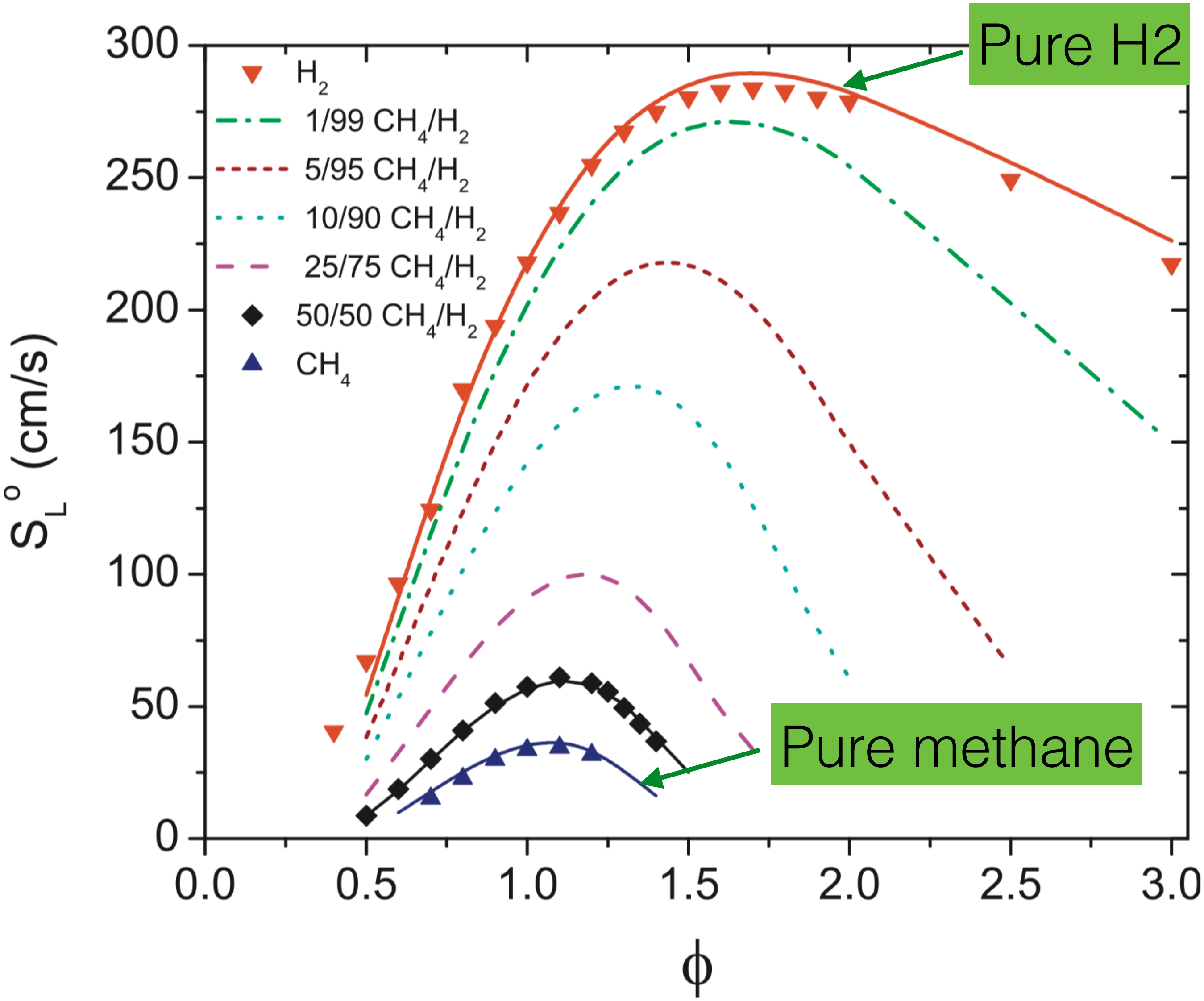
FLAMMABILITY LIMITS:

	LEAN FLAMMABILITY LIMIT	RICH FLAMMABILITY LIMIT
CH_4 methane	5 %	15 %
C_3H_8 propane	2,1 %	9,5 %

The MIE (minimum ignition energy) is also ten times less for H_2 than for other fuels

H2 BURNS MUCH FASTER THAN ALL FUELS: example in air

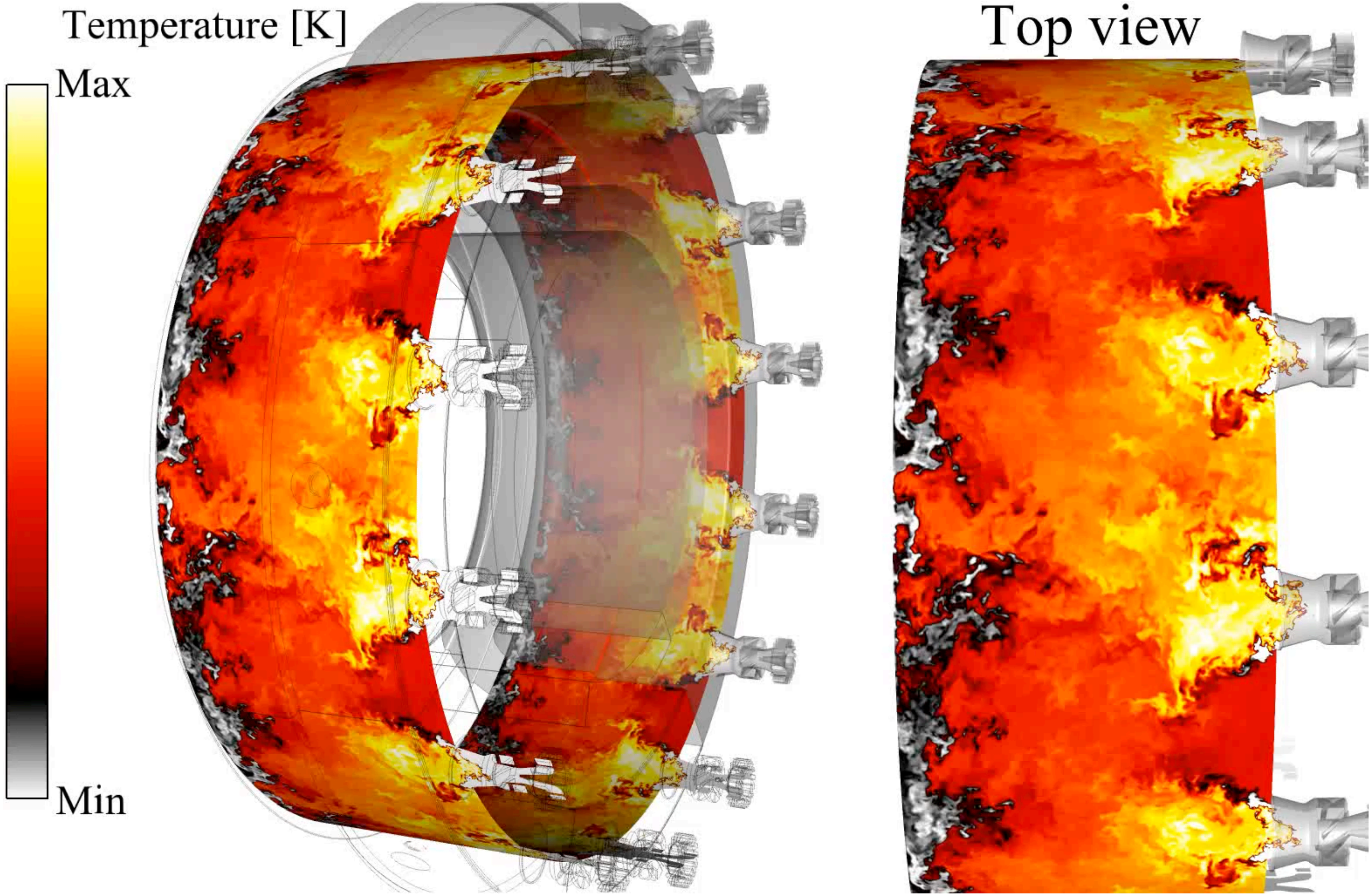
Flame speed as a function of equivalence ratio



– Computational Fluid Dynamics (CFD) codes: compute scenarios instead of (or in connection with) experiments

– The example of the simulations performed at CERFACS in Toulouse with a software called AVBP:

WHAT IS CFD ?



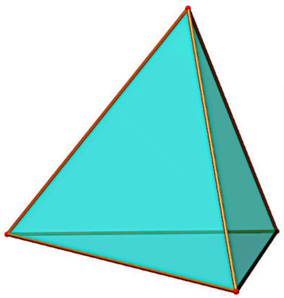
CONSERVATION EQUATIONS: COUNTING...

This morning, I had … €

Tonight, I have … €

This is a balance of € on one day

COUNTING IN CFD…



At time t, I had this amount of H2

IN

SMALL ELEMEN
(tetrahedron)

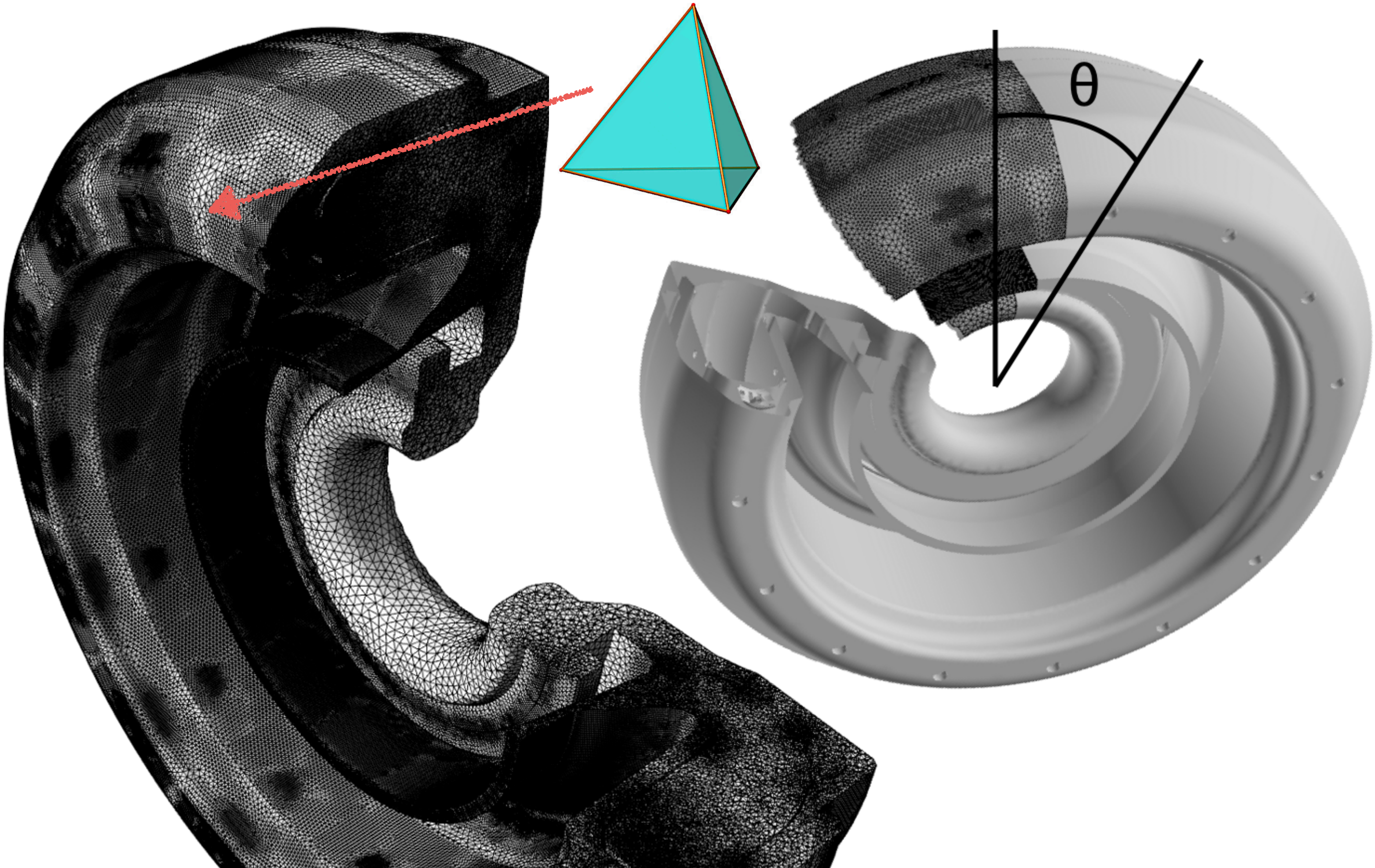
OUT

BURN

At time t+dt, I have this amount of H2

This is a balance of H2 for this hexahedron on a time step dt

WE CUT SPACE INTO BILLIONS OF SMALL TETRAHEDRAL ELEMENTS



COMPUTATIONAL FLUID DYNAMICS CODES ARE COUNTING SPECIES, MASS AND ENERGY (not Euros…sorry)

- For each element of the mesh, make a balance of mass, energy and all chemical species. The size of each mesh element is less than a mm.
- The time step is typically 10 to 100 nanoseconds
- Each simulation creates approximately 10^{16} real numbers
- The code is based on first principles of physics, not on correlations
- Expensive but precise -> predictive

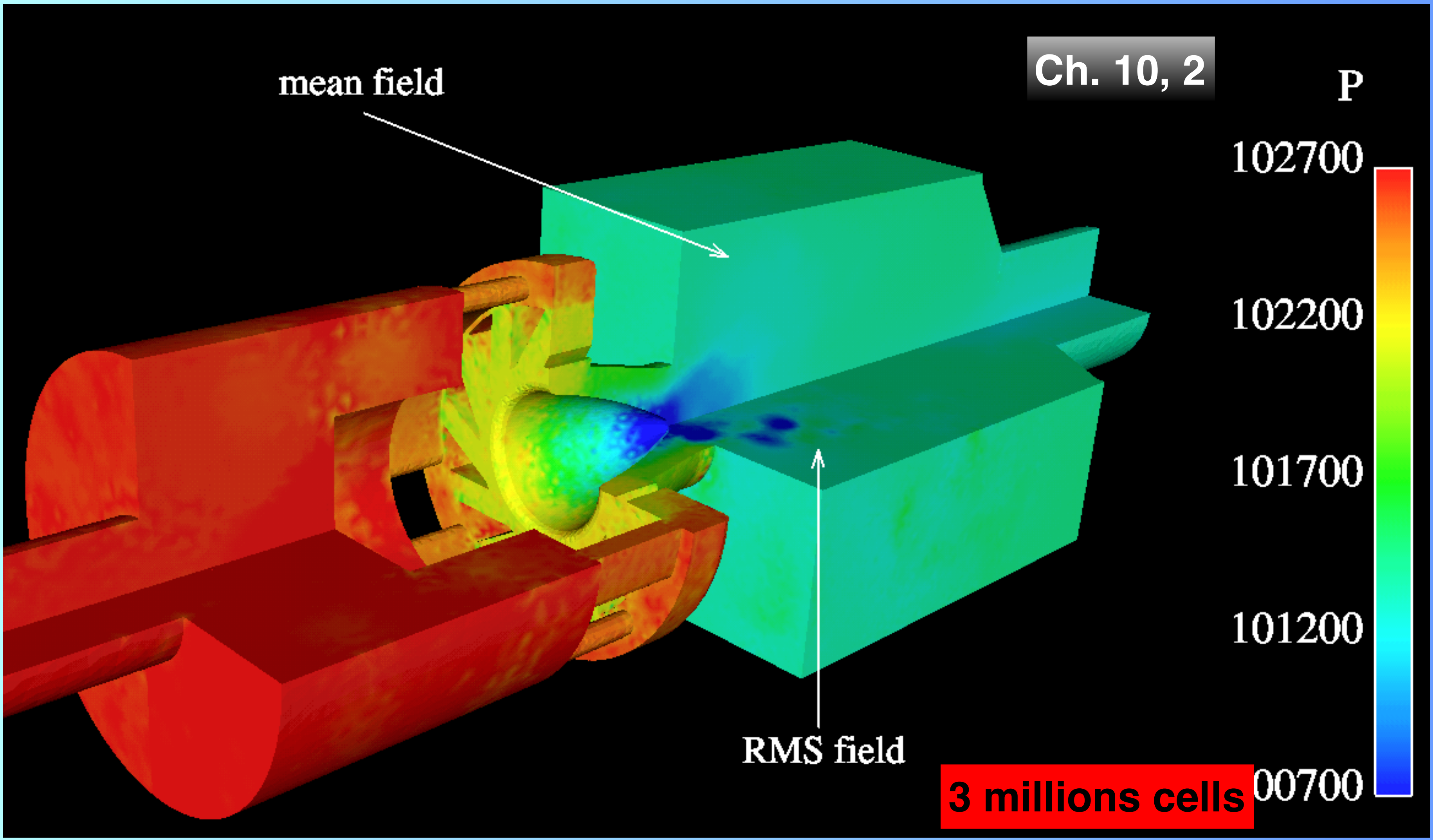
BUT THIS TAKES A SIGNIFICANT CPU POWER AS WELL AS HUMAN POWER:

HOW DO YOU SIMULATE COMBUSTION WITH CFD ?

CERFACS uses a code (AVBP) developed for aerospace applications:

- **1000 man years of work and 30 developers**
- **200 users in SAFRAN HELICOPTER ENGINES, SAFRAN AIRCRAFT ENGINES, ARIANEGROUP, AIR LIQUIDE, TOTALENERGIES, TU MUNICH, TU BERLIN, CENTRALESUPELEC, IMF TOULOUSE, LMFA Lyon, Un SHERBROOKE…**
- **1 million lines of codes**
- **massively parallel: can run on 200 000 processors**
- **VALIDATED ON HUNDREDS OF CASES (thanks to the AEROSPACE industry which has provided validation cases) published in refereed journals**

LPP (aero gas turbine). Gaseous fuel /air (DLR)

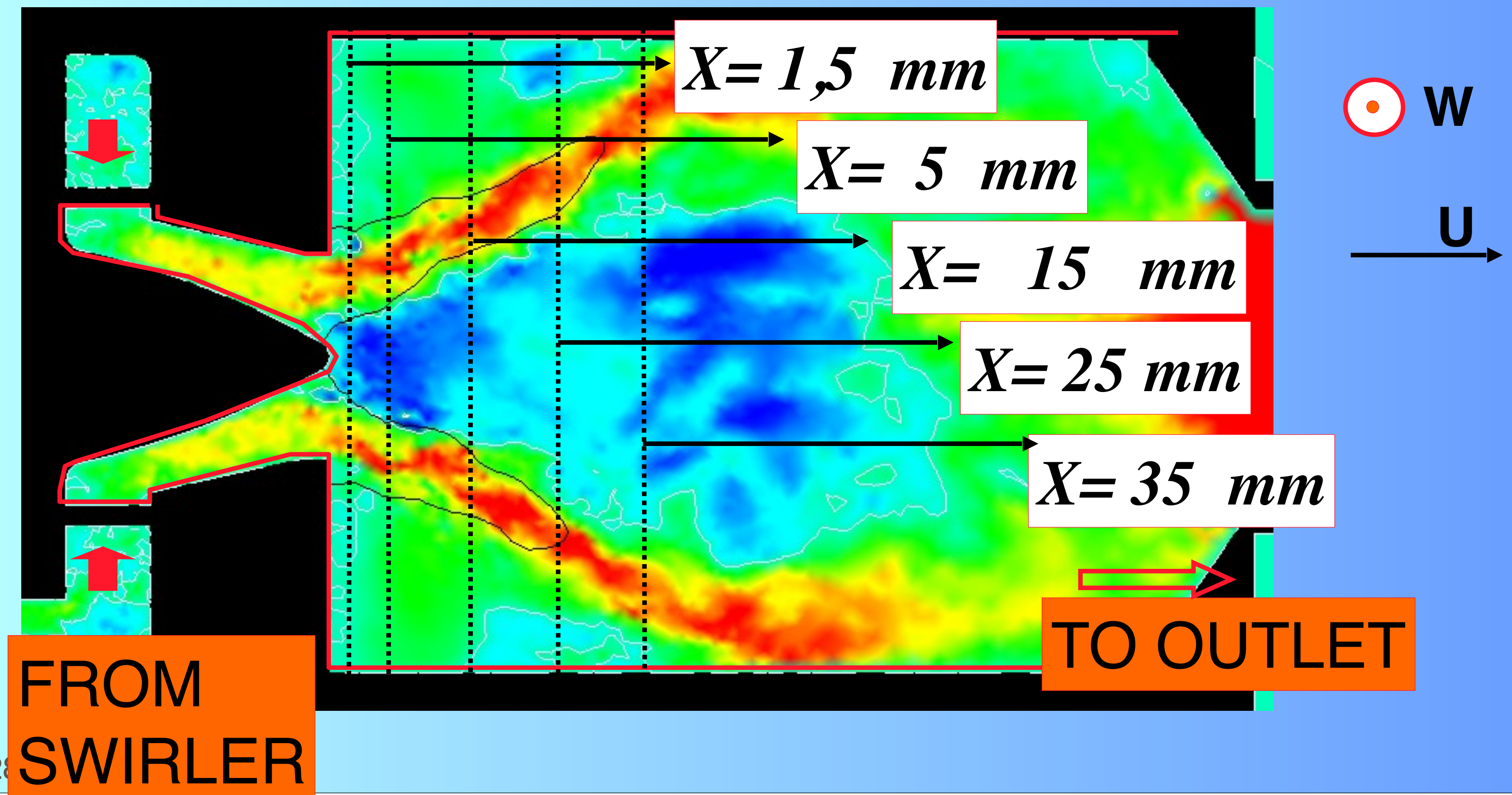


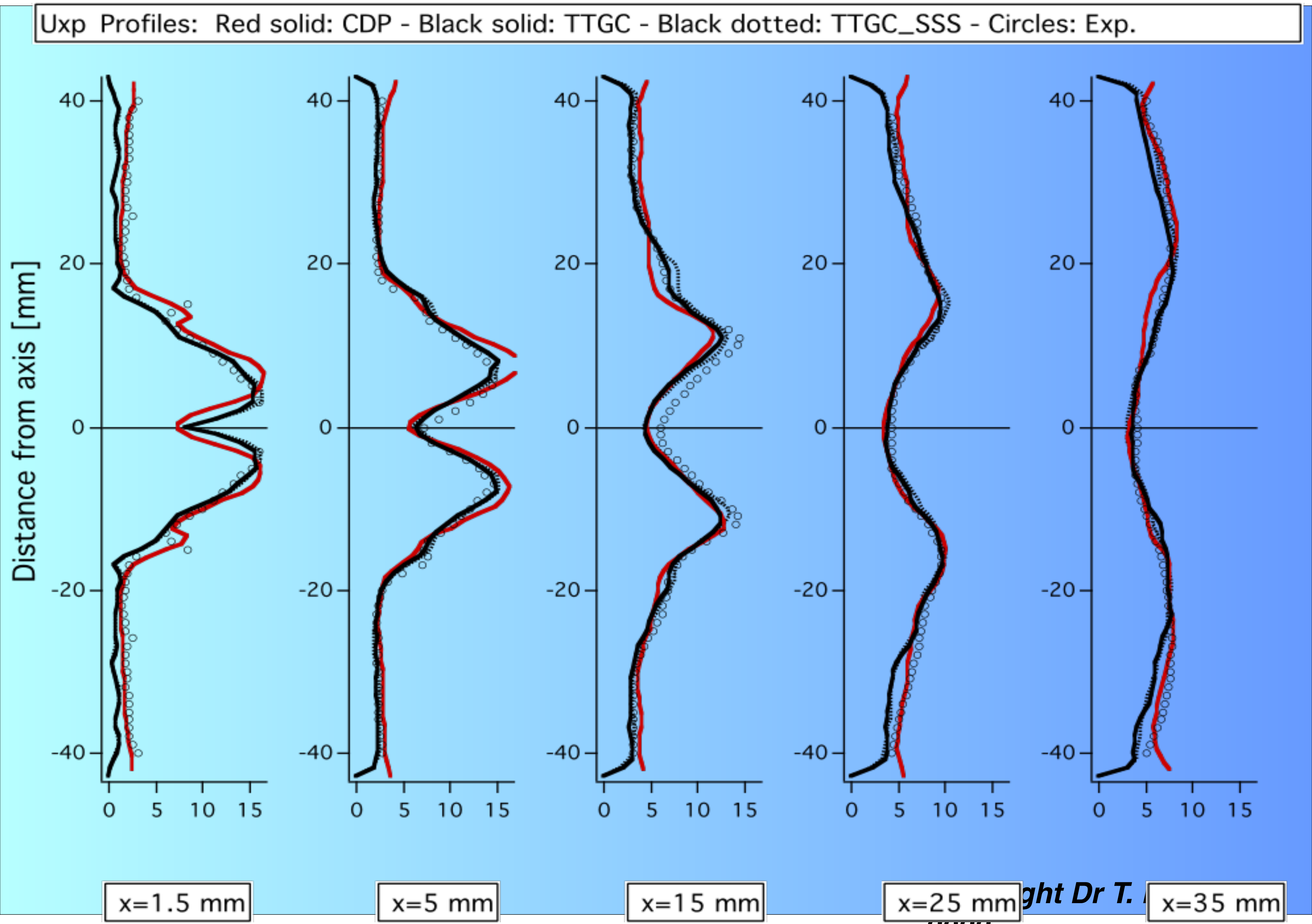
Roux, Lartigue, Poinsot, Meier and Bérat *Comb and Flame 141, 2005*

Comparison of mean velocity fields

All LES are compared with measurements DLR (LDA):

- **Velocity profiles are compared at five stations along the burner.**
- **Comparison for axial, tangential and radial velocities (mean and RMS)**

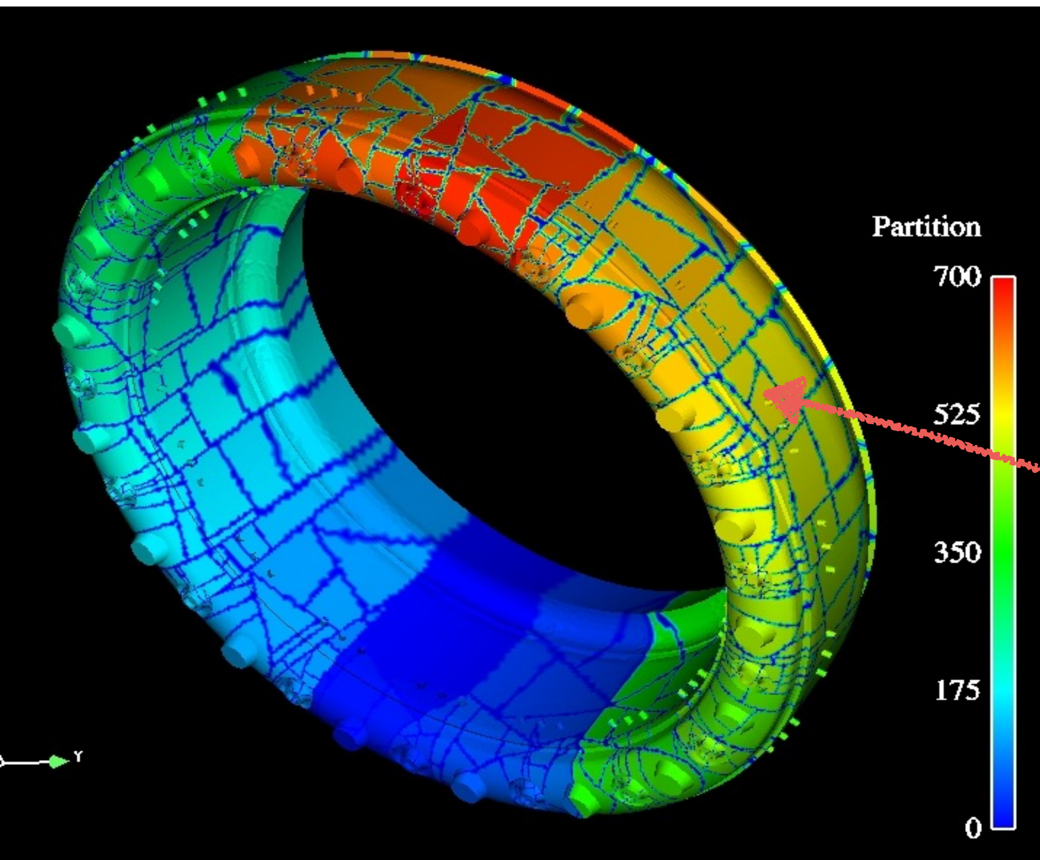


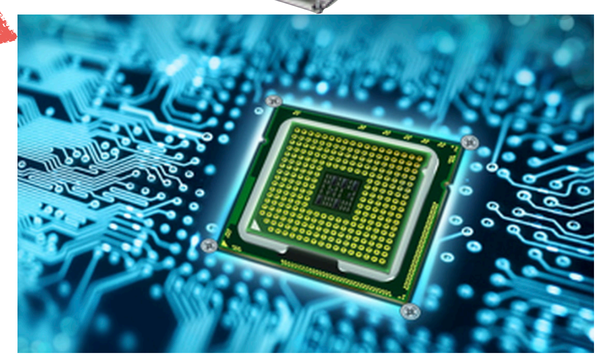


Uxp Profiles: Red solid: CDP - Black solid: TTGC - Black dotted: TTGC_SSS - Circles: Exp.
Distance from axis [mm]
40
20
0
-20
-40
0 5 10 15
x=1.5 mm
x=5 mm
x=15 mm
x=25 mm
x=35 mm
ght Dr T.
2022

CPU TIME AND MACHINES:

- A single simulation can require 1000 years of CPU.
- Cannot be done on a single processor computer
- On 100 000 cores, only a few days….

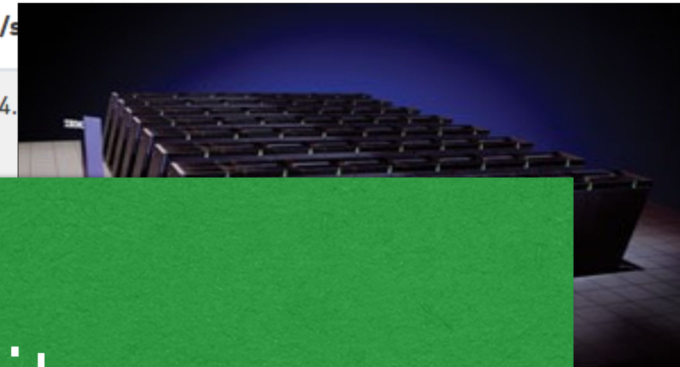




SUPER COMPUTERS

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s	Power
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, **Fujitsu** RIKEN Center for Computational Science	7,299,072	415,530.0	513,854.	
2					
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, **IBM / NVIDIA / Mellanox** DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
4	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, **NRCPC** National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
5	**Tianhe-2A** - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000, **NUDT** National Super Computer Center in Guangzhou China	4,981,760	61,444.5	100,678.7	18,482

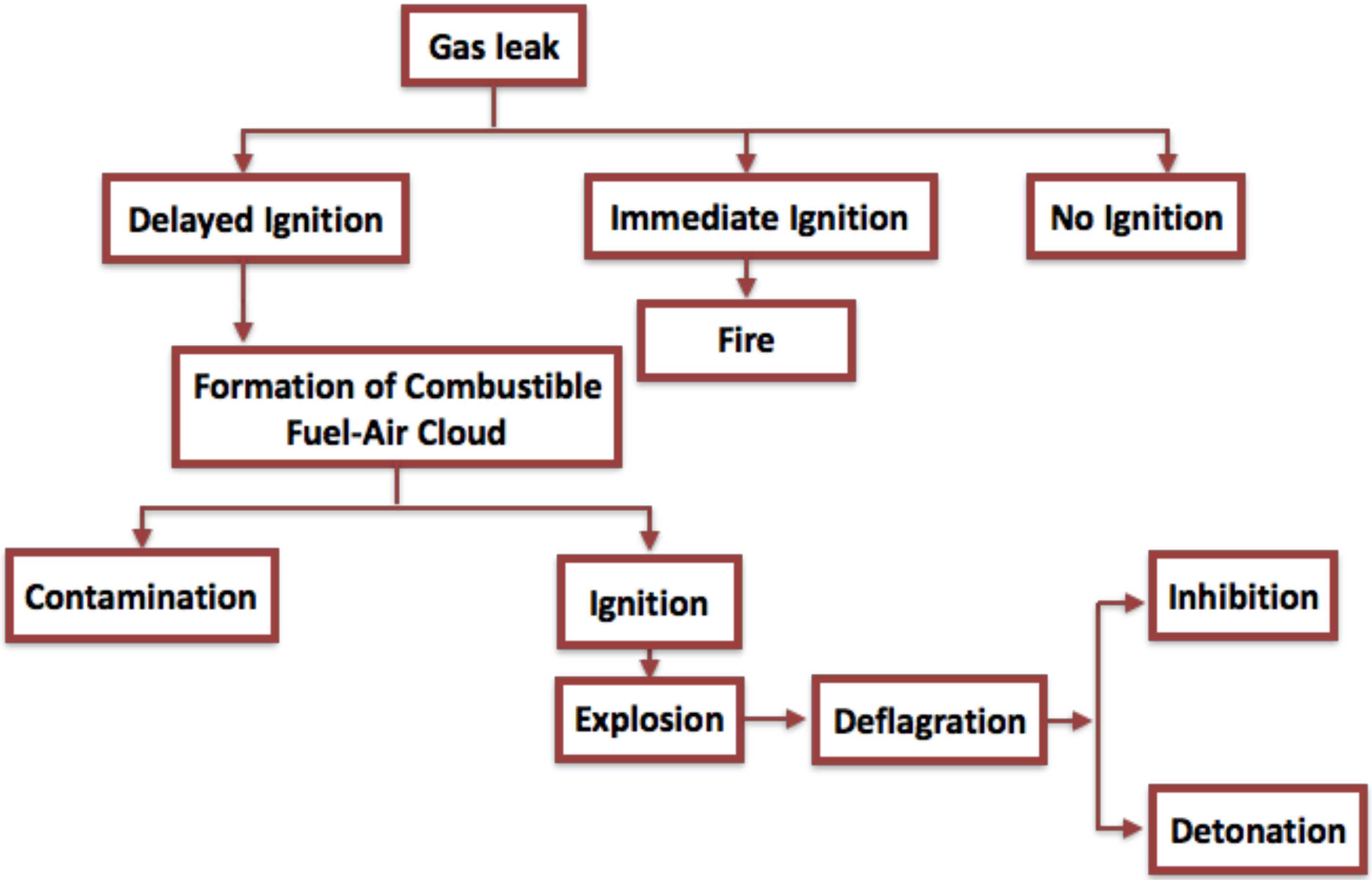
- 100 Meuros
- 20 Meuros of electricity per year



COMPLICATED TASK.

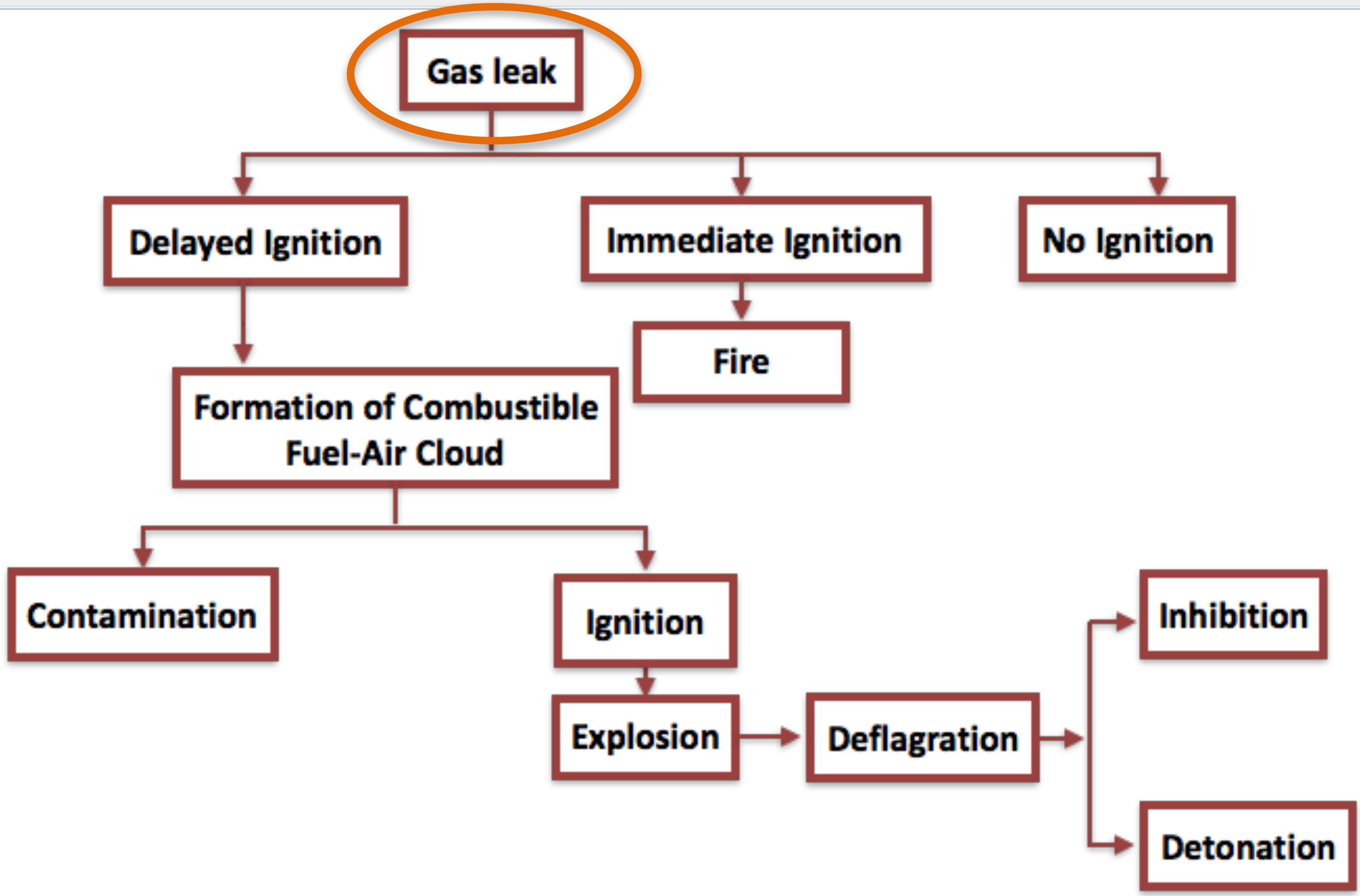
1 million musicians

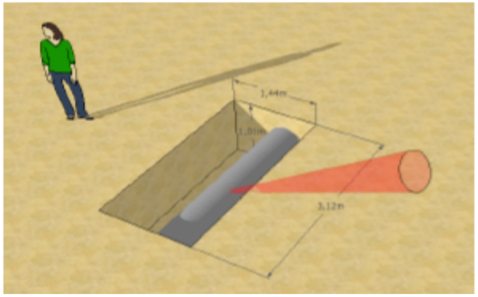
Computing safety scenarios

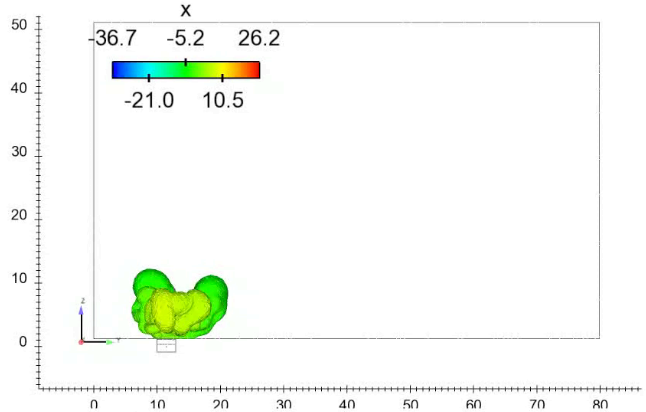


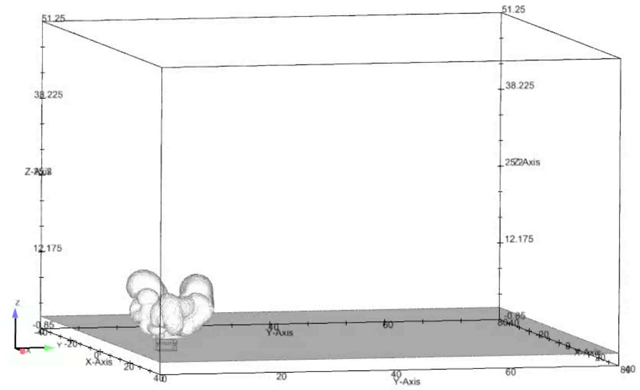
ALL THESE EVENTS CAN BE SIMULATED WITH CFD

Safety activity at CERFACS

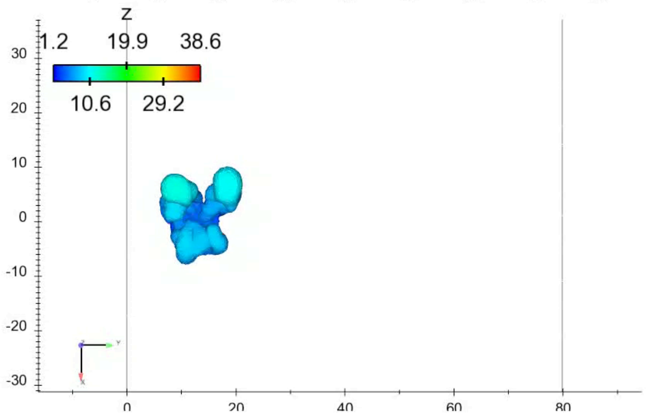


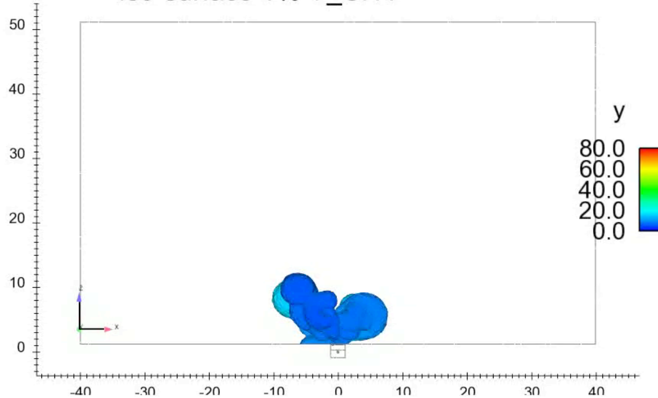




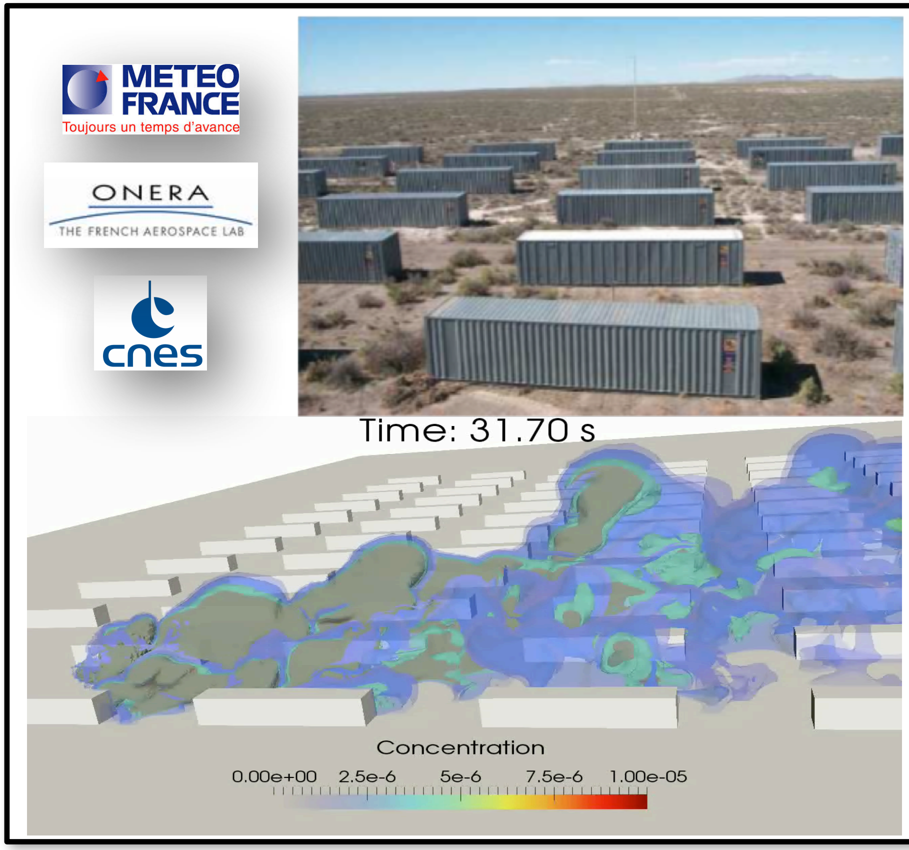


Iso-surface 1% Y_CH4

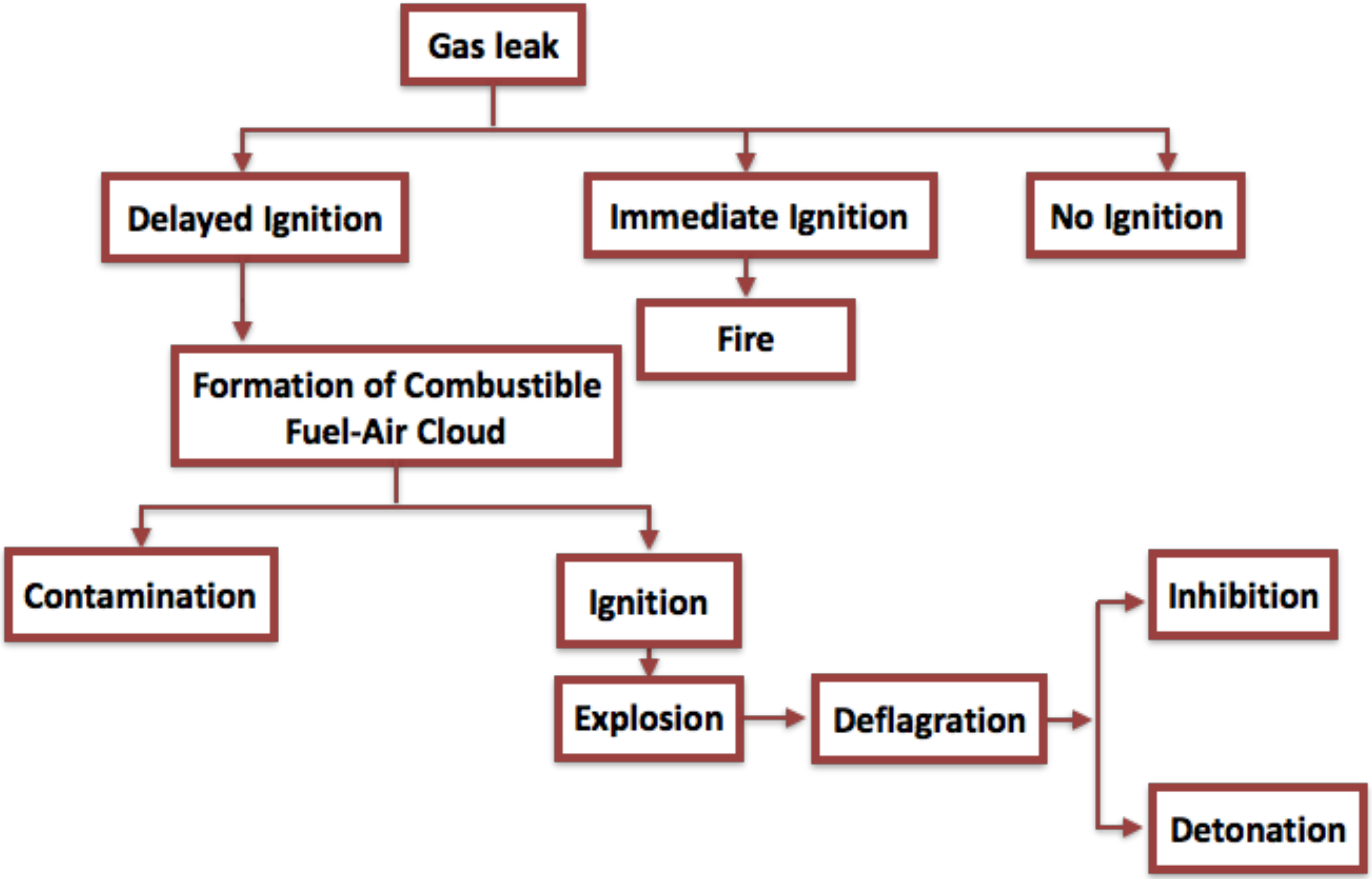


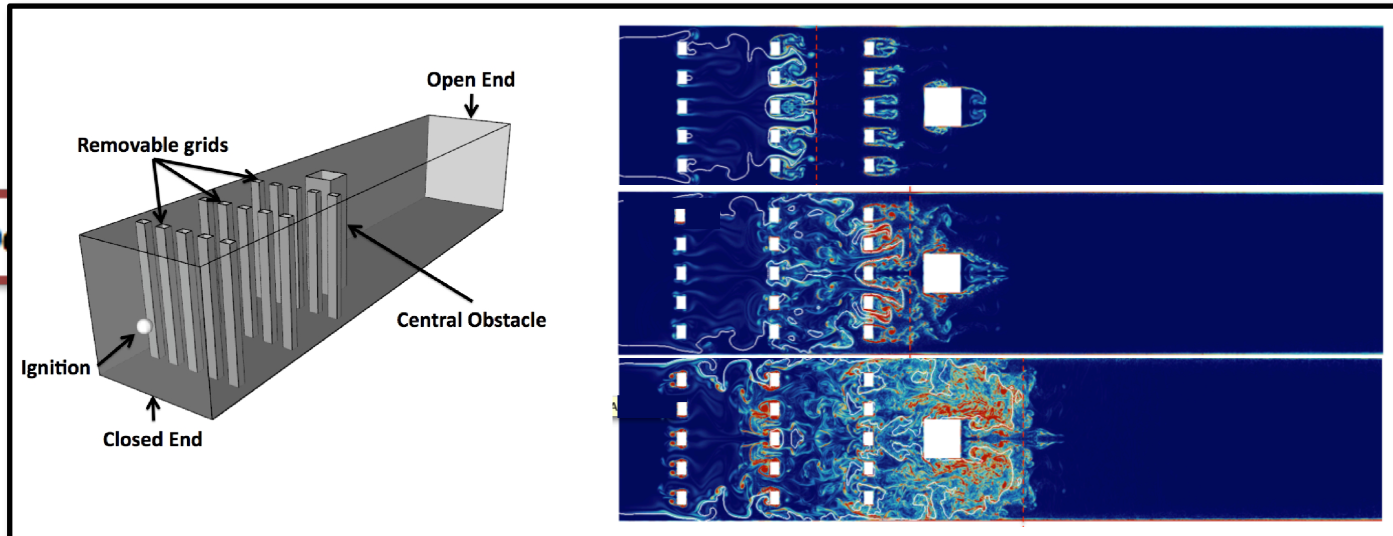


GDF SUEZ



HOW MUCH OF THIS FUEL IS MIXED WITH AIR BETWEEN THE LOW AND HIGH FLAMMABILITY LIMITS GIVES THE LEVEL OF GRAVITY OF A POTENTIAL EXPLOSION


Gas leak
Delayed Ignition
Immediate Ignition
No Ignition
Fire
Formation of Combustible Fuel-Air Cloud
Contamination
Ignition
Inhibition
Explosion
Deflagration
Detonation



Contamination

Ignition

Explosion

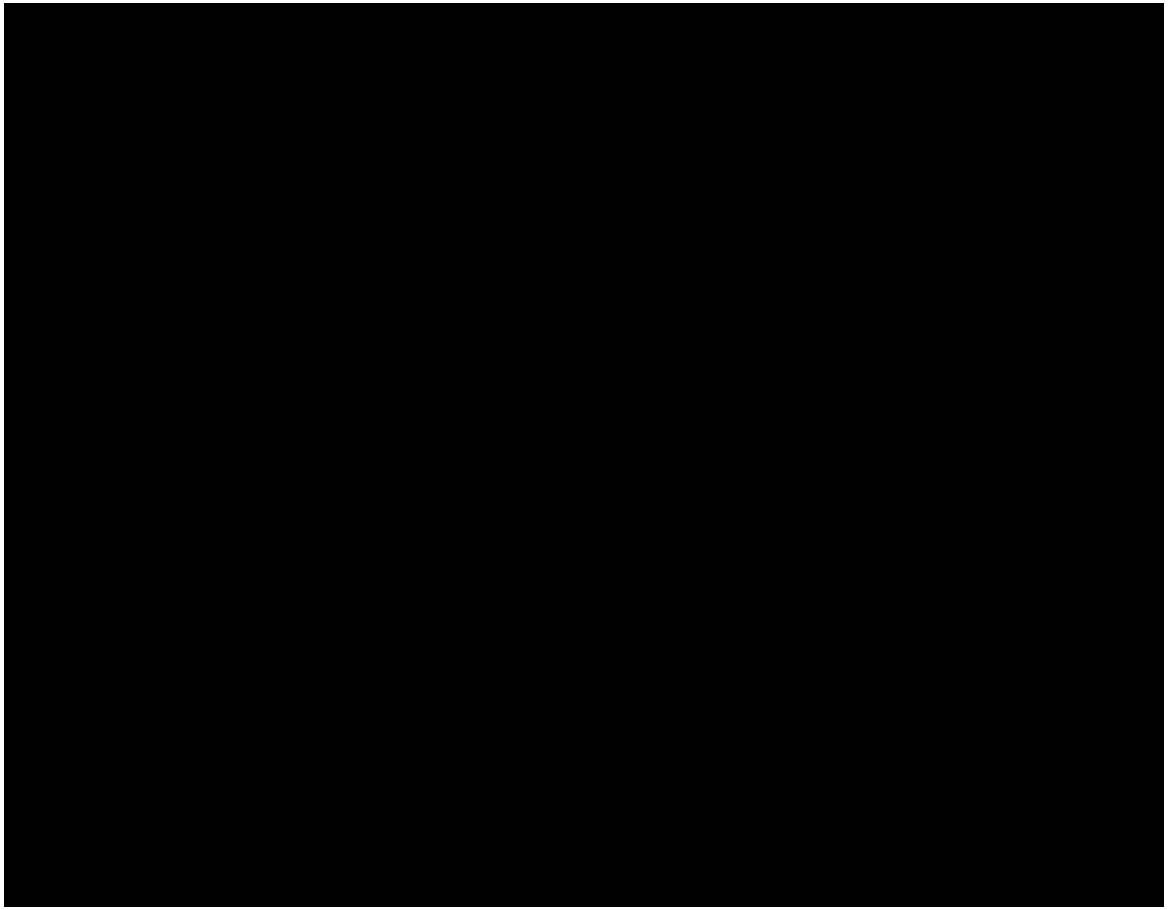
Deflagration

Inhibition

Detonation

DEFLAGRATION vs DETONATION:

- ★ ANY LEAK OF GAS INTO A CONFINED SPACE CAN LEAD TO EXPLOSIONS. DEFLAGRATION:



★DETONATION

NO NEED TO DISCUSS EFFECTS:

30 avril 2007	Mine illégale du village de Liujiacun, comté de Yuxian (Shanxi)[20]	Chine	14
05 mai 2007	Mine de Pudeng à Linfen, comté de Puxian (Shanxi)[21]	Chine	28
23 mai 2007	Mine Xinglong, comté de Luxian, ville de Luzhou (Sichuan)[22]	Chine	13
24 mai 2007	Mine Ioubileïnaïa, à Novokouznetsk (Sibérie)[23]	Russie	38
04 juin 2007	Mine de Niheling, comté de Jingle (Shanxi)[24]	Chine	13
25 juin 2007	Mine Komsomolskaïa à Vorkouta (Russie)[25]	Russie	11
08 novembre 2007	Mine de Qunli, province de Guizhou[26]	Chine	32
18 novembre 2007	Mine de Zasyadko (oblast de Donetsk)	Ukraine	101
06 décembre 2007	Mine au nord de la Chine	Chine	environ 100
22 février 2009	Mine de Tunlan (Shanxi)[27]	Chine	73
21 novembre 2009	houillère de Hegang dans la province chinoise du Heilongjiang[28]	Chine	au moins 104
23 février 2010	Mine d'Odakijy dans la province turque de Balikesir[29].		
05 avril 2010	Mine d'Upper Big Branch, dans l'état de Virginie[30]	États-Unis	29
16 octobre 2010	Mine de Yuzhc… Henan[31,32]		
26 janvier 2011	Mine La Precic…		
29 octobre 2011	Mine Xialiuchong à Hengyang	Chine	29
10 novembre 2011	Mine Shizong province du Hunan[35]	Chine	34

Worse accident: China, 1942, 1565 deaths

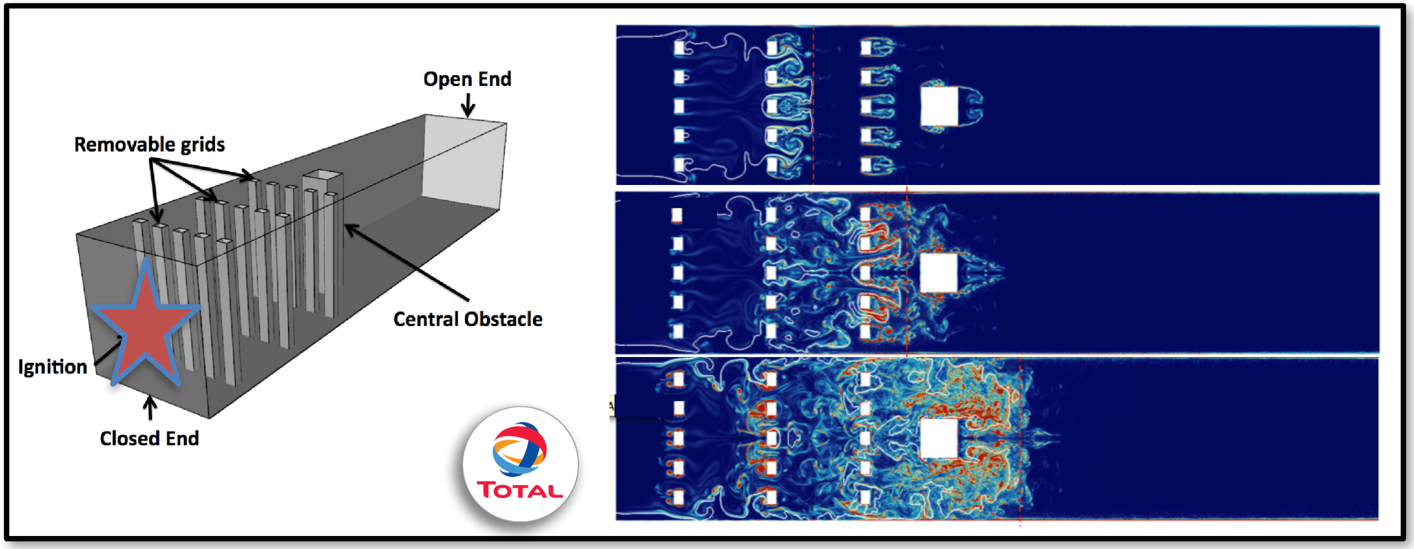
What is the main issue ?

When combustion proceeds in a building, pressure goes up : need to know the 'over pressure'

This over pressure depends directly on the speed of the turbulent combustion process

Computing the speed of combustion in a turbulent flow is the oldest problem for the combustion community and also the first unsolved one…

This is a FUNDAMENTAL RESEARCH problem



SELF-ACCELERATION OF FLAMES

Most flames start ‘slowly’ and move at a few meter/sec.

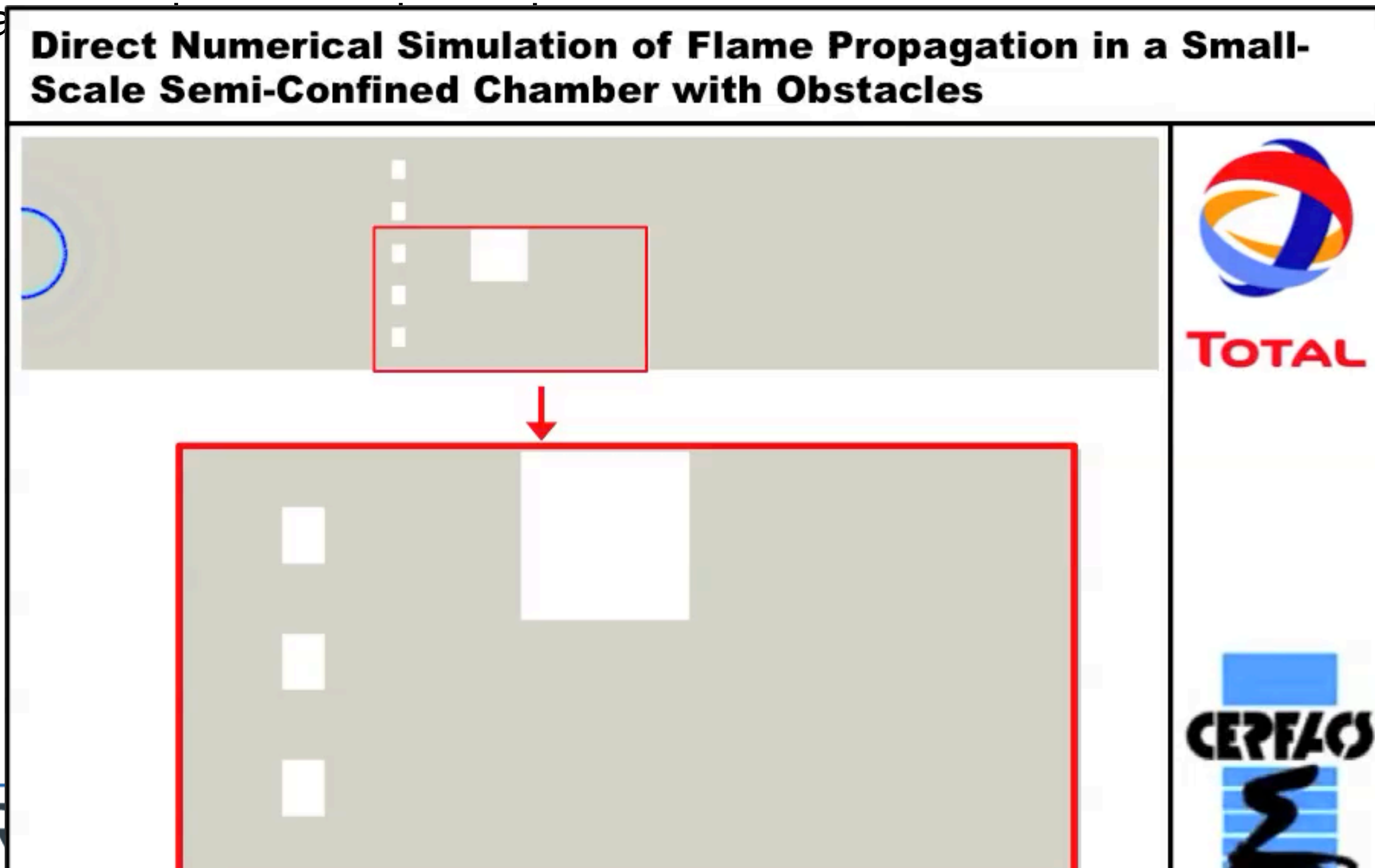
But they produce a **dilatation** effect which pushes gases away from them and creates turbulence

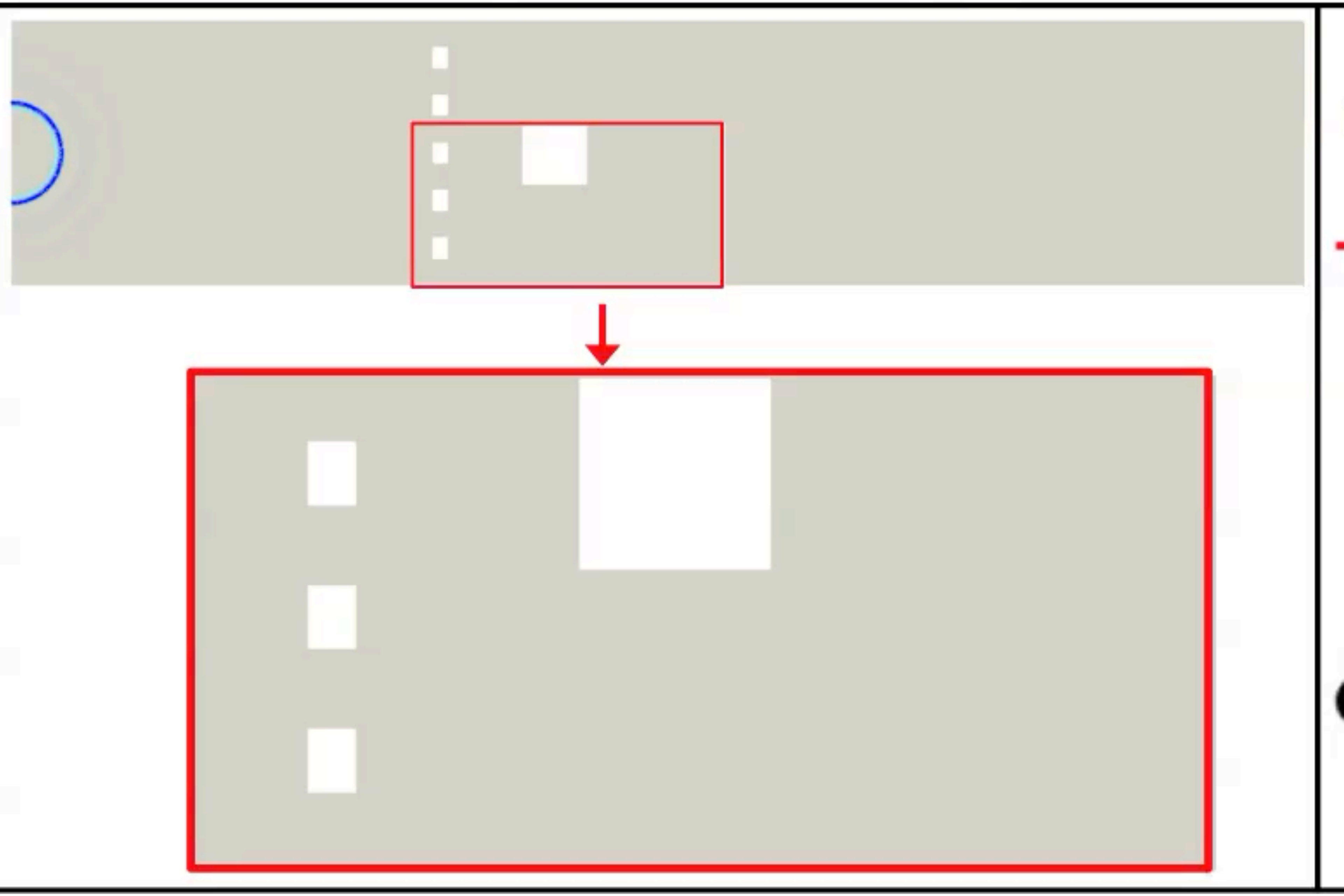
When flames enter the zone of turbulence they created, they accelerate.

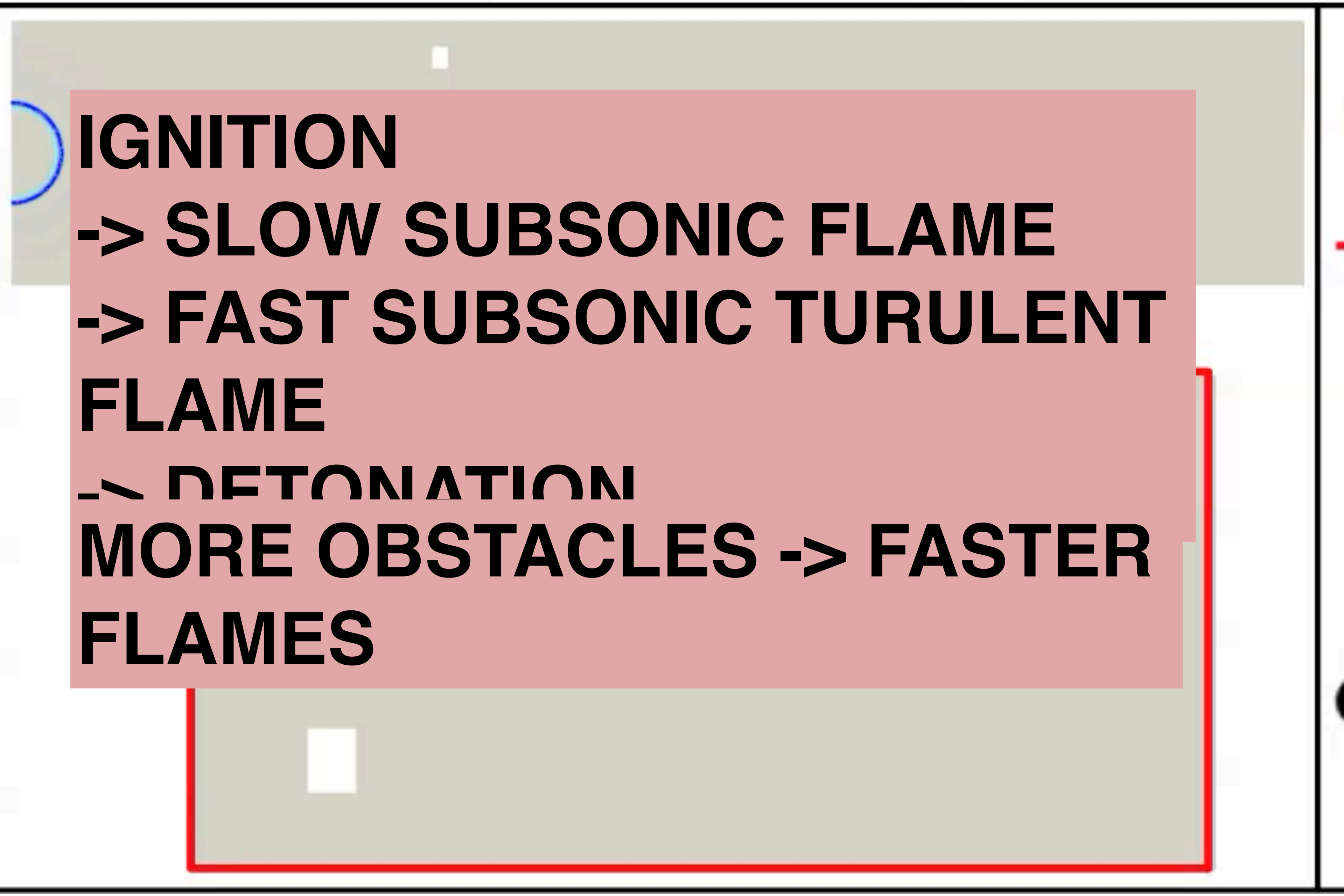
This process is **self sustained,** speeds the flame up from 0.5 m/s to hundreds of m/s

Then flames start moving fast enough to catch up on the acoustic wave in front of them

and the fla





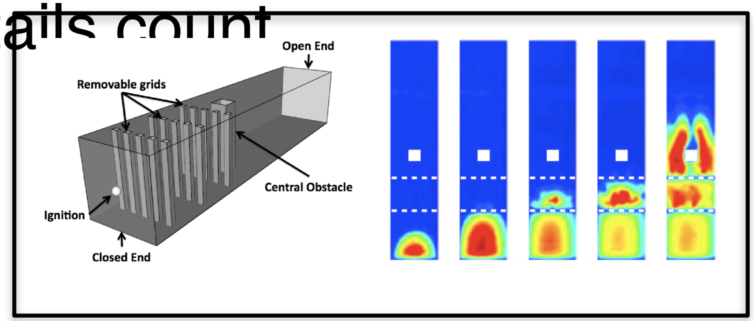


IGNITION
-> SLOW SUBSONIC FLAME
-> FAST SUBSONIC TURULENT FLAME
-> DETONATION

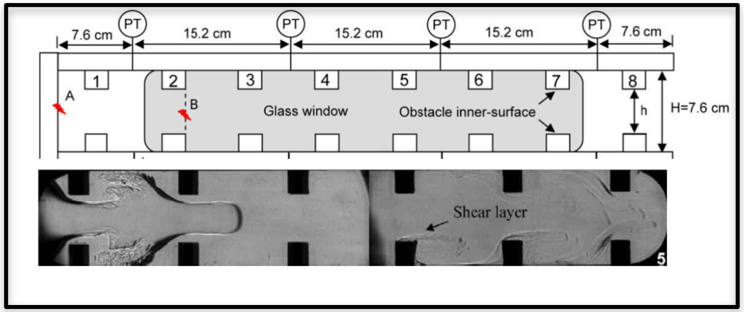
MORE OBSTACLES -> FASTER FLAMES

Deflagration scenarios in venting chambers

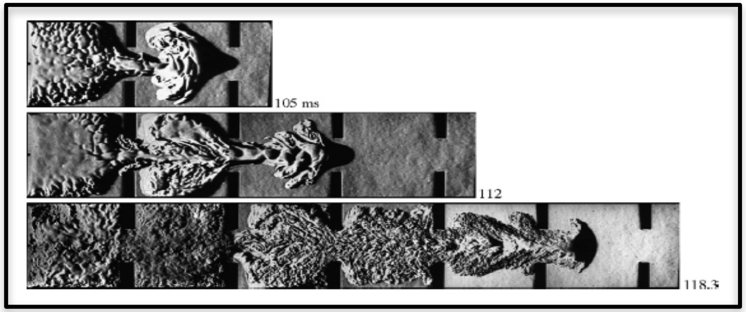
Use of small and simplified configurations: unfortunately, nothing is ‘generic’. Each case is special, all geometry details count



Sydney Univ.
Masri *et al.*, IECR 2012
Semi-confined
CH_4, C_3H_8, H_2



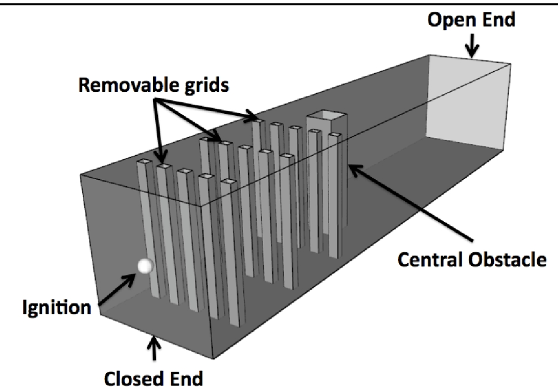
Queen’s Univ.
Johansen *et al.*, CF 2009
Confined
C_3H_8

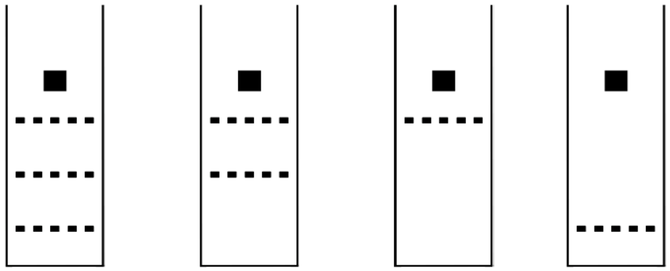


Gravent database, TU Munich
Vollmer *et al.*, CST 2012
Confined
H_2

Semi-confined explosion chamber from Sydney Univ.

- 5 x 5 x 25 cm
- Perfectly premixed fuel/air mixture
- Fuel :
  - C_3H_8
  - CH_4
  - H_2
- Flow initially at rest
- One central obstacle
- 3 (removable) baffle plates
- Laser ignition at the closed end
- Various geometric arrangements
- About 50 experimental shots for each configuration.

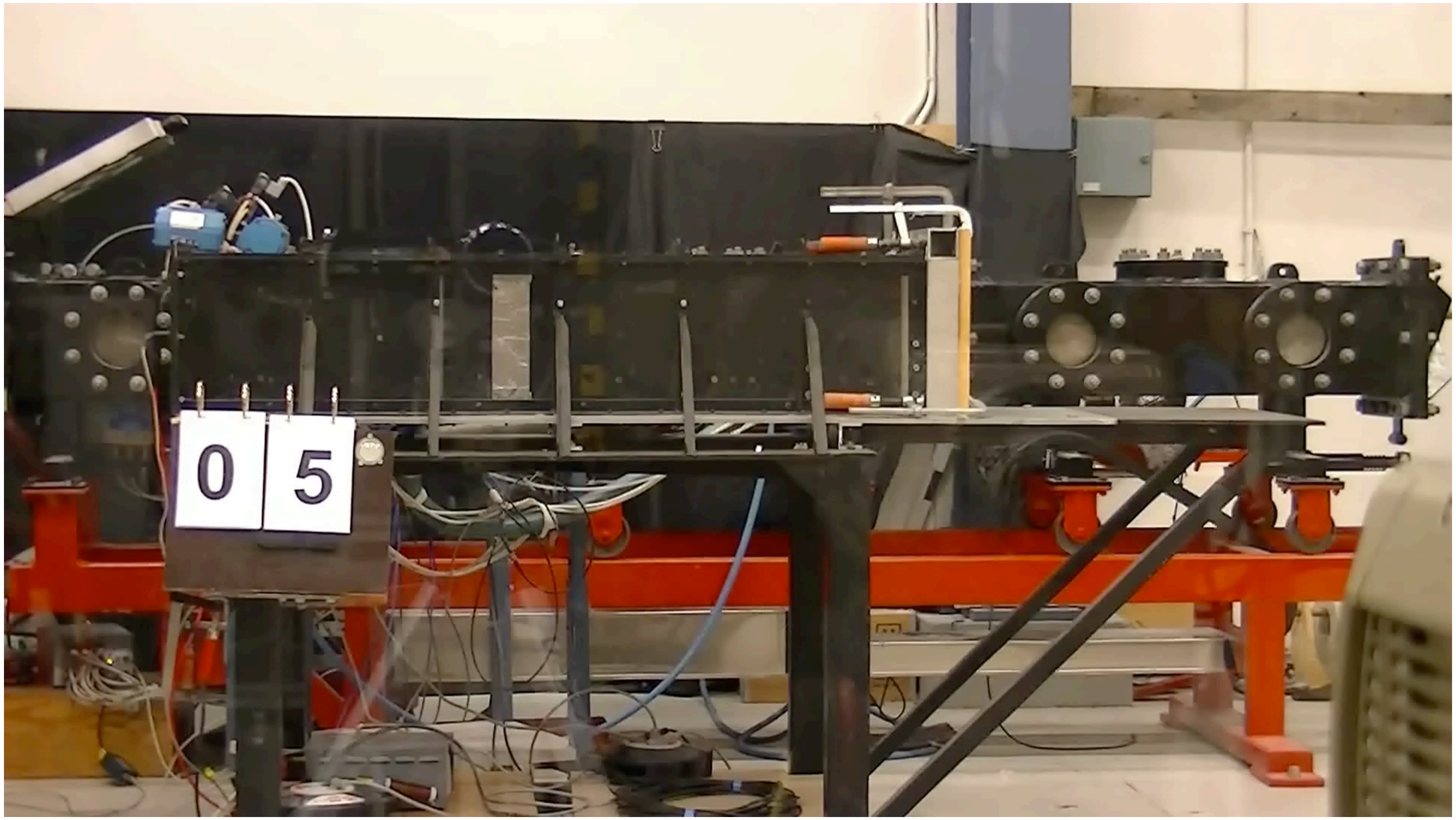




Small dimensions, a lot of experimental data, various configurations
➔ well suited for simulation validation!

A.R. Masri et al. IECR 2012

Visualisation of gas explosion

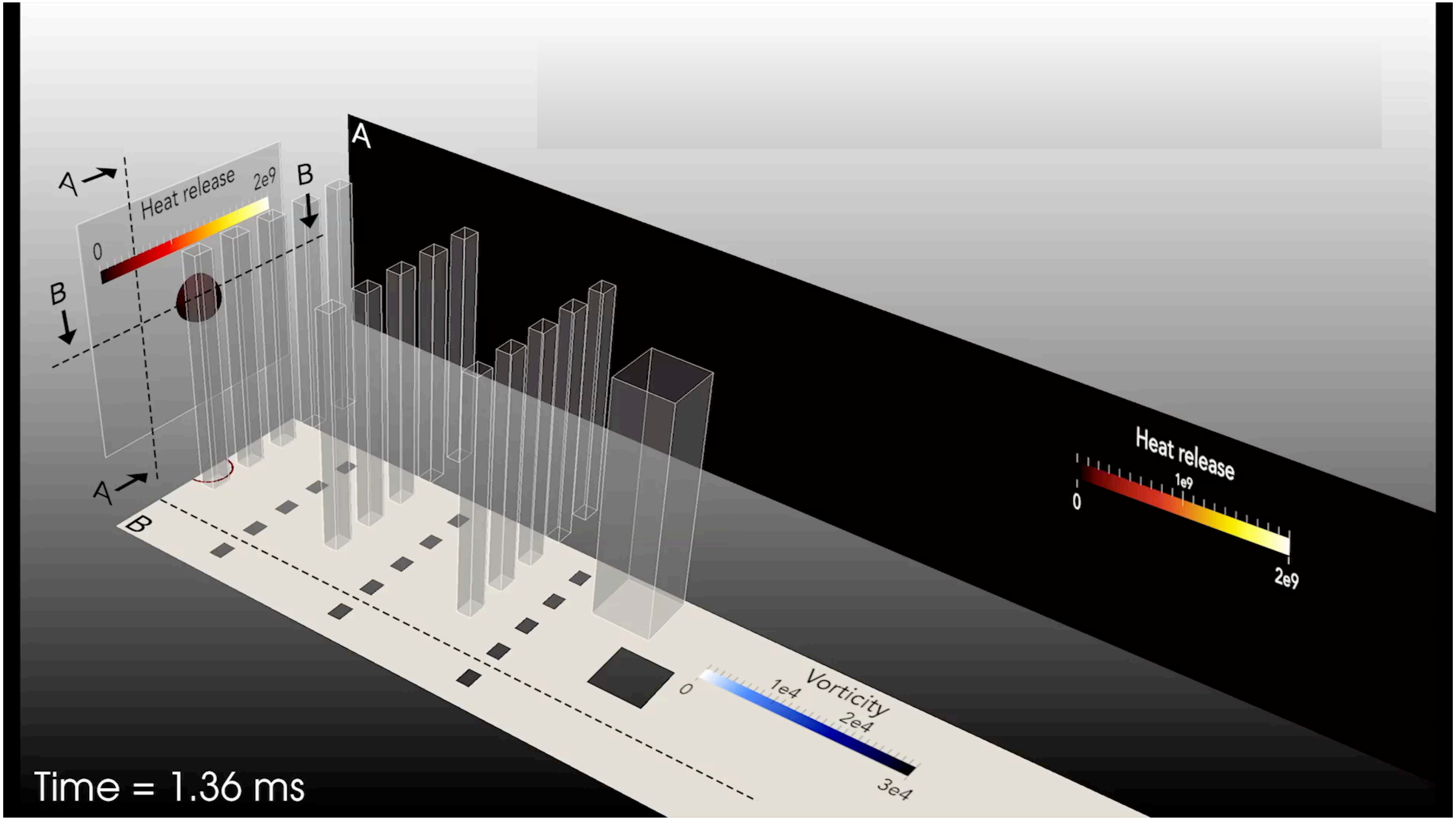


Experiments by GEXCON

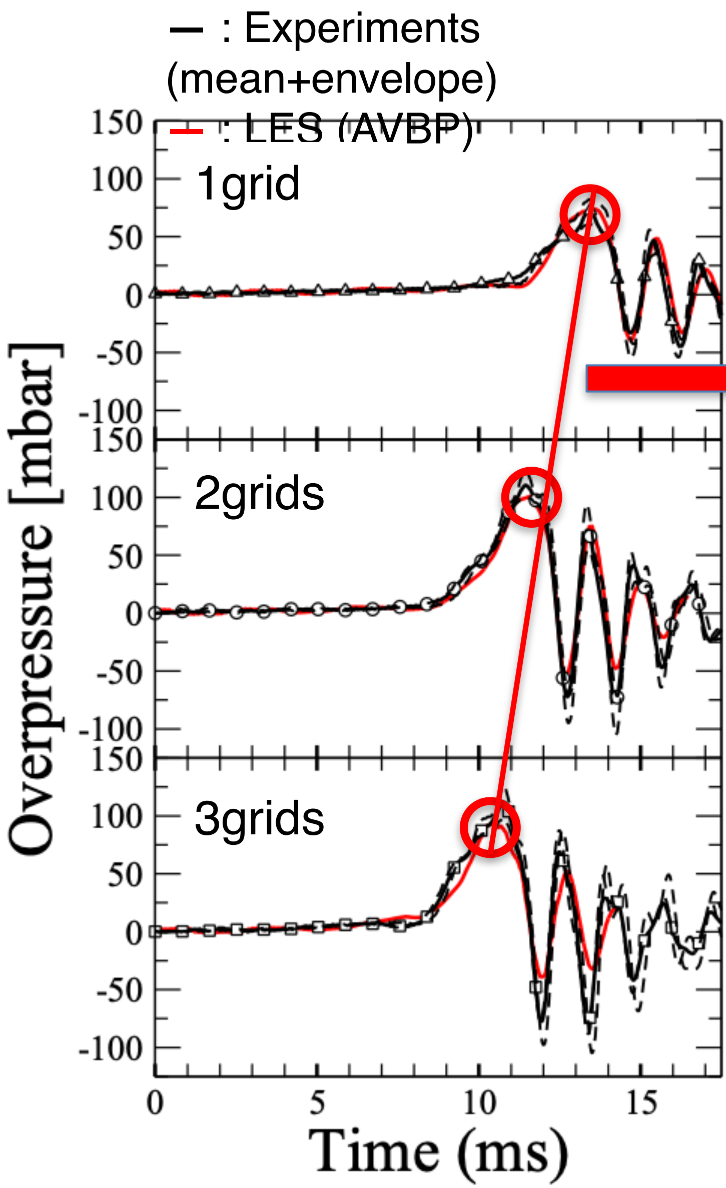
Visualisation of gas explosion

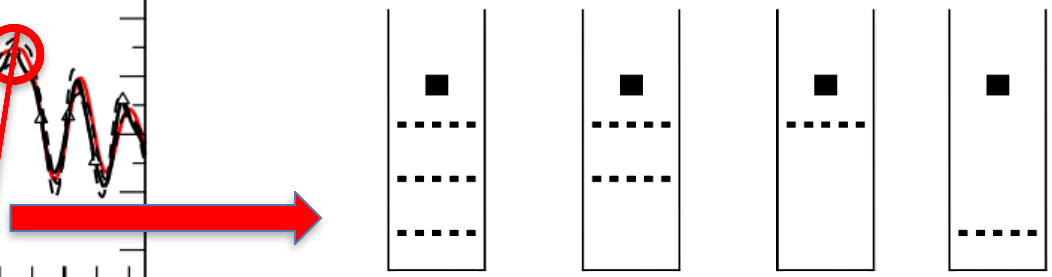
Experiments by GEXCON

Large Eddy Simulation with AVBP

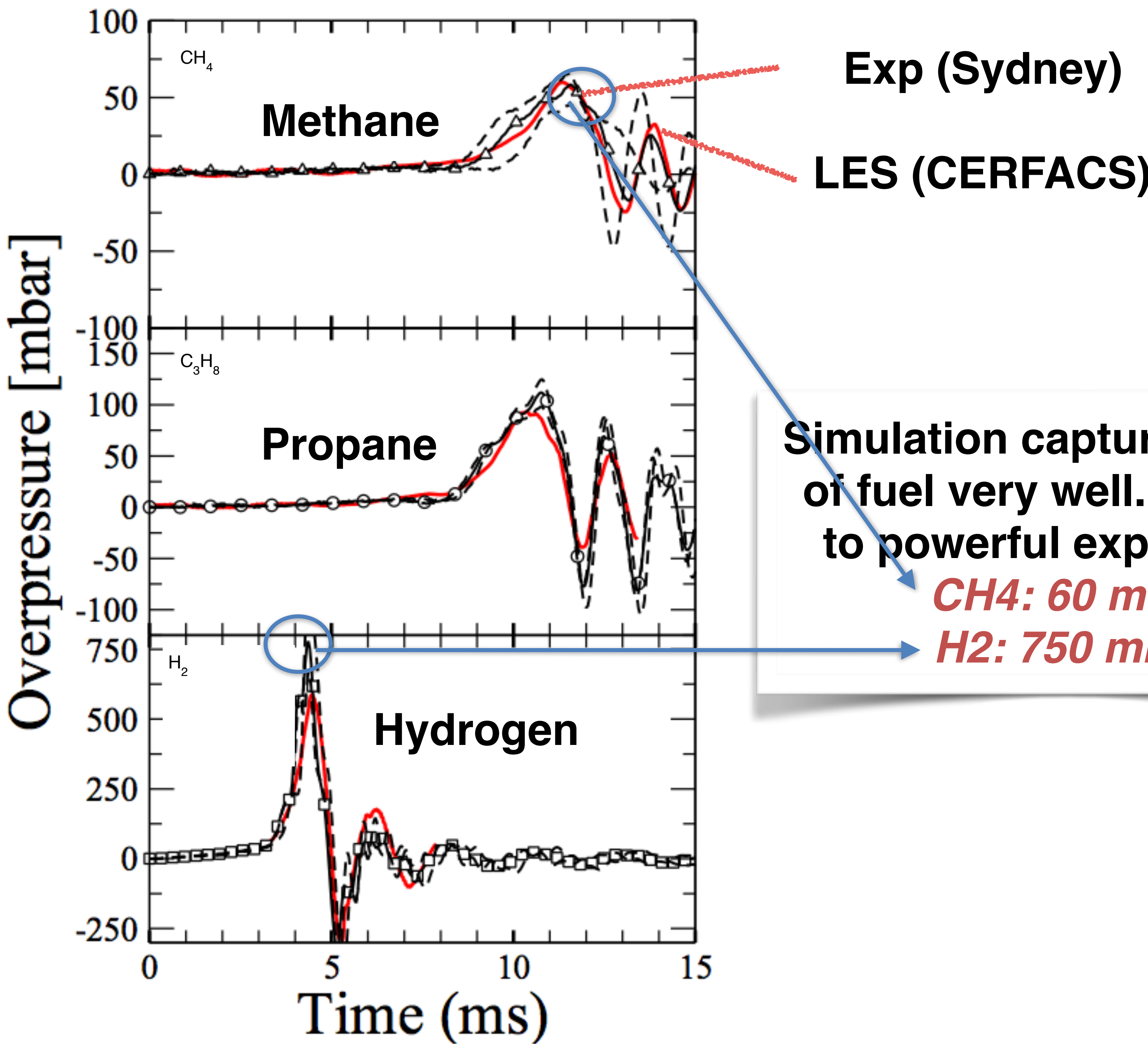


Influence of the number of grids (1, 2 or 3)





- → More obstacles: more danger
- → Simulations capture the maximum overpressure
- → Influence of the number of grids correctly predicted

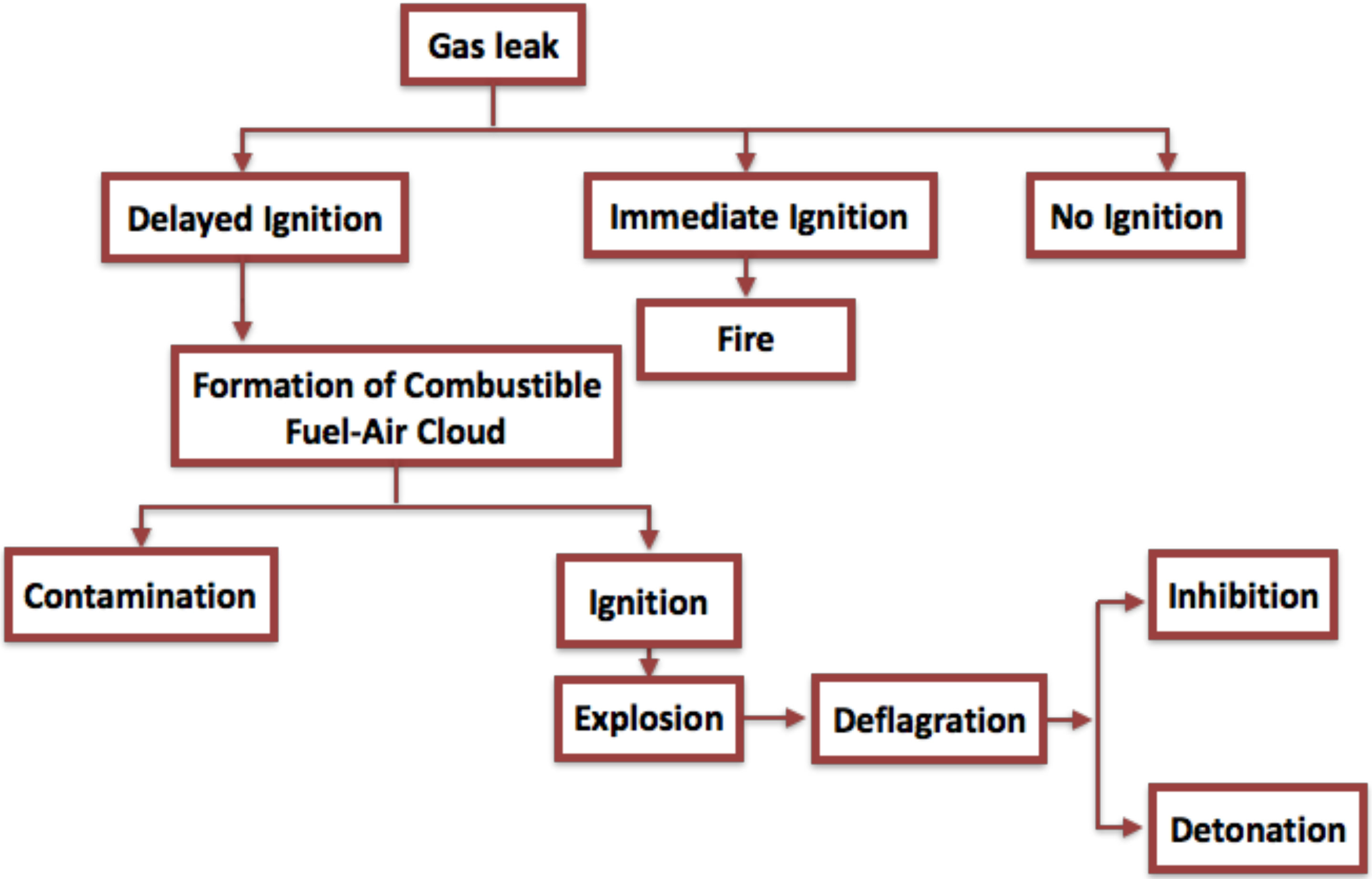


Simulation captures effects of fuel very well. H2 leads to powerful explosions:

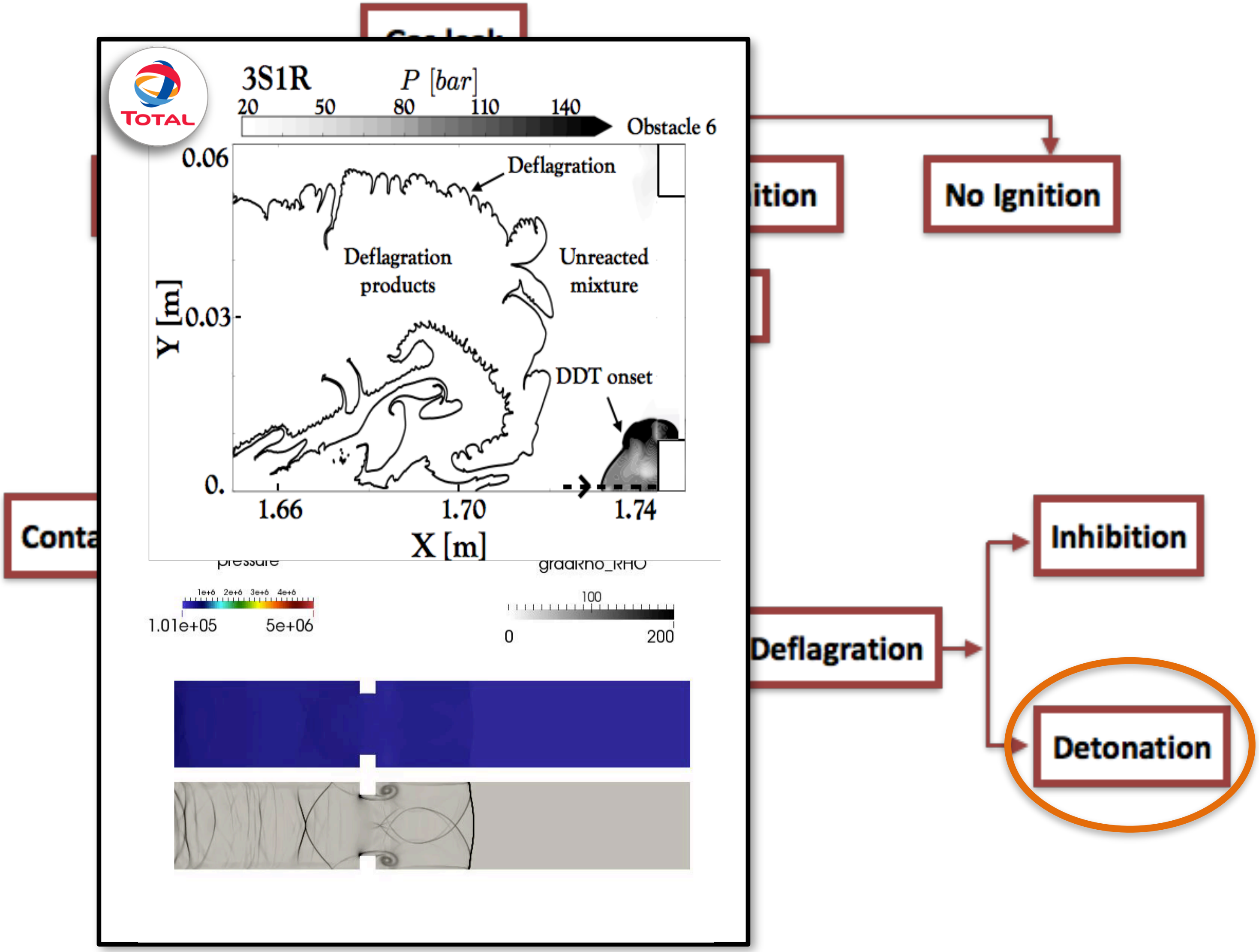
CH4: 60 mbar

H2: 750 mbar

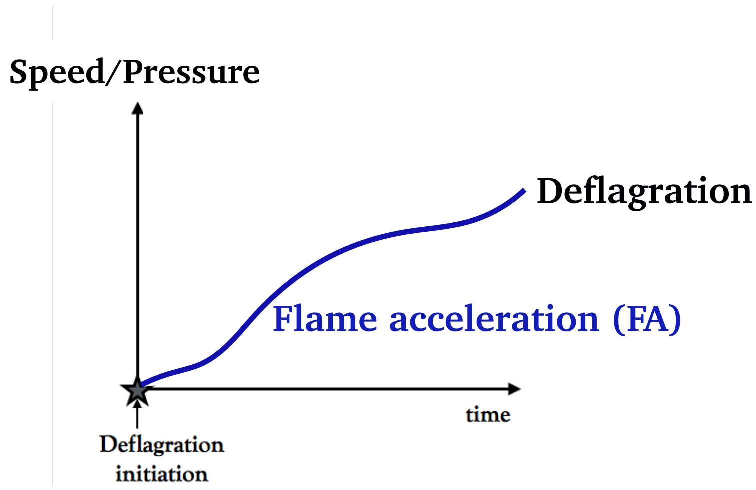
Safety activity at CERFACS

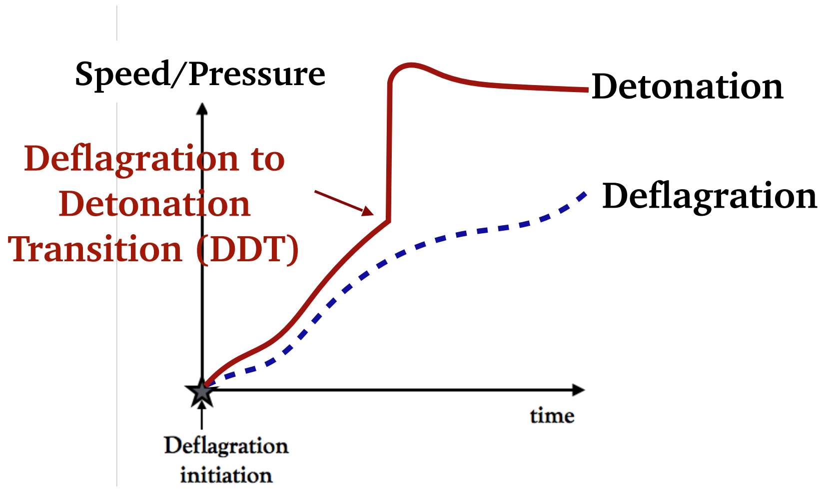


But things can get worse: detonations



Two different regimes of 'explosion'





Subsonic flames:

- Moderate velocities (0.5 m/s)
- Moderate overpressure (< a few bars)

Supersonic shock-flame association:

- High velocities (2 km/s)
- High overpressure (100 bars)

Going to detonation:

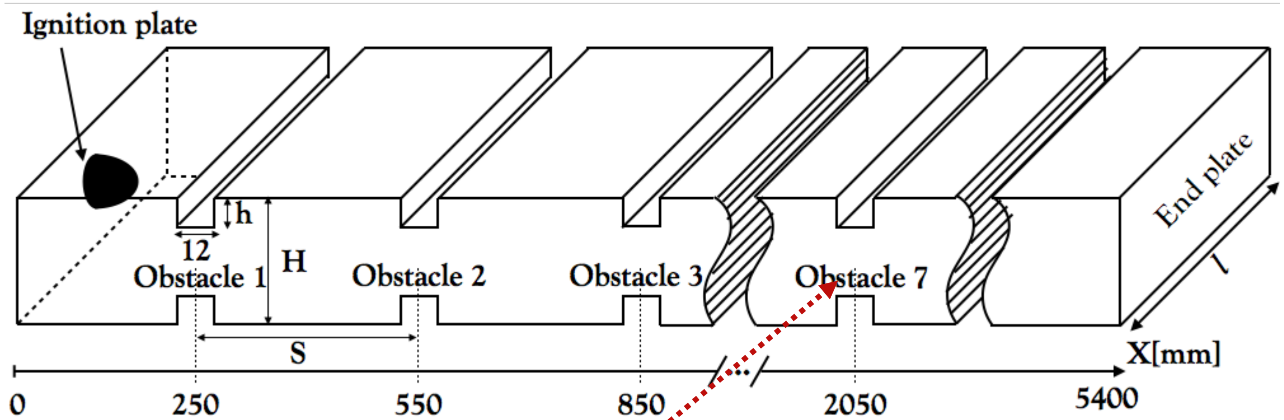
Predicting the speed of subsonic flames propagating in a turbulent flow is one of the main unsolved research topics for the combustion community. For these subsonic flames (deflagration), overpressure will be of the order of mbar to bar

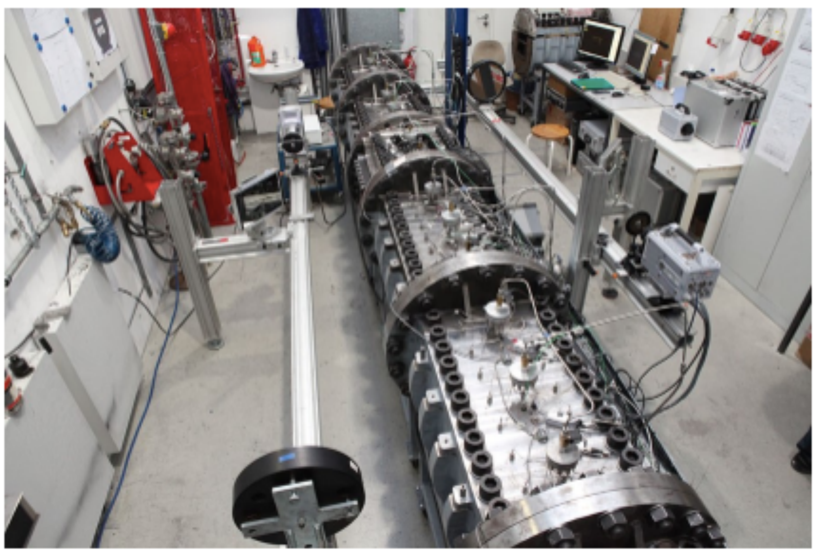
But going to detonation will lead to overpressure of 50 to 300 bars…

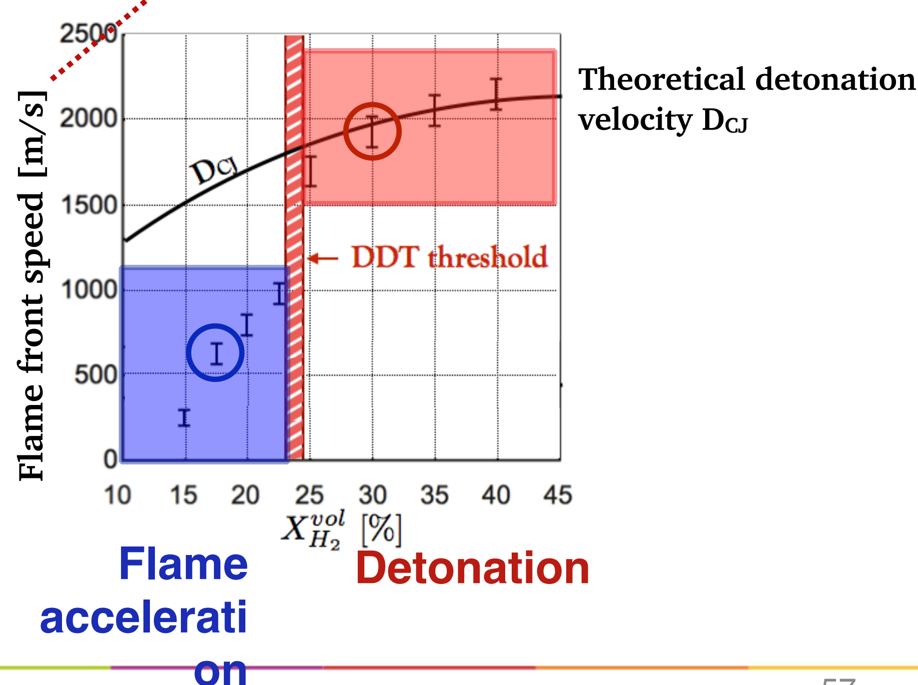
Predicting whether a subsonic flame will lead to detonation is the second unsolved problem of our community

Gravent database (TU Munich): example of deflagration and of detonation

- H_2/air mixture
- Blockage ratio 0.3



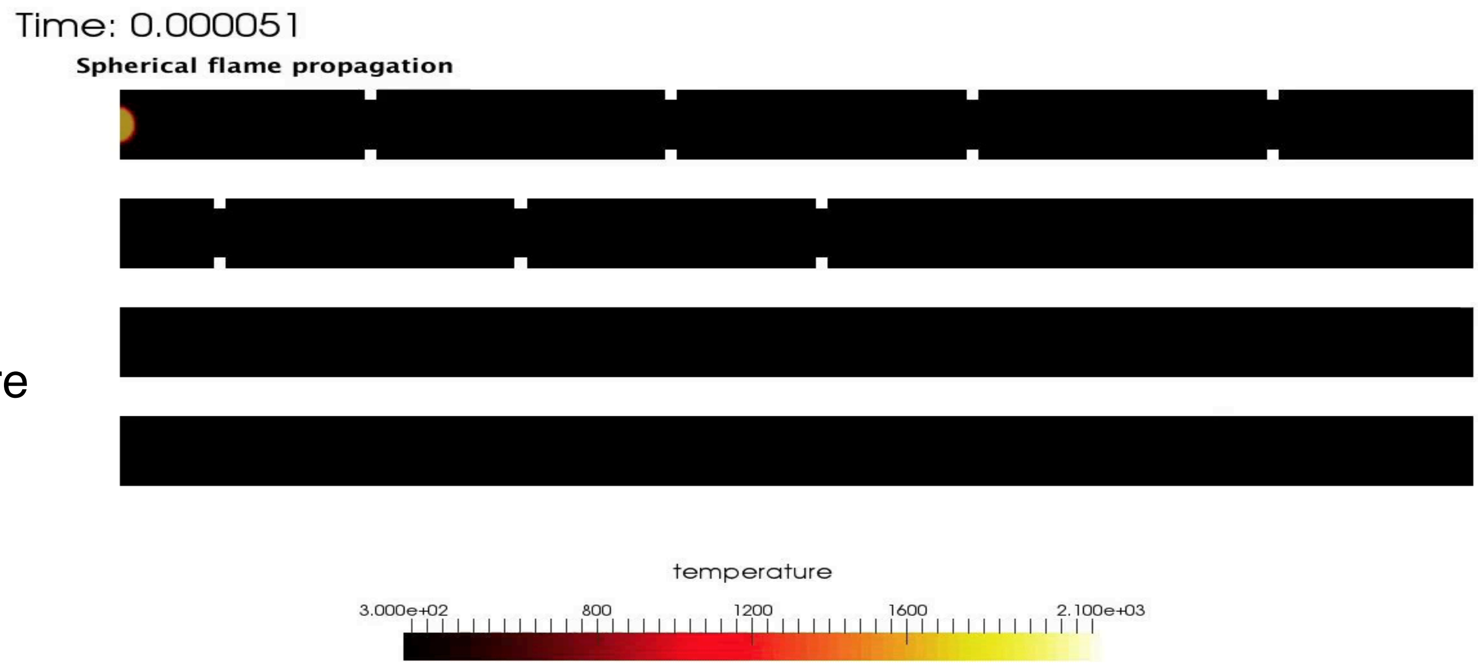




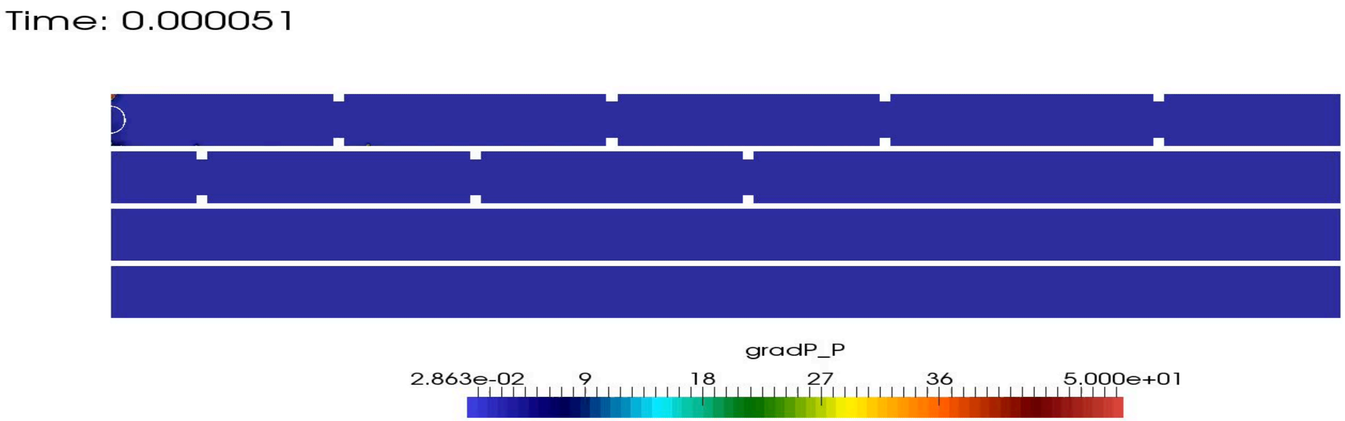
http://www.td.mw.tum.de/ddt/

Deflagration case (phi=0.52)

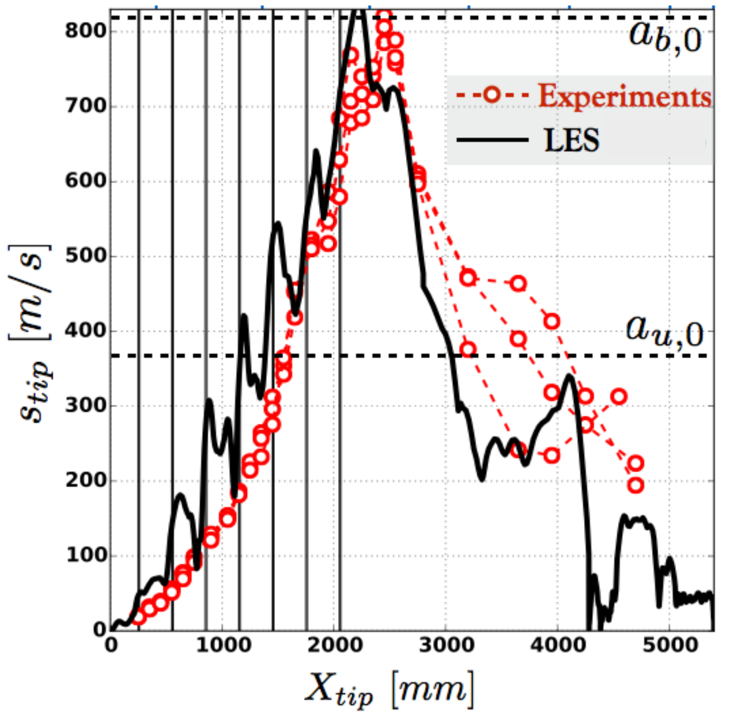
Temperature



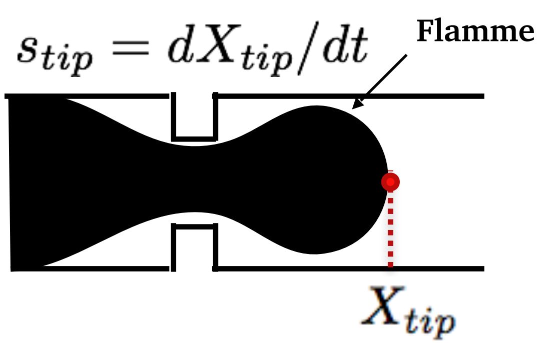
Grad(P) / P

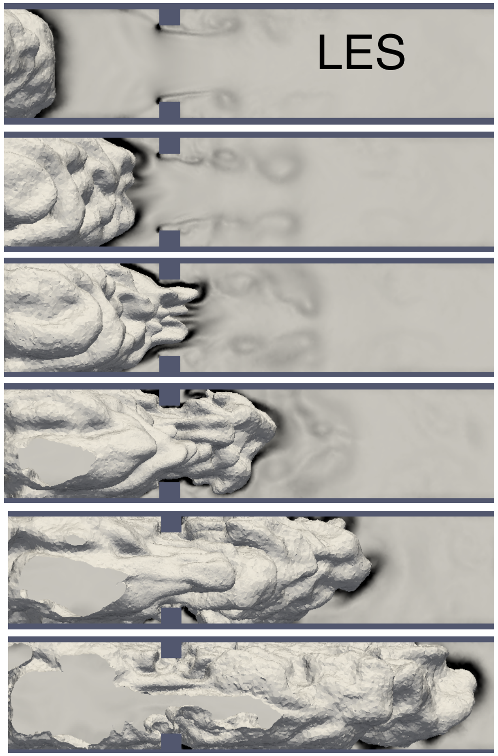


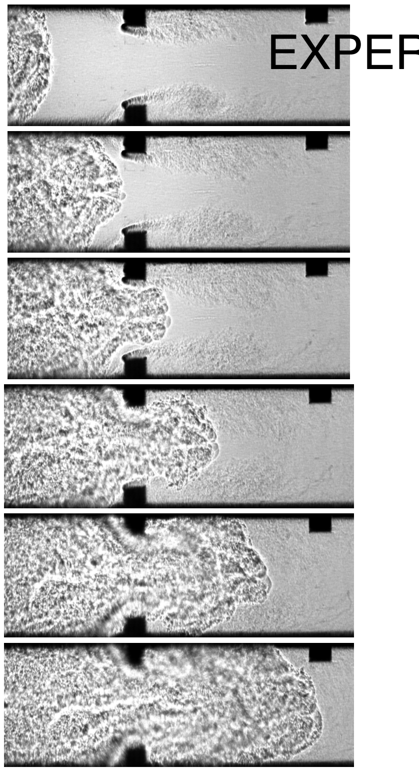
Deflagration case (phi=0.52)



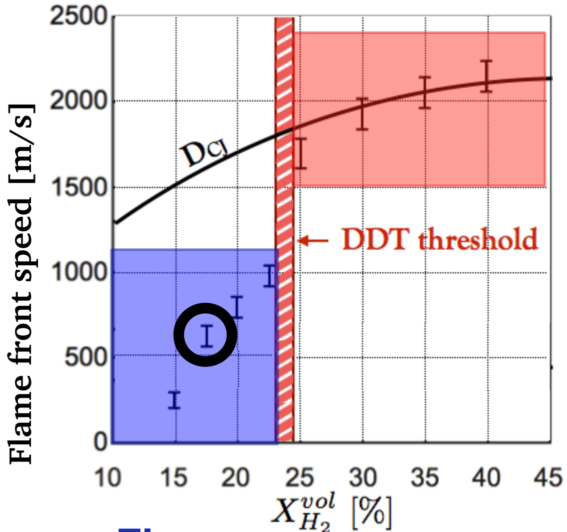
$$s_{tip} = dX_{tip}/dt$$







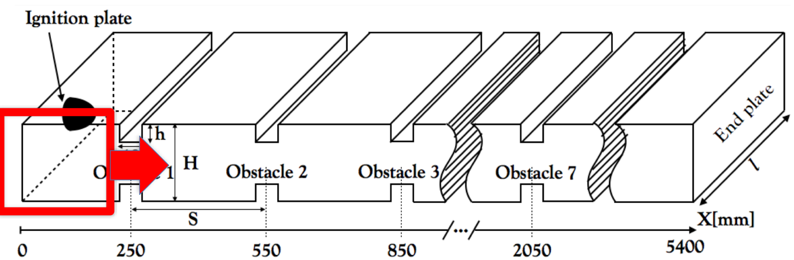
Detonation case (phi=1.0): put more H2 in the duct

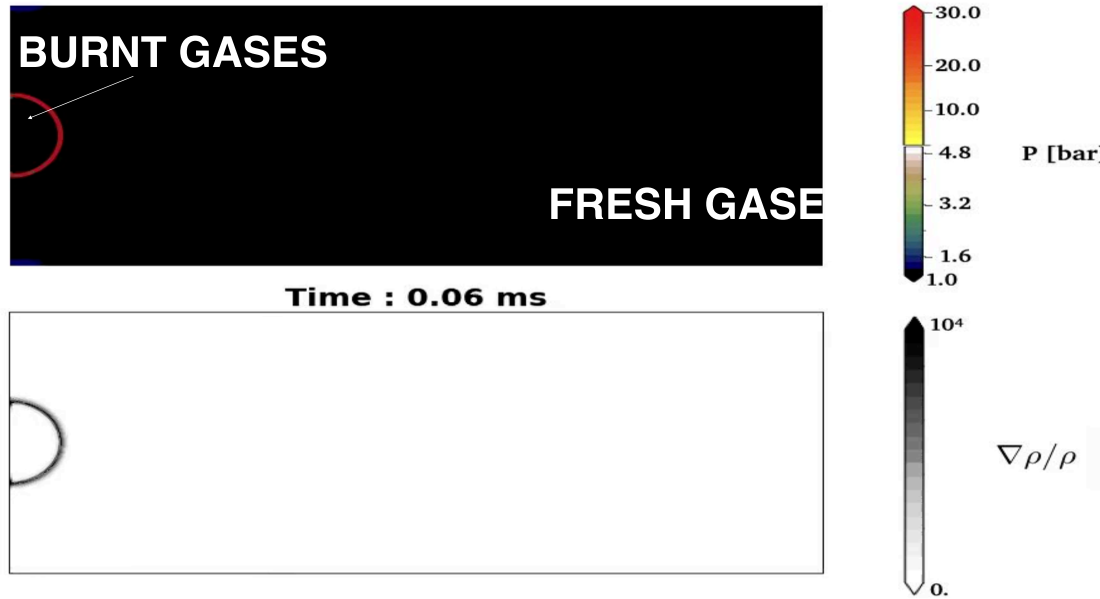


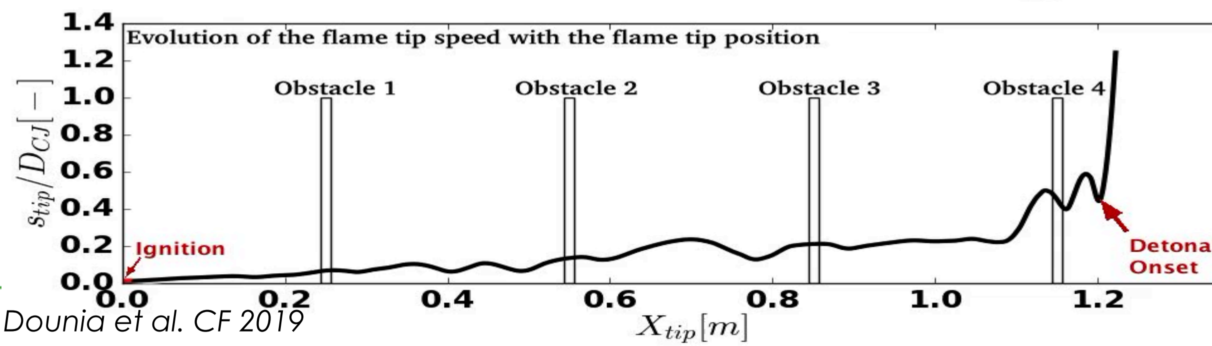
Flame acceleration

Detonation

Detonation case (phi=1.0)





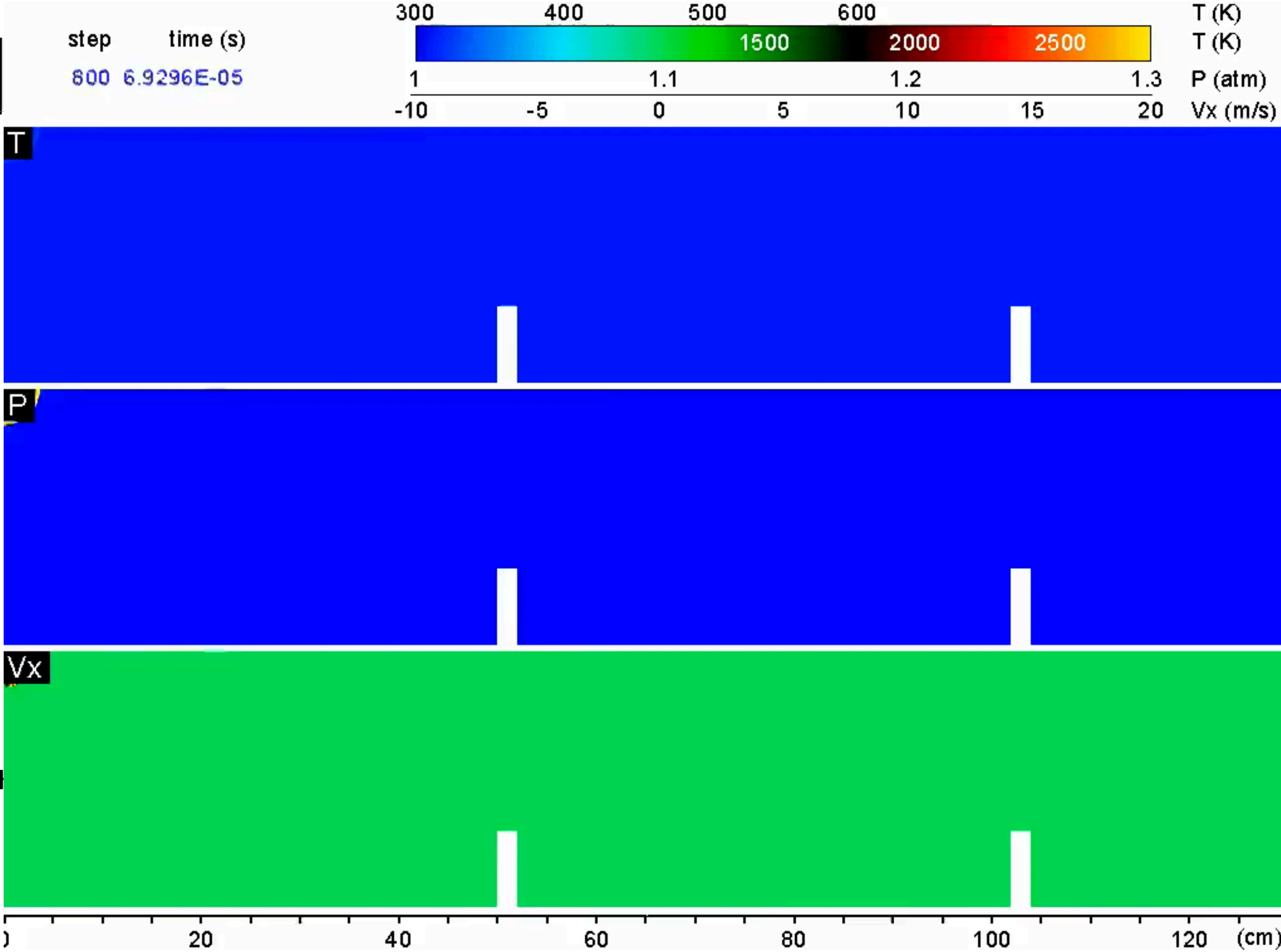


CERFACS

O. Dounia et al. CF 2019

O. Dounia, Q. Douasbin, O. Vermorel

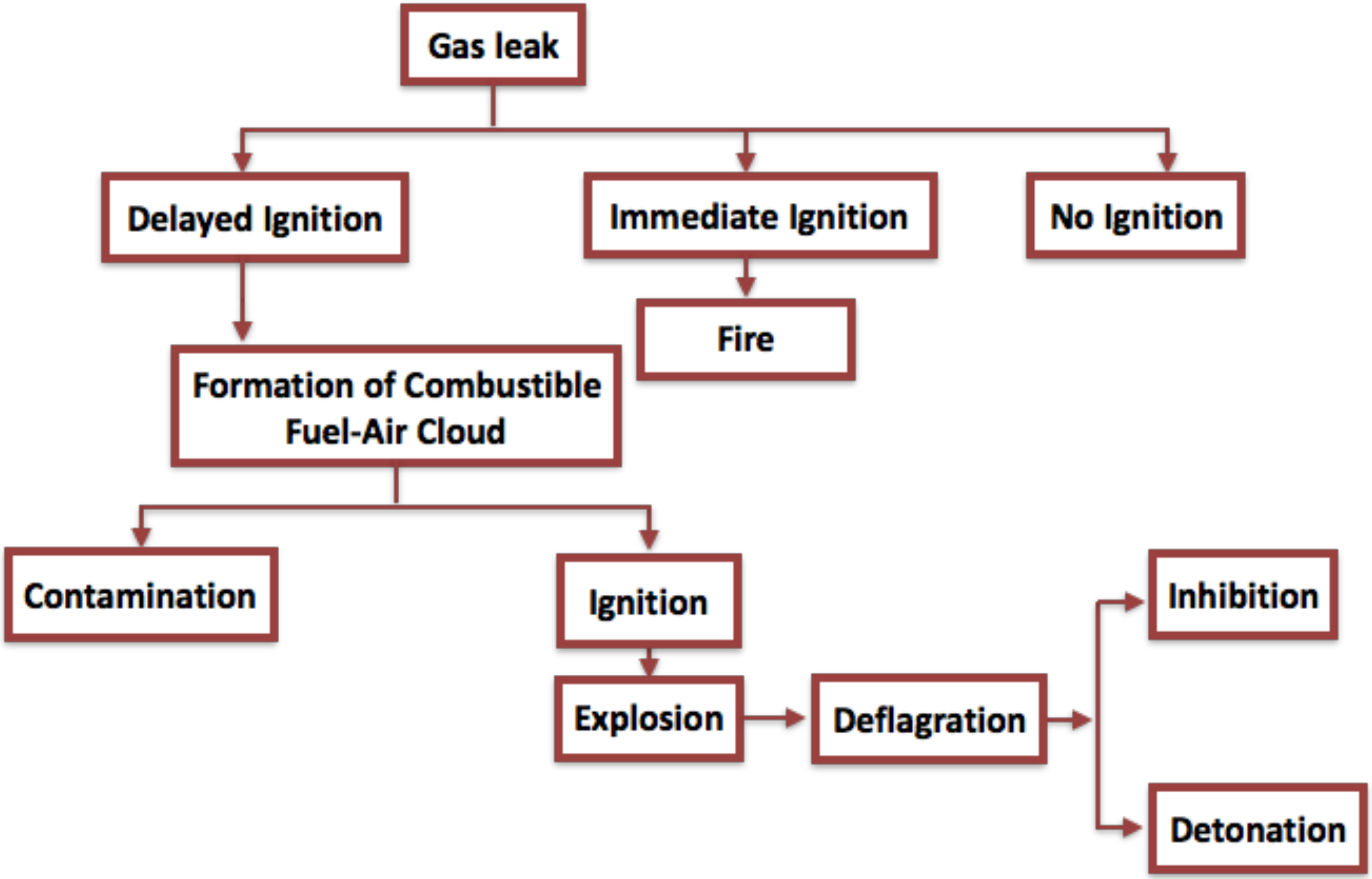
ANOTHER EXAMPLE (E. Oran)



On what does DDT depend ?

- On the composition
- On the mixing: stratified mixtures usually detonate faster (counter intuitive)
- On the geometry and the presence of obstacles

Mitigating flames ?



Mitigation: trying to limit the effects of flames

Objectives:
- stop the flame
- if impossible, let the flame propagate but slowly
- avoid detonation at all costs…

How:
- inject water mist
- inject powders
- inject inert gases (N_2, CO_2)
- add obstacles, flame arrestors

P. Hoorelbeke, *PhD, Brussel Univ. (2011)*

Mitigation: injecting powder into the air (TotalEnergies)

NOT TRYING TO AVOID COMBUSTION:
ONLY TO MAKE IT SLOWER AND LESS DESTRUCTIVE

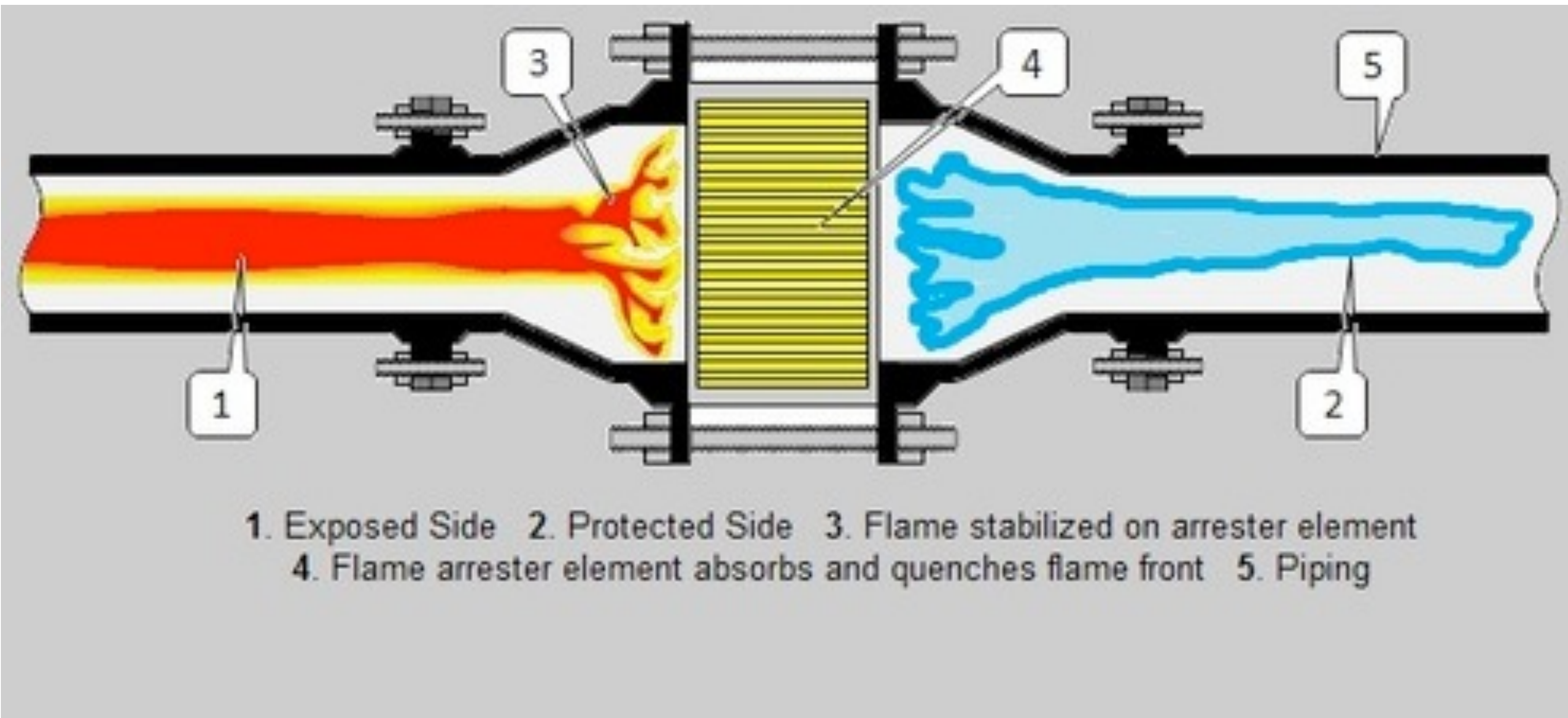
STANDARD CASE

WITH INHIBITORS BEFORE IGNITION

P. Hoorelbeke, *PhD, Brussel Univ. (2011)*

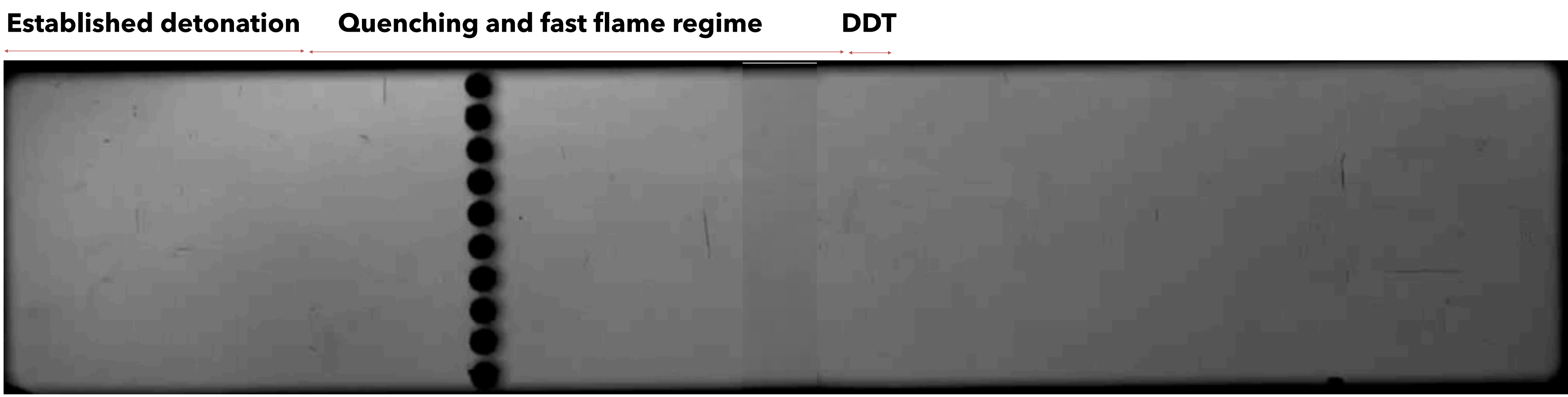
Can we stop detonations with obstacles ?

- We can stop deflagrations with special flame arrestor devices:



But that does not work so well with detonation…

- DDT obtained from the interaction with an obstacle (Radulescu, U. Ottawa)

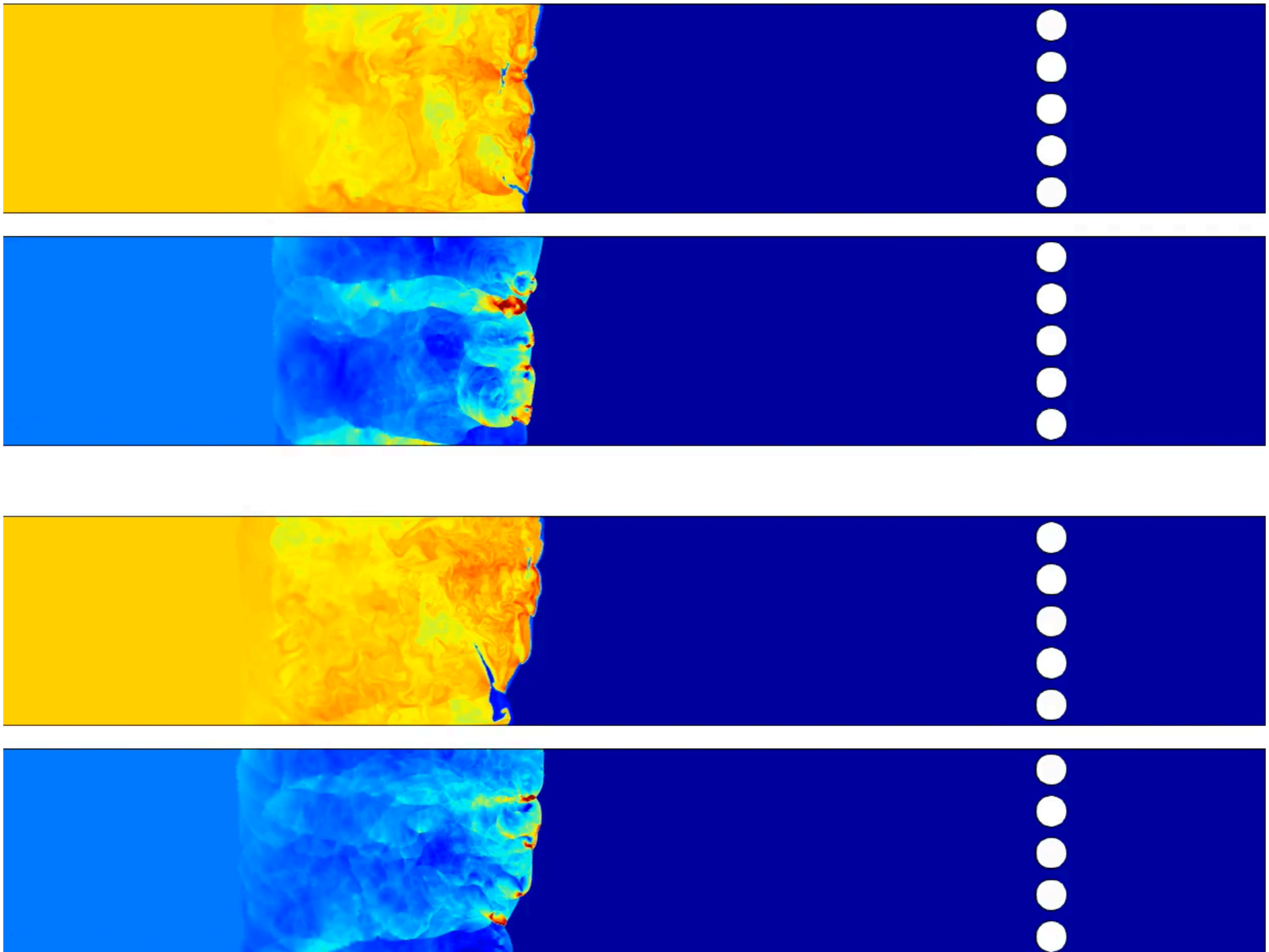


Experimental shadowgraph of reinitiation [ref]
($CH_4 + 2O_2$, P=8.2 kPa, 75% blockage ratio)

- In practice, very difficult. Once it has started it is too late
- Flame transmission through holes is another topic in itself…

Can we stop a detonation at 2 km/s ?

2D DNS of a similar case (O. Dounia, CERFACS)



Decarbonization of aviation

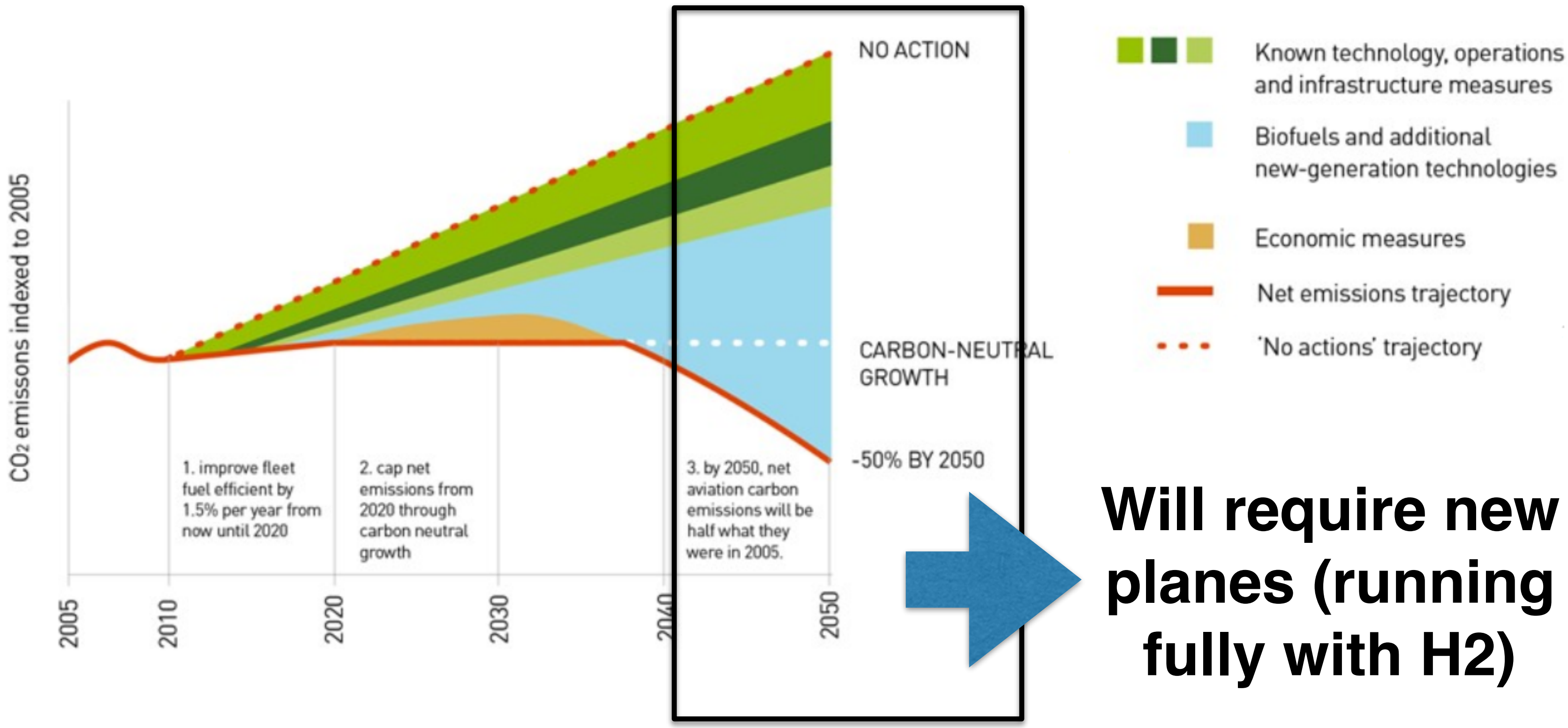
HYDROGEN AND AIRCRAFT

Yes, there will be hydrogen available almost everywhere

Which leads to the next question:

Can we make H2 fly ?

Airbus research focused to support sustainable growth (BEFORE COVID)



Will require new planes (running fully with H2)

Hundreds of engineers on the H2 air aircraft in Toulouse

BRING AND STORE H2 ON THE PLANE

H2 can be stored:

- **A: gaseous at high pressure (700 bar, 300 K)**
- **B: liquid, cryogenic (1 bar, 20 K)**

Problem: in both cases, H2 is not very dense

- **A: gaseous at high pressure**

High pressure (700 bars) H2 tanks are simply too heavy to fly… In a H2 car like the TOYOTA, the tank weight is 130 kgs to store a few kgs of H2

- **B: cryogenic at one bar but 20 K**

Here the problem is not mass but volume of the tank:

Kerosene creates LESS energy than H2 per kg. Heat of reaction of H2 = 2.2 PCI of kerosene for one kg. GOOD

Kerosene is MORE dense: Density of kerosene = 800 kg/m3 Density of liquid, cryogenic H2 = 70 kg/m3. NOT GOOD

=> Replacing 200 tons of kerosene (220 m3) by H2 will lead to 80 tons of H2 (1100 m3 … at 20 K)

BACK TO THE AIRCRAFT

- Suppose that we can build the engine itself

- What about the aircraft ?

- Safety issues rapidly come forward. Similar as those found for buildings and process industry except that H_2 is cryogenic and that it must fly
  - Filling H_2 tanks at -250 °C
  - Transporting and storing large quantities of H_2
  - Leaks of H_2 (gas OR liquid): detection and protection
  - Public relations in case of accidents -> sociology

HYDROGEN AND SAFETY

- **TWO EXAMPLES:**
  - ★ **EXPLOSIONS DUE TO A IGNITION AFTER A H2 LONG TIME LEAK AND ACCUMULATION (ENGINE COMPARTMENTS BUT EVEN AROUND THE AIRCRAFT): This is the problem we just discussed…**
  - ★ **FIRES DUE TO A FLAME STABILIZED ON A LEAKING ELEMENT RELEASING H2**

Explosions are not the only problem for H2: in many scenarios, if pressure goes up in the cryogenic tank, we may have to blow H2 out through a tube:

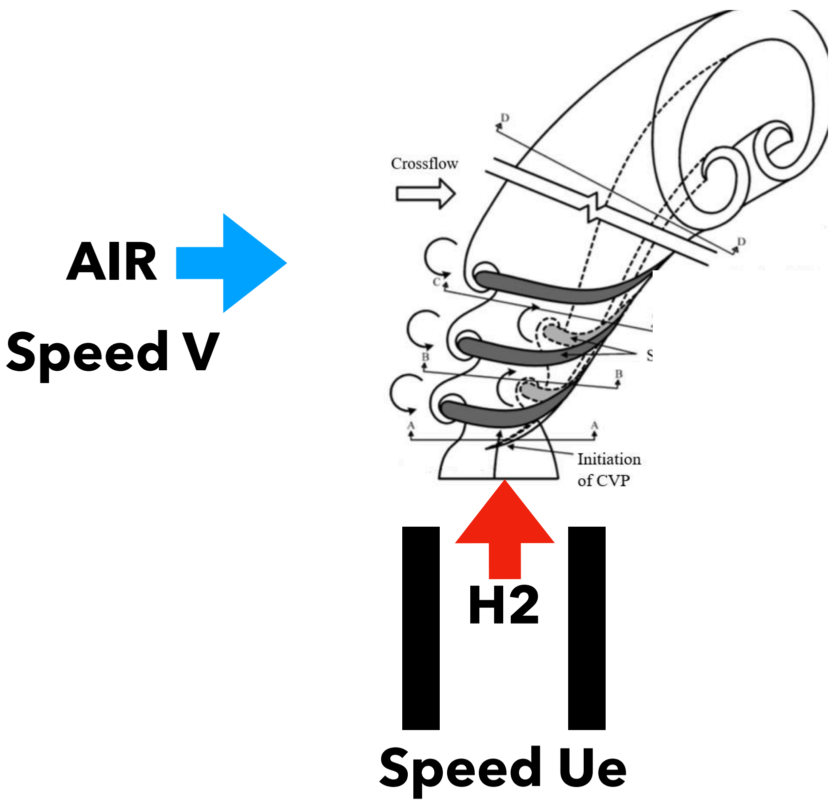
THEN TWO THINGS MAY HAPPEN WHEN H2 MEETS AIR:

NO IGNITION →

IGNITION →

REMEMBER A CASE OF ANCHORED FLAME ON AN AIRCRAFT:

What we know for a H2 jet into air:

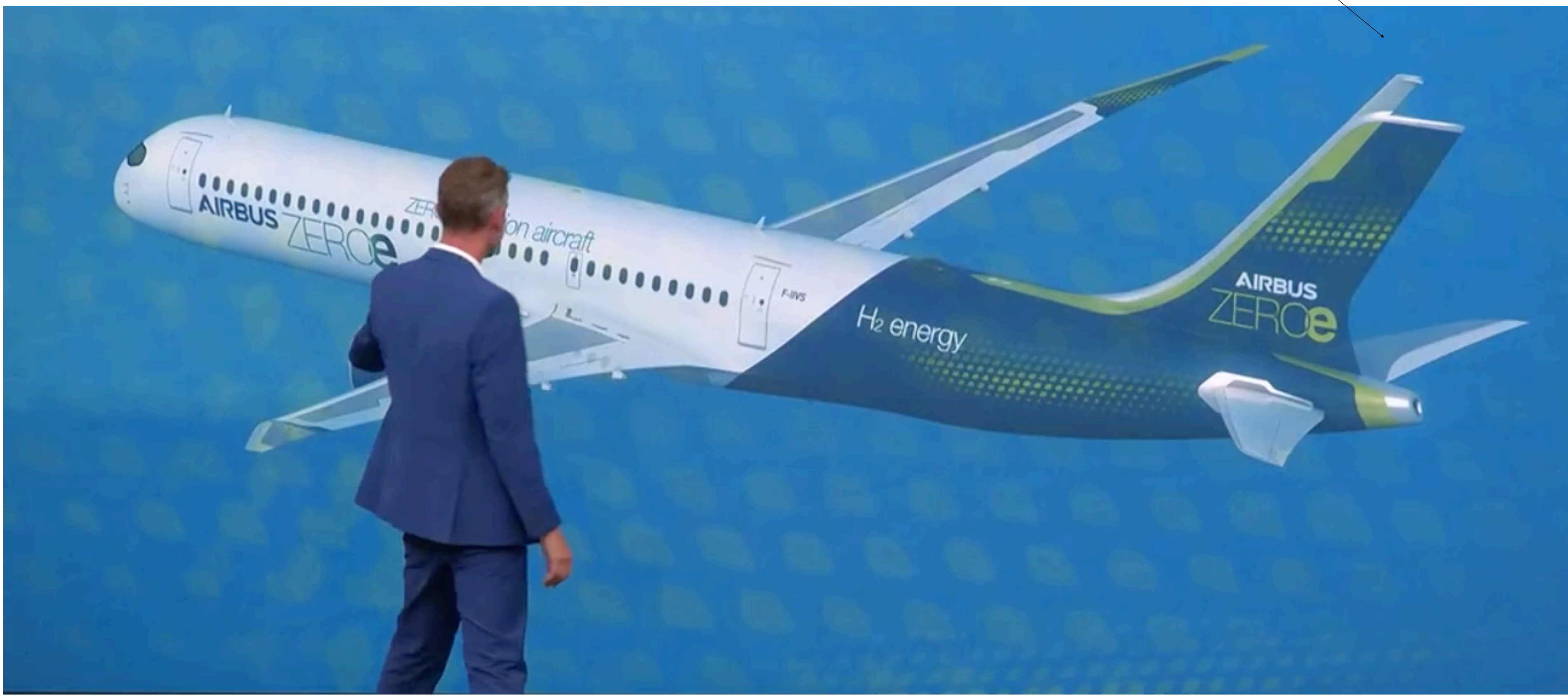


H2 jet flames will burn for all jet speeds Ue (other fuels don't)

We dont know yet at which speed V, a cross flow of air will quench a H2 flame but it is very large: a flame attached to a plane at Mach=0.5 will probably not quench

H2 jets can auto ignite if they are fast enough (tank pressure > 20 or 30 bar)

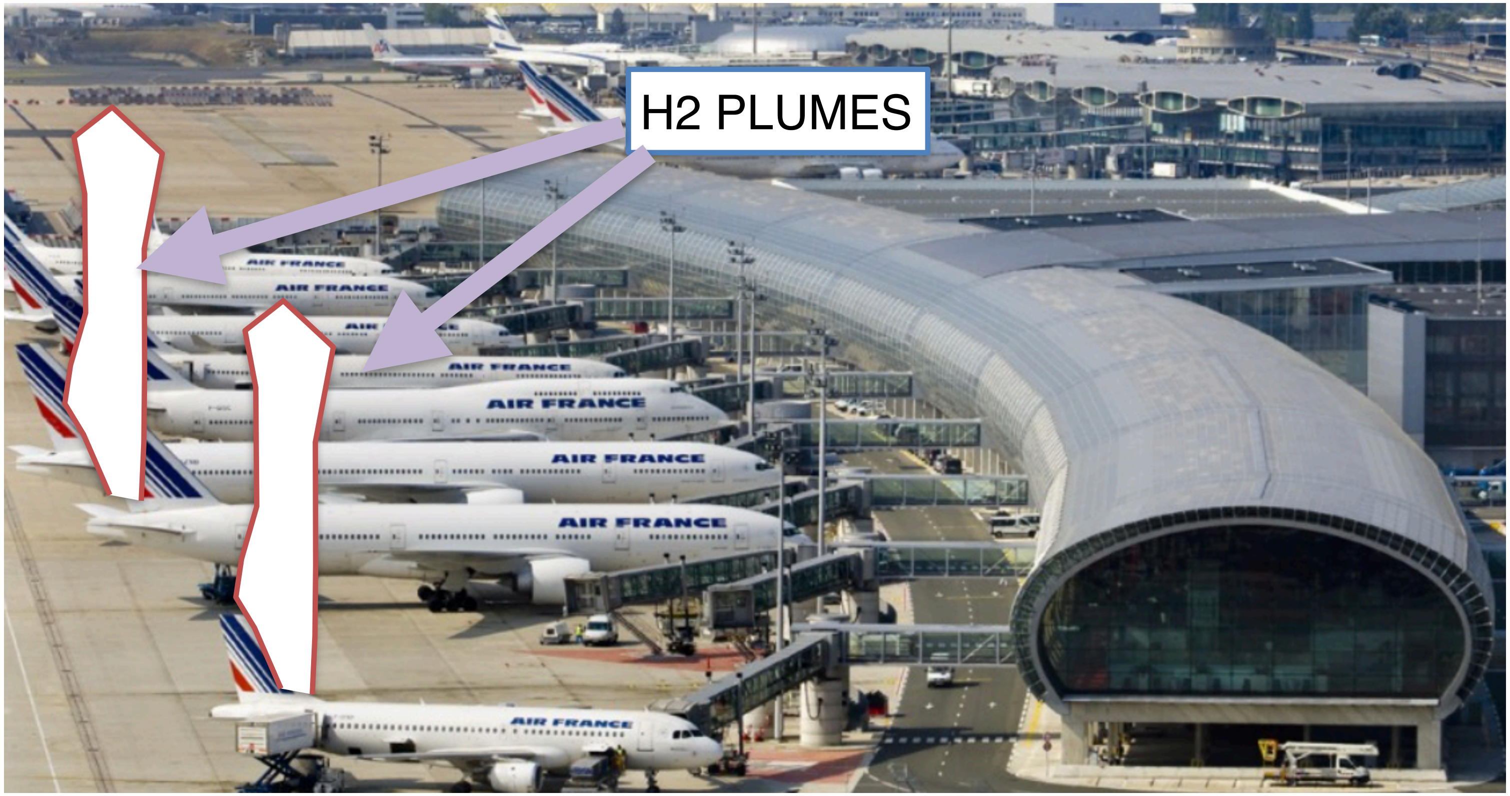
Designing an exhaust pipe for H2 which DOES NEVER allow anchoring will require some work



This is for a H2 jet produced at a place WE chose…

If we have a mechanical failure and the leak takes places anywhere in the engine for ex, similar problem… but more complicated to predict and control

Even if leaks are always produced through events we control, what about the overall effect of airliners releasing H2 in an airport ? Mixing with air will depend on weather conditions. Ignition sources will become an issue (no smoking…)



CONCLUSIONS

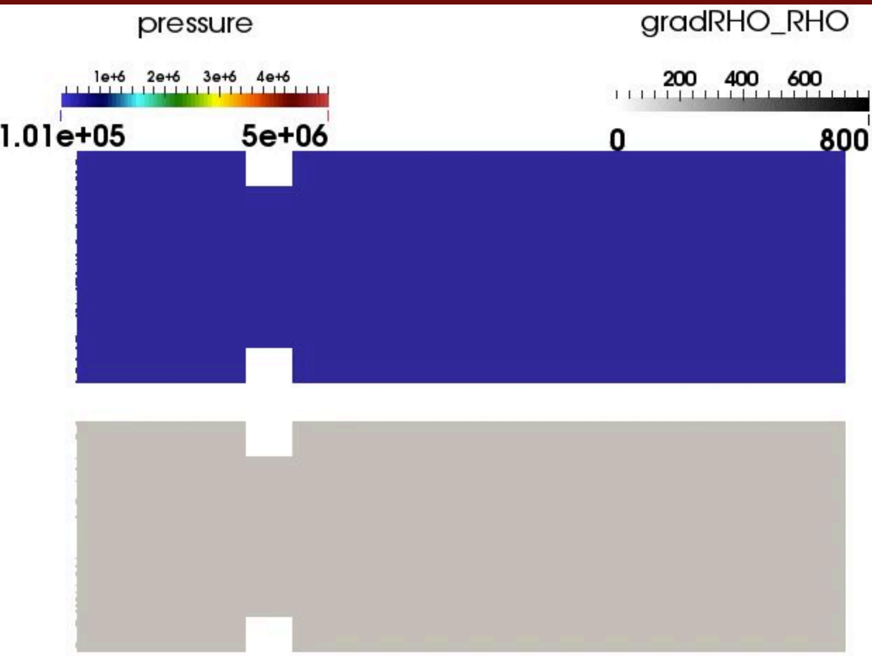
Numerical simulations of safety scenarios will grow, especially now that companies used to apply high-level, expensive CFD are involved (AIRBUS, SAFRAN)

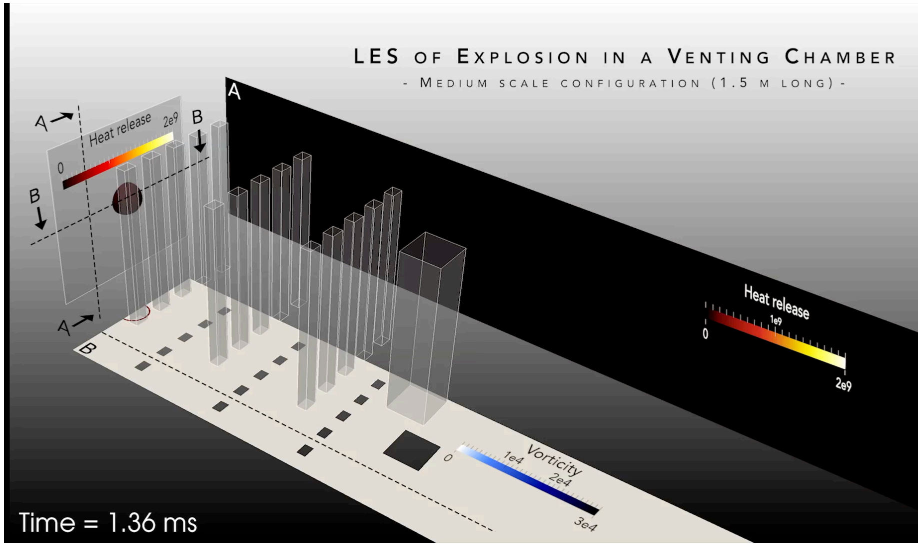
Specialized, well-validated codes will be available and used in conjunction with simple tools based on correlations, as observed for aerospace applications.

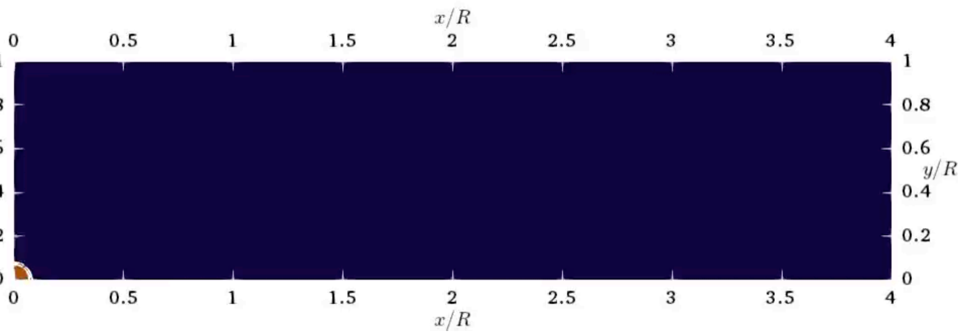
Using simulation to analyze safety scenarios is now possible but it still is expensive and relies on two difficult problems:

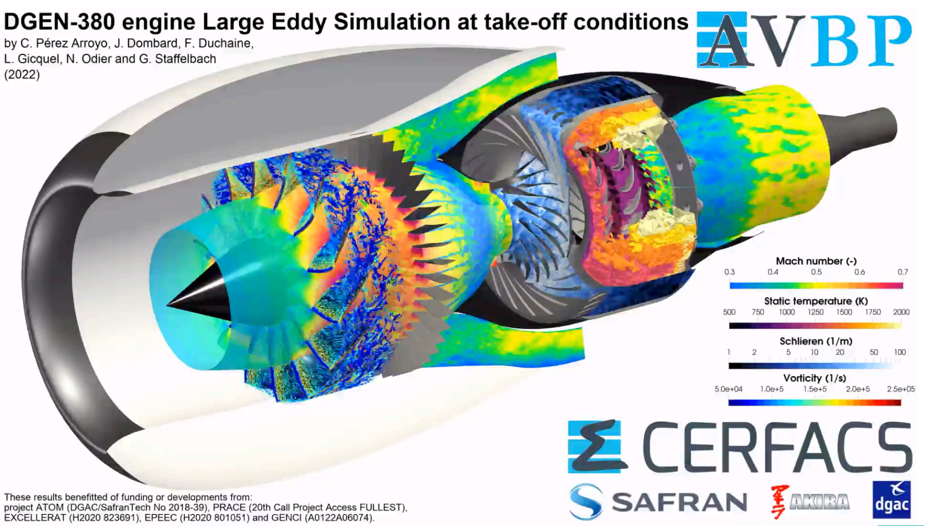
- **the speed of flames propagating in turbulent flows**
- **the transition from deflagration to detonation**

THANKS !


pressure
gradRHO_RHO
1e+6 2e+6 3e+6 4e+6
1.01e+05 5e+06
200 400 600
0 800


LES of Explosion in a Venting Chamber
- Medium scale configuration (1.5 m long) -
Heat release
Vorticity
Time = 1.36 ms


x/R
y/R
0 0.5 1 1.5 2 2.5 3 3.5 4
0 0.2 0.4 0.6 0.8 1


DGEN-380 engine Large Eddy Simulation at take-off conditions
by C. Pérez Arroyo, J. Dombard, F. Duchaine,
L. Gicquel, N. Odier and G. Staffelbach
(2022)
AVBP
Mach number (-)
Static temperature (K)
Schlieren (1/m)
Vorticity (1/s)
CERFACS
SAFRAN
dgac
These results benefitted of funding or developments from:
project ATOM (DGAC/SafranTech No 2018-39), PRACE (20th Call Project Access FULLEST),
EXCELLERAT (H2020 823691), EPEEC (H2020 801051) and GENCI (A0122A06074).