TSINGHUA-PRINCETON-COMBUSTION INSTITUTE

2026 SUMMER SCHOOL ON COMBUSTION

Theoretical and Numerical Combustion

Thierry Poinsot

Institut de Mécanique des Fluides de Toulouse, CNRS, France

July 06-10, 2026



TSINGHUA-PRINCETON-COMBUSTION INSTITUTE

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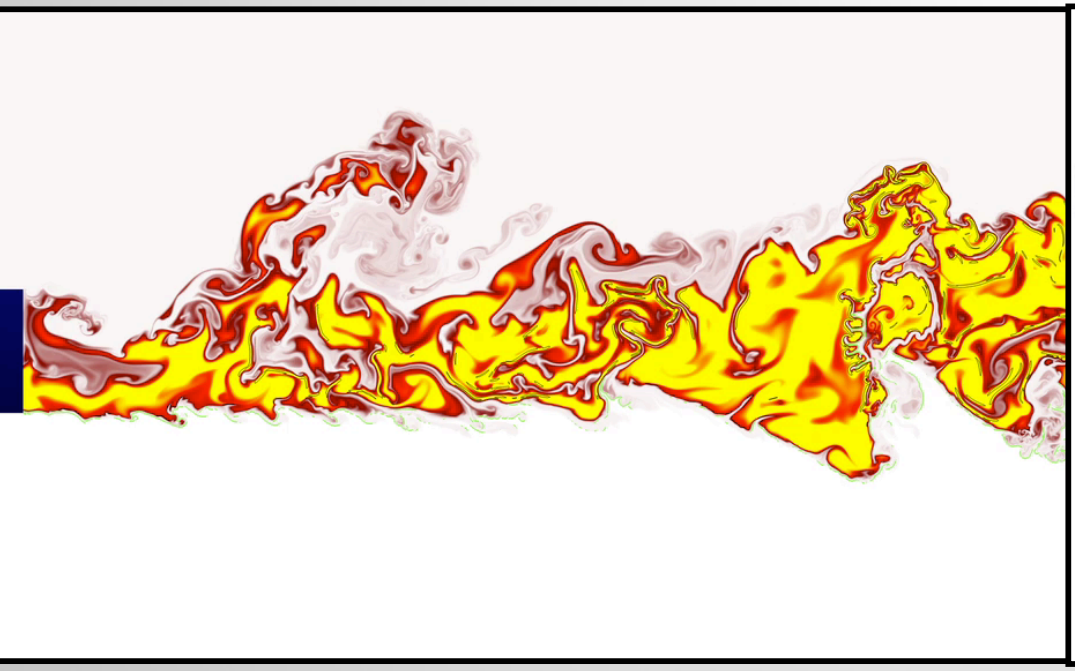
Key Activities / 重要活动			
July 5 (Sunday) /7 月 5 日 （周日）	10:00-17:30	Registration 注册	Northeast Gate, Lee Shau Kee Sci. and Tech. Building 李兆基科技大楼东北门
	18:30	Welcome Reception 开班仪式	A-278, Multifunction Room, Lee Shau Kee Sci. and Tech. Building 李兆基科技大楼多功能厅
Class Schedule / 课程安排			
Schedule 时间	Location 地点	Morning 上午 (9:00-9:50/10:00-10:50/11:00-11:50)	Afternoon 下午 (14:00-14:50/15:00-15:50/16:00-16:50)
July 6-10 (Monday-Friday) /7 月 6-10 日 （周一至周五）	Zone A, 6th Teaching Building 第六教学楼 A 区	**Theoretical and Numerical Combustion** **classroom: 6A018 (0th floor)** Thierry Poinsot	**Combustion Chemistry: From Fundamentals to Kinetic Modelling for Low-Carbon Technologies** **classroom: 6A018 (0th floor)** Alison Tomlin
July 6-7 (Monday-Tuesday) /7 月 6-7 日 （周一至周二）	Zone A, 6th Teaching Building 第六教学楼 A 区	**Spectroscopic Diagnostics for Combustion Chemistry** **classroom: 6A203 (2nd floor)** Pascale Desgroux	**Quantum Mechanics, Statistical Mechanics,and Machine Learning for Molecular Simulations** **classroom: 6A203 (2nd floor)** Alexandre Tkatchenko
July 8-10 (Wednesday-Friday) /7 月 8-10 日 （周三至周五）	Zone A, 6th Teaching Building 第六教学楼 A 区	**Introduction to Plasma-assisted Combustion** **classroom: 6A203 (2nd floor)** Deanna Lacoste	**AI for Combustion** **classroom: 6A016 (0th floor)** Matthias Ihme
Special Activities / 特殊活动			
July 5 (Sunday) /7 月 5 日 （周日）	13:30-17:30	Art Museum Visit / 艺术博物馆参观	Tsinghua University Art Museum 清华大学艺术博物馆
July 7 (Tuesday) /7 月 7 日 （周二）	17:00-18:00	Campus Tour / 校园游览	Tsinghua University 清华大学

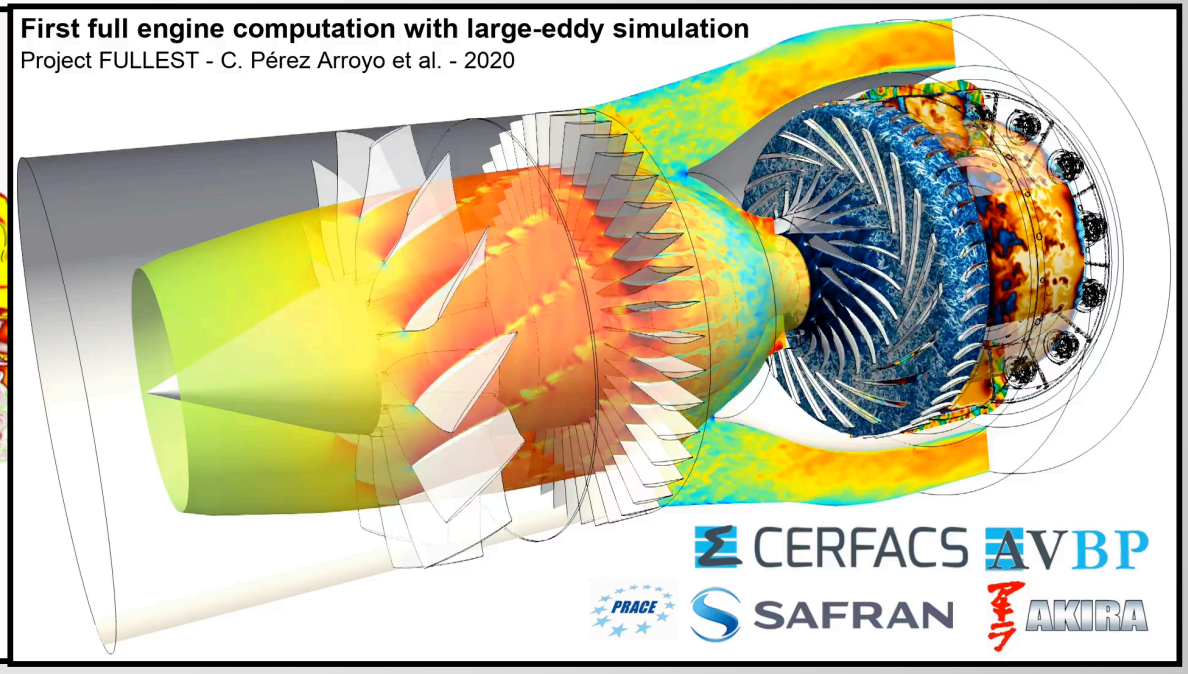
July 8 (Wednesday) /7 月 8 日 （周三）	17:00-17:30	Group Picture Taking / 暑期学校合影	Mong Man Wai Concert Hall 蒙民伟音乐厅
July 8 (Wednesday) /7 月 8 日 （周三）	18:30-19:30 19:30-21:00	Poster Presentation / 海报展示 Career Panel / 职业发展论坛	B-518, Lee Shau Kee Sci. and Tech. Building 李兆基科技大楼 B-518 会议室
July 9 (Thursday) /7 月 9 日 （周四）	18:00	Farewell Reception / 欢送会	Guan Chou Yuan Restaurant 观畴园餐厅
July 10 (Friday) /7 月 10 日 （周五）	8:00-18:00	Program Certificate Distribution / 学习证书发放	6th Teaching Building 第六教学楼
July 11 (Saturday) /7 月 11 日 （周六）	9:30-11:30	CCE Laboratory Tour / 燃烧能源中心实验室参观	Northeast Gate, Lee Shau Kee Sci. and Tech. Building 李兆基科技大楼东北门

Electronic version of all lecture materials are available at the summer school website

Theoretical and numerical combustion

Thierry Poinsot
Research Director, Institut de Mécanique des Fluides de Toulouse (IMFT, CNRS et INPT)
Senior researcher, CERFACS
Senior research fellow, STANFORD
French Academy of Sciences
Editor in chief, Combustion and Flame (with Pr F. Egolfopoulos, USC)
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https://www.cerfacs.fr/~poinsot

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Presentation… of todays's speaker

PhD in heat transfer for Michelin in 1983 at Ecole Centrale Paris (Heat transfer in tyres)

These d'Etat (second PhD) at Univ. Orsay in 1987 (combustion instabilities, Pr S. Candel)

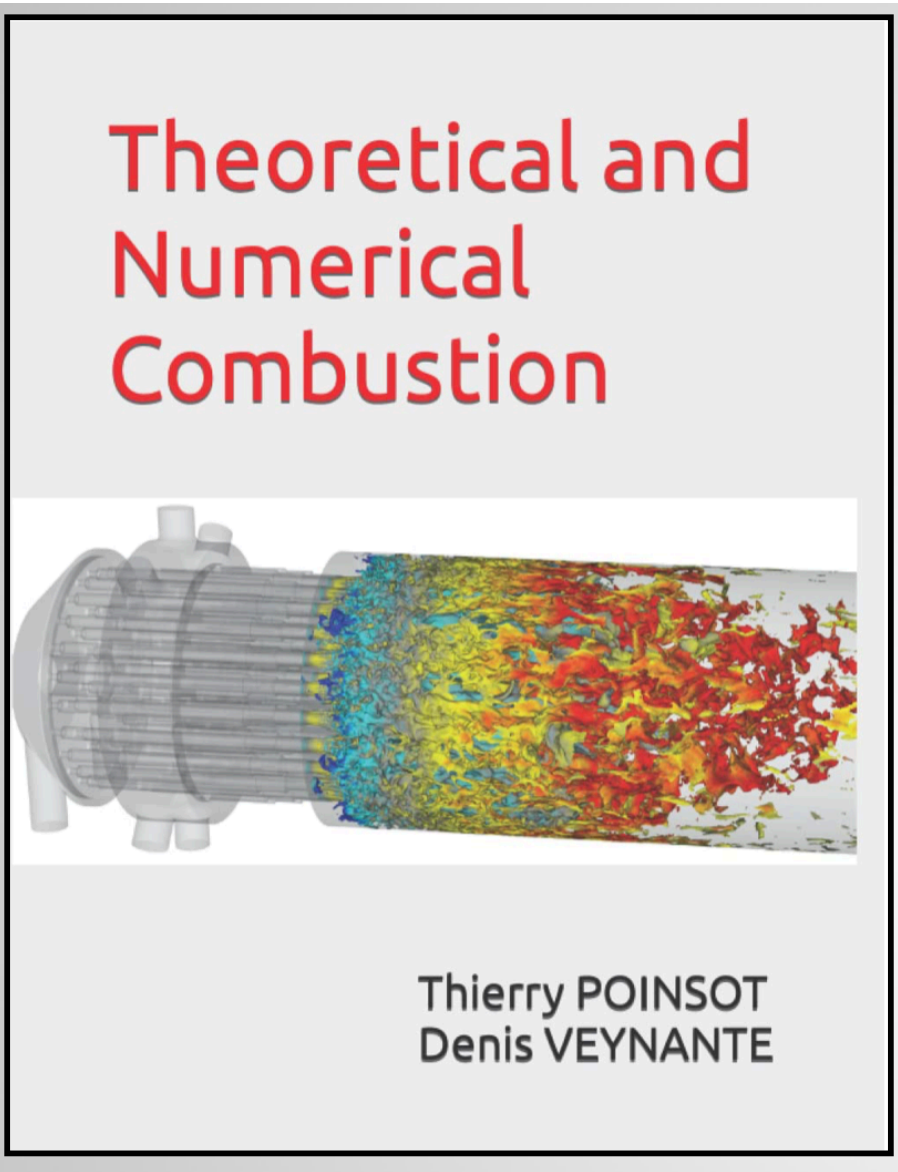
Presently:

- *Research Director at Institut de Mécanique des Fluides de Toulouse (CNRS and INPT)*
- *Senior adviser of CFD group at CERFACS, Toulouse, France*
- *French Academy of Sciences*
- *Editor in chief of Combustion and Flame (with Pr F. Egolfopoulos, USC)*

poinsot@cerfacs.fr
www.cerfacs.fr/~poinsot

OUTLINE OF PRESENTATIONS:

- Introduction. Energy policies. The impact of combustion, simulation methods, combustion regimes
- Laminar combustion concepts required to study turbulent flames
- Turbulent combustion models- RANS, LES and DNS. Short history and state of the art models
- Numerical methods: RANS, LES and DNS. Boundary conditions. High Performance Computing
- Waves: numerical, physical waves, acoustics, instabilities
- Instabilities: mechanisms, thermoacoustics
- Flame/wall interaction
- Ignition
- Hydrogen combustion



Textbook: «Theoretical and numerical combustion» by Poinsot and Veynante

english version available on Amazon

Electronic access here:

https://elearning.cerfacs.fr/combustion/onlinePoinsotBook/onlinethirdedition/index.php

Chinese version of the TNC book :

https://item.jd.com/13737793.html?bbtf=1

http://product.dangdang.com/29571730.html

京东

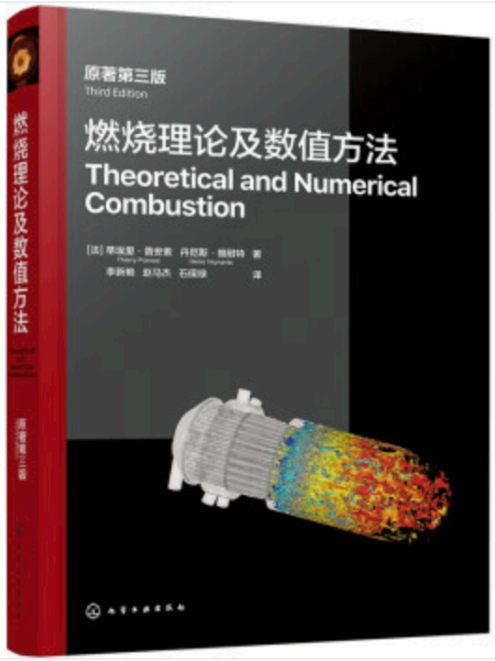
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Reference to TNC book in these lectures:

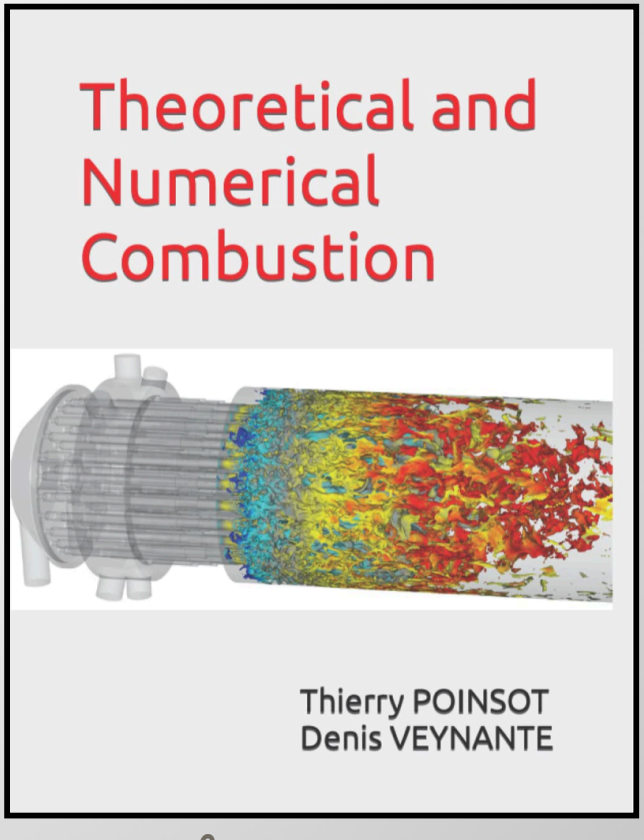
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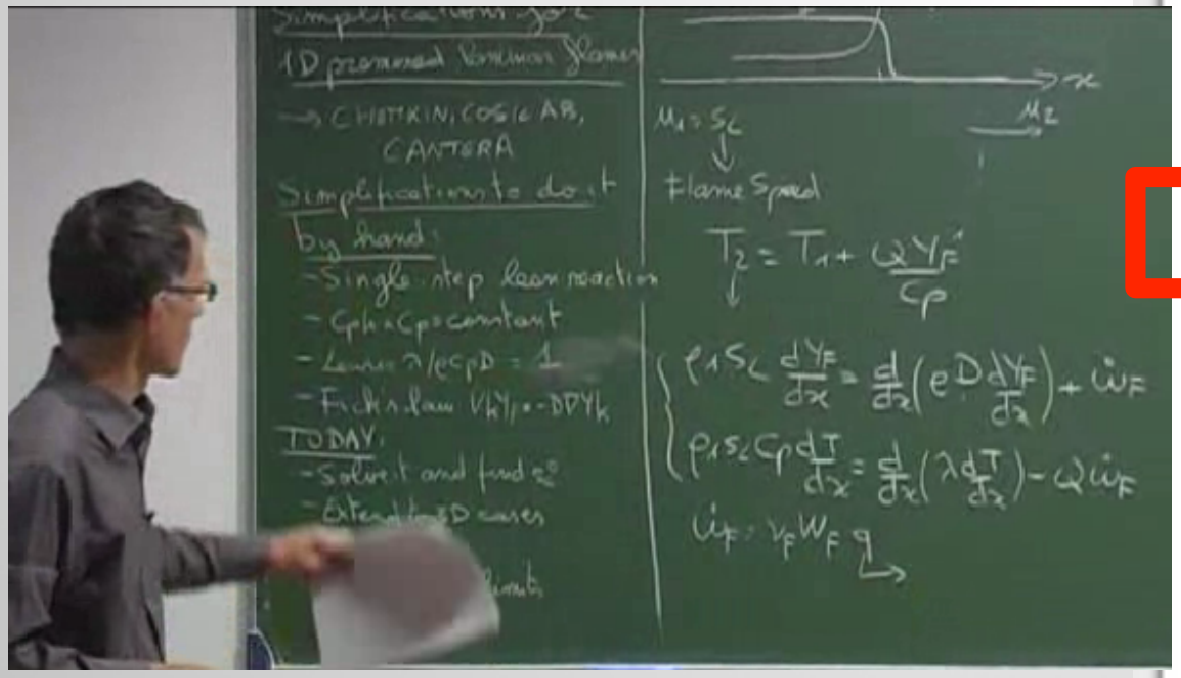
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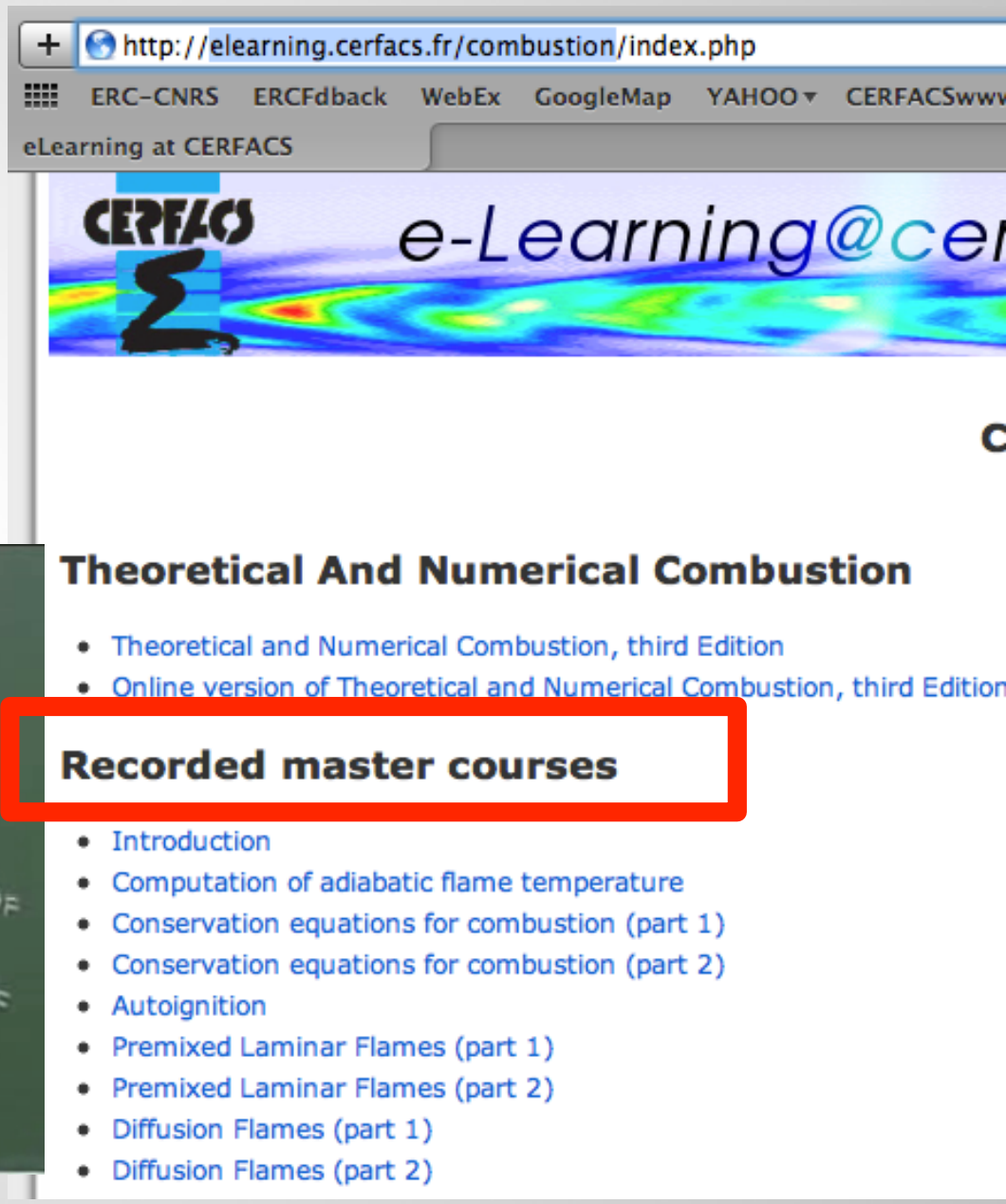


COURSES (in english):

https://elearning.cerfacs.fr/combustion

SLOW COURSE - you can copy it by hand to understand details





Elearning web site on combustion and CFD

https://elearning.cerfacs.fr

eLearning @ Cerfacs - Online Courses

Contents

CERFACS members collaborate to formation in multiple places (engineering schools and universities in Toulouse, Bordeaux and Paris, and specialized schools for PhDs and engineers such as Von Karmann Institut, College de Polytechnique, etc) and on many topics (numerical methods, high-performance computing, fortran, optimization, tutorial for Large Eddy Simulation of reacting flows, theoretical and numerical combustion, Computation Fluid Dynamics on massively parallel architectures, etc).

To ensure that students can have the best access to teaching materials (courses, hands-on exercices, links to various external sources, examples of exams), CERFACS has gathered data on this website where you can download all data related to the course they are following. You are welcome to use this site.

Topics

- Combustion
- Turbomachines
- Environmental science
- Numerical methods for CFD
- Advices for phD students
- Miscellaneous
- Coupling

Formations

- Computation of adiabatic flame temperature
- Stability, dispersion and dissipation
- Mesh and discretization
- Unstable modes of a combustor
- Tutorial on spectral analysis
- Calibration of a model parameter on the 1D diffusion equation
- Data Assimilation for flood wave propagation model

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Topics

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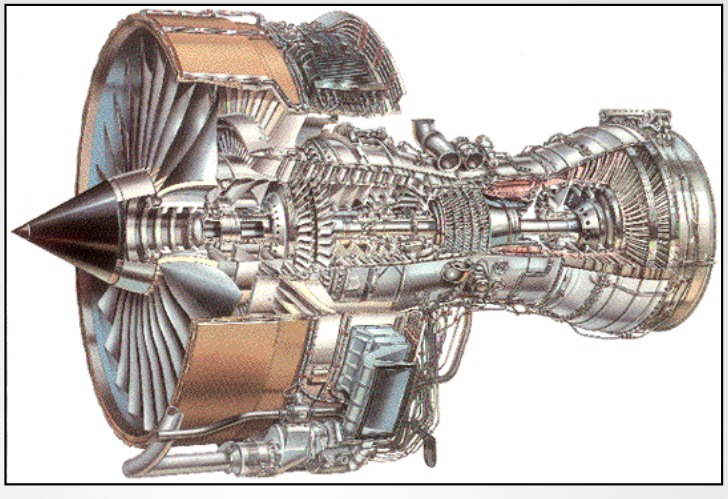
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Mesh and discretization
Unstable modes of a combustor
Tutorial on spectral analysis
Calibration of a model parameter on the 1D diffusion equation
Data Assimilation for flood wave propagation model
Convection Scheme
Exchanges of anlytical fields between LMDz and Orca2T

ENERGY POLICY SUMMARY:

ENERGY ON EARTH TODAY = COMBUSTION

Combustion: more than 85 percent of the energy produced on earth









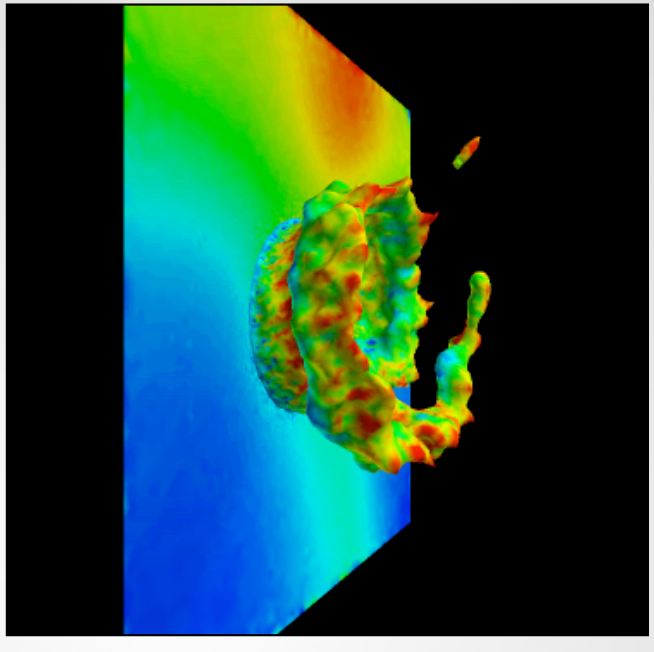


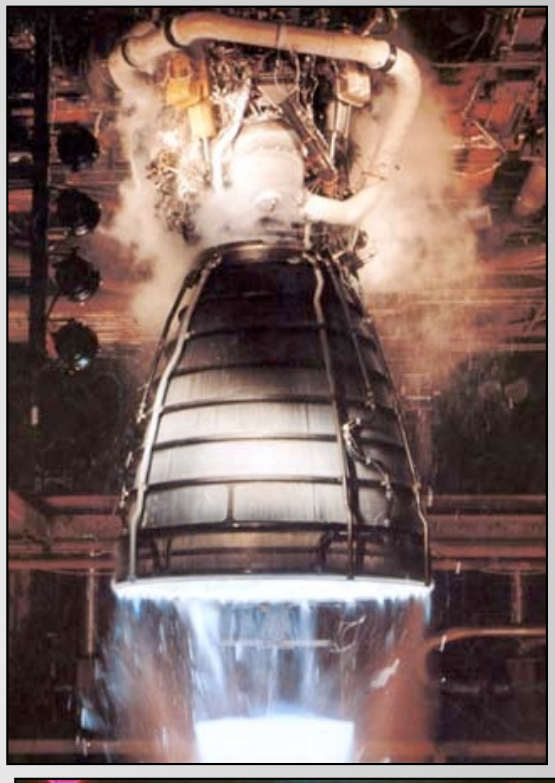


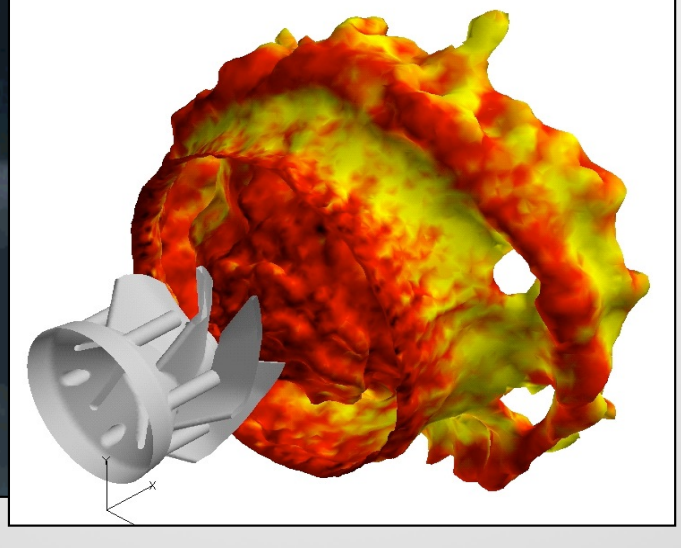


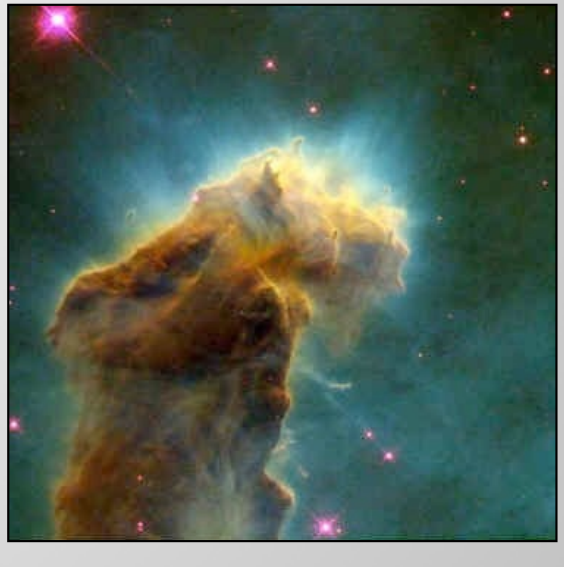




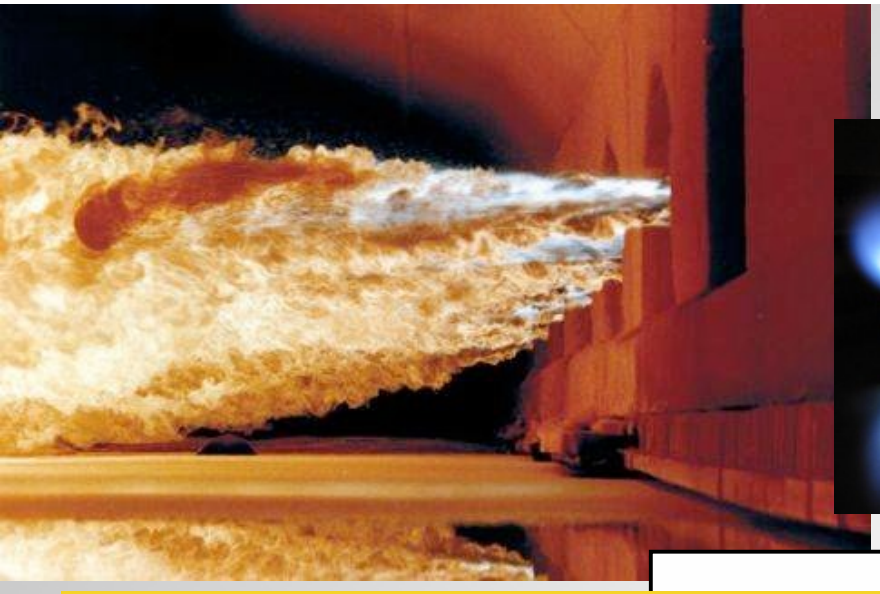








ASTROPHYSICS IS ALSO ABOUT COMBUSTION !







On average: 2 litres of oil burnt

- **per person**
- **per day**

worldwide








Satellites…
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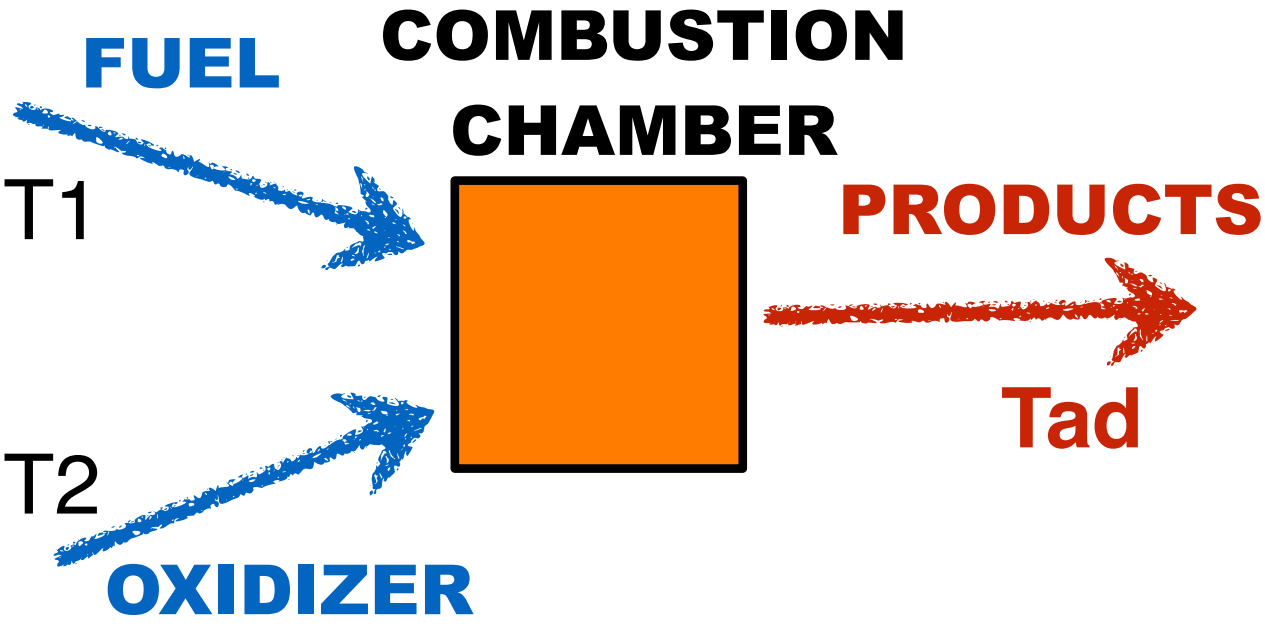

Ariane V


Delta IV
Photo by Thom Baur © The Boeing Company

What is combustion ?

Fuel + Oxidizer -> Products + ***Heat***

H2
CH4
C3H8
Octane
Kerosene



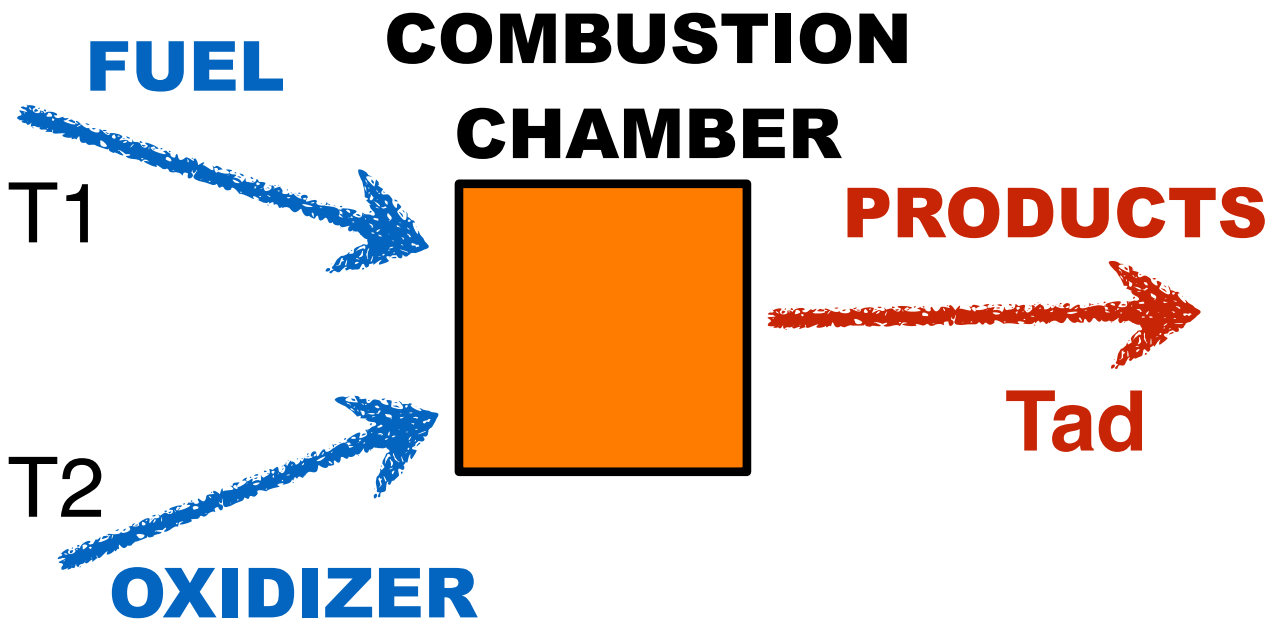
What is combustion ?

Fuel + Oxidizer -> Products + ***Heat***

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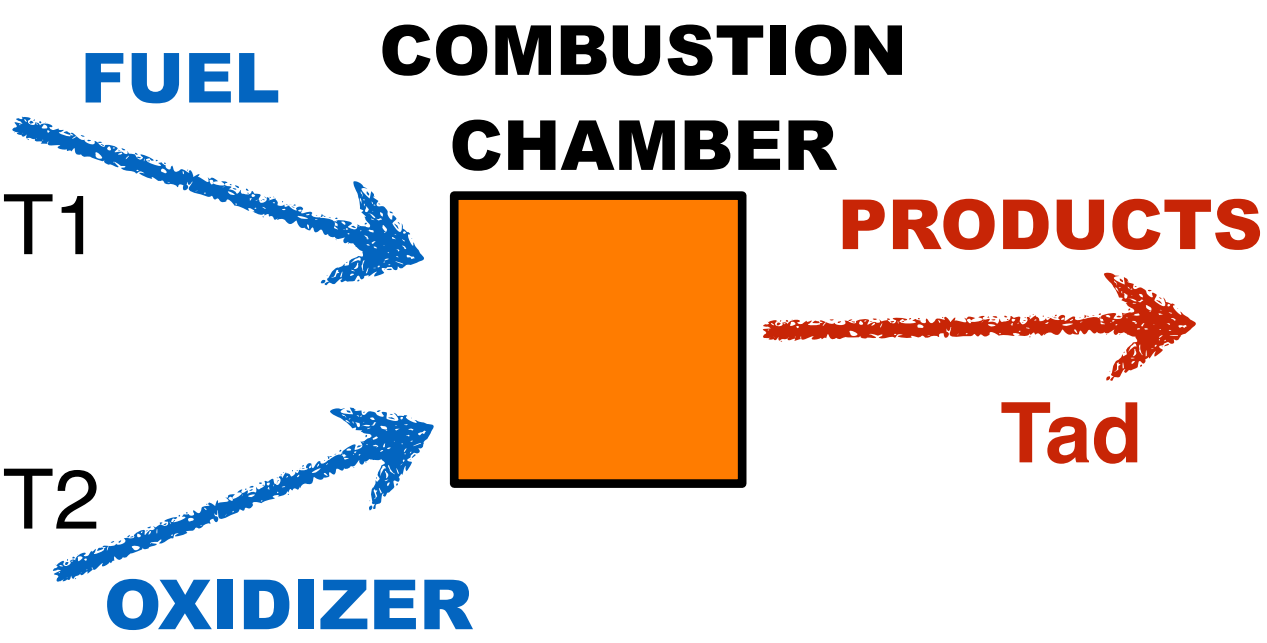
Air

Oxygen



What is combustion ?

Fuel + Oxidizer -> Products + ***Heat***



CO2
H2O
CO
NOx
Soot

Specificity of combustion ?

The heat released per mass of fuel burnt is enormous:

Fuel + Oxidizer -> Products + ***Heat***

For mos he heat
release f the
order of 50 MJ/kg (120 for H2).

One kg of kerosene
=
40 kg of batteries

COMBUSTION OVERVIEW

Two important equations:

ENERGY ON EARTH TODAY

=

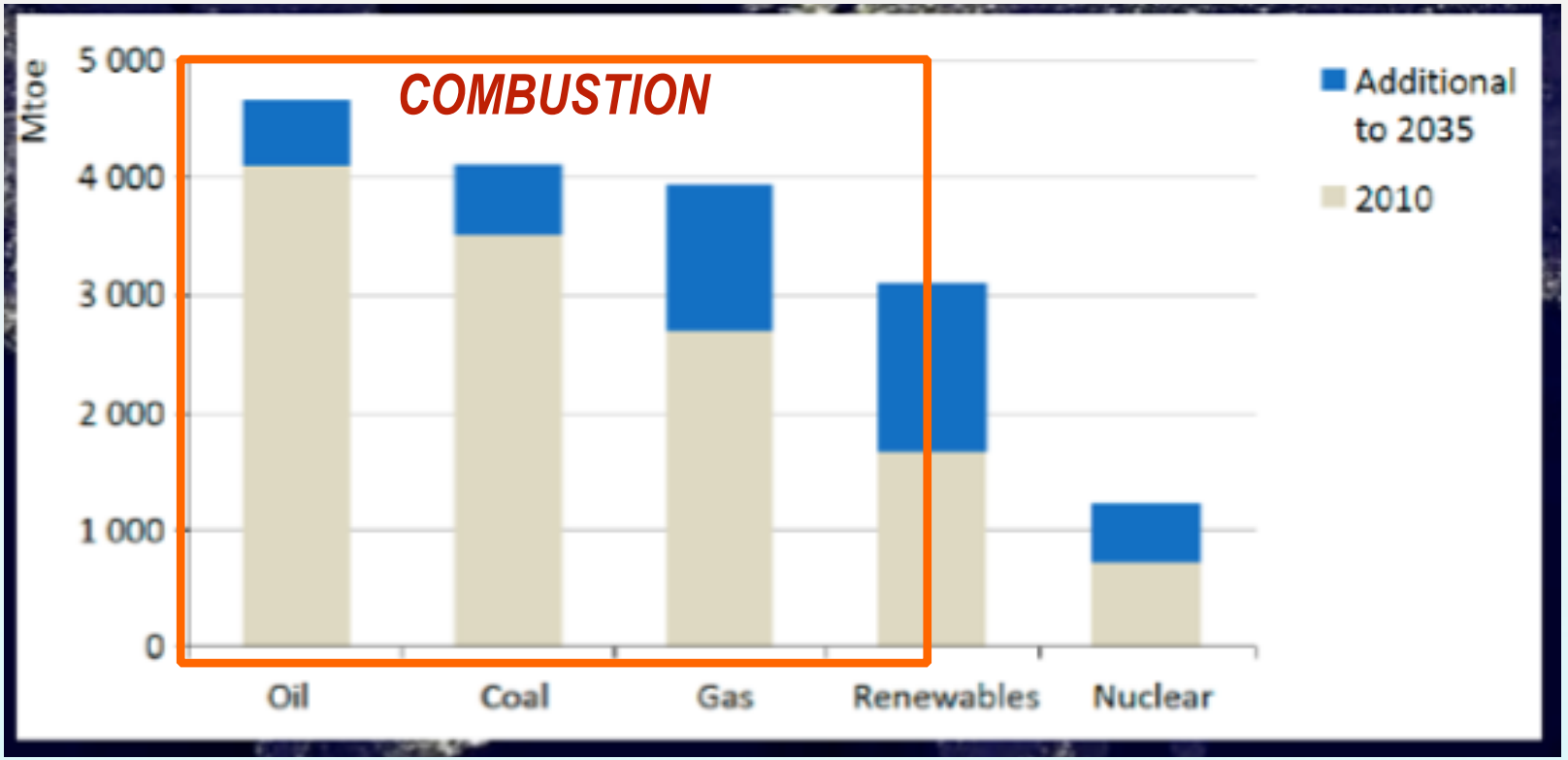
COMBUSTION

ENERGY ON EARTH TOMORROW

ALMOST =

COMBUSTION

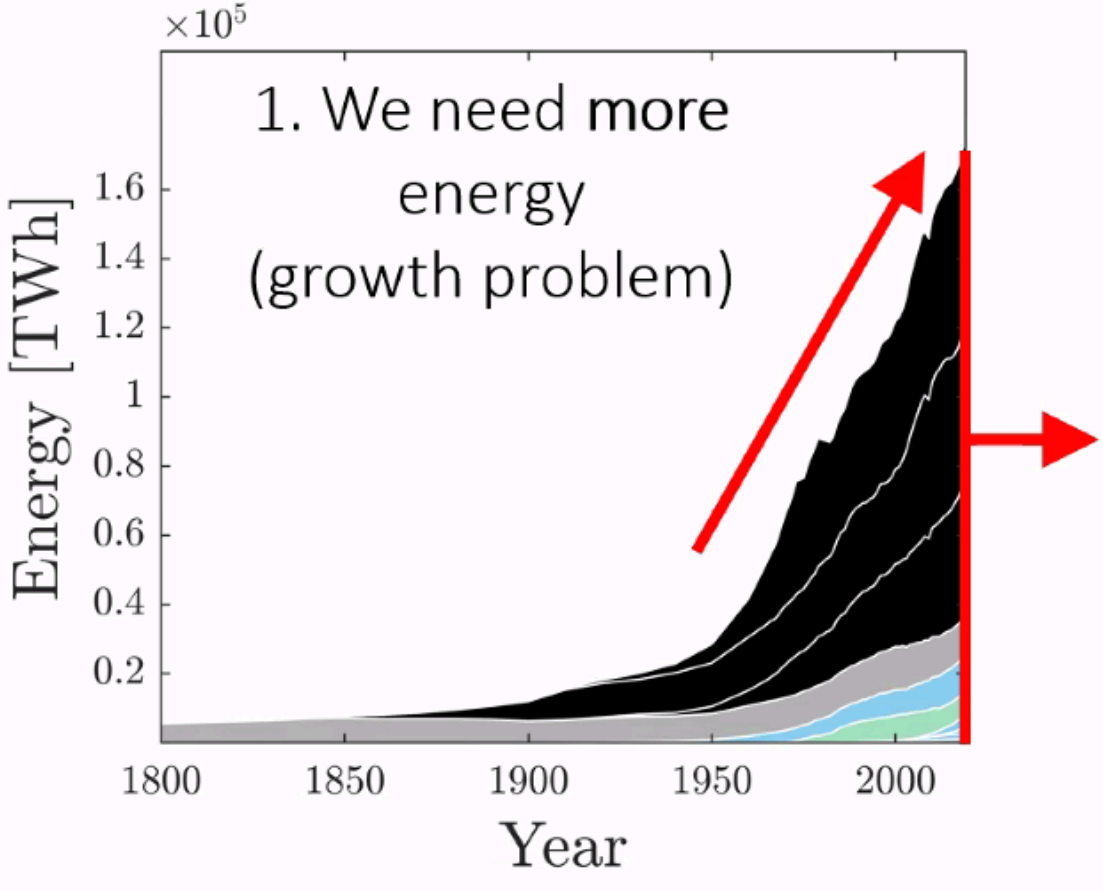
IN MOST SCENARIOS, THE ABSOLUTE ENERGY PRODUCTION USING COMBUSTION RISES BECAUSE THE INCREASE OF GLOBAL ENERGY NEEDS CANNOT BE SATISFIED BY RENEWABLES SOURCES ONLY…

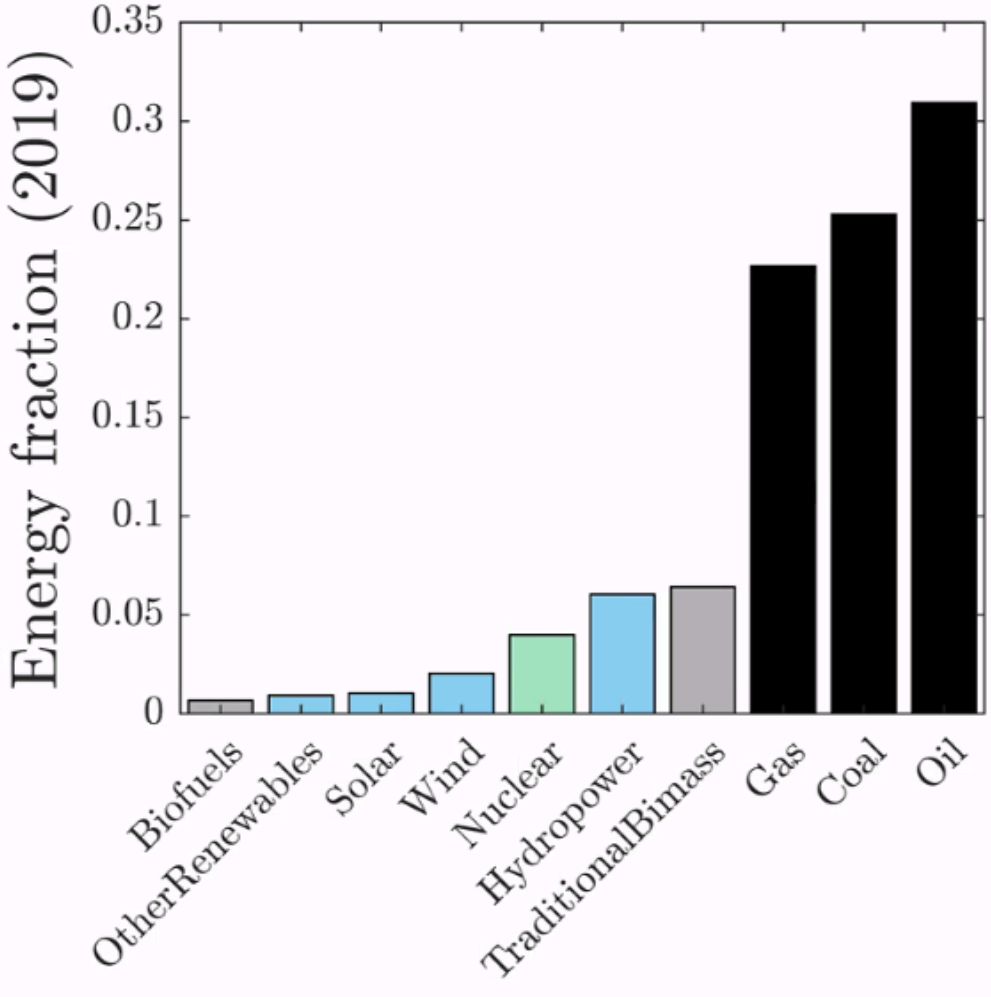


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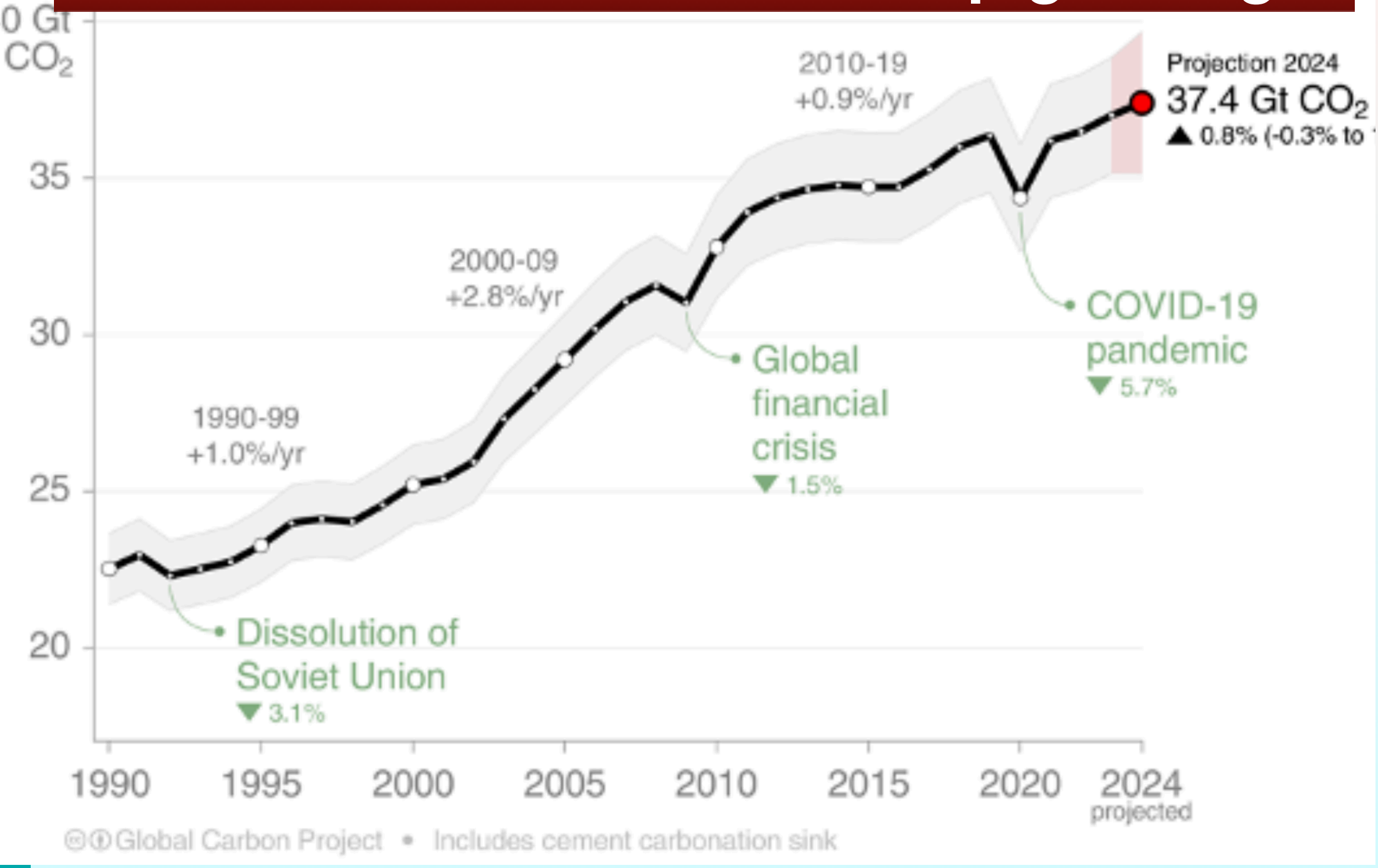
Whatever the scenario is, need the best combustion systems: optimize efficiency, minimize pollutants and CO2 emission

The global energy needs increase





So that CO2 emissions keep growing





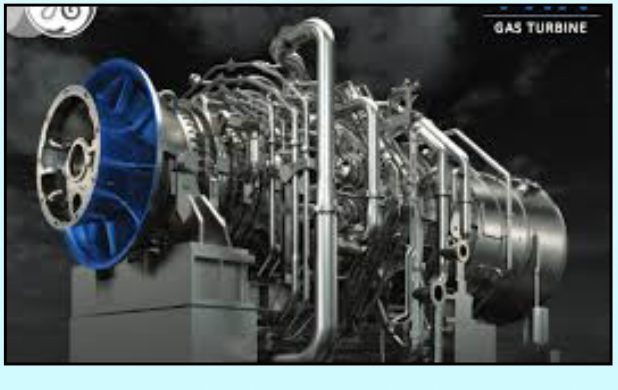
So combustion is the problem

It can also be the solution !

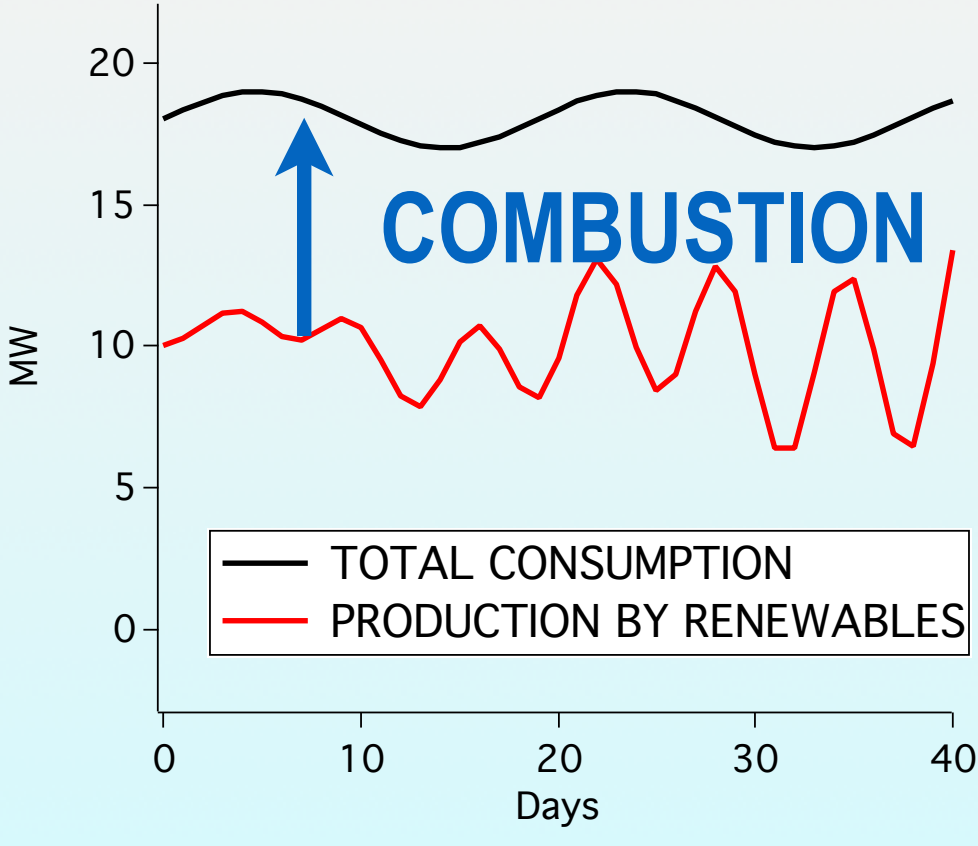
COMBUSTION IS A KEY ELEMENT IF WE WANT TO GO TO A MASSIVE USE OF RENEWABLE ENERGIES





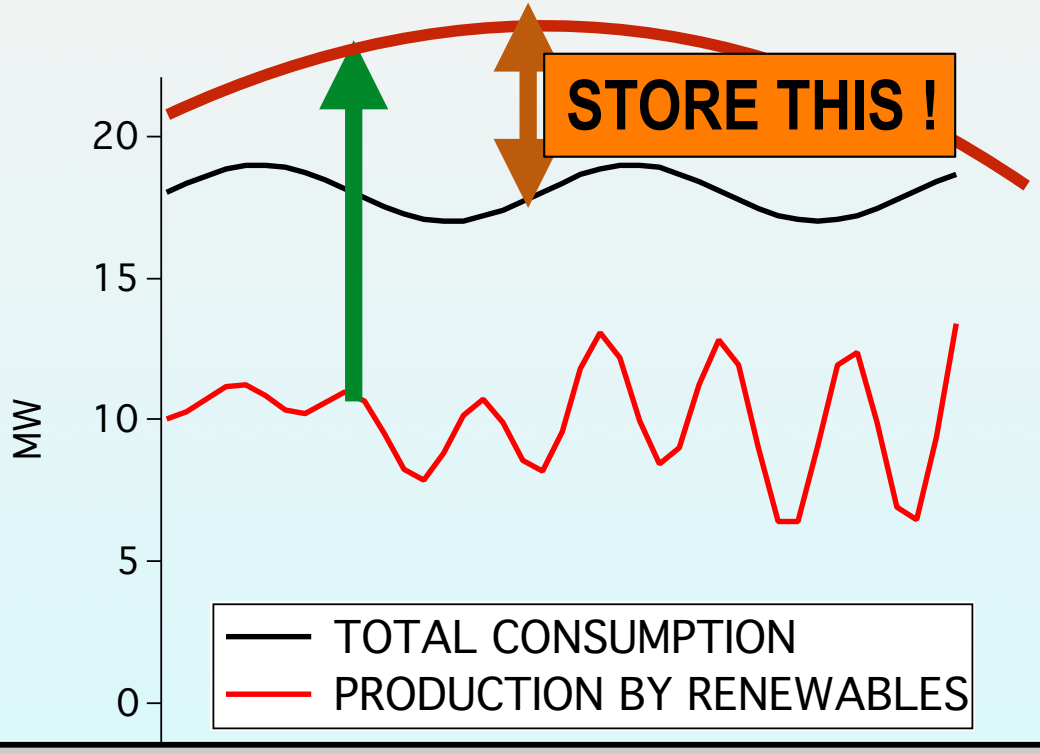


PRODUCTION = CONSUMPTION



WHAT HAPPENS WHEN WE HAVE TOO MUCH PRODUCTION BY RENEWABLE SOURCES ?





WE MUST BE ABLE TO STORE RENEWABLE ENERGIES

COMBUSTION IS AN EXCELLENT WAY TO STORE ENERGY:





TOO MUCH WIND
TOO MUCH SUN

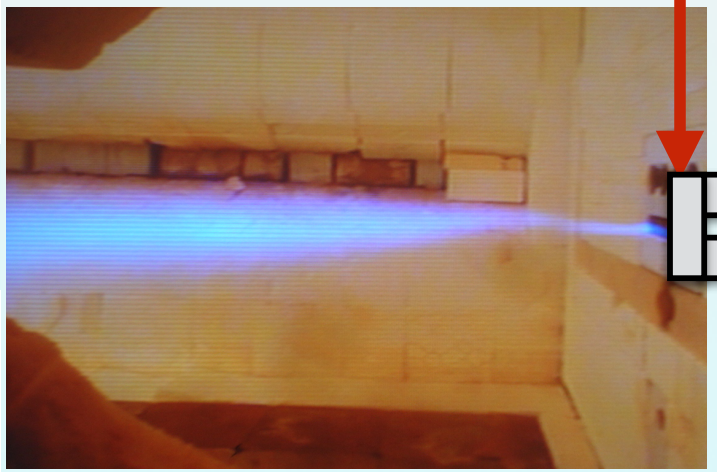
Electrolysis





Renewable fuel

Fossil fuel

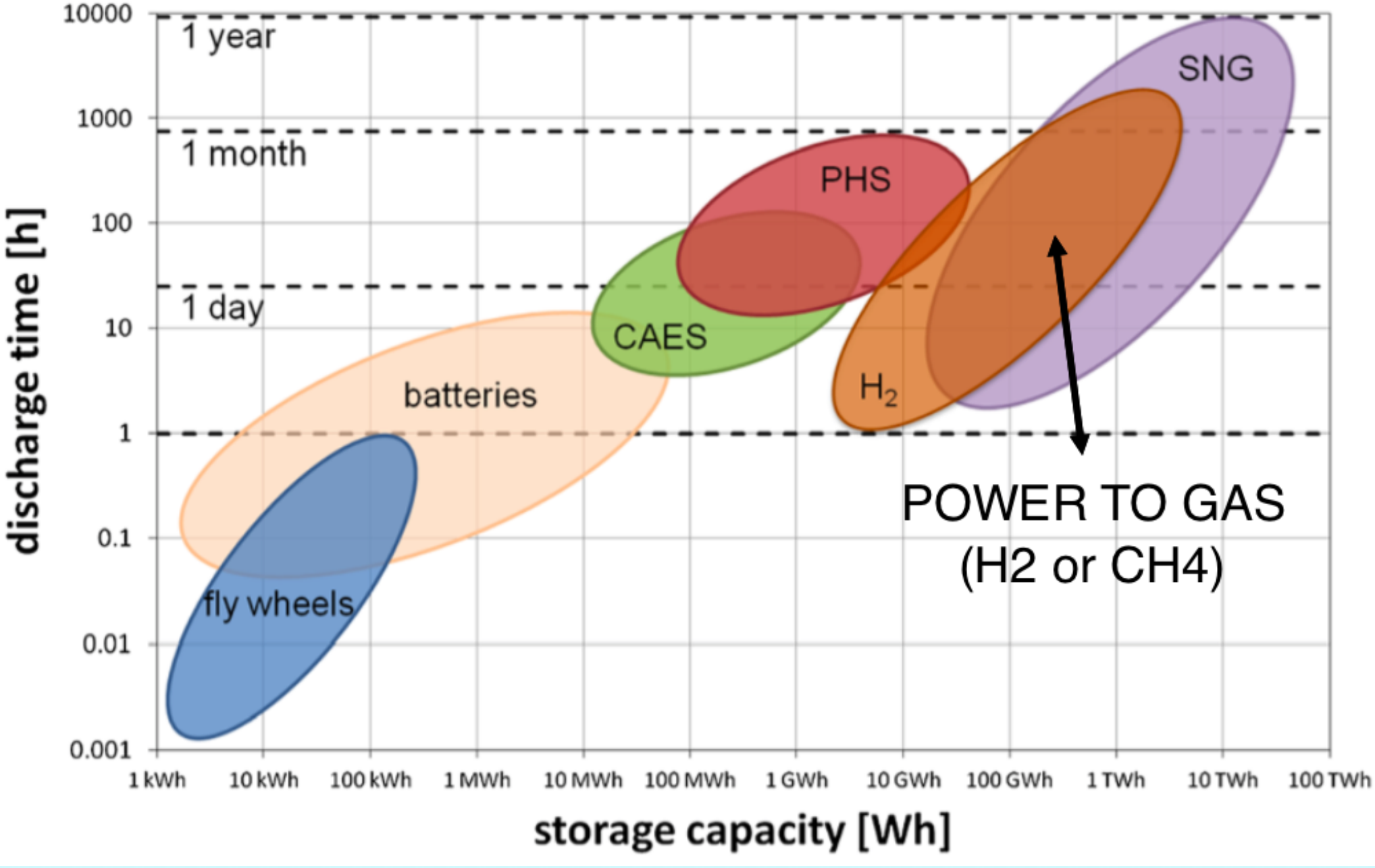


Air

Combustor

NO WIND
NO SUN

AND COMBUSTION CAN STORE MUCH MORE AND FOR MUCH LONGER TIMES



FOCUSING ON ELECTRICITY

- ★Electricity will be produced using wind, sun and nuclear power in 2050
- ★BUT a main issue is ‘reliability of electricity supply’. Are we ready to have no electricity during 0, 10 minutes, 10 hours per day ? We need storage… and combustion can do it

So:

★We burn a lot

★We will keep burning a lot

★We can use combustion to store energy

★COMBUSTION SCIENCE MUST ALLOW US TO DO THIS WITHOUT WASTING FUEL, INCREASING POLLUTION, KILLING PEOPLE AND CHANGING

Combustion is THE source of pollution: CO, NOx, CHx, SOx









Chemical species are not the only ‘pollution’ produced by combustion: NOISE is also a big issue





Too much noise can become a major issue for the structure: satellites



So:

★Combustion creates pollutants

★Combustion makes noise and can break structures

★Combustion also changes climate !



GLOBAL WARMING:



ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Proceedings of the Combustion Institute 32 (2009) 45–56

Proceedings of the Combustion Institute

www.elsevier.com/locate/proci

Science based policy for addressing energy and environmental problems

Robert F. Sawyer

Mechanical Engineering Department, University of California, Berkeley, CA 94720-1740, USA

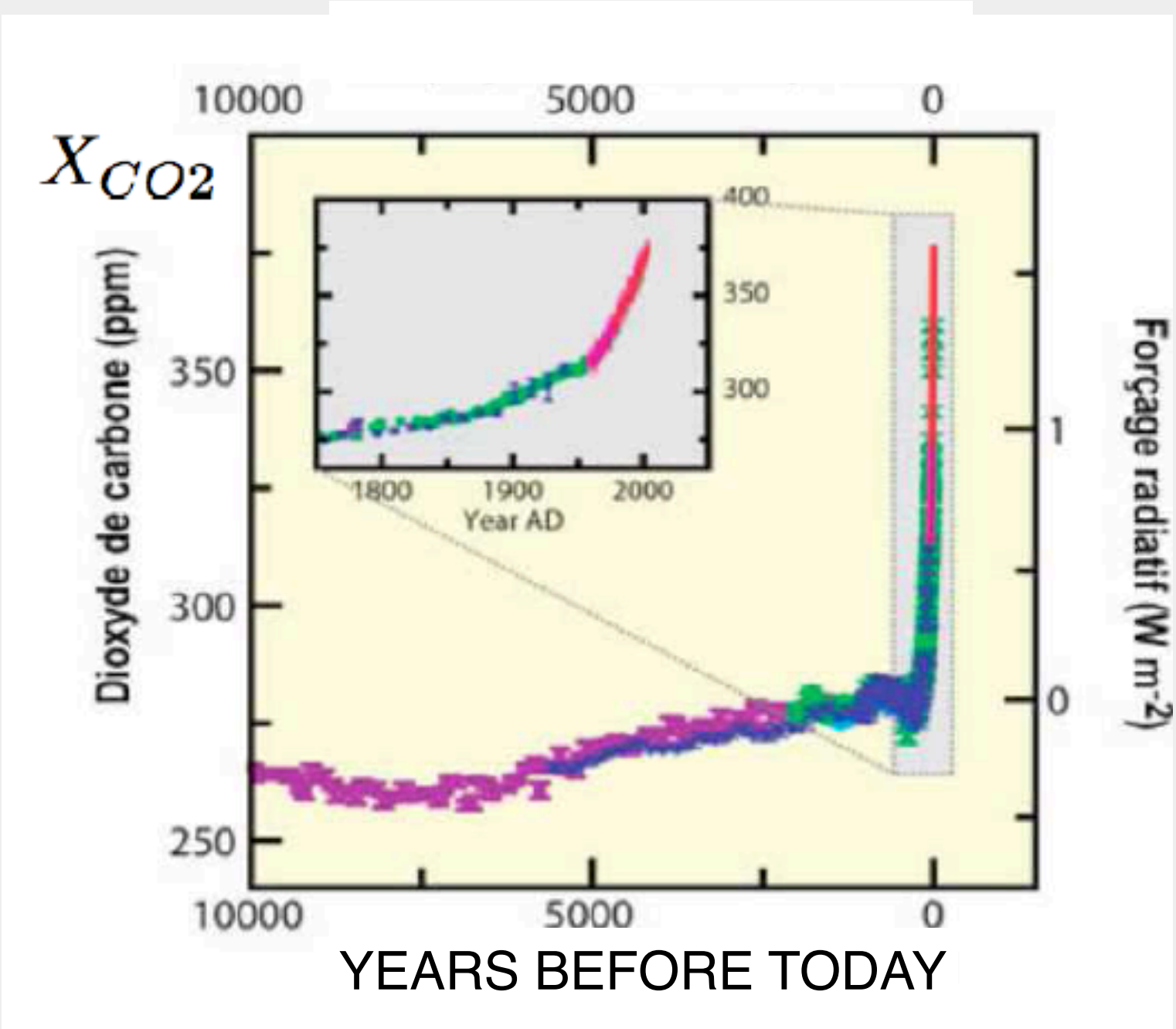
- CO2 in atmosphere->global warming...
- Combustion produces a lot of CO2

- Guessed by Fourier in 1824

- Role of CO2 shown by Arrhenius in 1896: doubling CO2 would raise earth temperature by 5 degrees

If you want to be more precise, talk to IPCC




X_{CO2}
10000
5000
0
Dioxyde de carbone (ppm)
350
300
250
400
350
300
1800
1900
2000
Year AD
1
0
Forçage radiatif (W m-2)
10000
5000
0
YEARS BEFORE TODAY

So:

★Combustion creates pollutants

★Combustion makes noise and can break structures

★Combustion also changes climate !

★Combustion is dangerous…

Dangerous technologies: control needed






FOTOSEARCH





So:

★Combustion creates pollutants

★Combustion makes noise and can break structures

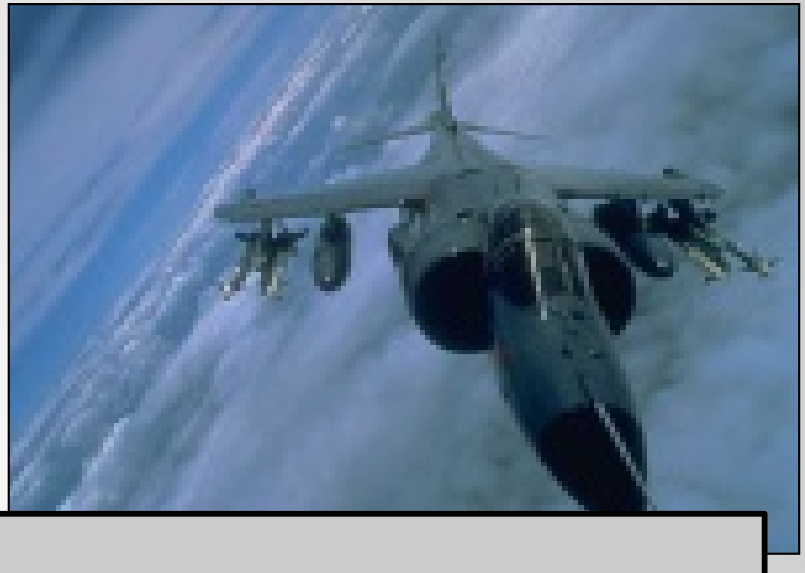
★Combustion also changes climate !

★Combustion is dangerous…

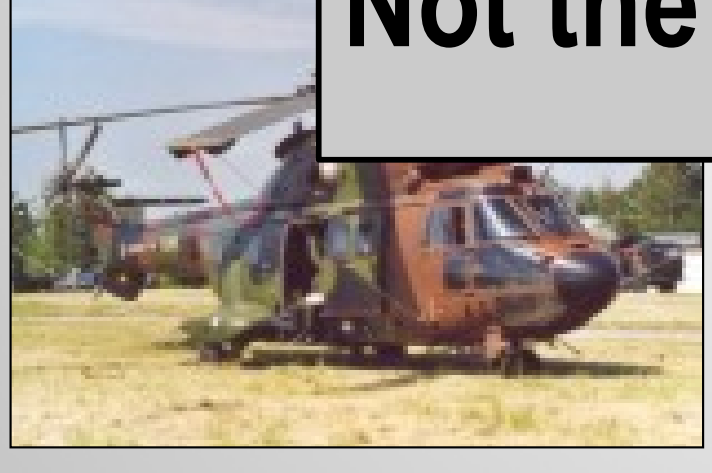
★Sometimes we use combustion to hurt people

Army applications





Not the main topic in this course





To do certain things like flying

- An aircraft engine produces typically 5 MW. 10 MW for an aircraft. Produced using kerosene

- Other ideas ?

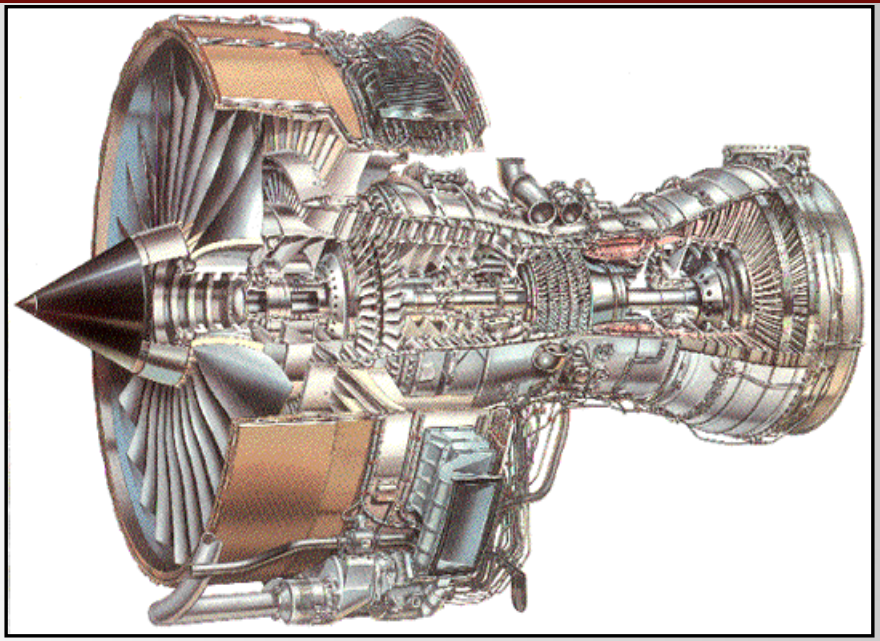
➡Solar: use sun power. 300 W/m2. We need a surface of 10 E6/300= 34 000 m2. 1 km per 34 m…. on sunny days. Forget it !

➡Battery: here the problem is weight. 40 times more than for kerosene. A330: 110 tons of kerosene to be replaced by 4400 tons of batteries ?

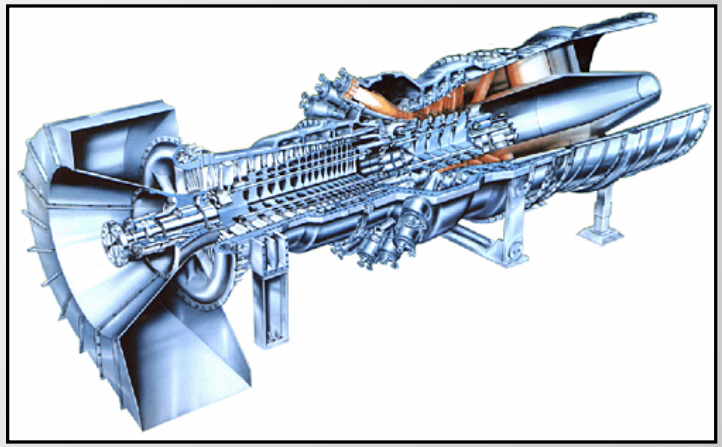
➡COMBUSTION NEEDED

In this course: many gas turbine examples

1/ No other way to propel aircraft



2/ Highly efficient (60%), cheap, flexible systems to produce electricity (certain days, there is no sun and no wind: for each windmill plant, you need a gas turbine)



The gas turbine market grows. The regulations become tougher => Optimization is mandatory !

OPTIMIZING SOMETHING WHICH HAS BEEN HERE FOR 70 YEARS IS DIFFICULT

- Example: the LOW NOX projects in Europe (1995-2005) lead to combustor designs which produced low NOX... but were unstable -> thermoacoustics
- Compromises (efficiency, pollution, noise, stability, cost) are difficult to find and experimental costs too high to test all possible designs

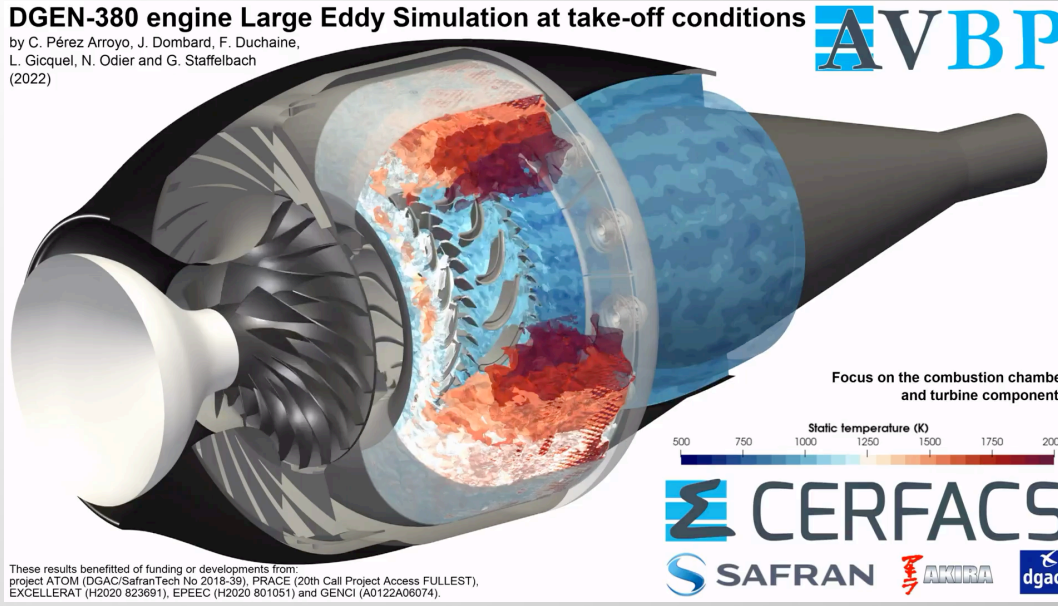


W2 engine



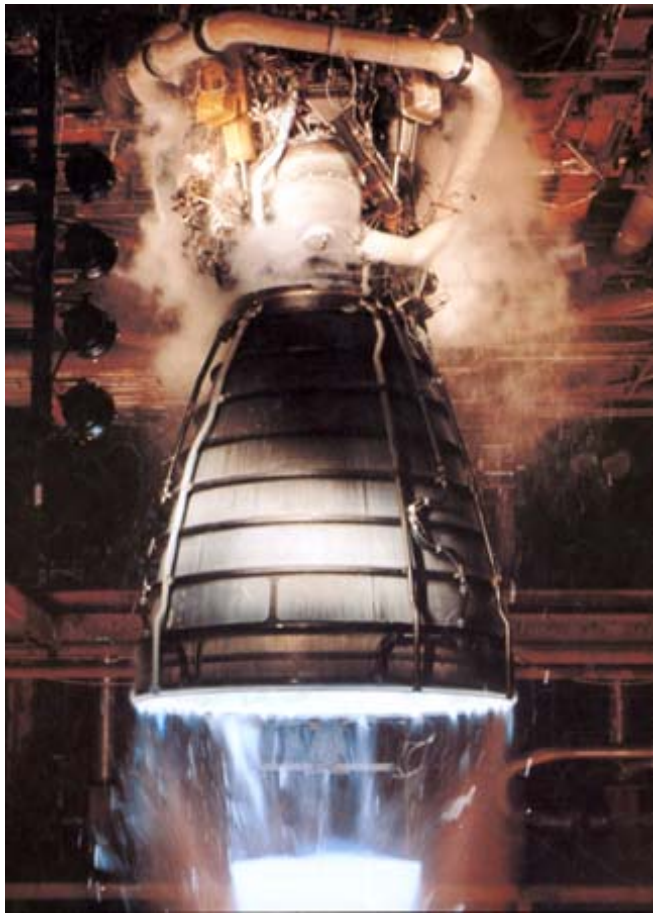
Sir F. Whittle

- Simulation has become essential: gas turbine companies now perform advanced CFD, including LES. Developing numerical tools which speed up developments is a key issue, and they must include possible coupling between all components of the engine.

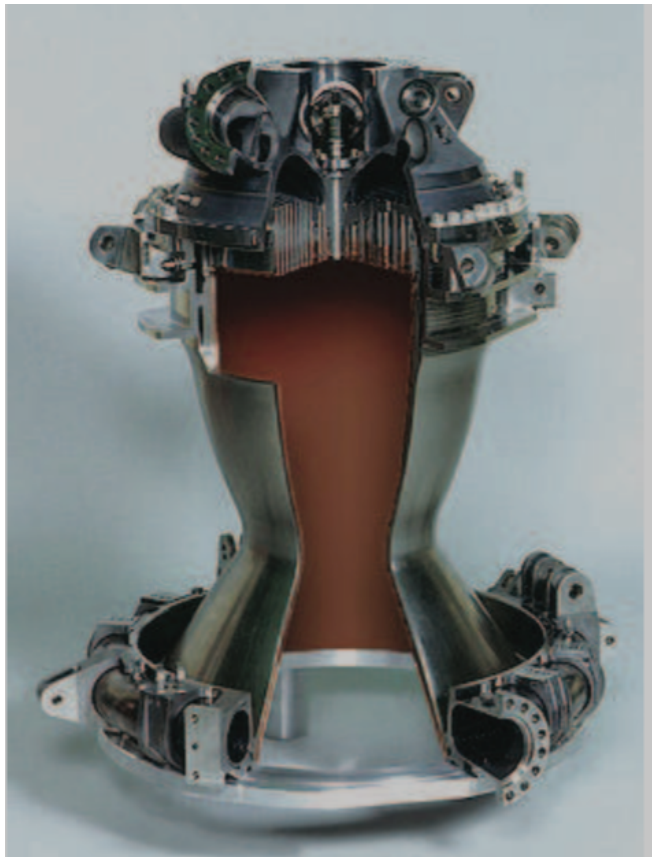


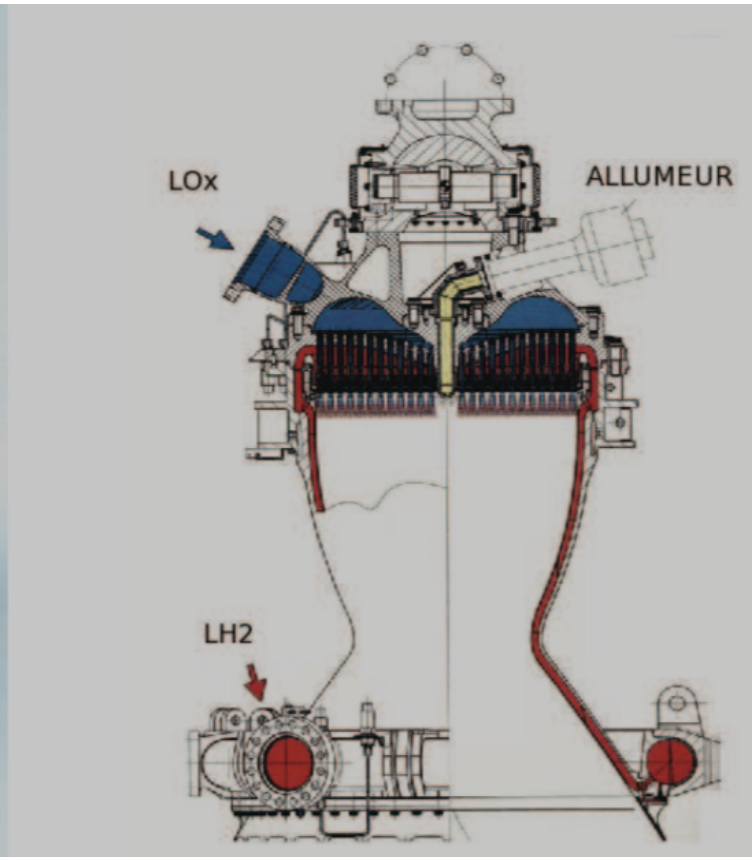
COMBUSTION: MULTISCALE -MULTIPHYSICS

MULTI SCALE PROBLEM →

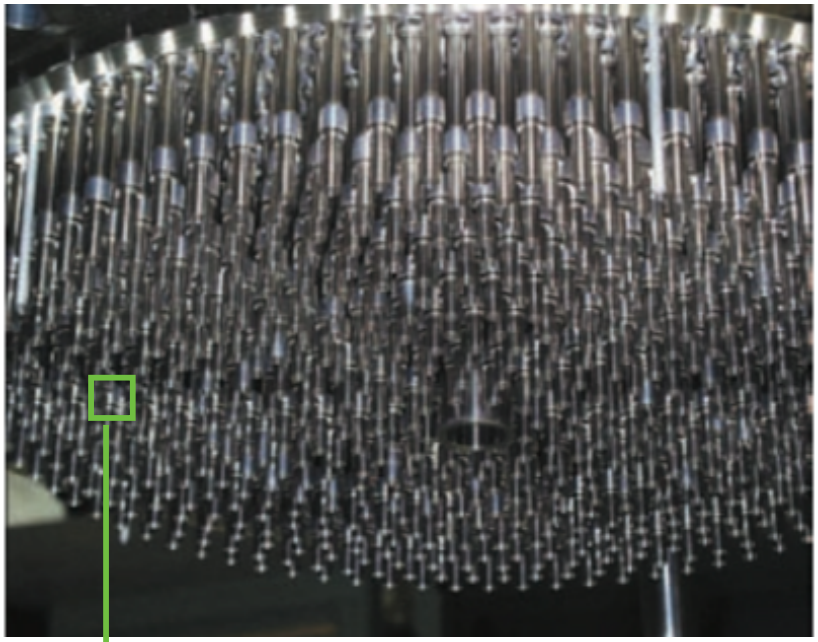


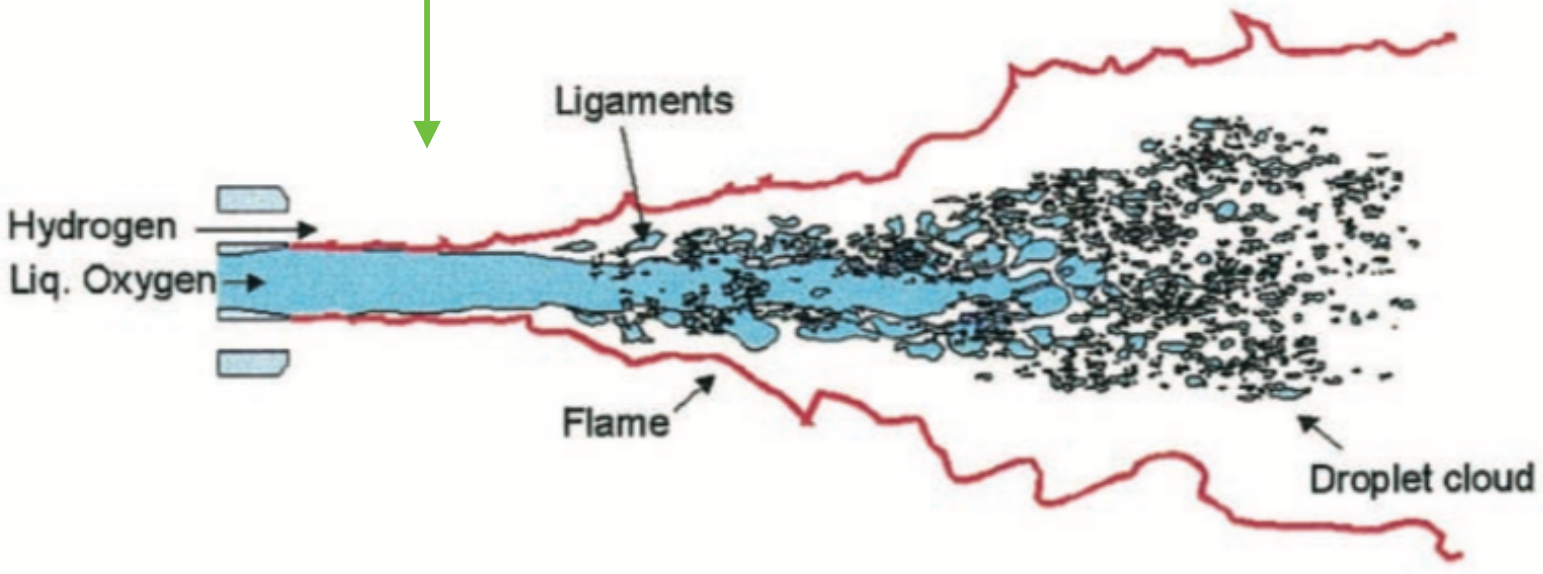
Combustion chamber:
meters and hours



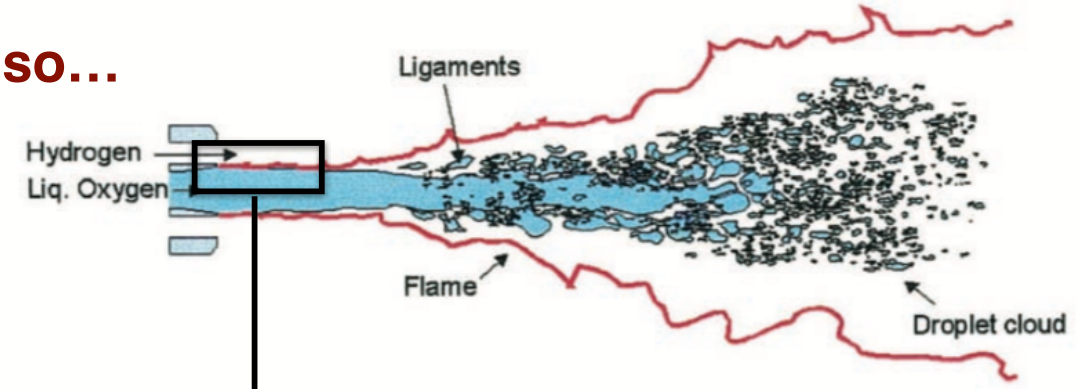


Five hundred injectors of cryogenic H2 and O2



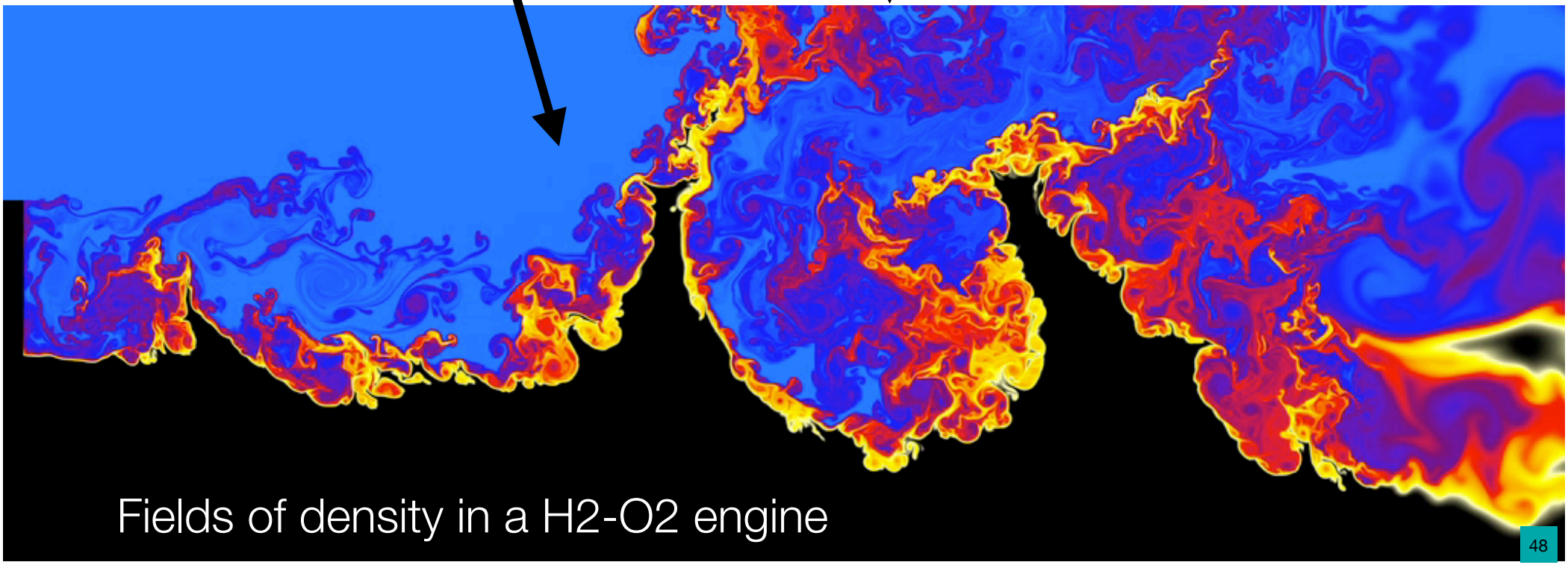


In this 1m diameter engine, we need to mesh a flame smaller than 0.1 micron.
This requires at least 10 million points in each direction if the mesh is regular and 10^21 points in 3D ?
This is impossible and will remain so…



Within the combustion chamber: nanoseconds and nanometers

1 cm



Fields of density in a H2-O2 engine

Very complex technologies:



Offering a huge range of powers

From small engines:

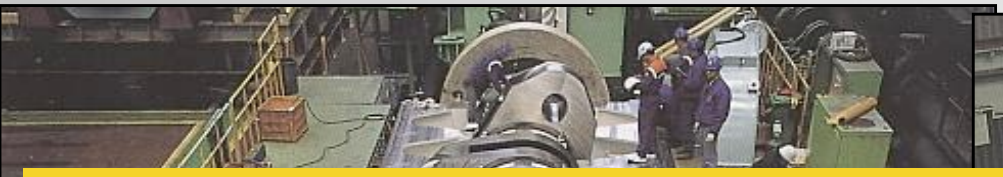


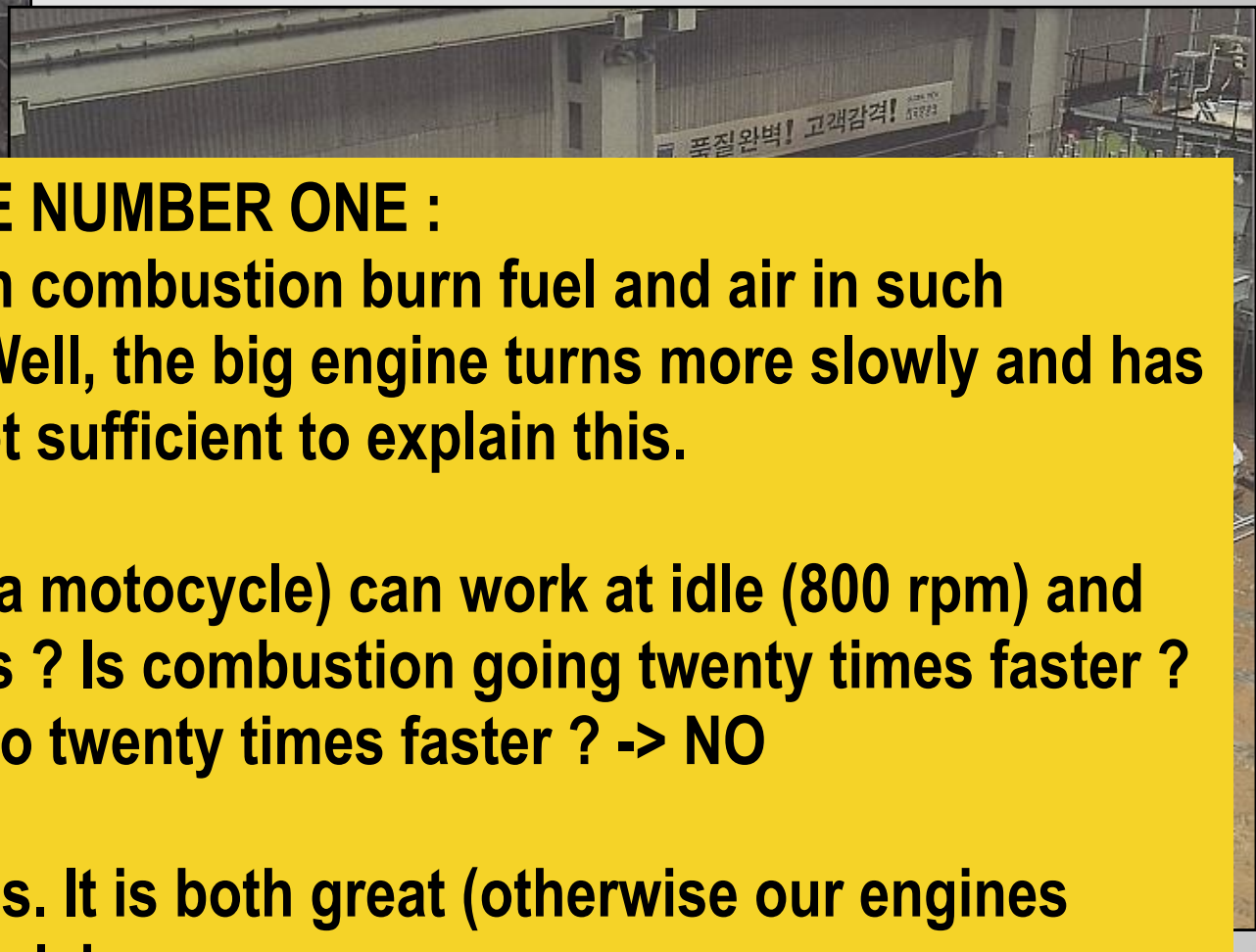




0.1 cm3
0.3 horsepower
25000 trs/min

to big engines:





TURBULENT COMBUSTION ISSUE NUMBER ONE :
(Engineer naive question) how can combustion burn fuel and air in such engines with so different sizes ? Well, the big engine turns more slowly and has more time to burn.... But that is not sufficient to explain this.

For example: the same engine (in a motocycle) can work at idle (800 rpm) and high speed (16000 rpm) conditions ? Is combustion going twenty times faster ? Does it mean that chemistry can go twenty times faster ? -> NO

Turbulent combustion explains this. It is both great (otherwise our engines would not work) and difficult to explain...



90 000 HP
100 trs/min
6000 liters/hour

From small gas turbines to big gas turbines

Efficiencies:

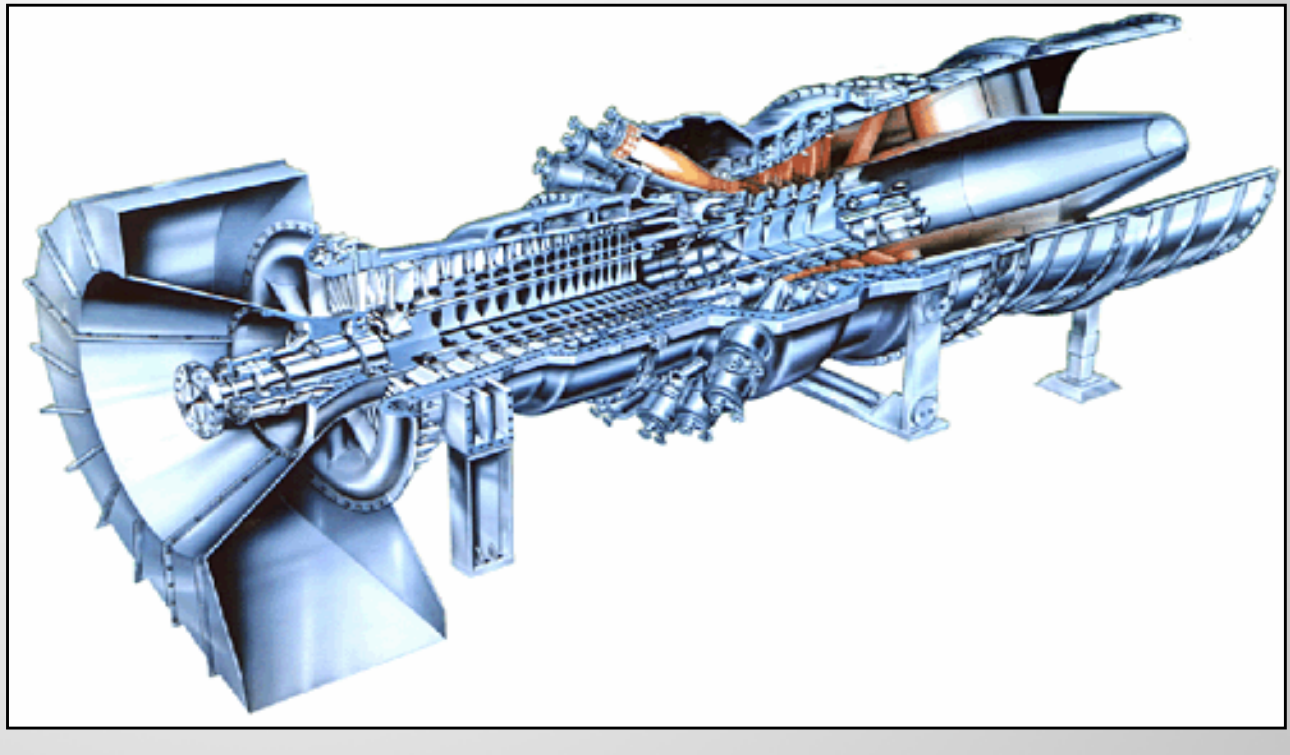
40% Electric

60% Combined Cycles

80% Cogeneration



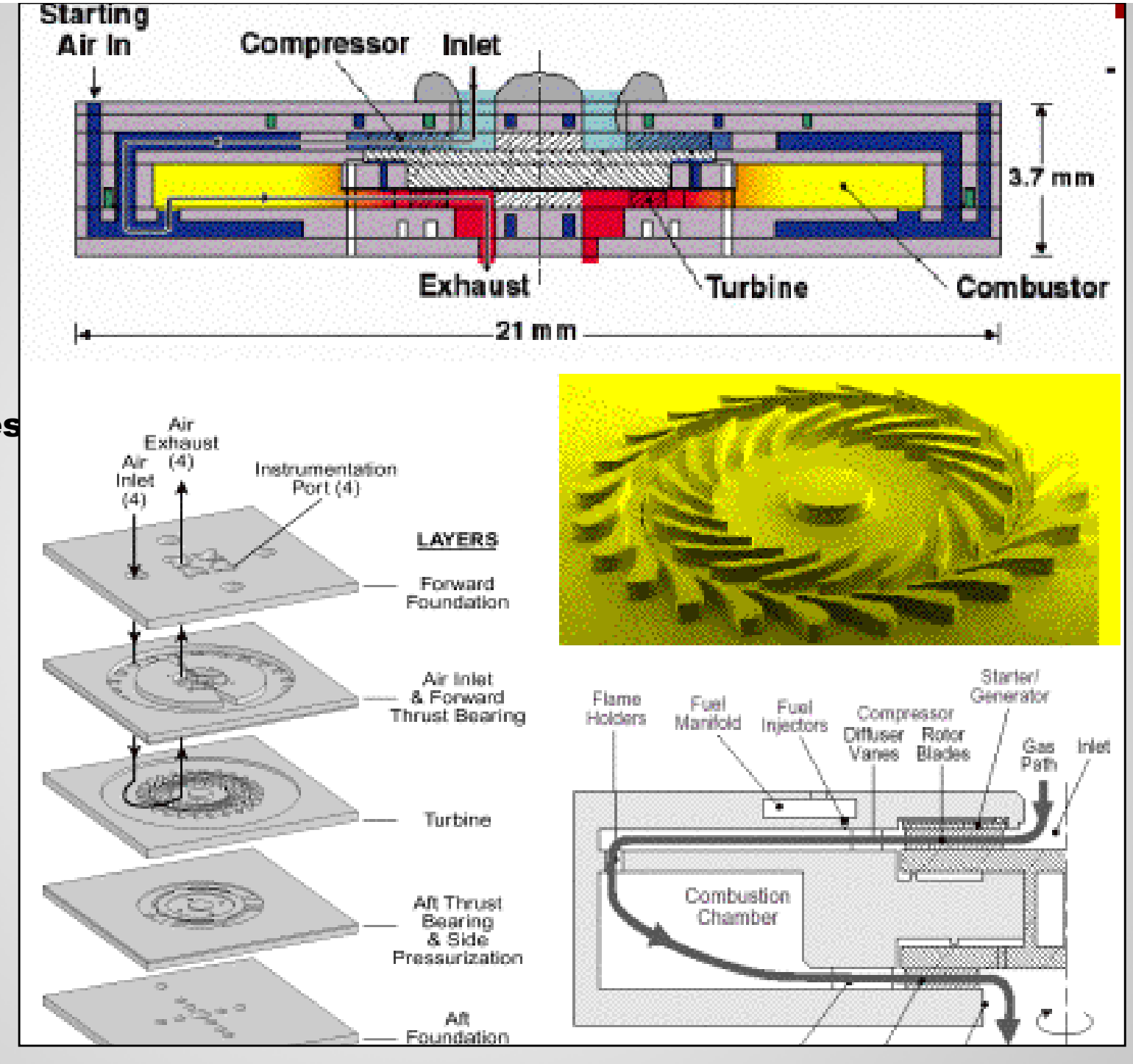
50W



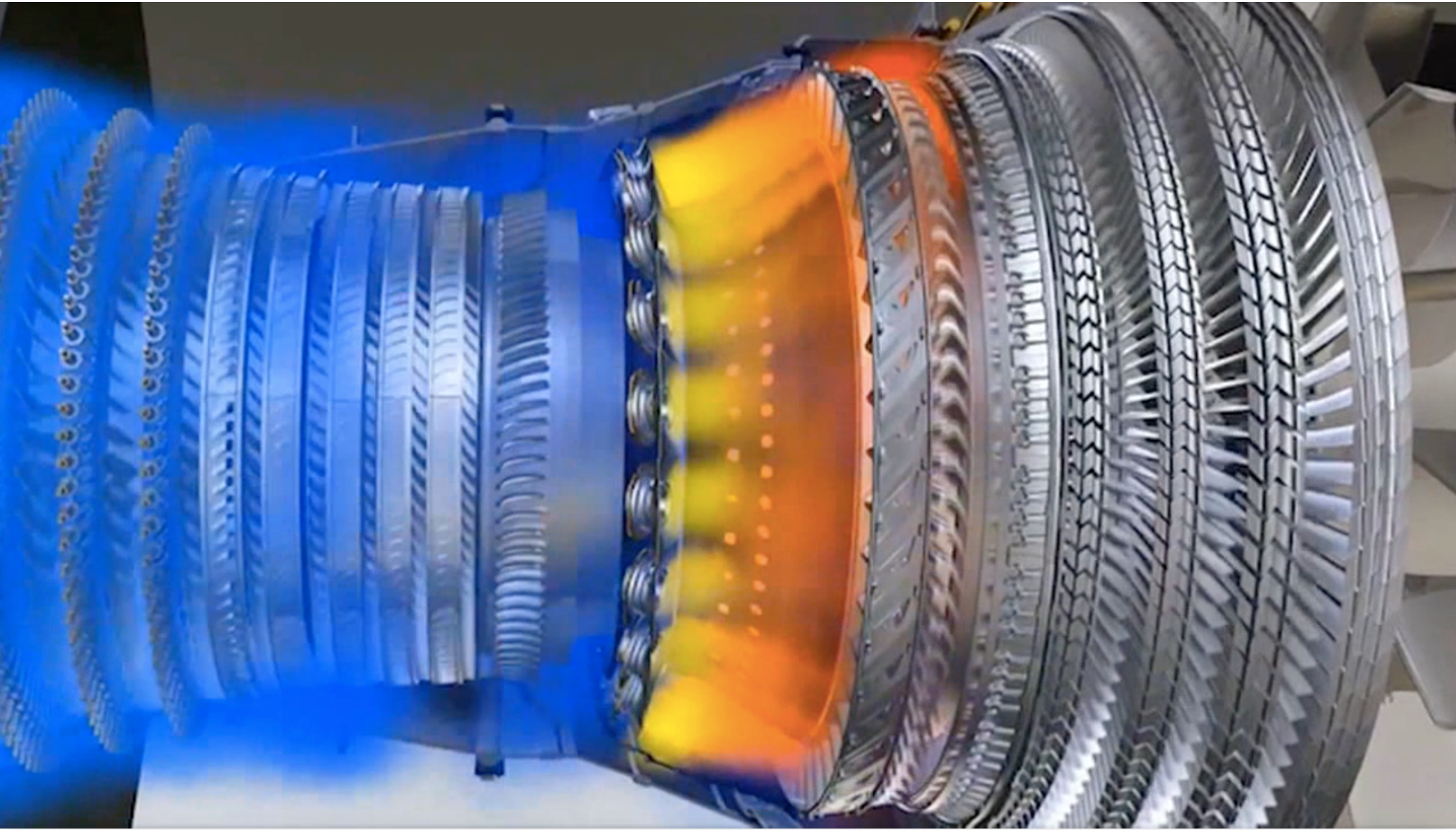
400 000 000 W

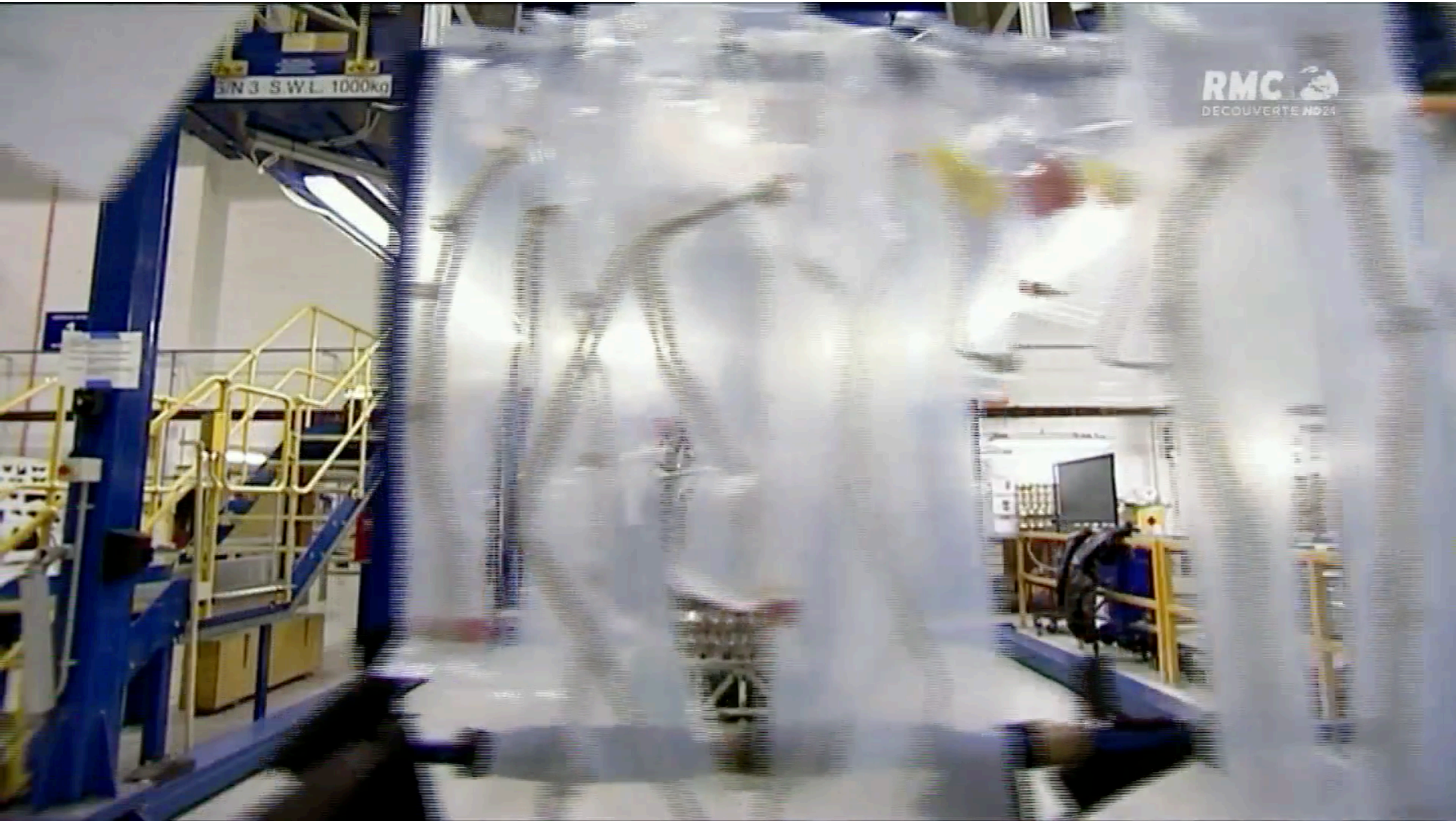
For soldiers and maybe for cell phones

100 g of CH4 = 15 times more energy than a 100 g battery

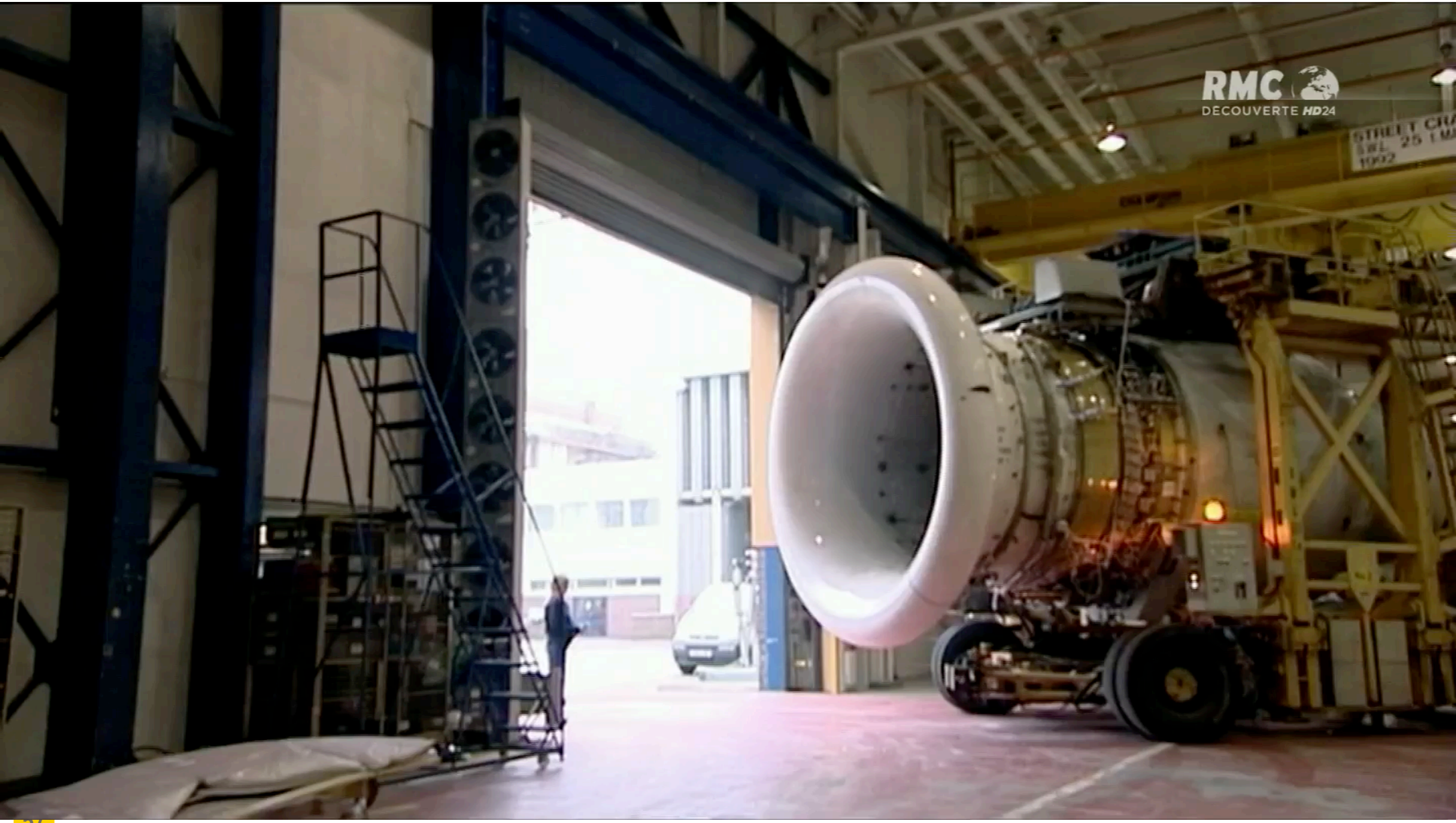



737
AIRCRAFT ENGINES

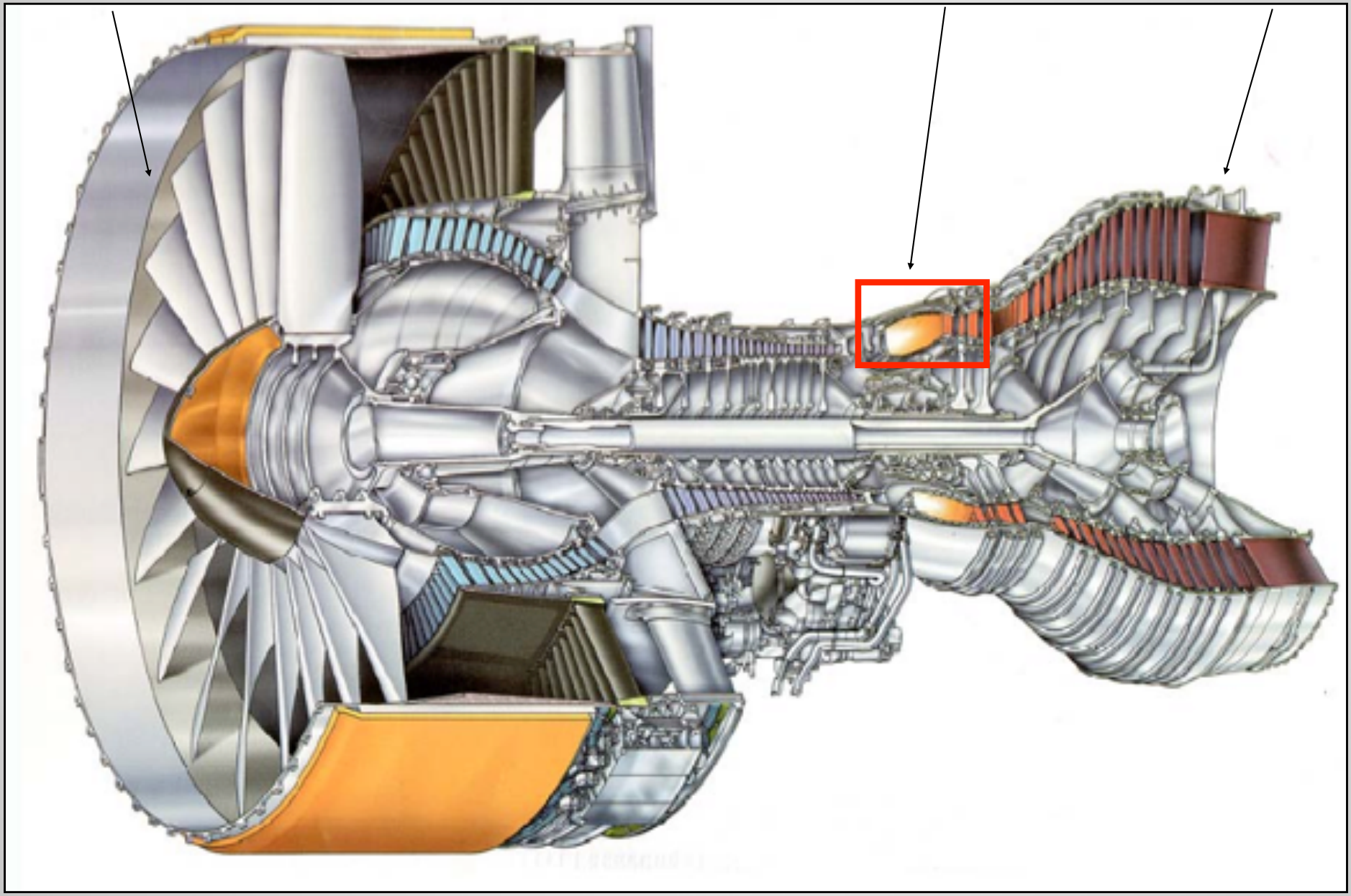



S/N 3 S.W.L. 1000kg
RMC
DECOUVERTE HD24

Big engines even on aircraft:

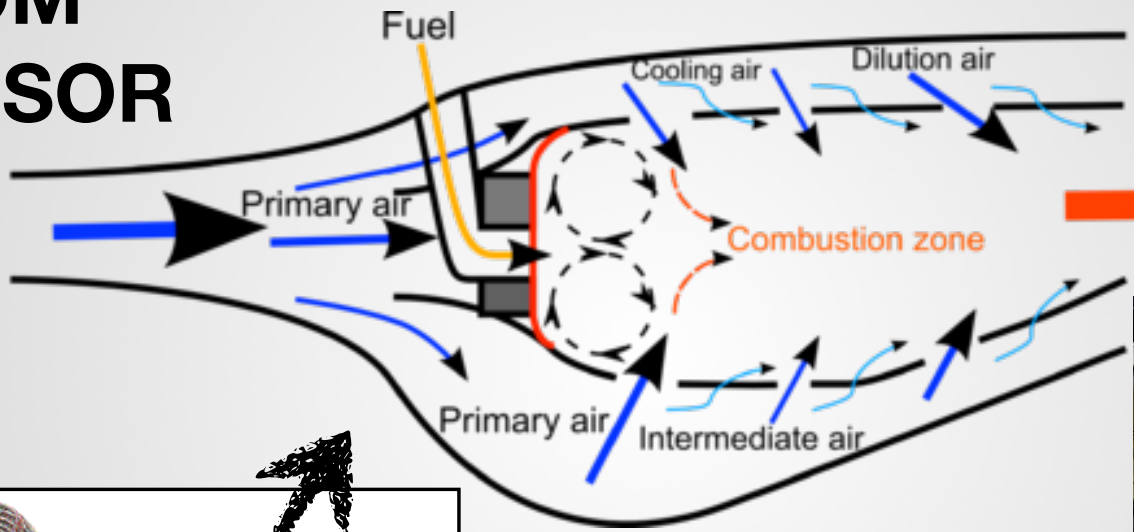


Compressor Combustor Turbine

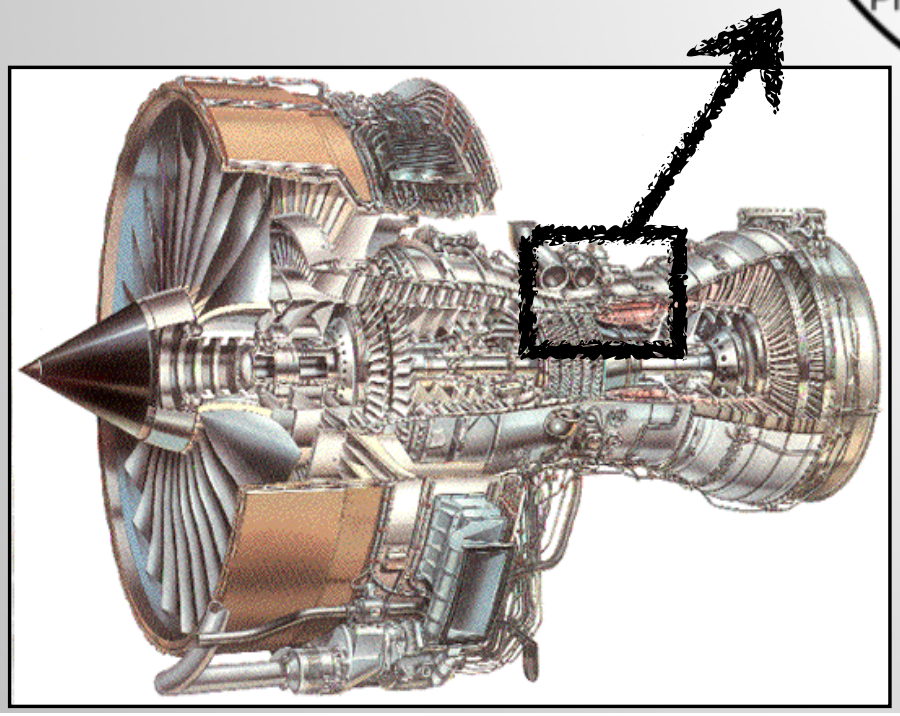


TERMINOLOGY:

AIR FROM COMPRESSOR



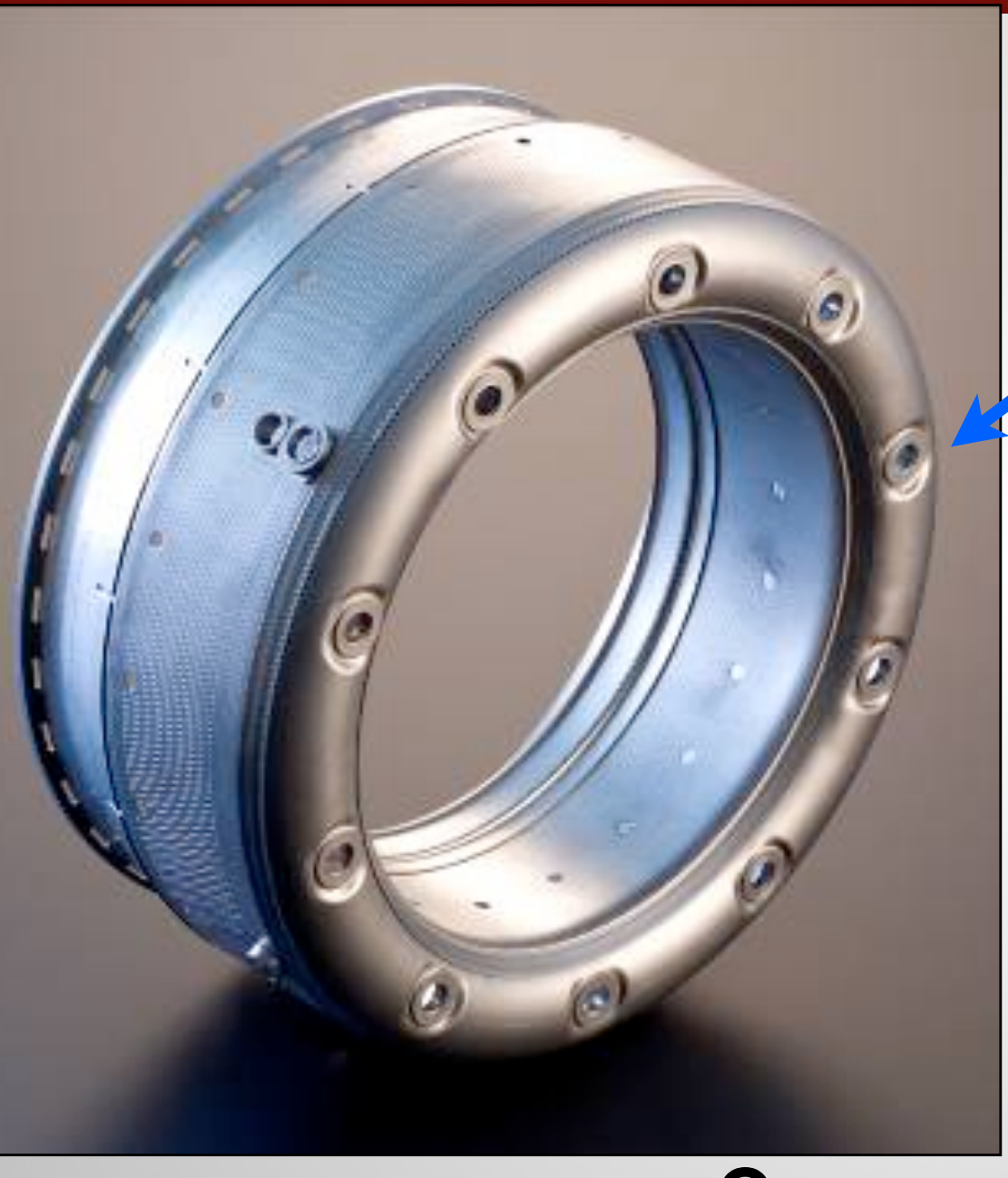
TO TURBINE



TURBINE AXIS

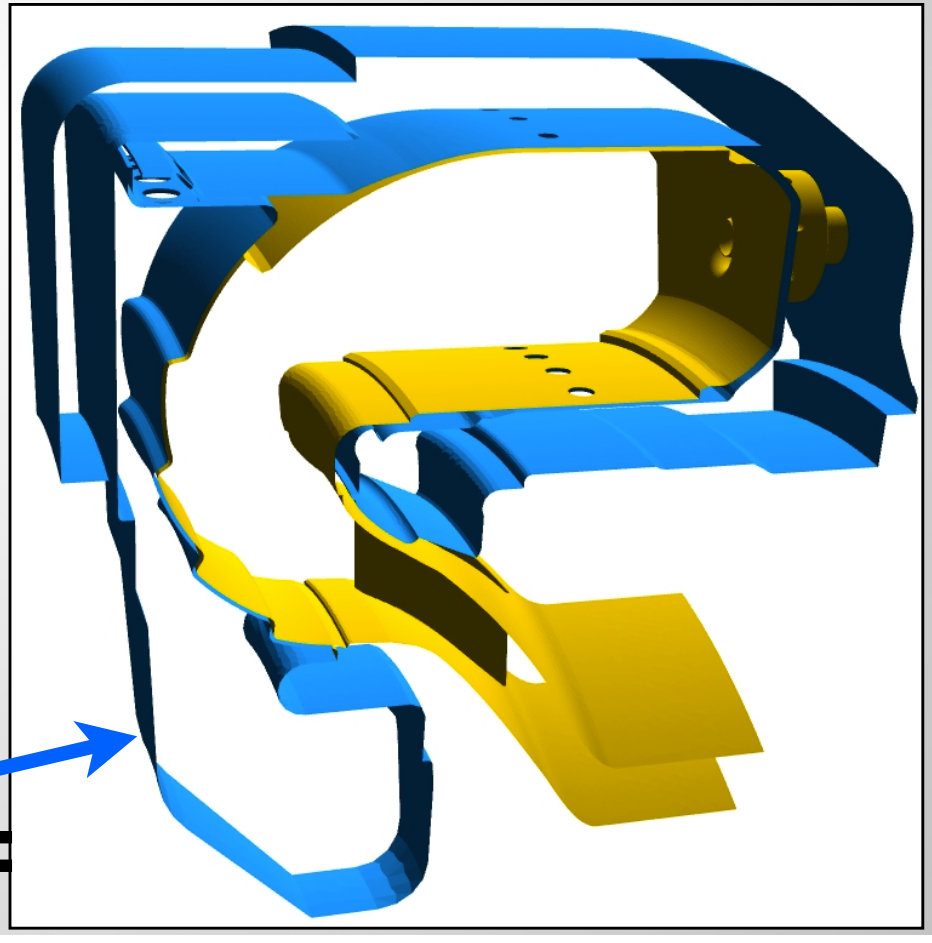


MORE TERMINOLOGY

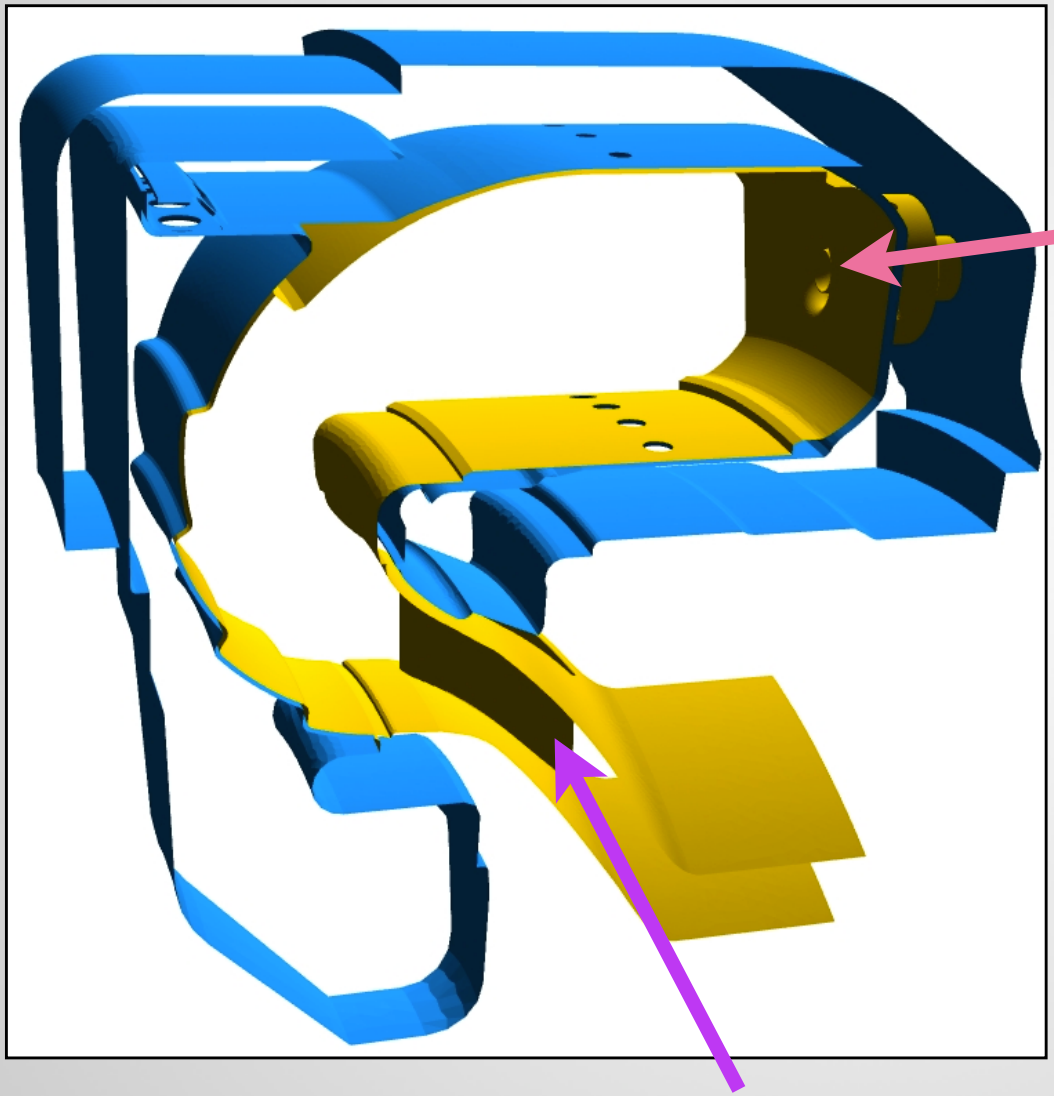


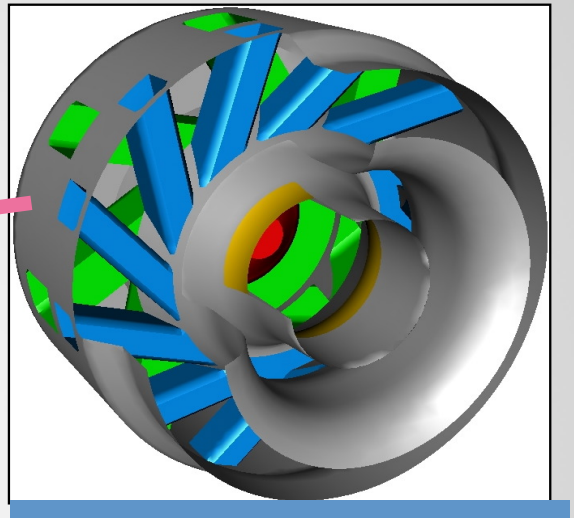
Full combustion chamber (10 to 24 ‘sectors’ or ‘burners’)

One sector :



FOR EACH SECTOR:
A SWIRLER AND A HPS



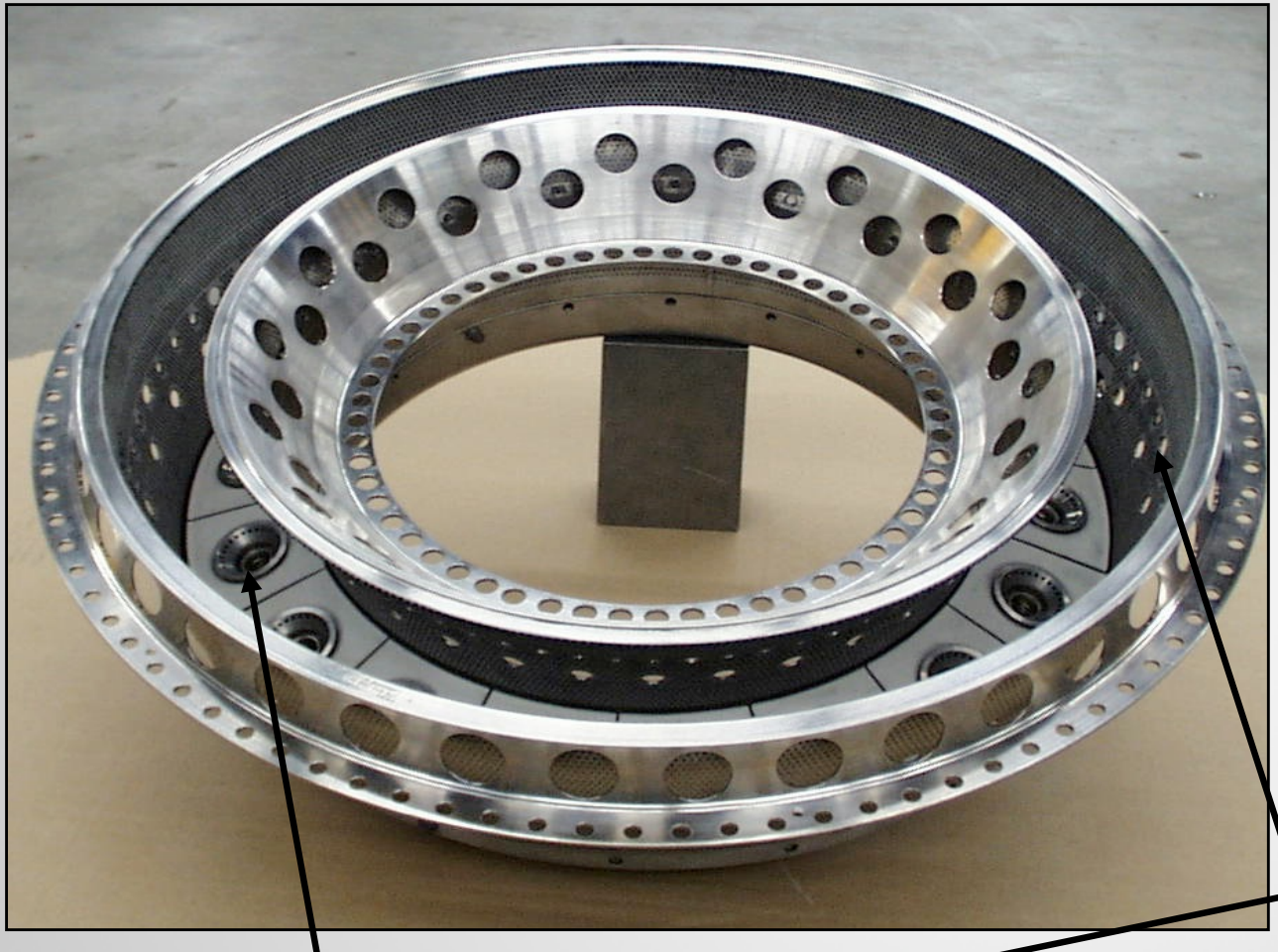


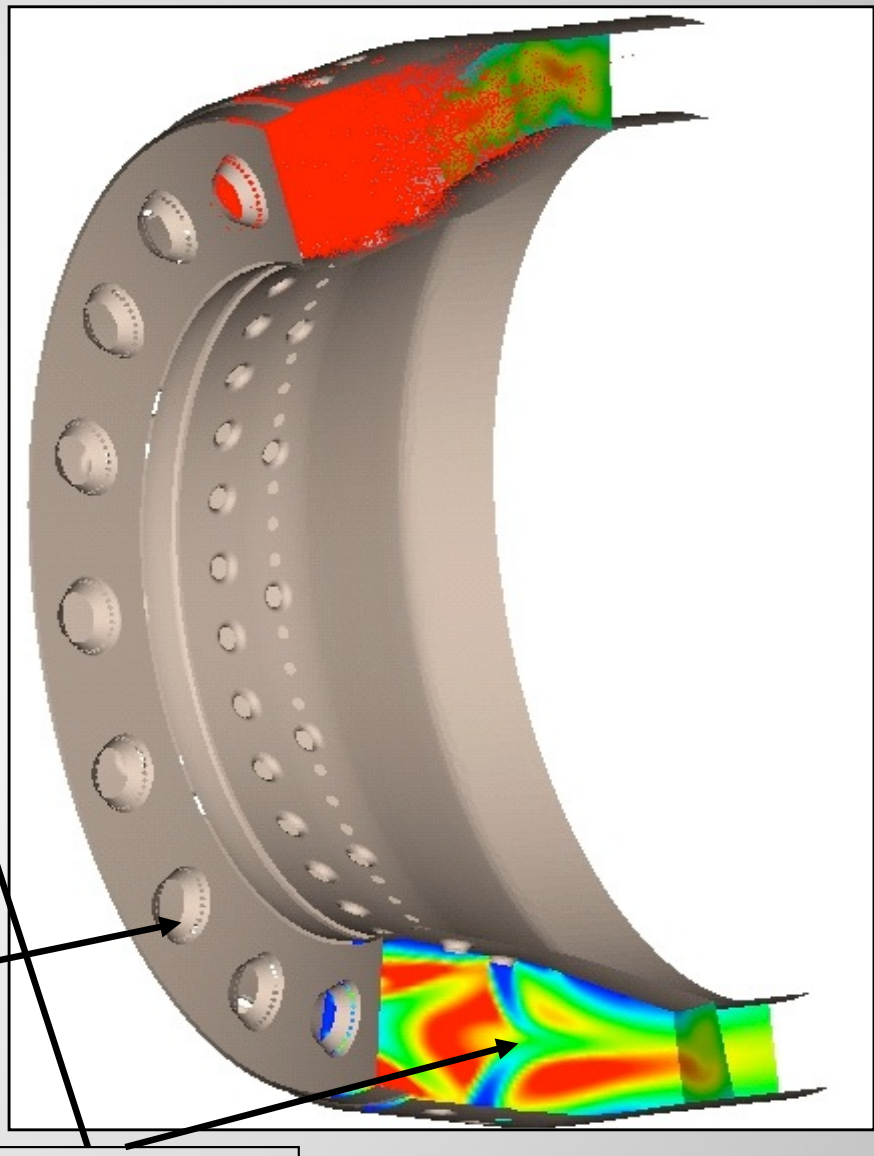
LPP injector

A swirler (one per secto

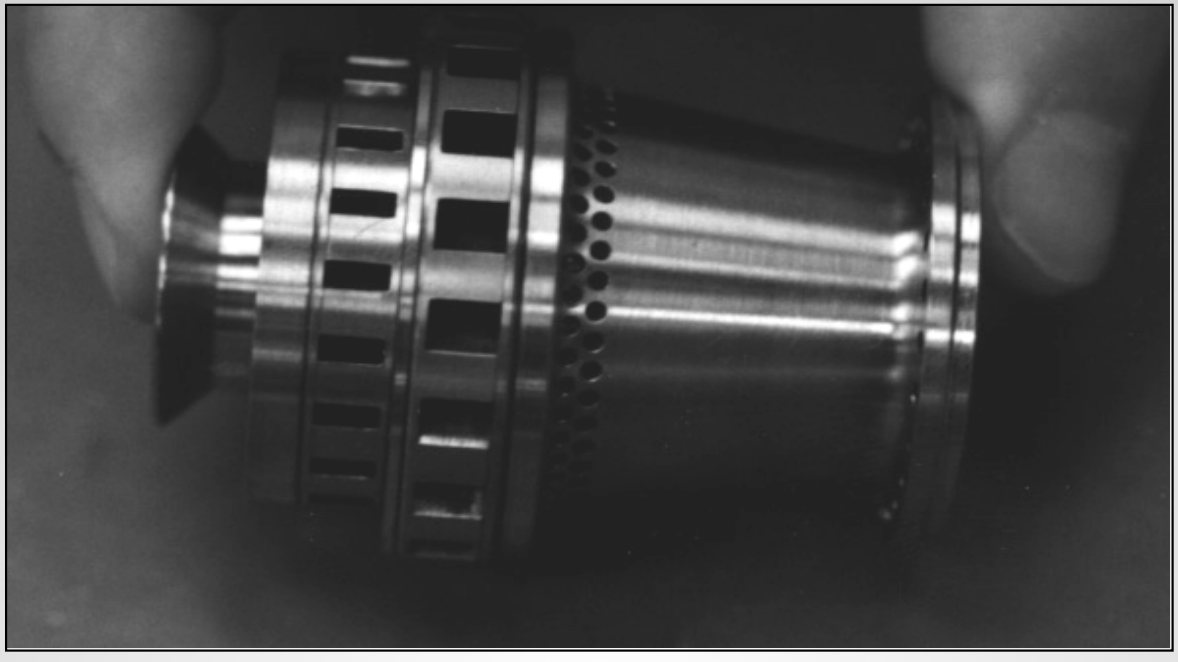
A HPS (High Pressure Stator: one per sector)

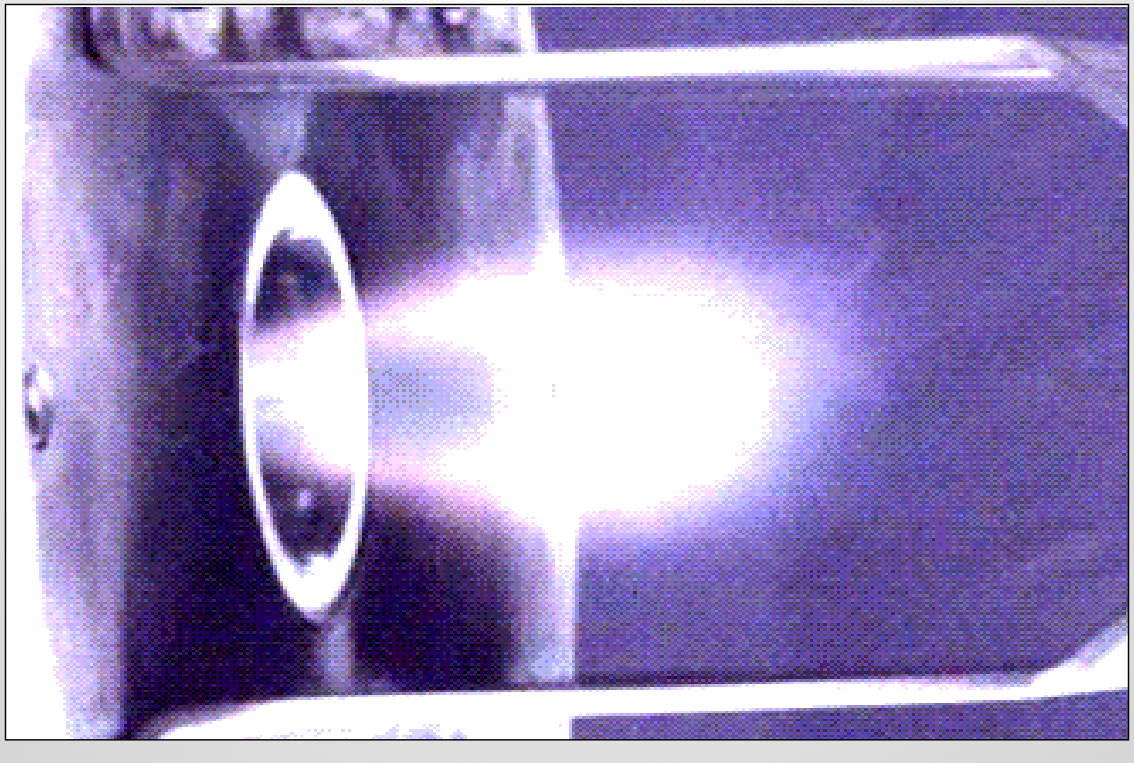
Example of combustion chamber





(BURNER) (COMBUSTION CHAMBER)



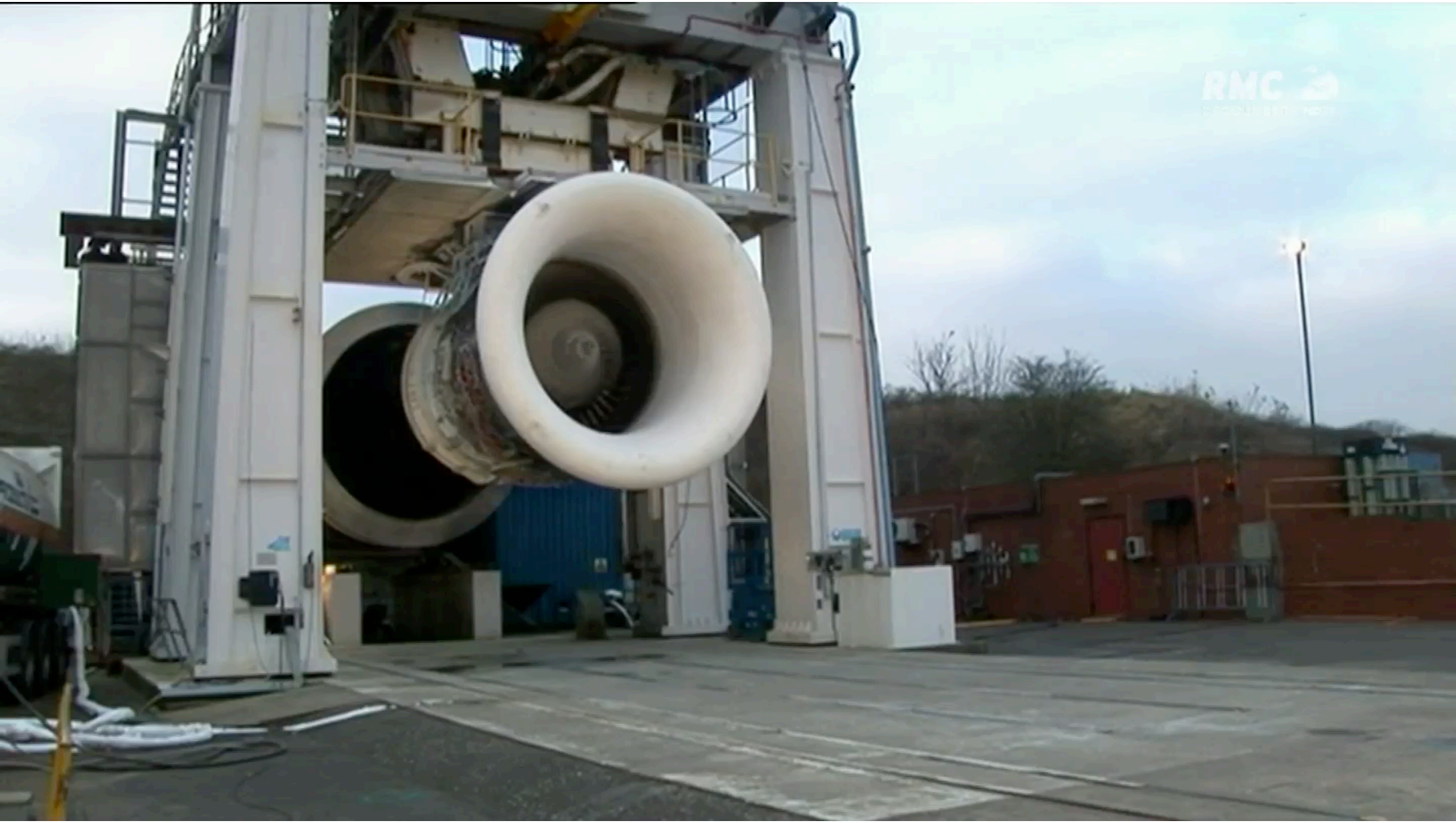


Additional issues

- The engine must work over a wide variety of conditions:
  - power
  - inlet temperature
  - pressure
  - water content
- It must be simple to ignite and reignite
- The engine must not quench

What is ‘quenching’ ?

- ★Quenching occurs when the flame stops (then the engine stops, then the plane falls…)
- ★Quenching can occur for all flames but obviously quenching in aircraft and helicopters is a major issue
- ★What causes quenching ?
  - Sudden change of operating conditions: when an helicopter pilot decreases power, the kerosene flow rate decreases fast but not the air flow rate -> the mixture might become too lean and the flame may quench
  - Outside conditions may also quench the flame: volcano ashes with less oxygen, rain or ice



140 tons/hour of water

Ignition ?

★Two types of ignition problems in aircraft:

- ➡ Need to start the engine on the ground before take off
- ➡ If the engine stops then we need to re ignite it during the flight -> this is actually the most stringent condition and a requirement for certification

★Helicopters: ignition must be possible at high altitude. Stop on a mountain at 5000 m and then restart the engine after a few hours.

Turbulent combustion

★Ultimately, steady as well as unsteady combustion (quenching like ignition) take place in turbulent flows

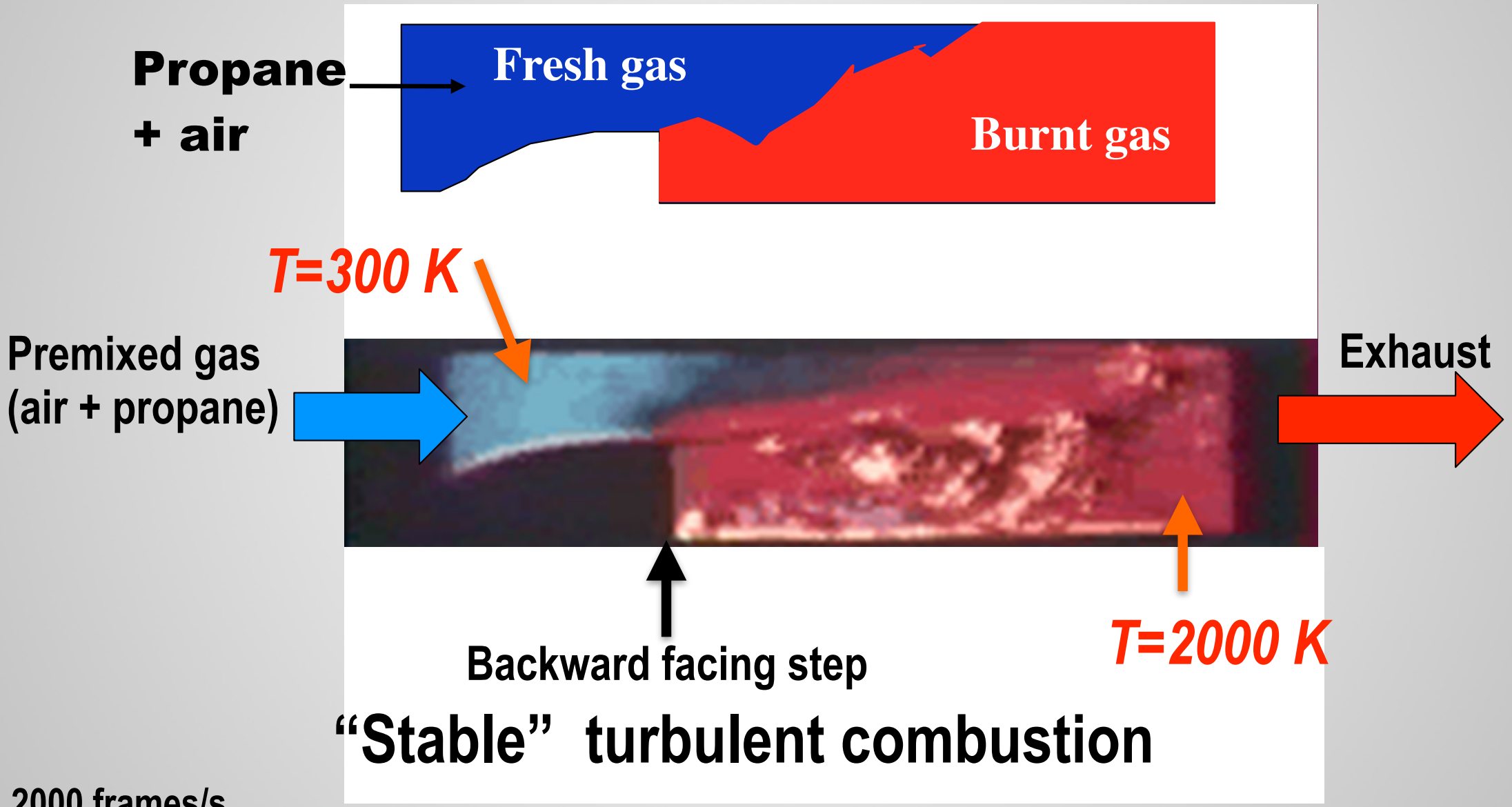
★The coupling between turbulence and chemistry becomes especially difficult to predict in these phenomena where a small change of chemistry can change the result -> prediction of quenching or of ignition is more difficult than the prediction of steady turbulent combustion.

So that:

- the optimization of a combustion chamber is a complex task requiring multiple iterations between different objectives. This is not only about computing one full power regime in terms of efficiency or pollutant emission. Ignition, quenching, noise are also important

- this optimization very often leads to a new problem which must be discussed now: **combustion instabilities**

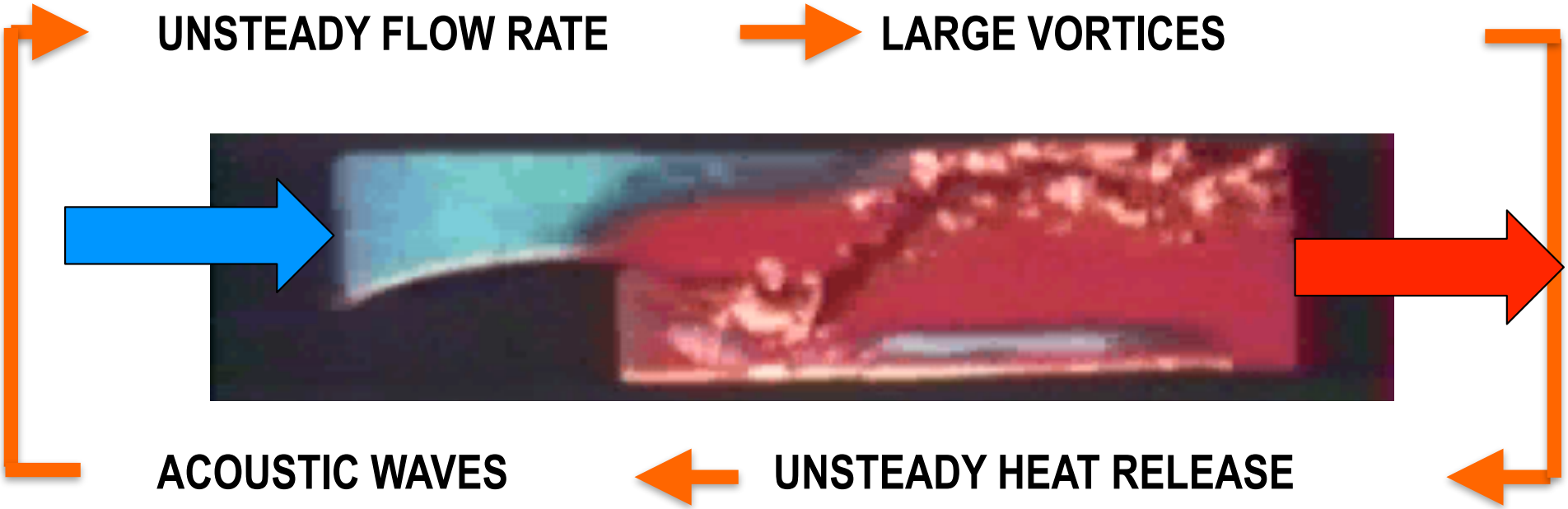
The classic example of the Berkeley backward facing step in the 80s (Pr Ghoniem PhD)



"Stable" turbulent combustion

2000 frames/s

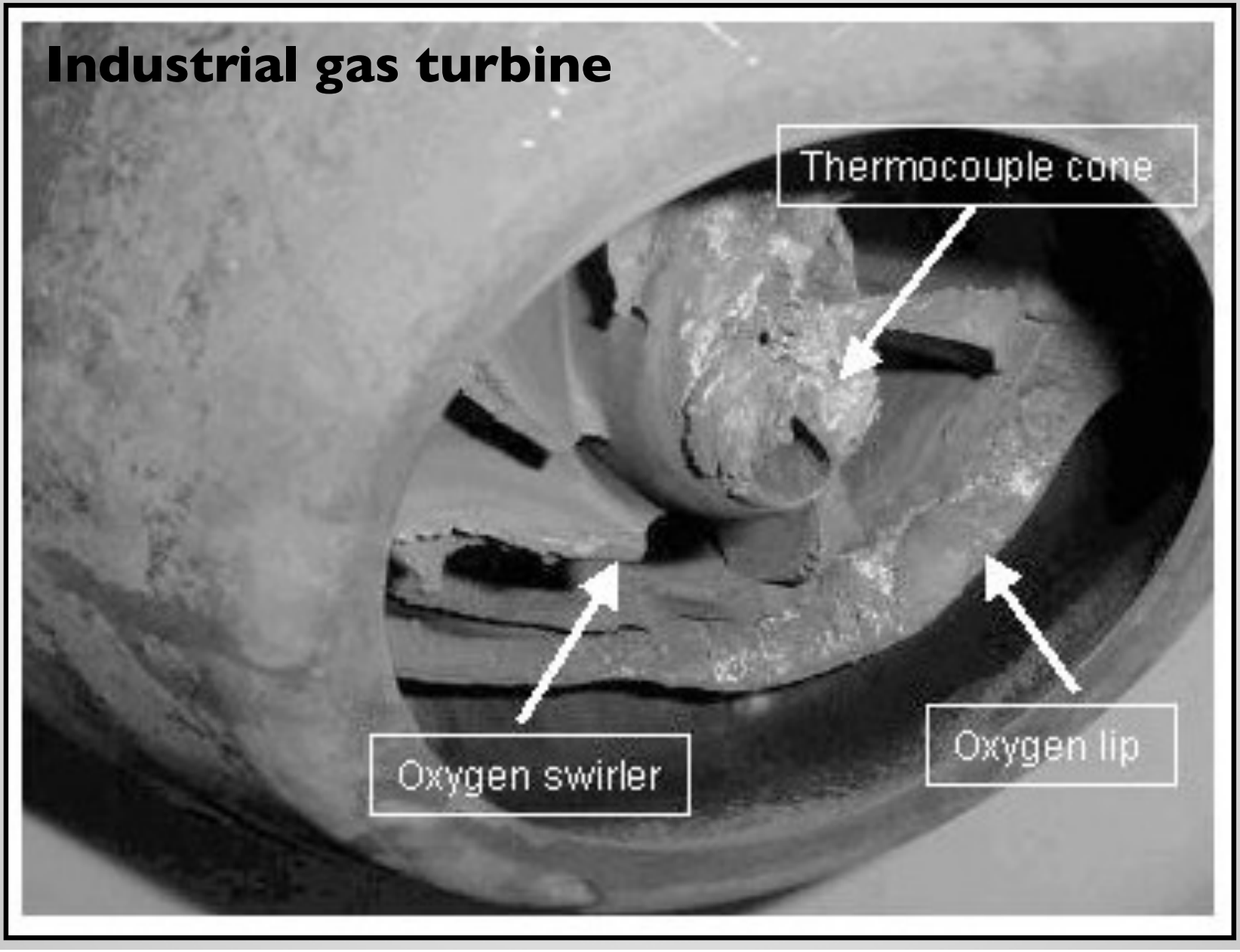
A small change of operating conditions (flow rates of fuel and air) can trigger instability:



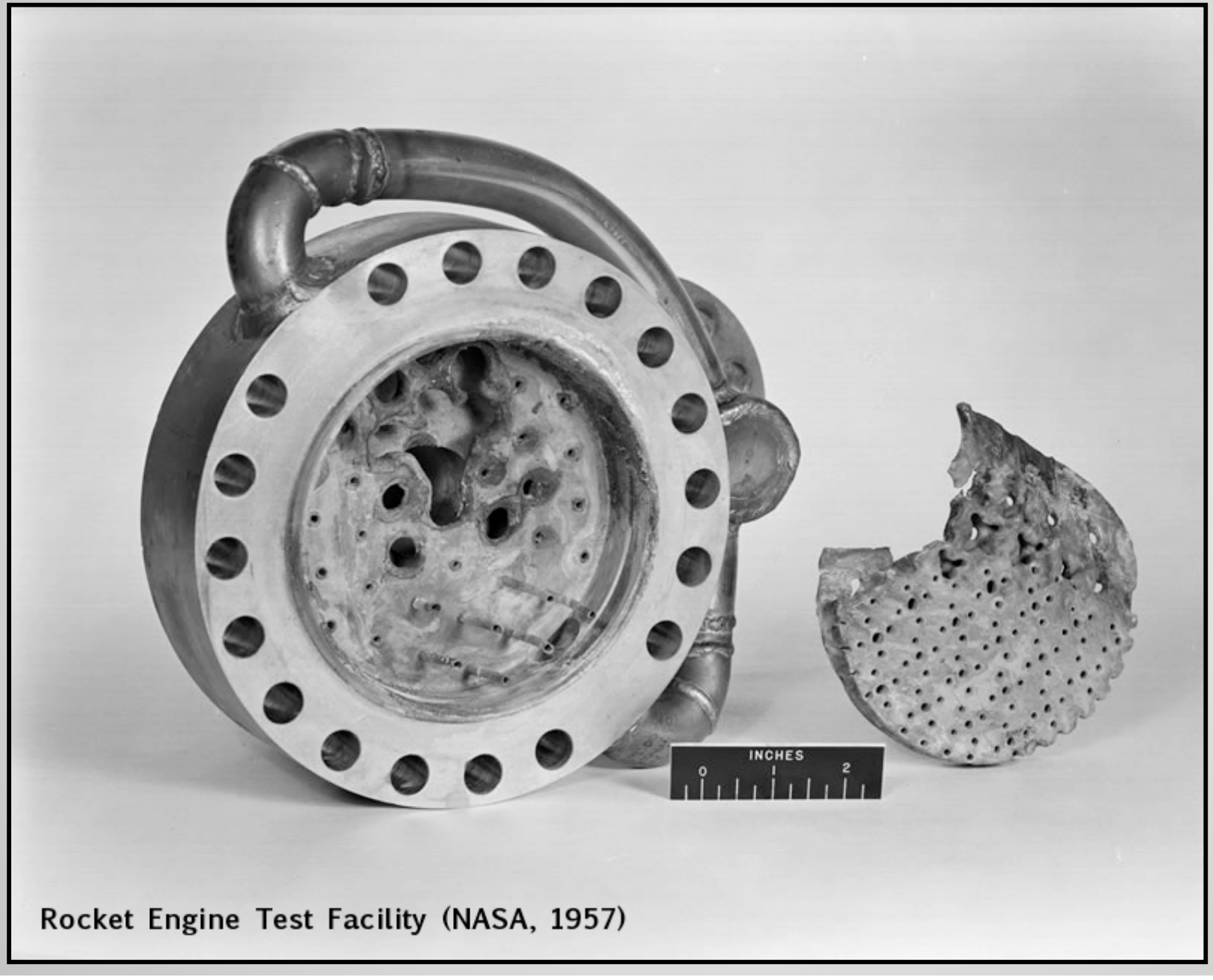
Combustion instabilities hurt:

- **Ariane IV**
- **Saturne F1 engine**
- **Post combustion**
- **Alstom**

Consequences of combustion instabilities



Consequences of combustion instabilities



Rocket Engine Test Facility (NASA, 1957)

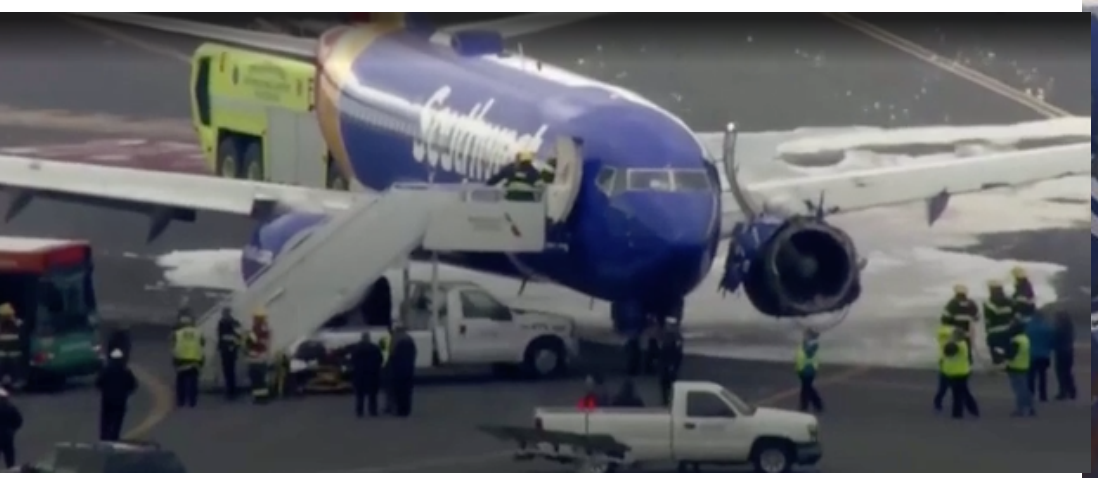
Nasa Injector (1957)

Instability -> Vibrations -> Breaking vanes…



It still happens...

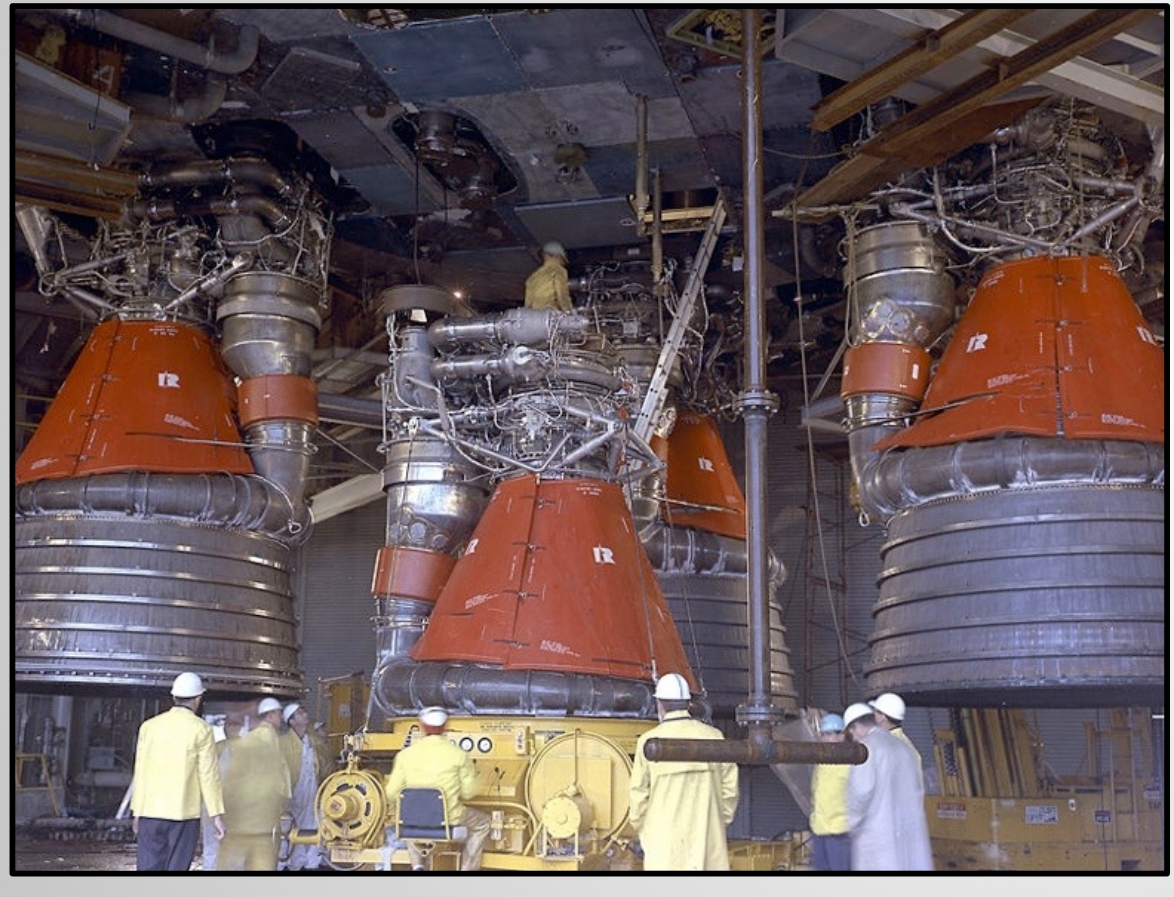
April 2018
Flight 1380 New York-Dallas Southwest Airlines

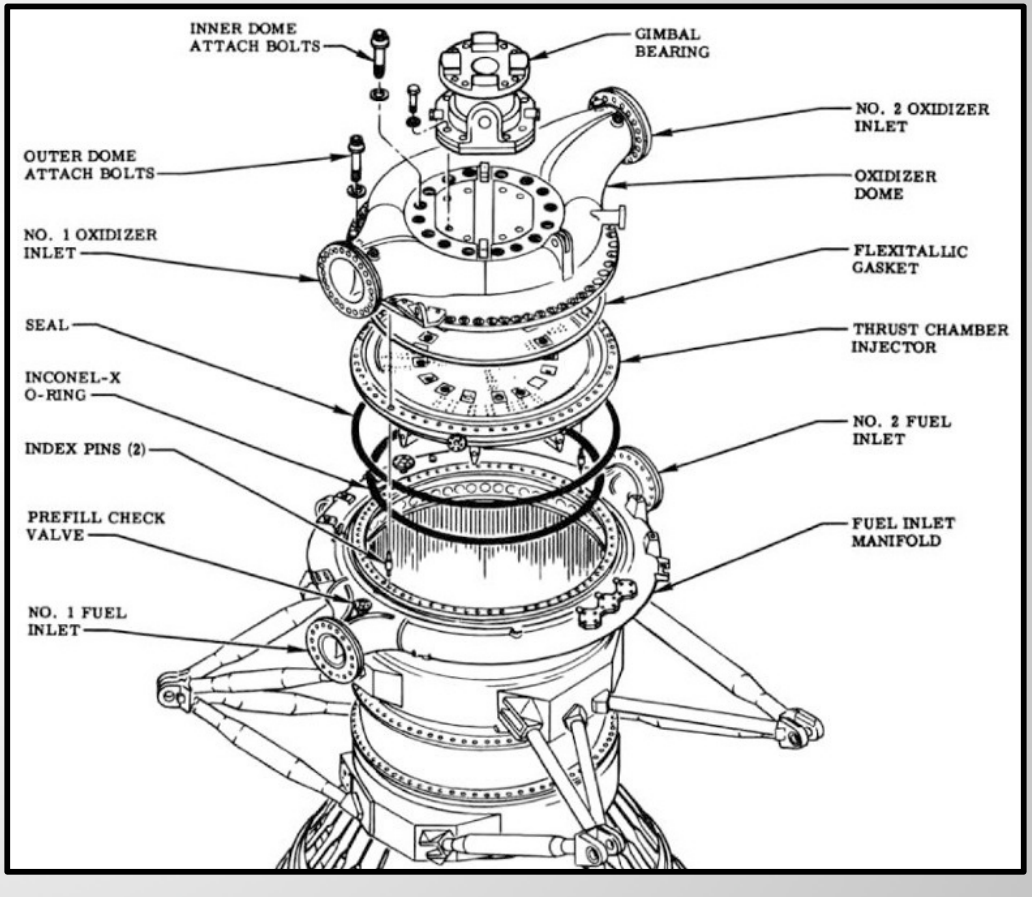




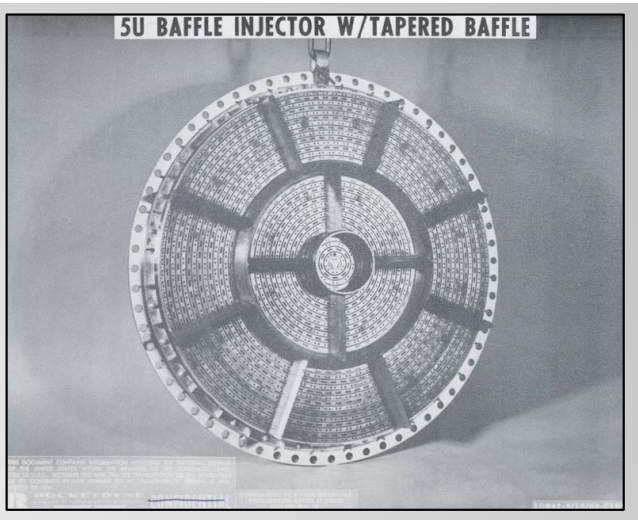
Curing instability problems:

Example: the F1 engine for Saturn V in the 60s. In most cases, trial and error remains the 'preferred' solution in practice...



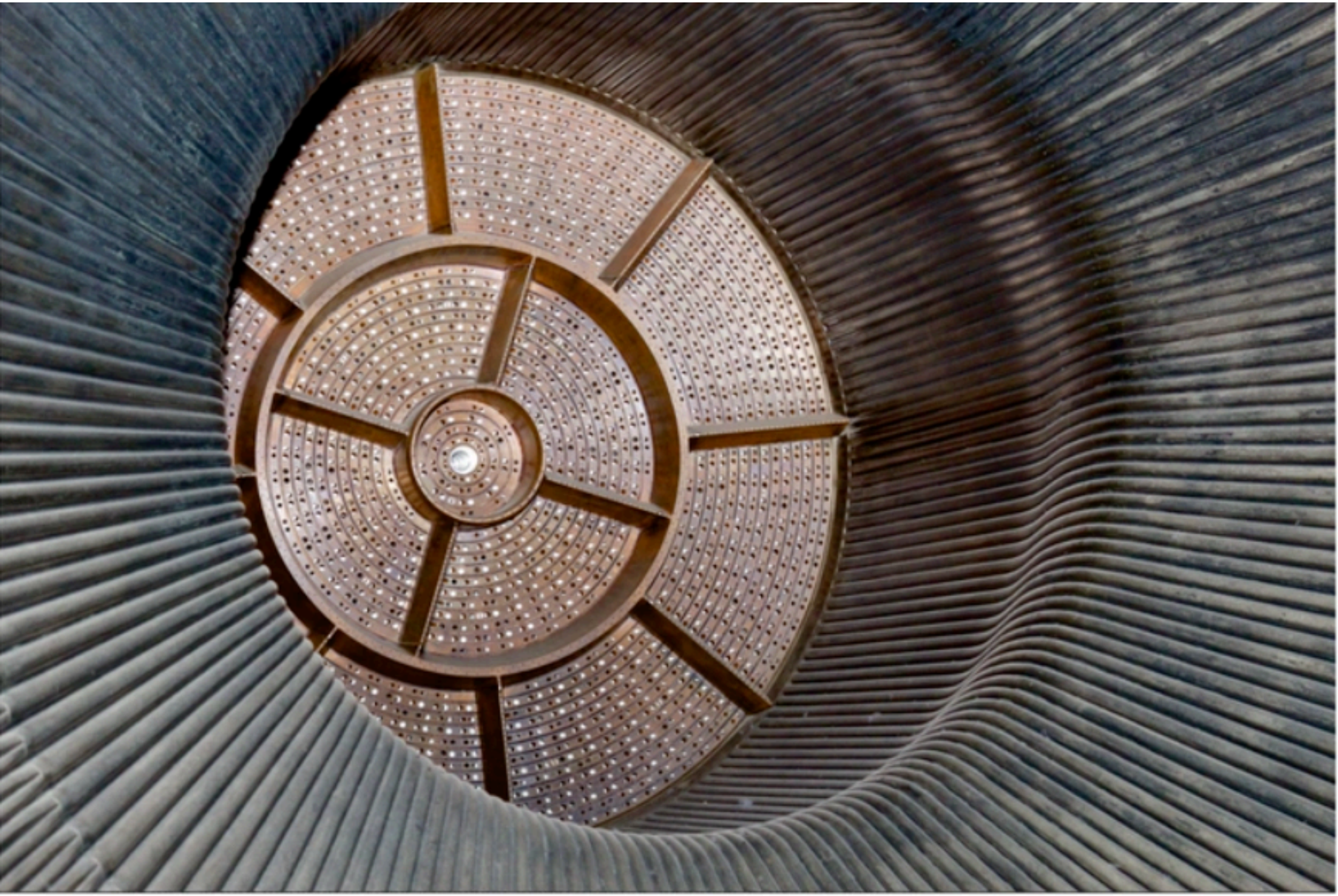


F1 engine design (thanks to Pr V. Yang, Georgia Tech)



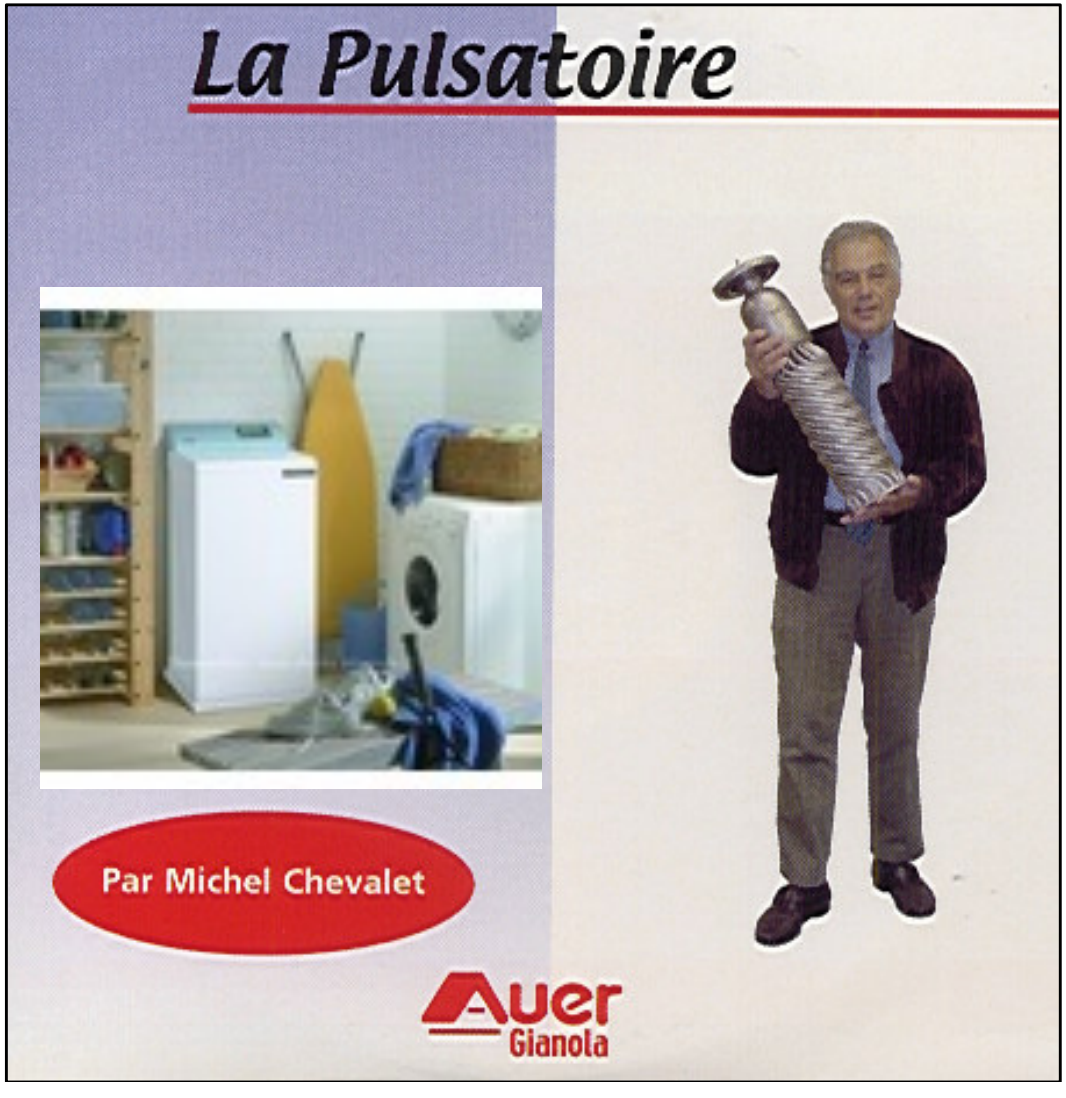
- ★ Initially unstable
- ★ The solution was to modify the fuel injectors and add baffles... but how ?
- ★ 1332 engine tests performed before 1966 to identify the stable solutions (which also had to deliver the other performances)
- ★ Billions of dollars spent
- ★ Incompatible with present programs
- ★ NEED TO BE ABLE TO PREDICT INSTABILITIES AND MORE GENERALLY UNSTEADY COMBUSTION -> *CFD OF REACTING FLOWS IS NEEDED*

Source: Pr Vigor Yang, Georgia Tech

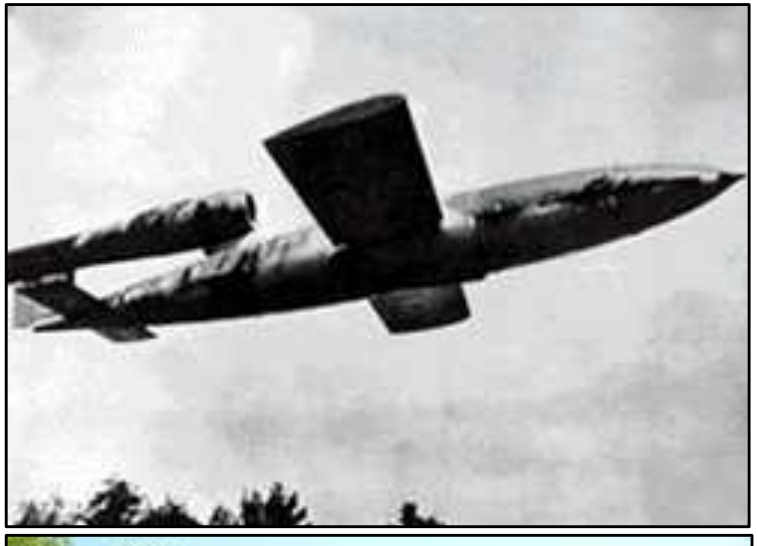


Combustion instabilities can sometimes be used on purpose:

Heaters (nowadays)



V1 (not useful)







BLACK AND WHITE IMAGES ARE REAL IMAGES FROM V1
COLORED IMAGES ARE FAKE

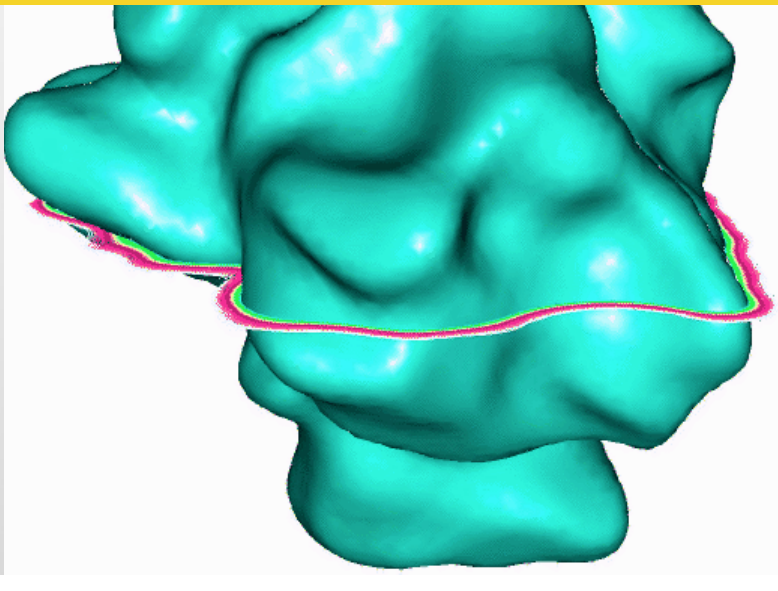
CFD and combustion

CFD is essential but not yet able to do its job:

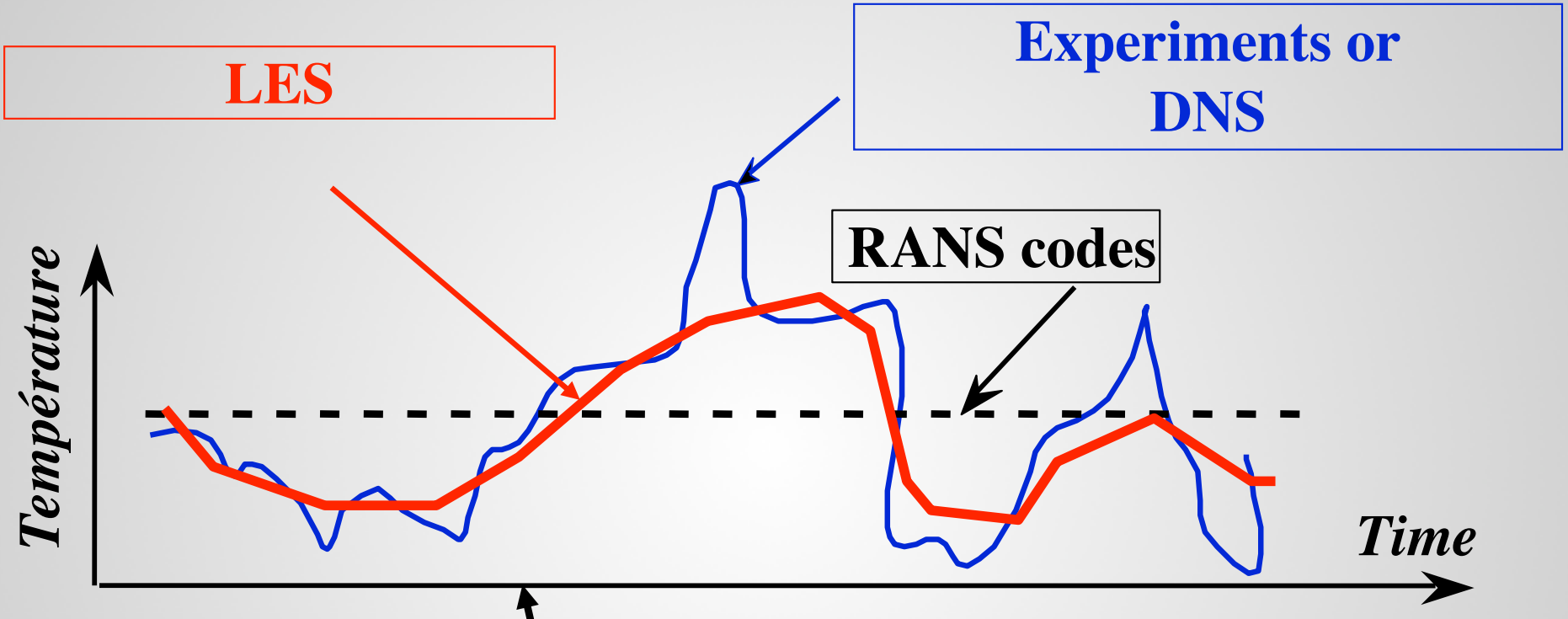
- kinetics + turbulence + radiation + heat transfer + structures

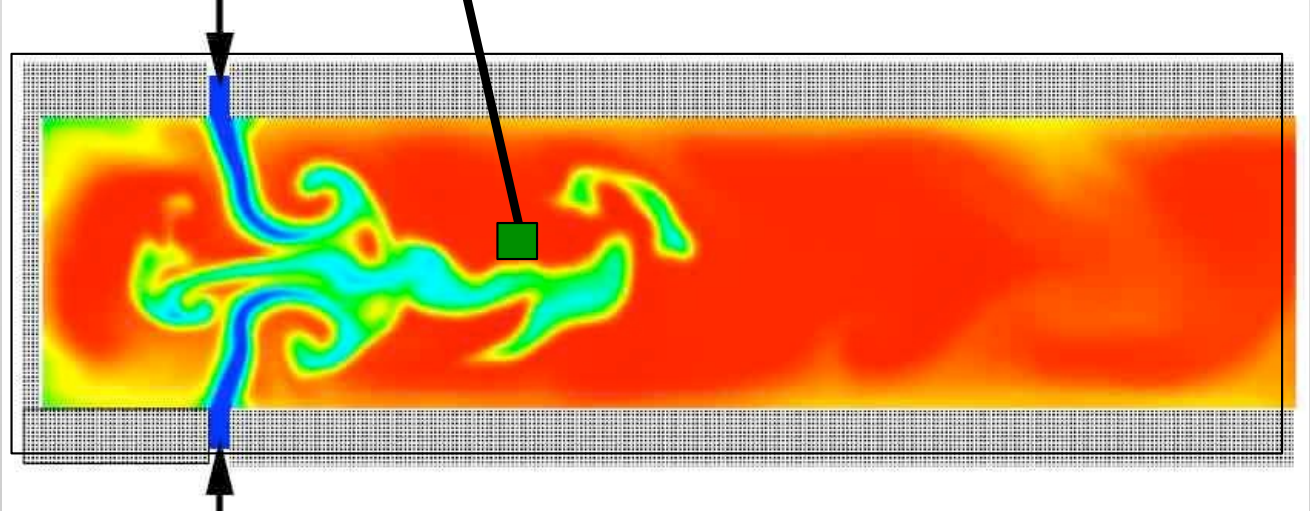
Experiments remain necessary

- non linear -> many (bad) surprises
+ quenching or non ignition
+ explosions and destructions
+ combustion instabilities



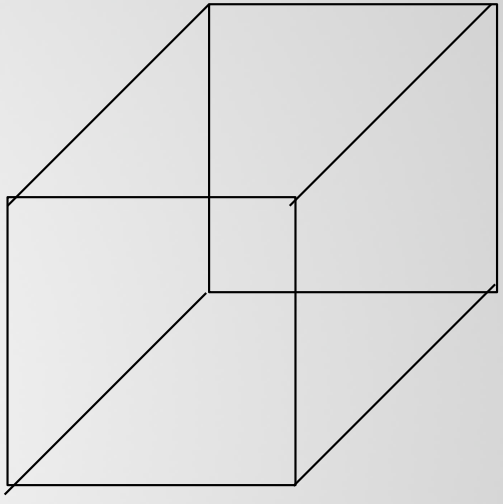
Turbulence remains a major problem





Do we really know what turbulence is ?

Visualization of vortices in a square box of isotropic turbulence (no combustion)
1 billion points



Vortices within vortices:
hierarchical nature of vortex tubes in turbulence

Kai Bürger[1], Marc Treib[1], Rüdiger Westermann[1],
Suzanne Werner[2], Cristian C Lalescu[3],
Alexander Szalay[2], Charles Meneveau[4], Gregory L Eyink[2,3,4]

Entry #: 84174

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[1] Informatik 15 (Computer Graphik & Visualisierung), Technische Universität München
[2] Department of Physics & Astronomy, The Johns Hopkins University
[3] Department of Applied Mathematics & Statistics, The Johns Hopkins University
[4] Department of Mechanical Engineering, The Johns Hopkins University

Fully unsteady

Three dimensional

Can we really compute this ?

AVERAGING: Instead of computing the 3D instantaneous field, we compute the 'average' values of all variables.

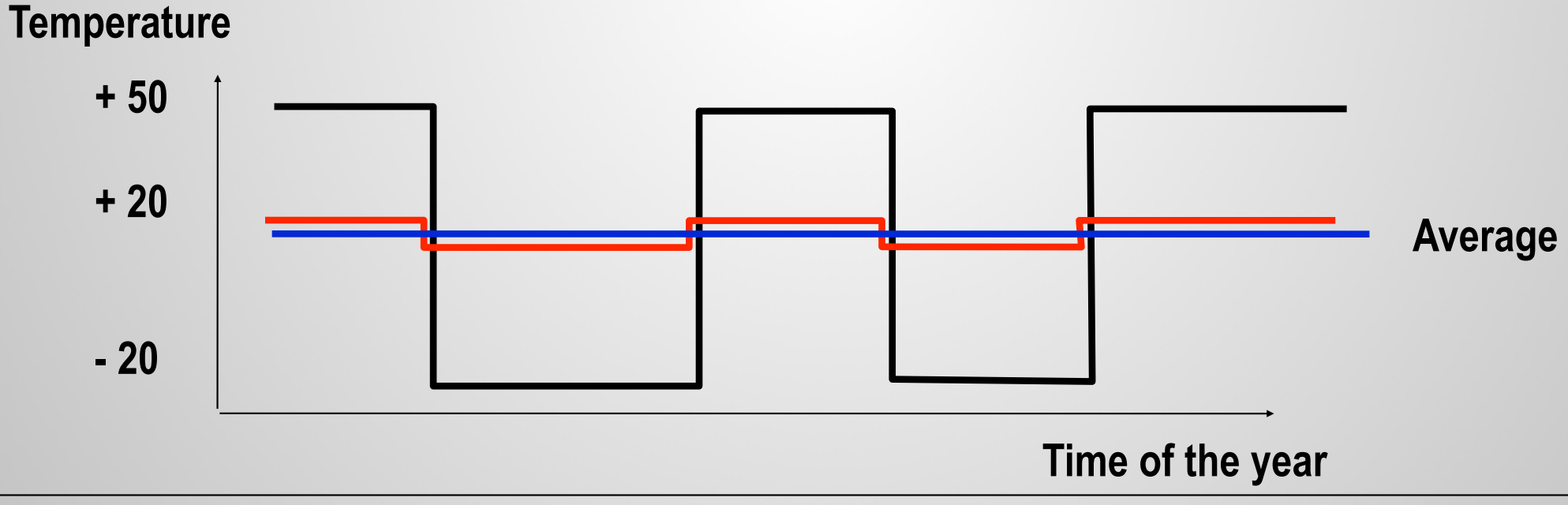
Can be performed in many ways:

- In a gas turbine: average over time. The average quantities depend on space only
- In a piston engine: average over cycle. The average quantities will then depend on space and on the crank angle

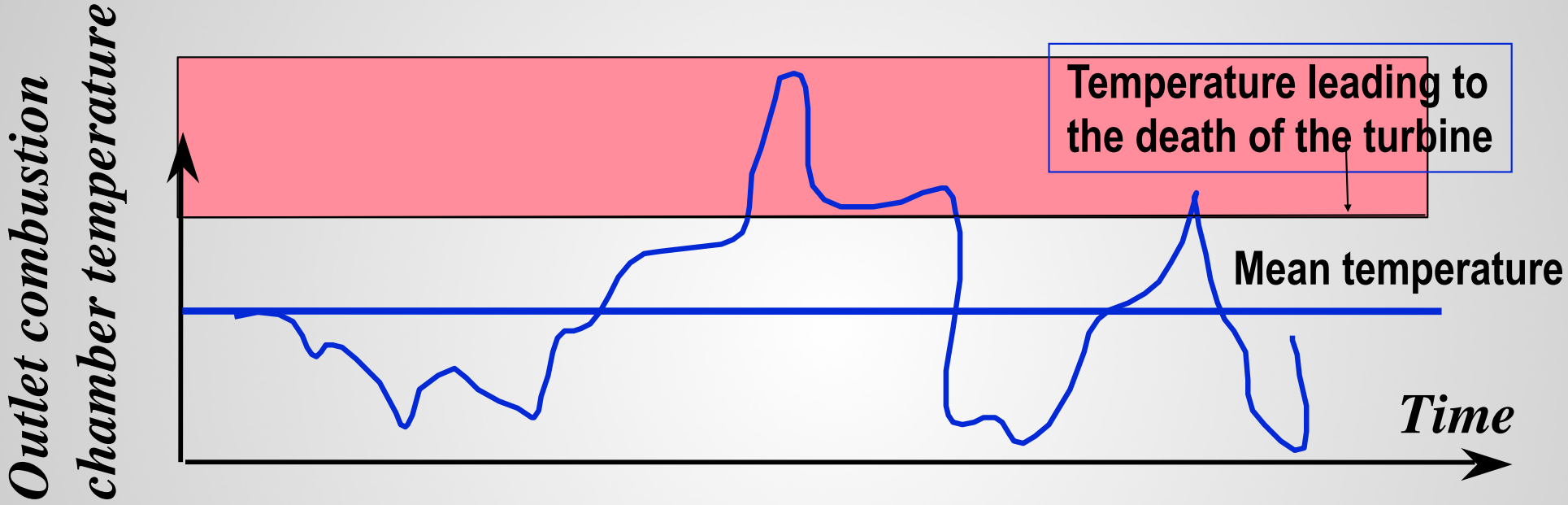
But is averaging a good idea ?

What does the ‘mean’ mean ?

Example: choose the place where you live:



In a turbine:



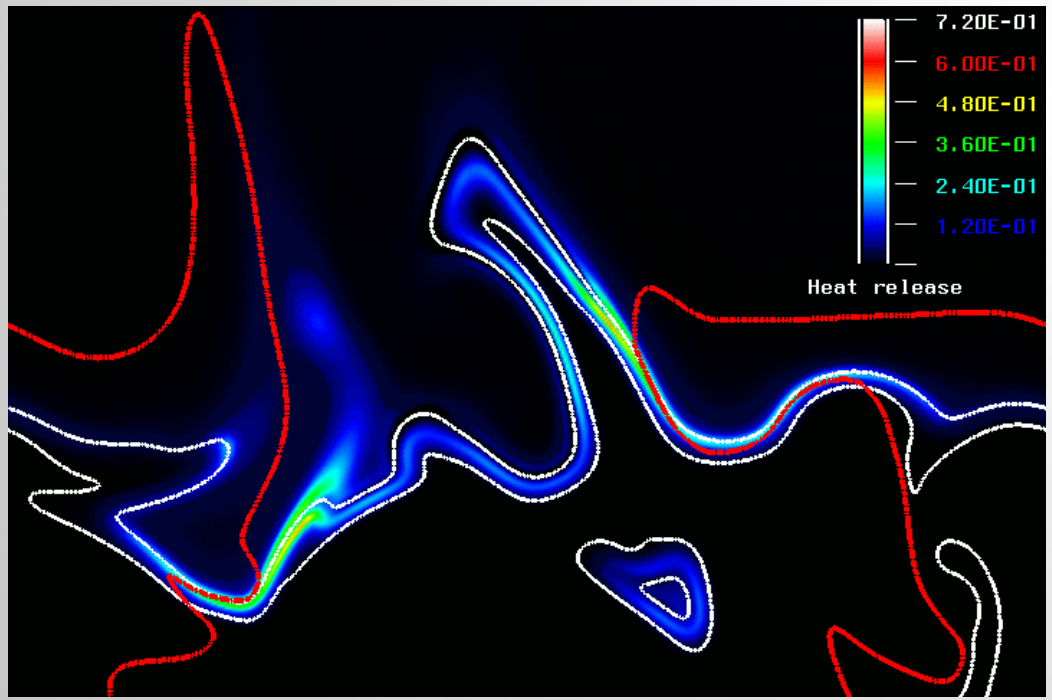
Computing averages is certainly not good but this was a reasonable compromise (and still is in many cases)

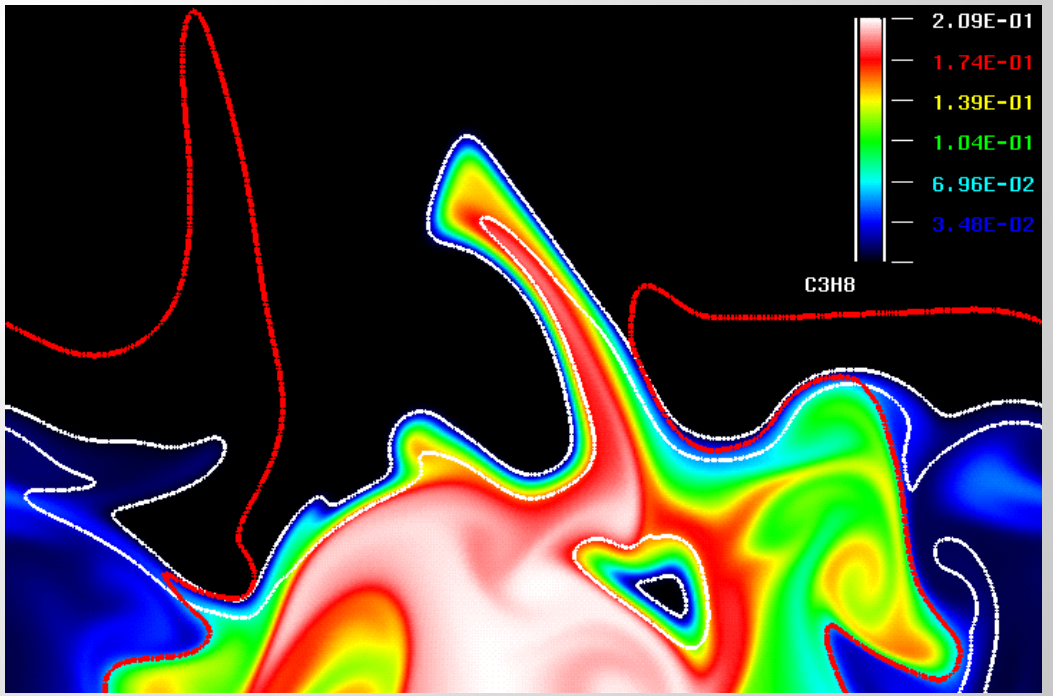
Computing the ‘mean’ only: RANS

- In labs in the 70s
- In industry and commercial codes since 1980: FLUENT, CONVERGE
- In open source codes: OPENFOAM
- Result conditioned by models describing everything we do not compute ie turbulent motions
- Difficult to provide predictive results for mean flows
- Impossible to address unsteady combustion (extinctions, flashbacks) or combustion oscillations

DNS is just on the opposite side: no averaging at all! 3D, UNSTEADY FLOWS

- In labs for reacting flows since 1980 (France / USA)
- No model
- Intrinsically unsteady
- Limited to small cubic boxes





0.1 to 3 mm

WHY IS COMPUTING 'MEAN' QUANTITIES, NOT ENOUGH FOR MANY CASES?

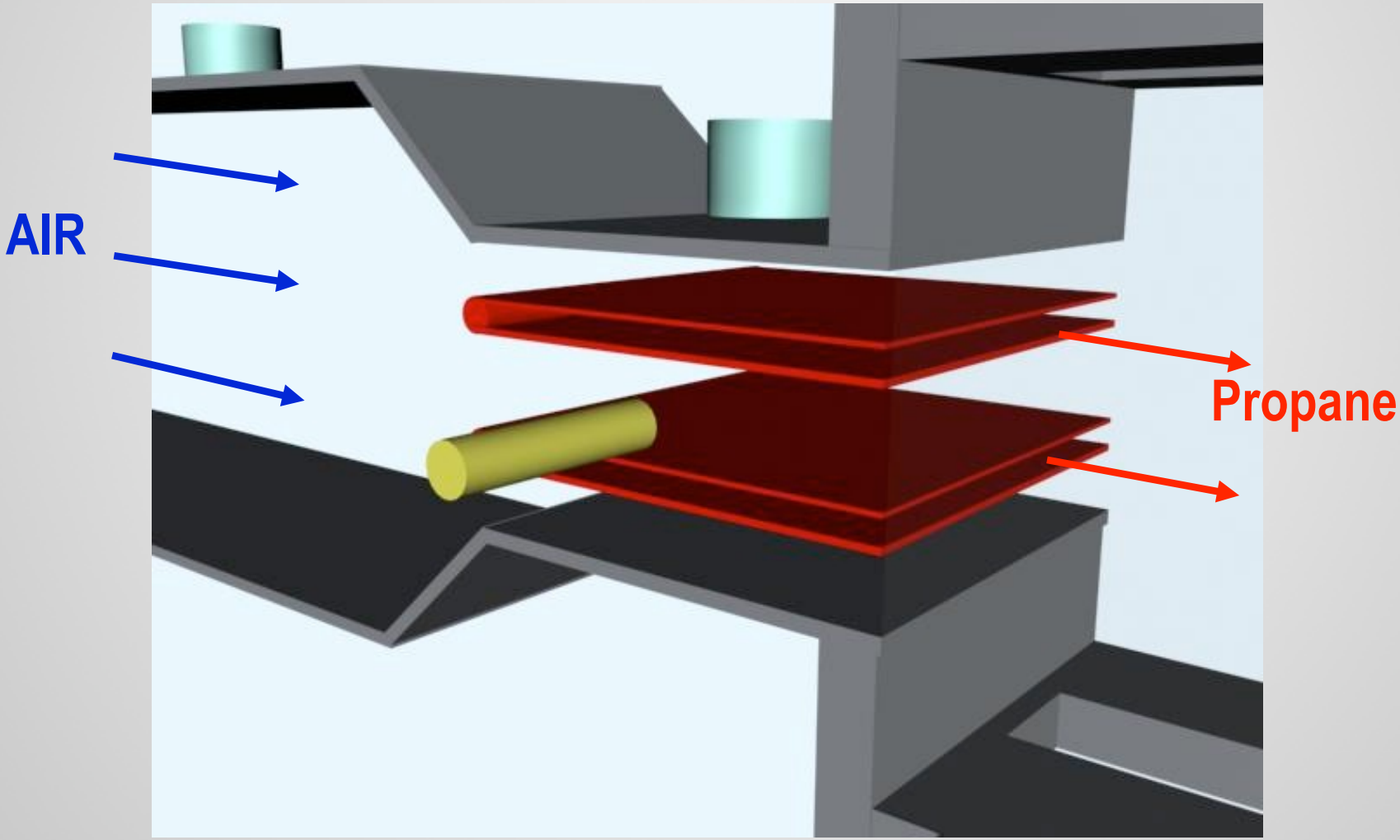
★ Two examples:

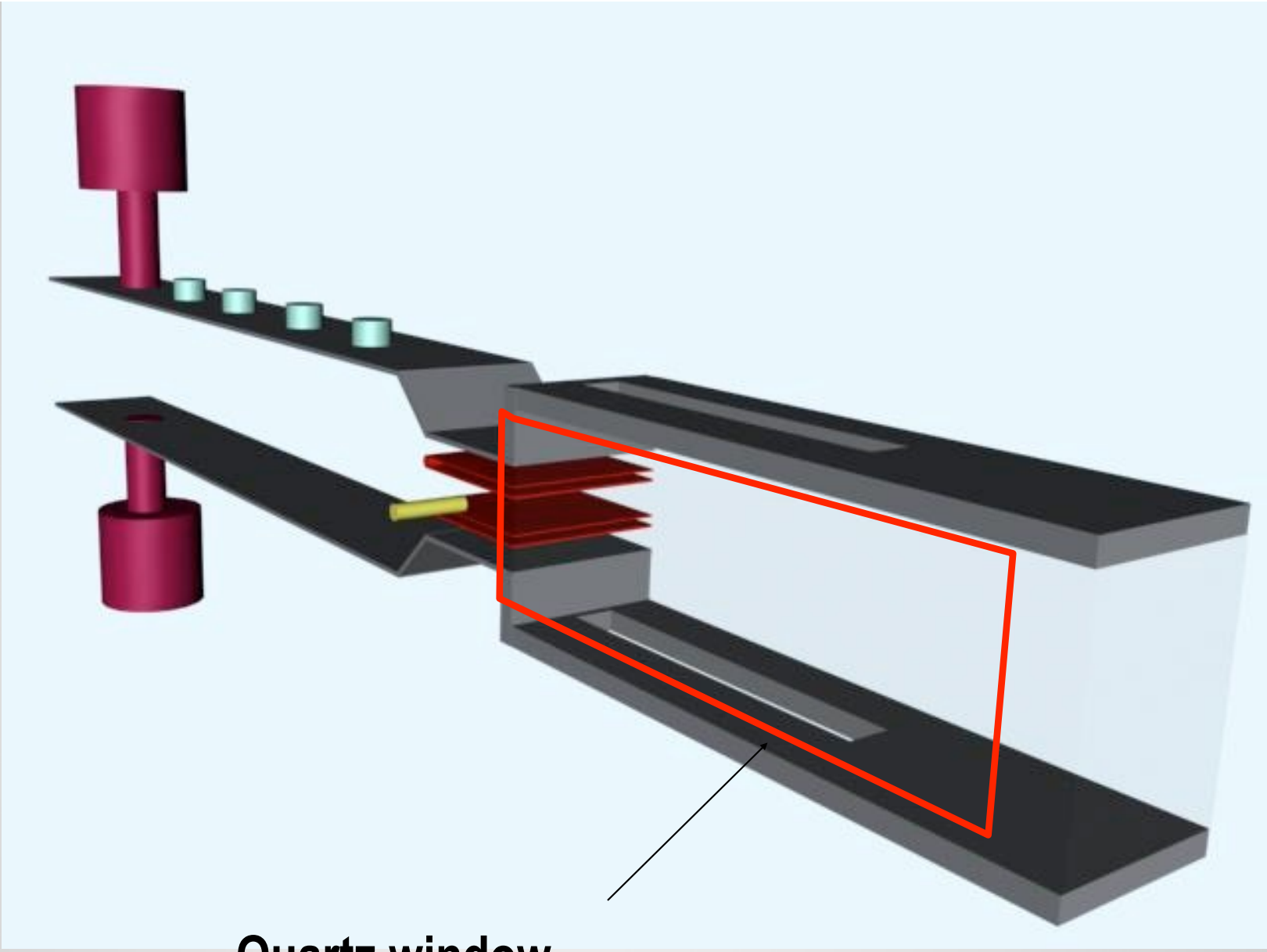
➡ A turbulent laboratory diffusion flame

➡ A piston engine

A comparison of RANS and LES

The ICLEAC burner (Ecole Centrale Paris): diffusion, 250 kW.

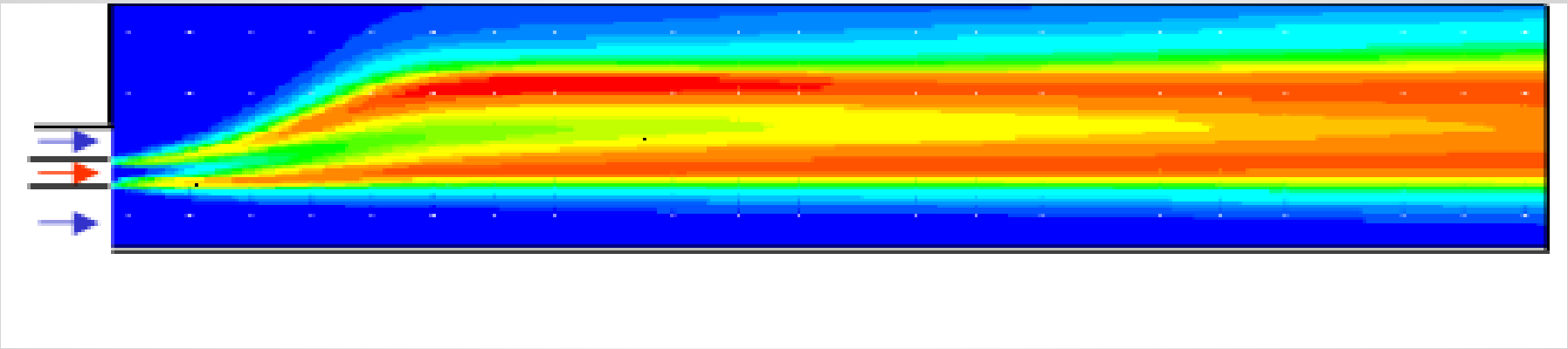




Quartz window

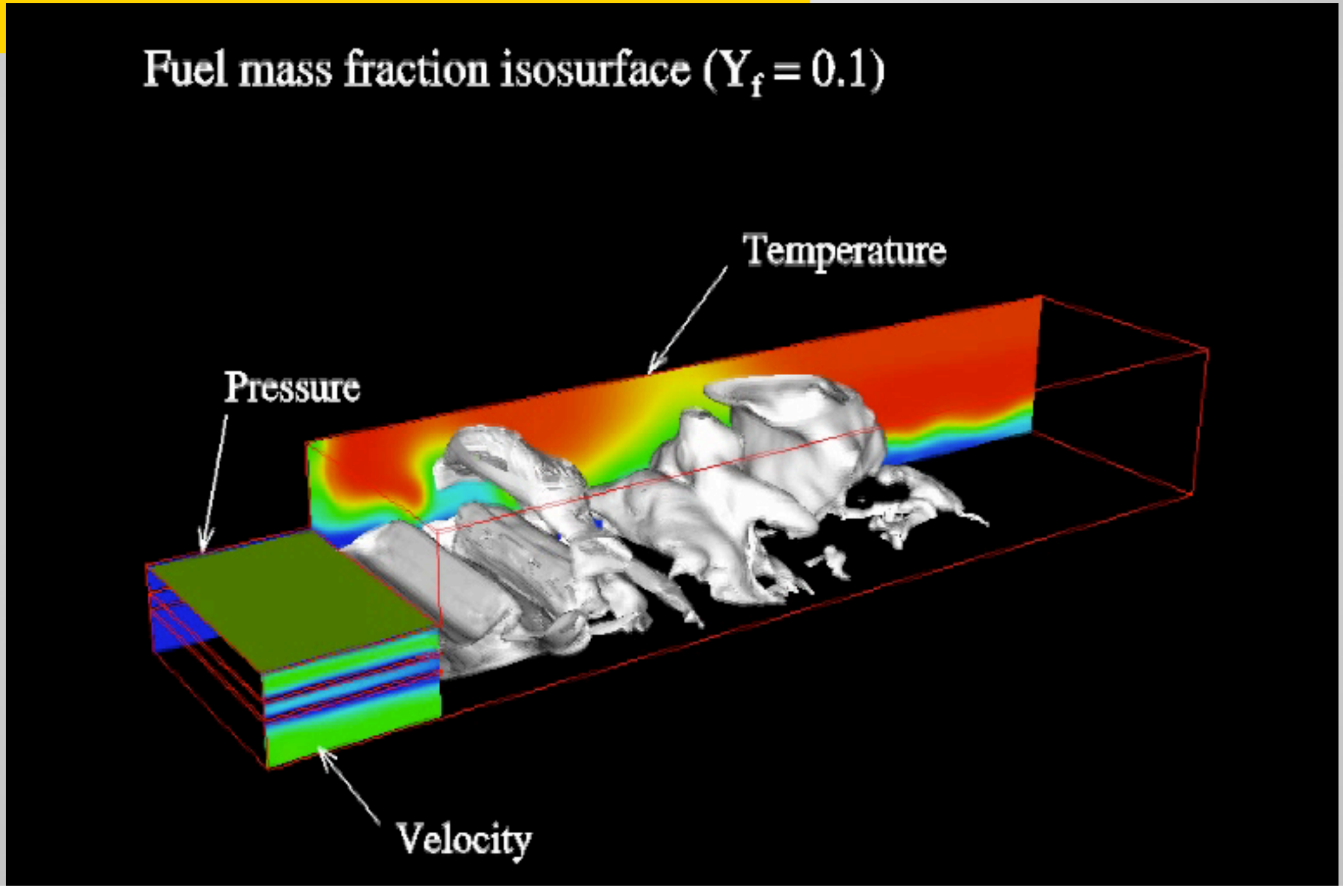
Typical RANS result: one field of ‘averaged’ values (here temperature)

Régime	FUEL(g/s)	AIR(g/s)
B	4,5	62,5



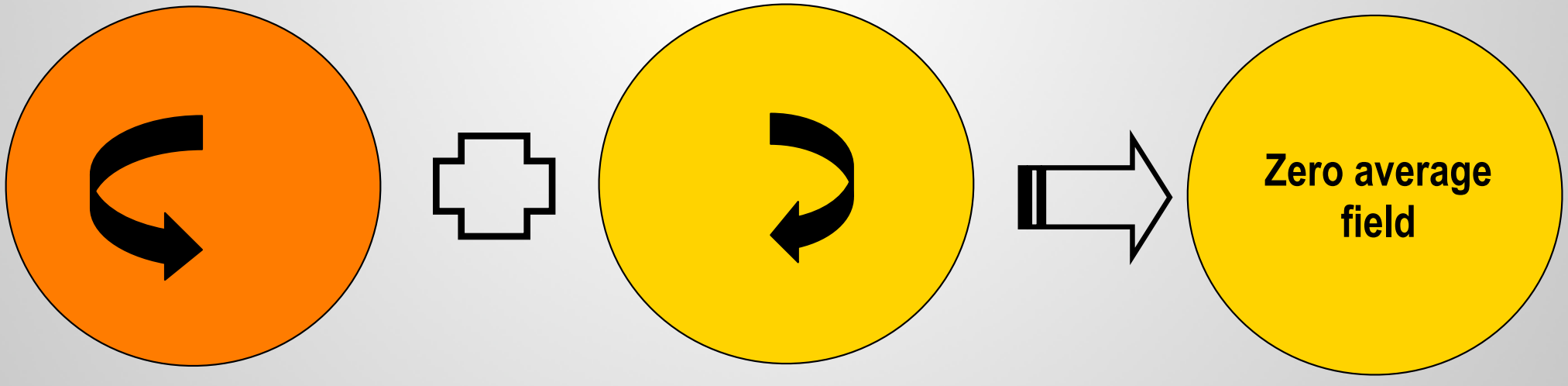
LES gives a very different image of the flame:

K. Truffin, CERFACS



Same problem in piston engines where we average over cycles.
However, cycle-to-cycle variations are a major issue
They are also a major problem for modeling:

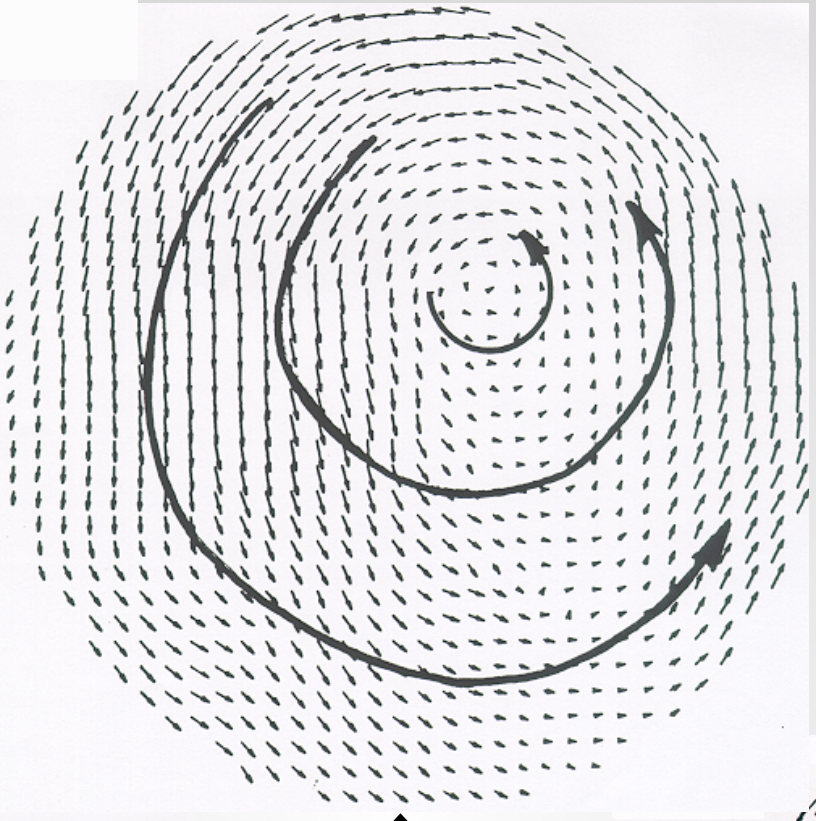
Example of an extreme case:



500 cycles followed by 500 cycles

PIV data

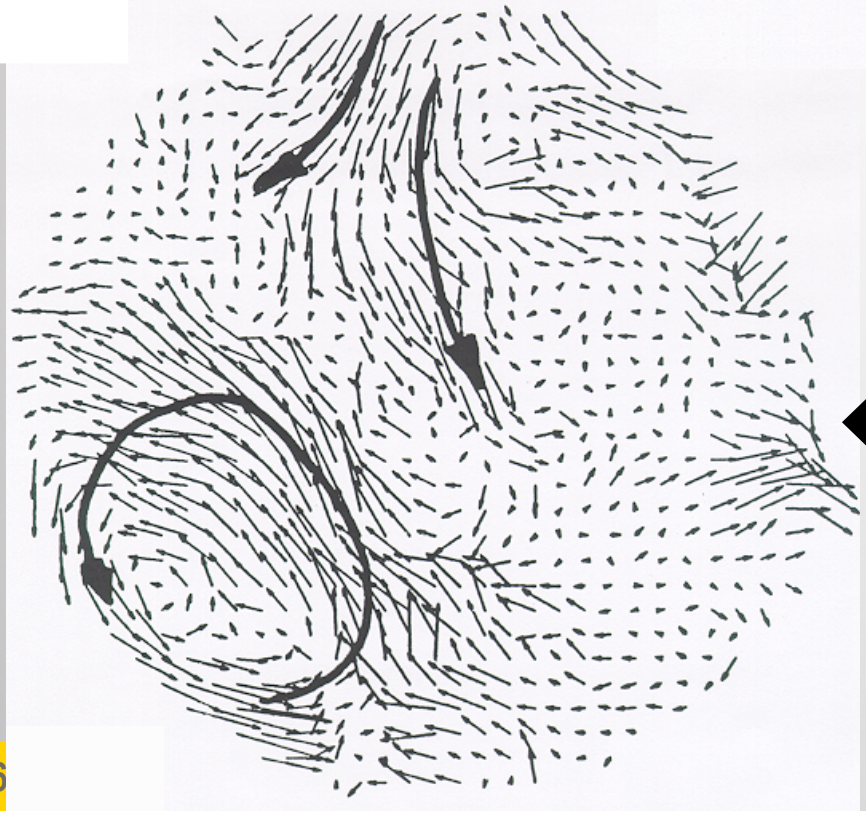
Reuss (1998)
Reuss (2000)



1,200 r/min
40 kPa MAP
standard valve

TDC
z = - 6.1 mm
~70 mm circle
in 92 mm bore

90-cycle mean

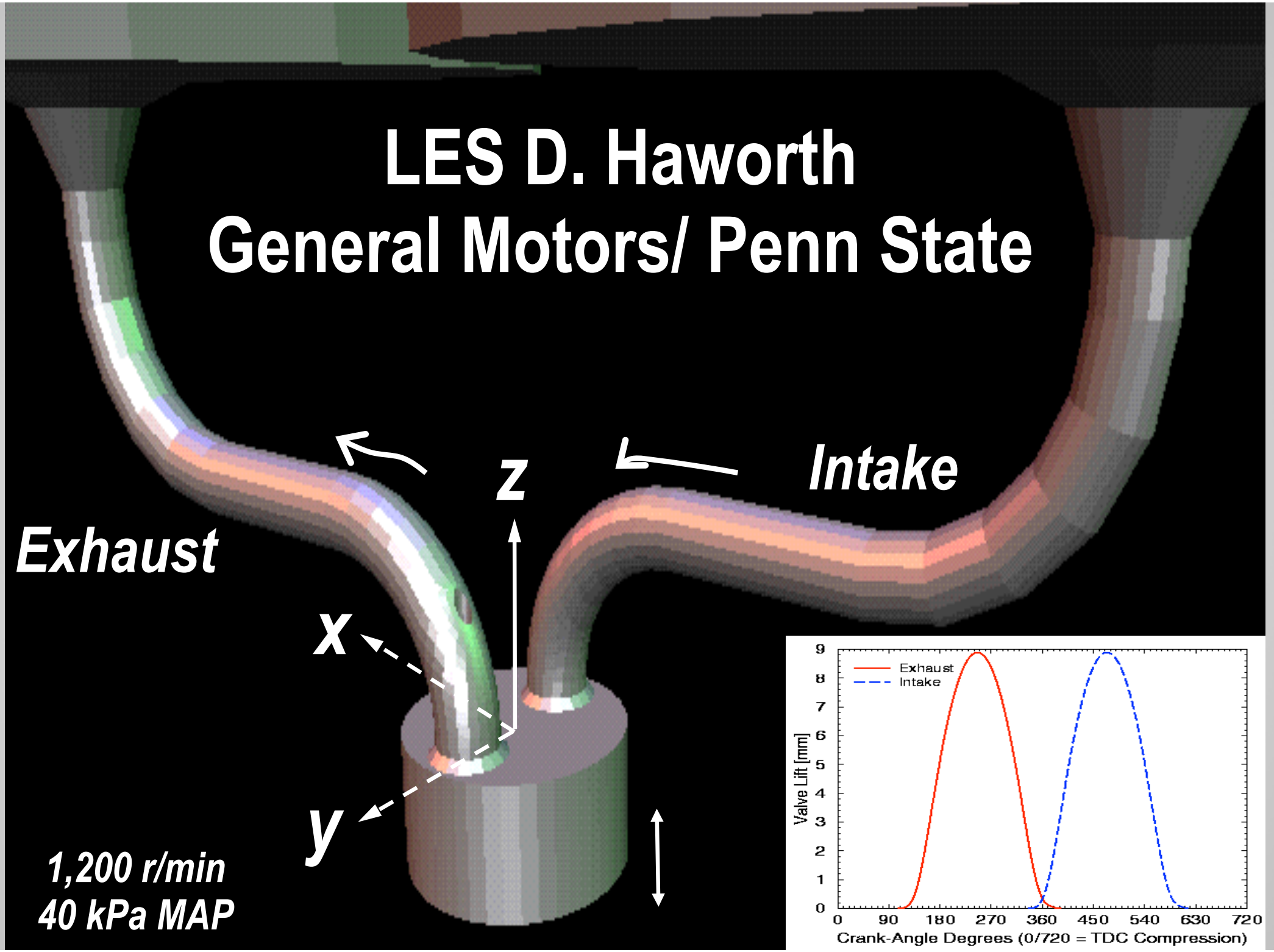


two individual cycles



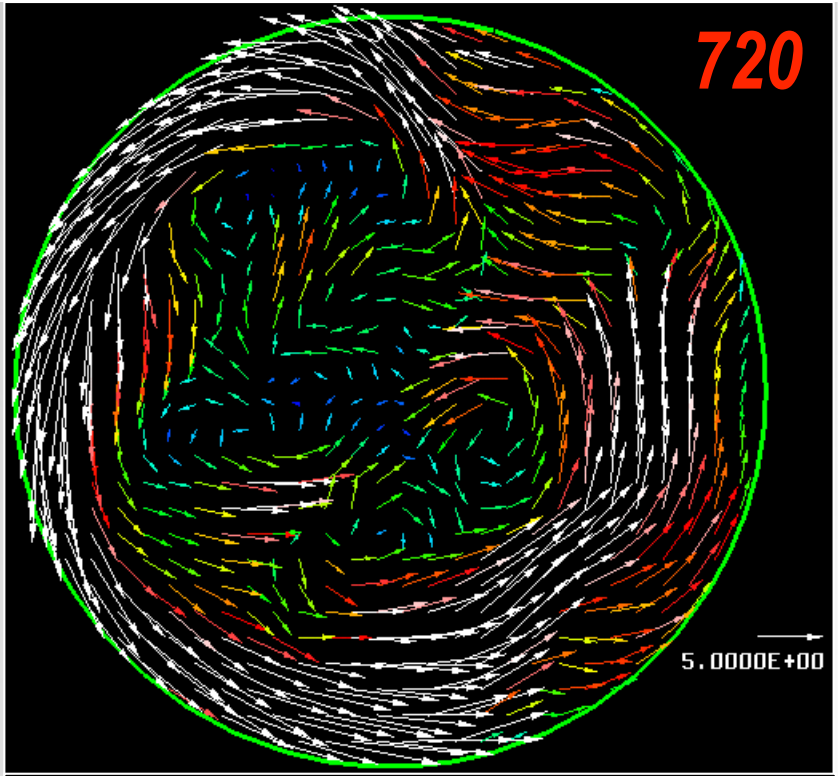
5 m/s

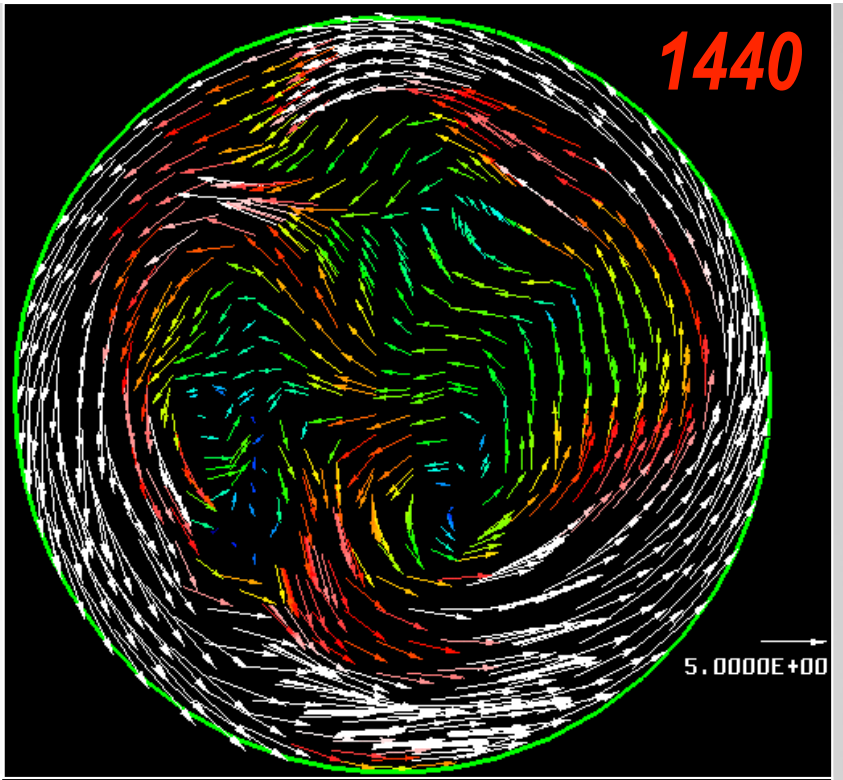
LES D. Haworth
General Motors/ Penn State

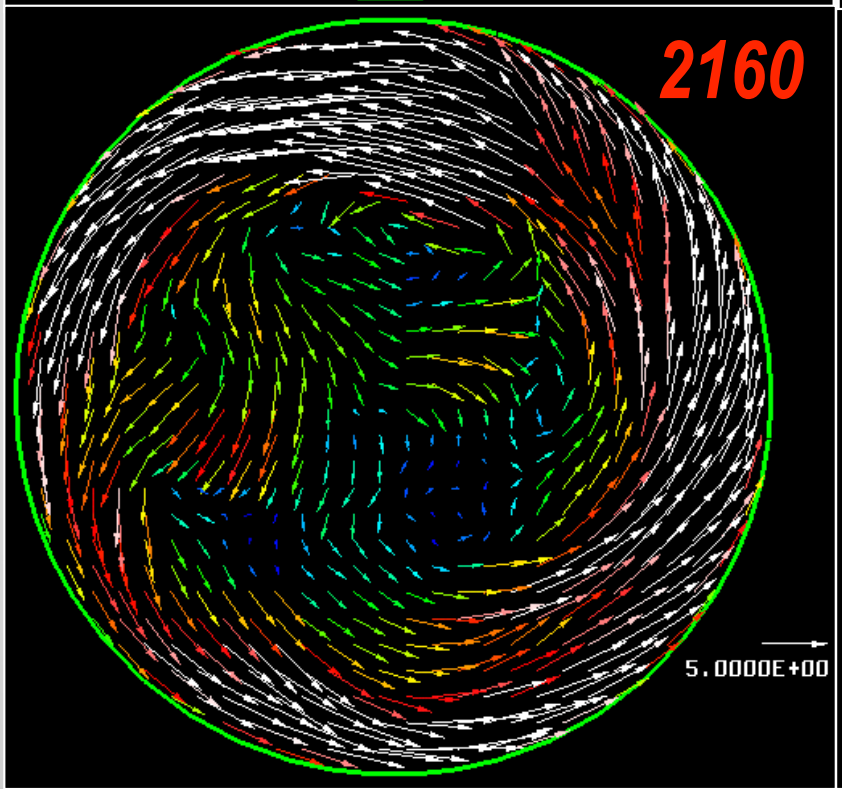


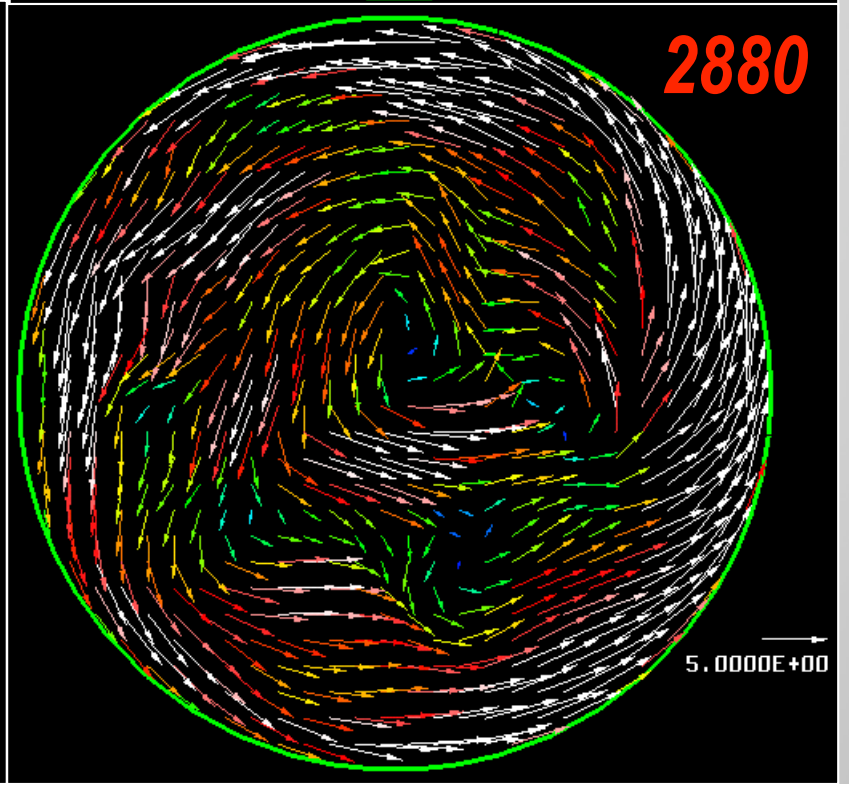
TCC LES

TDC
z = -6.1 mm
1,200 r/min
40 kPa MAP
motored









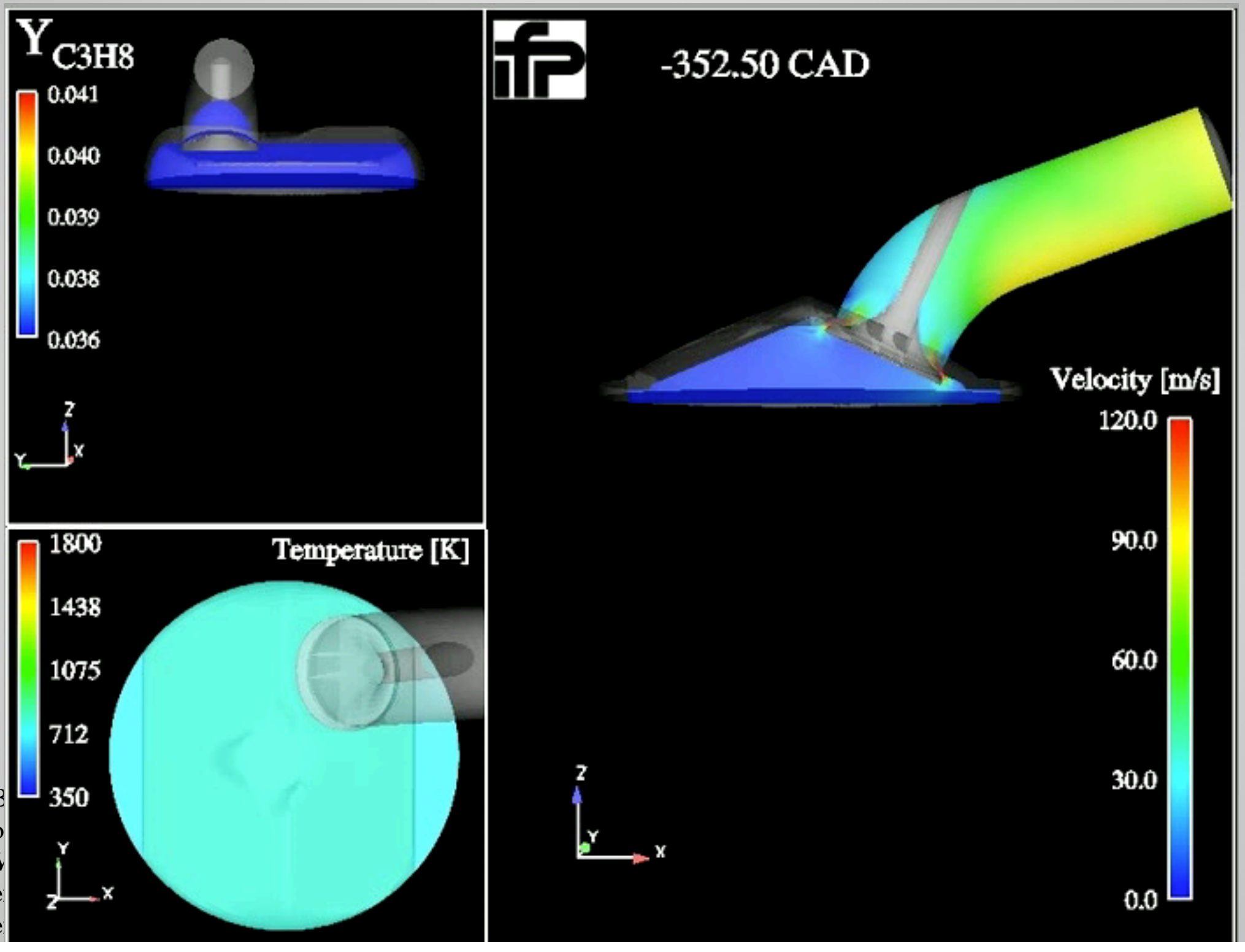
tccles3
DCH
04-29-99

LES of engine combustion captures cycle to cycle variations:



B. Enaux, V. Granet, O. Vermorel, C. Lacour, C. Pera, C. Angelberger, and T. Poinsot, "LES and experimental study of cycle-to-cycle variations in a spark ignition engine", *Proc. of the Combustion Institute* 33, 3115-3122, 2011

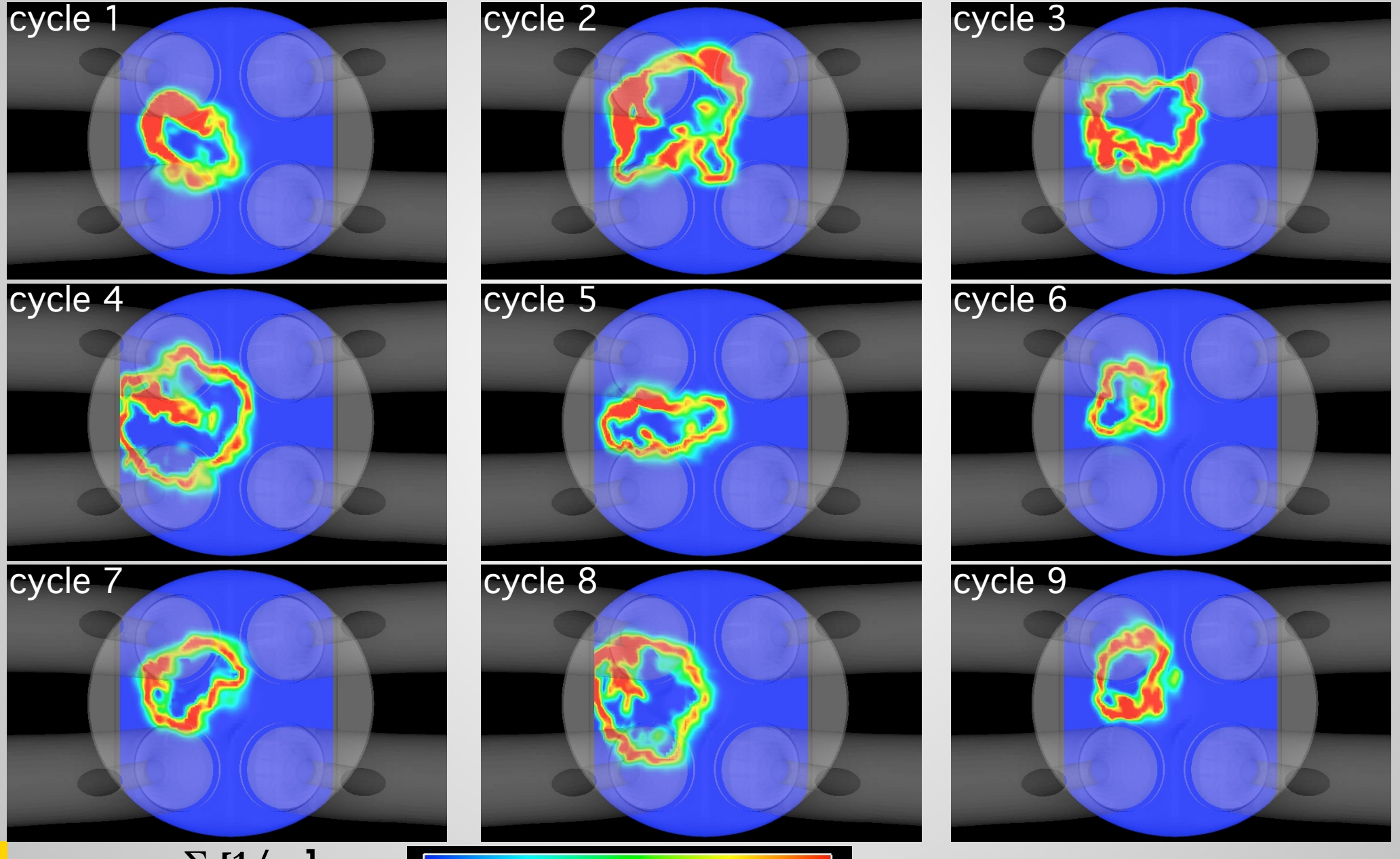
V. Granet, O. Vermorel, C. Lacour, B. Enaux, V. Dugué and T. Poinsot, "Large Eddy Simulation and experimental study of cycle-to-cycle variations of stable and unstable operating points in a spark ignition engine", *Comb. Flame* 159, 4, 1562-1576, 2012.


Y C3H8
0.041
0.040
0.039
0.038
0.036
Z
Y
X
-352.50 CAD
Velocity [m/s]
120.0
90.0
60.0
30.0
0.0
Z
Y
X
1800
1438
1075
712
350
Temperature [K]
Y
Z
X

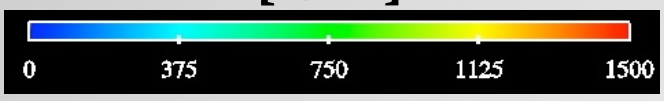
B
o
V
e
e

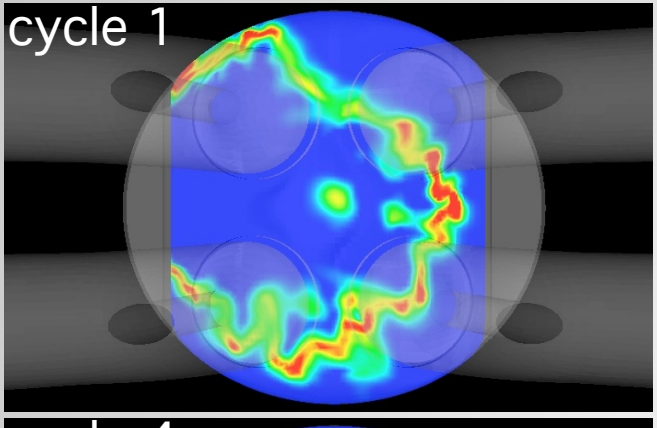
LES predicts that all cycles differ

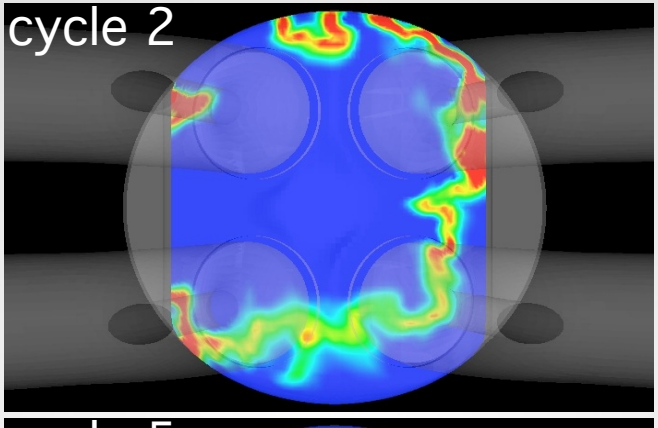
Flame surface density Σ -5 CAD

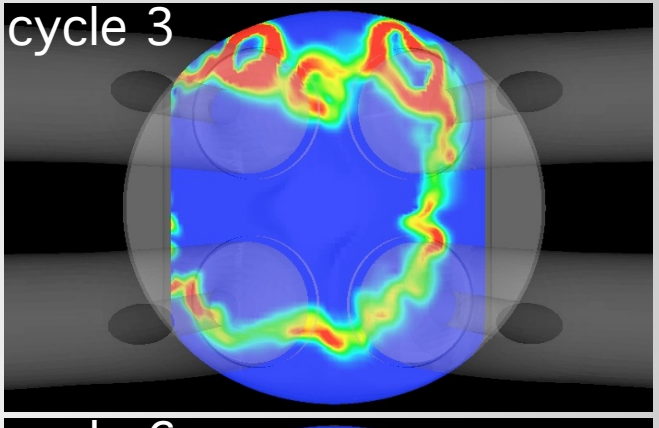


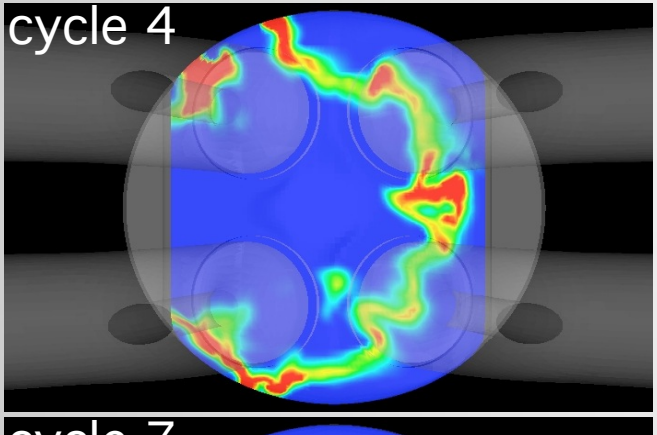
Flame surface density Σ
+10 CAD

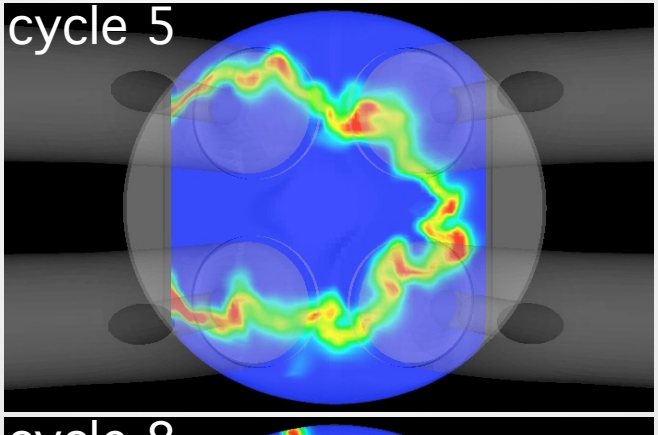


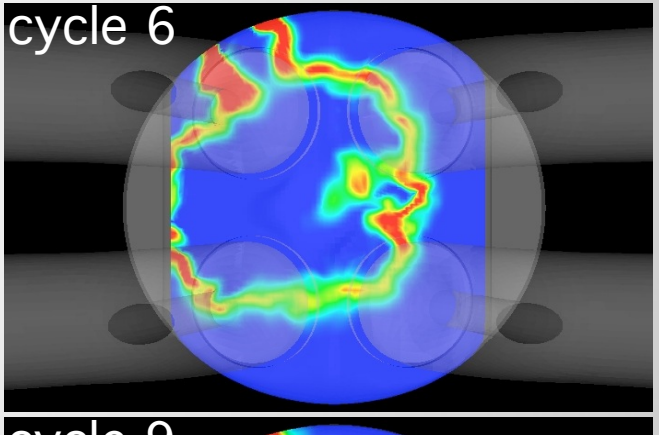


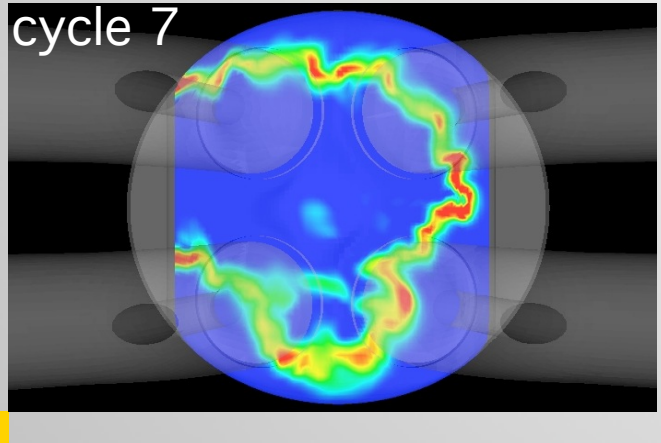


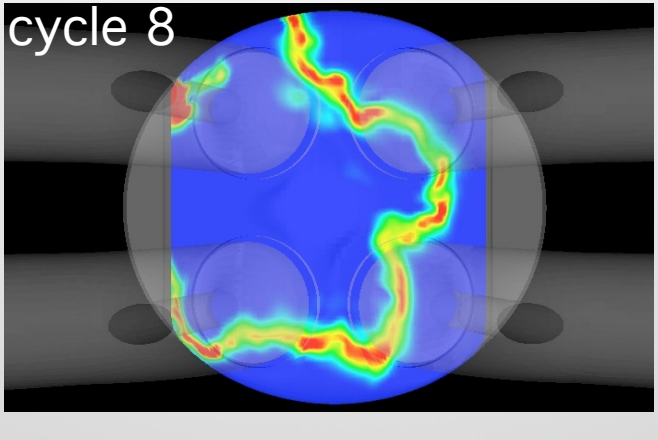


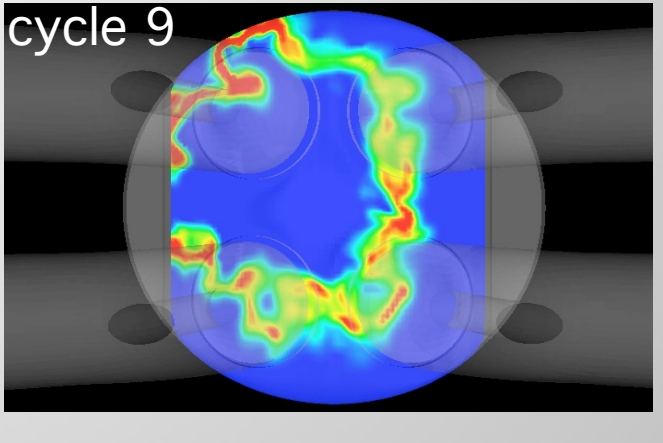




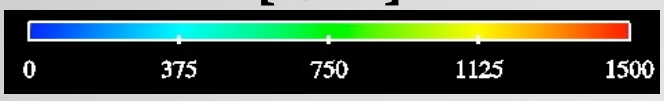


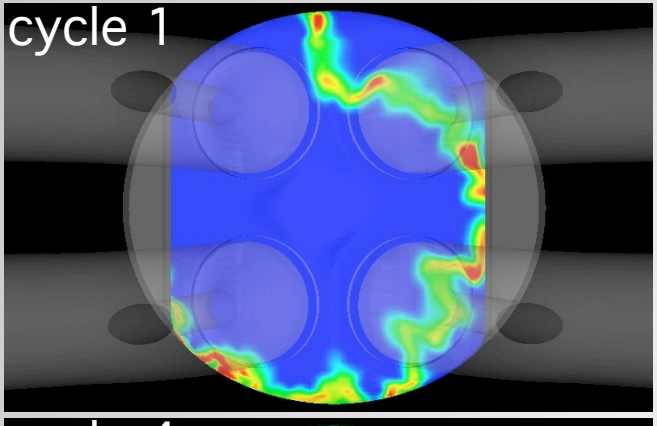


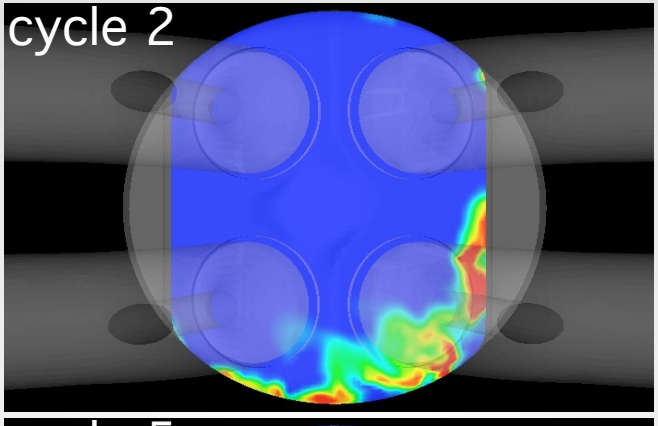


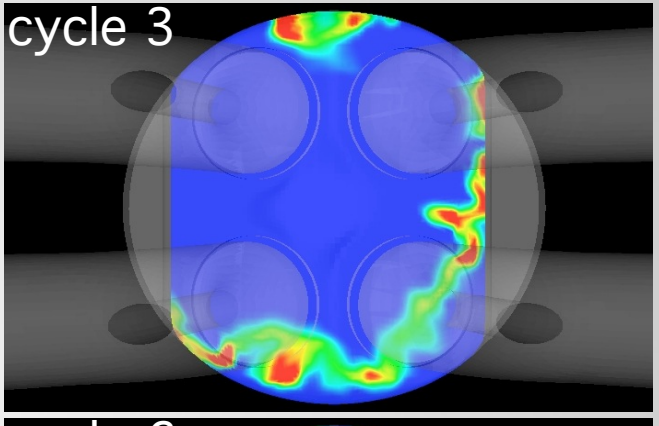


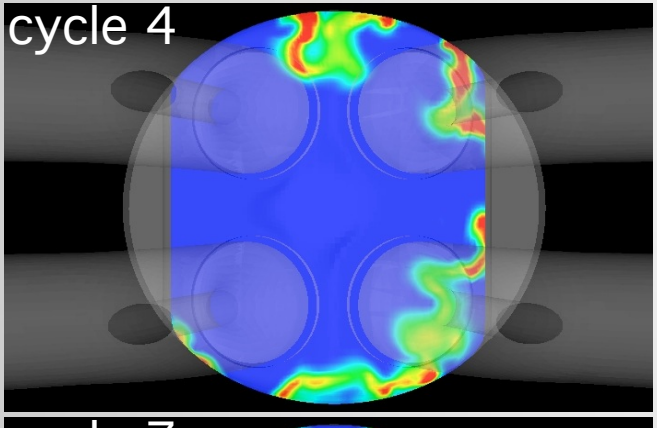
Flame surface density Σ
+20 CAD

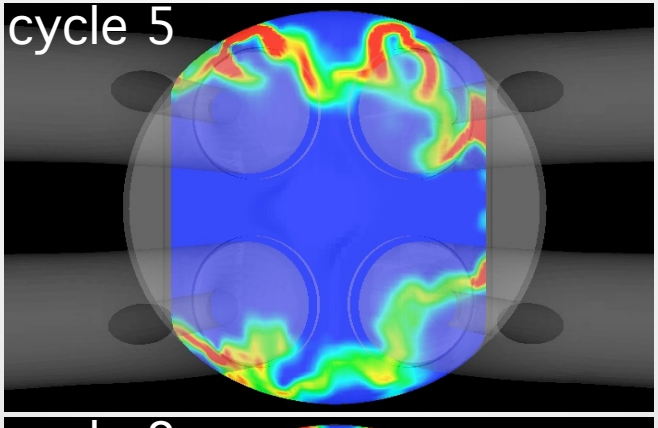


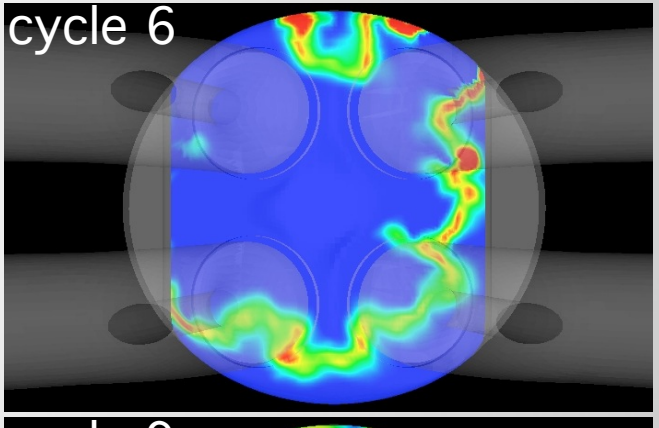


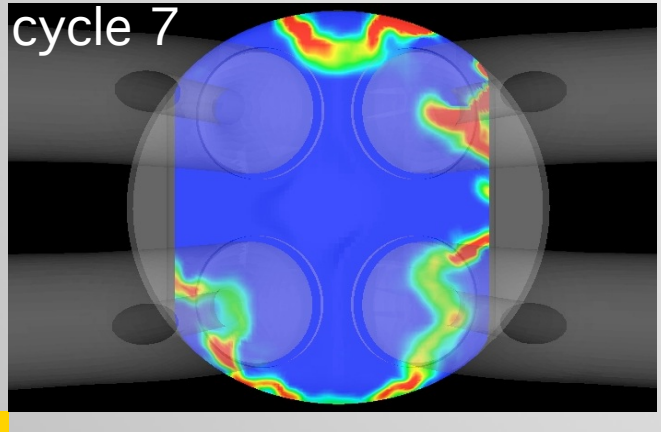


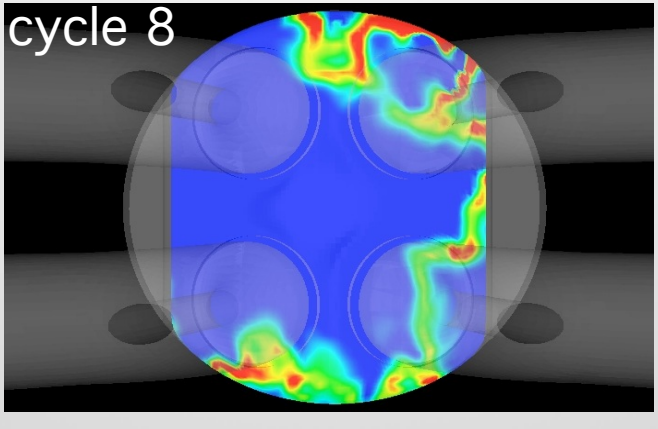


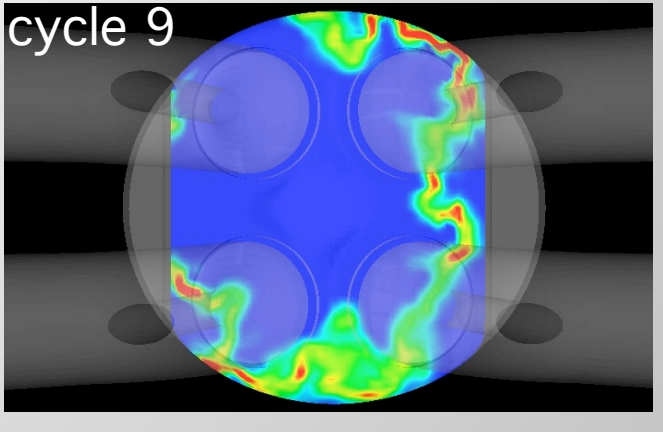




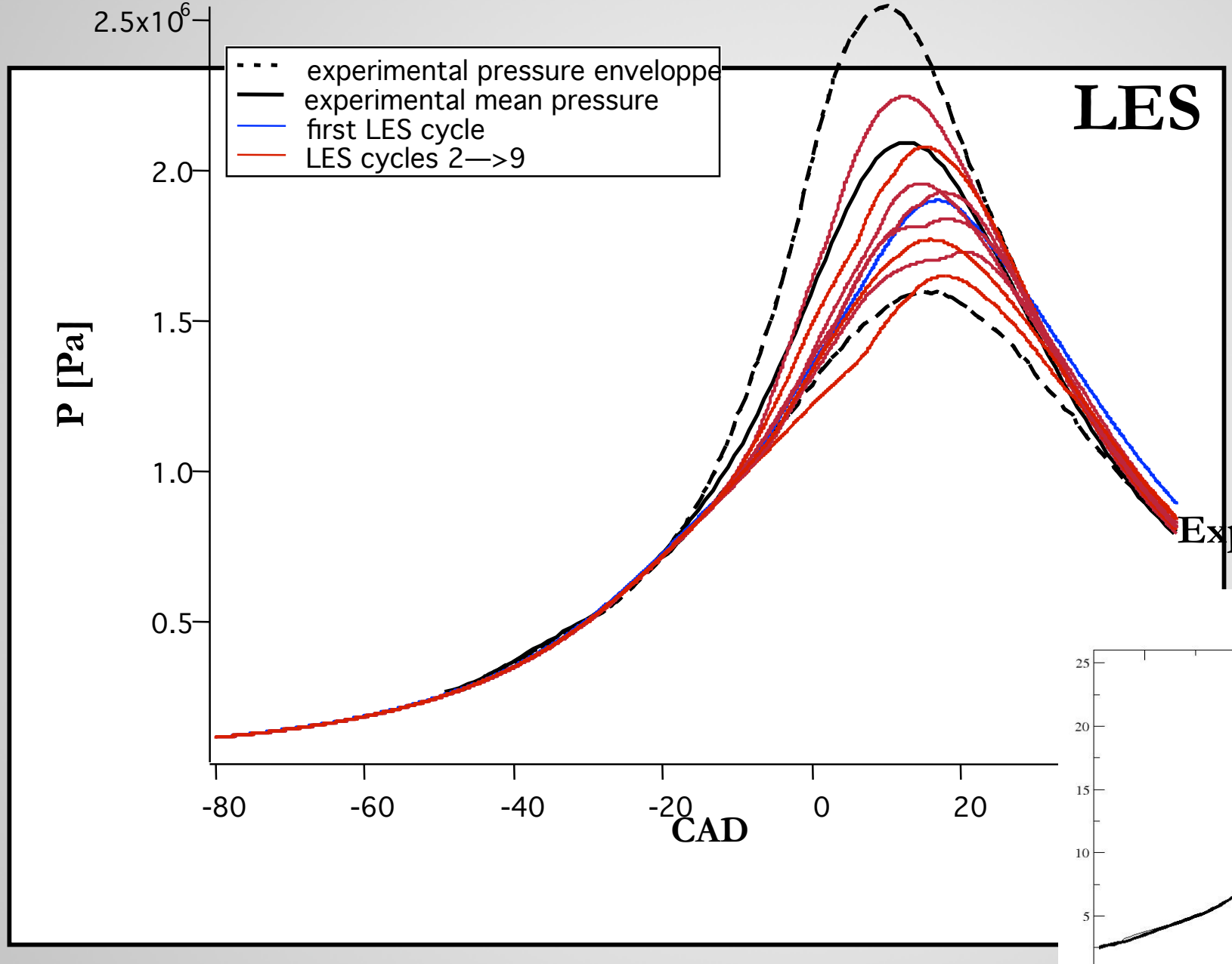




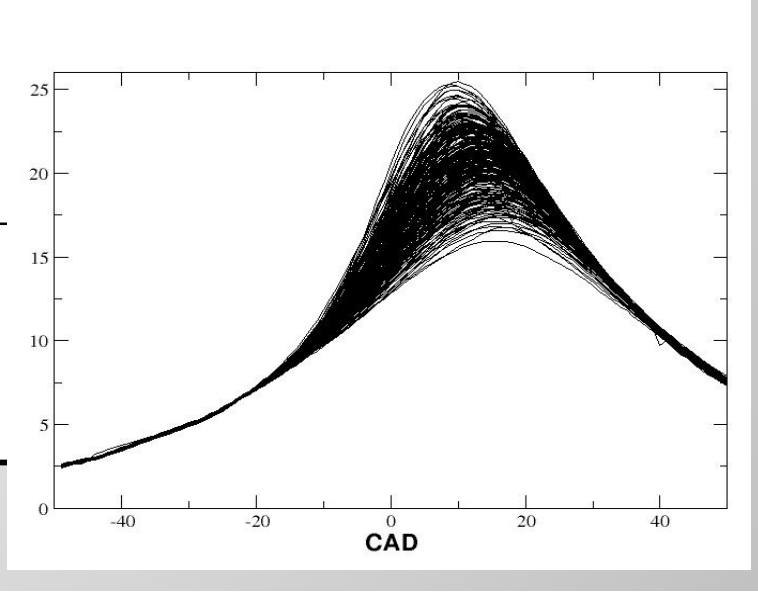




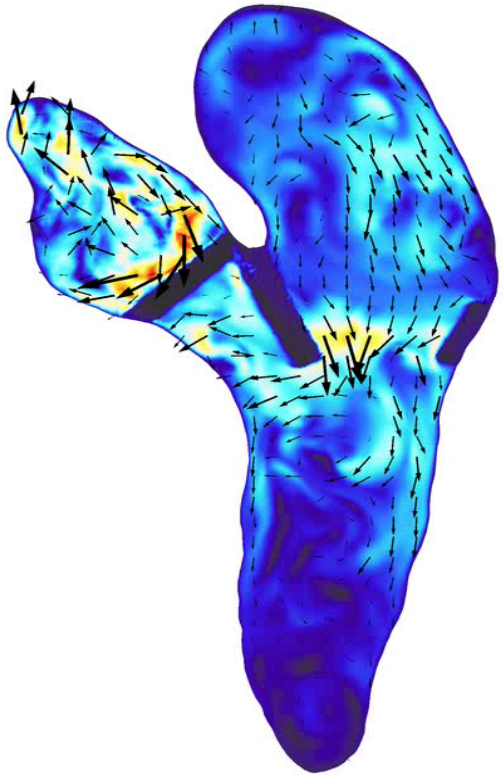
Each cycle is different: the pressure curves all differ

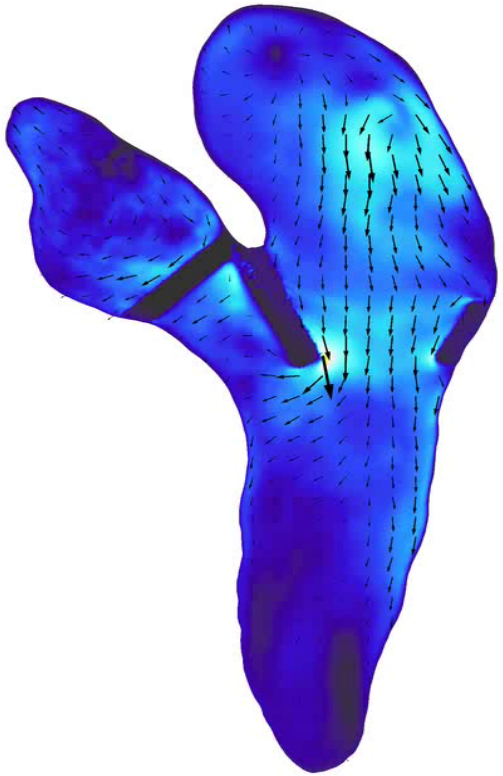


Experimental data



Your heart also has cycle to cycle variations:

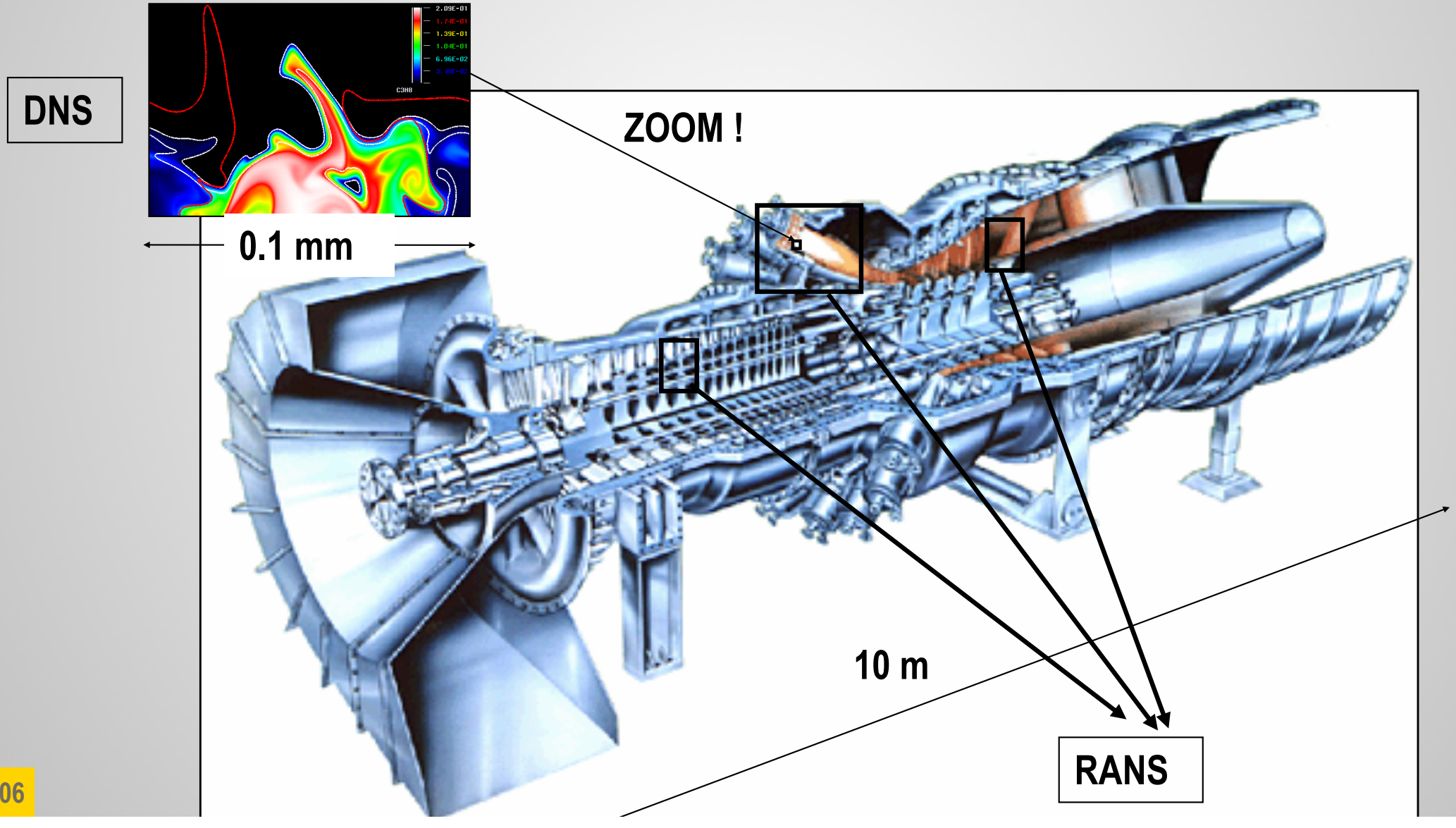




Instantaneous cycle **Averaged cycle**

So that we can do:

- bad RANS on real engines
- good DNS on very small imaginary boxes



This is why we turn now to LES: Large Eddy Simulations

LES combines RANS and DNS:

- Model small structures but keep the large ones — DNS

- Diminish impact of models

- in REAL CONFIGURATIONS — RANS

WE WILL DESCRIBE THESE METHODS IN DETAILS

SO, what do we need to build these CFD models for combustion ?

FIRST POINT: chemistry...

Combustion is the chemical reaction of a fuel with an oxidizer

	FUELS	OXIDIZERS
Gas	H2	AIR or OXYGEN
	CH4 methane	
	C3H8 propane	
	CxHy and mixtures of CxHy	
Liquids	Gasoline	
	Kerosene	

Will not talk about solids here

Global chemistry and equivalence ratio:

Consider a moles of A (fuel) burning with b moles of B (air):

$$aA + bB \rightarrow P \quad \text{(global reaction)}$$

Stoichiometric ratio:

$$s = (bW_B) / (aW_A)$$

It takes *s* grams of B to burn *1* gram of A.

Example:

$$H2+1/2O2 \rightarrow H20$$

*s = 1/2 * 32/2= 8.*

It takes 8 g of oxygen to burn one gram of hydrogen

Equivalence ratio:

aA + bB --> P (global reaction)

The equivalence ratio is defined by:

$$\phi = \frac{\frac{Y_A}{Y_B}}{\left(\frac{Y_A}{Y_B}\right)_{st}} = s\frac{Y_A}{Y_B}$$

Where ϕ = 1: the reaction is 'stoichiometric'. After combustion, no A or B will be left

If ϕ < 1, combustion is 'lean' ==> oxidizer (B) left after combustion.

If ϕ > 1, combustion is 'rich' ==> we waste fuel. There is unburnt fuel (A) in the burnt gases.

Detailed chemistry:

Consider A + B --> C (global reaction)
Example: H2+1/2O2 --> H20
At which speed does it progress ?

$$\dot{\omega} = A Y_A^{\nu_A} Y_B^{\nu_B} exp(-T_a/T)$$

Need
- A
- B
- temperature

A, Ta are provided by kinetics.
It takes *three ingredients* to burn: A, B and a high temperature

Chemical kinetics: the true story ?

H2 never meets O2 to produce H20…

```
ELEMENTS
 H  O  N
END
SPECIES
H2 O2 OH O H H2O HO2 H2O2 N N2 NO
END
REACTIONS
H2+O2=OH+OH                    1.700E13   0.0    47780.
H2+OH=H2O+H                    1.170E09   1.30    3626.
H+O2=OH+O                      5.130E16  -0.816  16507.
O+H2=OH+H                      1.800E10   1.0     8826.
H+O2+M=HO2+M                    2.100E18  -1.0       0.
  H2/3.3/ O2/0./ N2/0./  H2O/21.0/
H+O2+O2=HO2+O2                  6.700E19  -1.42      0.
H+O2+N2=HO2+N2                  6.700E19  -1.42      0.
OH+HO2=H2O+O2                   5.000E13   0.0     1000.
H+HO2=OH+OH                    2.500E14   0.0     1900.
O+HO2=O2+OH                    4.800E13   0.0     1000.
OH+OH=O+H2O                    6.000E08   1.3        0.
H2+M=H+H+M                     2.230E12   0.5    92600.
  H2/3./ H/2./  H2O/6.0/
O2+M=O+O+M                     1.850E11   0.5    95560.
H+OH+M=H2O+M                    7.500E23  -2.6       0.
  H2O/20.0/
HO2+H=H2+O2                    2.500E13   0.0      700.
HO2+HO2=H2O2+O2                  2.000E12   0.0       0.
H2O2+M=OH+OH+M                   1.300E17   0.0    45500.
H2O2+H=H2+HO2                  1.600E12   0.0     3800.
H2O2+OH=H2O+HO2                  1.000E13   0.0     1800.
END
```

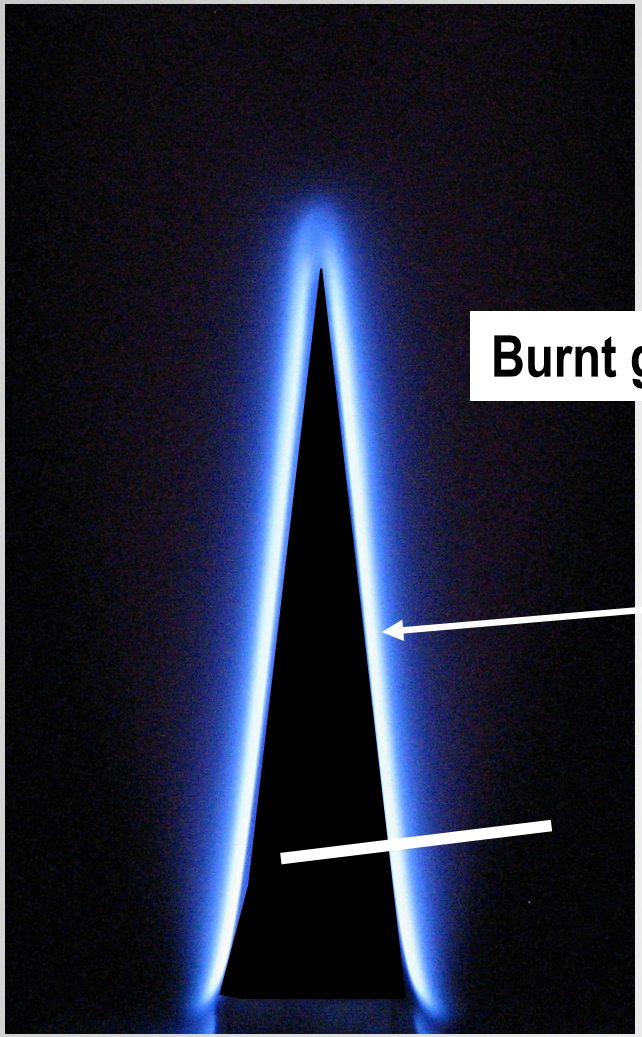
Standard CHEMKIN

$$\dot{\omega} = A Y_A^{\nu_A} Y_B^{\nu_B} exp(-T_a/T)$$

Other problem: all the exciting things occur in thin fronts: 'flames'



Example: the laminar Bunsen flame



WHAT IS THE STRUCTURE OF THIS FRONT ?
HOW THICK IS THIS FRONT ?
DOES IT HAVE A SPEED ?

« DETONATIONS ? »

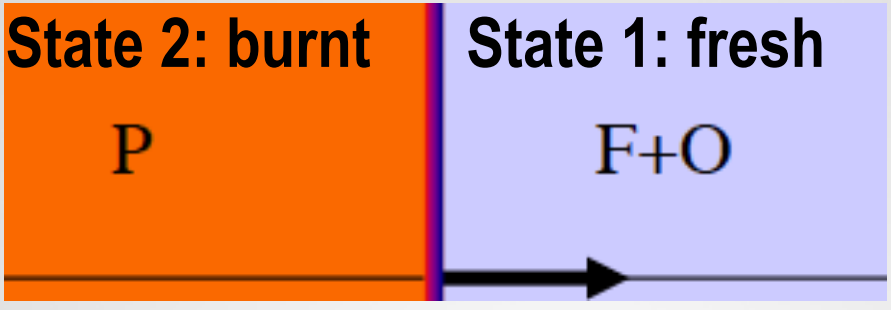
We consider a gas where air and gaseous fuel are mixed

If we ignite this gas, a flame front will propagate. It can be a deflagration or a detonation.

A very simple and elegant theory allows to understand the basics of this phenomenon.

A 'must know' for engineers

TWO TYPES OF FLAME FRONTS: DEFLAGRATION VS DETONATION



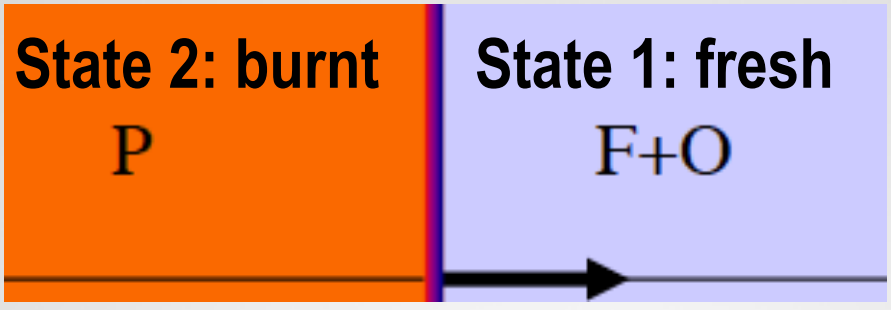
For fronts separating states 1 and, we can write global balance equations between states 1 and 2:

- continuity
- momentum
- total enthalpy



Source: Pr Kasimov, MIT

JUMP CONDITIONS (in the front reference frame):



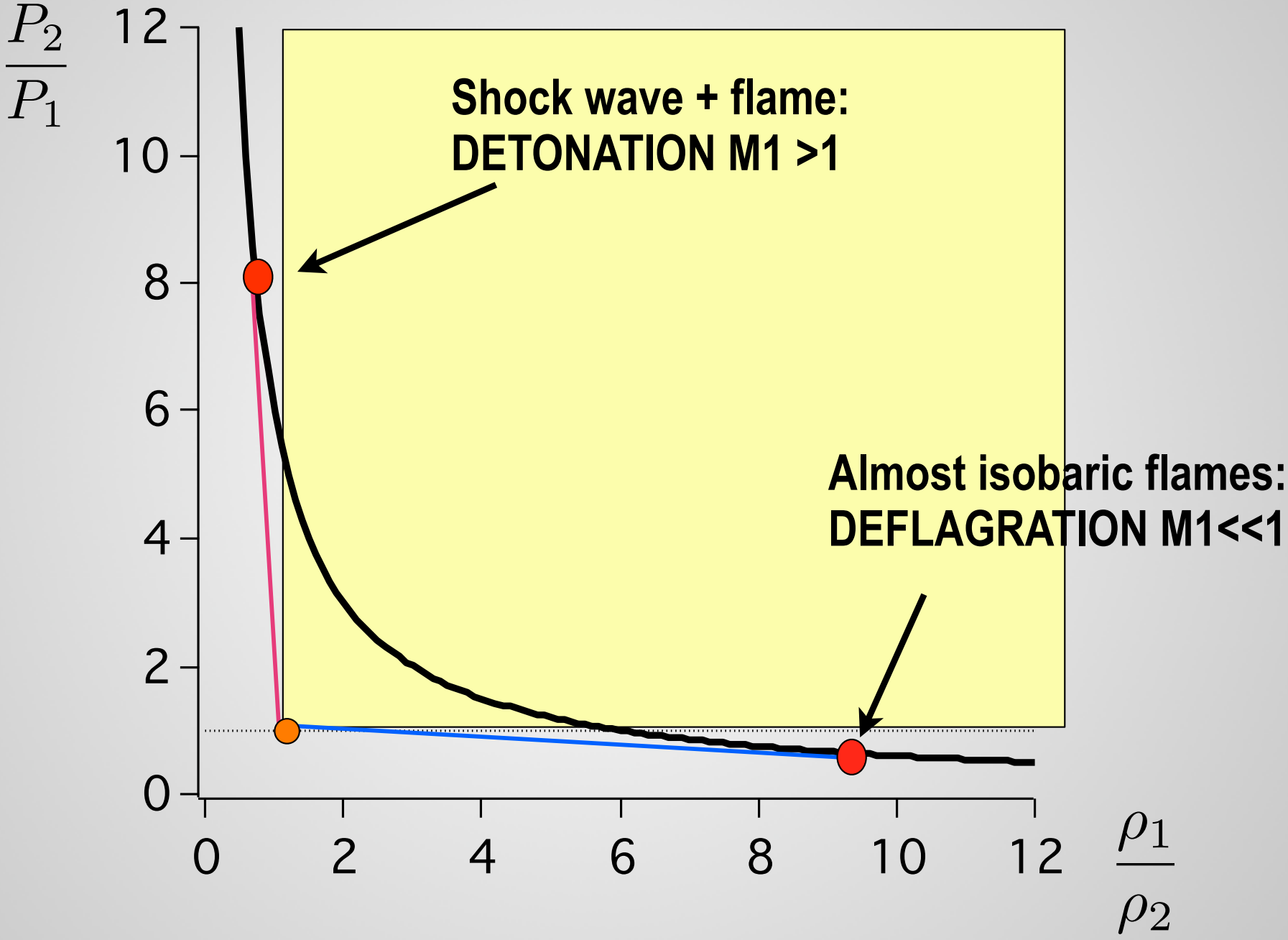
WRITE CONSERVATION OF:

- **MASS**
- **MOMENTUM**
- **ENERGY**

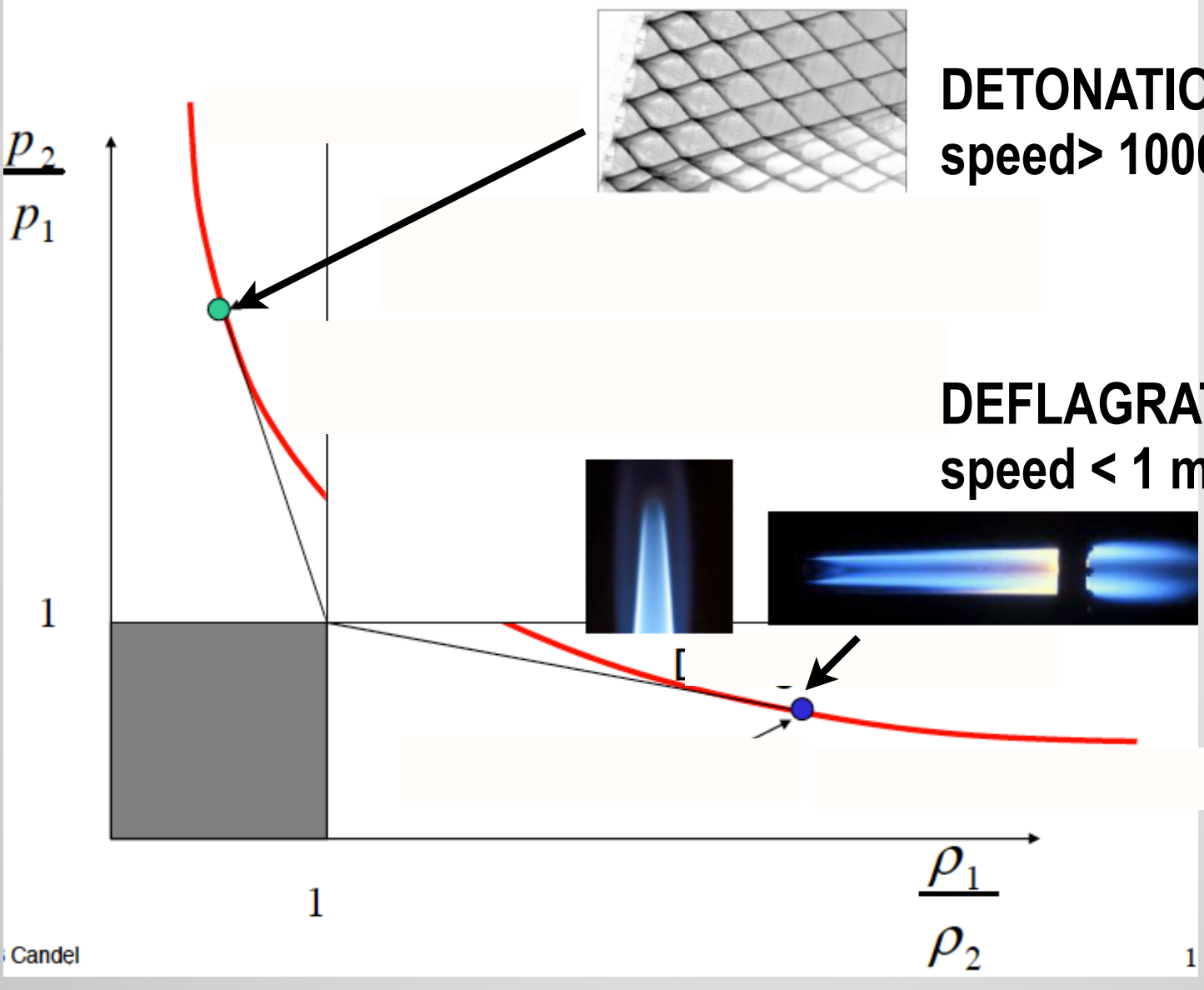
FROM STATE 1 TO STATE 2

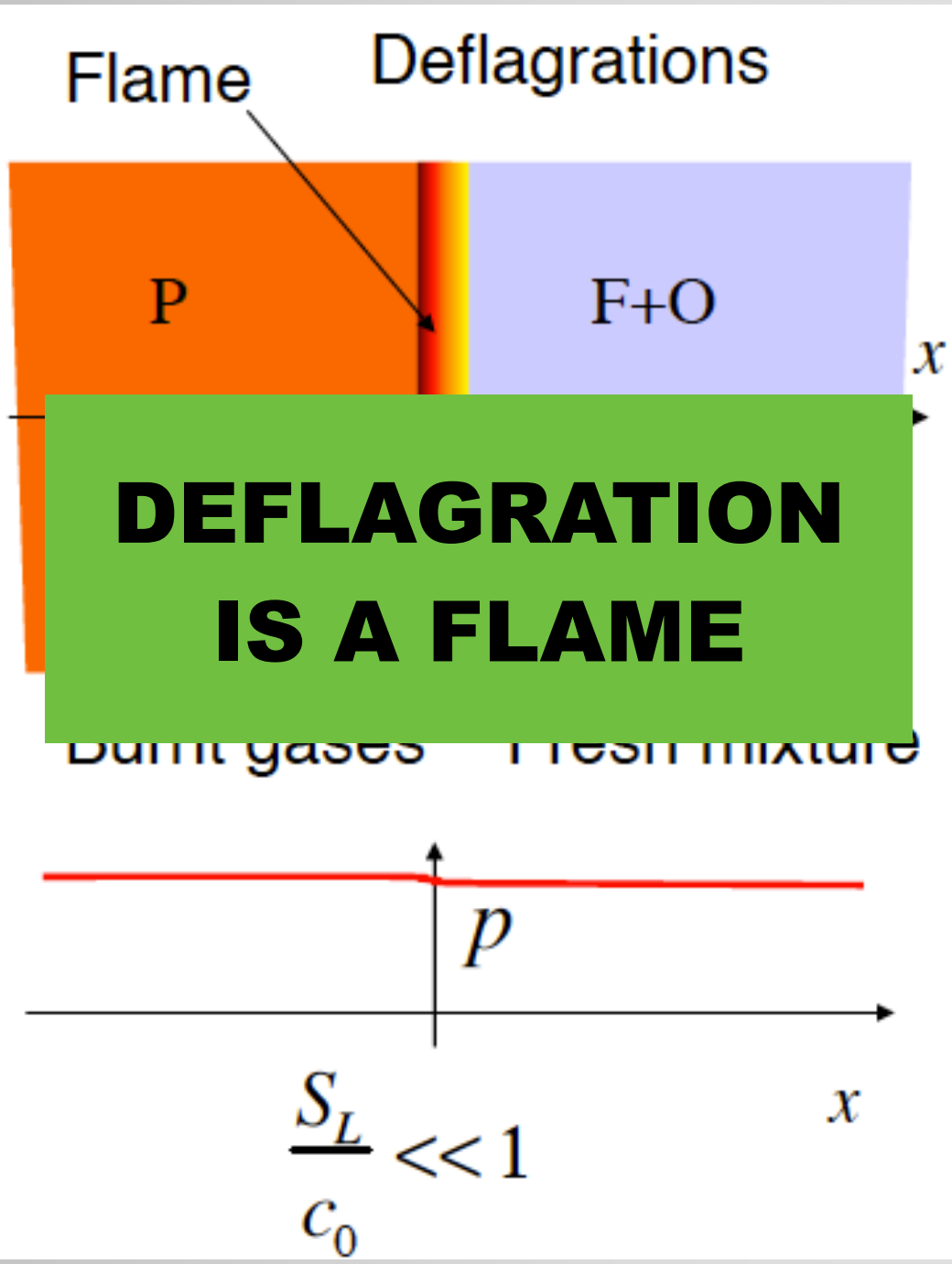
THREE SOLUTIONS:

- **NO FLAME: STATE 1 = STATE 2**
- **DEFLAGRATION: SLOW FLAME**
- **DETONATION: FAST FLAME Boom**

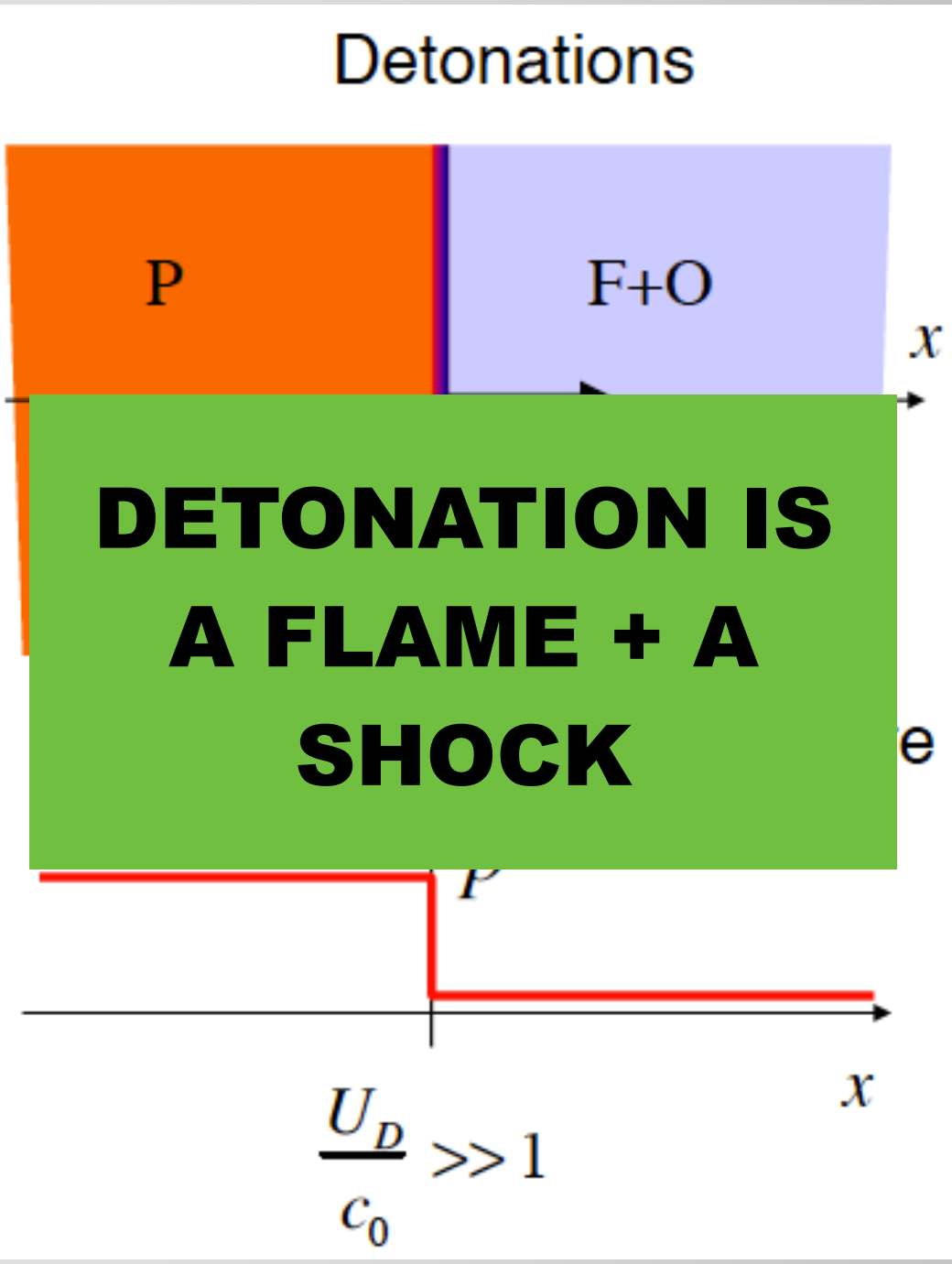

$\frac{P_2}{P_1}$
12
10
8
6
4
2
0
0
2
4
6
8
10
12
$\frac{\rho_1}{\rho_2}$
Shock wave + flame:
DETONATION M1 >1
Almost isobaric flames:
DEFLAGRATION M1<<1

Two solutions in a density ratio / pressure ratio diagram:





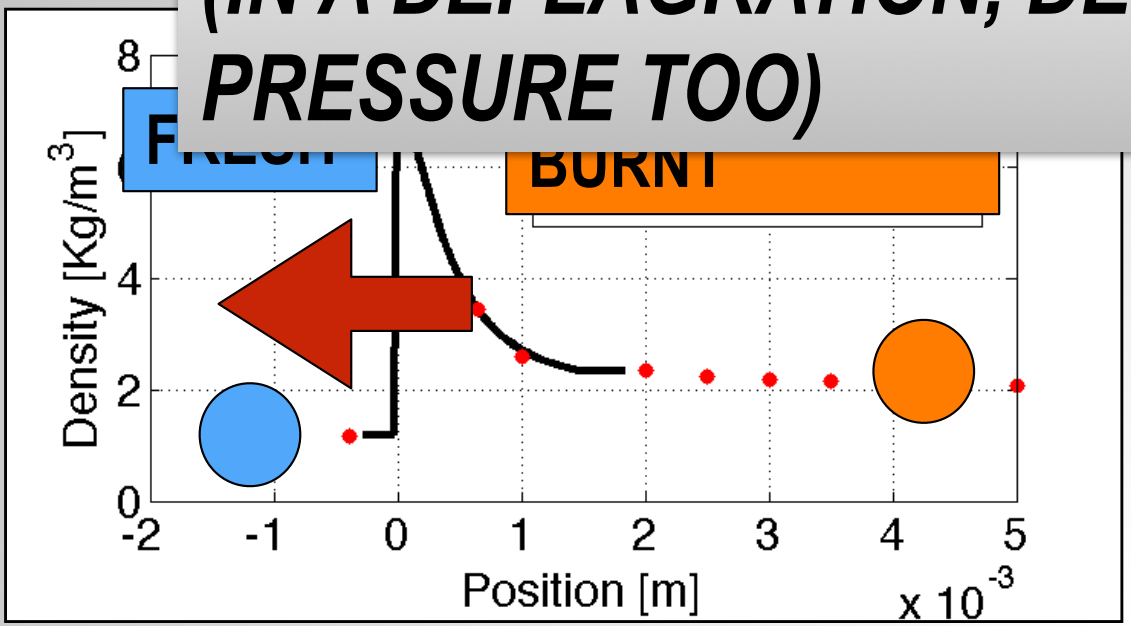
DEFLAGRATION IS A FLAME

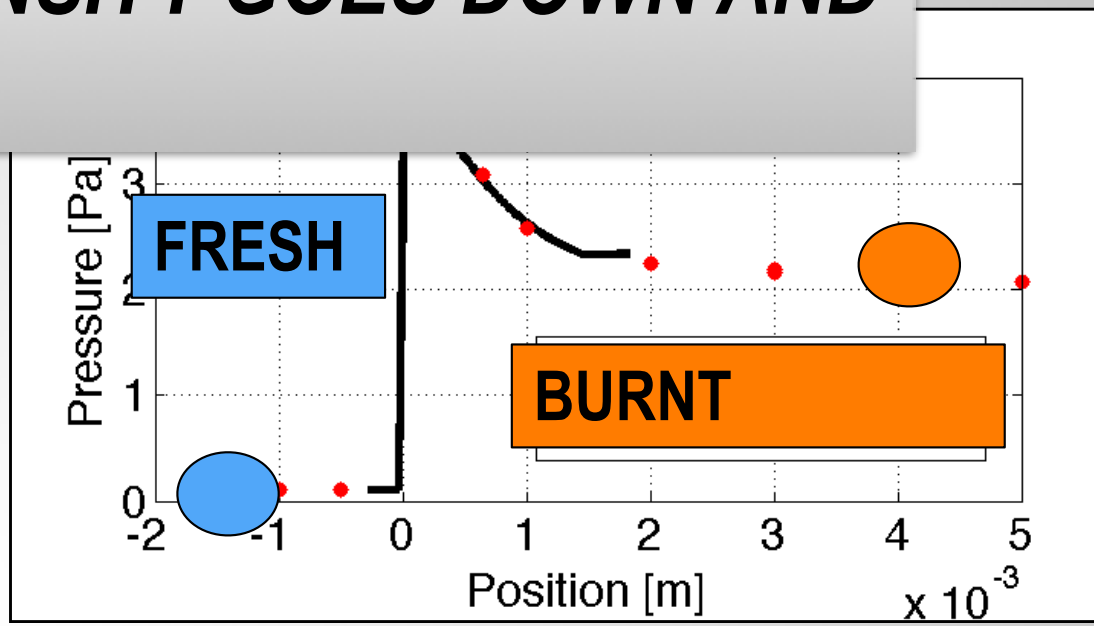


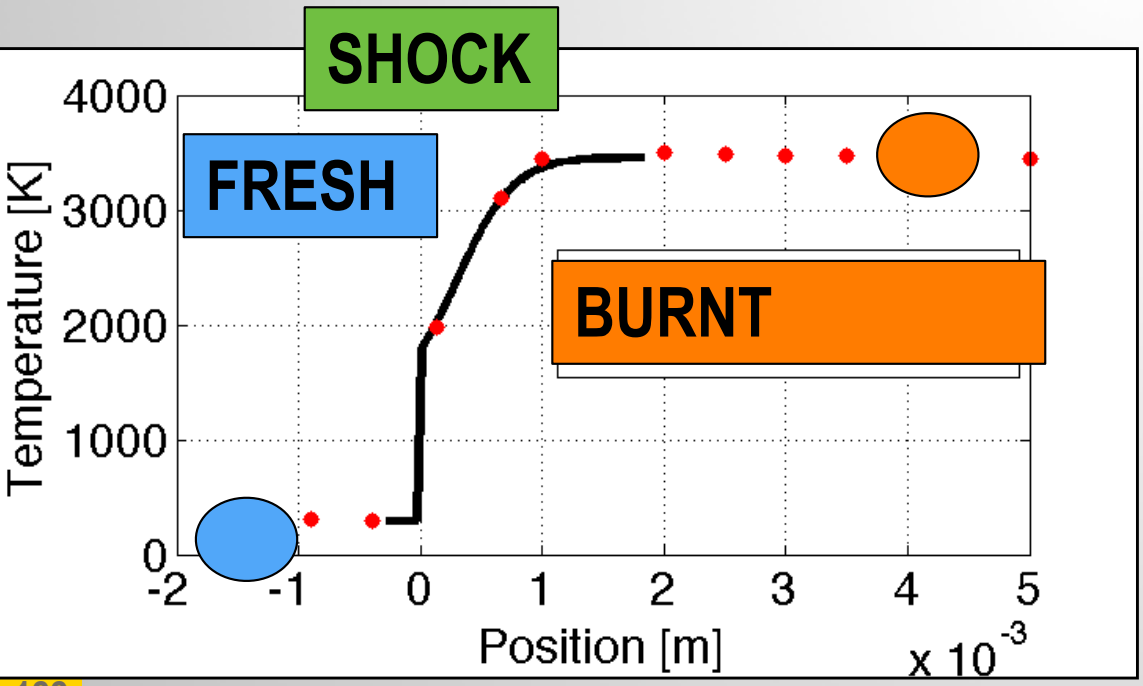
DETONATION IS A FLAME + A SHOCK

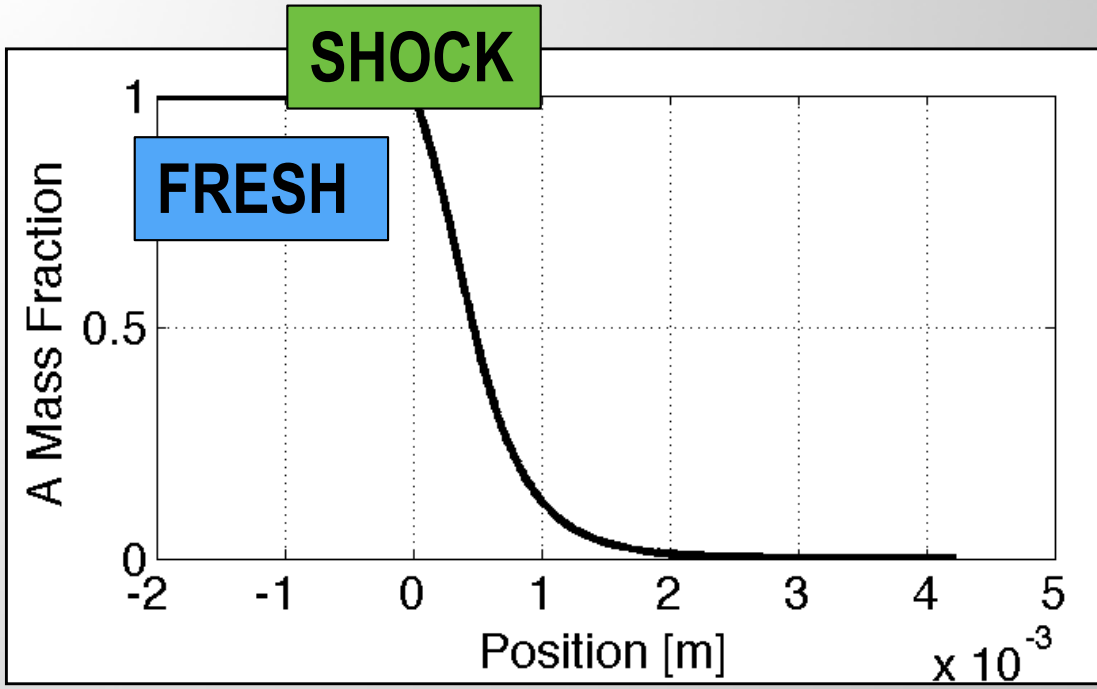
Source: Pr S. Candel, EM2C

DENSITY, PRESSURE AND TEMPERATURE GO UP (IN A DEFLAGRATION, DENSITY GOES DOWN AND PRESSURE TOO)



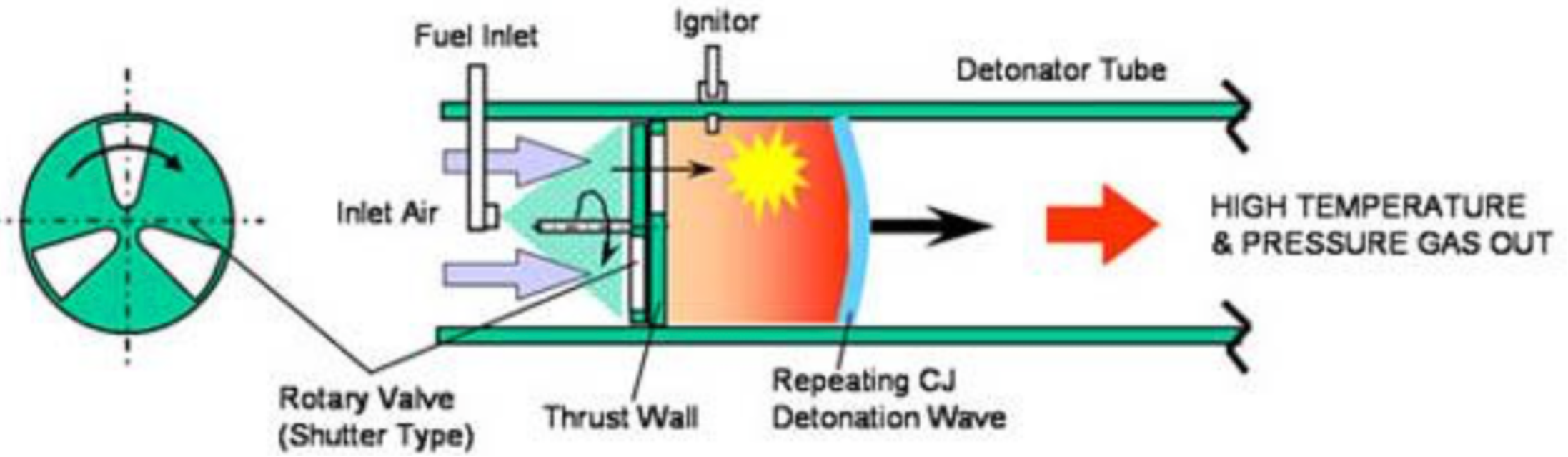




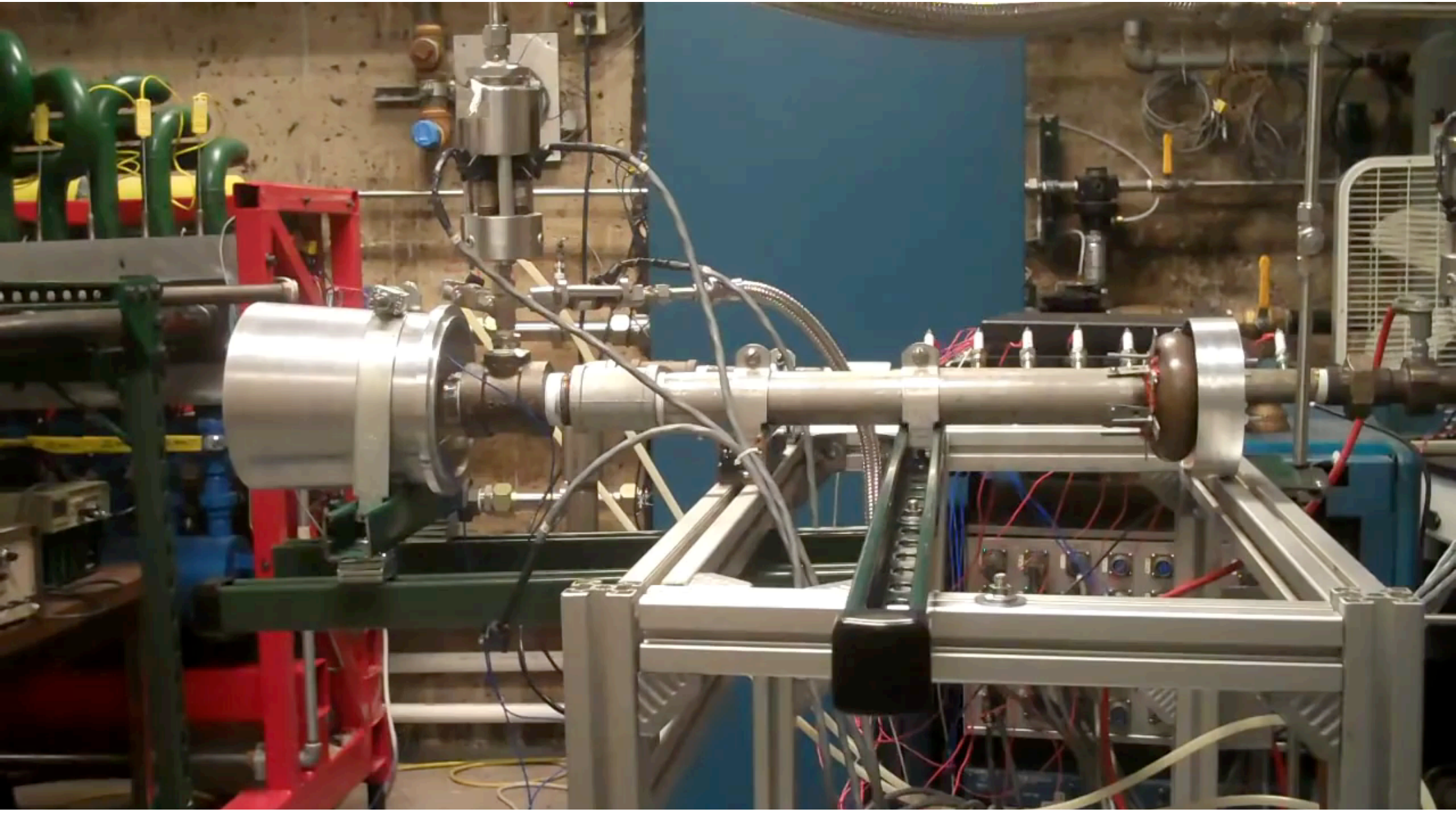


Detonations can be used in engines:

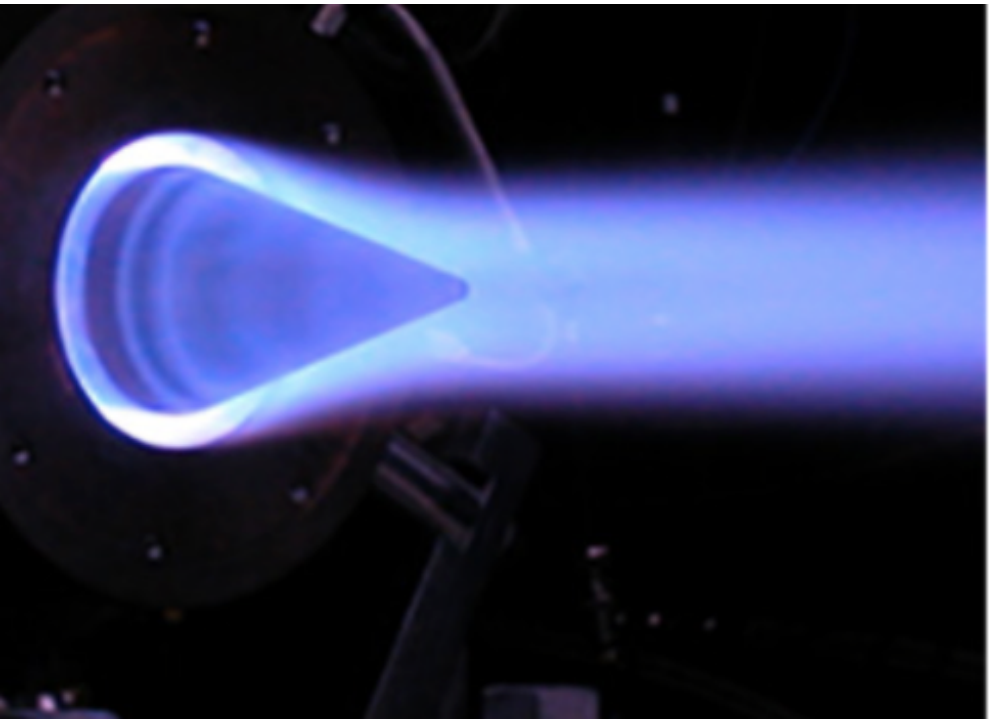
1/ the PDE - Propagating Detonation Engine:

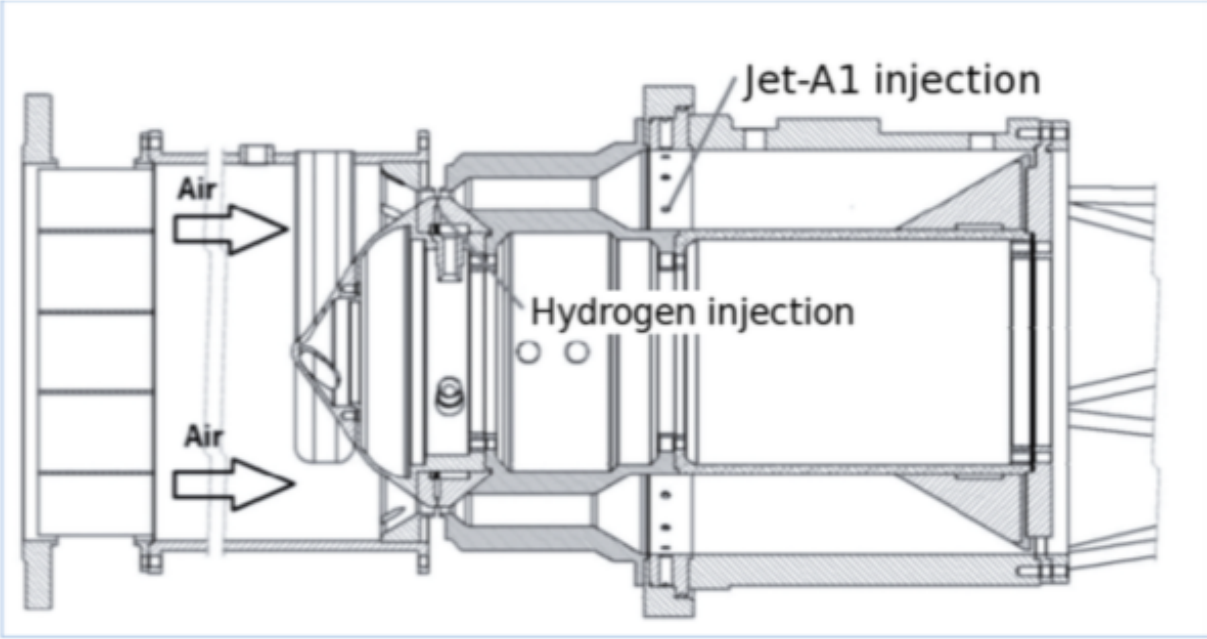


Propagating Detonation Engine:

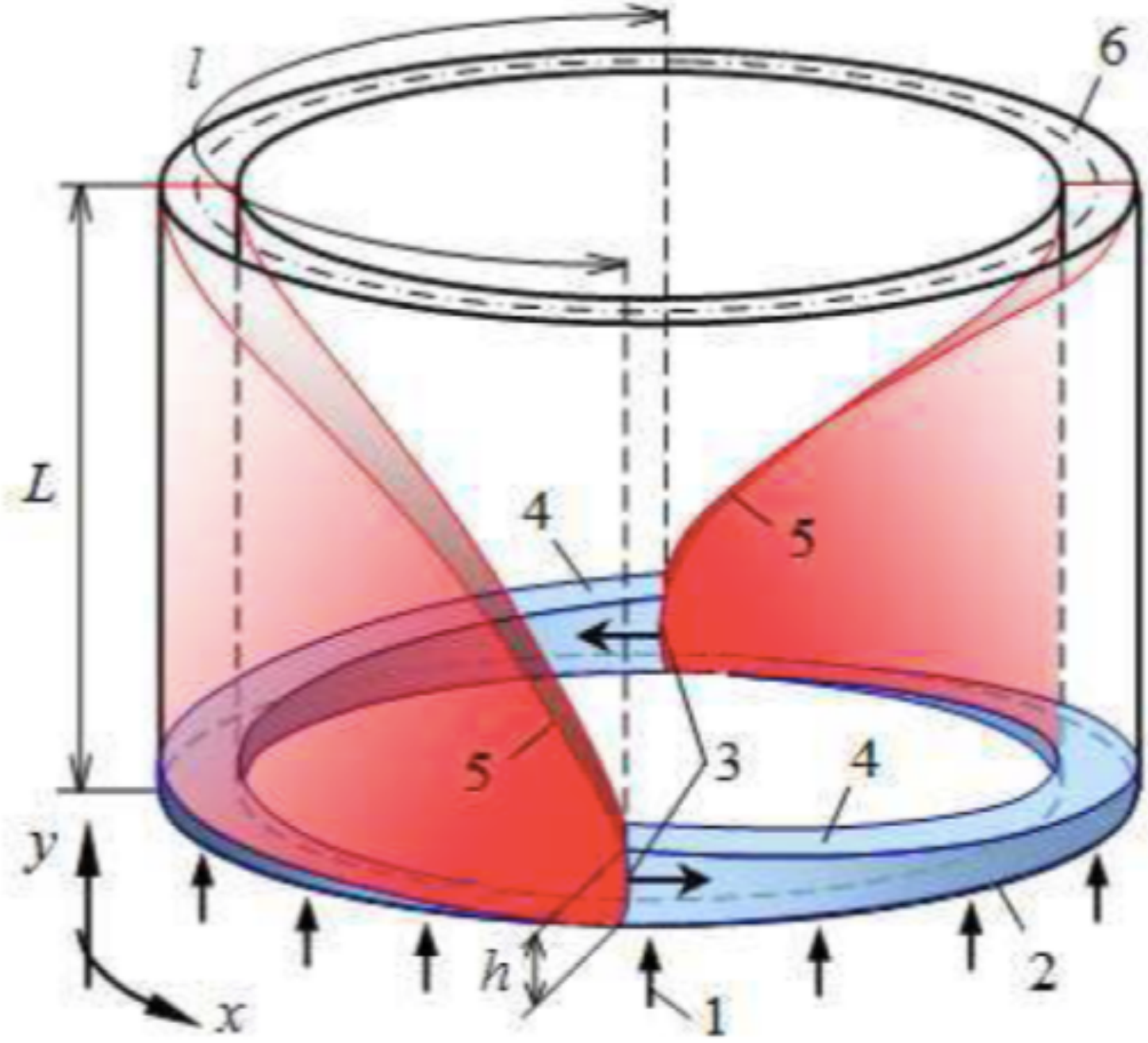


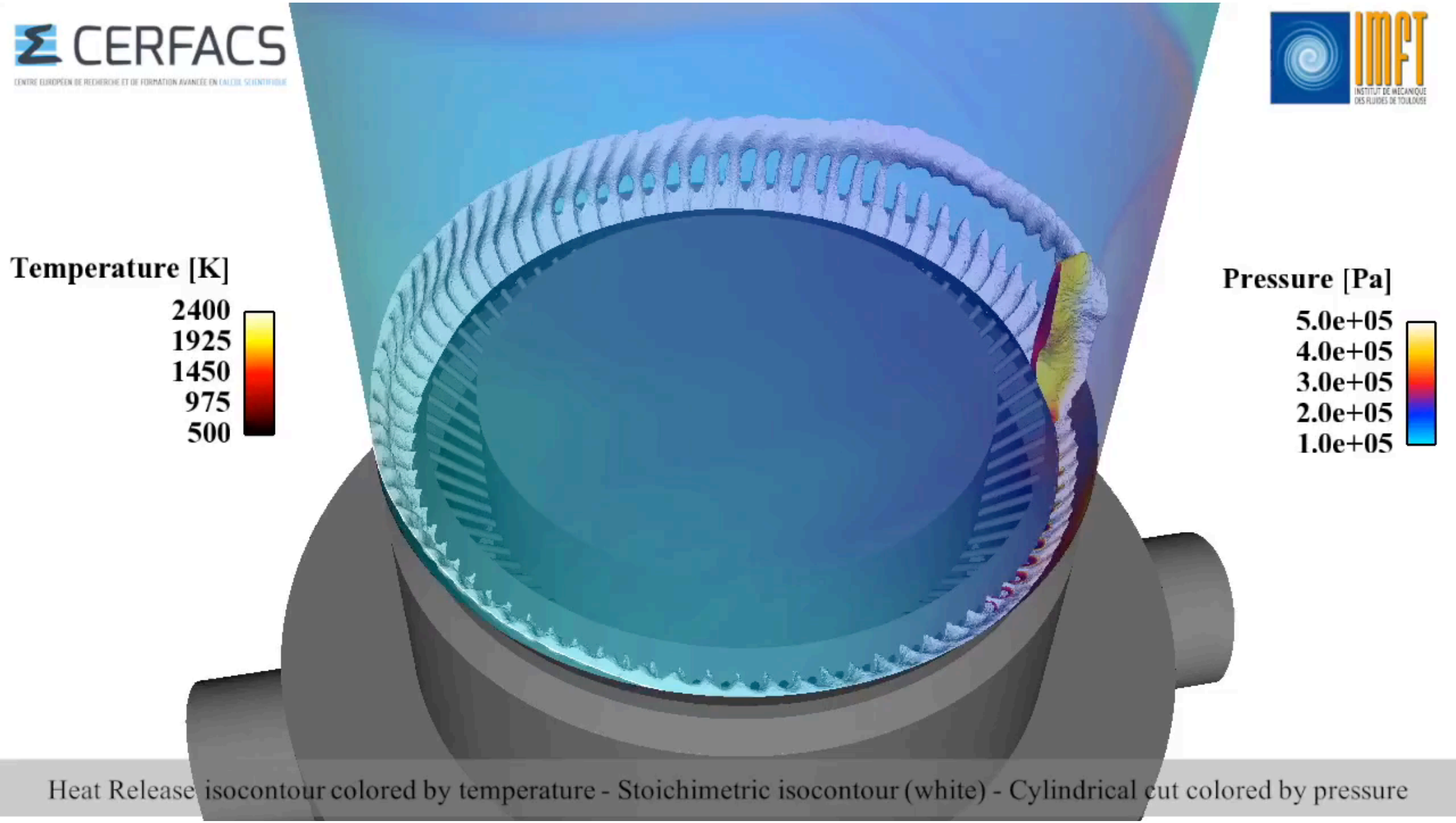
Detonations can be used in engines: 2/ the RDE - Rotating Detonation Engine:





RDE





Heat Release isocontour colored by temperature - Stoichimetric isocontour (white) - Cylindrical cut colored by pressure

But the main issue with detonation is safety and explosions

- Let us look at examples in one specific field: flames ignited in a building full of air + reactants (safety issues)

- We will also introduce ‘transitions’: deflagrations can become detonations (also called DDT: deflagrations to detonation transitions)

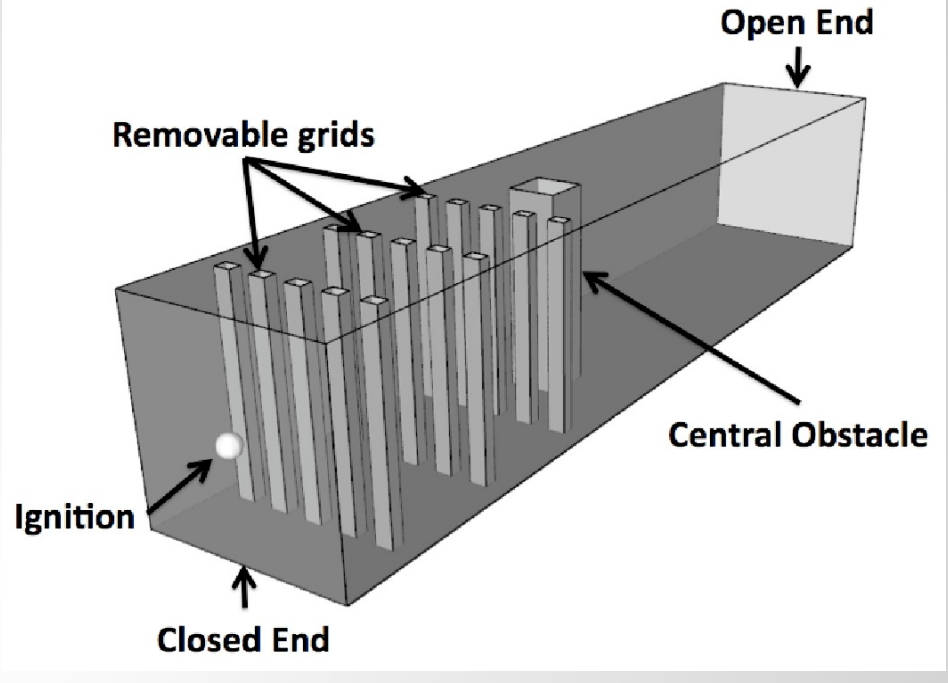
Example of deflagration



Exemple of DETONATION



DDT OFTEN DUE TO TURBULENT COMBUSTION:





DEFLAGRATION or/and DETONATION

FLAMES HAVE TWO TYPES OF SOLUTIONS:

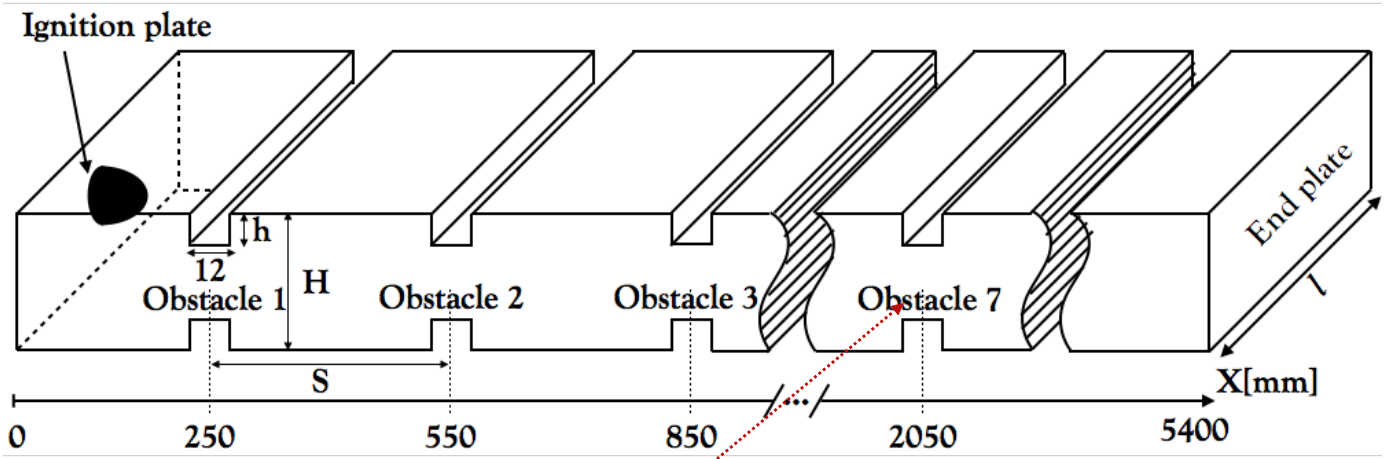
- DEFLAGRATION
- DETONATION

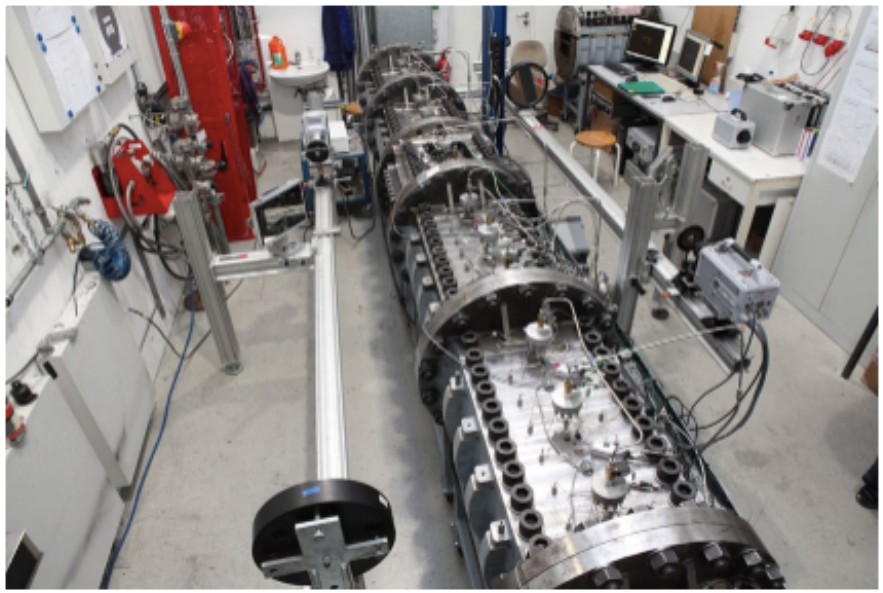
BOTH SOLUTIONS CAN APPEAR IN THE SAME SETUP

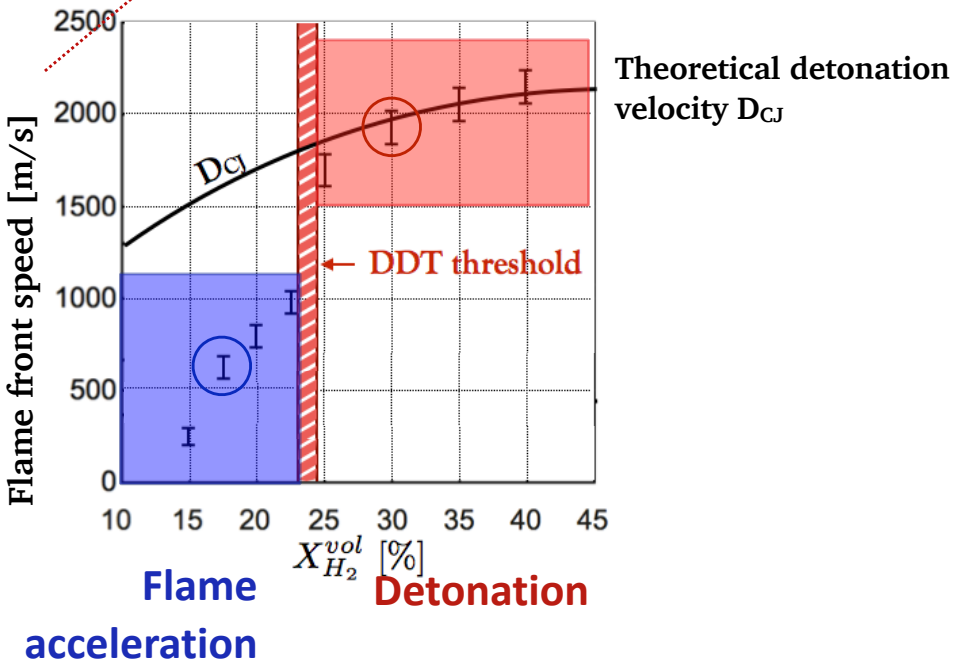
Copyright T. Poinsot 2023

Simulation of Deflagration to Detonation in the Gravent experiment (TU Munich)

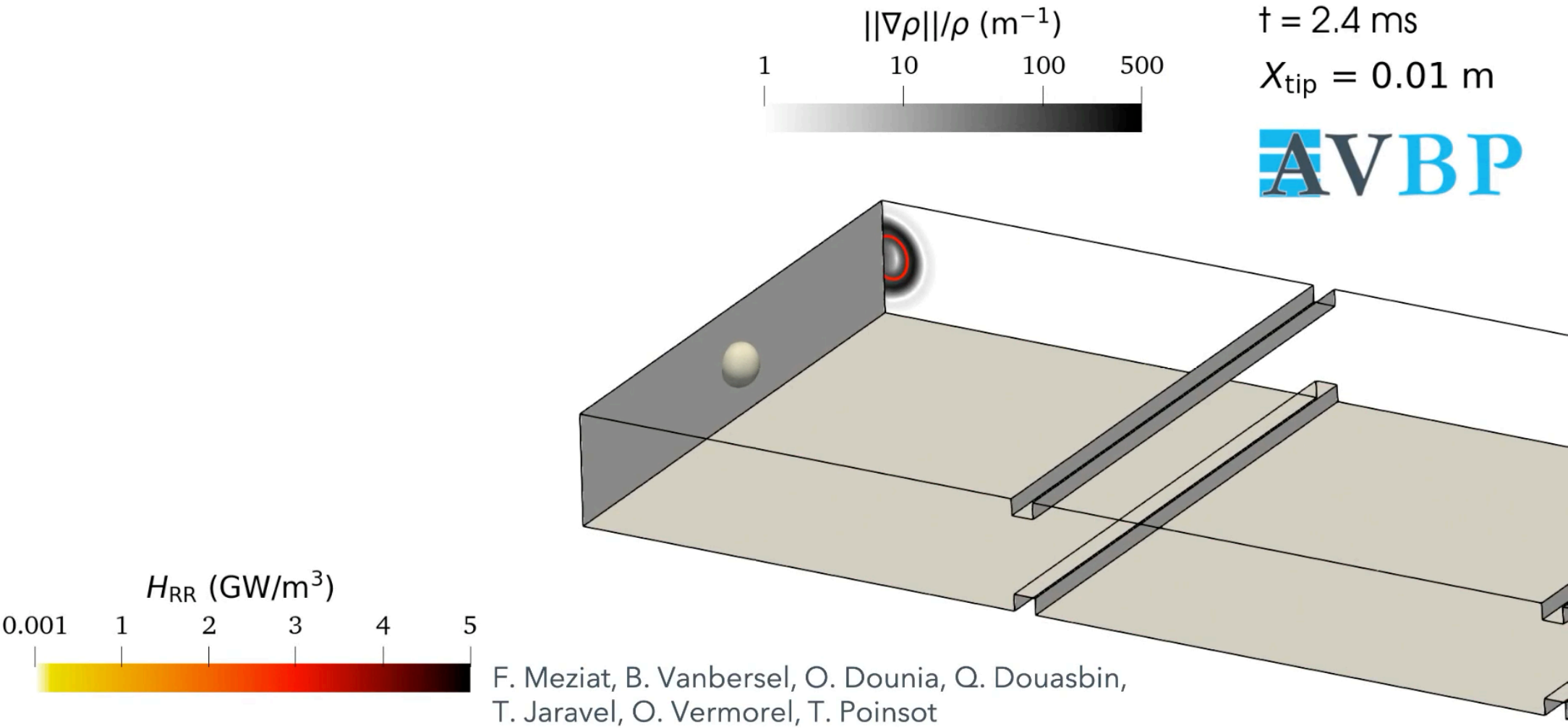
- H_2/air mixture
- Blockage ratio 0.3





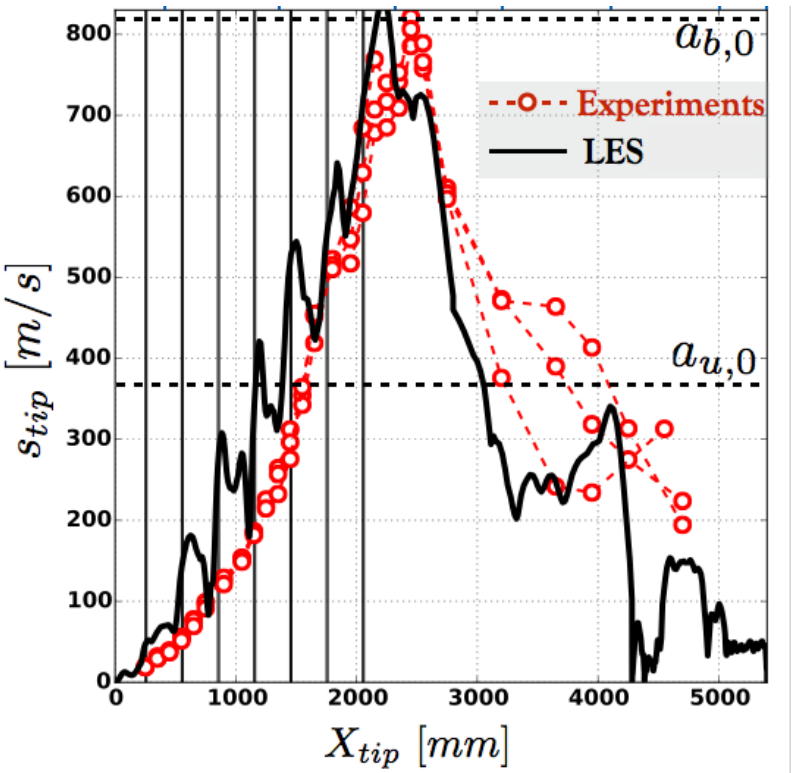


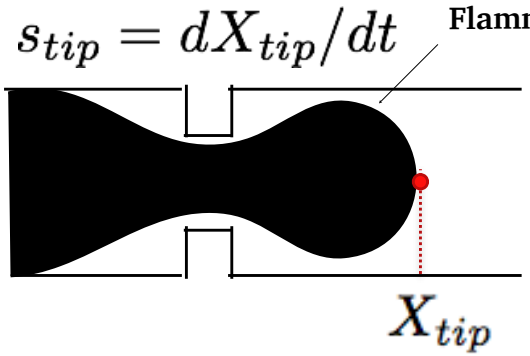
Deflagration case (phi=0.52)

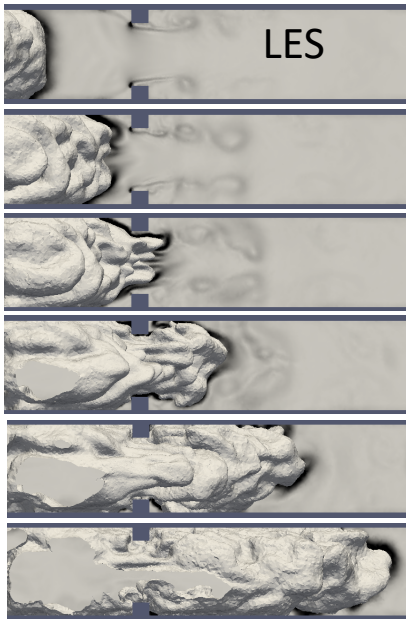


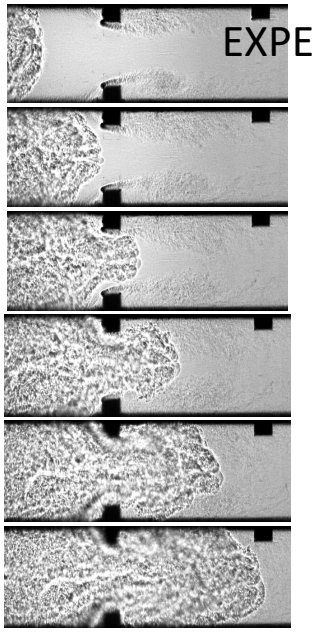
F. Meziat, B. Vanbersel, O. Dounia, Q. Douasbin, T. Jaravel, O. Vermorel, T. Poinsot

Deflagration case (phi=0.52)

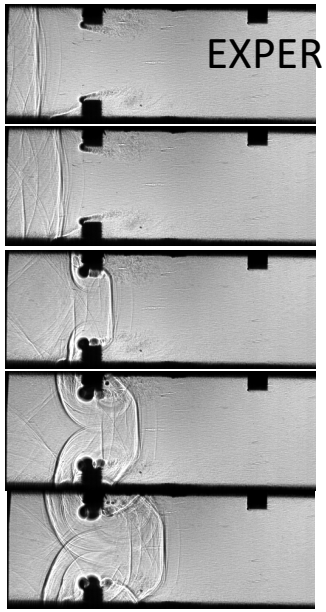




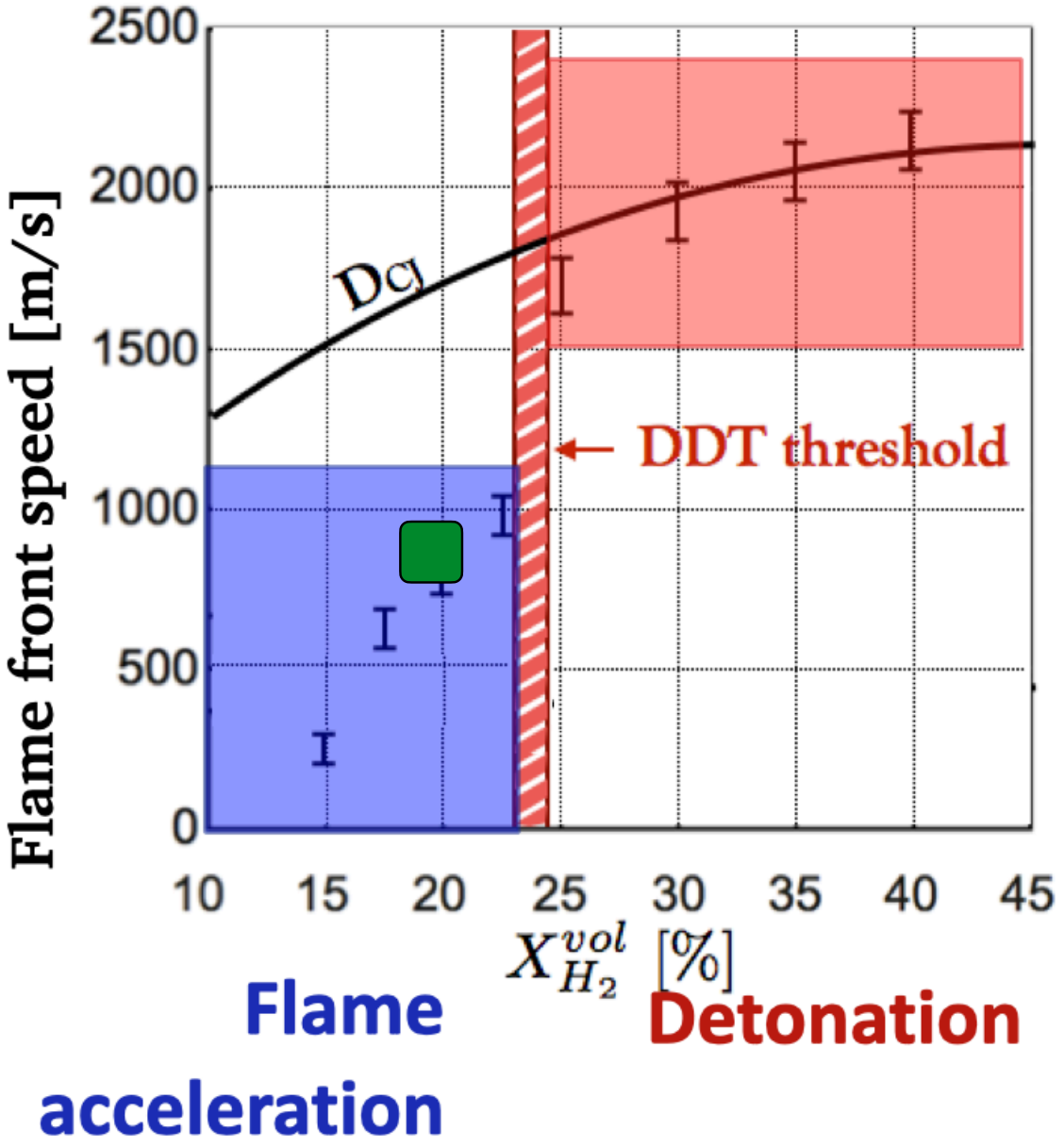






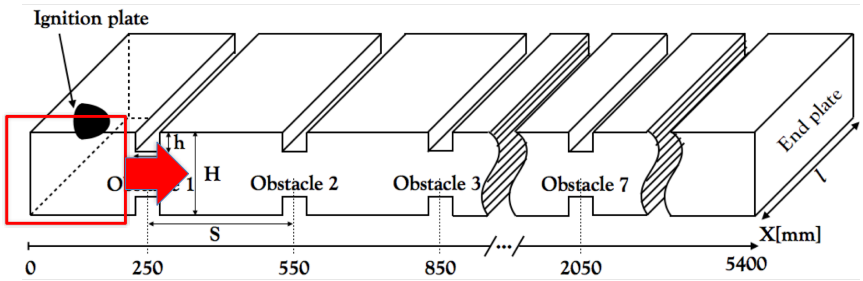


Detonation case (phi=1.0): put more H2 in the duct

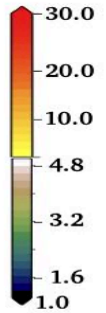


O. Dounia et al. CF 2019

Detonation case (phi=1.0)

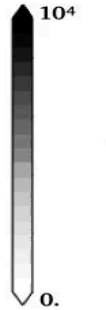


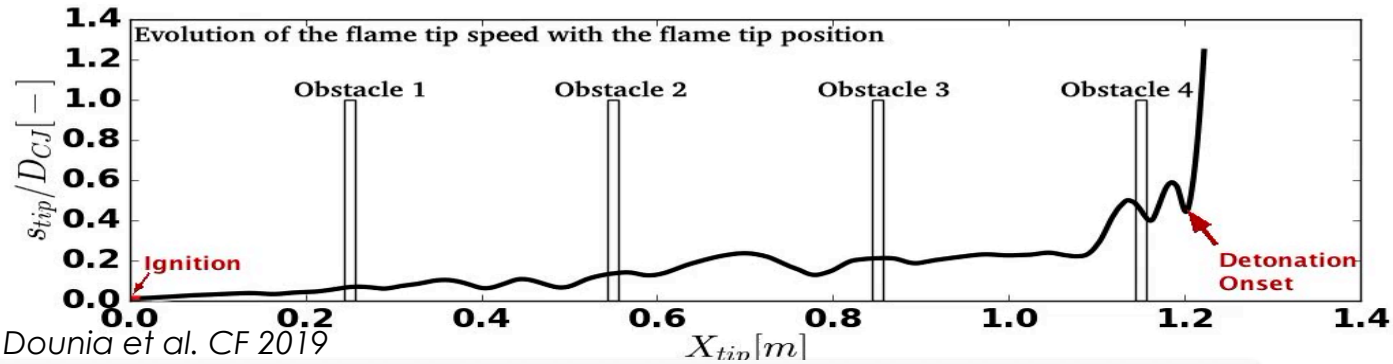




Time : 0.06 ms







CERFACS

O. Dounia et al. CF 2019

SHOCK AND FLAME 'LOCK IN': DETONATION

O. Dounia, Q. Douasbin, O. Vermorel

PLANAR FLAMES ?

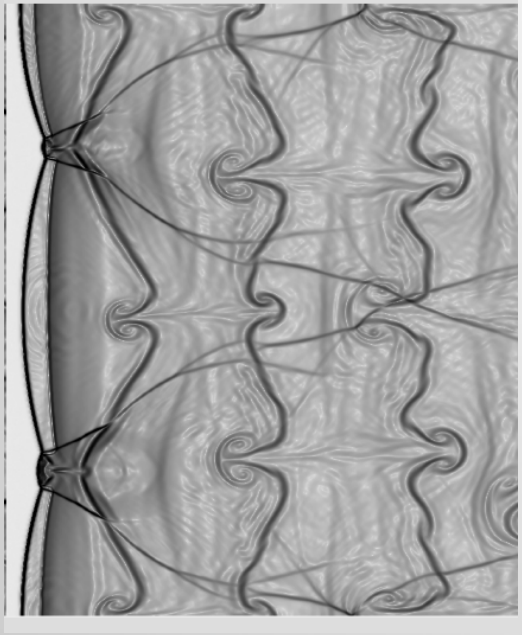
- All theories begin by describing fronts as planar 1D waves (this is what we just did for detonations)

- Is it true ? NO… flames do not usually remain flat

PLANAR FLAMES ?

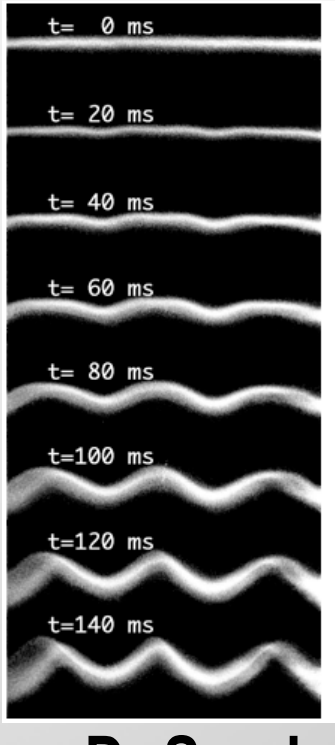
★ REAL DETONATIONS AND DEFLAGRATIONS ARE RARELY 'PLANAR':

- ➡ ONE-D DETONATIONS ARE ALMOST ALWAYS UNSTABLE.
- ➡ DEFLAGRATIONS ARE UNSTABLE TOO: MOST OF THEM DEVELOP INSTABILITIES:



DETONATION

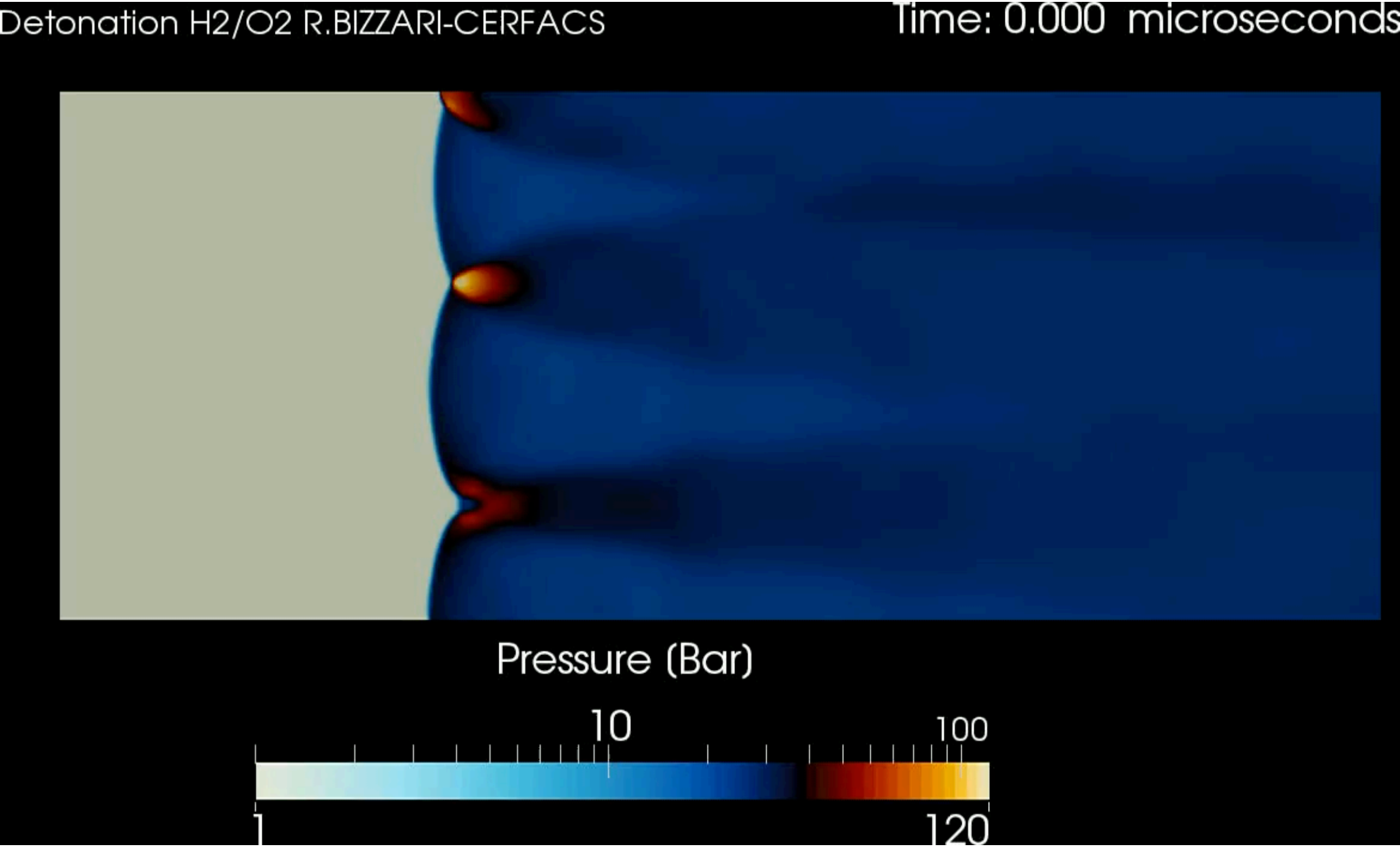
DEFLAGRATION



Source: Pr Bauwens

Source: Dr Searby

A detonation makes cells:



FLAME REGIMES

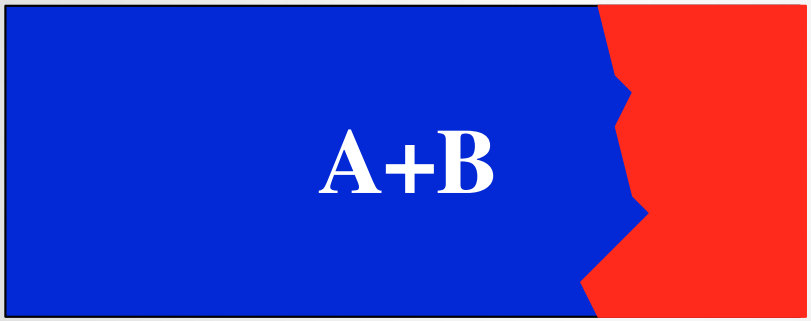
Since the reaction rate is written:

$$\dot{\omega} = A Y_A^{\nu_A} Y_B^{\nu_B} exp(-T_a/T)$$

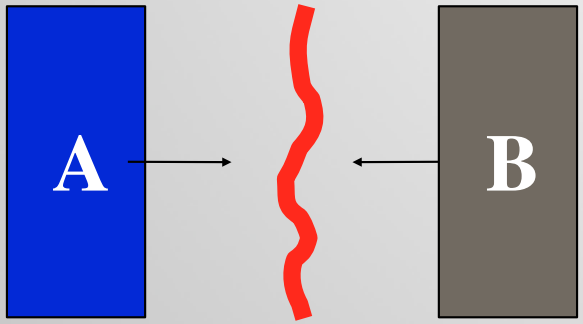
it takes three ingredients to burn: A, B and high temperature.

Regimes depend on A and B mixing:

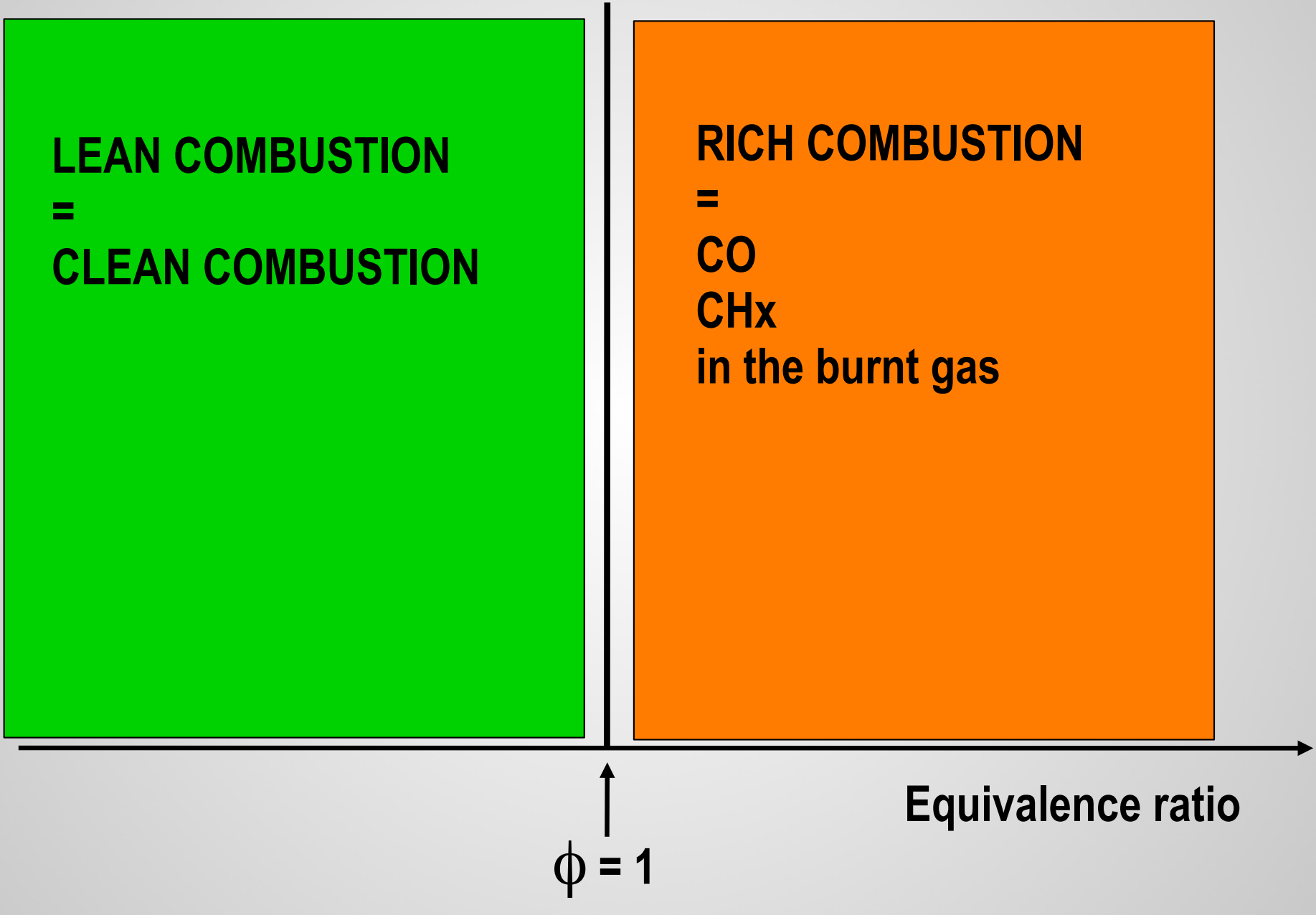
PREMIXED: A and B are mixed first and burnt afterwards



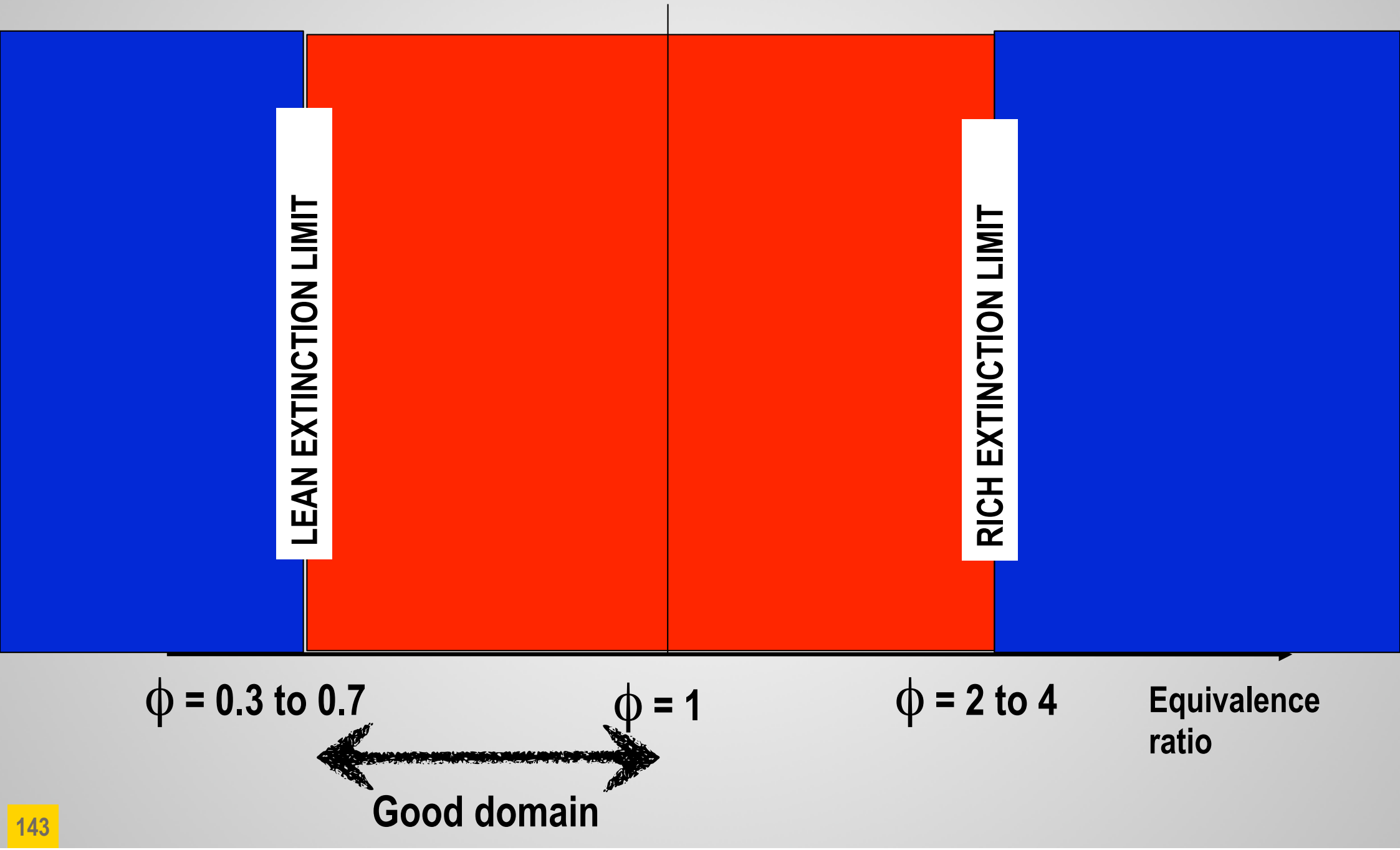
DIFFUSION: A and B are stored separately. They mix AND burn at the same time



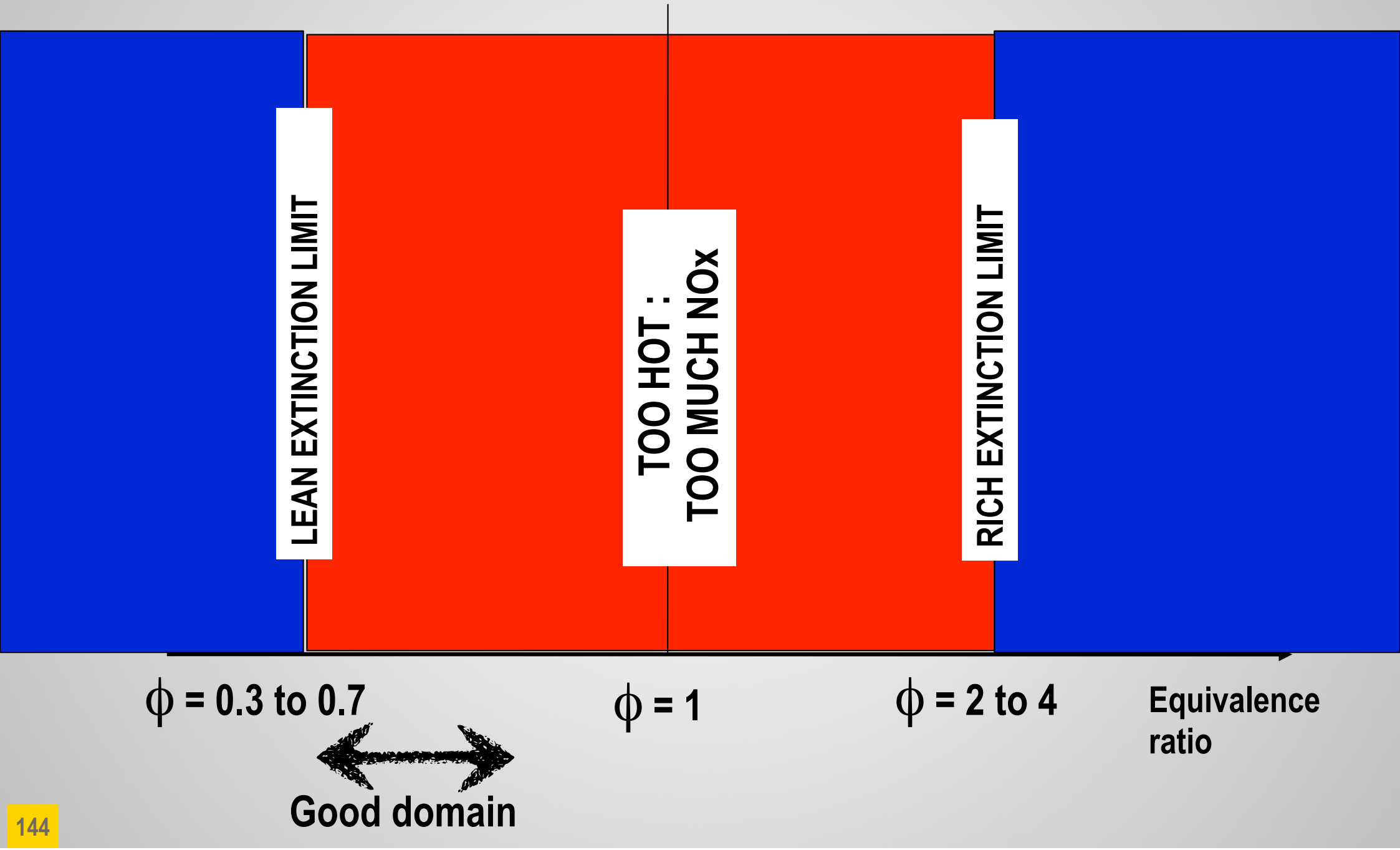
PREMIXED FLAME REGIMES:



FLAMMABILITY DOMAIN FOR A PERFECTLY PREMIXED GAS



FLAMMABILITY DOMAIN FOR A PERFECTLY PREMIXED GAS







Premixed combustion can be rich or lean….

If we premix fuel and air before combustion… Sometimes we don’t

But not all flames are premixed:

PREMIXED:

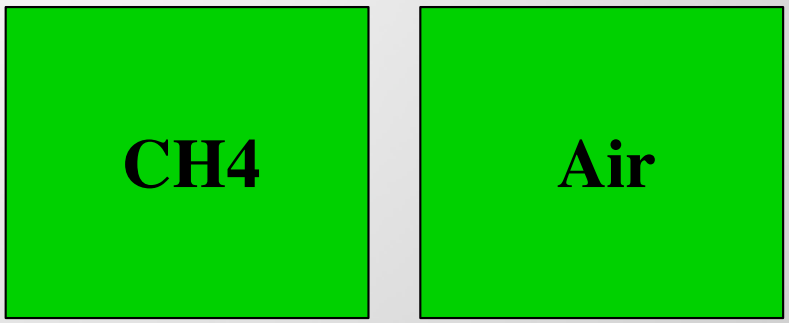
The most efficient
The cleanest
The most dangerous



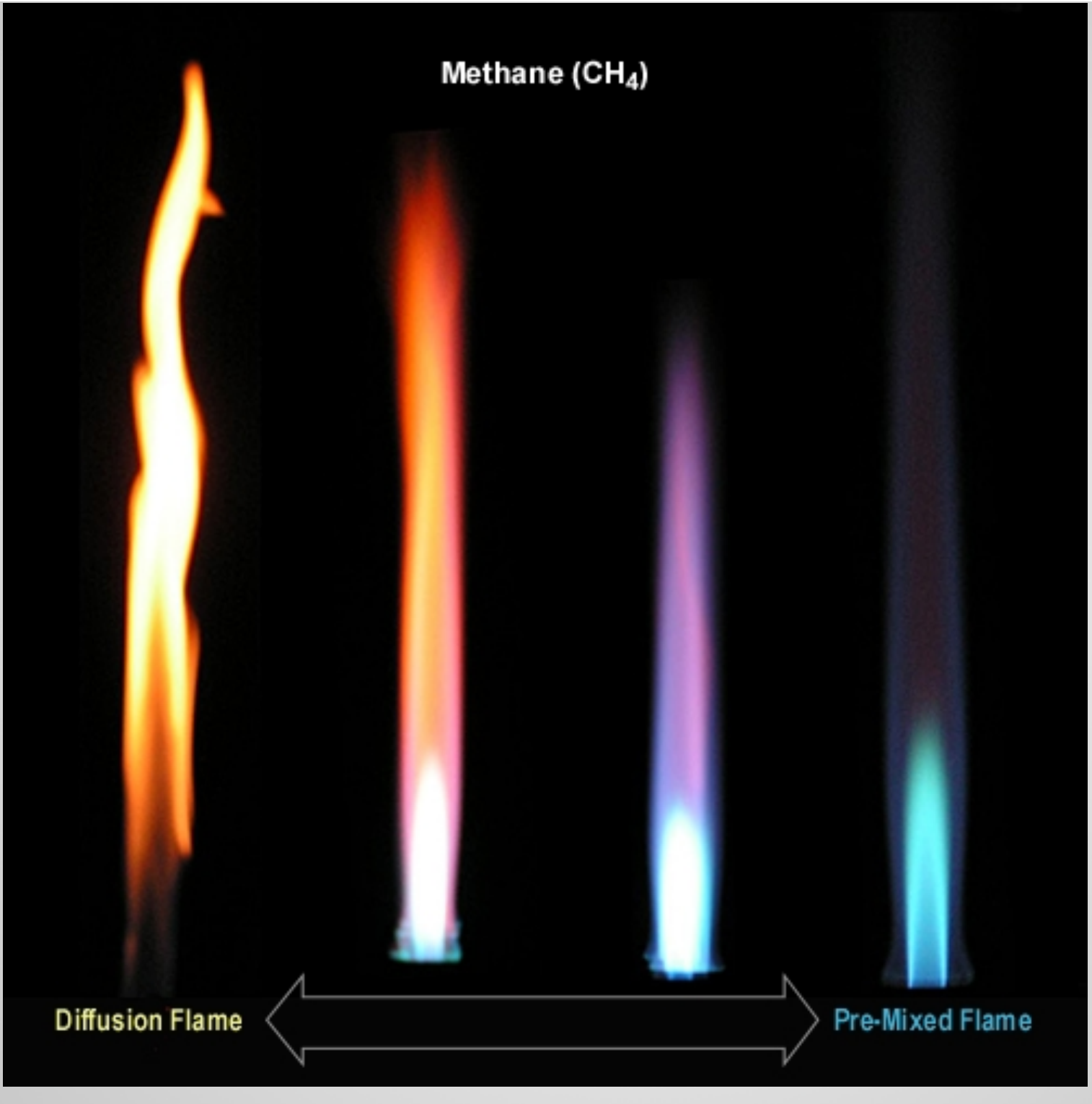
No smoking...

DIFFUSION (also called non premixed):

Always stoichiometric
Less efficient
Less clean
Less dangerous



No possible uncontrolled ignition


Methane (CH_4)
Diffusion Flame
Pre-Mixed Flame

IN PRACTICE, WE WOULD LIKE TO:

- **Store reactants separately for safety**

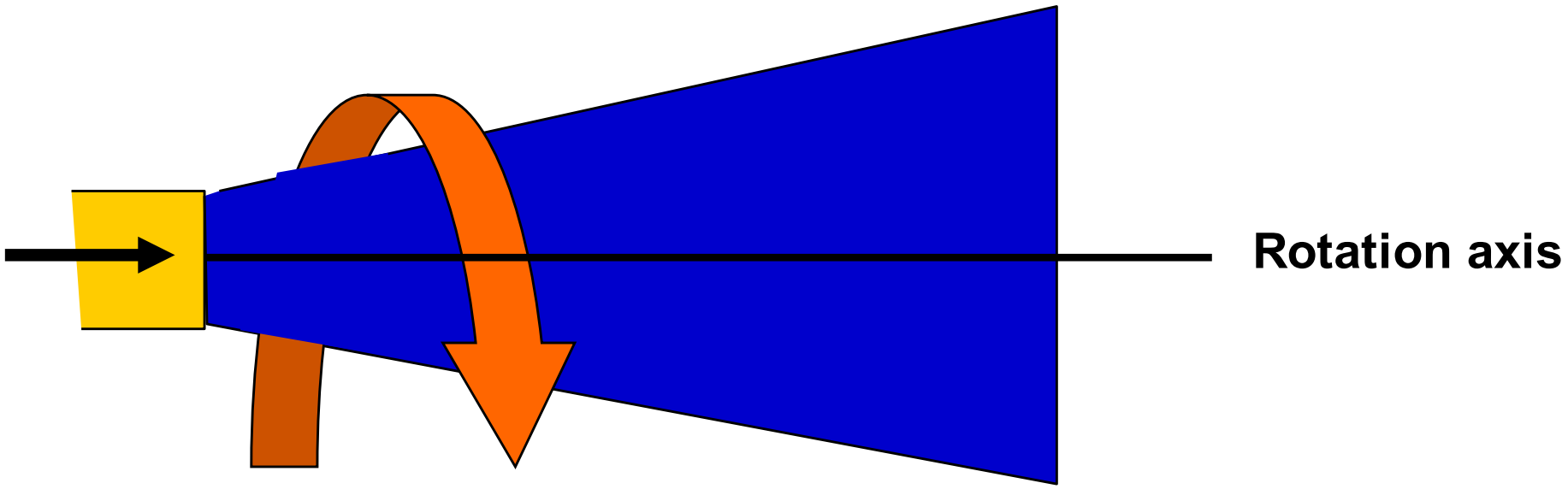
BUT, AT THE SAME TIME,

- **Burn in a premixed mode for performance and pollution**

This requires special devices for fuel and air injection to create fast mixing

➢ **SWIRL IS ONE OF THE MOST COMMON**

« SWIRL »: a very common flow feature in combustion used to increase mixing and stabilize flames



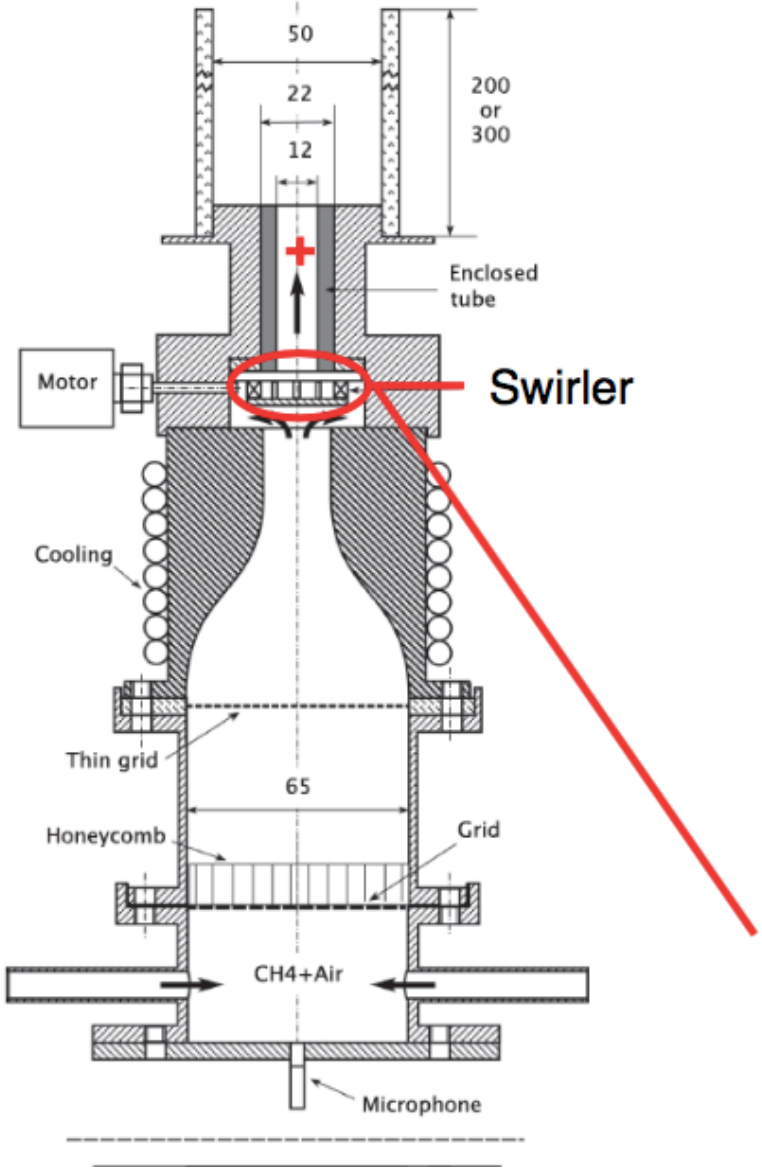
Initiation to ‘swirl’



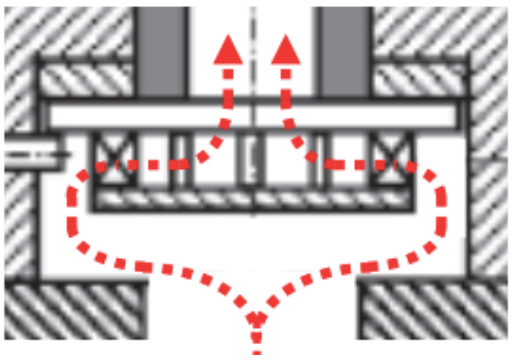
Initiation to ‘swirl’ but… bigger !



In the laboratory: a flame with variable swirl (EM2C, Centralesupelec)



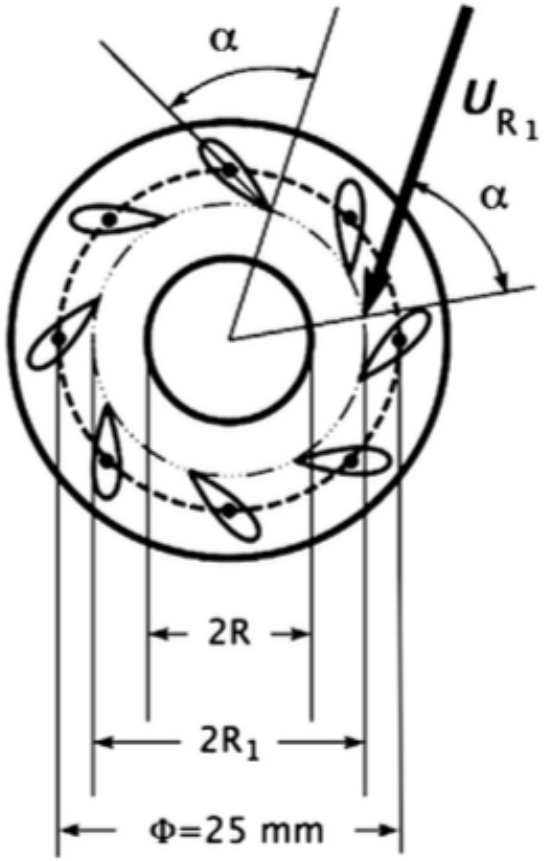
- premixed mixture CH_4 / Air : $\phi = 0.7$
- bulk velocity in the injection tube (+): $U_b = 11\ m.$
- $Re = 8800$
- thermal power $Q = 2.85\ kW$
- 2 confinement tubes (CT):
  - $L = 200\ mm\ (stable\ flame)$
  - $L = 300\ mm\ (unstable\ flame)$



Flow direction

Adjustable blades are used to change the swirl number

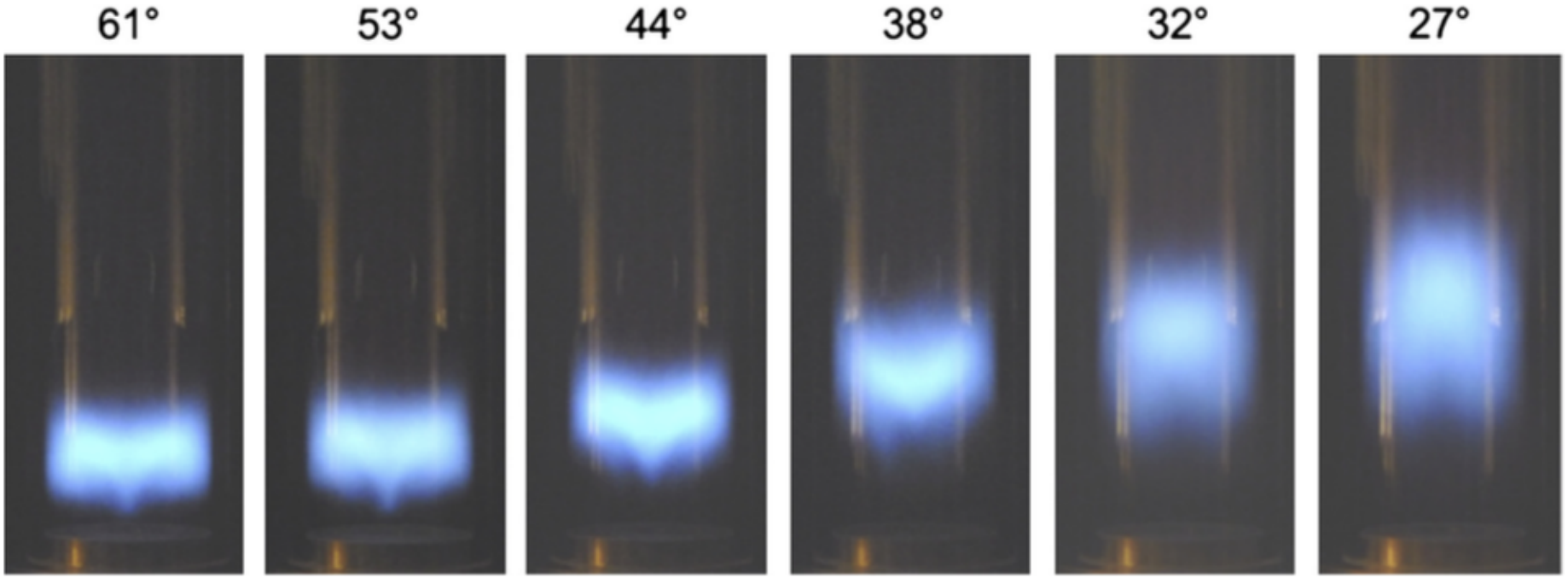




Swirler design

- purely radial swirler
- 8 blades
- blade angle $\alpha = 22\ to\ 61°$
- average diameter $D = 25\ mm$
- inner tube radius $D_{in} = 2R = 12\ mm$
- passage height : $h = 4.25\ mm$

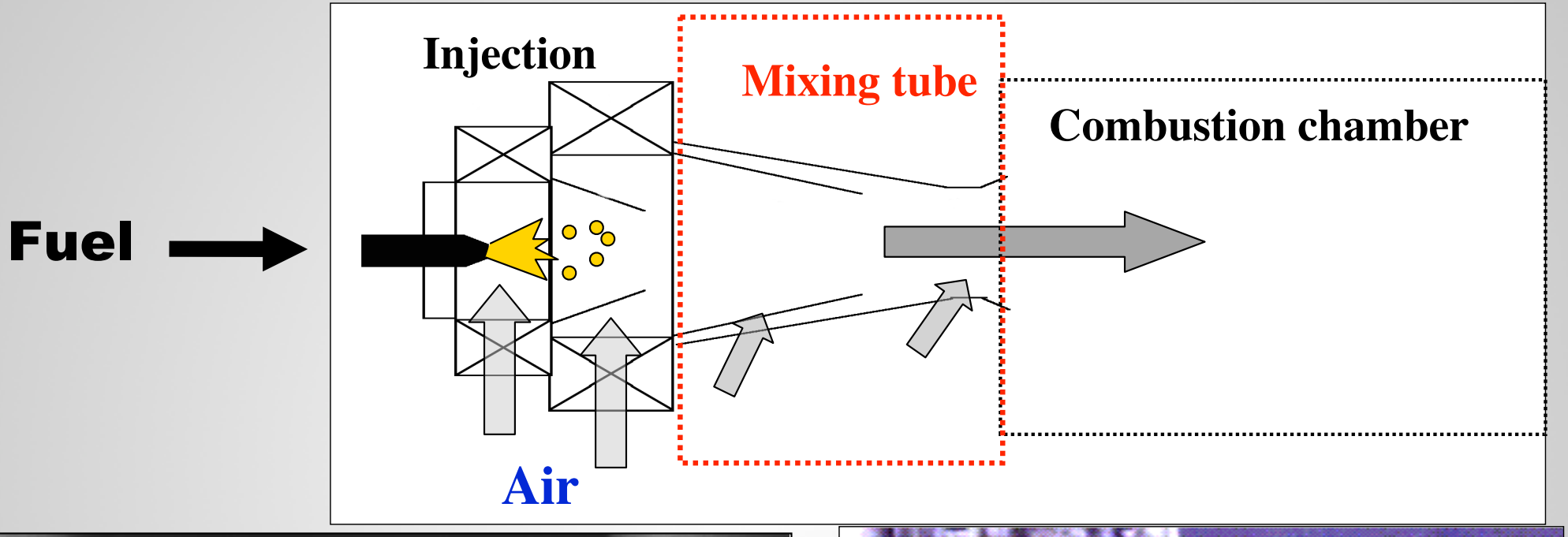
Long exposure time flame images with the 200mm exhaust tube

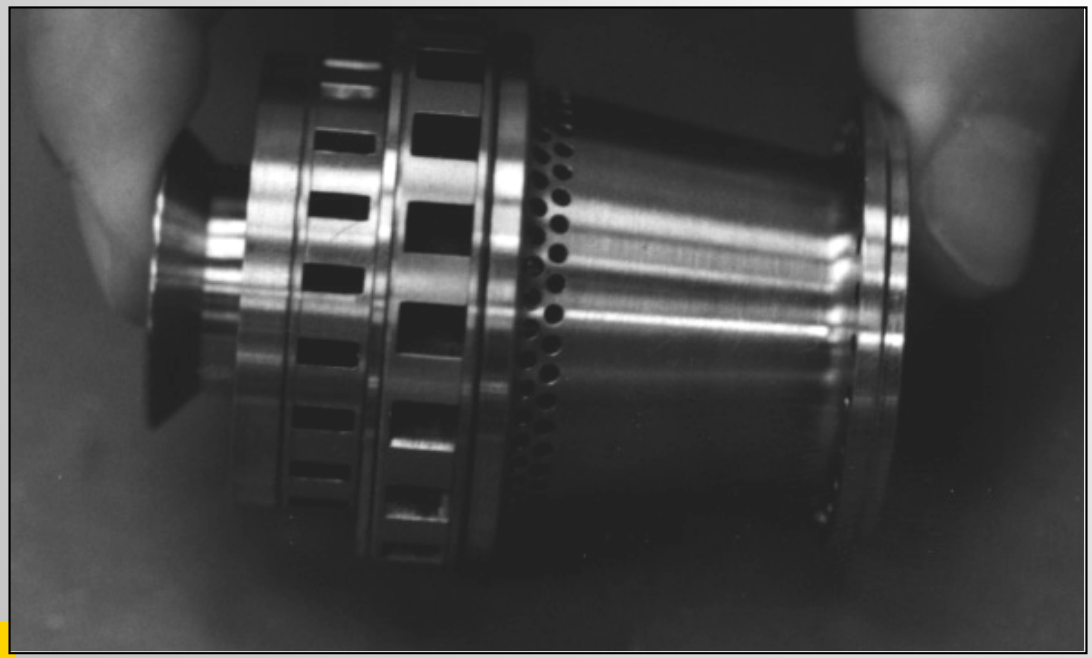


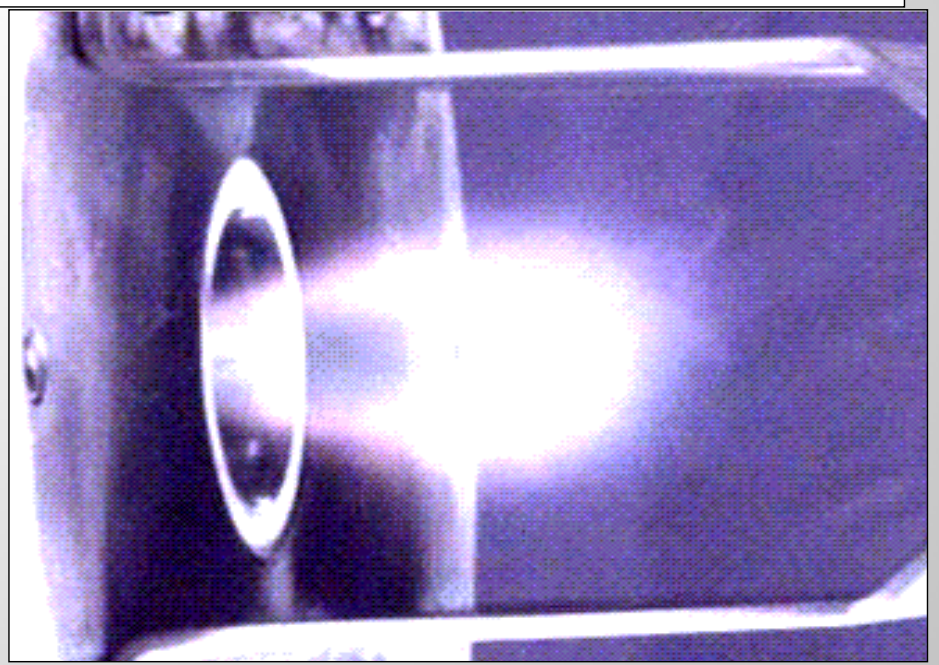
Swirl level

Increasing swirl makes flames more compact and more efficient

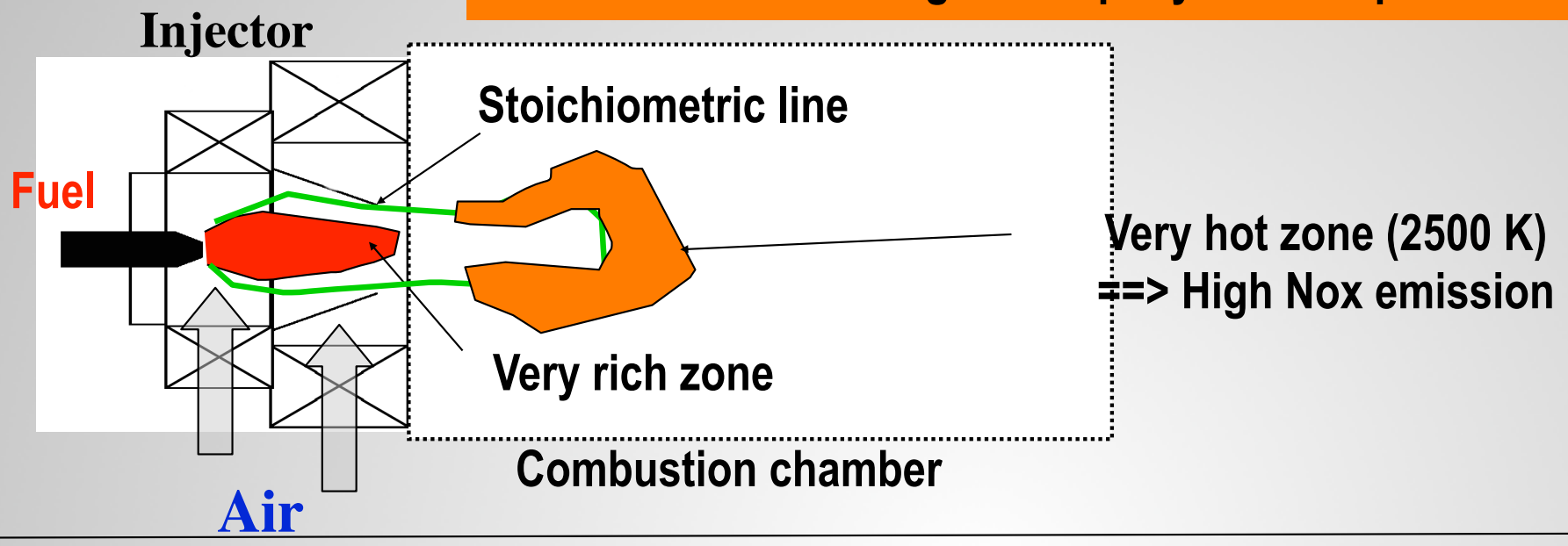
This strategy can lead to problems. Ex: flashback in LPP (Lean Premixed Prevaporized) systems.

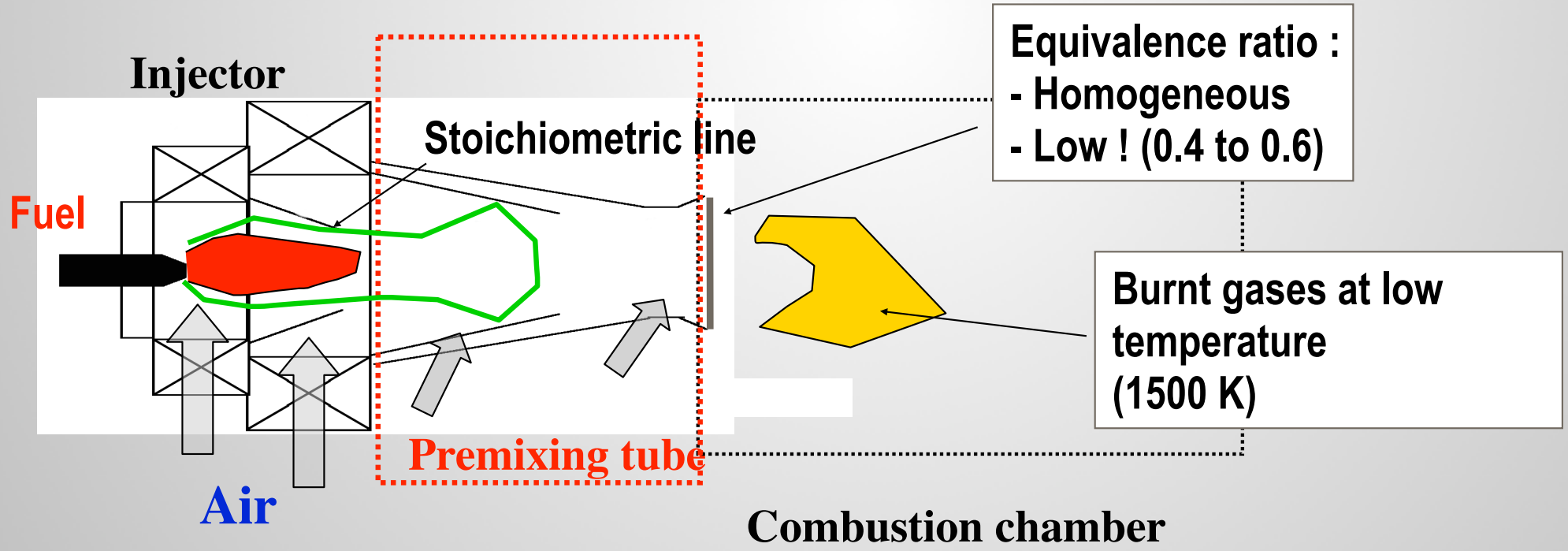




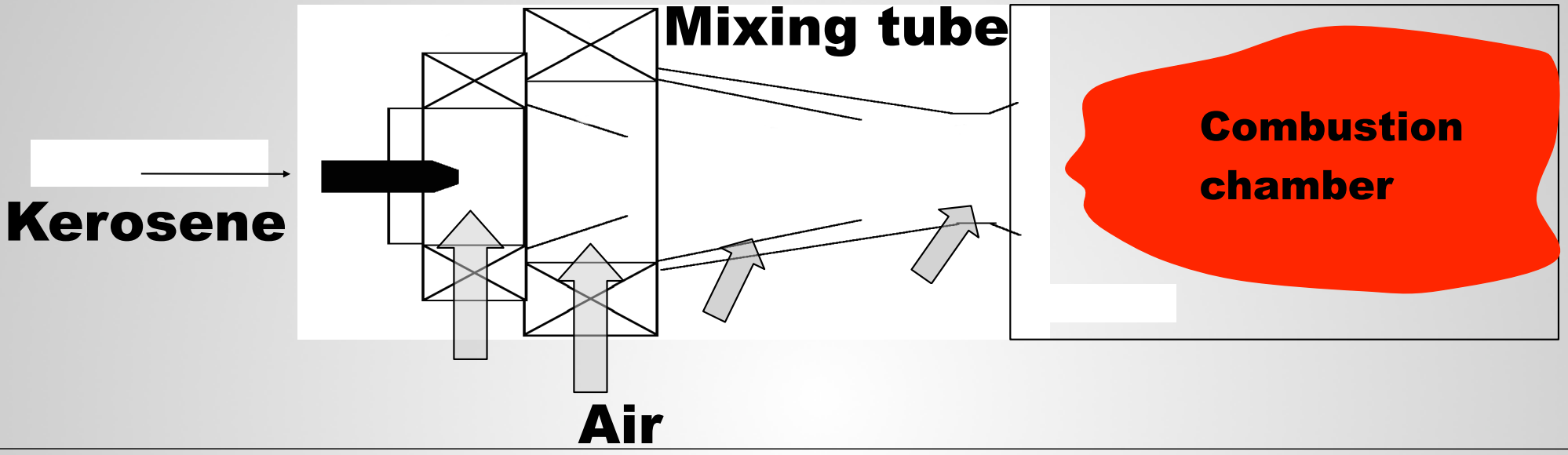


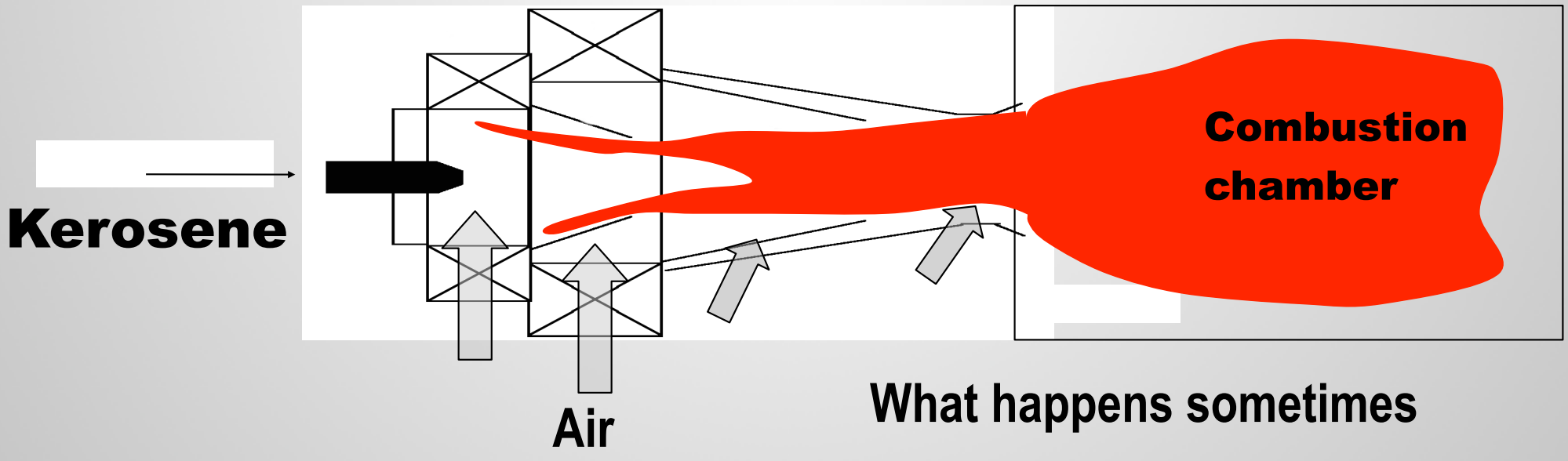
WHY LPP ?: Nox grows rapidly with temperature





What engineers expected:





What happens sometimes

Another classification of flames, important for CFD

We can classify flames in many ways:

- ★premixed vs non premixed (diffusion) flames
- ★swirled vs unswirled

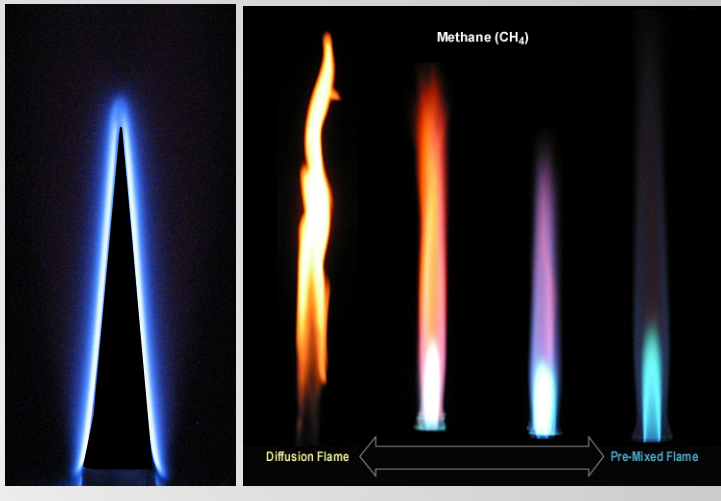
But there is another way to classify flames when doing CFD:

★**UNCONFINED FLAMES:** many theoretical approaches assume 'free' flames (the 1D premixed laminar flame, the perfect strained planar diffusion flame, the turbulent jet flames of the TNF workshop (see www.sandia.gov/TNF))

★**CONFINED FLAMES:** in practice, 99 % of the useful flames are confined either to recover heat (furnaces) or mechanical power (engine)

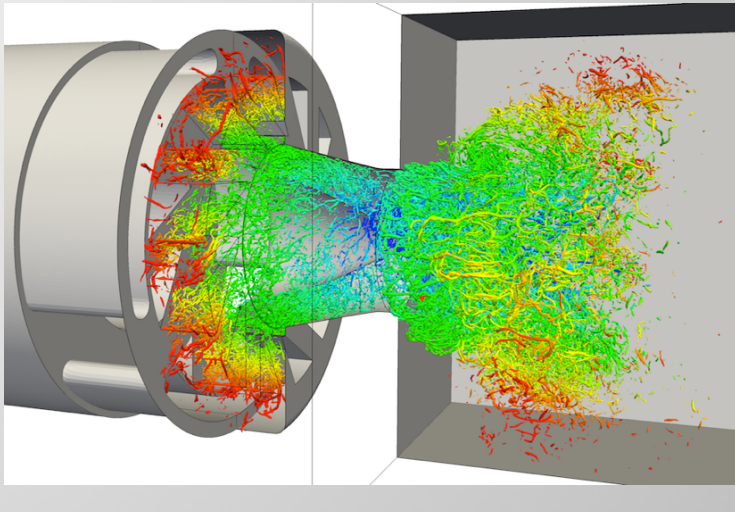
Confined vs unconfined flames: what is the difference ?

- ★ The velocity fields are different because of density changes due to dilatation
- ★ Walls everywhere in confined flames ==> Heat transfer becomes important
- ★ Acoustics can become important and induce combustion instabilities which are a problem in multiple present programs
- ★ In CFD codes: taking into account the complex geometry forces us to change (completely) our codes !



UNCONFINED

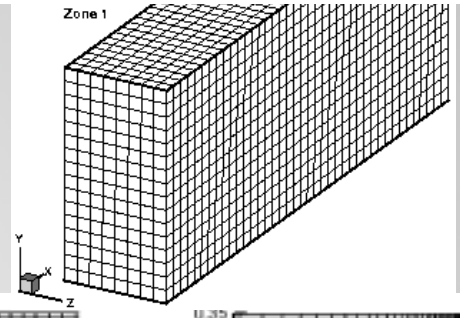
CONFINED

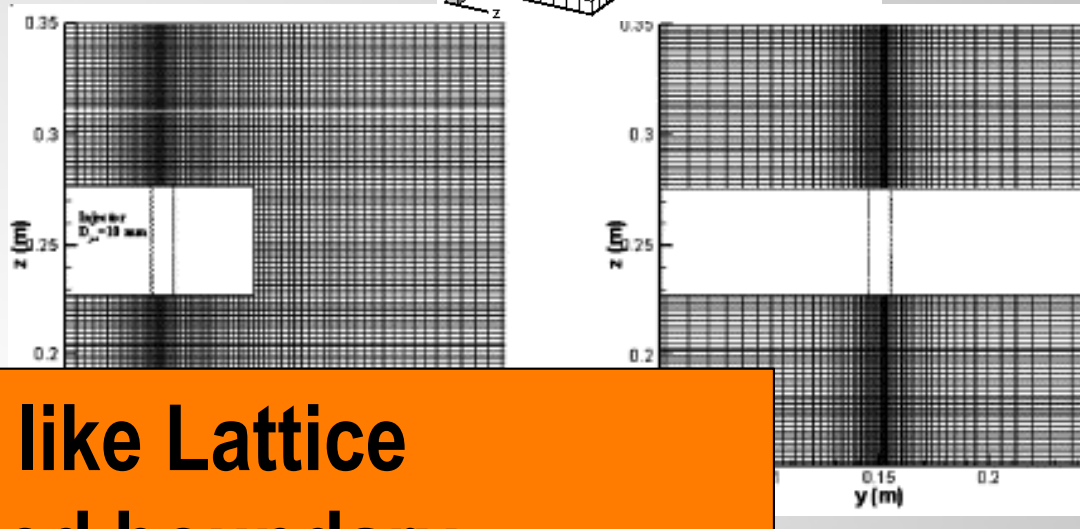


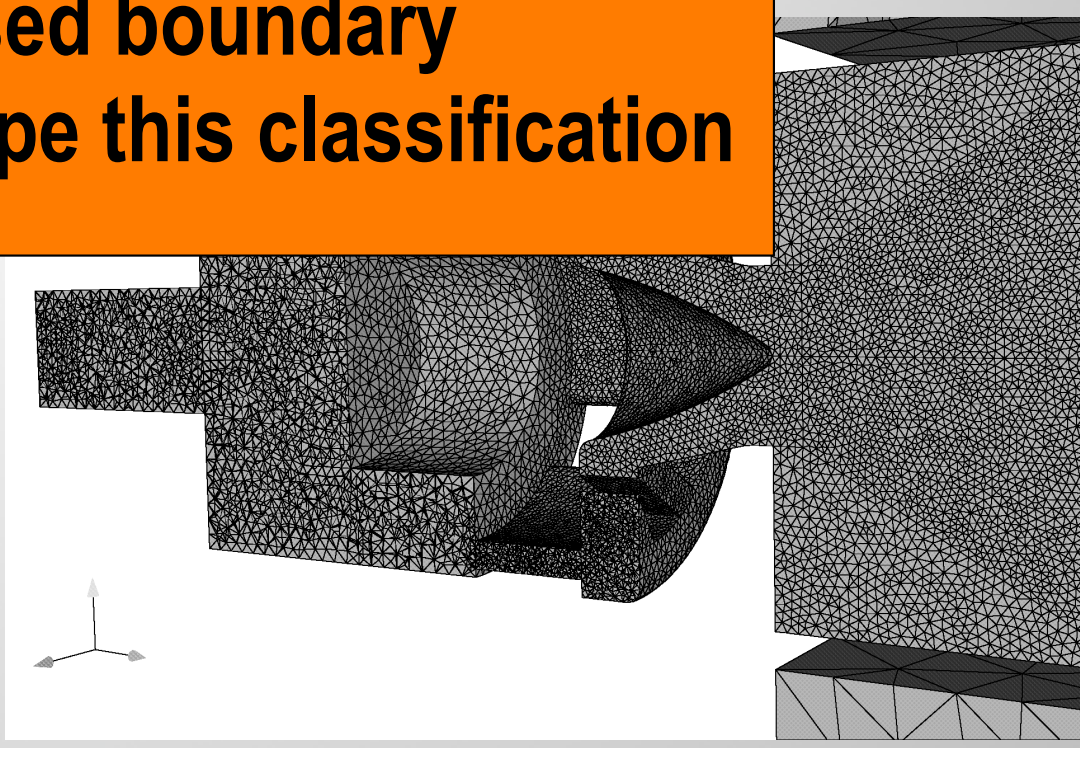
Meshes and codes:

- ★ ‘SIMPLE’ GEOMETRIES (UNCONFINED):
  - ★ STRUCTURED MESHES
  - ★ HIGH ORDER IS EASY
- ★ REAL FLAMES (CONFINED)
  - ★ UNSTRUCTURED MESHES
  - ★ HIGH ORDER IS TOUGH
  - ★ ==> NEW CODES !

Recent CFD methods like Lattice Boltzmann or Immersed boundary techniques may escape this classification

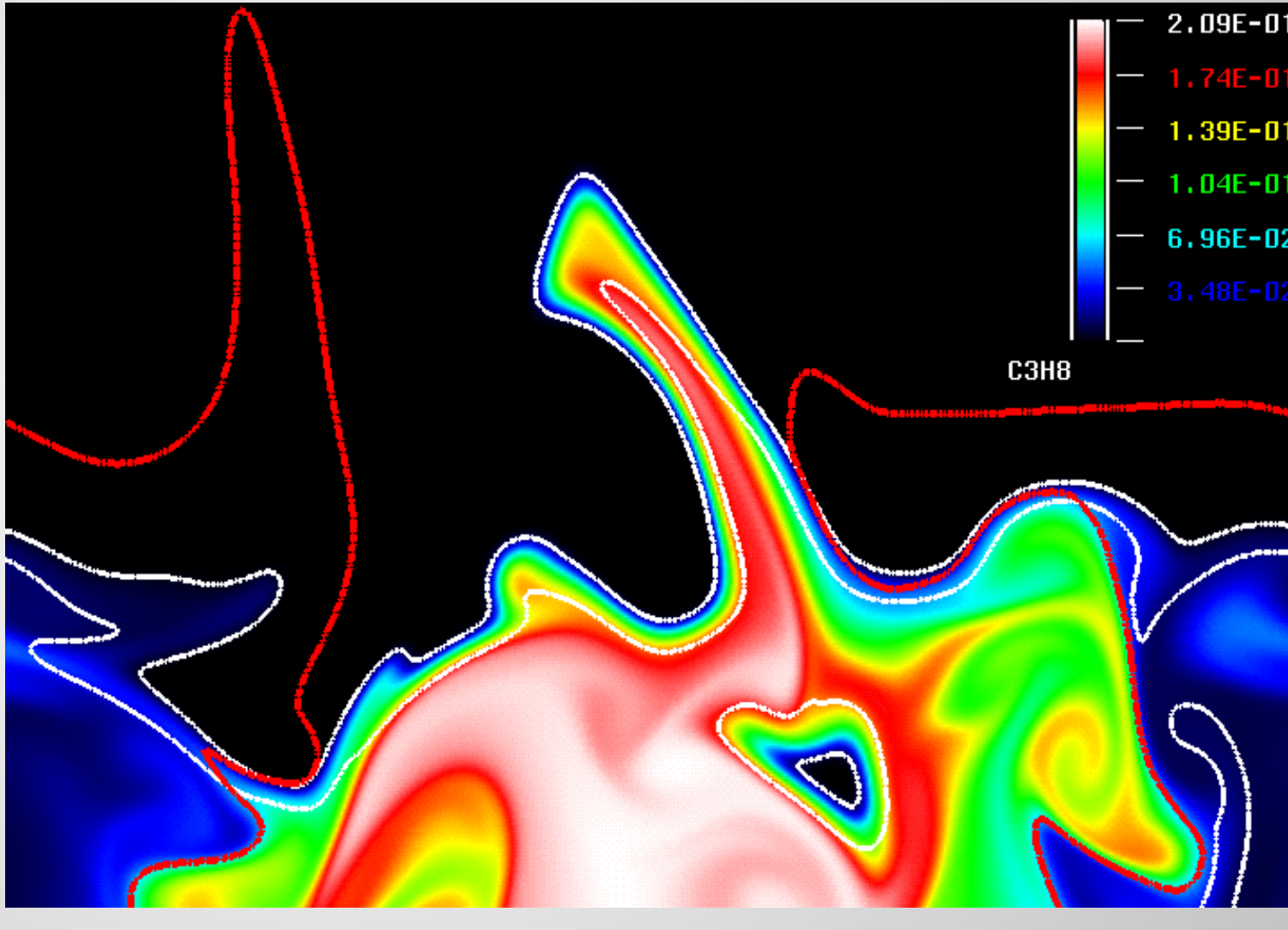


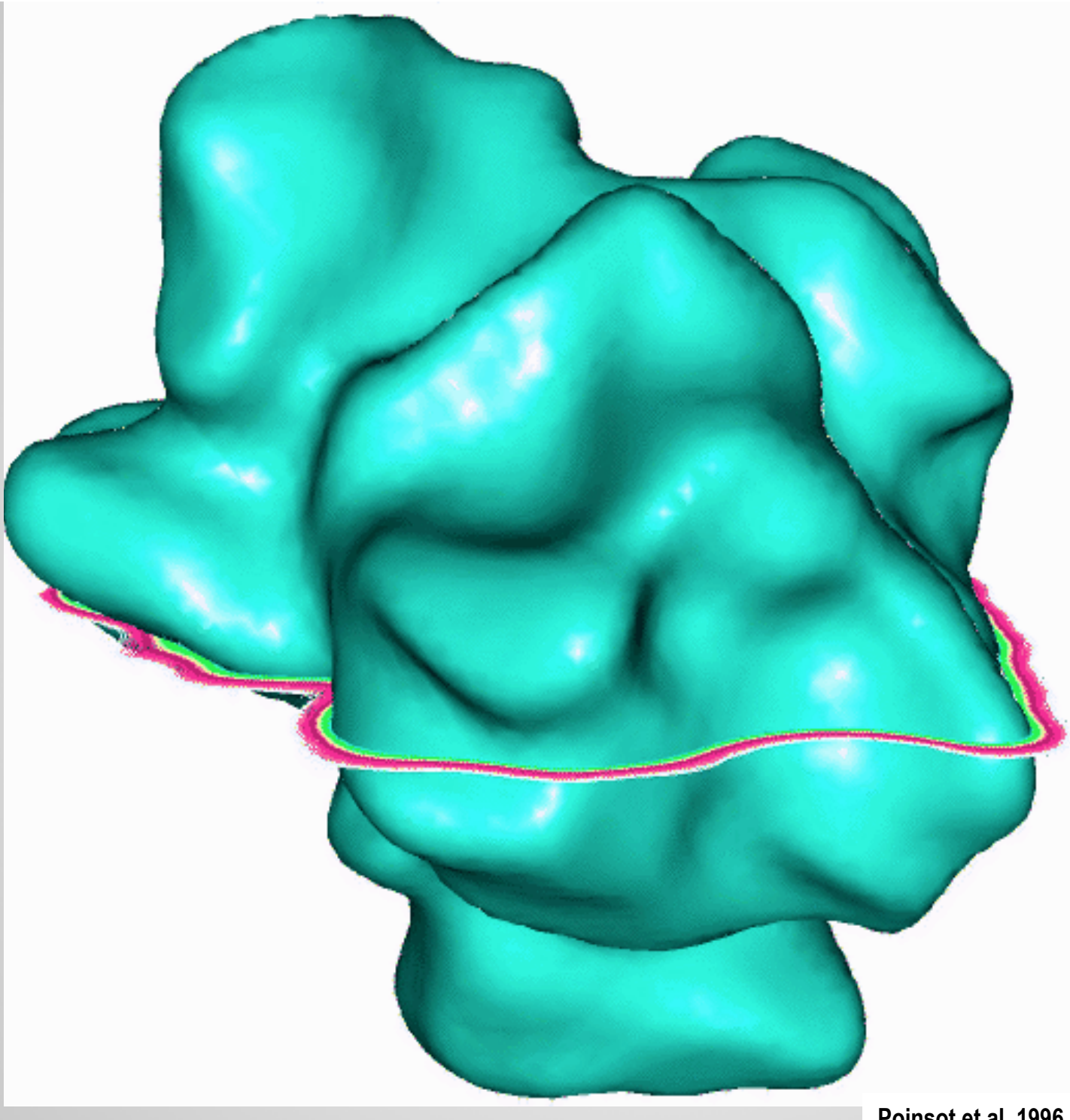




DNS usually performed in unconfined cases and cubic boxes

C3H8/air flame DNS
Full chemical scheme
Jimenez et al, Comb and Flame 2002.





Poinsot et al, 1996. 26th Symp. (Int.) on Comb. Naples. Plenary session on DNS for reacting flows

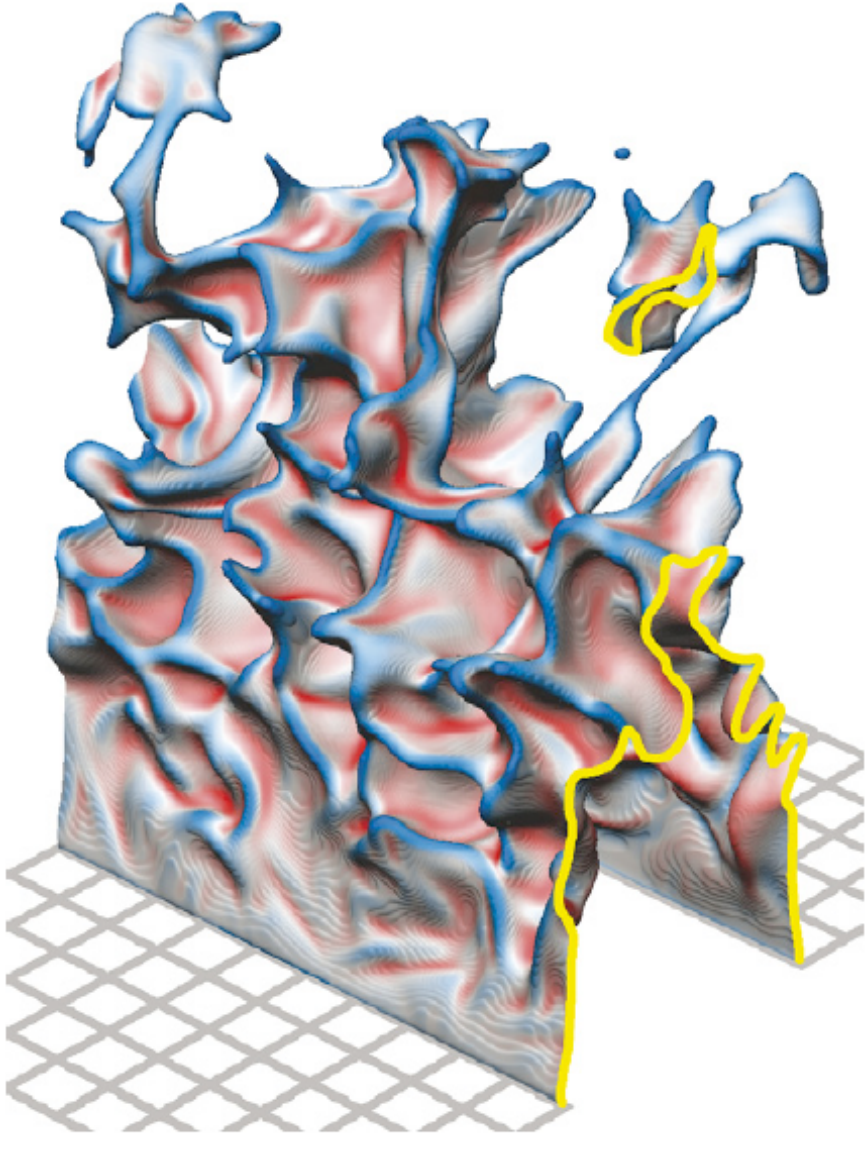
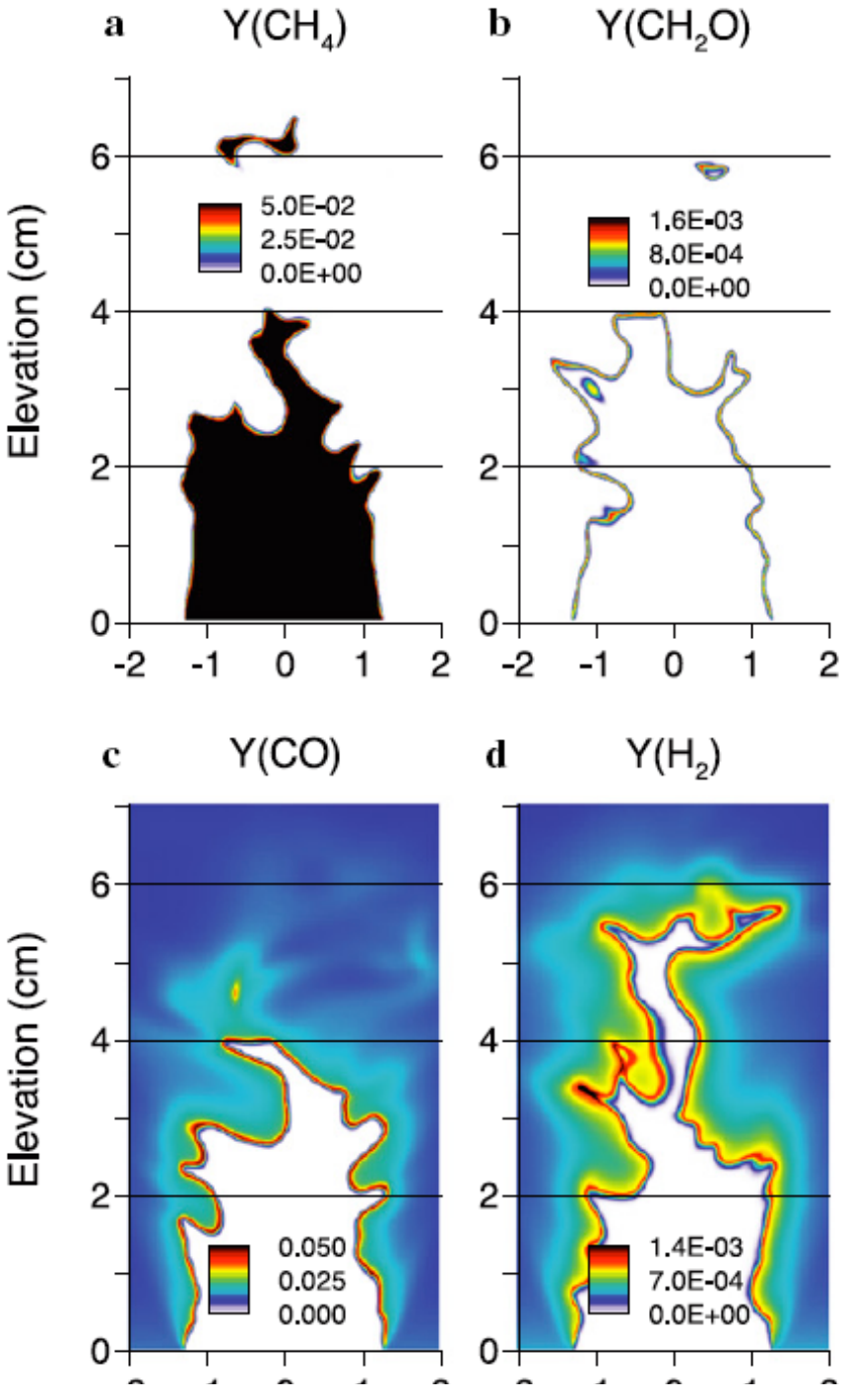
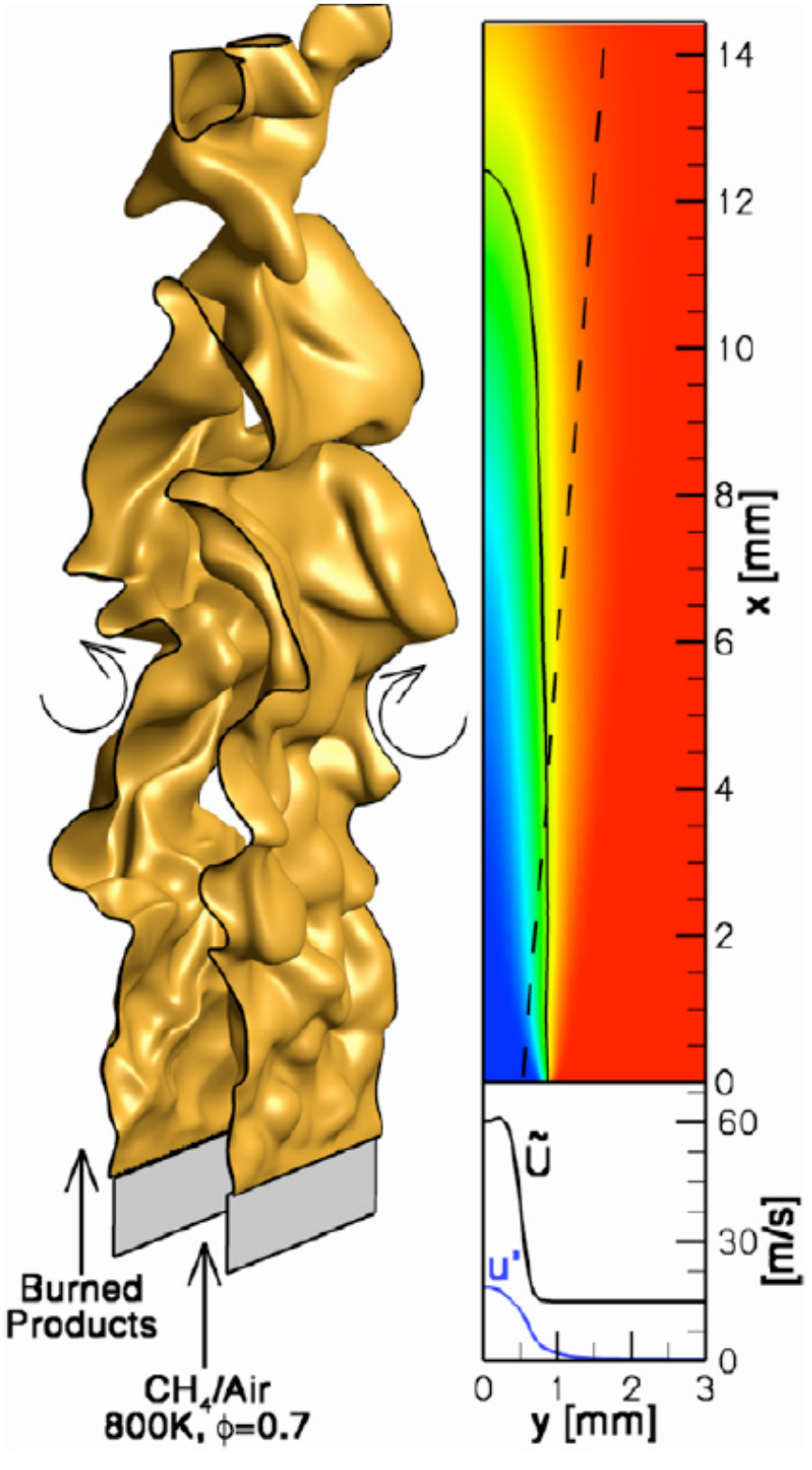


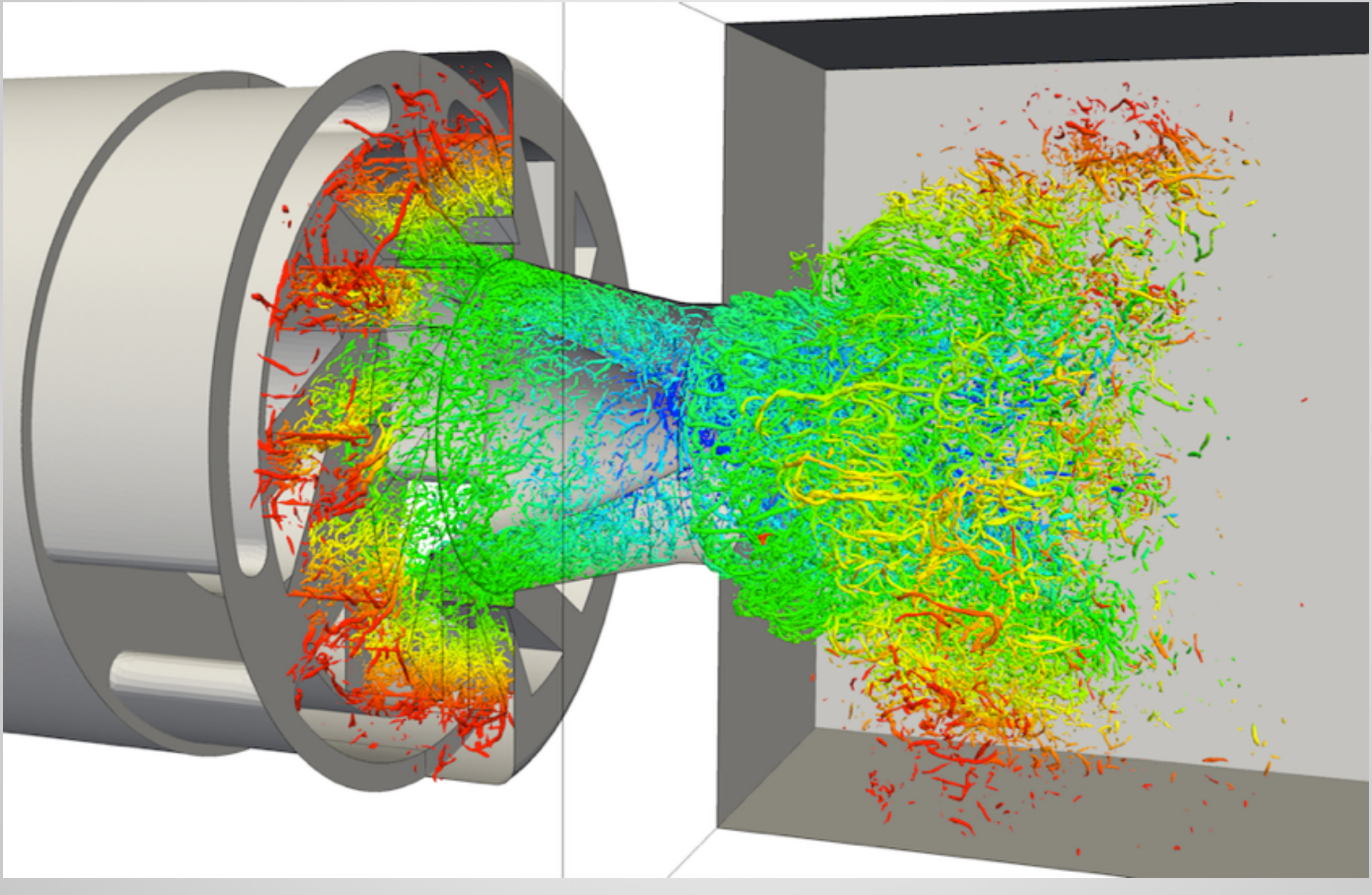
Fig. 1. Simulated instantaneous flame surface represented by the isotherm at 1684 K that coincides with peak heat release in a simulation of the flat, laminar flame. The flame surface is colored by the mean curvature where blue is negative and red is positive. Tiles marking the coflow are 0.5 cm squares.





Chen et al
31st Symp.

LES in confined domains...



Moureau et al Comb. Flame 2011

So… what are we going to discuss here ?

- ★ TURBULENT COMBUSTION (INCLUDING FLAME INSTABILITIES)
- ★ NUMERICAL COMBUSTION (INCLUDING CODES DESCRIPTIONS AND MODELS)
- ★ THIS WILL REQUIRE THEORETICAL BASIS ON COMBUSTION AND LAMINAR FLAMES WHICH WE WILL DISCUSS FIRST

WE WILL ALSO DISCUSS ‘COMPLEXITIES’ IN COMBUSTION:

- ★ The classical topics studied in combustion courses do not correspond to the everyday life of engineers studying real combustors
- ★ Other phenomena have to be taken into account: complexity (of geometries and of multiphysics) is the first one
- ★ A short overview of what is done in practice in codes:

WHAT DO WE CALL COMPLEXITY ?:

Complex chemistry
Simple geometry
Simple flows
Flows only

Complex chemistry
Complex geometry
Complex flows
Multiphysics

FROM





TO



LET US PRESENT NUMERICAL TOOLS BY GROWING COMPLEXITY

ZERO DIMENSIONAL FLAMES (PSR): ALL VARIABLES VARY ONLY WITH t

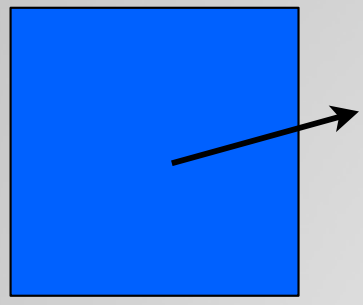
FUEL + AIR

$$\rho \mathbf{C_P} \frac{\mathbf{dT}}{\mathbf{dt}} = \dot{\omega}_{\mathbf{T}}$$

$$\frac{d(\rho Y_k)}{dt} = \dot{\omega}_k$$

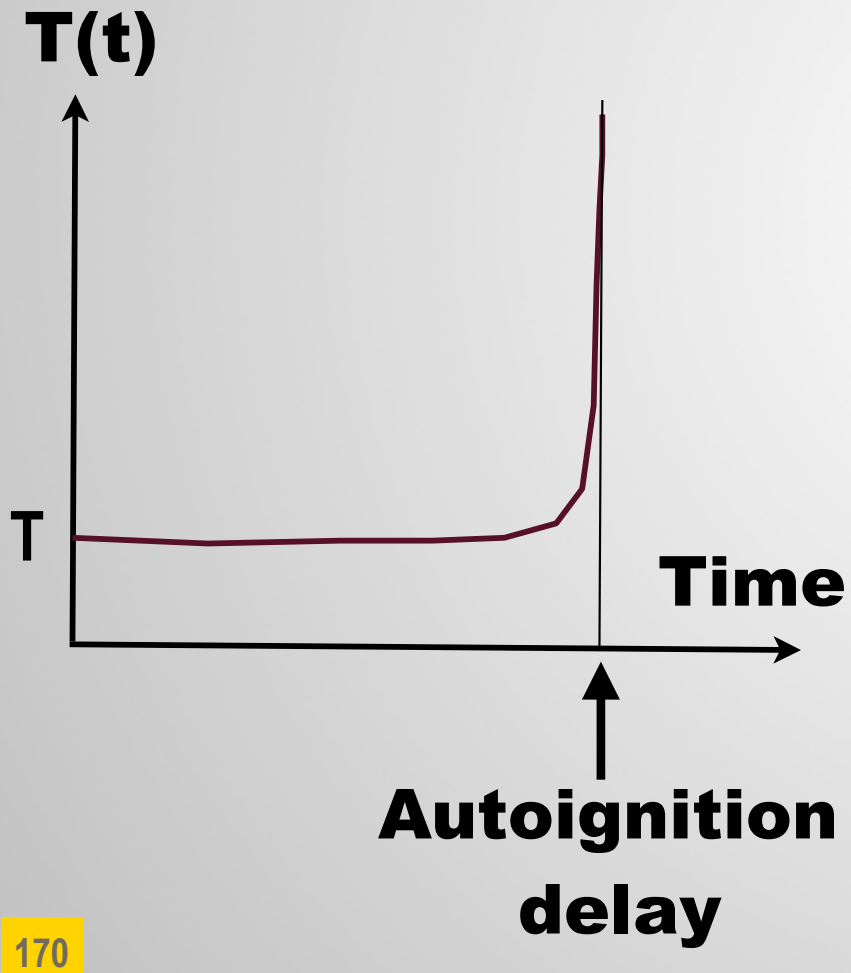
Kinetics

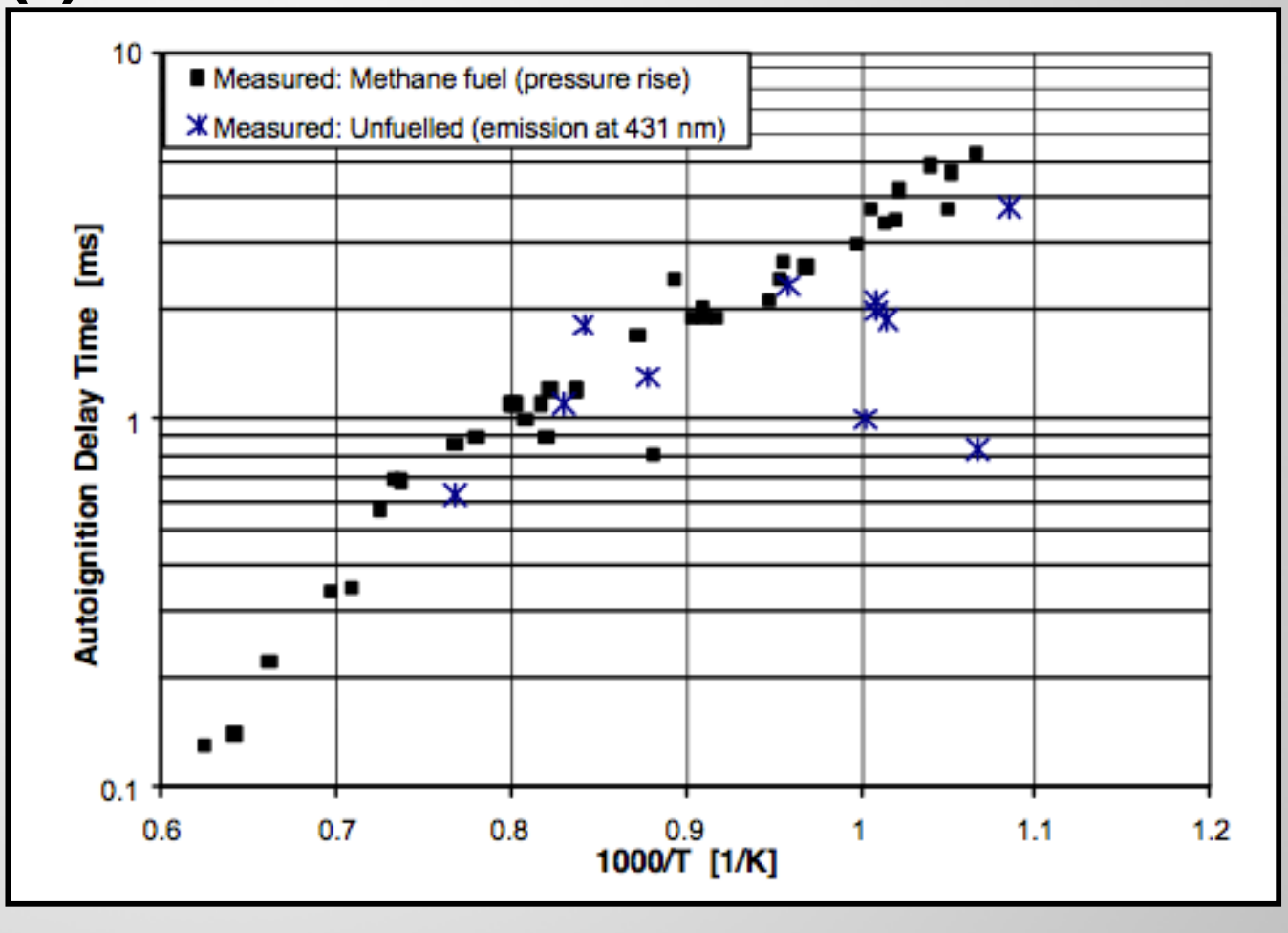
Thermo chemistry



Well mixed box with fresh premixed gas at initial temperature T (preferred set up of kinetics experts)

Solve for T(t)

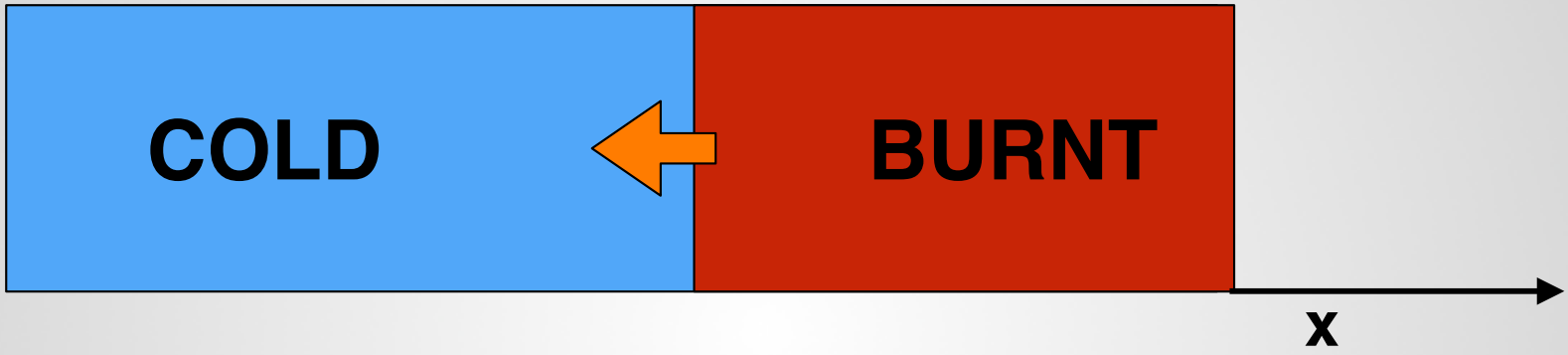




Important point for kinetics

- The autoignition problem is usually the place where kinetics experts… stop !
- They compute autoignition times for very complex schemes (O(10000) reactions)
- But they never compute a FLAME ! (by flame: we mean a flame front which has an internal structure and depends on time AND space): to compute a flame, you need:
  - Chemical kinetics
  - Molecular transport models for diffusion, viscosity
  - Flow description

STEADY 1D LAMINAR FLAMES: ALL VARIABLES DEPEND ON x ONLY



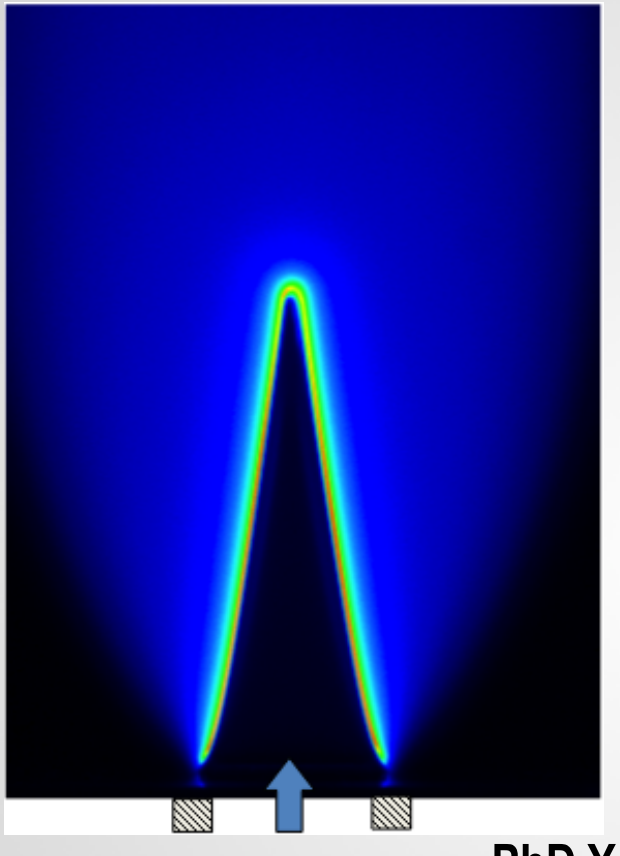
Kinetics

Transport

Thermo chemistry

(CANTERA/CHEMKIN/COSILAB)

MULTI-DIMENSIONAL LAMINAR FLAMES: ALL VARIABLES DEPEND ON x,y,z



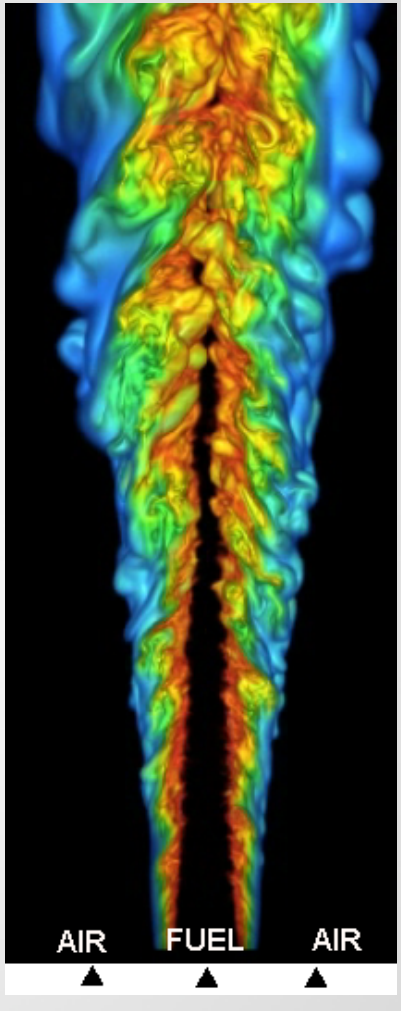
PhD Y. Dhue IMFT

Kinetics | Transport | Thermo chemistry | Fluid mechanics

TURBULENT UNCONFINED FLAMES: VARIABLES DEPEND ON x,y,z,t

Turbulence

Kinetics | Transport | Thermo chemistry | Fluid mechanics



Sandia



EM2C Paris

TURBULENT UNCONFINED FLAMES

‘Industry type’



Turbulence
High Re

Radiation

Kinetics

Transport

Thermo
chemistry

Fluid
mechanics

AFTER THIS POINT: FORGET SIMPLE GEOMETRIES

- ★ As soon as complicated shapes must be computed, the whole code has to be rewritten
- ★ The implications of this statement on modeling are very strong: the problem becomes now a coupled problem of modeling + numerical accuracy
- ★ Numerical accuracy and especially our capacity to mesh precisely the geometry become the first-order difficulty

TURBULENT CONFINED FLAMES

Acoustics

Turbulence

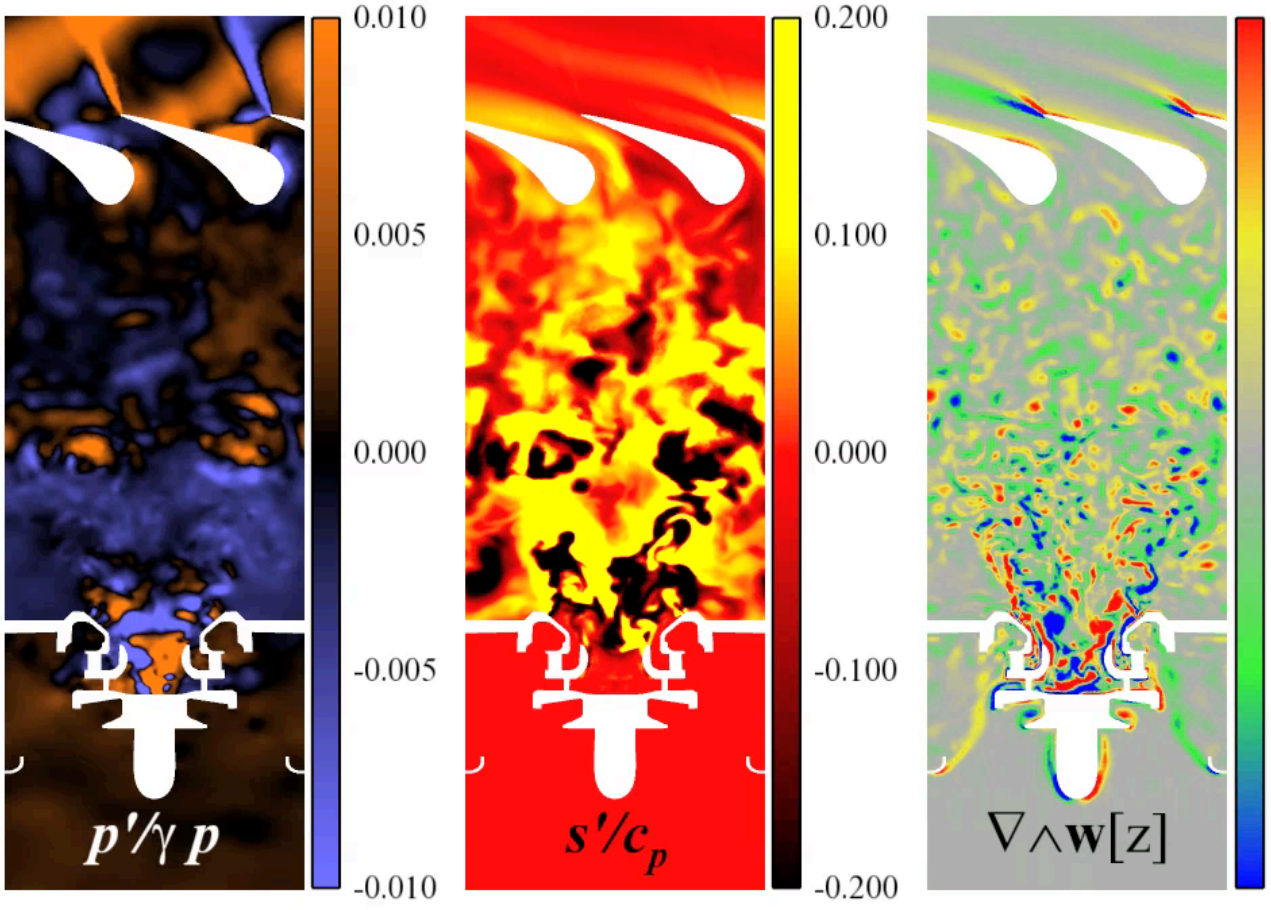
Radiation

Kinetics

Transport

Thermo chemistry

Fluid mechanics



PhD M. Leyko CERFACS

TURBULENT CONFINED FLAMES AND IMPACT ON WALLS

Acoustics

Heat transfer

Turbulence

Radiation

Kinetics

Transport

Thermo chemistry

Fluid mechanics



TURBULENT CONFINED FLAMES AND IMPACT ON WALLS... WHEN WALLS MOVE !

Fluid/structure interaction

Acoustics

Heat transfer

Turbulence

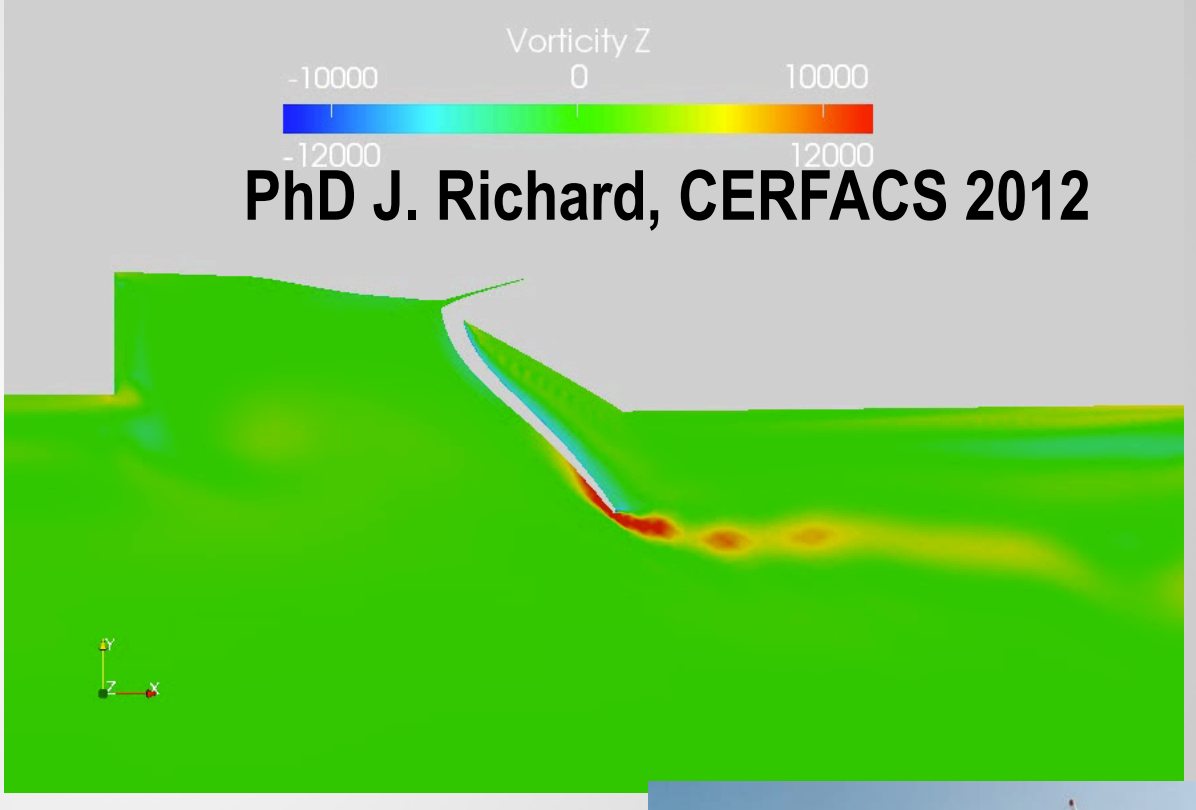
Radiation

Kinetics

Transport

Thermo chemistry

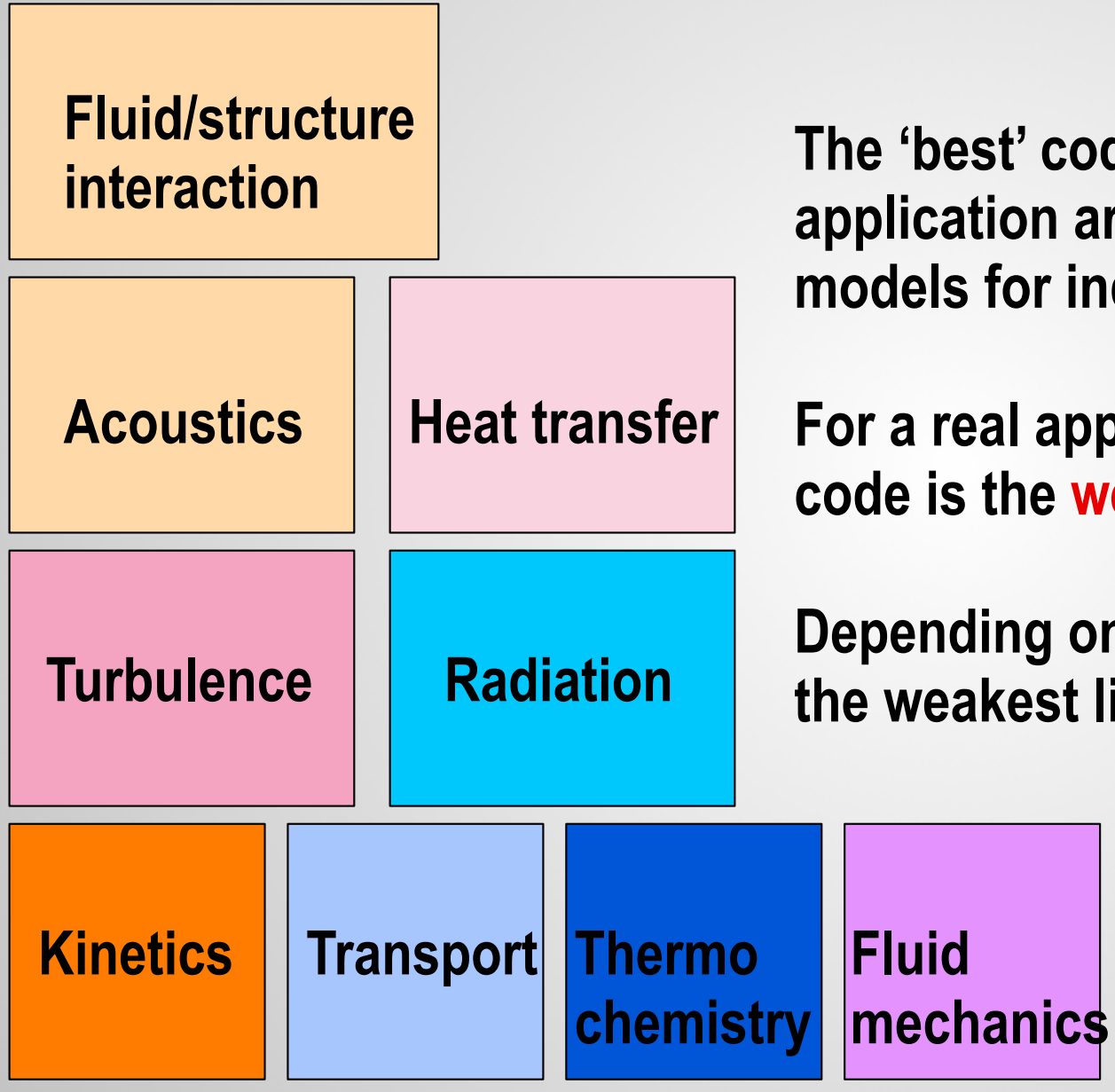
Fluid mechanics



PhD J. Richard, CERFACS 2012



IMPLICATIONS FOR CODES AND MODELS:



The 'best' codes and models for a real application are not always the best codes and models for individual problems.

For a real application, the limiting part of the code is the weakest element of all of them.

Depending on your background, you will see the weakest link at different places...

IF WE INCLUDE NUMERICAL METHODS:

Fluid/structure interaction

Acoustics

Heat transfer

Turbulence

Radiation

Kinetics

Transport

Thermo chemistry

Fluid mechanics

Mesh type (structured/ unstructured)

Spatial order (high-order?)

Time integration (implicit/explicit)

Finite volume/ elements/ differences Others?

Boundary conditions

High Performance Computing capacities (massively //)

Maintenance, adaptability

Coupling (multiphysics)

AND ALSO THEMES WHICH MIX COMBUSTION AND MATHS:

Fluid/structure interaction

Mesh type (structured/ unstructured)

Spatial order (high-order?)

Time integration (implicit/explicit)

Acoustics

Heat transfer

Finite volume/ elements/ differences Others?

Boundary conditions

Turbulence

Radiation

Optimization Quantification of uncertainties Data assimilation

High Performance Computing capacities (massively //)

Kinetics

Transport

Thermo chemistry

Fluid mechanics

Maintenance, adaptability

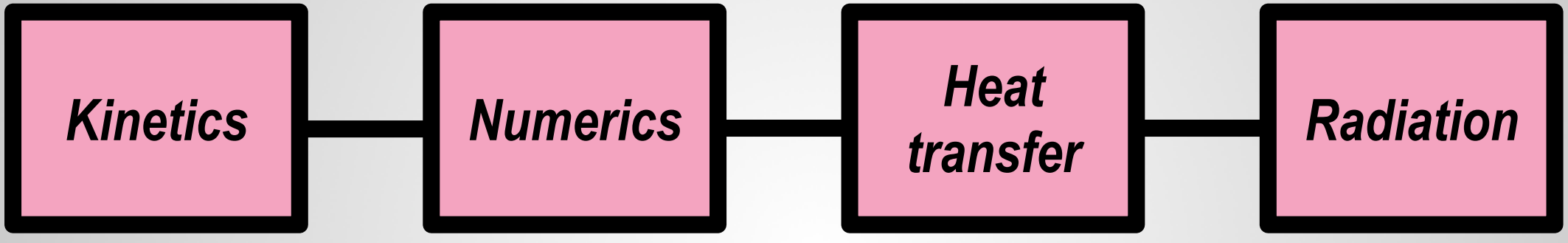
Coupling (multiphysics)

« DONT BE A PERFECTIONIST…"

P. O'Rourke - KIVA Manual (the 1st serious combustion CFD code)

DONT FOCUS ON PHENOMENA JUST BECAUSE YOU KNOW THEM.... FOCUS ON THE WEAKEST LINK

Weakest link:



Excellent * Excellent * Bad * Excellent

= Bad…

To relax for 3 minutes:

« What is a flame ? »

A movie for children but full of useful information

An example of combustion seen by a CERFACS former PhD, now working at SPACE X: G. Lacaze



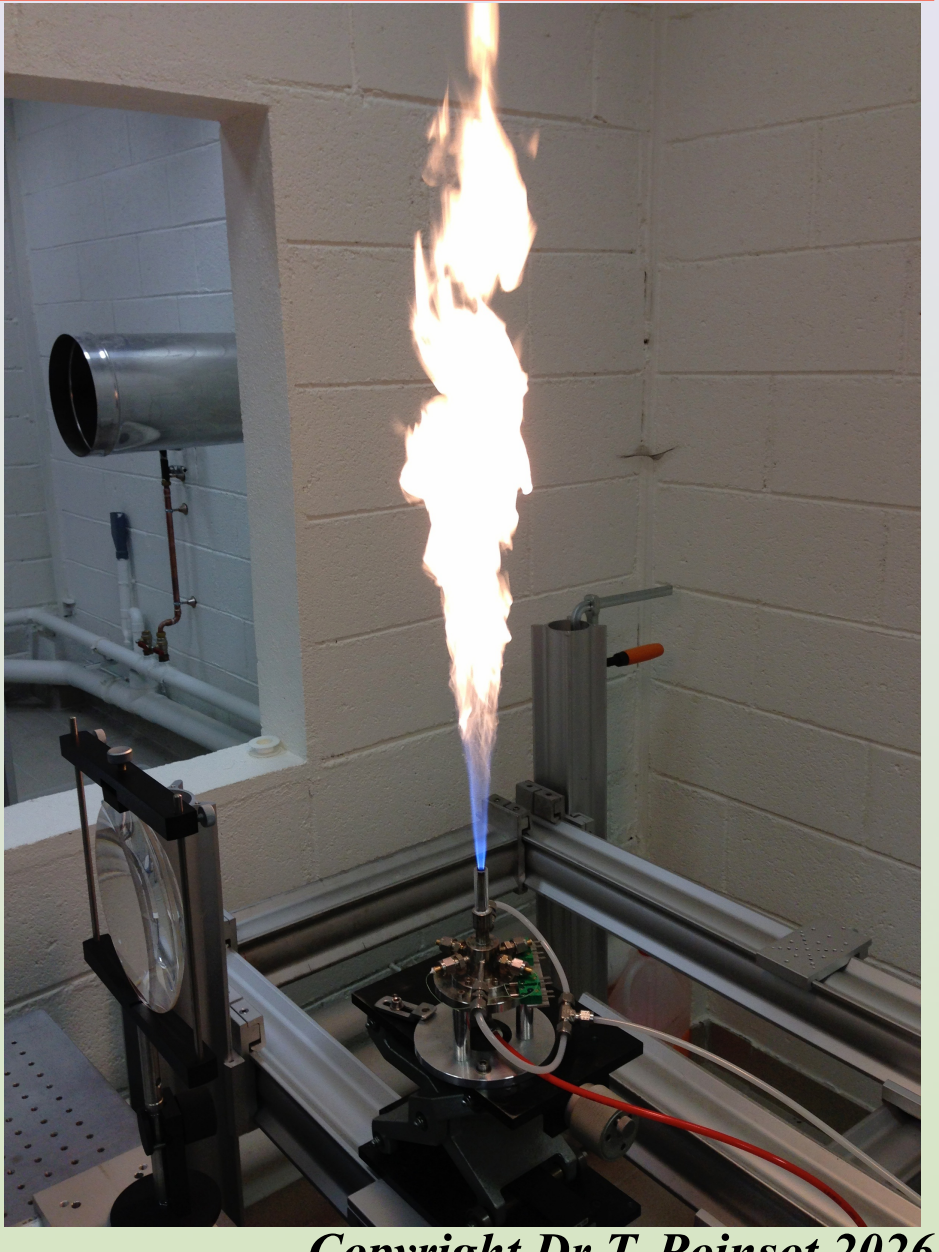
Combustion basics

T. Poinsot

The things you should know to understand the following courses

Mainly elements of laminar flame theory for premixed and diffusion flames

Most equations expressed so that you can code them directly …



Copyright Dr T. Poinsot 2026

OUTLINE

CONSERVATION EQUATIONS FOR REACTING FLOWS — Ch. 1

PREMIXED FLAMES — Ch. 2

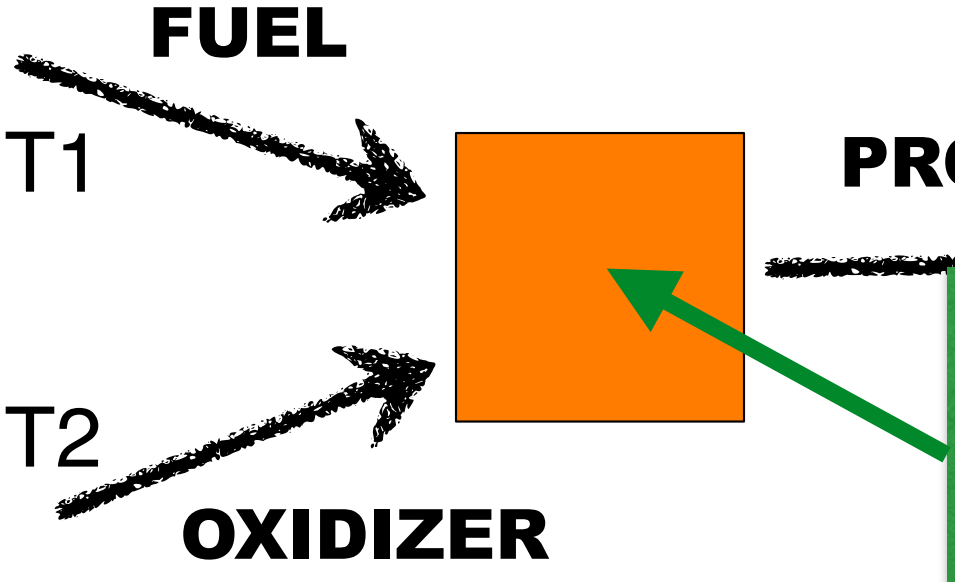
DIFFUSION FLAMES — Ch. 3

OTHER FLAMES: PARTIALLY PREMIXED, TRIPLE FLAMES — Ch. 6

Why talk about laminar flames since we are interested in turbulent combustion ?

Because:

REASON 1: certain things do not change when the flame becomes turbulent: thermochemistry, for example. The temperature of burnt gases (T_{ad}) is the same for laminar and turbulent flames (if combustion really took place and was complete)

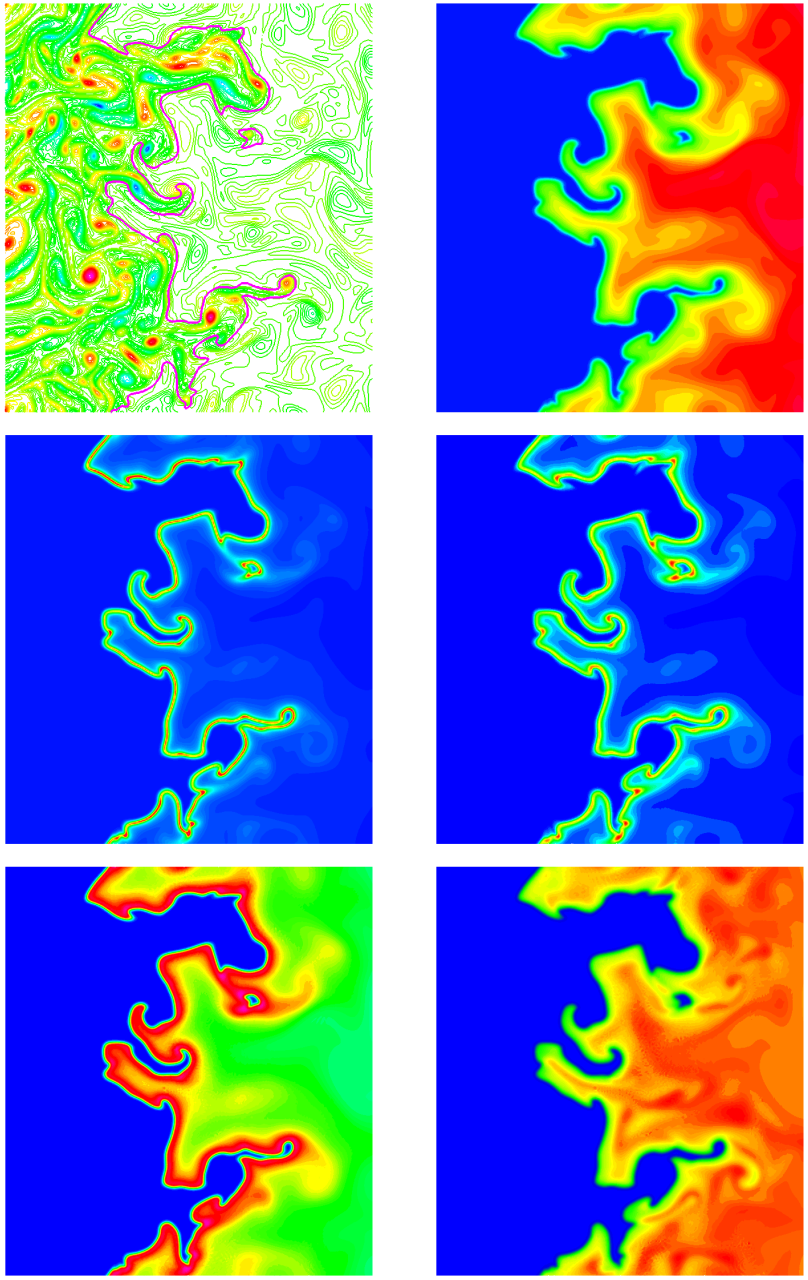


ANYTHING CAN TAKE PLACE HERE, LAMINAR OR TURBULENT. IF ALL THE FUEL BURNS THEN T_{ad} IS THE SAME

REASON 2: models !

- flamelet models: we hope that a turbulent flame is close to a collection of small laminar flames called ‘flamelets’

- knowing how a laminar flame reacts to strain or curvature will help us for turbulent combustion models



DNS of H2/air flames M. Baum PhD thesis CERFACS

Why this might be misleading ?

We do see multiple examples where turbulent flames are very different from laminar flames.

Deciding how species are transported in turbulent flames is one example: the issue of species Lewis number

$$Le_k = \frac{\lambda}{\rho C_p D_k} = \frac{D_{th}}{D_k}$$

Heat diffusivity

Species k diffusivity

Molecular transport vs turbulent transport

In laminar flames, species are transported by molecular processes (collisions between molecules): small species (H2) diffuse faster than big ones (CO2, CxHy).

In turbulent flows, species are transported by eddies which carry all species at the same speed.

So that a good question is: in turbulent flames, which model should we use for diffusion ?

- ➡ **a molecular one with different diffusion speeds or**
- ➡ **a turbulent one with equal speeds, controlled by the turbulent velocity ?**

OUTLINE

CONSERVATION EQUATIONS FOR REACTING FLOWS

Ch. 1

PREMIXED FLAMES

DIFFUSION FLAMES

OTHER FLAMES: PARTIALLY PREMIXED, TRIPLE FLAMES

CLASSICAL AERODYNAMICS WITH « AIR » AS THE ONLY FLUID:

- AIR IS ONE MOLE OF O2 FOR 3.76 MOLES OF N2:

- THE AVERAGE MOLECULAR WEIGHT OF AIR IS:

$$W = \frac{W_{O_2} + W_{N_2} * 3,76}{4,76} = 0,029 kg/mole$$

- O2 like N2 ARE DIATOMIC GAS. KINETIC THEORY SAYS THAT IN THE PERFECT GAS LIMIT, THEIR MOLAR HEAT CAPACITIES ARE:

$$C_v^m = \frac{5}{2}R \qquad C_p^m = \frac{7}{2}R \qquad R = 8.32 uSI$$

- **SO THAT:** $C_p^m = 3.5 * 8.32 = 29,1 J/Kmol$
- **AND THE RATIO OF HEAT CAPACITIES IS:** $\gamma = \frac{7}{5} = 1.4$

- **MOST 3D CFD CODES WORK WITH MASS HEAT CAPACITIES:**

$$C_p = \frac{C_p^m}{W} \qquad C_p = \frac{29,1}{0,029} = 1004 J/Kkg$$

- **SO MUCH FOR AIR. ITS COMPOSITION DOES NOT CHANGE.** C_p **CHANGES ONLY WITH T.**
- **THIS IS NOT TRUE ANY MORE IN A FLAME WHERE COMPOSITION CHANGES !**

For flames: need to know the composition of the gases in the flow. Two ways to measure this composition: molar or mass quantities. For each species $k = 1$ to N:

Molar fractions $X_k = \dfrac{N_k}{N}$ — N_k: *NBR OF MOLES k*; N: *TOTAL NBR OF MOLES*

Mass fractions $Y_k = \dfrac{\rho_k}{\rho}$ — ρ_k: *MASS OF k*; ρ: *TOTAL MASS*

From molar to mass fractions:

Mass of species k (N_k moles of mass W_k)

$$Y_k = \frac{N_k W_k}{NW} = \frac{W_k}{W} X_k$$

Total mass

We are discussing gaseous combustion in a mixture of perfect gases containing N species indexed by k=1 to N:

$$p = \sum_{k=1}^{N} p_k \quad \text{where} \quad p_k = \rho_k \frac{R}{W_k} T$$

$$\rho = \sum_{k=1}^{N} \rho_k \qquad p = \rho \frac{R}{W} T$$

How do we obtain the mean molecular weight W ?

Ch. 1

If you have X_k:

$$W = \sum_{k=1}^{N} W_k X_k$$

If you have Y_k:

$$\Sigma X_k = 1$$

$$X_k = (Y_k / W_k) W$$

$$\Sigma X_k = 1 = \Sigma (Y_k / W_k) W$$

or:

$$\frac{1}{W} = \Sigma_{k=1}^{N} \left(\frac{Y_k}{W_k} \right)$$

Are there cases where the perfect gas assumption fails ? :

yes, at high pressures (more than 60 bars). Rocket engines or Diesel engines require to replace:

$$p = \rho \frac{R}{W} T$$

by a more complex equation of state.

Each species k has a molecular weight W_k, a mass fraction Y_k, a mole fraction X_k. The mixture of the N species has a mean molecular weight W.

Quantity	Definition	Useful relations
Mass fraction Y_k	Mass of species k / Total Mass	Y_k
Mole fraction X_k	Moles of species k / Total moles	$X_k = \frac{W}{W_k} Y_k$
Molar concentration $[X_k]$	Moles of species k / Unit volume	$[X_k] = \rho \frac{Y_k}{W_k} = \rho \frac{X_k}{W}$

Of course, since the composition changes with space and time, W changes also with space and time. And it can change a lot.

$W_{H_2} = 0.002$ $W_{H_2O} = 0.018$



$W_{O_2} = 0.032$

IN A H_2/O_2 FLAME,THE MEAN MOLECULAR WEIGHT CHANGES BY A FACTOR OF 16

STOECHIOMETRY AND EQUIVALENCE RATIO:

$$\nu'_F F + \nu'_O O \rightarrow Products$$

$$\left(\frac{Y_O}{Y_F}\right)_{st} = \frac{\nu'_O W_O}{\nu'_F W_F} = s$$

Stoechiometric ratio

$$\phi = s\frac{Y_F}{Y_O} = \left(\frac{Y_F}{Y_O}\right) / \left(\frac{Y_F}{Y_O}\right)_{st}$$

Equivalence ratio

HOME WORK FOR BEGINNERS

- **WHAT ARE THE MASS FRACTIONS IN A FUEL/AIR MIXTURE BEFORE COMBUSTION, WHERE THE EQUIVALENCE RATIO ϕ IS IMPOSED:**

$$\phi = s\frac{Y_F}{Y_O} = \left(\frac{Y_F}{Y_O}\right) / \left(\frac{Y_F}{Y_O}\right)_{st}$$

- **AIR IS ONE MOLE OF O2 FOR 3.76 MOLES OF N2:**

$$Y_{N_2} = 3.76\frac{W_{N_2}}{W_{O_2}}Y_{O_2}$$

- **WE NEED TO FIND Y_{O_2}, Y_{N_2}, Y_F. Their sum is one:**

$$Y_{O_2} + Y_{N_2} + Y_F = 1$$

FUEL / AIR COMBUSTION COMPOSITION AT EQUIVALENCE RATIO ϕ

$$Y_F = \frac{1}{1 + (1 + 3.76 W_{N_2}/W_{O_2})\, s/\phi}$$

At stoechiometry: $(\phi = 1)$

Global reaction	s	Y_F^{st}
$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2$	4.00	0.055
$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2$	3.63	0.060
$2C_8H_{18} + 25(O_2 + 3.76N_2) \rightarrow 16CO_2 + 18H_2O + 94N_2$	3.51	0.062
$2H_2 + (O_2 + 3.76N_2) \rightarrow 2H_2O + 3.76N_2$	8.00	0.028

Air/fuel mixtures used in flames contain typically 95 % of... air !
This is useful for theory: a combustible premixed air/fuel gas will have the same properties (density, viscosity, conductivity) as pure air.

LET US START DISCUSSING CFD:

- What do we have to solve for in a combustion code ?
- How complicated is this compared to classical aerodynamics (like computing the flow around a foil) ?

CFD:

- In a non-reacting compressible flow (aerodynamics around an aircraft), we have 5 variables:
  - 3 velocities
  - pressure or temperature or enthalpy or entropy
  - density
- In a reacting compressible flow, we have 5 + (N-1) variables to determine:
  - 3 velocities
  - pressure or temperature or enthalpy or entropy
  - density
  - N species -> actually N-1 since their sum is unity
- So in combustion, we need 5 + (N-1) equations:
  - Momentum (3)
  - Energy, or enthalpy or entropy or temperature
  - Continuity for each species (or for N-1 species + total mass)

Momentum equations (3)

Ch. 1 Sec 1.1.2

Viscous stress ↓ **Total stress** ↓

$$\frac{\partial}{\partial t}\rho u_j + \frac{\partial}{\partial x_i}\rho u_i u_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} = \frac{\partial \sigma_{ij}}{\partial x_i}$$

Total stress ⟶ $\sigma_{ij} = -p\delta_{ij} + \tau_{ij}$ ⟵ **Viscous stress**

↑ **Pressure stress**

$\delta_{ij} = 0$ **if** $i \neq j$

$\delta_{ij} = 1$ **if** $i = j$

$$\frac{\partial}{\partial t}\rho u_j + \frac{\partial}{\partial x_i}\rho u_i u_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i}$$

Same form as in non-reacting flows.

Except that:

- **density here has very strong gradients**
- **the dynamic viscosity μ changes rapidly with T**

$$\tau_{ij} = -\frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

CHANGES LIKE T

TOTAL MASS:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

Combustion does not create or destroy TOTAL mass

Diffusion velocities: careful...

(Williams 1985 or Ern and Giovangigli 1994)

- The V_k's are obtained by solving this system:

$$\nabla X_p = \sum_{k=1}^{N} \frac{X_p X_k}{\mathcal{D}_{pk}} (V_k - V_p) + (Y_p - X_p)\frac{\nabla P}{P} + \frac{\rho}{p}\sum_{k=1}^{N} Y_p Y_k (f_p - f_k) \quad \text{for} \quad p = 1, N$$

- In these N equations, the diffusion velocities V_ks are the unknown -> it is « the diffusion matrix » which must be inverted at each point at each instant...
- But almost no one does it. We use simplified forms:

$$\mathbf{V}_k = -D_k \frac{\nabla Y_k}{Y_k}$$

- FICK's law

$$\mathbf{V}_k = -D_k \frac{\nabla X_k}{X_k}$$

- HIRSCHFELDER's law

What are the D_ks ?

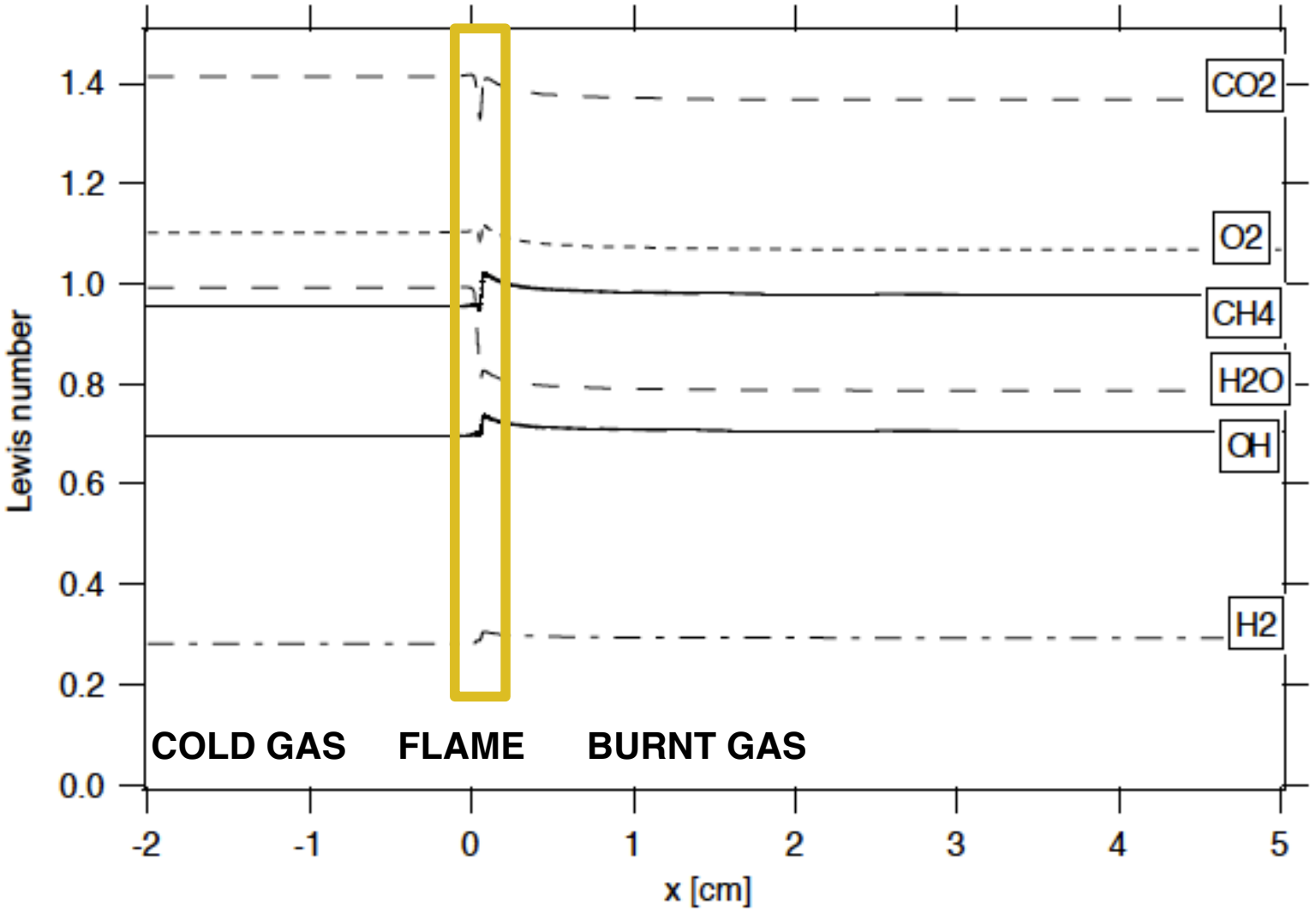
- D_k is the diffusion coefficient of species k in the MIXTURE
- D_k is not the binary diffusion coefficient D_{jk} of kinetic gas theory but the D_k's are obtained from the D_{jk}'s by:

$$D_k = \frac{1 - Y_k}{\Sigma_{j \neq k} X_j / \mathcal{D}_{jk}}$$

- All D_k's are different in general...
- D_k's vary significantly BUT their ratios to thermal diffusivity D_{th} vary much less. The D_k's can be obtained from the heat diffusivity D_{th} and the Lewis number of each species:

$$Le_k = \frac{\lambda}{\rho C_p D_k} = \frac{D_{th}}{D_k}$$

Lewis numbers are not intrinsic parameters of a species. They depend on the mixture:



Ch. 1 Sec 1.1.4

Lewis numbers of main species in a stoechiometric laminar CH4/air premixed flame (1 bar, 300 K)

The need for correction velocities if Lewis numbers are different:

$$Le_k = \frac{\lambda}{\rho C_p D_k} = \frac{D_{th}}{D_k}$$

The D_k's are not equal if Le_k differ

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}(\rho(u_i + V_{k,i})Y_k) = \dot{\omega}_k \qquad V_k = -D_k \frac{\nabla X_k}{X_k}$$

Summing the species equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho \sum_{k=1}^{N} D_k \frac{W_k}{W} \frac{\partial X_k}{\partial x_i}\right)$$

which is not zero if all Lewis numbers and molar weights are not equal (which is never the case).

A correction velocity V_c is required:

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}(\rho(u_i + V_{k,i})Y_k) = \dot{\omega}_k$$

Replace: $$V_k = -D_k \frac{\nabla X_k}{X_k}$$

By: $$V_k = -D_k \frac{\nabla X_k}{X_k} + V_c$$

Adding all species equations gives:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho \sum_{k=1}^{N} D_k \frac{W_k}{W} \frac{\partial X_k}{\partial x_i} - \rho V_i^c \right)$$

so that V_c can be chosen to ensure mass conservation:

$$V_i^c = \sum_{k=1}^{N} D_k \frac{W_k}{W} \frac{\partial X_k}{\partial x_i}$$

and the proper expression of the diffusion velocity is:

$$V_k = -D_k \frac{\nabla X_k}{X_k} + V_c = -D_k \frac{\nabla X_k}{X_k} + \frac{1}{W} \sum_{k=1}^{N} D_k W_k \nabla X_k$$

Conclusion: careful of codes using simplified expressions for diffusion velocities with non-equal Lewis numbers.

Last but not least: energy

Ch. 1, Sec. 1.1.5

- Each code uses a different form for energy, enthalpy or temperature
- All forms are equivalent (should be...)
- Beware of simplified forms taken from one code to another..
- Compressible vs incompressible is one source of confusion. ‘Total’ versus other forms of energy is another one
- Full summary in TNC Chapter 1, p 22

USUAL SOURCE OF PROBLEMS: MOLAR VS MASS

- ENERGIES/ENTHALPIES ARE DEFINED:

h_k^m	OR	h_k
PER MOLE		PER UNIT MASS

$$h_k = \frac{h_k^m}{W_k}$$

- CODES USE... BOTH:
  - MOST 0D AND 1D CODES WORK WITH MOLAR QUANTITIES.
  - MOST 3D CODES USE MASS QUANTITIES

DEFINITION OF ENERGIES/ENTHALPIES.

h is not $h = C_p T$ anymore like in air

- FOR SPECIES k:

$$h_k = \underbrace{\int_{T_0}^{T} C_{pk}\, dT}_{\text{sensible}} + \underbrace{\Delta h^o_{f,k}}_{\text{chemical}}$$

TABULATED

Ch. 1 Sec 1.1.5

- FOR THE MIXTURE:

$$h = \sum_{k=1}^{N} Y_k h_k$$

FORMATION ENTHALPIES $\Delta h^{o}_{f,k}$ and $\Delta h^{o,m}_{f,k}$:

Substance	Molecular weight W_k (kg/mole)	Mass formation enthalpy $\Delta h^{o}_{f,k}$ (kJ/kg)	Molar formation enthalpy $\Delta h^{o,m}_{f,k}$ (kJ/mole)
CH_4	0.016	−4675	−74.8
C_3H_8	0.044	−2360	−103.8
C_8H_{18}	0.114	−1829	−208.5
CO_2	0.044	−8943	−393.5
H_2O	0.018	−13435	−241.8
O_2	0.032	0	0
H_2	0.002	0	0
N_2	0.028	0	0

Formation enthalpies (gaseous substances) at $T_0 = 298.15\,K$.

Homework for tonight:

- Compute the energy release Qm by the complete combustion of one mole of CH4 with oxygen. Then deduce the energy release Q by the combustion of one kg of CH4 with oxygen.

- Answer: Qm= 802 kJ/mole and Q= 50100 kJ/kg

So much for formation enthalpies.

Let us go to heat capacities C_p^m

- For ‘cold’ air (O2 + 3,76 N2):

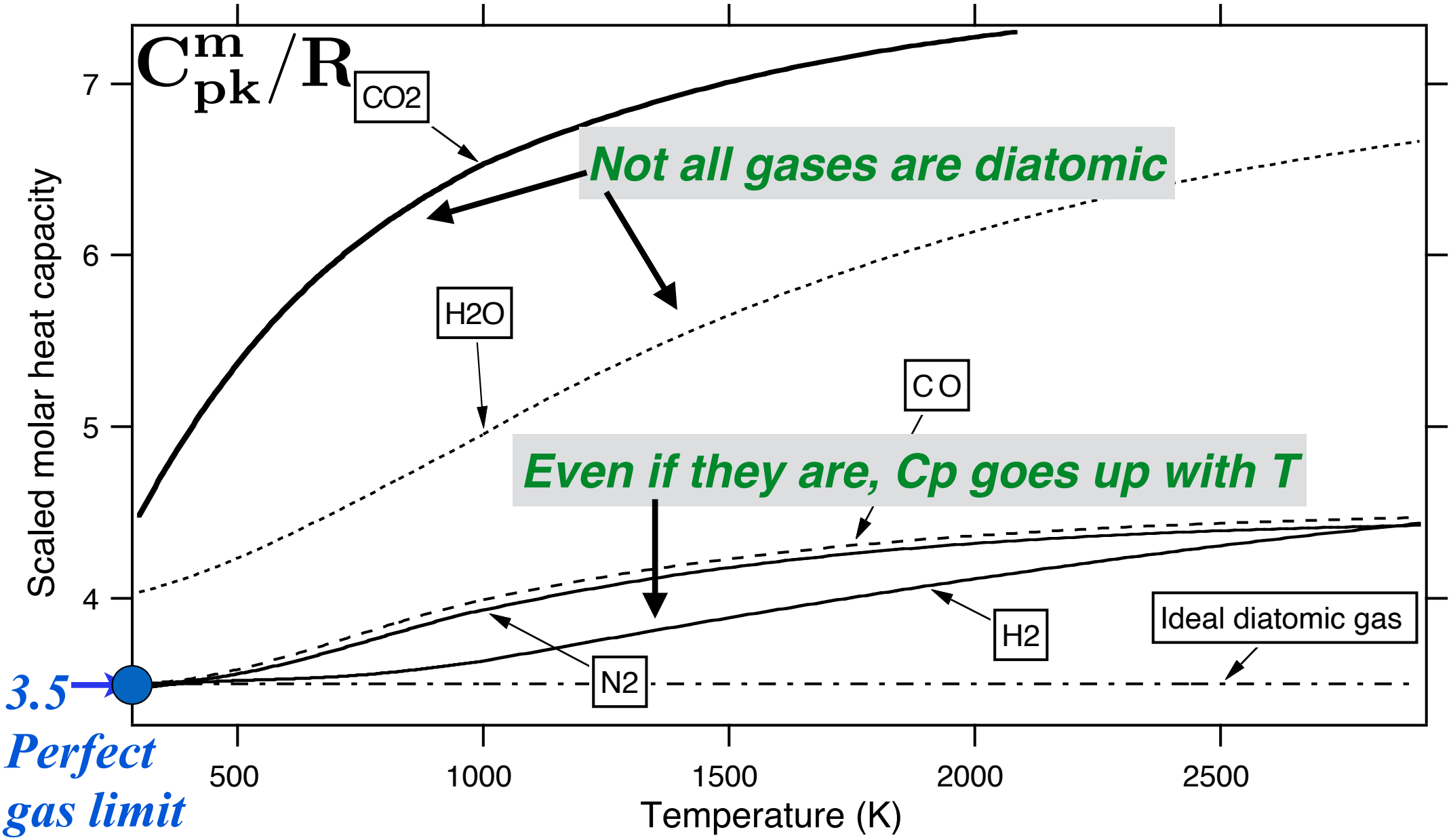
$$C_p^m = \frac{7}{2}R \qquad C_v^m = \frac{5}{2}R$$

$$\gamma = \frac{C_p}{C_v} = 7/5 = 1.4 \qquad R = 8.31\text{uSI}$$

- Most codes for aerodynamics use

$$C_p^m = \frac{7}{2}R = 29,1\text{uSI} \qquad C_p = \frac{7}{2}\frac{R}{W_{air}} = 1004\text{uSI}$$

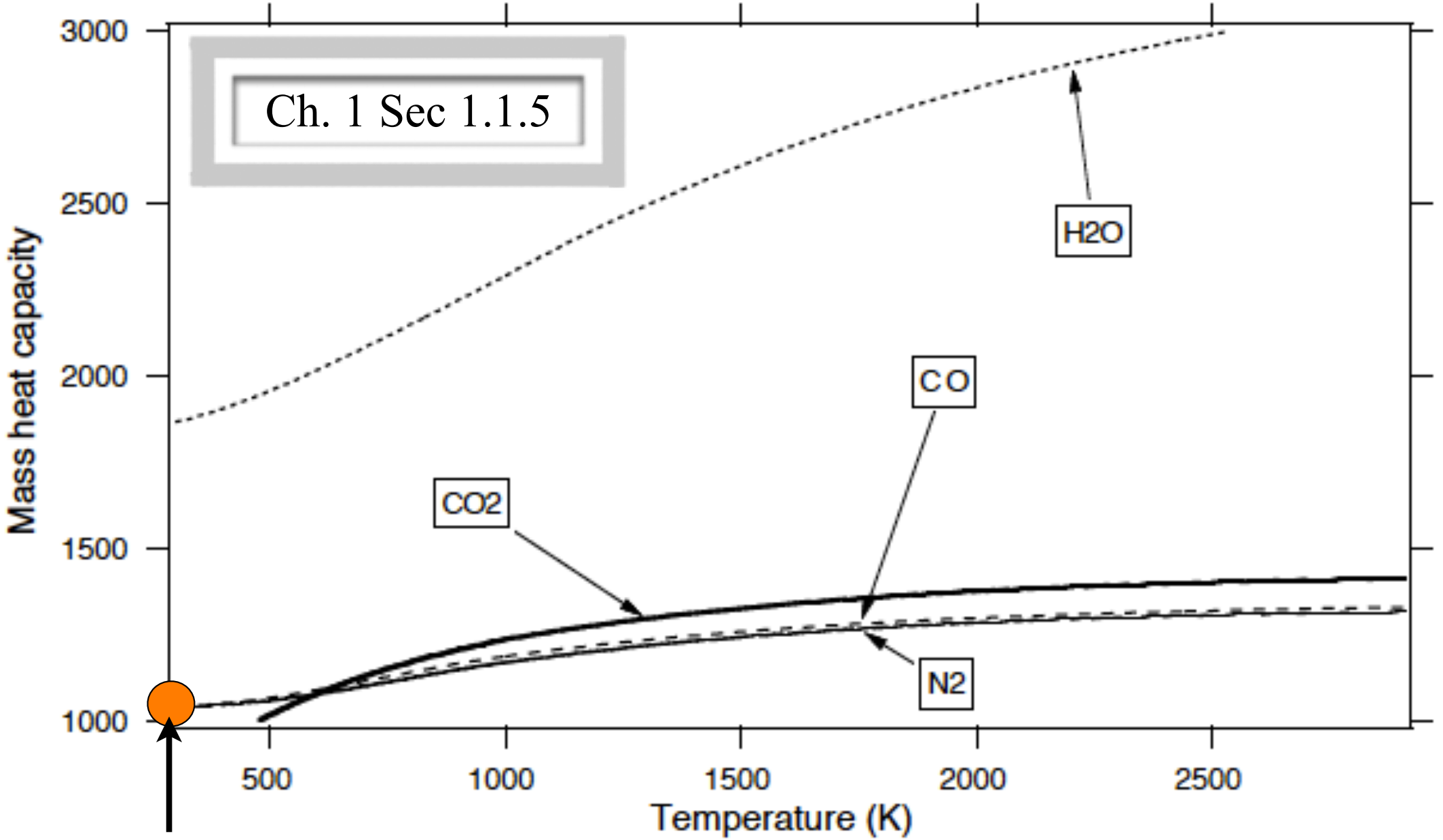
This is not sufficient in reacting flows:



Molar heat capacities change with (1) species and (2) temperature

Mass heat capacities:

$$C_{pk} = \frac{C_{pk}^{m}}{W_k}$$



The usual value for air at 300 K

ADIABATIC FLAME TEMPERATURES

DO WE REALLY NEED TO ACCOUNT FOR VARIABLE HEAT CAPACITIES C_{pk}?:

- In most codes we have to. CHEMKIN, CANTERA, COSILAB, most 3D codes use tables or polynomes to account for the changes of heat capacities C_{pk} with temperature

- For theory, we usually dont because it makes analytical resolutions almost impossible and does not change the major conclusions of analytical studies.

- **If we assume constant C_p^k :**
  - **Adiabatic flame temperatures are over- or underpredicted depending on which C_p^k value we take: 300 K errors are usual**
  - **Pollutant levels are very wrong: 5000 %…NO for example is extremely sensitive to temperature. Errors on temperature of 50 K can double NO levels.**
  - **The rest of the physics (stretch effects, heat losses, ignition) is unchanged**

EQUATIONS AND VARIABLES NEEDED FOR A CFD COMBUSTION CODE

- VARIABLES (5 + N-1): Density, U, V, W, ENERGY , Partial density of the N species

- WE HAVE DERIVED ALL EQUATIONS (CONTINUITY, MOMENTUM, SPECIES) EXCEPT ONE FOR ENERGY

- NOW: LET US LOOK AT ENERGY (WHICH CAN ALSO BE ENTHALPY, ENTROPY, PRESSURE, TEMPERATURE: ANY OF THEM WOULD WORK BECAUSE THEY ARE ALL RELATED)

ENTHALPIES:

- Non reacting flows:
  - Enthalpy

$$C_p T$$

  - Total enthalpy

$$C_p T + \frac{1}{2} u_i u_i$$

- Combustion

  Enthalpy (sensible)

$$h_s = \int_{T_0}^{T} C_p dT$$

  - Enthalpy sensible + formation

$$h = h_s + \sum_{k=1}^{N} \Delta h^o_{f,k} Y_k$$

  - Total enthalpy including heat of formation and kinetic energy

$$h_t = h + \tfrac{1}{2} u_i u_i$$

  - Total enthalpy including kinetic energy but no heat of formation

$$H = h_s + \tfrac{1}{2} u_i u_i$$

Energy: 4 forms.
Enthalpy: 4 forms + one (T)

Ch. 1, Sec. 1.1.5

Form	Energy	Enthalpy
Sensible	$e_s = \int_{T_0}^{T} C_v dT - RT_0/W$	$h_s = \int_{T_0}^{T} C_p dT$
Sensible+Chemical	$e = e_s + \sum_{k=1}^{N} \Delta h^o_{f,k} Y_k$	$h = h_s + \sum_{k=1}^{N} \Delta h^o_{f,k} Y_k$
Total Chemical	$e_t = e + \frac{1}{2} u_i u_i$	$h_t = h + \frac{1}{2} u_i u_i$
Total non Chemical	$E = e_s + \frac{1}{2} u_i u_i$	$H = h_s + \frac{1}{2} u_i u_i$

$$C_p = \sum_{k=1}^{N} C_{pk} Y_k = \sum_{k=1}^{N} C^m_{pk} \frac{Y_k}{W_k} \qquad e = h - \frac{p}{\rho}$$

The C_{pk}'s depend on temperature so that C_p depends both on temperature (through the C_{pk}'s) and on composition (the Y_k's)

➡ **Good starting point: total energy e_t**

$$\frac{\partial \rho e_t}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i e_t) = -\frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_j}(\sigma_{ij} u_i)$$

$$\sigma_{ij} = \tau_{ij} - p\delta_{ij}$$

careful with the heat flux. It is not:

$$q_i = -\lambda \frac{\partial T}{\partial x_i}$$

but is also includes the flux transported by species diffusion:

$$q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{k=1}^{N} h_k Y_k V_{k,i}$$

IN MOST FLAMES (no volume forces or sources):

e_t	$\rho \frac{De_t}{Dt} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_j}(\sigma_{ij} u_i)$ -
h_t	$\rho \frac{Dh_t}{Dt} = \frac{\partial p}{\partial t} - \frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij} u_i)$
e	$\rho \frac{De}{Dt} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ij} \frac{\partial u_i}{\partial x_j}$
h	$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} - \frac{\partial q_i}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_j}$
e_s	$\rho \frac{De_s}{Dt} = \dot{\omega}_T + \frac{\partial}{\partial x_i}(\lambda \frac{\partial T}{\partial x_i}) - \frac{\partial}{\partial x_i}(\rho \sum_{k=1}^{N} h_{s,k} Y_k V_{k,i}) + \sigma_{ij} \frac{\partial u_i}{\partial x_j}$
h_s	$\rho \frac{Dh_s}{Dt} = \dot{\omega}_T + \frac{Dp}{Dt} + \frac{\partial}{\partial x_i}(\lambda \frac{\partial T}{\partial x_i}) - \frac{\partial}{\partial x_i}(\rho \sum_{k=1}^{N} h_{s,k} Y_k V_{k,i}) + \tau_{ij} \frac{\partial u_i}{\partial x_j}$
E	$\rho \frac{DE}{Dt} = \dot{\omega}_T + \frac{\partial}{\partial x_i}(\lambda \frac{\partial T}{\partial x_i}) - \frac{\partial}{\partial x_i}(\rho \sum_{k=1}^{N} h_{s,k} Y_k V_{k,i}) + \frac{\partial}{\partial x_j}(\sigma_{ij} u_i)$
H	$\rho \frac{DH}{Dt} = \dot{\omega}_T + \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}(\lambda \frac{\partial T}{\partial x_i}) - \frac{\partial}{\partial x_i}(\rho \sum_{k=1}^{N} h_{s,k} Y_k V_{k,i}) + \frac{\partial}{\partial x_j}(\tau_{ij} u_i)$ -

$$\tau_{ij} = -\frac{2}{3}\mu \frac{\partial u_k}{\partial x_k}\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \qquad \sigma_{ij} = \tau_{ij} - p\delta_{ij}$$

The heat release rate $\dot{\omega}_T$ and the N reaction rates of species $\dot{\omega}_k$:

- There are N reaction rates $\dot{\omega}_k$ in the species equations (one for each species k)

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}(\rho(u_i + V_{k,i})Y_k) = \dot{\omega}_k$$

10 kg/m3/s

- But only one heat release term in the energy equation:

$$\dot{\omega}_T = -\sum_{k=1}^{N} \dot{\omega}_k \Delta H_{fk}^0$$

1E9 W/m3

Many of us like to work with the temperature equation.

If pressure is constant:

$$\rho C_p \frac{DT}{Dt} = \dot{\omega}'_T + \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) - \rho \frac{\partial T}{\partial x_i}\left(\sum_{k=1}^{N} C_{p,k} Y_k V_{k,i}\right)$$

Careful with this new 'heat release'

$$\dot{\omega}'_T = -\sum_{k=1}^{N} h_k \dot{\omega}_k$$

Two 'reaction rate' terms $\dot{\omega}_T$ and $\dot{\omega}'_T$: same name in the literature but NOT equal

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i E) = \dot{\omega}_T + \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) + \frac{\partial}{\partial x_j}(\sigma_{ij} u_$$

$$\dot{\omega}_T = -\sum_{k=1}^{N} \dot{\omega}_k \Delta H^0_{fk}$$

$$\rho C_p \frac{DT}{Dt} = \dot{\omega}'_T + \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) - \rho \frac{\partial T}{\partial x_i}\left(\sum_{k=1}^{N} C_{p,k} Y_k V_{k,i}\right)$$

$$\dot{\omega}'_T = -\sum_{k=1}^{N} h_k \dot{\omega}_k = -\sum_{k=1}^{N} h_{sk} \dot{\omega}_k - \sum_{k=1}^{N} \Delta H^0_{fk} \dot{\omega}_k$$

$$\dot{\omega}'_T = -\sum_{k=1}^{N} h_k \dot{\omega}_k = -\sum_{k=1}^{N} h_{sk} \dot{\omega}_k - \sum_{k=1}^{N} \Delta H^0_{fk} \dot{\omega}_k = \boxed{-\sum_{k=1}^{N} h_{sk} \dot{\omega}_k} + \dot{\omega}_T$$

Careful when you compute reaction rates

If the Cp,k s are equal: $C_{p,k} = C_p$

$$h_{sk} = \int C_{pk} dT = \int C_p dT = h$$

so that $\Sigma_{k=1}^{N} h_{sk} \dot{\omega}_k = h_k \Sigma_{k=1}^{N} \dot{\omega}_k = 0$

$$\dot{\omega}_T = \dot{\omega}'_T$$

And if the Cp,k s are equal: $C_{p,k} = C_p$

$$\sum_{k=1}^{N} C_{p,k} Y_k V_{k,i} = C_p \sum_{k=1}^{N} Y_k V_{k,i} = 0$$

so that the temperature equation:

$$\rho C_p \frac{DT}{Dt} = \dot{\omega}'_T + \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) - \rho \frac{\partial T}{\partial x_i}\left(\sum_{k=1}^{N} C_{p,k} Y_k V_{k,i}\right)$$

becomes:

$$\rho C_p \frac{DT}{Dt} = \dot{\omega}_T + \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right)$$

Another useful simplified form : the « single reaction »

Suppose that we have only ONE global reaction:

Q tells us how many Joules are released when one kilogram of fuel burns: 120 MJ/kg for H2 for example.

Since the $\dot{\omega}_k$ are all linked to $\dot{\omega}_F$:

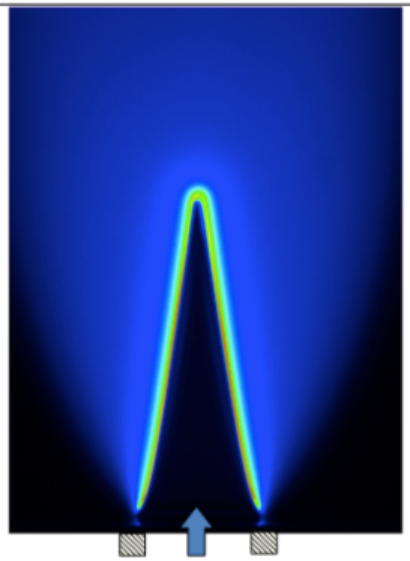
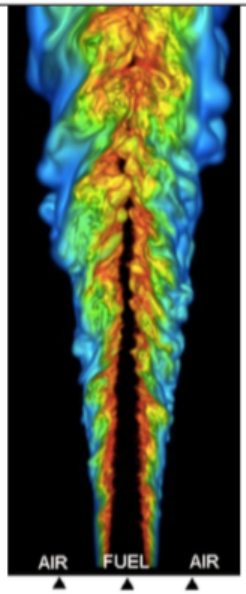
$\dot{\omega}_k = -\nu_k W_k \dot{\omega}_F$ **we can write the heat release as:**

$$\dot{\omega}_T = -\sum \Delta H^0_{fk} \dot{\omega}_k = -(\sum \Delta H^0_{fk} \nu_k W_k)\dot{\omega} = -Q\dot{\omega}_F$$

where Q is the heat of reaction: $Q = -(\sum \Delta H^0_{fk} \nu_k W_k)/(\nu_F W_f)$

SUMMARY:

- We have the basic equations of combustion. We could stop here… if these equations were simple to solve. But they are not !
- We are going to have difficulties with:
  - Kinetics
  - Turbulence
  - Very large domains
- We are going to need models. Better: we are going to need understanding...
- To do this we need to study academic (canonical) cases even if it means simplifying things a little bit.

	LAMINAR FLAMES	***TURBULENT FLAMES***
PREMIXED FLAMES	 Chapter 2	 Chapters 4 and 5
NON-PREMIXED FLAMES (DIFFUSION)	 Chapter 3	 Chapters 4 and 6

d

So… canonical cases are needed to understand the basic flame features. The two most usual ones are:

- The premixed laminar flame — Ch. 2
- The laminar diffusion flame — Ch. 3

OUTLINE

CONSERVATION EQUATIONS FOR REACTING FLOWS

PREMIXED FLAMES

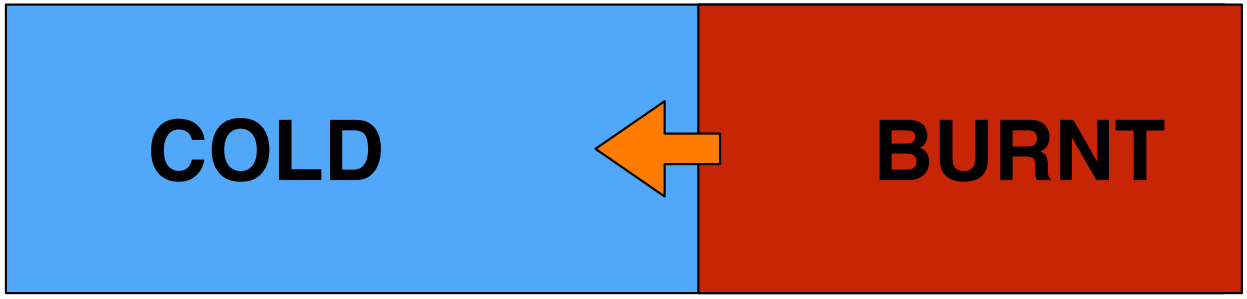
Ch. 2

DIFFUSION FLAMES

OTHER FLAMES: PARTIALLY PREMIXED, TRIPLE FLAMES

PREMIXED LAMINAR FLAME

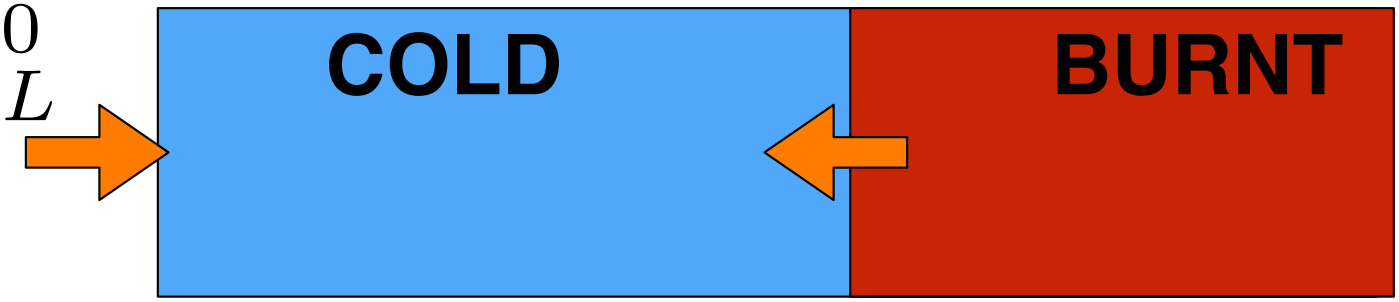
- Under certain assumptions, an explicit resolution of the previous equations is possible
- This is the case for the 1D premixed laminar flame:

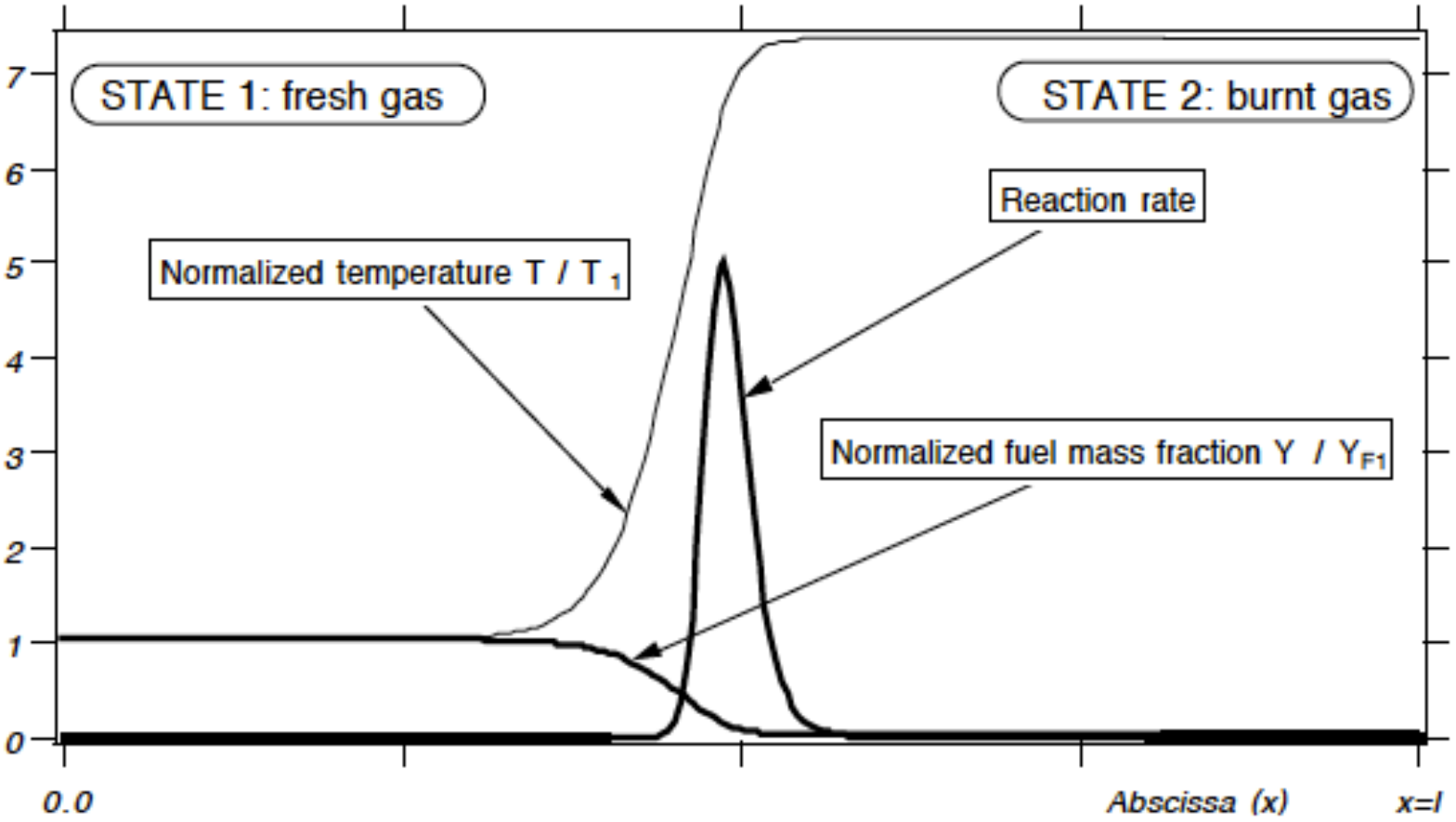


- Flame moves at a constant speed called the laminar flame speed s_L^0 - > this helps:
  - In a reference frame moving with the flame, the flow is steady.
  - In this reference frame, the flow enters the domain at the flame speed s_L^0

IN THE REFERENCE FRAME OF THE FLAME:

$$u = s_L^0$$





A one-dimensional steady problem in the reference frame of the flame

Ch. 2, Sec 2.3

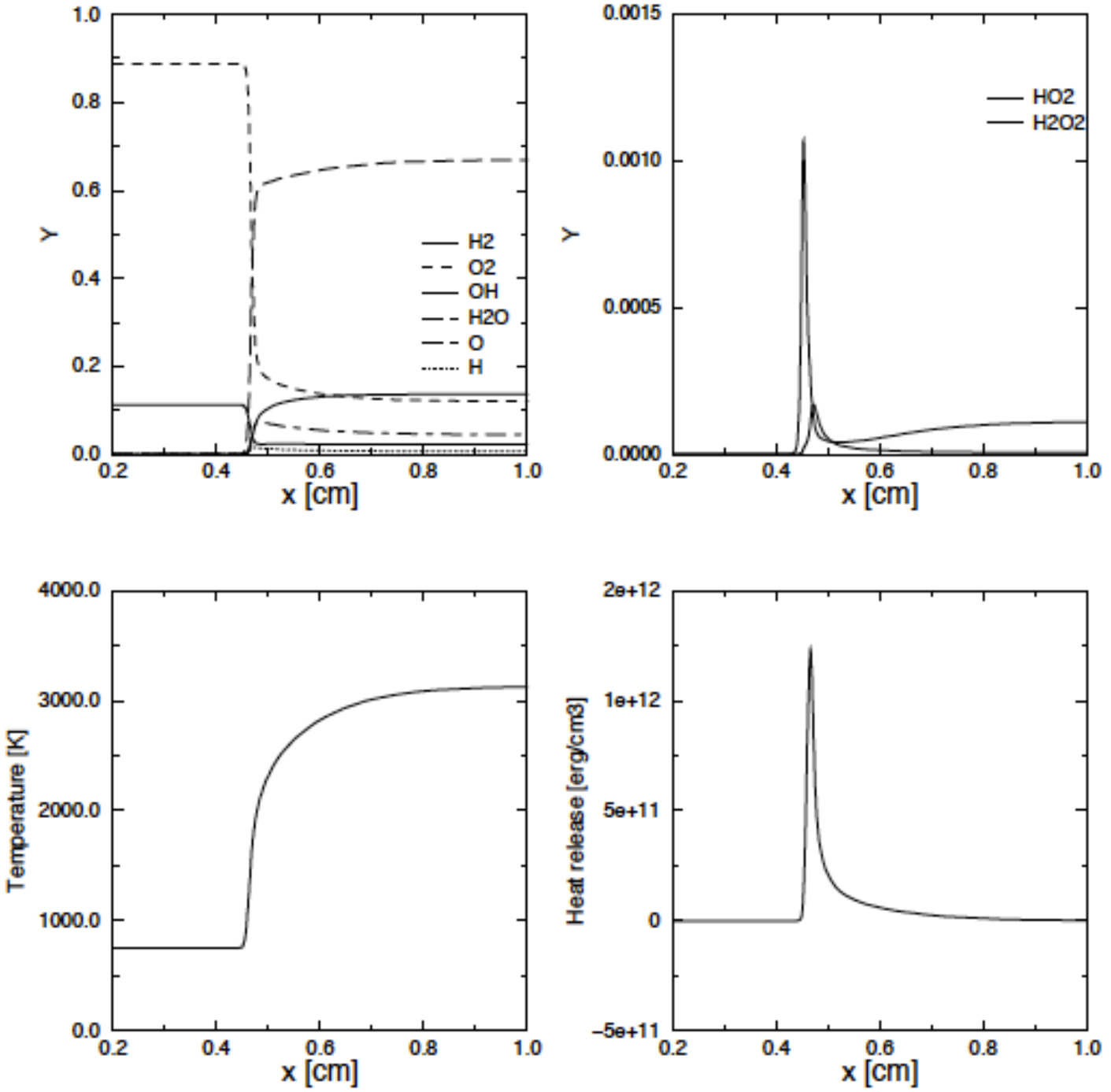
$$\rho u = \text{constant} = \rho_1 s_L$$

$$\frac{\partial}{\partial x}(\rho(u + V_k)Y_k) = \dot{\omega}_k$$

$$\rho C_p u \frac{\partial T}{\partial x} = \dot{\omega}'_T + \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) - \frac{\partial T}{\partial x}\left(\rho \sum_{k=1}^{N} C_{p,k} Y_k V_k\right)$$

No momentum equation needed: need it only to find pressure.
This equation can be solved for a large number of species numerically (CHEMKIN, COSILAB, CANTERA, FLAME MASTER)

CHEMKIN computation for H2/ O2 flame.



But doing so does not tell us much. Let us keep simplifying

Additional assumptions to obtain an explicit solution

Ch. 2 Sec 2.4

- Suppose we have a single reaction in a lean flame. General expression for fuel reaction rate

$$\dot{\omega}_F = A Y_F Y_O e^{-\frac{T_a}{T}}$$

Almost constant in a lean flame

$$\dot{\omega}_F = A' Y_F e^{-\frac{T_a}{T}} \quad \text{with } A' = A Y_O^0$$

- Instead of N mass fractions, we can track one only: the fuel mass fraction Yf. We assume that $Y_O = Y_O^0 = cst$ and do not need to compute Yo anymore

Ch. 2 Sec 2.4

$$\rho u = \text{constant} = \rho_1 u_1 = \rho_1 s_L$$

$$\rho_1 s_L \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F$$

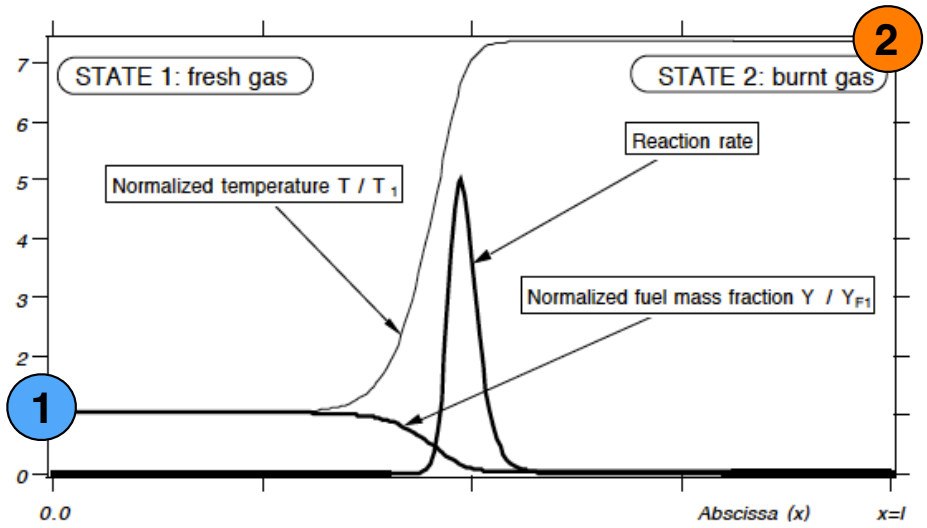
$$\rho_1 C_p s_L \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) - Q\dot{\omega}_F$$

➡ **Can solve this by hand ! -> famous field for mathematicians/combustion experts (Williams, Clavin, Linan, Matalon)**

Before solving it, let us integrate these 2 equations from cold to hot side:

$$\rho_1 s_L \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F$$

$$\rho_1 C_p s_L \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) - Q\dot{\omega}_F$$



$$\rho_1 s_L [Y_f^2 - Y_f^1] = [\rho D \nabla Y_f]_1^2 + \int \dot{\omega}_F dx$$

$$\rho_1 C_p s_L [T_2 - T_1] = [\lambda \nabla T]_1^2 - Q \int \dot{\omega}_F dx$$

Total fuel combustion rate

$$\rho_1 s_L Y_F^1 = -\boxed{\int \dot{\omega}_F dx}$$

$$\rho_1 s_L C_p (T_2 - T_1) = -Q\boxed{\int \dot{\omega}_F dx}$$

$$\rho_1 s_L Y_F^1 = -\boxed{\int \dot{\omega}_F dx}$$

Total combustion rate

The inlet fuel flux: all fuel entering the flame… burns

$$\rho_1 s_L C_p (T_2 - T_1) = -Q \boxed{\int \dot{\omega}_F dx}$$

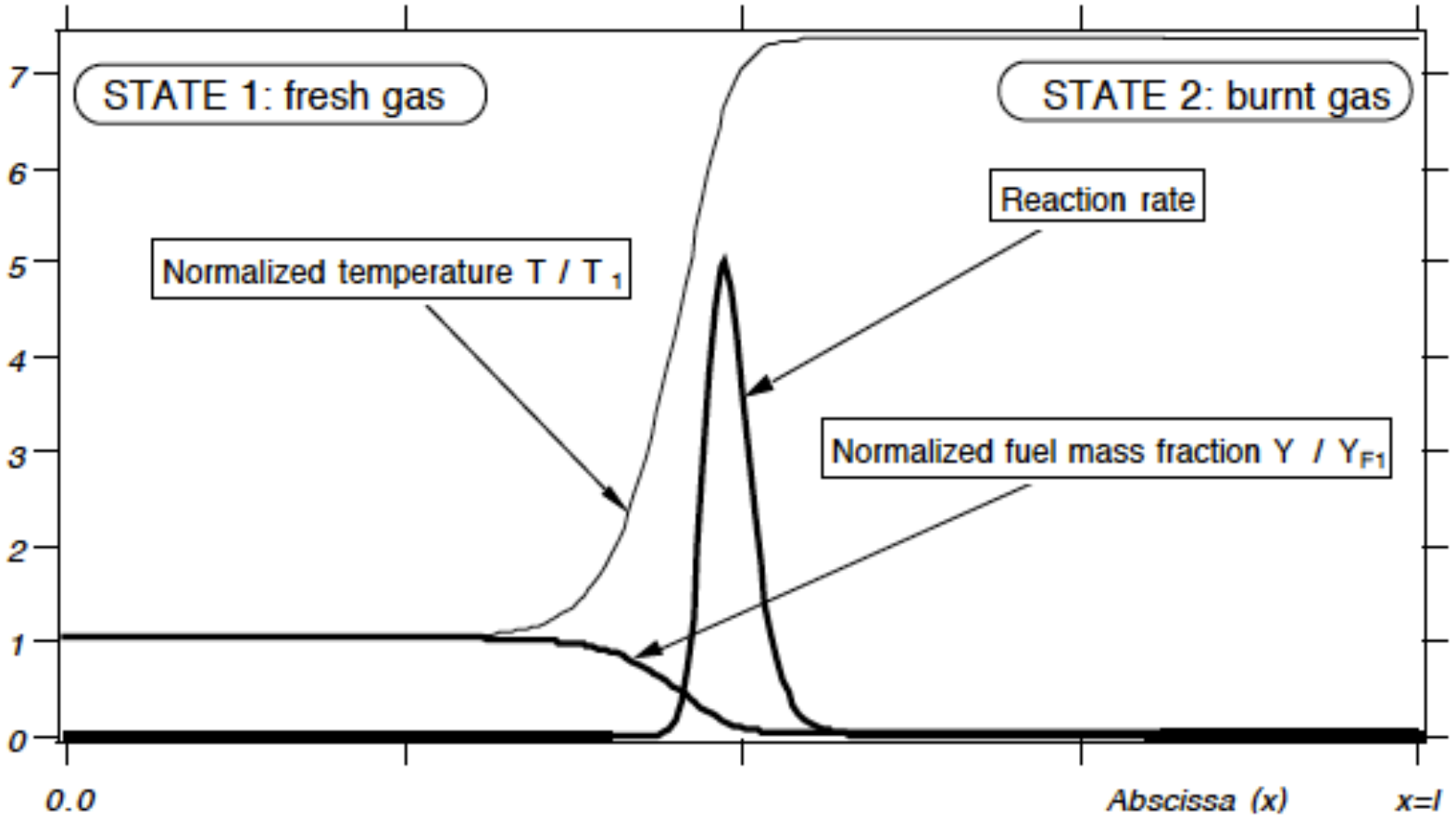
The fuel which has burnt in the flame, has released Q Joule per unit mass

Eliminate the total reaction rate: $\int \dot{\omega}_F dx$

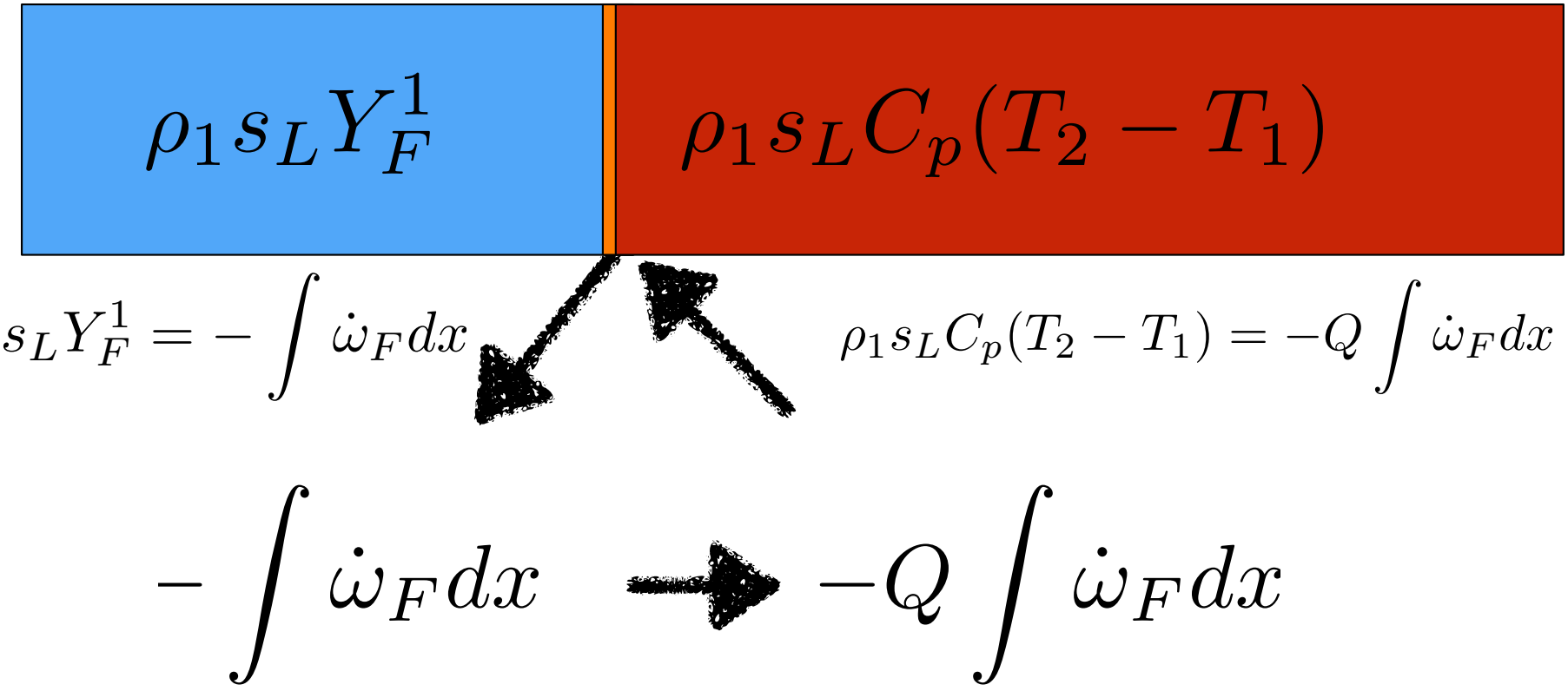
BURNT GAS TEMPERATURE AND FUEL MASS FRACTION

COLD	BURNT
u_1, T_1, Y_F^1	$u_2, T_2, Y_F^2 = 0$

$$C_p(T_2 - T_1) = QY_F^1$$



VISUALIZATION OF WHAT A PREMIXED FLAME DOES



Let us solve these equations now.

First change variables: instead of Y_F and T, use scaled variables Y and θ:

$$\boxed{Y = Y_F / Y_F^1} \quad \text{and} \quad \boxed{\Theta = \frac{C_p(T - T_1)}{QY_F^1} = \frac{T - T_1}{T_2 - T_1}}$$

Boundary conditions:

	Cold gas	Hot gas
Y	1	0
θ	0	1

➡ **Lewis number equal to unity:** $Le = \lambda/(\rho C_p D) = 1$

$$/Y_F^1 \Rightarrow \rho_1 s_L \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F$$

$$/C_p(T_2 - T_1) \Rightarrow \rho_1 C_p s_L \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) - Q\dot{\omega}_F$$

$$\rho_1 s_L \frac{d(Y+\theta)}{dx} = \frac{d}{dx}\left(\lambda \frac{d(Y+\theta)}{dx}\right)$$

Boundary conditions:

	Cold gas	**Hot gas**
Y	1	0
θ	0	1
$Y+\theta$	1	1

Solution: $\theta + Y = 1$

Ch 2 used in Ch. 4, 5, 6

- If Lewis = 1 temperature and fuel mass fractions are directly linked. No need to solve for both of them !

- In terms of physics: simple interpretation:

$$\theta + Y = 1$$

sensible enthalpy + chemical enthalpy = constant

- We are left with only one variable to solve for: the reduced temperature θ (also called progress variable c)

Master equation for laminar premixed flames:

$$\rho_1 s_L \frac{d\Theta}{dx} = \frac{d}{dx}\left(\frac{\lambda}{C_p}\frac{d\Theta}{dx}\right) - \underbrace{B_1 \left(T_1 + \Theta(T_2 - T_1)\right)^{\beta_1} \rho(1-\Theta) \exp\left(-\frac{T_{a1}}{T_1 + \Theta(T_2 - T_1)}\right)}_{\dot{\omega}_T}$$

This is where asymptotics enter the field. This equation can be solved completely analytically. Suppose $\beta_1 = 0$

The reaction rate depends only on θ :

$$\dot{\omega}_T = B_1 \rho (1-\theta) exp(-\frac{T_{a1}}{T_1 + (T_2 - T_1)\theta})$$

Constant pressure:

$$\rho T = \rho_1 T_1$$

$$\rho = \frac{\rho_1}{1 + (\frac{T_2}{T_1} - 1)\theta}$$



$$\dot{\omega}_T = B_1 \frac{\rho_1}{1 + (\frac{T_2}{T_1} - 1)\theta} (1-\theta) exp(-\frac{T_{a1}}{T_1 + (T_2 - T_1)\theta})$$

$$\dot{\omega}_T = B_1 \frac{\rho_1}{1 + (\frac{T_2}{T_1} - 1)\theta}(1 - \theta)exp(-\frac{T_{a1}}{T_1 + (T_2 - T_1)\theta}$$

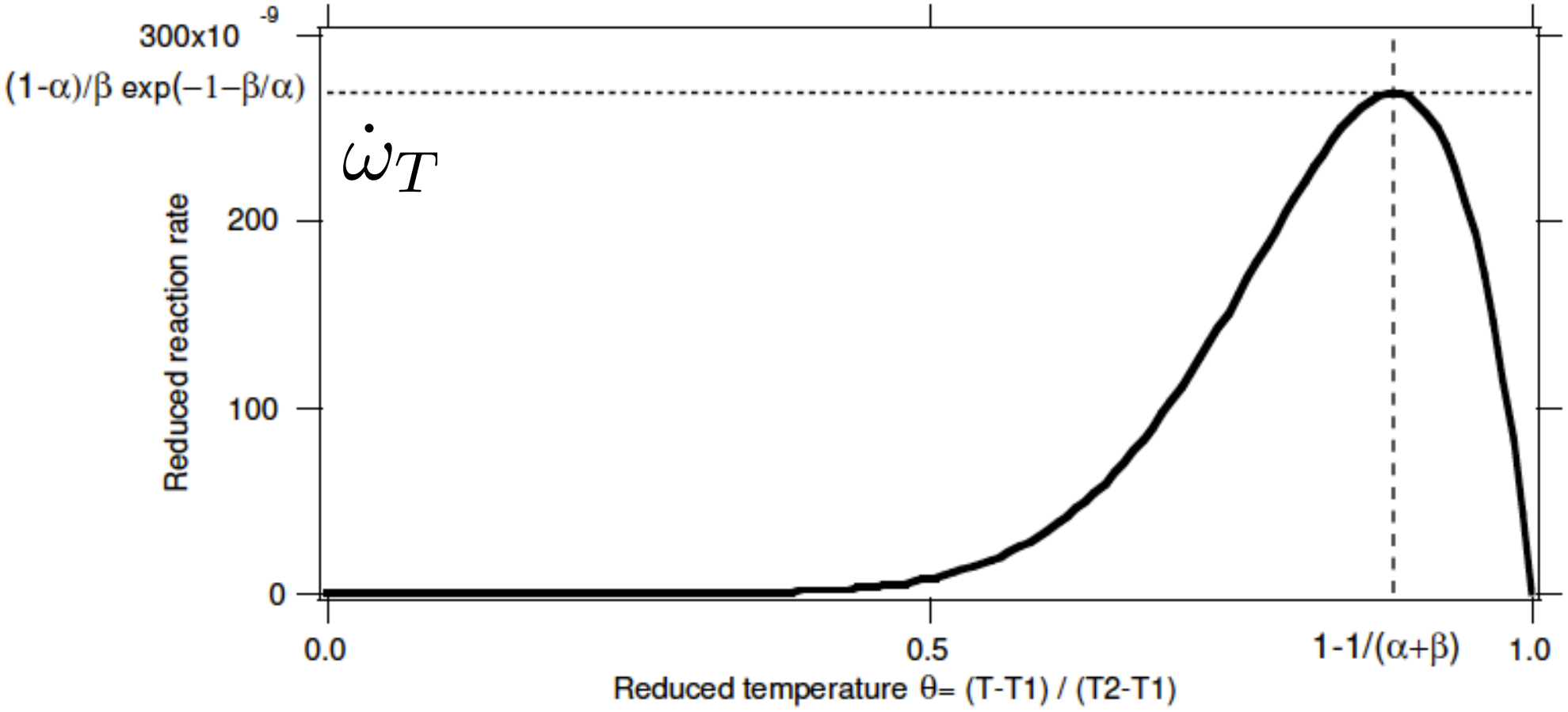
This expression is the baseline one for turbulent combustion in premixed flames.

Useful but be careful - valid only when:

- **constant pressure**
- **single reaction**
- **unity Lewis number**
- **adiabatic flows**

The reaction rate depends only on θ:

$$\dot{\omega}_T = B_1 \frac{\rho_1}{1 + (\frac{T_2}{T_1} - 1)\theta}(1 - \theta)exp(-\frac{T_{a1}}{T_1 + (T_2 - T_1)\theta})$$



The temperature at which the reaction rate is maximum can be obtained by searching for:

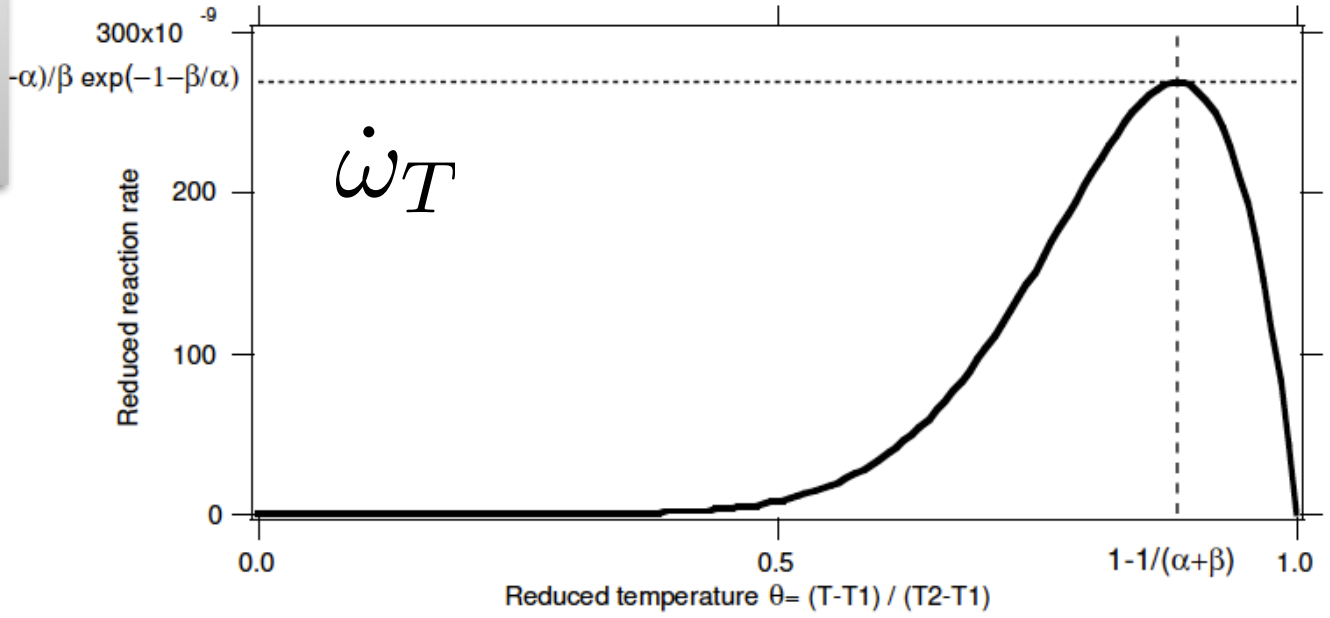
$$\frac{d\dot{\omega}_T}{d\theta} = 0$$

$$\theta_c = 1 - \frac{1}{\alpha + \beta} \simeq 1 - \frac{1}{\beta}$$

$$\alpha = (T_2 - T_1)/T_2$$

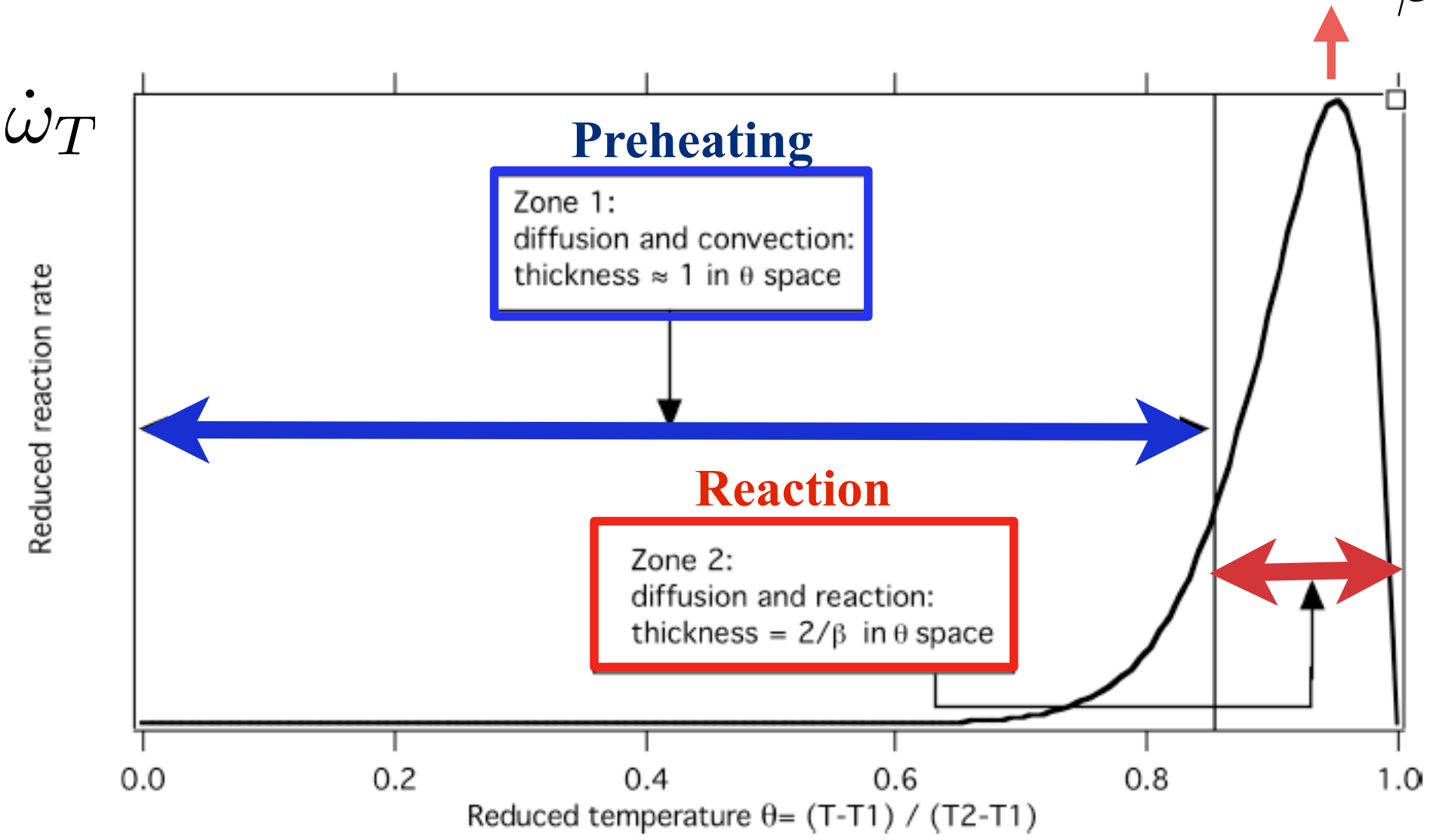
$$\beta = \alpha T_{a1}/T_2$$

$$\alpha \simeq 0.9 \quad \beta \simeq 12$$

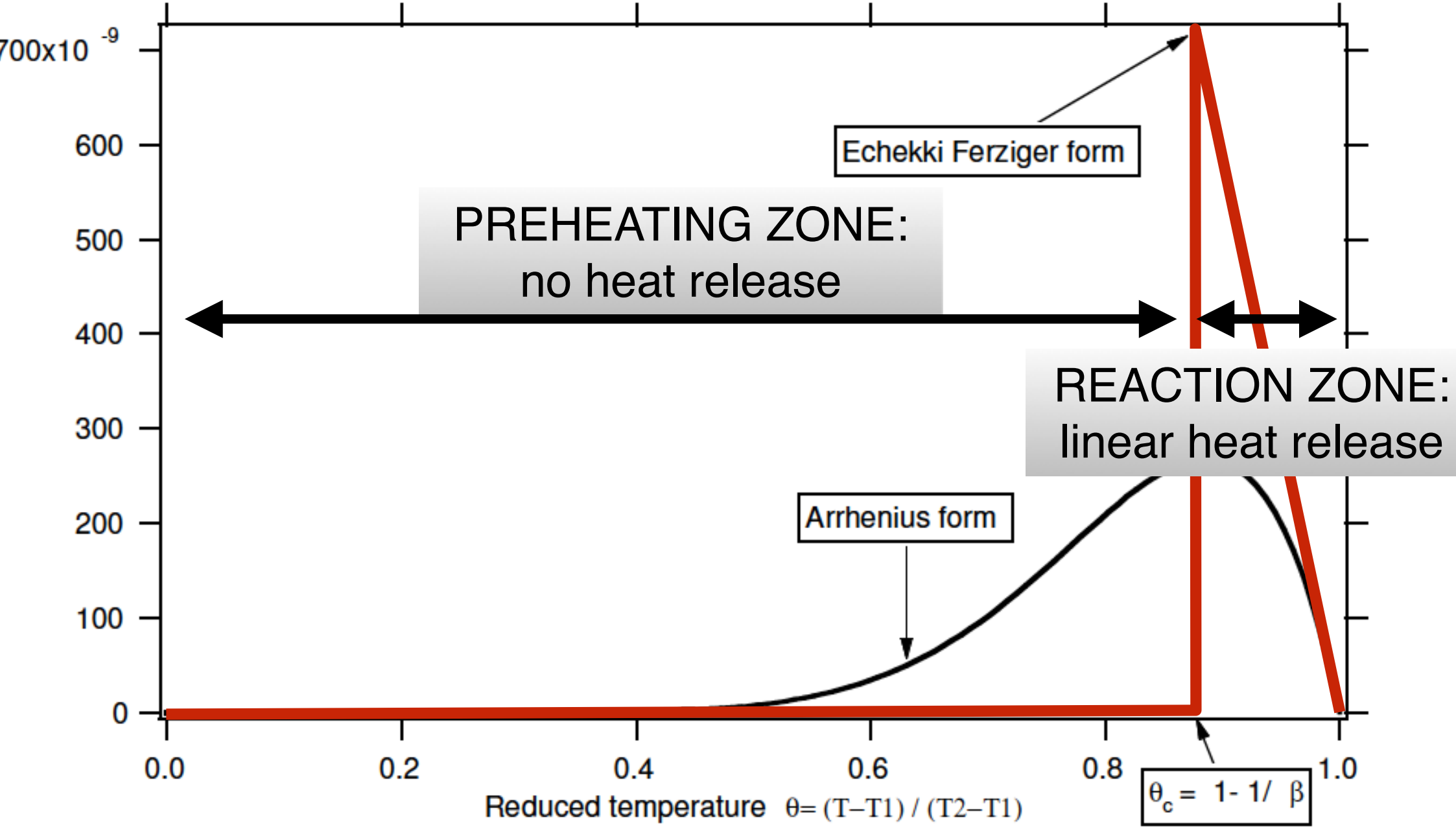


The laminar flame can be decomposed in two zones: a preheating region and a reaction zone

$$\theta_c = 1 - \frac{1}{\beta}$$



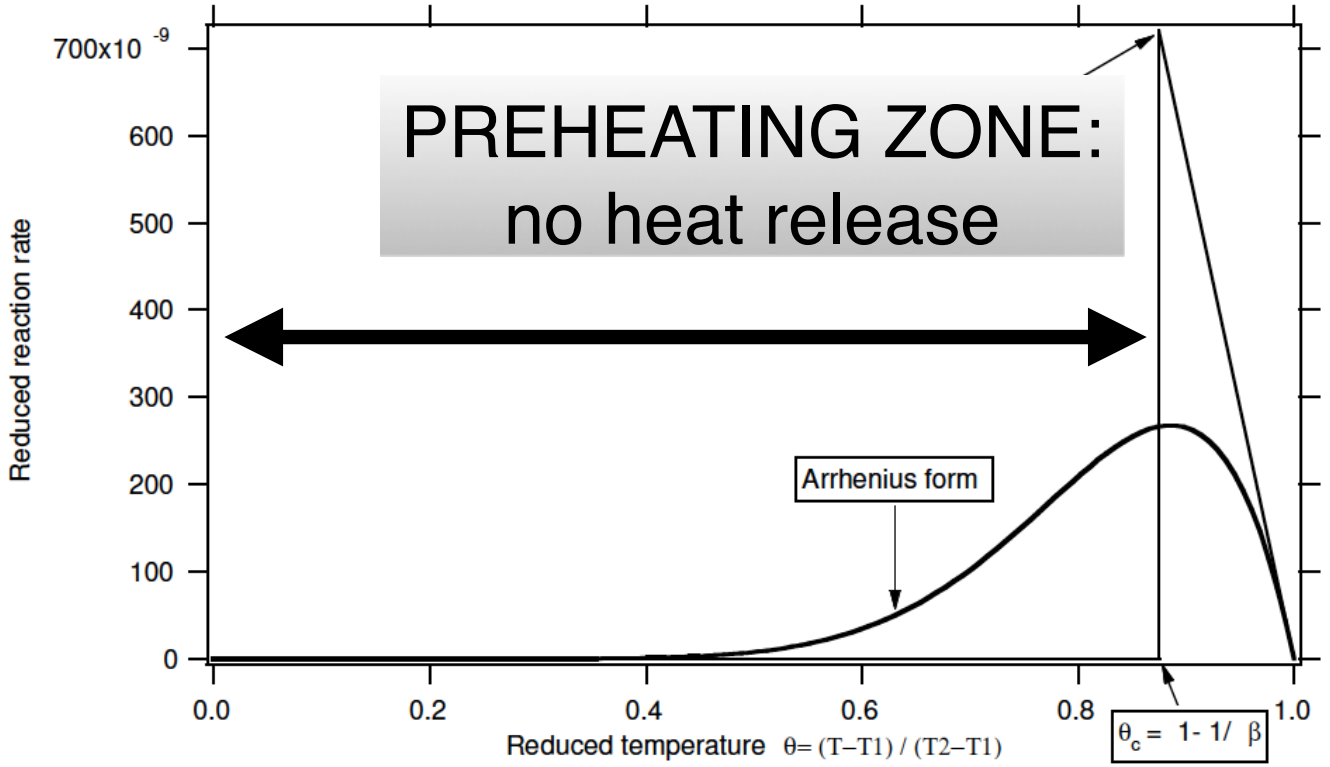
The Echekki Ferziger model: a simple solution for deflagrations



The Echekki Ferziger model:

- An elegant method to solve the problem analytically
- Based on a change of expression for the heat release which allows a fully analytical solution
- Extensions to more complex flames in Echekki, Comb. Flame 172, 280, 2016
- Full derivations with Arrhenius chemistry: see Matalon's and Clavin's papers

STEP 1: INTEGRATE IN THE PREHEATING ZONE



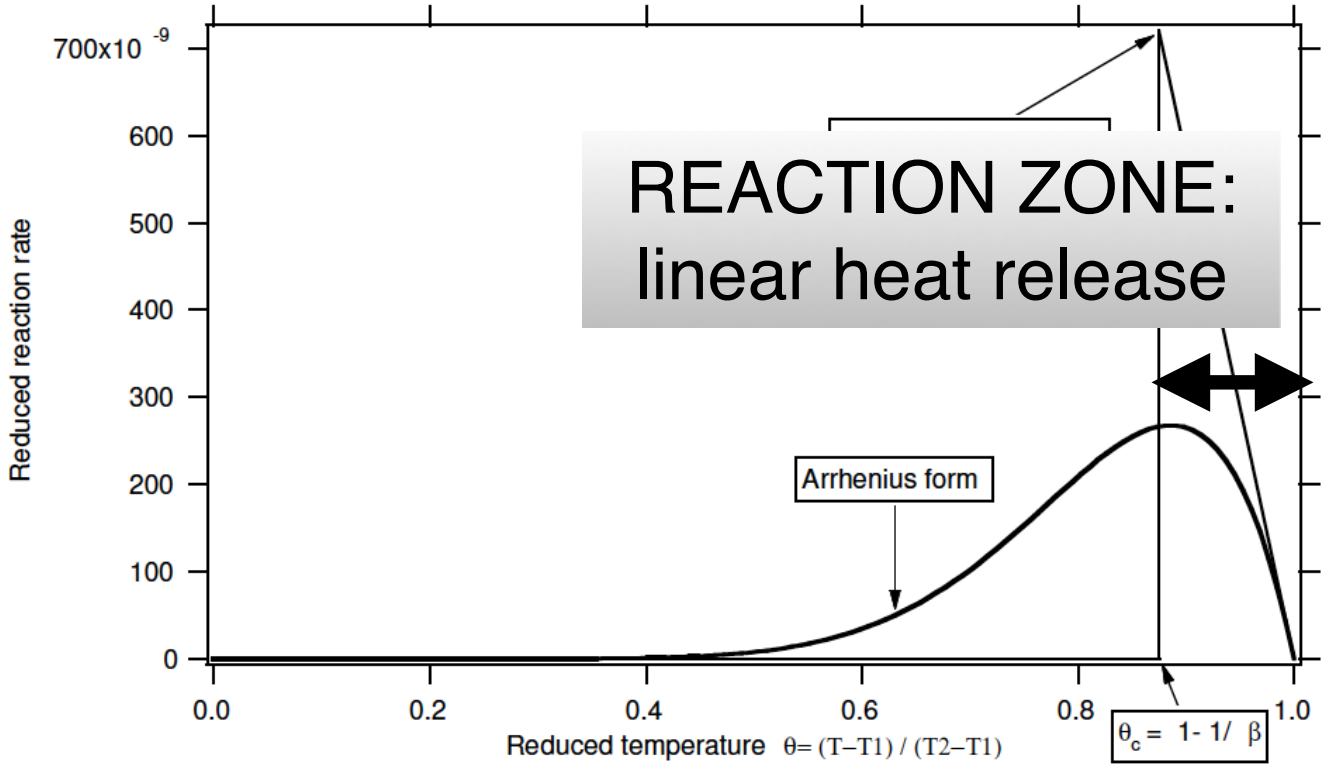
$$\rho_1 s_L \frac{d\Theta}{dx} = \frac{d}{dx}\left(\frac{\lambda}{C_p}\frac{d\Theta}{dx}\right) \qquad \begin{aligned} \Theta &= 0 \quad if \quad x \to -\infty \\ \Theta &= \theta_c \quad if \quad x \to 0 \end{aligned}$$

$$\Theta = \theta_c e^{x/\delta} = \left(1 - \frac{1}{\beta}\right) e^{x/\delta}$$

$$\delta = D_{th}^1 / s_L$$

δ **IS A FLAME THICKNESS**

STEP 2: INTEGRATE IN THE REACTION ZONE



$$\rho_1 s_L \frac{d\Theta}{dx} = \frac{d}{dx}\left(\frac{\lambda}{C_p}\frac{d\Theta}{dx}\right) + \rho_1 R(1-\theta)$$

$$\Theta = \theta_c \quad if \quad x \to 0$$

$$\Theta = 1 \quad if \quad x \to \infty$$

STEP 2: INTEGRATE IN THE REACTION ZONE: search the solution as $\theta = 1 - be^{\Gamma x}$ with $\Gamma < 0$. This means that $d\theta/dx = -b\Gamma e^{\Gamma x}$ and $d^2\theta/dx^2 = -b\Gamma^2 e^{\Gamma x}$

Inject this into the θ equation :

$$\rho_1 s_L \frac{d\Theta}{dx} = \frac{d}{dx}\left(\frac{\lambda}{C_p}\frac{d\Theta}{dx}\right) + \rho_1 R(1-\theta)$$

$$\theta = 1 - be^{\Gamma x} \qquad -s_L\Gamma = D^1_{th}\Gamma^2 + R$$

$$\Gamma = \frac{1}{2\delta}\left[1 - \left(1 + 4\frac{R\delta}{s_L}\right)^{1/2}\right] \qquad \delta = D^1_{th}/s_L$$

We still need b. Just apply the boundary condition at $x = 0$

$$\theta(x = 0) = \theta_c = 1 - 1/\beta = 1 - b$$

So that b must be $1/\beta$

$$\boxed{\Theta = 1 - \frac{1}{\beta}e^{\Gamma x}}$$

SO: IF THE GAS HAS A THERMAL DIFFUSIVITY D_{th}^1 AND A CHEMISTRY CONSTANT R ,THE TEMPERATURE PROFILE IS KNOWN:

$$\delta = D_{th}^1 / s_L$$

$$\Gamma = \frac{1}{2\delta}\left[1 - \left(1 + 4\frac{R\delta}{s_L}\right)^{1/2}\right]$$

$$\Theta = \left(1 - \frac{1}{\beta}\right) e^{x/\delta}$$

IN THE PREHEAT ZONE

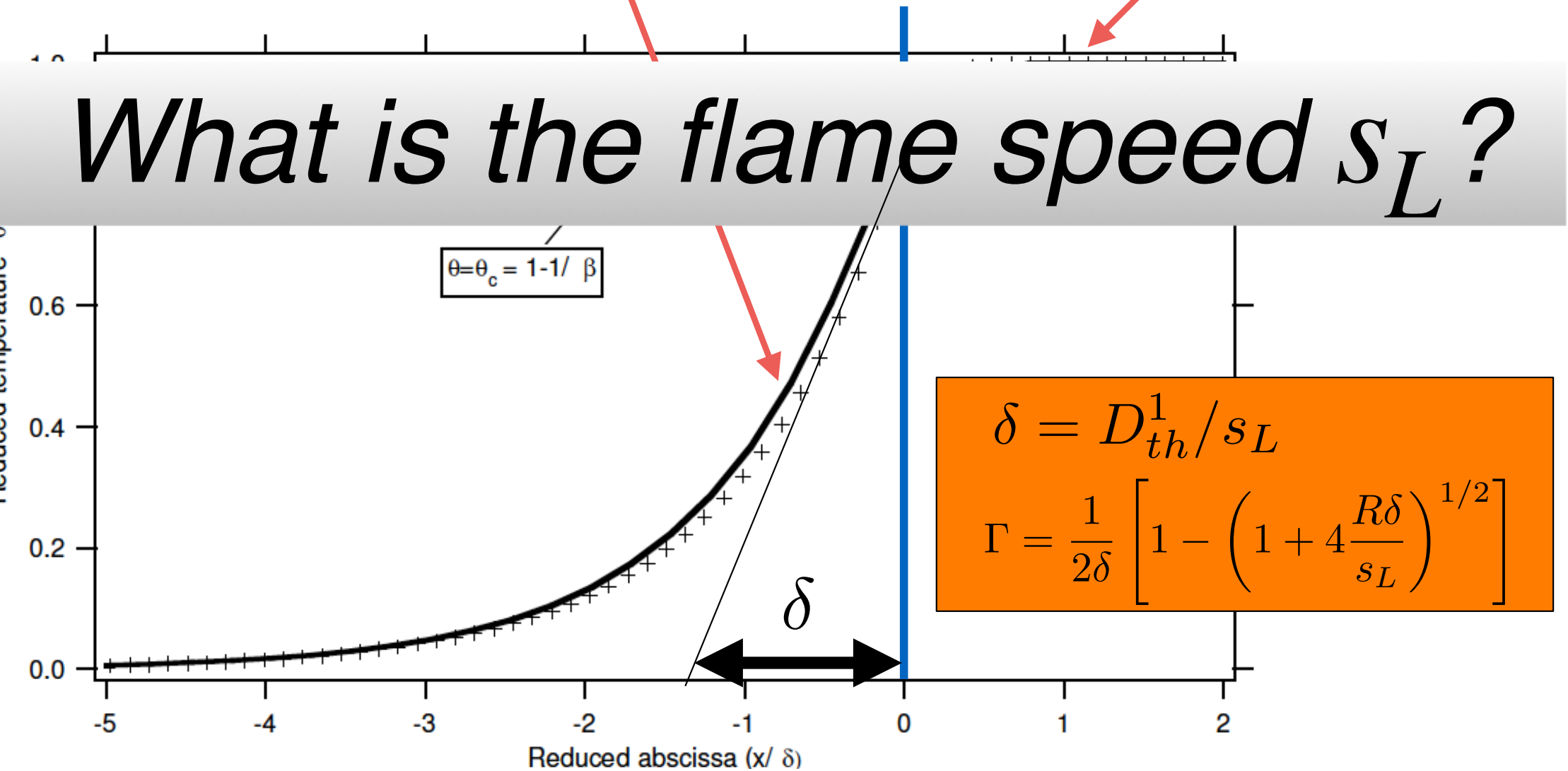
$$\Theta = 1 - \frac{1}{\beta} e^{\Gamma x}$$

IN THE REACTION ZONE

STEP 3: SO WE HAVE EVERYTHING. OR DO WE ?

$$\Theta = \left(1 - \frac{1}{\beta}\right) e^{x/\delta} \qquad \Theta = 1 - \frac{1}{\beta} e^{\Gamma x}$$

What is the flame speed s_L ?



$$\delta = D_{th}^1 / s_L$$

$$\Gamma = \frac{1}{2\delta}\left[1 - \left(1 + 4\frac{R\delta}{s_L}\right)^{1/2}\right]$$

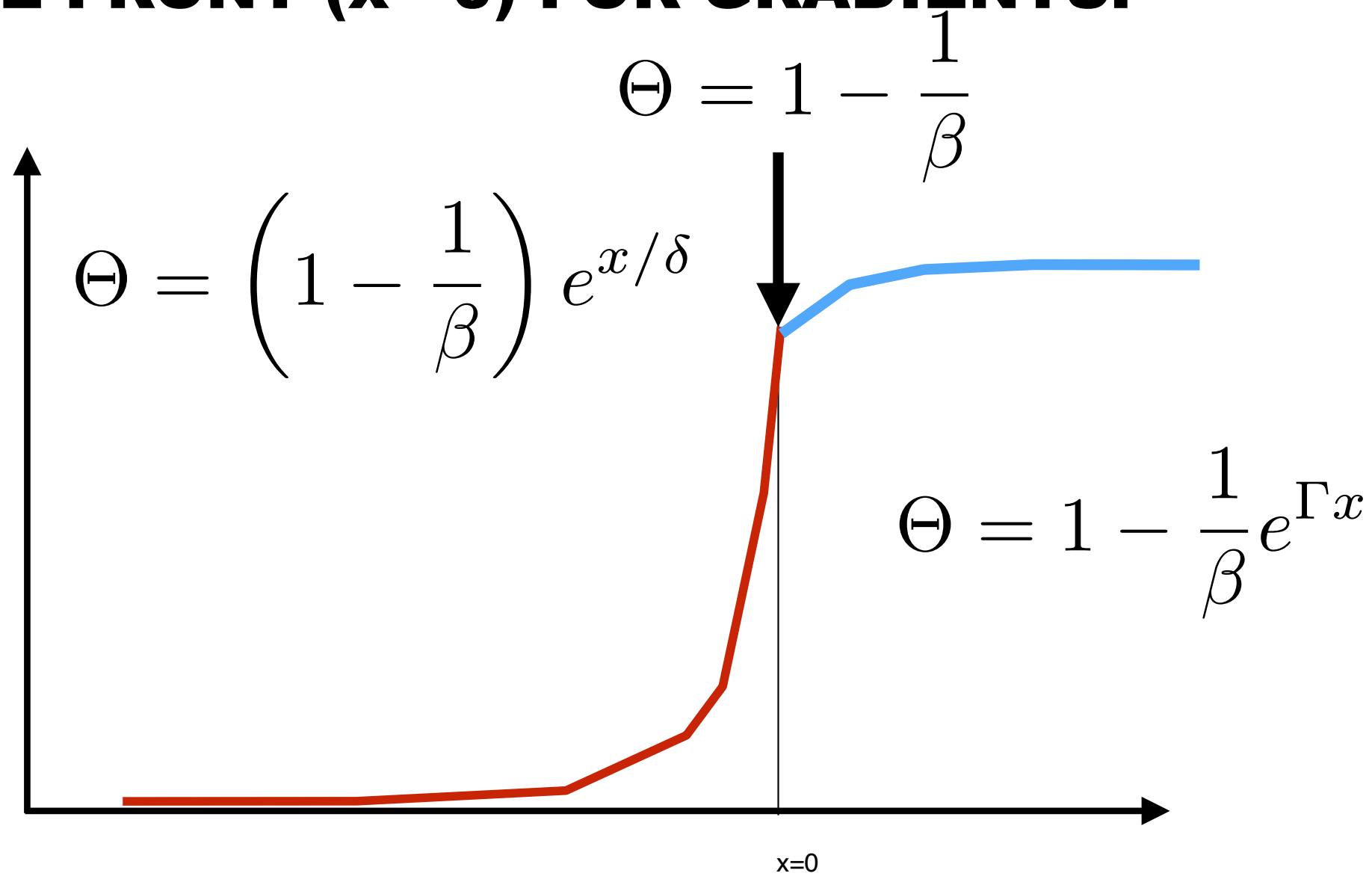
SINCE WE BEGAN, WE HAVE SAID 'LET US SIT IN THE REFERENCE FRAME OF THE FLAME AT SPEED s_L'

BUT WE DID NO SAY OR KNOW WHAT s_L WAS !
s_L IS THE EIGENVALUE OF THIS PROBLEM

SO WE ARE NOT DONE YET: WE NEED TO DETERMINE s_L

THIS CAN BE DONE BY NOTING THAT WE HAVE IMPOSED TEMPERATURE θ TO BE CONTINUOUS AT THE FLAME BUT NOT ITS GRADIENT $\nabla\theta$

FOR THE MOMENT OUR TWO SOLUTIONS FOR T ARE NOT NECESSARILY COMPATIBLE AT THE FLAME FRONT (x =0) FOR GRADIENTS:



STEP 3: At x=0, we now want continuity of the temperature gradient. Matching left and right heat fluxes can be obtained for only one value of s_L:

$$\Theta = \left(1 - \frac{1}{\beta}\right) e^{x/\delta} \qquad \Theta = 1 - \frac{1}{\beta} e^{\Gamma x}$$

$$\left(\frac{d\theta}{dx}\right)_{x=O^-} = \left(\frac{d\theta}{dx}\right)_{x=O^+}$$

$$s_L = \left(\frac{1}{\beta(\beta-1)} \frac{\lambda_1 R}{\rho_1 C_p}\right)^{1/2} = \frac{1}{(\beta(\beta-1))^{1/2}} (D_{th}^1 R)^{1/2}$$

SUMMARY:

- **A premixed flame has a thickness given by**

$$\delta = \frac{\lambda_1}{\rho_1 C_p s_L} = \frac{D_{th}^1}{s_L}$$ ← Heat diffusivity in the fresh gas

- **or** $$\frac{\delta s_L}{D_{th}^1} = 1$$

- **The Reynolds number of the flame is unity:**

$$\mathrm{Re_{flame}} = \frac{\delta \mathrm{s_L^0}}{\nu} = 1$$

- **And a flame speed :**

$$s_L = \left(\frac{1}{\beta(\beta-1)} \frac{\lambda_1 R}{\rho_1 C_p} \right)^{1/2} = \frac{1}{(\beta(\beta-1))^{1/2}} (D_{th}^1 R)^{1/2}$$

- **This is the result for the Echekki Ferziger model for reaction rate but other models would lead to similar results**

This flame speed depends on the form assumed for reaction rate and molecular diffusion:

Ch. 2 Sec 2.4.5

Model	Fuel reaction rate $\dot{\omega}_F$ in Eq. (2.22)	Transport assumptions	Flame speed s_L
ZFK	$B_1 T^{\beta_1} \rho Y_F e^{-T_a/T}$	$\lambda = \lambda_1 (T/T_1)^{1-\beta_1}$	$\frac{1}{\beta} e^{-\frac{\beta}{2\alpha}} (2 \lvert B_1 \rvert T_1^{\beta_1} D_{th}^1)^{1/2}$
Williams	$B_1 T^{\beta_1} \rho Y_F e^{-T_a/T}$	$\lambda = \lambda_1 (T/T_1)^{1-\beta_1}$	$\frac{1}{\beta} e^{-\frac{\beta}{2\alpha}} (2 \lvert B_1 \rvert T_1^{\beta_1} D_{th}^1)^{1/2} (1 + \frac{1.34-3\alpha}{\beta})$
Van Kalmthout	$B_1 \rho Y_F Y_O e^{-T_a/T}$	$\lambda = \lambda_1 T/T_1$	$\frac{1}{\beta} e^{-\frac{\beta}{2\alpha}} (2 \lvert B_1 \rvert Y_O^1 D_{th}^1 \frac{2}{\beta})^{1/2}$
Echekki	$\rho R_r (1-\Theta) H(\Theta - \Theta_c)$	$\lambda = \lambda_1 T/T_1$	$\left(\frac{1}{\beta(\beta-1)} D_{th}^1 R_r \right)^{1/2}$
This book	$\rho_1 R_r (1-\Theta) H(\Theta - \Theta_c)$	$\lambda = \lambda_1$	$\left(\frac{1}{\beta(\beta-1)} D_{th}^1 R_r \right)^{1/2}$

You can find the results in the TNC book and in asymptotic papers but let us focus on an important result:

In all premixed flame speed expressions:

$$s_L \propto (D_{th}^1 R_r)^{1/2}$$

Ch. 2 Sec 2.4.6

Heat diffusivity

Kinetics constant

- **Flame propagation is the combination of both molecular diffusion D_{th}^1 and reaction R_r**
- **Multiply the kinetics constant by 4 : it will increase the flame speed by two**
- **Without heat (or species) diffusivity… no premixed flame. This is specific of deflagrations**

A useful feature of premixed flames: the possibility of thickening it for simulations

$$s_L \propto (D_{th}^1 R_r)^{1/2}$$

$$s_L \approx (F D_{th}^1 \frac{R_r}{F})^{1/2}$$

Heat diffusivity *Kinetics constant*

$$\delta = \frac{\lambda_1}{\rho_1 C_p s_L} = \frac{D_{th}^1}{s_L}$$

$$\delta = F \frac{D_{th}^1}{s_L}$$

A useful feature of premixed flames:

- Divide the kinetics constant by a factor F>1 and multiply the diffusivity by F. You will get the *same* flame speed.

- But the thickness will be *larger* by a factor F:

Ch. 5 Sec 5.4.3

$$\delta = \frac{D_{th}^1}{s_L} \Rightarrow \delta = \frac{\mathbf{F} D_{th}^1}{s_L}$$

- This is the basis of the Thickened Flame model

A useful property in codes: thicken the flame (O'Rourke and Bracco JCP 1979+ CERFACS 90s)

$$d/dt(\rho Y_k) = \frac{\partial}{\partial x_i}(\rho D \frac{\partial Y_k}{\partial x_i}) + A\rho Y_1 Y_2 ... Yn \exp(-\frac{T_a}{T})$$

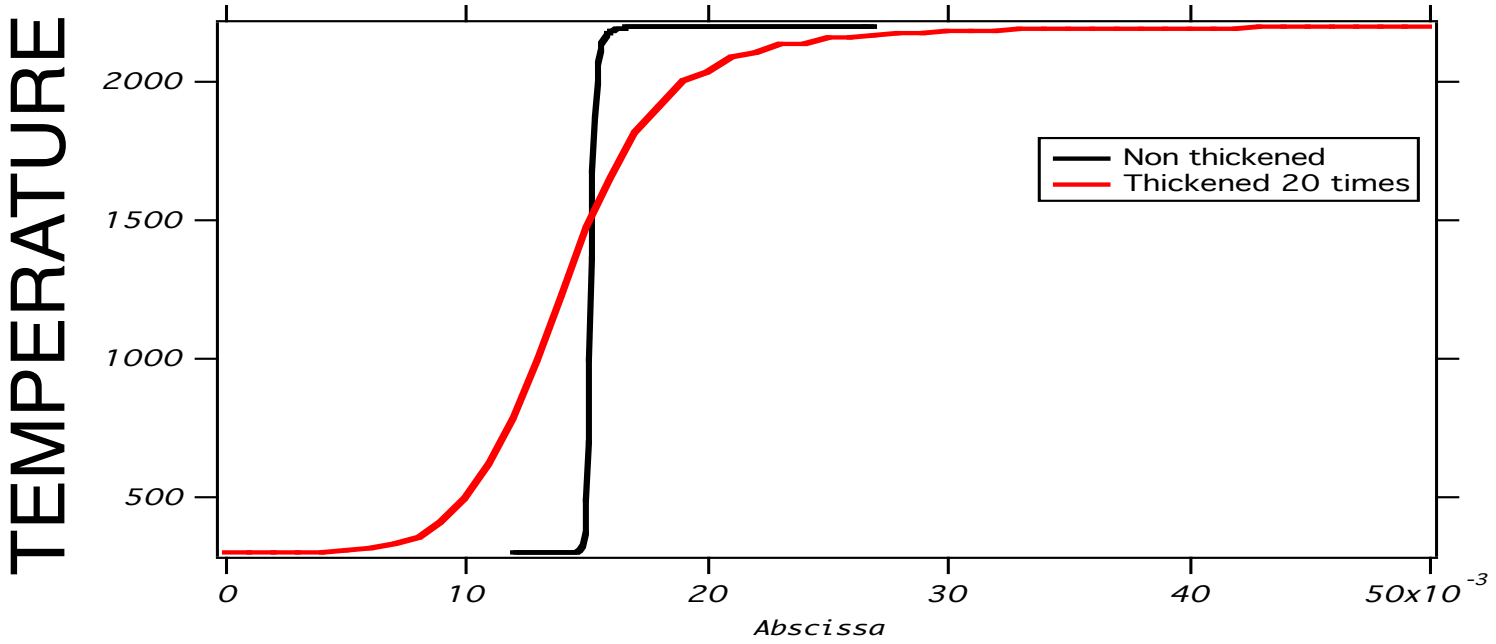
$$\delta = \frac{D_{th}^1}{s_L}$$

$$d/dt(\rho Y_k) = \frac{\partial}{\partial x_i}(\rho D \mathbf{F} \frac{\partial Y_k}{\partial x_i}) + \frac{A}{\mathbf{F}}\rho Y_1 Y_2 ... Yn \exp(-\frac{T_a}{T})$$

$$\delta = \frac{\mathbf{F} D_{th}^1}{s_L}$$

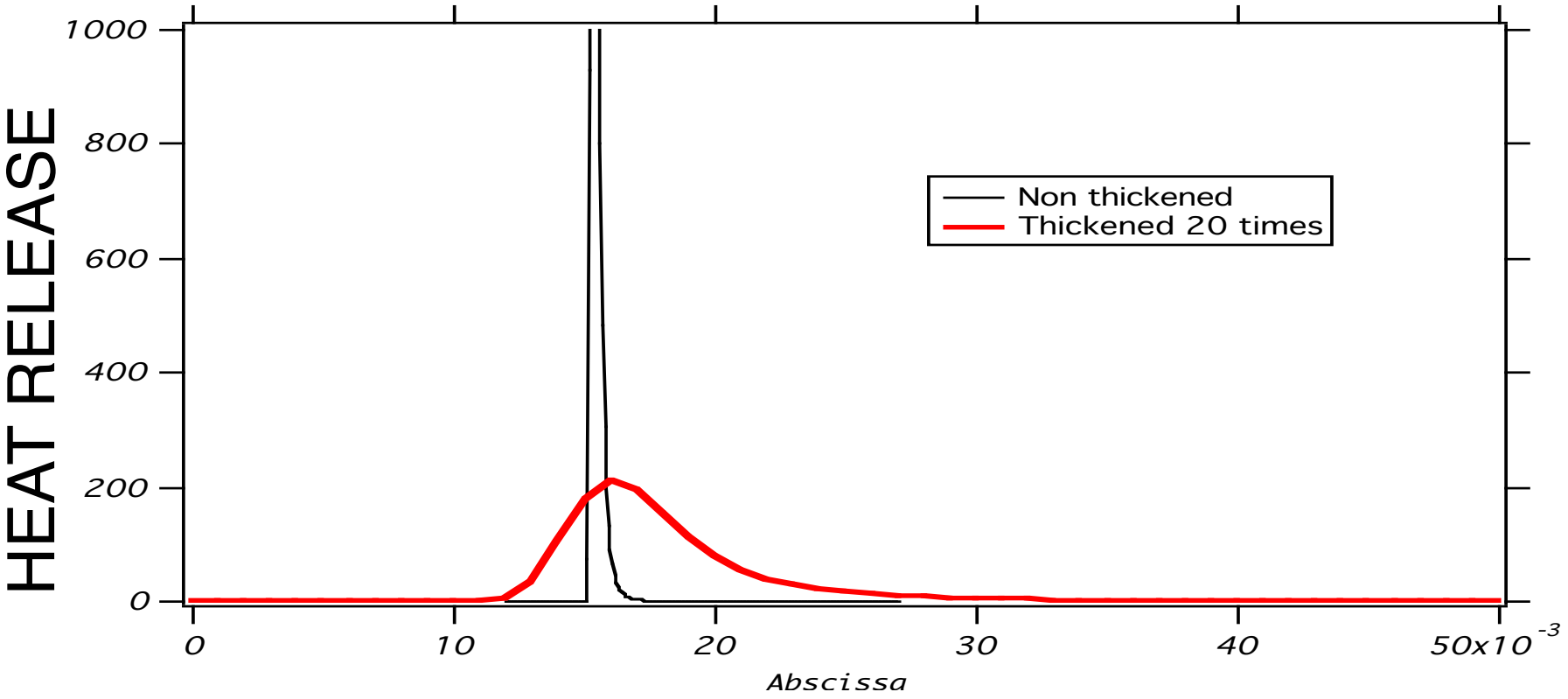
Same flame speeds with both equations !

In a numerical world where we fight with resolution… this can help !



Thickened and unthickened (F=20) flames for CH4/air premixed flames

For heat release: it is much easier when the flame is thick...



For turbulent flames: this property is the basis for the TFLES (thickened flame) model

FLAME SPEED OR FLAME SPEEDS ?

Ch. 2.7

★ **There are many flame speeds:**

★ **Absolute speed** s_a

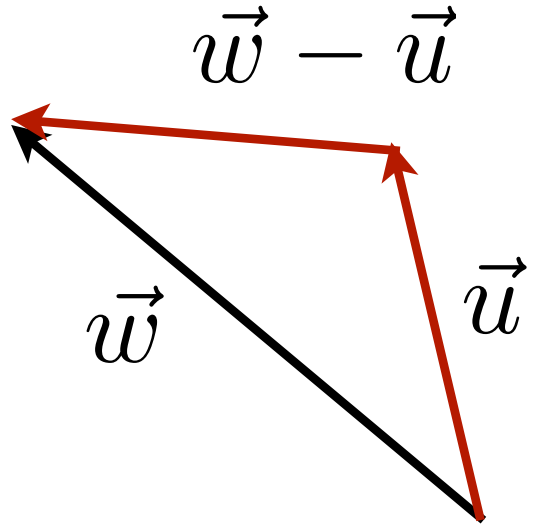
★ **Displacement speed** s_d **(here we use only the speed vs fresh gas)**

★ **Consumption speed** s_c

Identification	Definition
Absolute	Flame front speed relative to a fixed reference frame
Displacement	Flame front speed relative to the flow
Consumption	Speed at which reactants are consumed

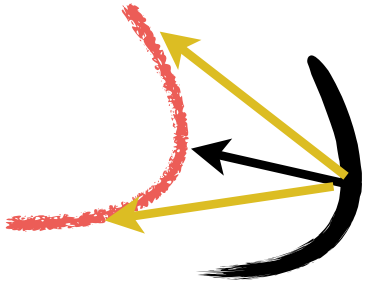
SPEEDS ARE .. VECTORS !

- At each point in the flow:
  - The flow moves with a speed $\vec{u}$
  - The flame moves with a speed $\vec{w}$
  - A good flame speed should measure the relative velocity of the flame compared to the flow

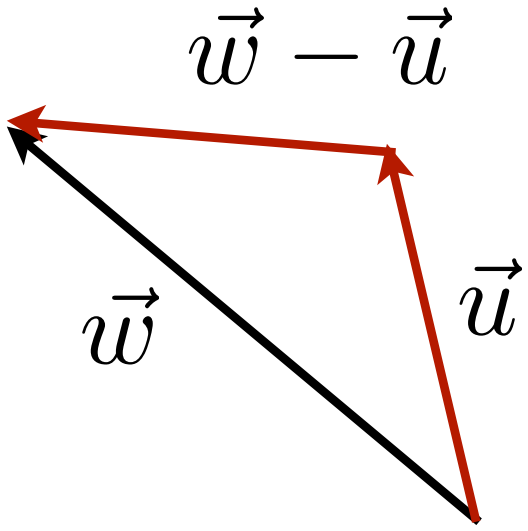


BUT THE SPEED OF A SURFACE (THE FLAME) IS NOT A 'STANDARD' SPEED:

- ONLY THE DISPLACEMENT OF THE FRONT NORMAL TO ITSELF IS IMPORTANT:



- USE FLAME NORMAL POINTING TOWARDS FRESH GAS:

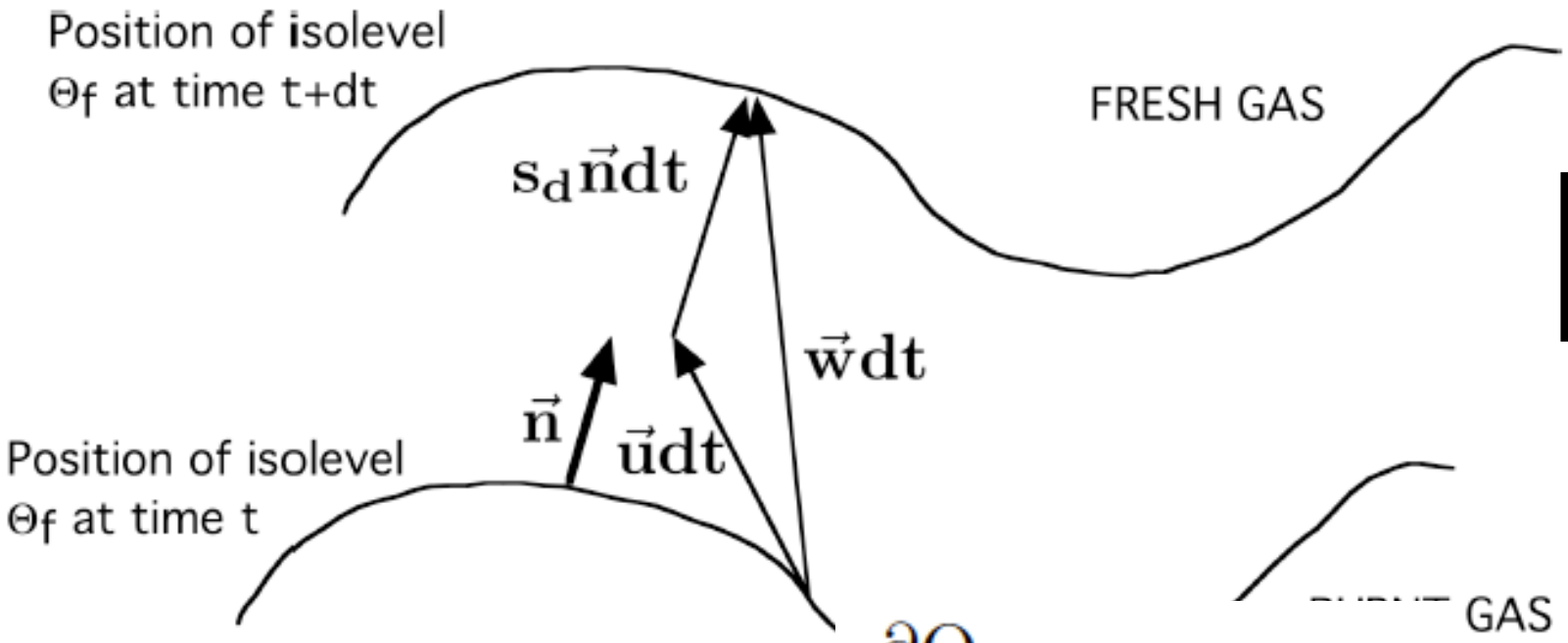


$$\vec{\mathbf{n}} = -\frac{\nabla\theta}{|\nabla\theta|}$$

$$s_a = \vec{w}.\vec{n}$$

$$s_d = (\vec{w} - \vec{u}).\vec{n}$$

THE ABSOLUTE FLAME SPEED s_a



$$s_a = \vec{w}.\vec{n}$$

An iso theta line follows:

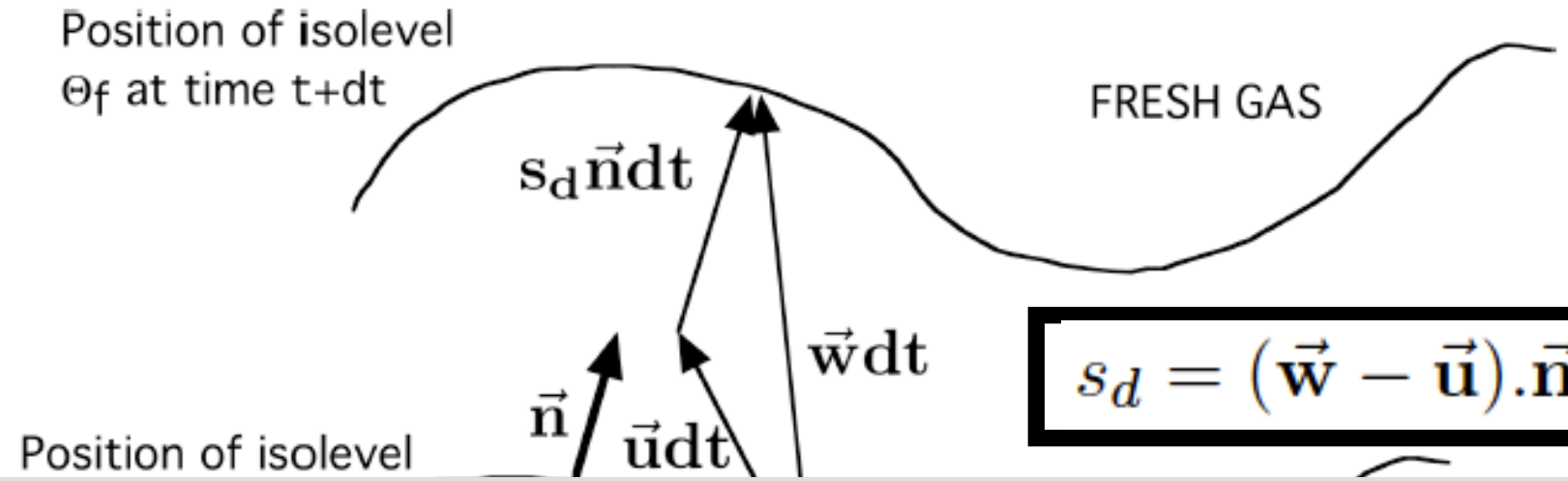
$$\frac{\partial \Theta}{\partial t} + \vec{\mathbf{w}}.\nabla\Theta = 0$$

$$\vec{\mathbf{n}} = -\frac{\nabla\theta}{|\nabla\theta|}$$

$$s_a = \vec{\mathbf{w}}.\vec{\mathbf{n}} = \frac{1}{|\nabla\Theta|}\frac{\partial\Theta}{\partial t}$$

EASY TO MEASURE EXPERIMENTALLY

THE DISPLACEMENT FLAME SPEED s_d



$$s_d = (\vec{\mathbf{w}} - \vec{\mathbf{u}}).\vec{\mathbf{n}} = s_a - \vec{\mathbf{u}}.\vec{\mathbf{n}}$$

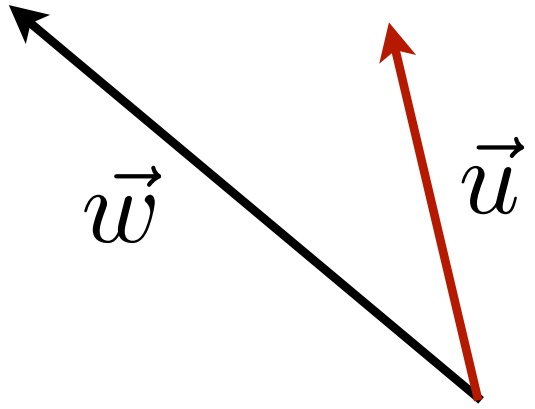
THIS IS THE SPEED USED IN G-EQUATION MODELS FOR TURBULENT FLAMES

$$s_d = \vec{\mathbf{w}}.\vec{\mathbf{n}} - \vec{\mathbf{u}}.\vec{\mathbf{n}} = \frac{1}{|\nabla\Theta|}\frac{\partial\Theta}{\partial t} + \vec{\mathbf{u}}\frac{\nabla\Theta}{|\nabla\Theta|} = \frac{1}{|\nabla\Theta|}\frac{D\Theta}{Dt}$$

DIFFICULT TO MEASURE EXPERIMENTALLY

DISPLACEMENT AND ABSOLUTE SPEEDS DEPEND ON THE POINT ON THE FLAME WHERE THEY ARE MEASURED:

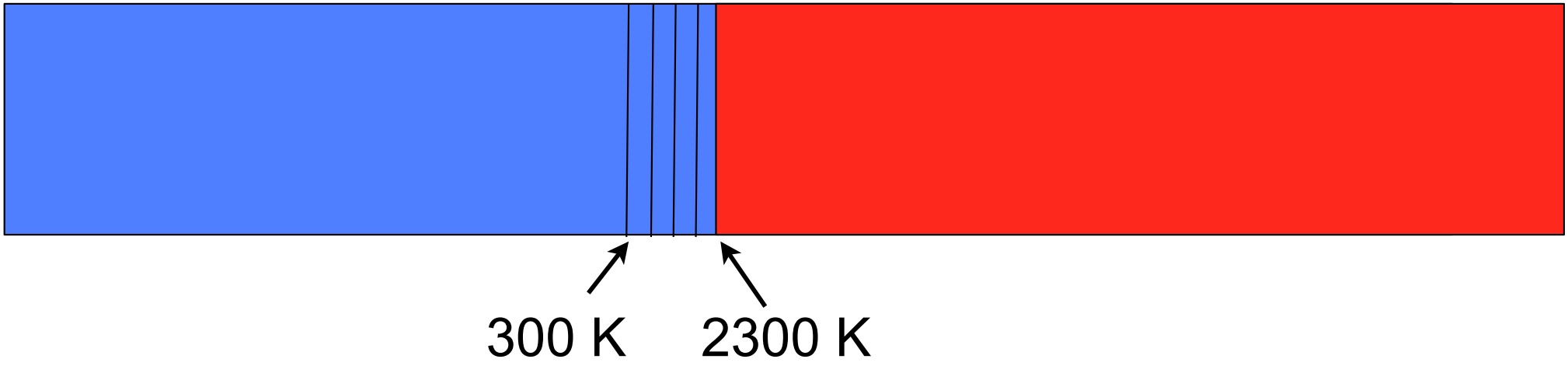
- ★Front speeds are usually defined as the speed of an iso-‘something’ (temperature, species, etc)
- ★This velocity varies strongly with the choice of the isolevel chosen to define it because the flow velocity varies strongly through the flame front (previous slide)



- ★All problems come from the fact that density changes through the flame. A constant density flame is much easier

DISPLACEMENT FLAME SPEEDS ARE AMBIGUOUS:

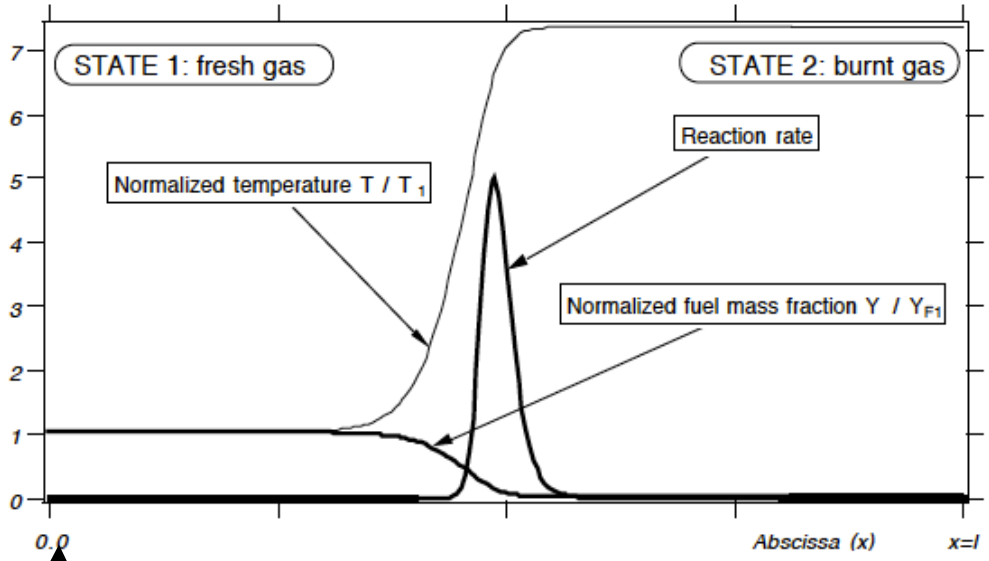
- **In a flame which keeps a constant thickness, *absolute* flame speeds of all isocontours are equal.**



- **Therefore since the FLOW speed changes significantly through the flame front, the *displacement* speed will depend strongly on the isocontour where it is measured…**
- **Big source of problems**

Example in the reference frame of a premixed laminar planar flame

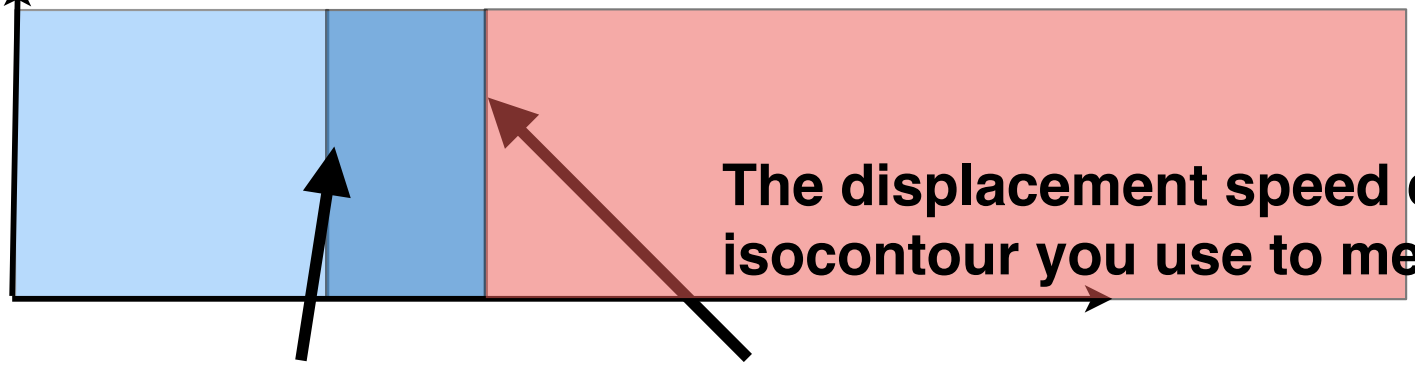
All isocontours of the flame front move at the same speed (thickness is constant)=> the absolute speed sa is constant. In this case it is zero



$$s_a = 0$$

$$s_d = (\vec{\mathbf{w}} - \vec{\mathbf{u}}).\vec{\mathbf{n}} = s_a - \vec{\mathbf{u}}.\vec{\mathbf{n}}$$

Since u depends on the position in the flame ie on θ :



$$s_d = f(\theta)$$

The displacement speed depends on the isocontour you use to measure it

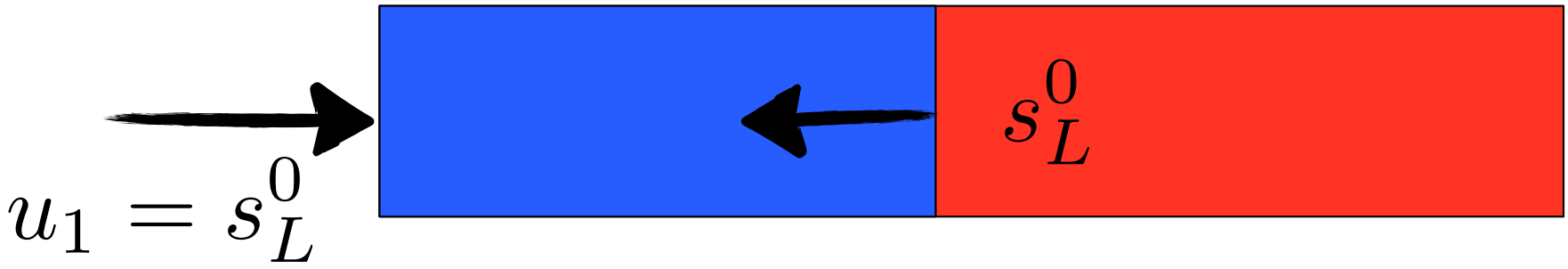
$\theta = 0.01$ $\theta = 0.99$

THE CONSUMPTION FLAME SPEED s_c

DEFINED FROM THE INTEGRAL OF THE REACTION RATE USING THE FLAME REFERENCE FRAME:

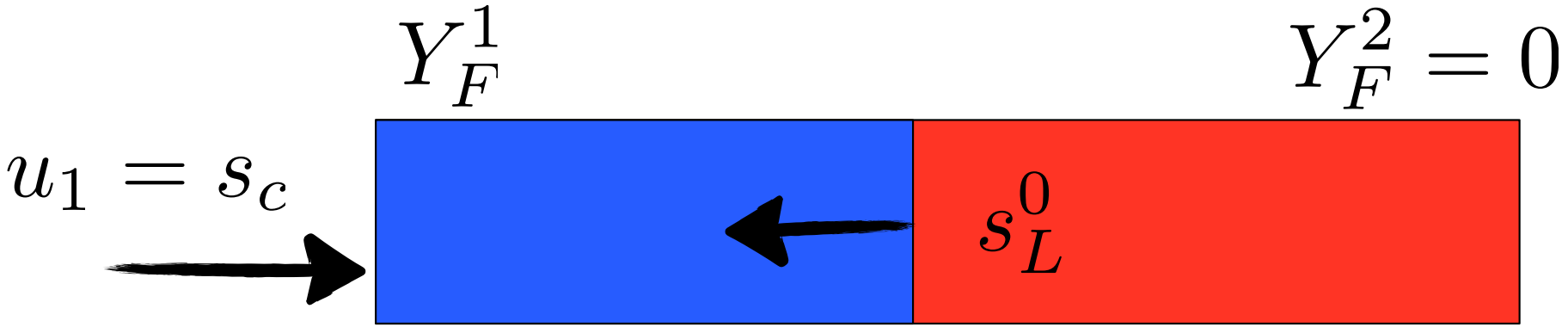
$$\rho u = \text{constant} = \rho_1 s_L$$

$$\rho_1 s_L \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F$$



INTEGRATE ALONG x FROM STATE 1 (fresh) TO STATE 2 (burnt):

$$\rho_1 s_L^0 (Y_F^2 - Y_F^1) = \int \dot{\omega}_F dx$$



$$s_c = -\frac{1}{\rho_1 Y_F^1} \int_{-\infty}^{+\infty} \dot{\omega}_F d\mathbf{n}$$

for lean flames

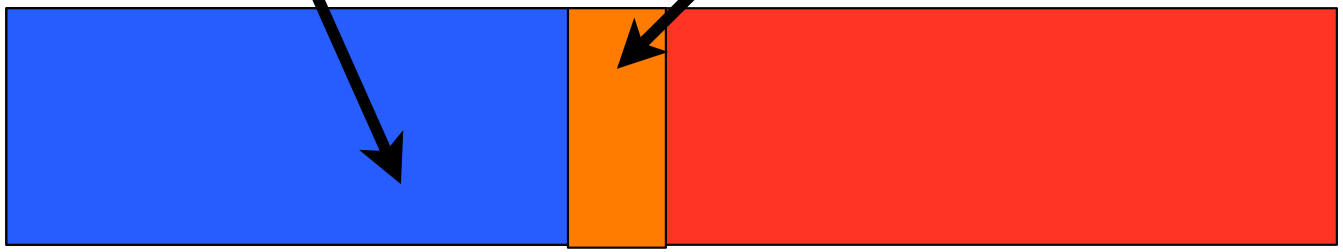
INDEPENDENT OF THE FRAME OF REFERENCE

CONSUMPTION SPEED: MEASURING THE INTEGRATED REACTION RATE

$$\rho_1 s_c Y_{F1} = -\int \dot{\omega}_F dx$$

Flux of fuel entering a unit area of flame

Fuel burnt in the flame front per unit area

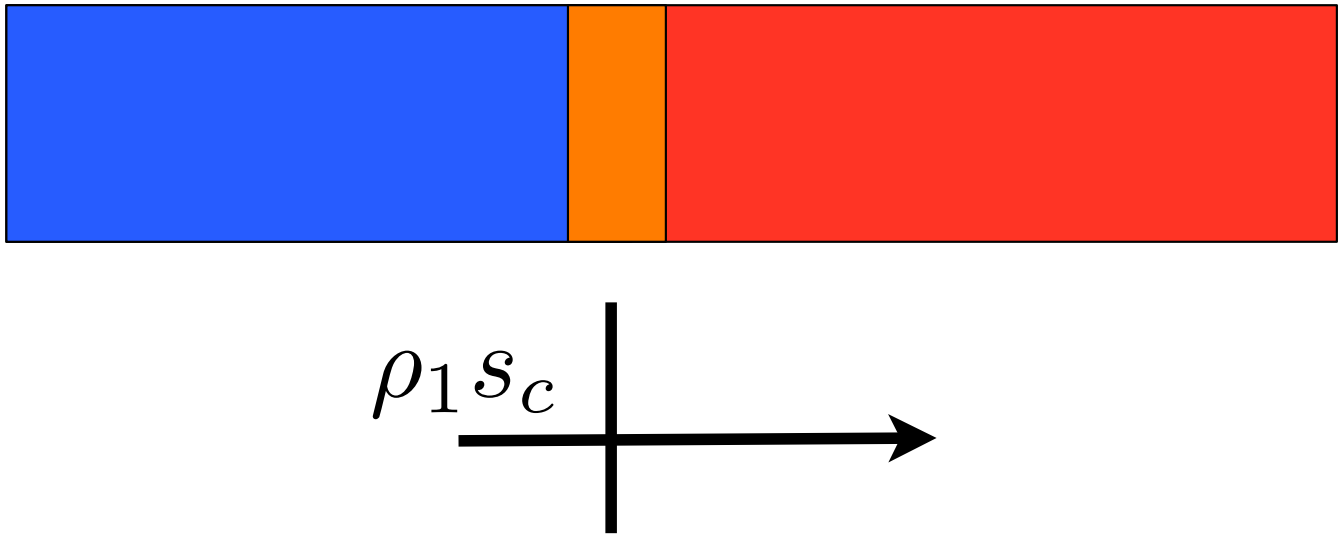


CONSUMPTION SPEED: VIEW THE FLAME AS A MEMBRANE WITH IMPOSED FLUX

Flux of fuel per unit area of flame: $\rho_1 s_c Y_{F1}$

Total flux of mass per unit area: $\rho_1 s_c$

Total flux of CO2 leaving the flame: $\rho_1 s_c Y_{CO_2}$



MULTIDIMENSIONAL EXTENSION:

- IF A FLAME HAS A TOTAL SURFACE Σ (WHATEVER ITS SHAPE IS)
- AND THE MEAN CONSUMPTION SPEED ALONG THE SURFACE IS s_c
- THE TOTAL FUEL CONSUMPTION RATE IS KNOWN:

$$(s_c \rho_1 Y_F^0)\Sigma$$

(BASELINE EQUATION FOR FLAMELET MODELS)

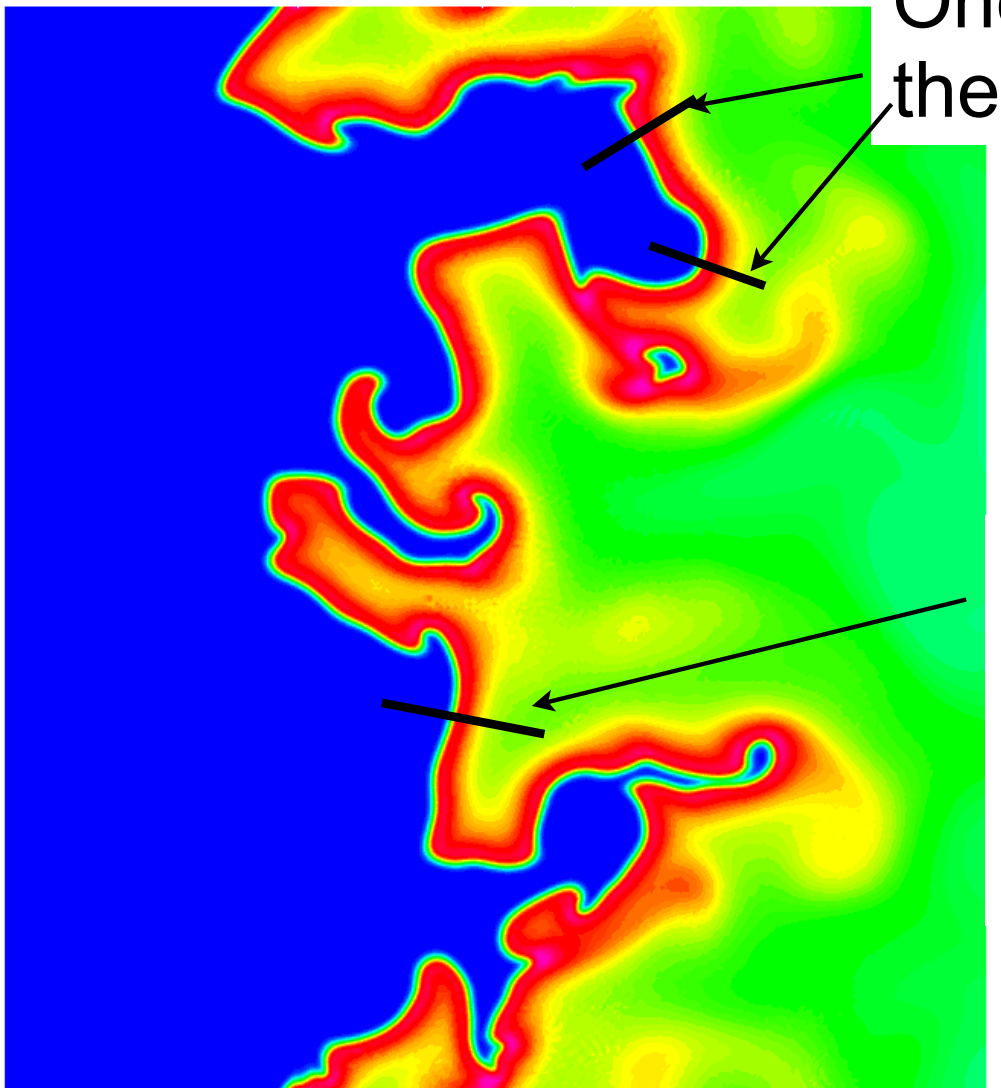
DIFFERENT CONCEPTS:

★THE CONSUMPTION SPEED IS AN INTEGRATED VALUE ALONG THE FLAME NORMAL. IT CAN CHANGE ALONG THE FLAME SURFACE BUT DOES NOT DEPEND ON THE POSITION NORMAL TO THE FLAME FRONT

★THE DISPLACEMENT AND ABSOLUTE SPEEDS CHANGE ALONG THE FLAME SURFACE BUT ALSO DEPEND ON THE VALUE OF THE ISOCONTOUR WHERE THE MOVEMENT IS MEASURED.

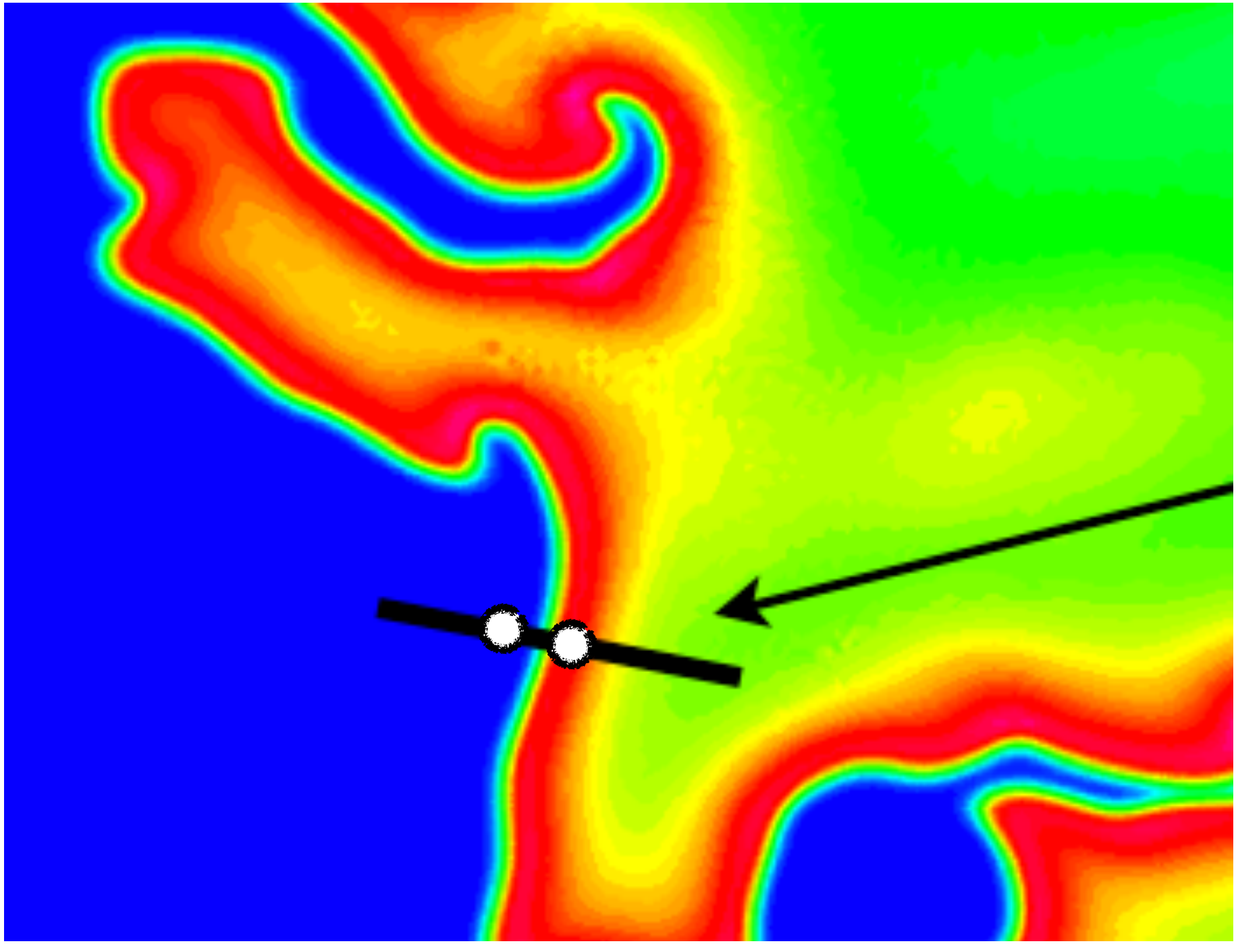
$$s_d = (\vec{\mathbf{w}} - \vec{\mathbf{u}}).\vec{\mathbf{n}} = s_a - \vec{\mathbf{u}}.\vec{\mathbf{n}}$$

DEPENDENCE OF SPEEDS WITH SPACE



One s_c for each location on the surface

Multiple s_d's for each location on the surface (one per isolevel)



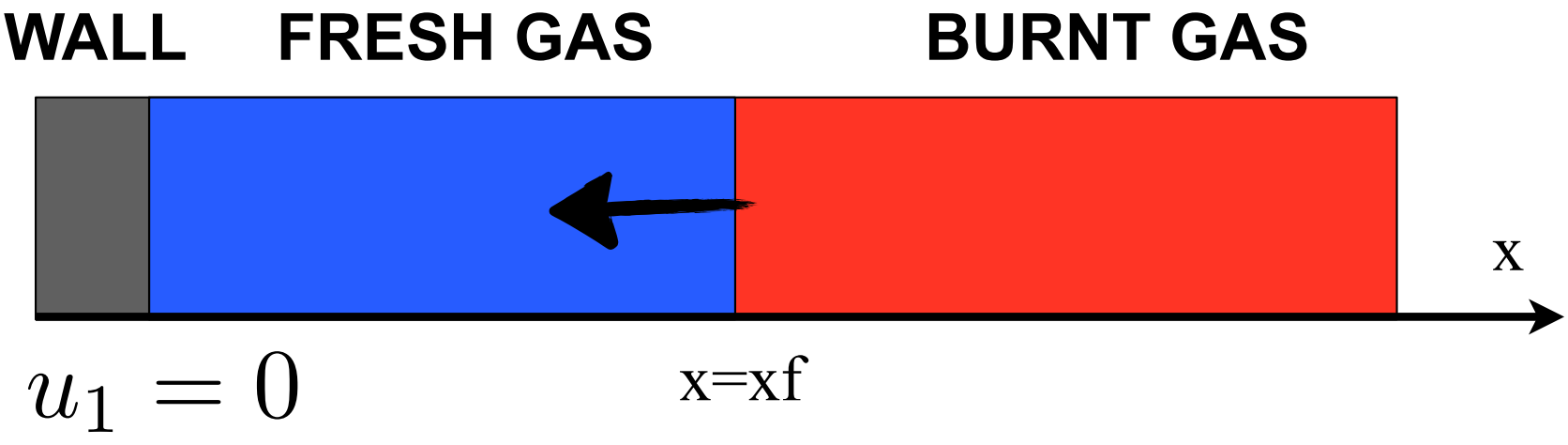
FOR PLANAR UNSTRETCHED FLAMES:

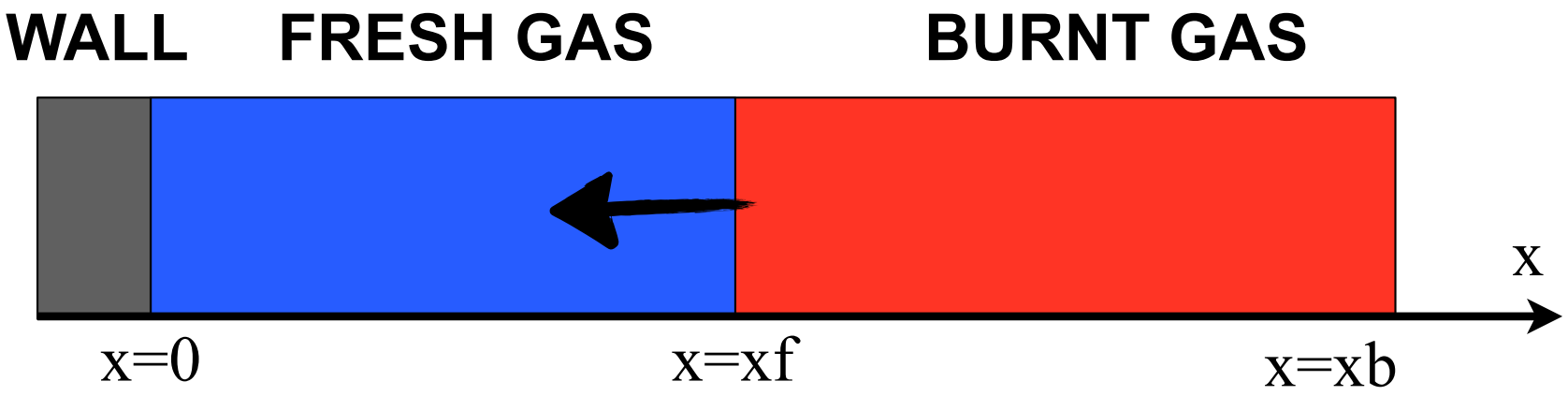
Let us study three cases:

- **Flame in a fixed frame of reference propagating towards a wall** $\longrightarrow u_1 = 0$
- **Flame in its own frame of reference** $\longrightarrow u_1 = s_L^0$
- **Frame propagating away from a wall** $\longrightarrow u_2 = 0$

FOR ALL THESE FLAMES, ASSUME THAT THE CONSUMPTION SPEED IS THE SAME AND EQUAL TO THE UNSTRETCHED LAMINAR FLAME SPEED

1/ IN A FIXED FRAME OF REFERENCE: A FLAME GOING TOWARDS A WALL





$$\frac{\partial \rho Y_F}{\partial t} + \frac{\partial (\rho u Y_F)}{\partial x} = \frac{\partial}{\partial x}(\rho D \frac{\partial Y_F}{\partial x}) + \dot{\omega}_F$$

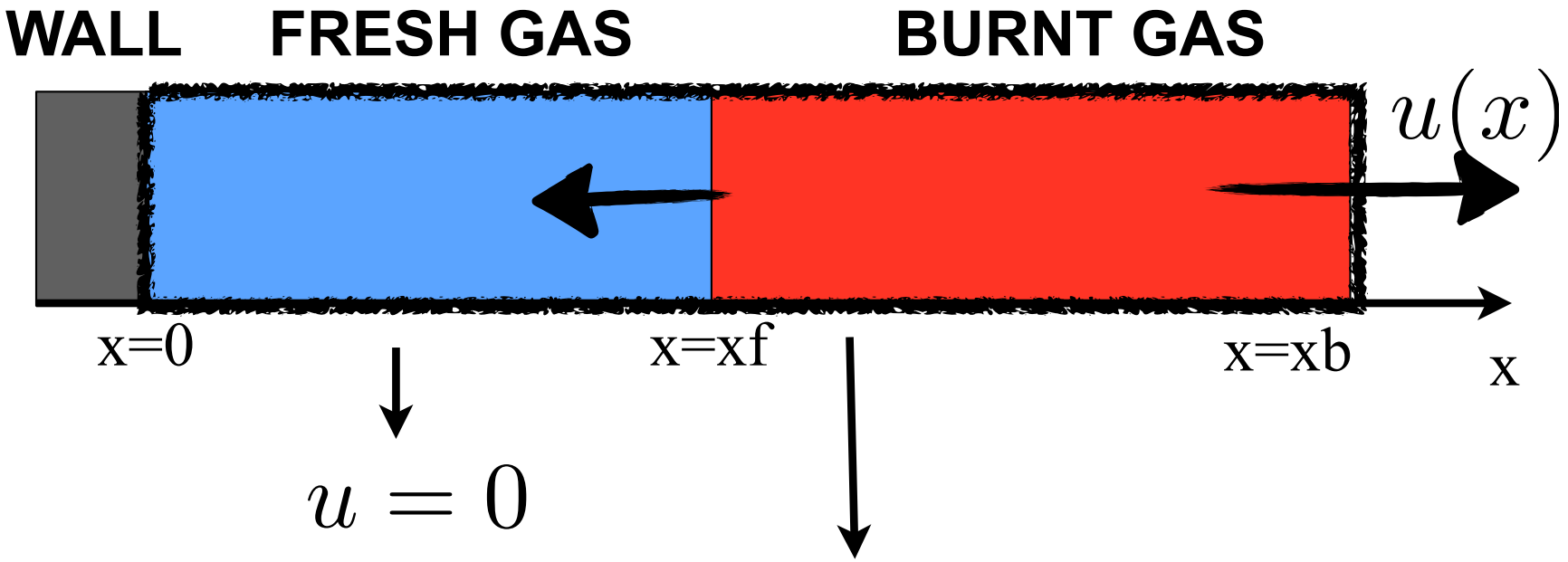
INTEGRATE BETWEEN WALL (x=0) AND BURNT GAS (x=xb):

$$\frac{\partial m_F}{\partial t} + [\rho u Y_F]_{x=0}^{x=x_b} = [\rho D \frac{\partial Y_F}{\partial x}]_{x=0}^{x=x_b} + \int_{x=0}^{x=x_b} \dot{\omega}_F dx$$

$$\rho_1 Y_{F1} \frac{dx_f}{dt} \qquad 0 \qquad 0 \qquad -\rho_1 Y_{F1} s_c$$

$$\boxed{\frac{dx_f}{dt} = -s_c}$$

WHAT IS THE FLOW SPEED ?



For any position in the burnt gas xb:

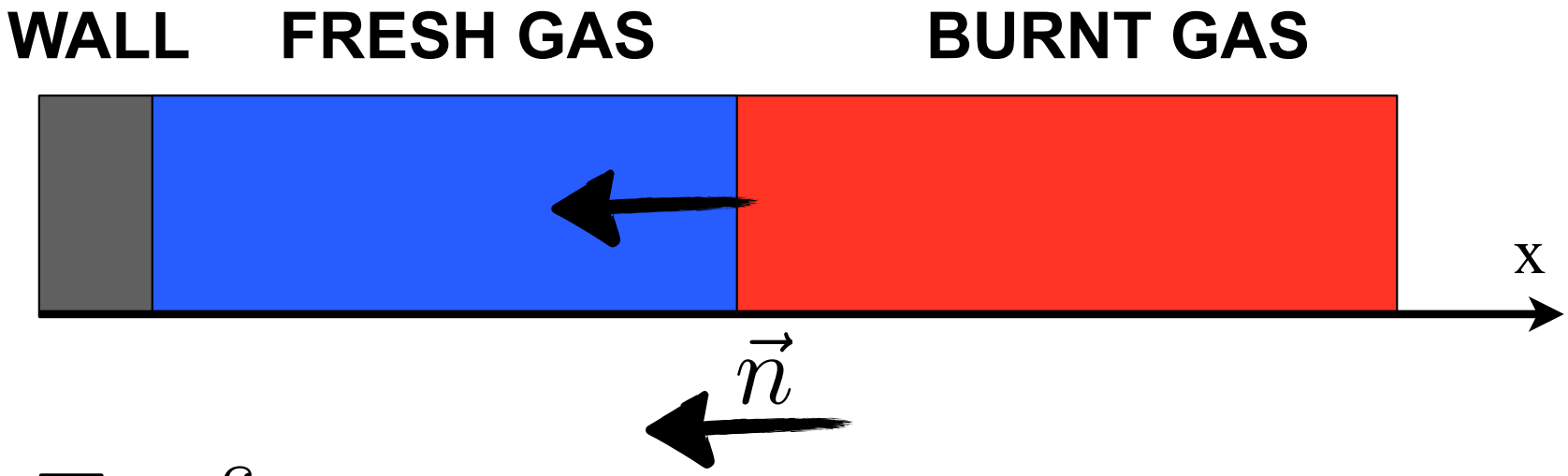
$$M = \rho_1 x_f + \rho_2 (x_b - x_f)$$

$$\frac{dM}{dt} = -\rho_2 u$$

$$\frac{dx_f}{dt} = -s_c$$

$$u(x_b) = (\frac{\rho_1}{\rho_2} - 1) s_c$$

WHAT IS THE DISPLACEMENT SPEED ?



$$\frac{dx_f}{dt} = -s_c$$

$$s_a = \vec{w}.\vec{n} = \frac{dx_f}{dt}\vec{x}.\vec{n} = s_c$$

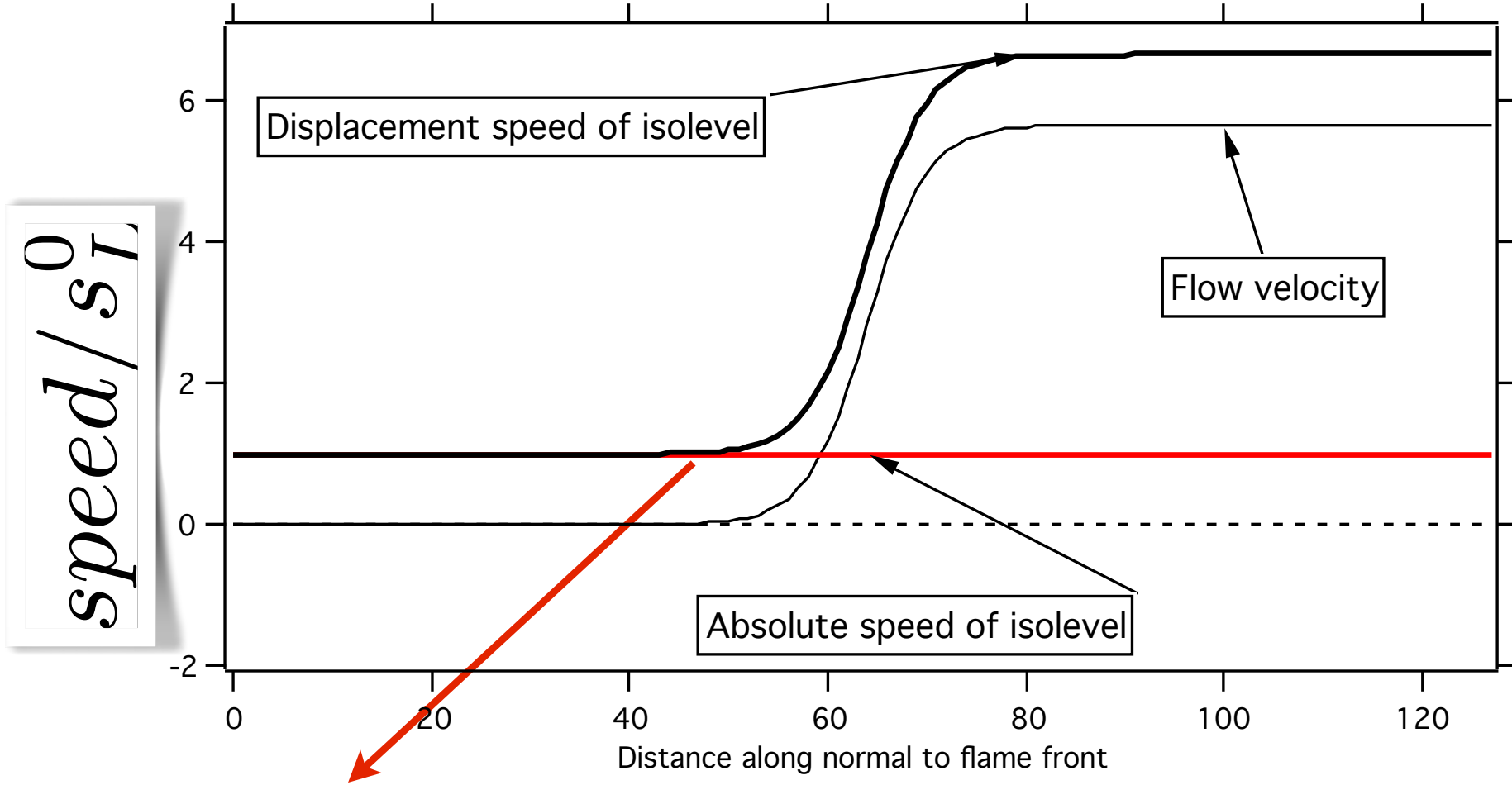
$$s_d = s_a - \vec{u}.\vec{n} = s_c + (\frac{\rho_1}{\rho} - 1)s_c = \frac{\rho_1}{\rho}s_c$$

Displacement (in the fresh gas), absolute and consumption speeds are equal. This is the only case where this is true

$s_d(\theta = 0) = s_a = s_c = s_L^0$ **Unstretched laminar flame speed**

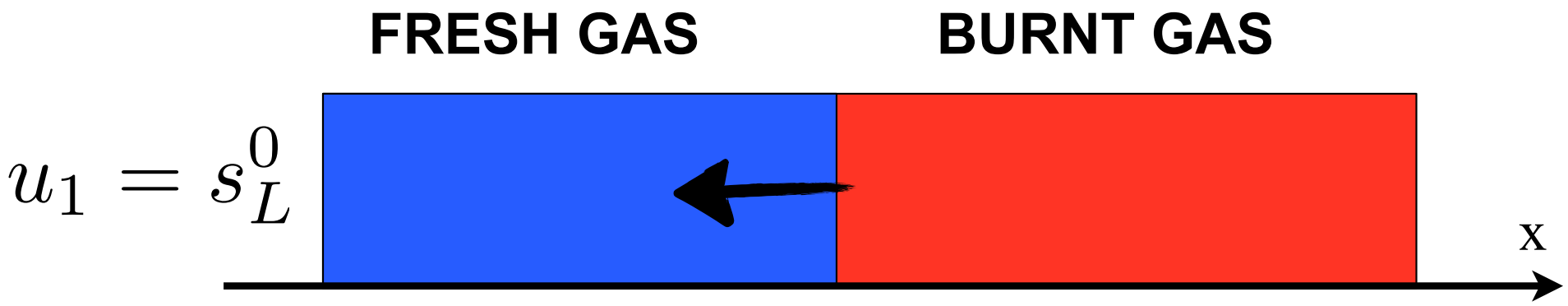
SPEEDS IN A FLAME PROPAGATING TOWARDS A WALL

$$\frac{\rho_1}{\rho_2} = \frac{T_2}{T_1} = 7$$



Note the very large variations of the displacement speed
The only place where it is equal to s_c is in the fresh gas

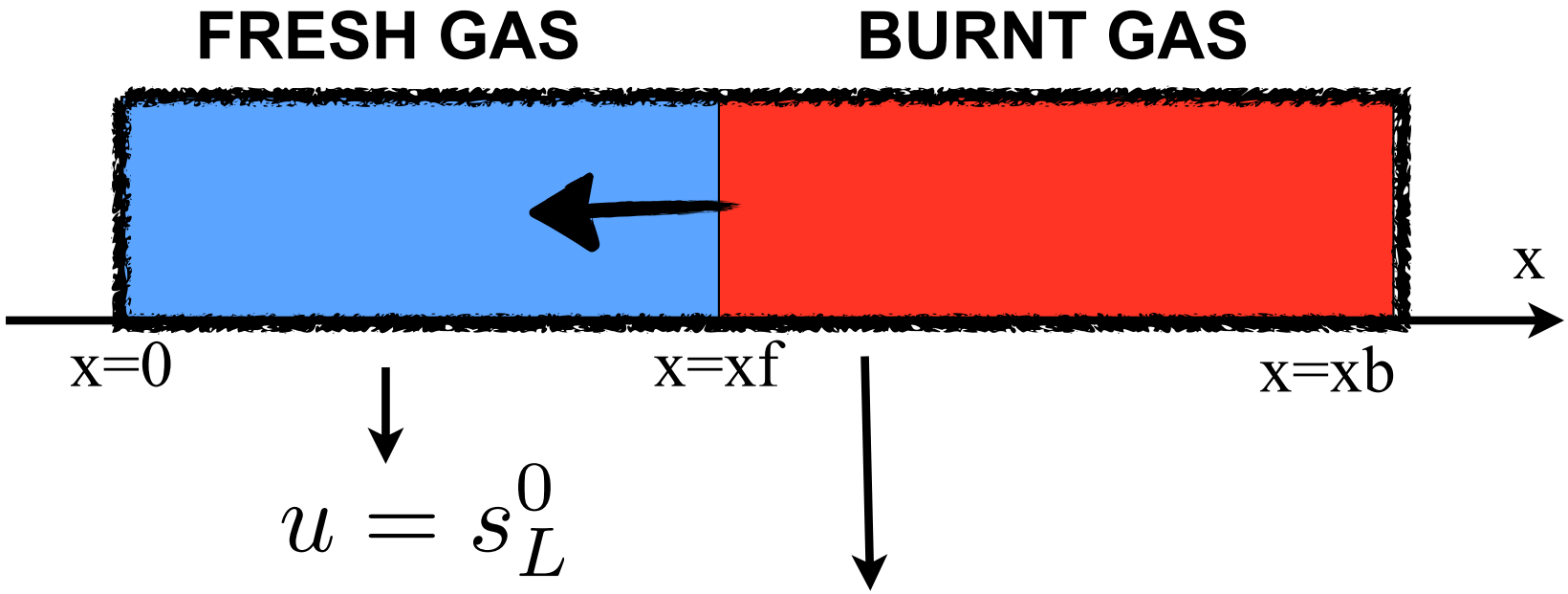
2/ A FIXED FLAME (IN ITS FRAME OF REF.)



The absolute speed is zero

$$s_a = \frac{dx_f}{dt} = 0$$

WHAT IS THE FLOW SPEED ?

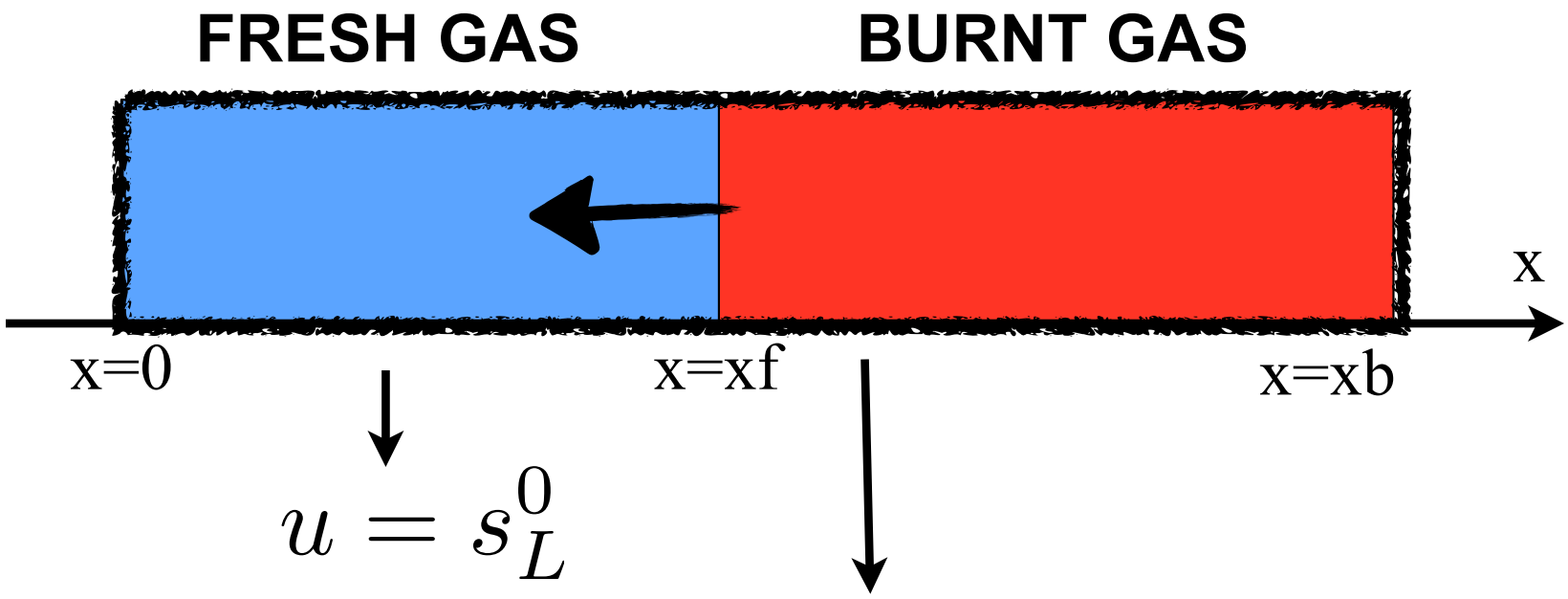


For any position in the burnt gas xb:

$$\rho_1 s_L^0 = \rho u$$

$$u = \frac{\rho_1}{\rho} s_L^0$$

WHAT IS THE DISPLACEMENT SPEED ?

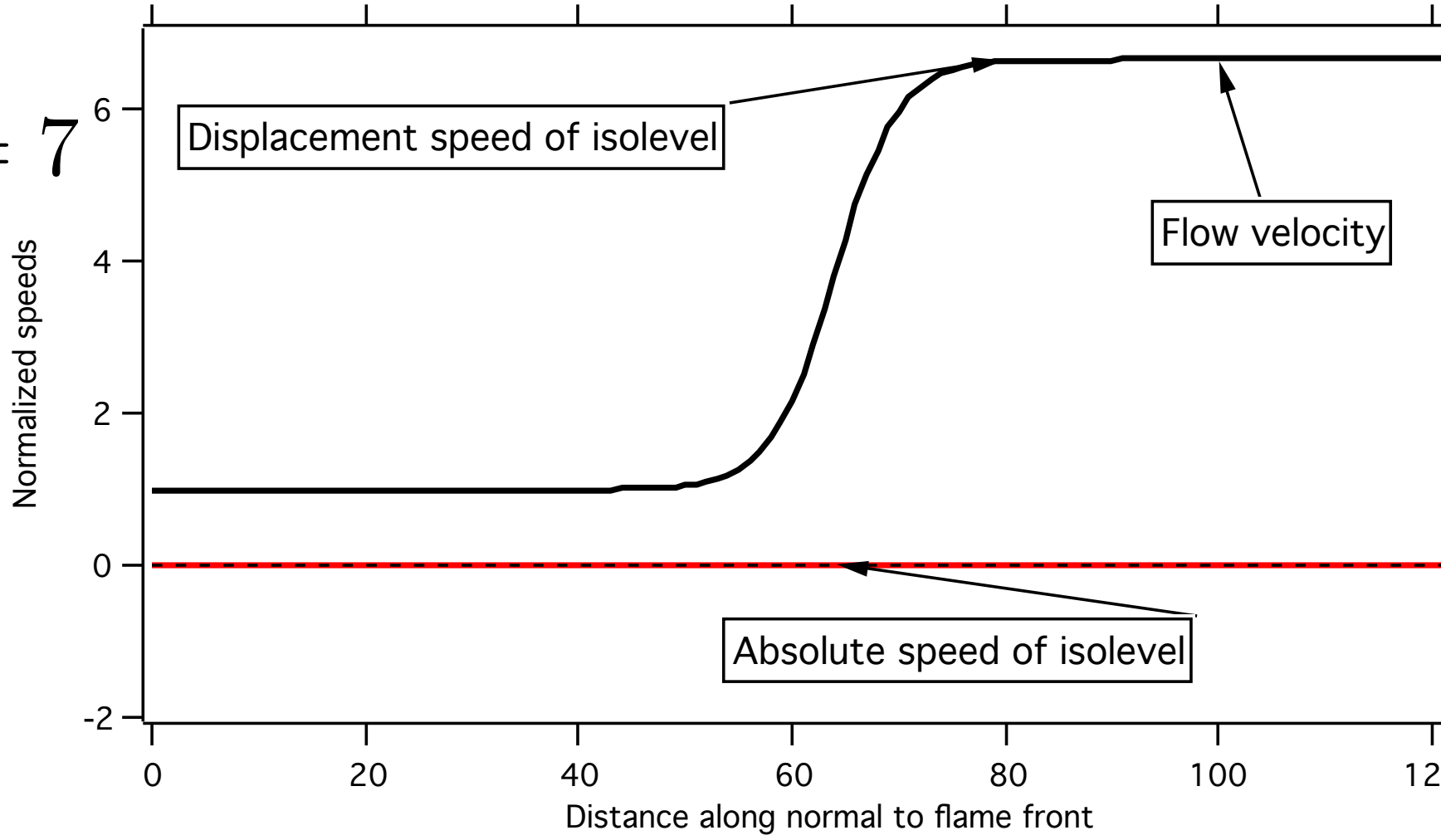


$$s_d = s_a - \vec{u}.\vec{n} = 0 - \frac{\rho_1}{\rho} s_c(-1) = \frac{\rho_1}{\rho} s_c$$

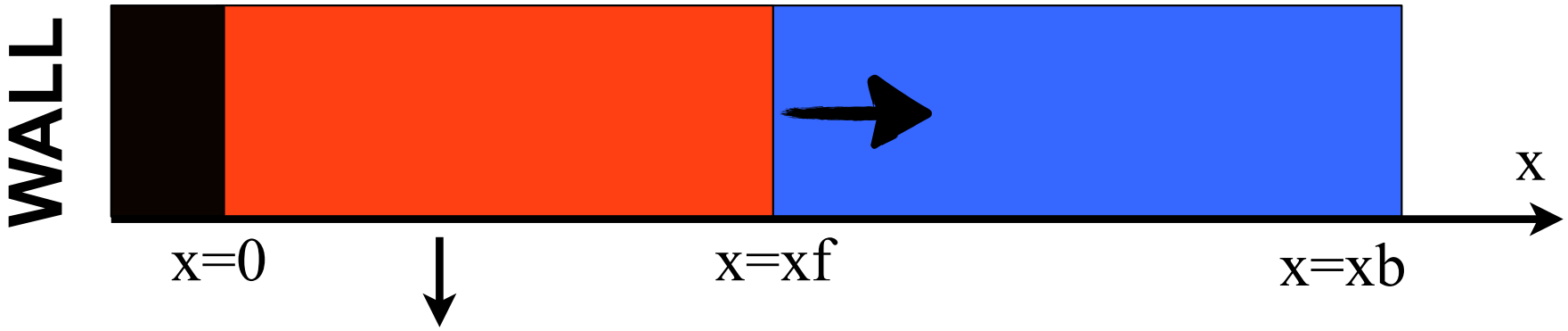
Careful: we 'count' absolute speeds along the normal from burnt to fresh gas

SPEEDS IN A FIXED FLAME:

$$\frac{\rho_1}{\rho_2} = \frac{T_2}{T_1} = 7$$

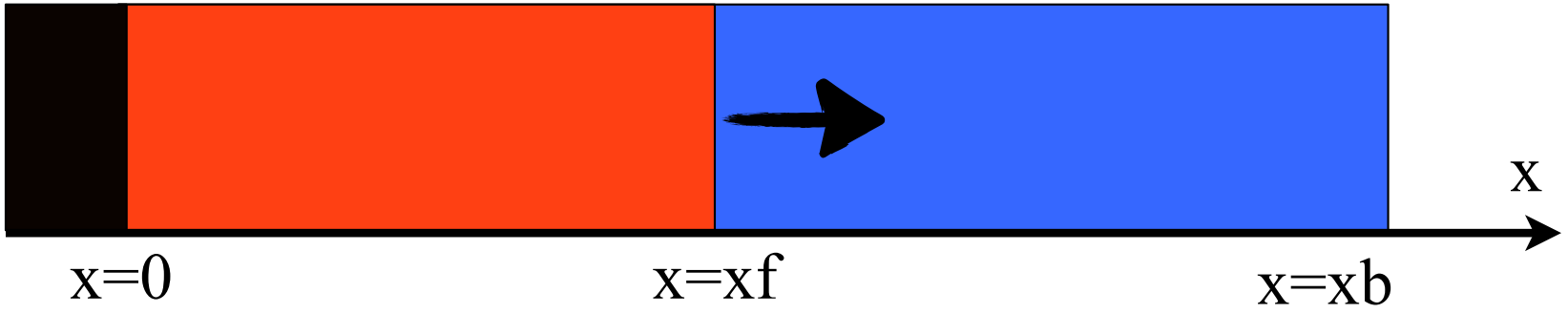


3/ A PLANAR PREMIXED FLAME PROPAGATING AWAY FROM A WALL



Burnt gas cant move: $u = 0$

The consumption speed is still the same: $s_c = s_L^0$



What is the absolute speed of the front?

$$M_{CO_2} = x_f \rho_2 Y_{CO_2}$$

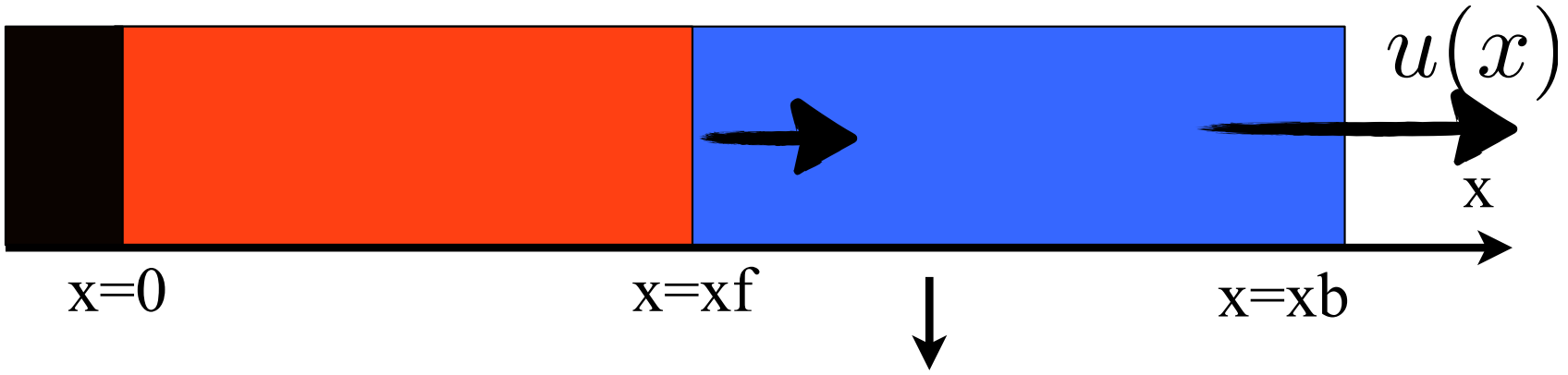
$$\frac{dM_{CO_2}}{dt} = \rho_1 Y_{CO_2} s_c$$

$$\frac{dx_f}{dt} = \frac{\rho_1}{\rho_2} s_c$$

$$s_a = \frac{dx_f}{dt} = \frac{\rho_1}{\rho_2} s_c$$

The flame 'moves' much faster than the flame speed. It is propelled by dilatation.

Careful: we 'count' absolute speeds along the normal from burnt to fresh gas



What is the flow speed in fresh gases ?

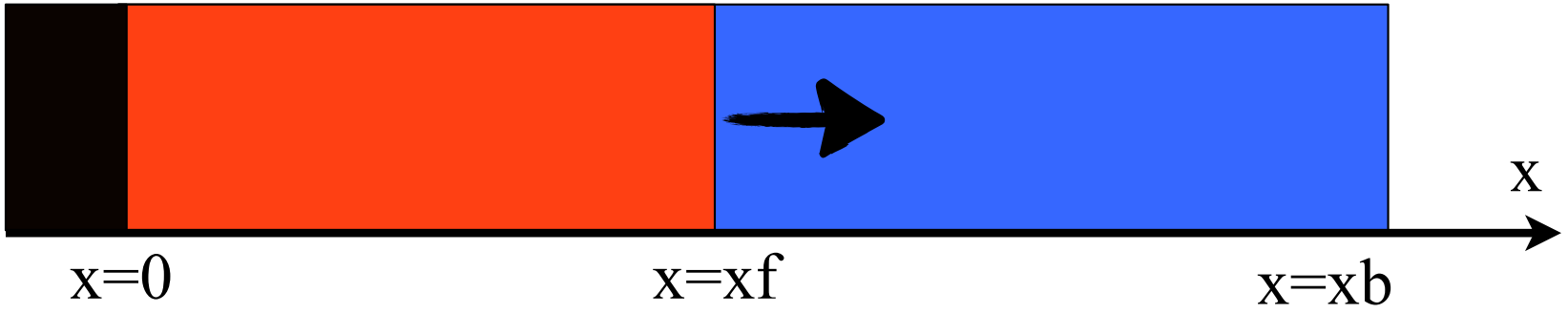
$$M = x_f \rho_2 + (x_b - x_f)\rho_1$$

$$\frac{dM}{dt} = -\rho_1 u$$

$$\frac{dx_f}{dt} = \frac{\rho_1}{\rho_2} s_c$$

$$u(x_b) = (\frac{\rho_1}{\rho_2} - 1)s_c$$

The flame pushes the fresh gases away



What is the displacement speed of the front at the flame location ?

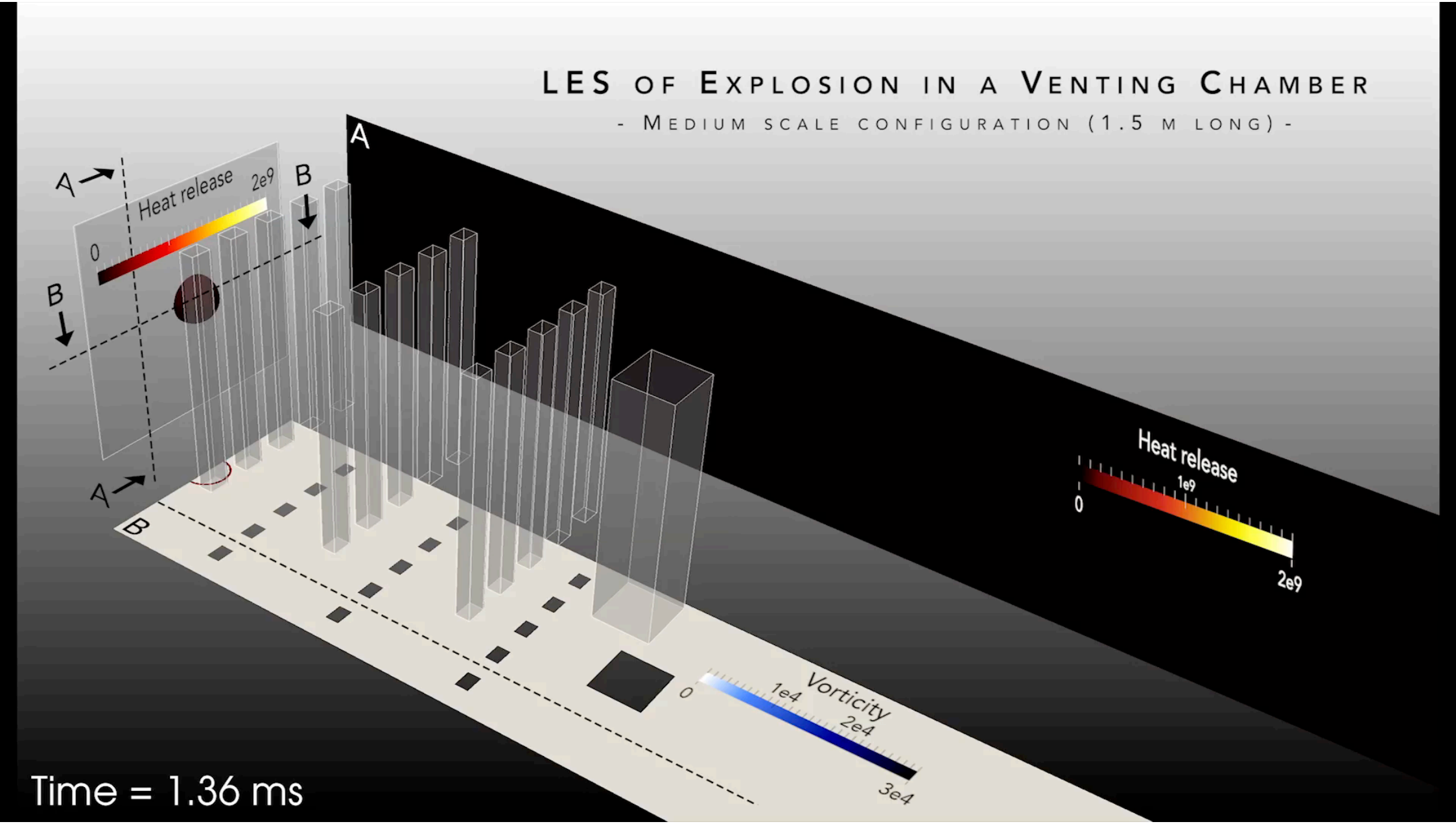
$$s_a = \frac{dx_f}{dt} = \frac{\rho_1}{\rho_2} s_c$$

$$u(x_b) = (\frac{\rho_1}{\rho_2} - 1) s_c$$

$$s_d = s_a - \vec{u}.\vec{n} = s_c$$

POSSIBLE ‘COMPLICATIONS’

- FRESH GASES FAR AWAY FROM THE FLAME FRONT ARE ACCELERATED (DILATATION EFFECT)
- IF THERE ARE OBSTACLES IN THIS REGION, THIS ACCELERATION CAN CREATE VORTICES, MAKE THE FLOW TURBULENT
- THIS ALLOWS THE FLAME TO ACCELERATE TOO WHEN IT WILL REACH THESE ZONES. THE FLAME CREATES ITS OWN TURBULENCE AND SPEED: « SELF ACCELERATION »
- THE FLAME MAY BECOME FASTER THAN THE SOUND SPEED
- A FLAME WHICH STARTS AT 30 cm/s CAN END UP AS A DETONATION AT 1600 m/s


LES OF EXPLOSION IN A VENTING CHAMBER
- MEDIUM SCALE CONFIGURATION (1.5 M LONG) -
A
B
A
B
Heat release
0
2e9
Heat release
0
1e9
2e9
Vorticity
0
1e4
2e4
3e4
Time = 1.36 ms

GENERAL CONCLUSIONS ON SPEEDS:

THE ABSOLUTE SPEED HAS NO GENERIC VALUE: IT DEPENDS ON THE FRAME OF REFERENCE

THE CONSUMPTION AND DISPLACEMENT SPEEDS ARE DIFFERENT. THE DISPLACEMENT SPEED IS OFTEN DIFFICULT TO USE

THE CONSUMPTION SPEED HAS A SIMPLE INTERPRETATION AND IS THE USEFUL QUANTITY TO USE FOR TURBULENT COMBUSTION MODELS: IT MEASURES THE REACTION RATE PER UNIT SURFACE

A few examples of more complicated laminar premixed flame speeds:

The oblique flame and the stagnation point flame: flames which dont move

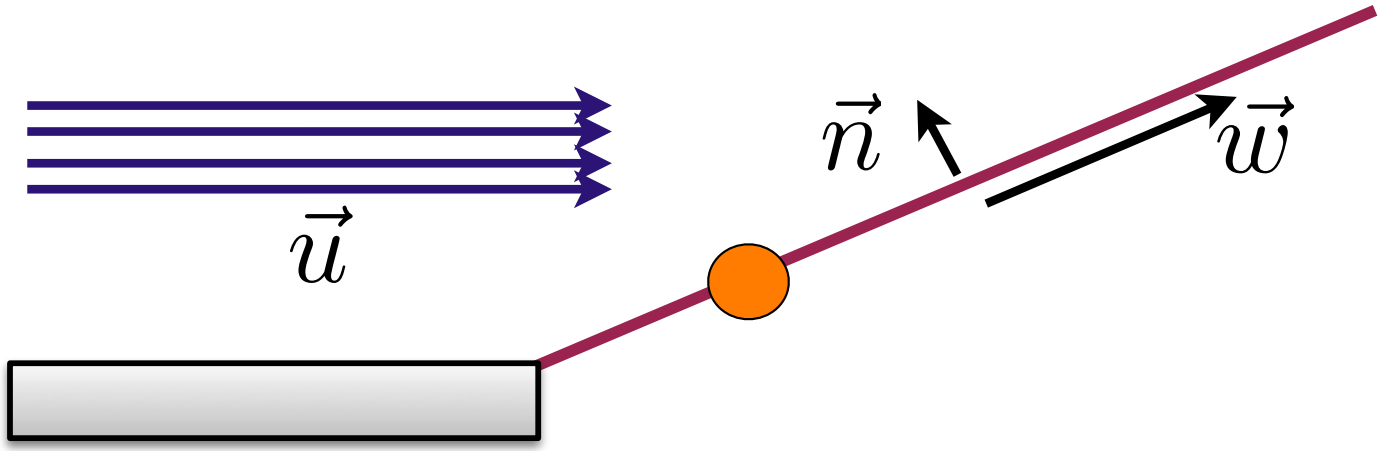
The flame tip

Flame cusps

Spherical flame

FLAMES WHICH DO NOT MOVE

Oblique premixed flame

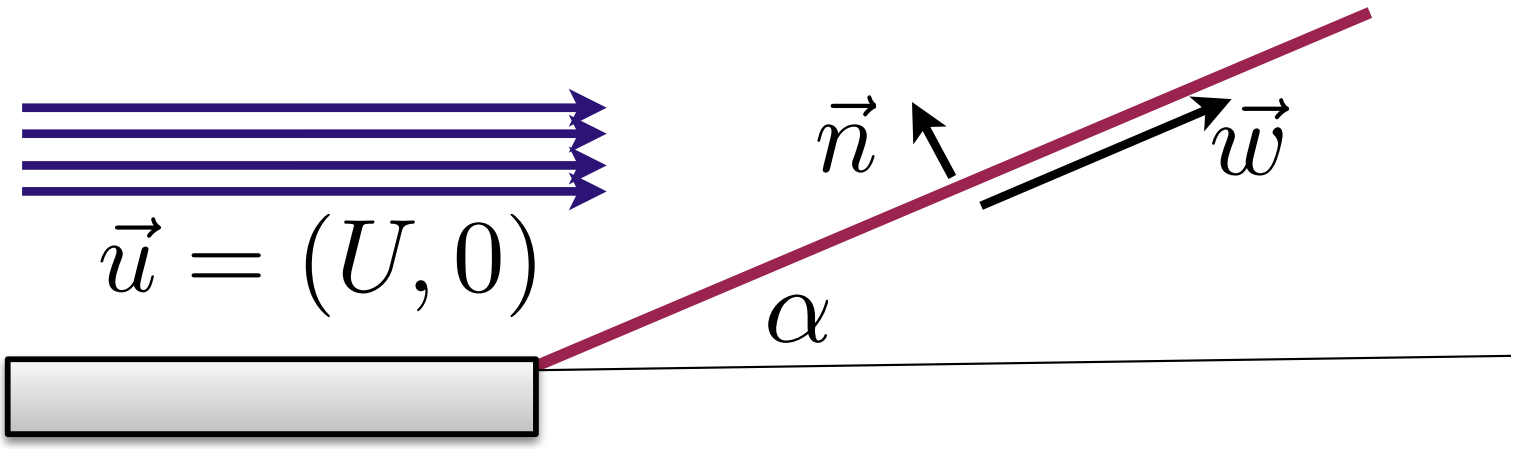


This flame does not move. It does not mean: $\vec{w} = \vec{0}$

It only means that: $\vec{w}.\vec{n} = 0$

FLAME ANGLE:

Oblique premixed flame



$\vec{w} = \vec{u} + s_d\vec{n}$ **and** $\vec{w}.\vec{n} = 0$

$\vec{u}.\vec{n} = -s_d$

$\vec{n} = (-sin(\alpha), cos(\alpha))$

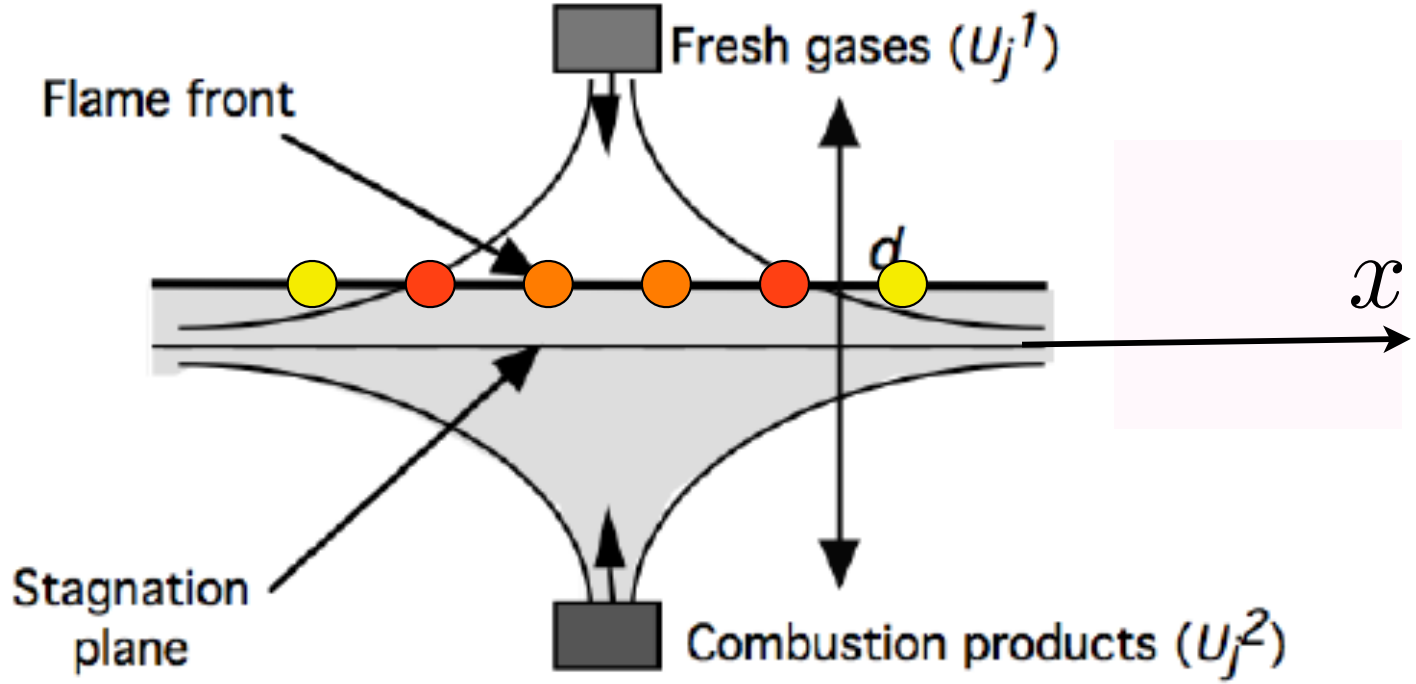
$sin(\alpha) = s_d/U$

STAGNATION POINT FLAME

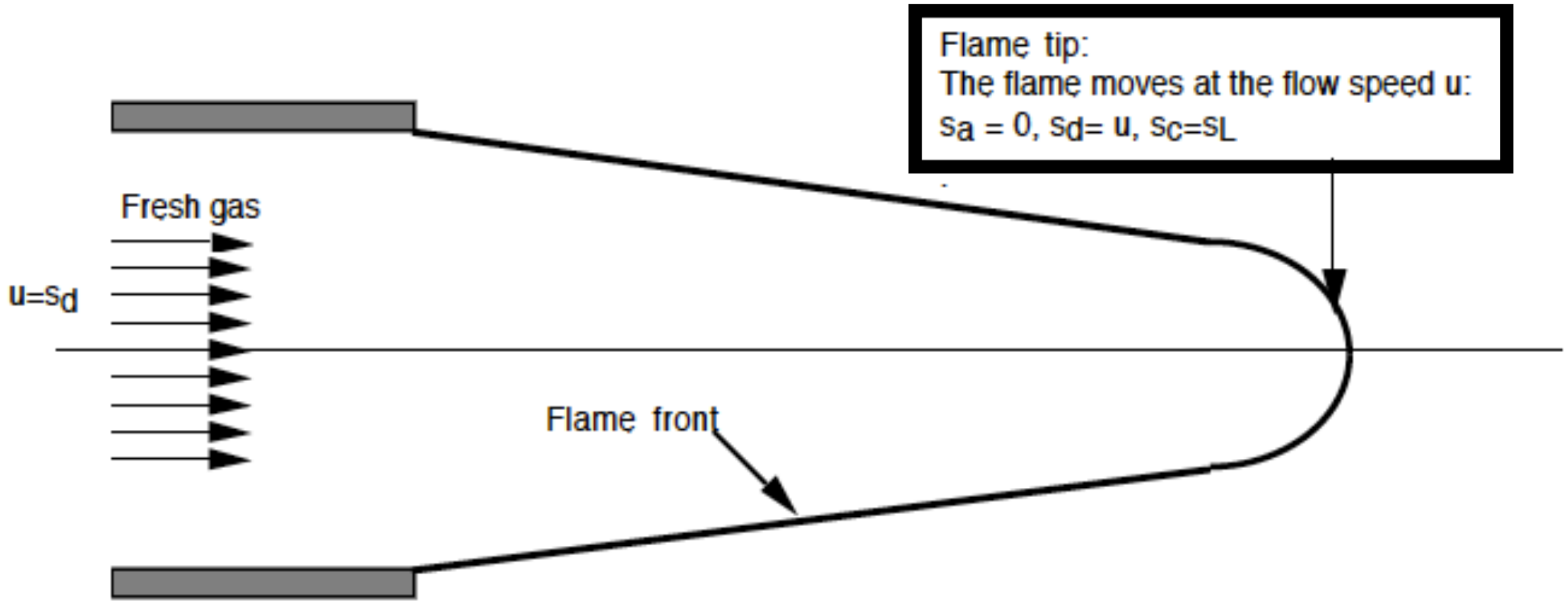
The flame does not move: $\vec{w}.\vec{n} = 0$

Particles do move along the flame front: $\vec{u}.\vec{n} \neq 0$

Particles get separated: the flame is stretched $\dfrac{\partial u_x}{\partial x} \neq 0$

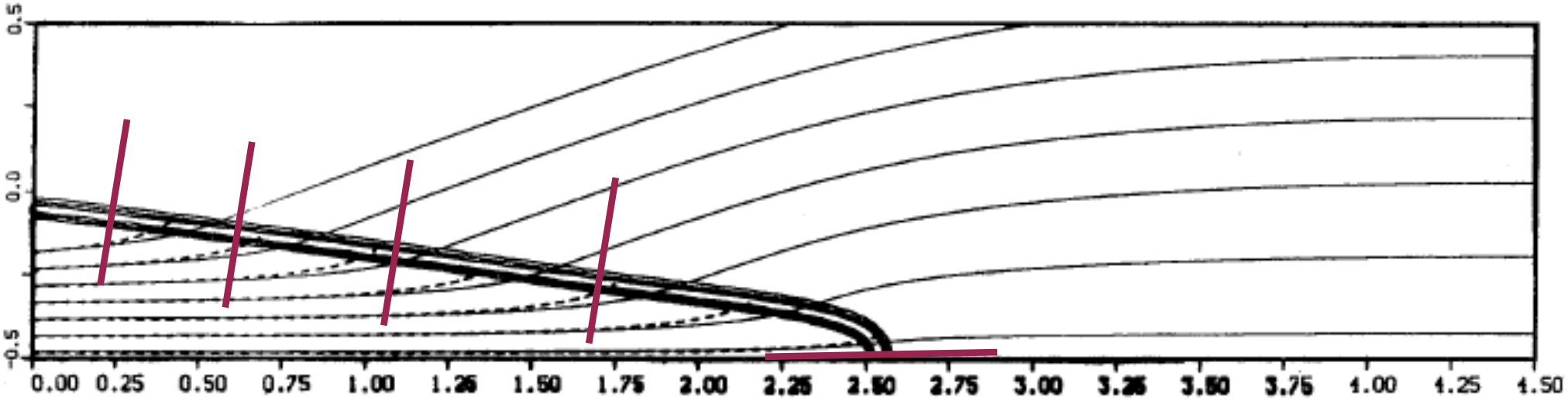


THE EXAMPLE OF THE FLAME TIP



The flow speed on the axis is 10 times larger than the flame speed.
The displacement speed at the tip is equal to the flow speed

$$s_d = u = 10 s_L^0$$

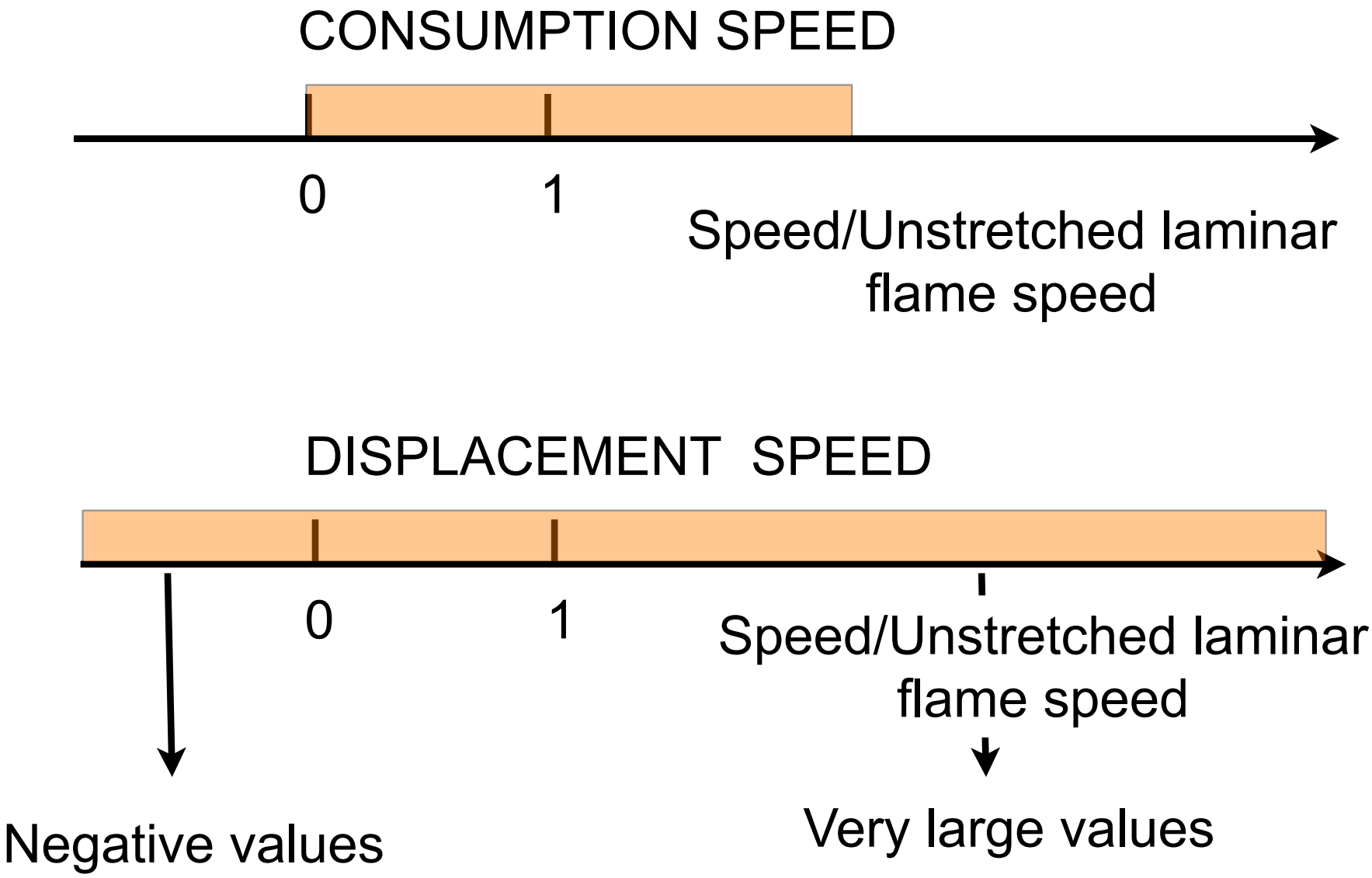


DNS of the flame tip for a flame with Lewis=1 (Poinsot, Echekki and Mungal, Comb. Sci. Tech, 1992, 81): streamlines and contours of reaction rate.

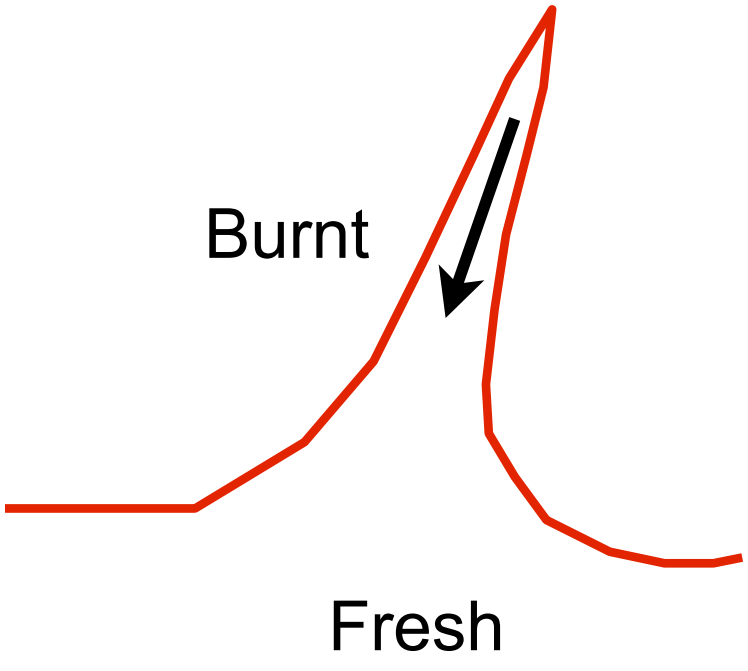
The consumption speed is the same along the flame front

It is equal to the laminar flame speed: $s_c = s_L^0$

The variations of flame speeds:



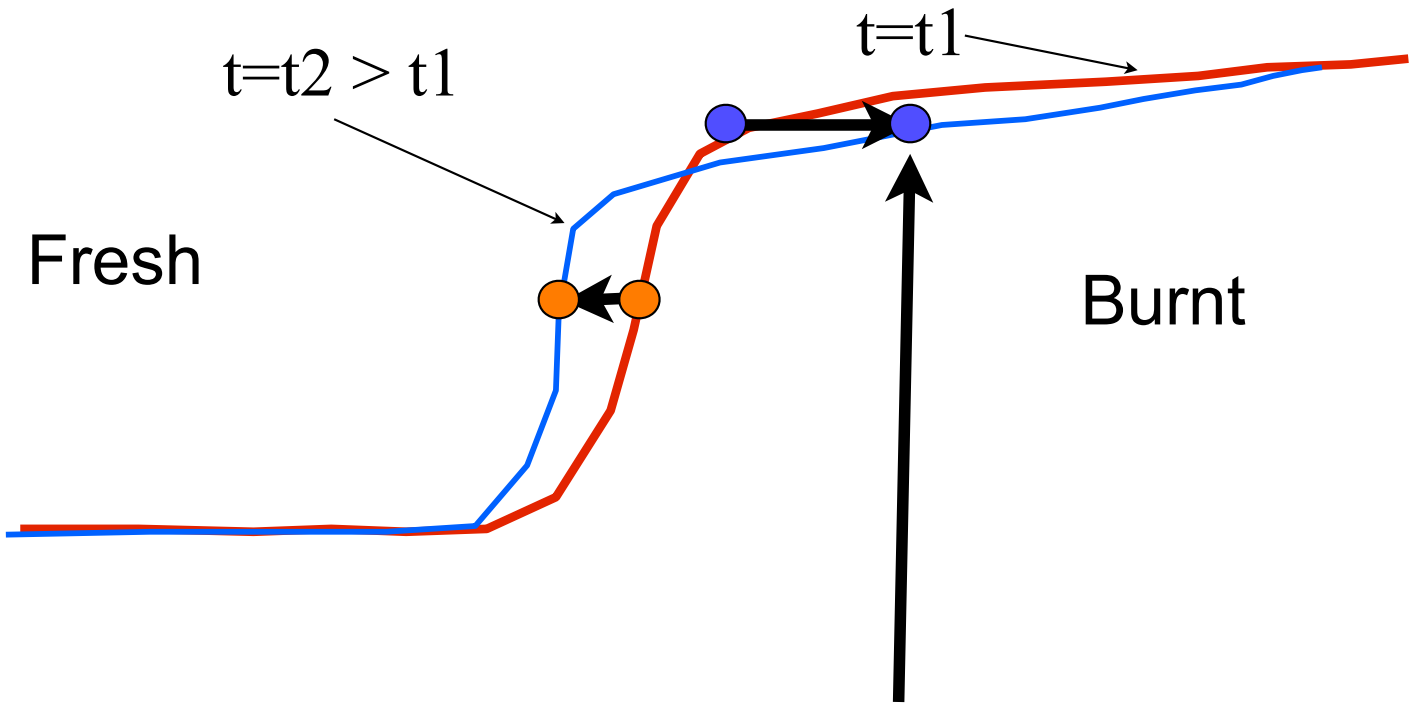
LARGE VALUES OF DISPLACEMENT SPEED: FLAME CUSPS



This point can move VERY FAST

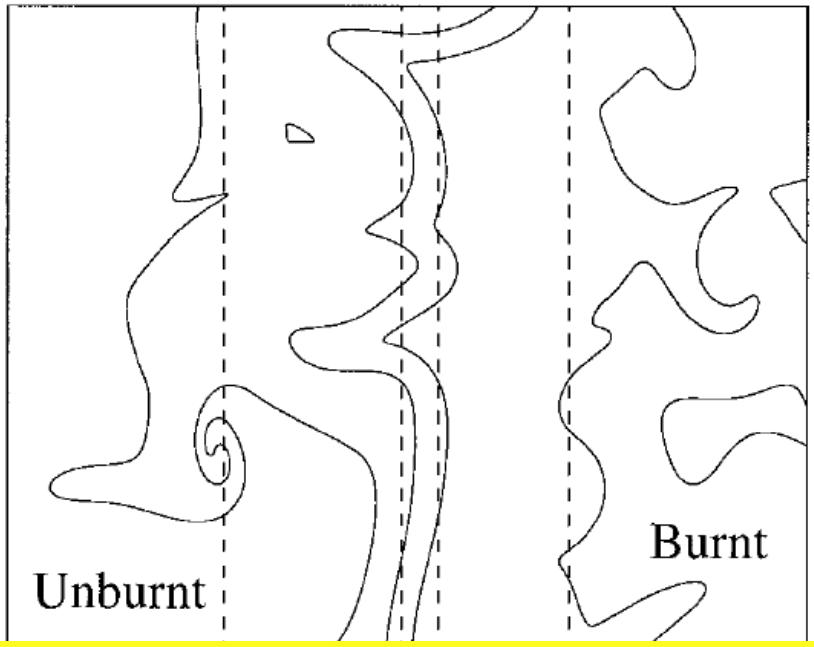
It will also be a problem for numerical methods using the displacement speed such as the G equation

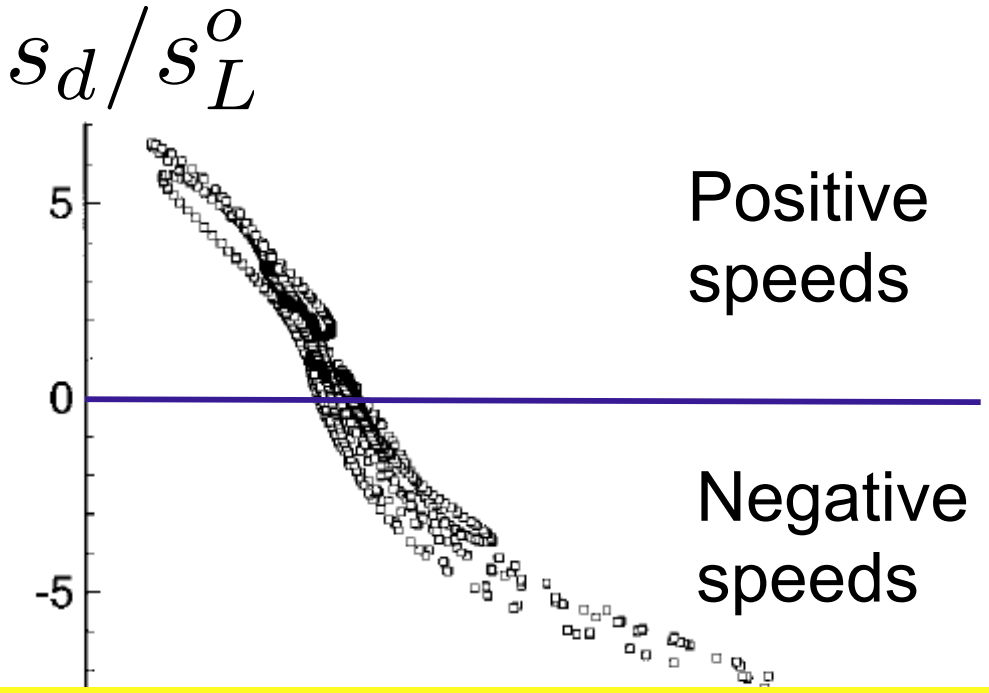
NEGATIVE VALUES OF DISPLACEMENT SPEED: VARYING THICKNESS



If the flame gets thicker, certain points can have negative velocities. This is often seen in DNS

DNS: displacement speed scatter plot vs curvature for the isoline Y_{CH4}=0.02

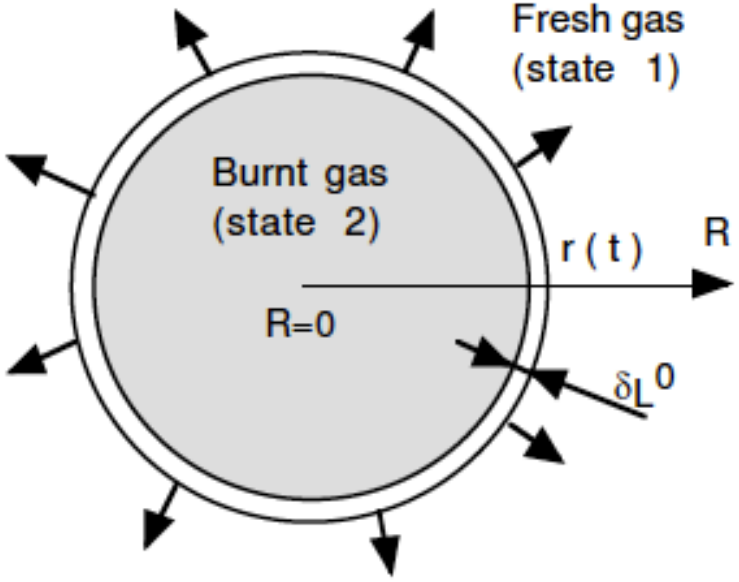




The displacement speed is a difficult quantity to manipulate. You may prefer the consumption speed

SPHERICAL FLAMES: ASSUME ZERO FLAME THICKNESS

Ch. 2, Sec 2.7.3



Write mass conservation of CO2

$$M_{CO_2} = \frac{4}{3}\pi r(t)^3 \rho_2 Y_{CO_2}$$

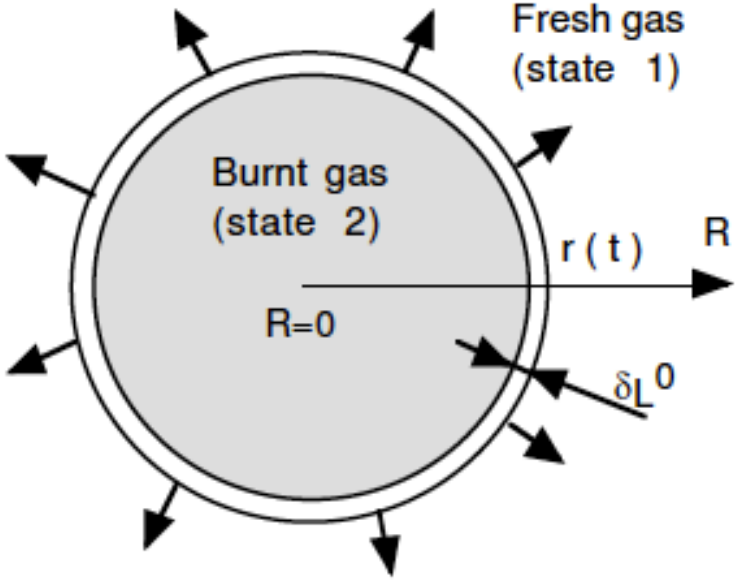
$$\frac{dM_{CO_2}}{dt} = \rho_1 s_c Y_{CO_2} 4\pi r(t)^2$$

Flux of CO2 produced in the front

SPEEDS IN A SPHERICAL FLAME:

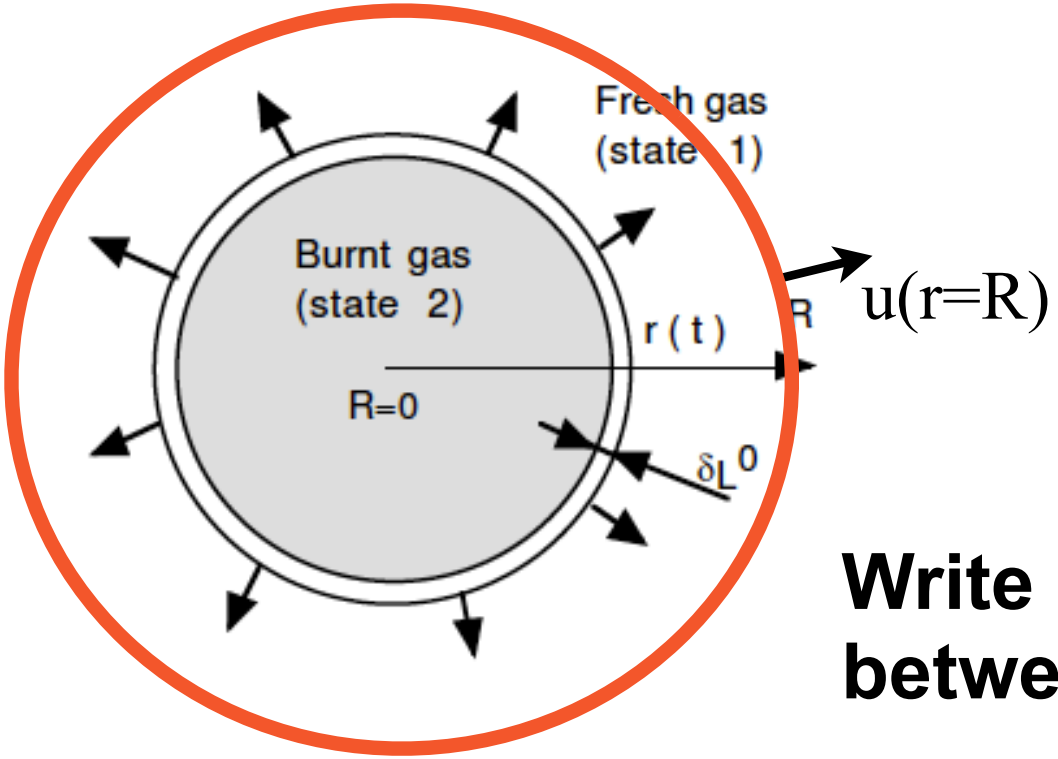
$$\frac{dr}{dt} = \frac{\rho_1}{\rho_2} s_c$$

s_a



The absolute speed of the flame is what you observe with your eyes.
It is much larger than the flame speed: this is the quantity observed in experiments

WHAT IS THE FLOW SPEED ?

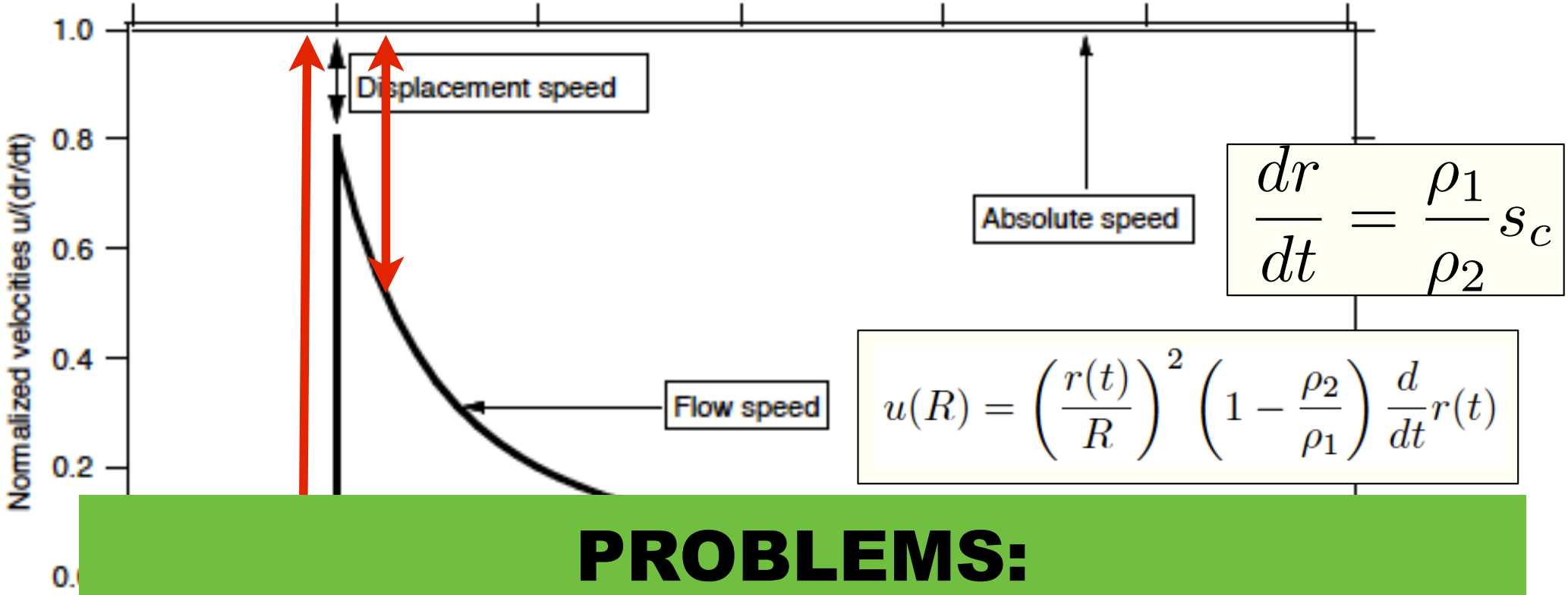


Write global mass conservation between r=0 and r=R:

$$\frac{d}{dt}\left(\frac{4}{3}\pi\rho_2 r(t)^3 + \frac{4}{3}\pi\rho_1\left(R^3 - r(t)^3\right)\right) = -4\pi R^2\rho_1 u(R)$$

$$u(R) = \left(\frac{r(t)}{R}\right)^2\left(1 - \frac{\rho_2}{\rho_1}\right)\frac{d}{dt}r(t)$$

WHAT IS THE DISPLACEMENT SPEED ?



$$\frac{dr}{dt} = \frac{\rho_1}{\rho_2} s_c$$

$$u(R) = \left(\frac{r(t)}{R}\right)^2 \left(1 - \frac{\rho_2}{\rho_1}\right) \frac{d}{dt} r(t)$$

PROBLEMS:

1/ HOW CAN WE MEASURE $u(r = R)$

2/ SINCE THE REAL FLAME IS NOT THIN, WHERE DO WE MEASURE u

$$s_d = \qquad\qquad s_c$$

IN REAL SPHERICAL FLAMES

MEASURING THE CONSUMPTION SPEED IS IMPOSSIBLE EXPERIMENTALLY (NO ACCESS TO REACTION RATE)

MEASURING THE DISPLACEMENT SPEED IS DIFFICULT: ONLY THE ABSOLUTE SPEED dr/dt CAN BE MEASURED EASILY. COMBINING PIV FOR THE FLOW ($\vec{u}$. $\vec{n}$) AND TOMOGRAPHY FOR THE FLAME ($\vec{w}$. $\vec{n}$) MAY WORK

SOURCE OF MULTIPLE CONTROVERSIES IN THE PAST (see papers by Faeth, Searby, Poinsot, Renou, Halter)

FINITE THICKNESS

IN ALL PREVIOUS DERIVATIONS OF SPEED, WE ASSUMED THAT THE THICKNESS OF THE FRONT WAS ZERO

IF IT IS NOT, THINGS BECOME MORE COMPLEX

IF IT CHANGES WITH TIME (AND THIS IS THE CASE), THINGS BECOME VERY COMPLEX...

Ch. 2, Sec 2.7.3

HOW TO OBTAIN A LAMINAR FLAME SPEED ?

THE VALUE OF THE LAMINAR FLAME SPEED IS *THE MAIN* INPUT TO EVERYTHING IN COMBUSTION

WHAT SHOULD YOU DO WHEN YOU NEED IT ?

A COMPUTATION: We can compute 1D flames with full chemistry. But in almost all cases, these codes (transport models) have been tuned to match experimental values ! So we still will be relying on a measurement

EXTRAPOLATING A COMPUTATION: if we have a reliable computation in one case, we can use the codes to have flame speeds for another case.

MEASURE A LAMINAR FLAME SPEED ?

HOW DO WE MEASURE A LAMINAR FLAME SPEED ?
THIS IS ACTUALLY :

1/ One of the oldest problems in combustion science

2/ One of the most difficult if you want to be precise

EXAMPLES OF EXPERIMENTAL METHODS TO MEASURE LAMINAR FLAME SPEEDS:

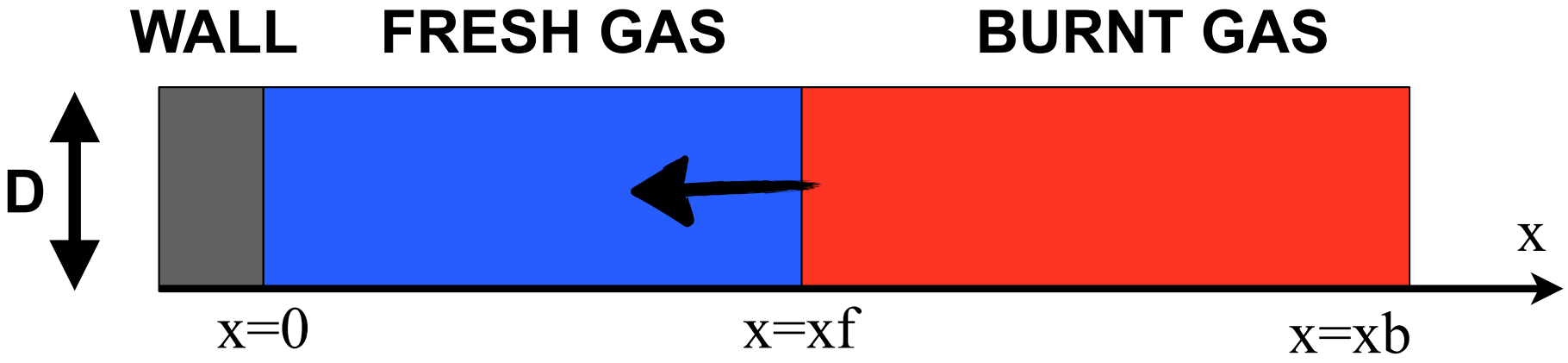
The straight tube

The spherical flame

The stagnation point flame

The Bunsen flame

FLAME SPEEDS IN A TUBE:



Measure dxf/dt and you have the flame speed

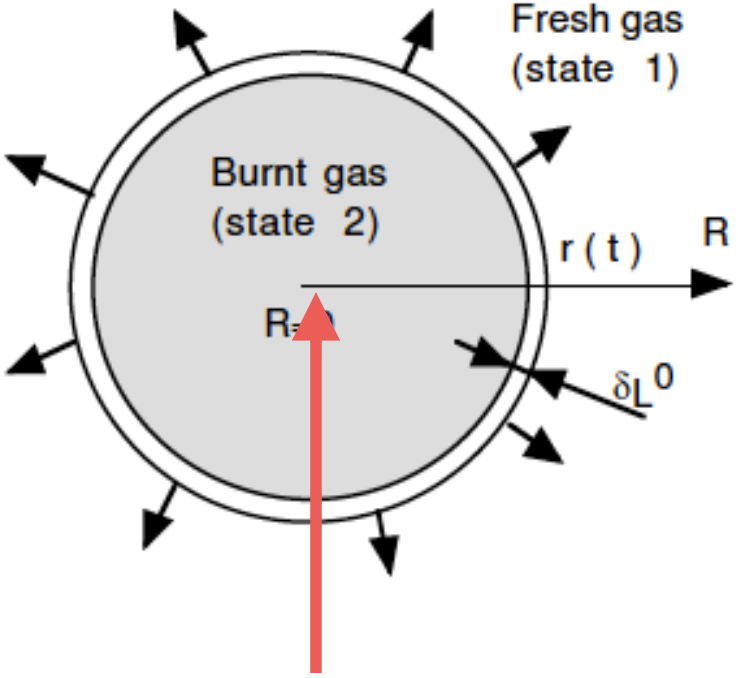
Problems: this speed will depend on the tube size D:

- **When the tube is too small, the flame speed is affected by flame wall interaction -> it took years around 1900 to figure this out**
- **When the tube is larger, the flame becomes unstable**

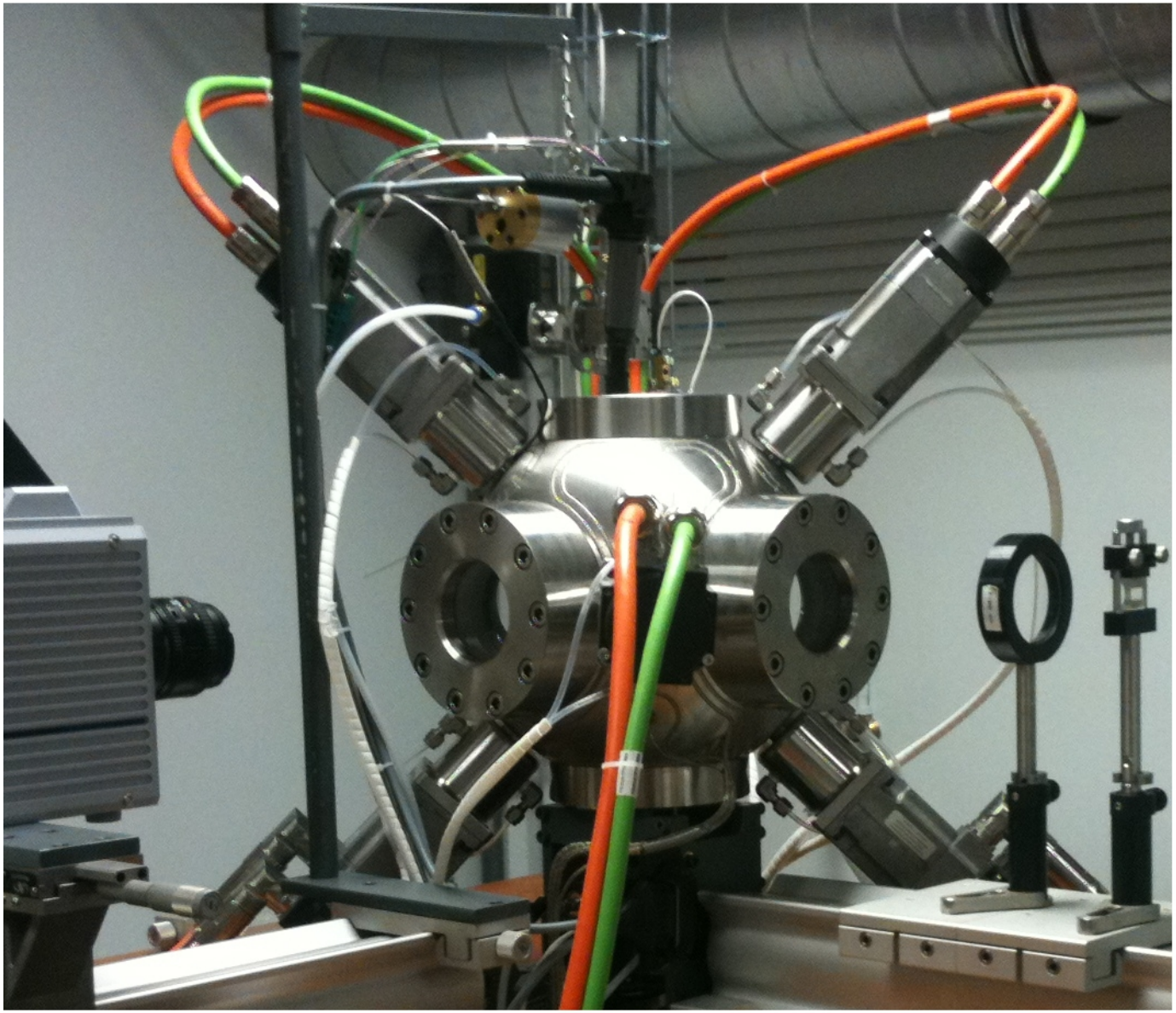
Trying to measure flame speeds in a duct:



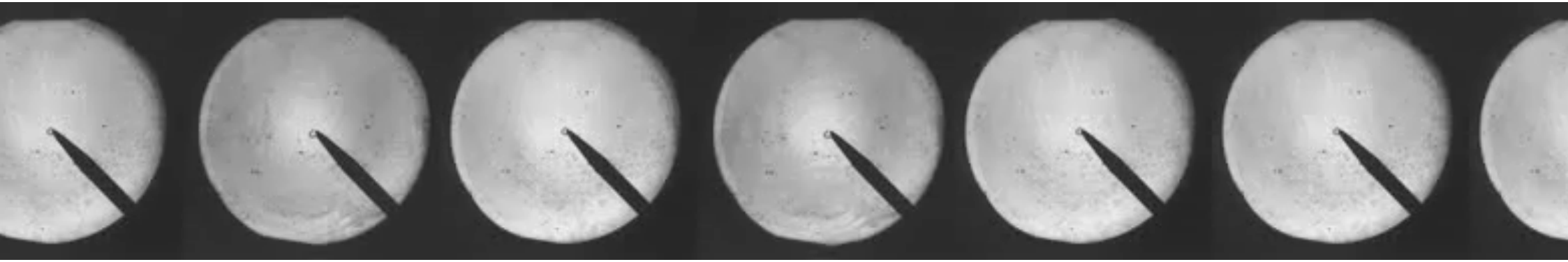
FLAME SPEEDS IN A SPHERICAL FLAME:



Spark ignition

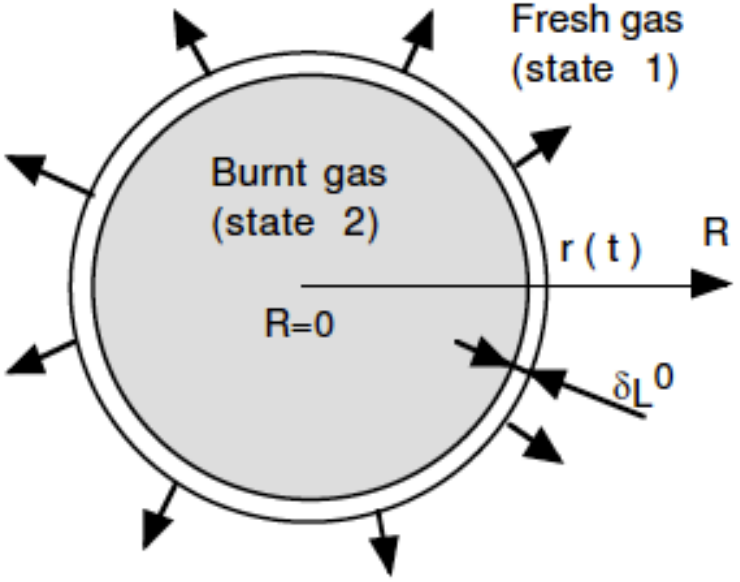


<- LEAN STOECHIO RICH ->



Malcolm Lawes, Matthew P. Ormsby, Chris G.W. Sheppard, Robert Woolley, The turbulent burning velocity of iso-octane/ air mixtures, Combustion and Flame, Volume 159, Issue 5, May 2012, Pages 1949-1959

FLAME SPEEDS IN A SPHERICAL FLAME:



Measure dr/dt, the absolute flame speed

Deduce the flame speed from dr/dt:

$$\frac{dr}{dt} = \frac{\rho_1}{\rho_2} s_c \qquad s_c = \frac{\rho_2}{\rho_1} \frac{dR}{dt}$$

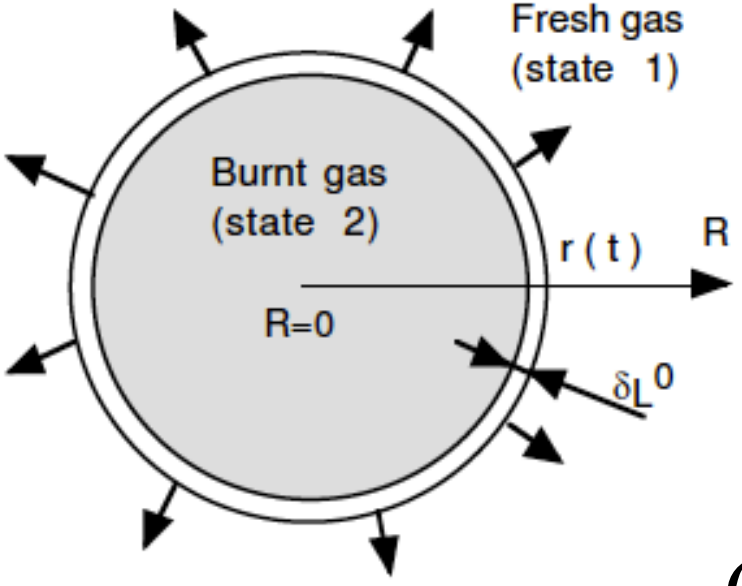
This requires a model for the density ratio:

$\frac{\rho_2}{\rho_1}$

→ **Burnt gases density -> make an equilibrium computation to have T2 and deduce the density**

→ **Fresh gases density (take the initial fresh gases density)**

PROBLEMS

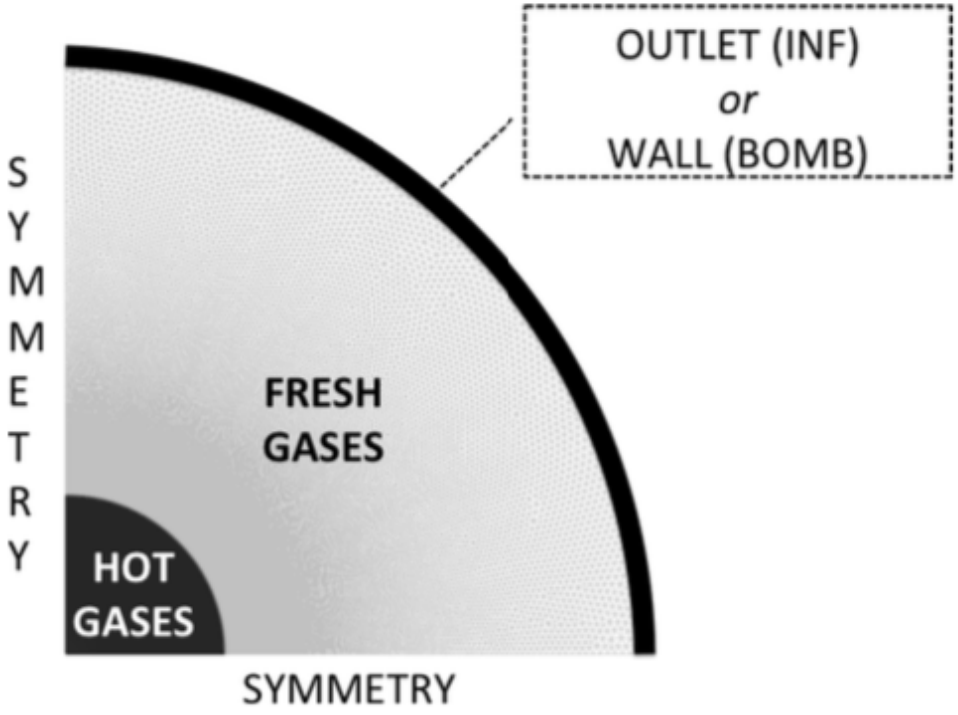


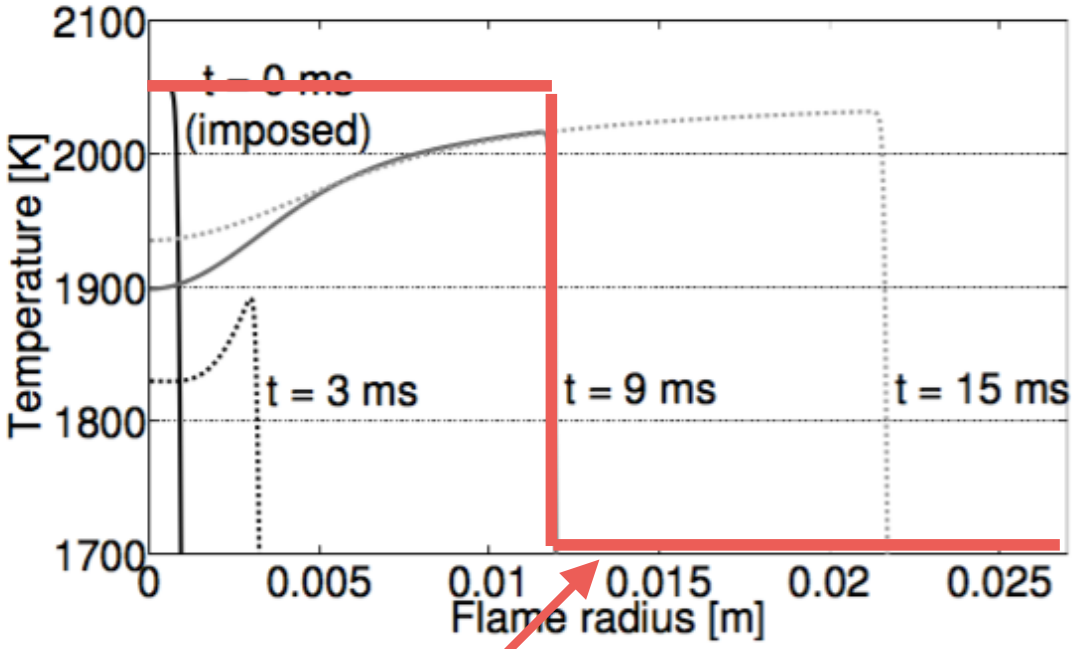
$\frac{\rho_2}{\rho_1}$ → **Burnt gas density: using equilibrium is a model. Results will depend on it. What about radiation for ex ?**

It is a bomb. Pressure goes up…so does density

The expression $\frac{dr}{dt} = \frac{\rho_1}{\rho_2} s_c$ **is also a model !**

Valid only if the flame is thin, and burnt gases are homogeneous: constant density and temperature

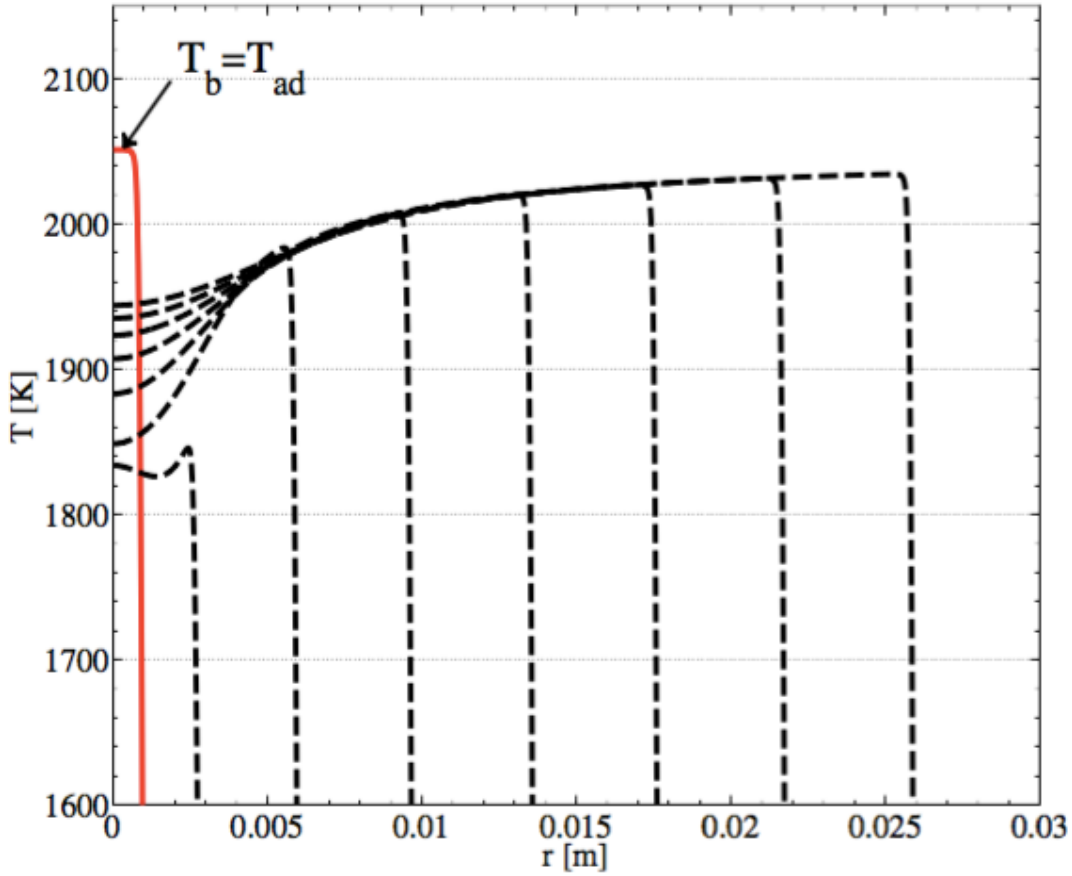




MODEL USED TO WRITE $\dfrac{dr}{dt} = \dfrac{\rho_1}{\rho_2} s_c$

A. Bonhomme, L. Selle and T. Poinsot. Curvature and confinement effects for flame speed measurements in laminar spherical and cylindrical flames. *Comb. Flame*. 160, 7, 1208-1214, 2013.

Simulation of a spherical flame:

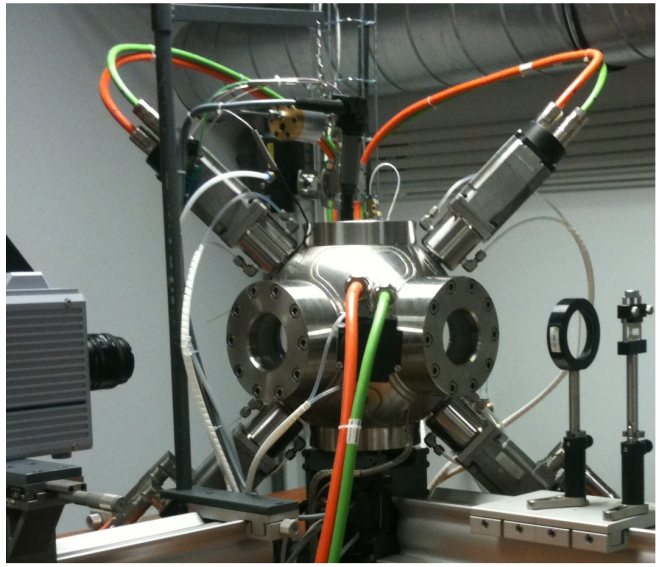


Figu
propa
to t =

The fact that the burnt kernel is not homogeneous in density or temperature is due to stretch effects

A fects
fo mes.
C

Measuring flame speeds in vessels/bombs:



Advantages:

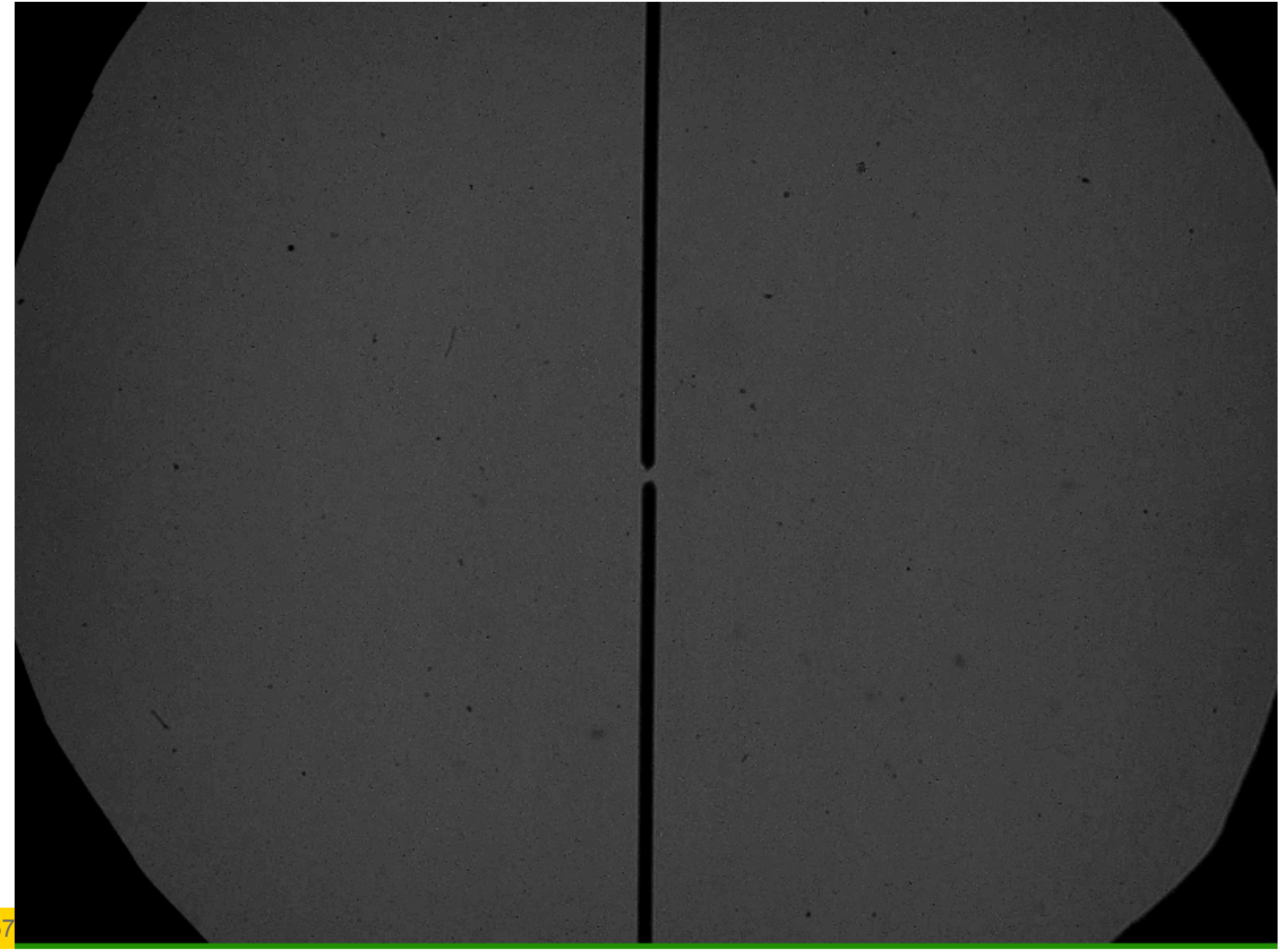
Can be used at high pressures

Drawbacks:

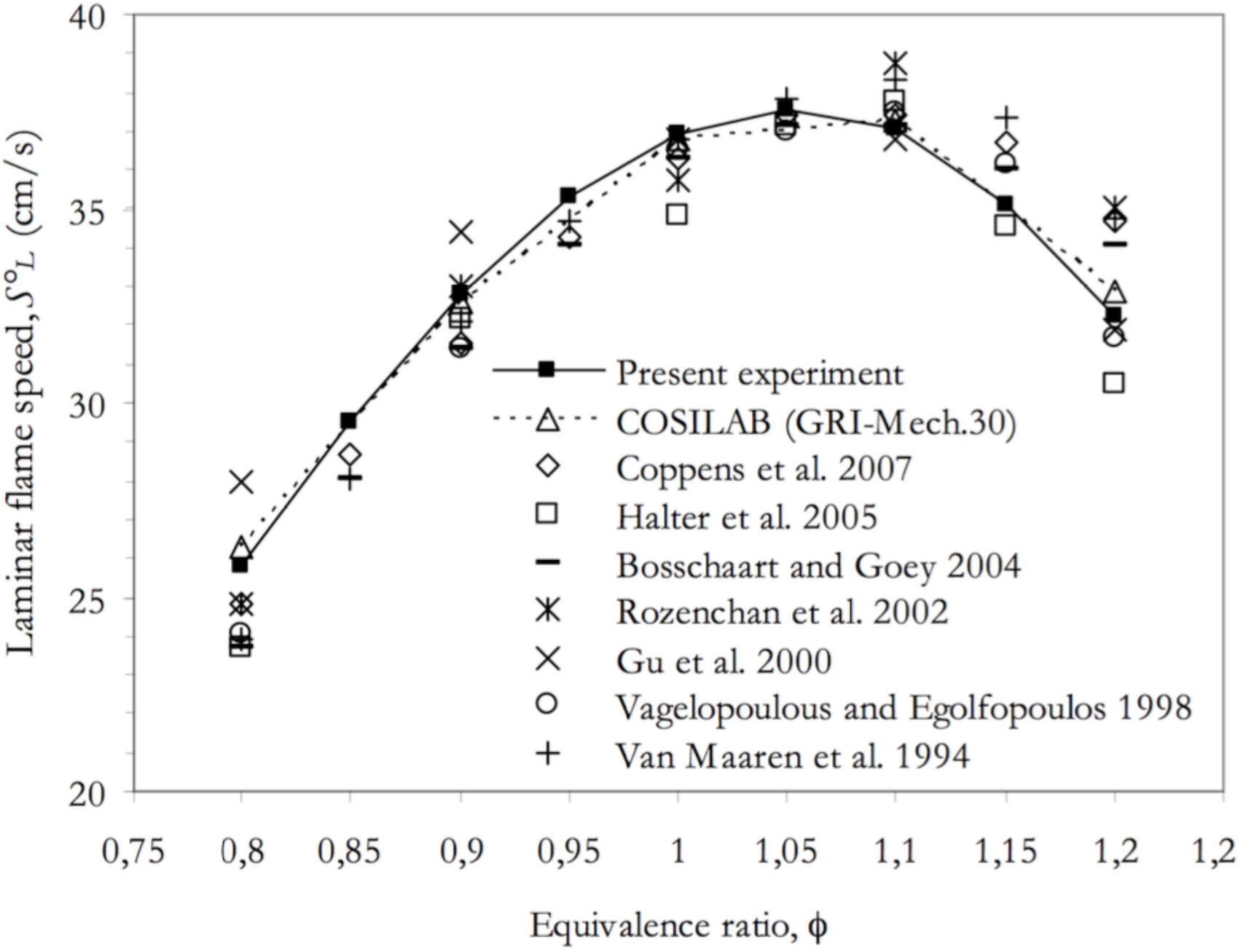
Just after ignition, flame is affected by the spark

Long after ignition, the pressure starts rising and the flame speed is not reliable anymore

The flame can also become unstable for rich cases and high pressures



Uncertainties on flame speeds:



CH4/air
1 bar
T1=300 K

Stretch

One additional notion is required to understand turbulent flames: stretch

Stretch measures the rate (s^{-1}) at which the flame area increases:

$$\kappa = \frac{1}{A}\frac{dA}{dt}$$

Intuition tells us that 'stretching' a flame must have a limit. You cannot increase the surface of something as fast as you want !

Stretch and premixed flames

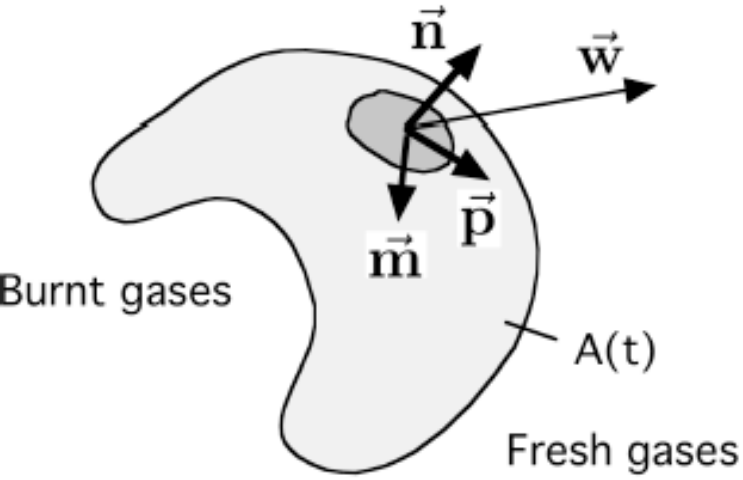
Strain in the tangent plane to the flame

Strain due to flame propagation

$$\kappa = \nabla_t \cdot \vec{\mathbf{u}} - s_d \left(\frac{1}{\mathcal{R}_1} + \frac{1}{\mathcal{R}_2} \right) = \nabla_t \cdot \vec{\mathbf{u}} + s_d \nabla_t \cdot \vec{\mathbf{n}}$$

Displacement speed

Front curvature

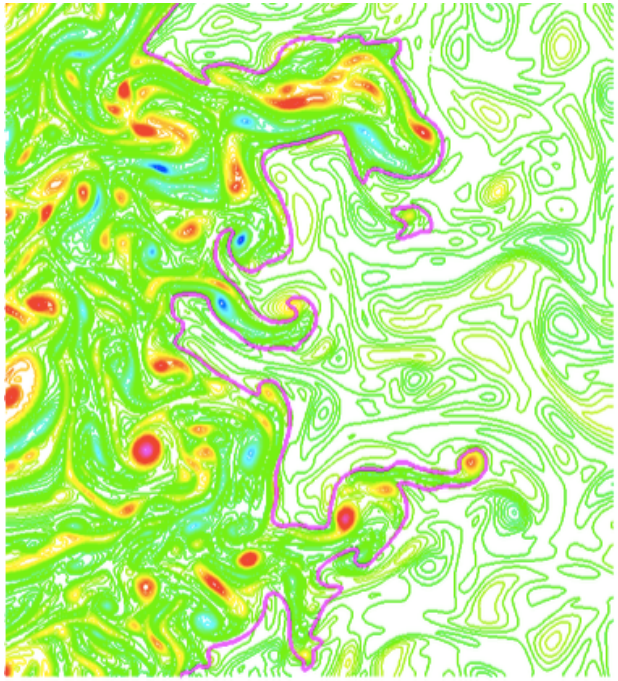


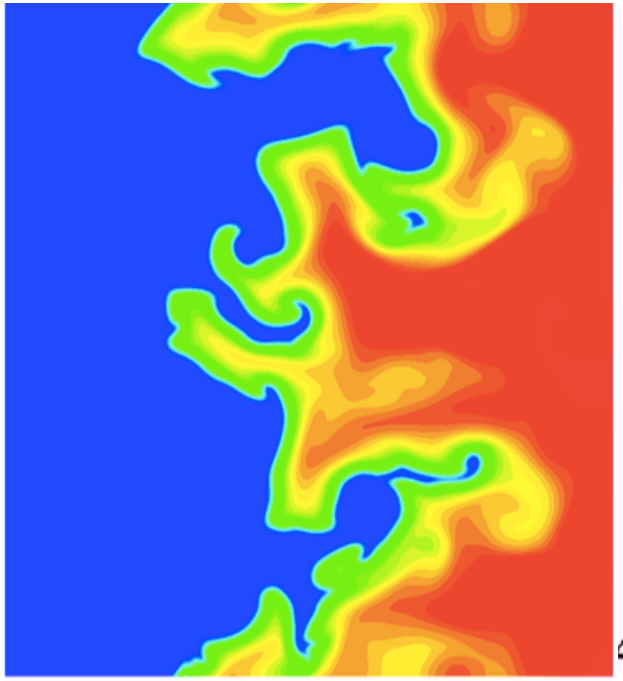
Ch. 2.6

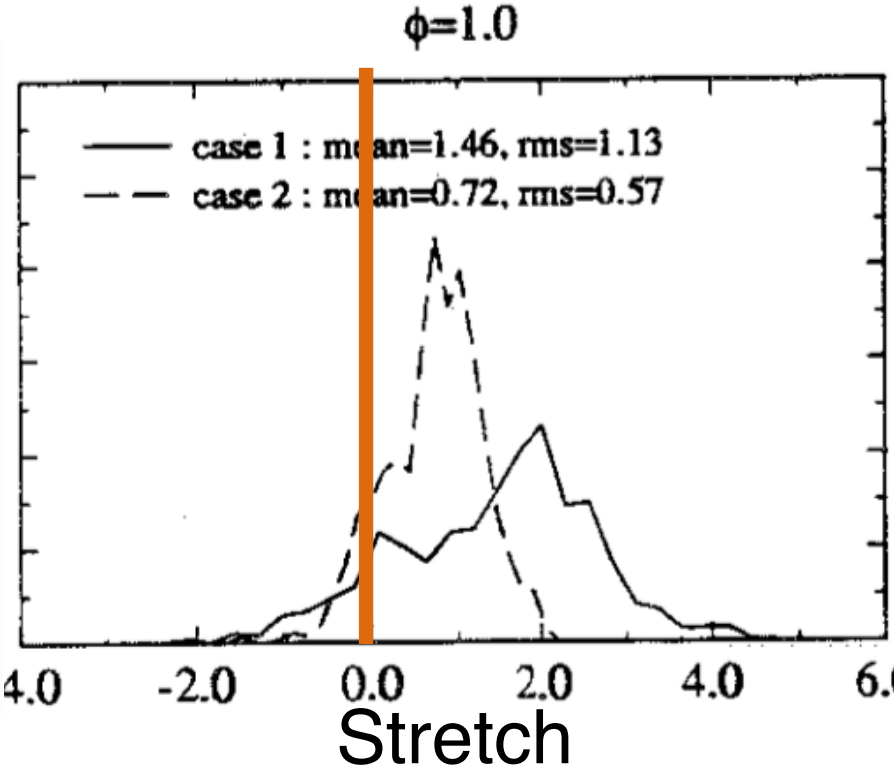
S. M. Candel and T. Poinsot. Flame stretch and the balance equation for the flame surface area. Combust. Sci. Tech., 70:1-15, 1990.

Stretch is essential for turbulent flames

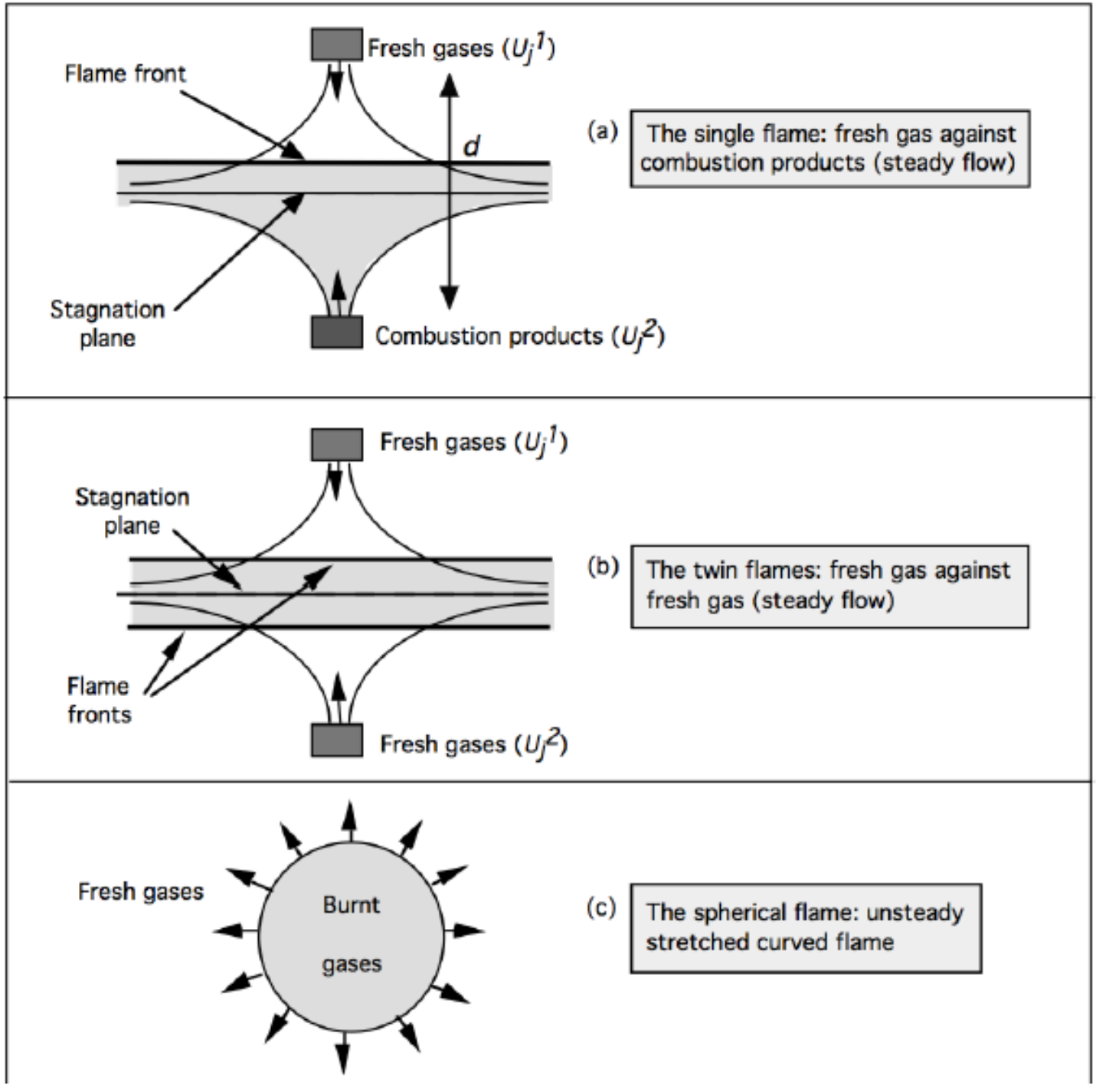
Stretch is what makes a 1m2 flame become a 2m2 flame !
Turbulence acts like a flame surface « multiplier »: in turbulent combustion models, estimating stretch will be our main goal.
Stretch is local: it can be negative or positive. But on average in a flame, it is positive: this is why the total surface grows

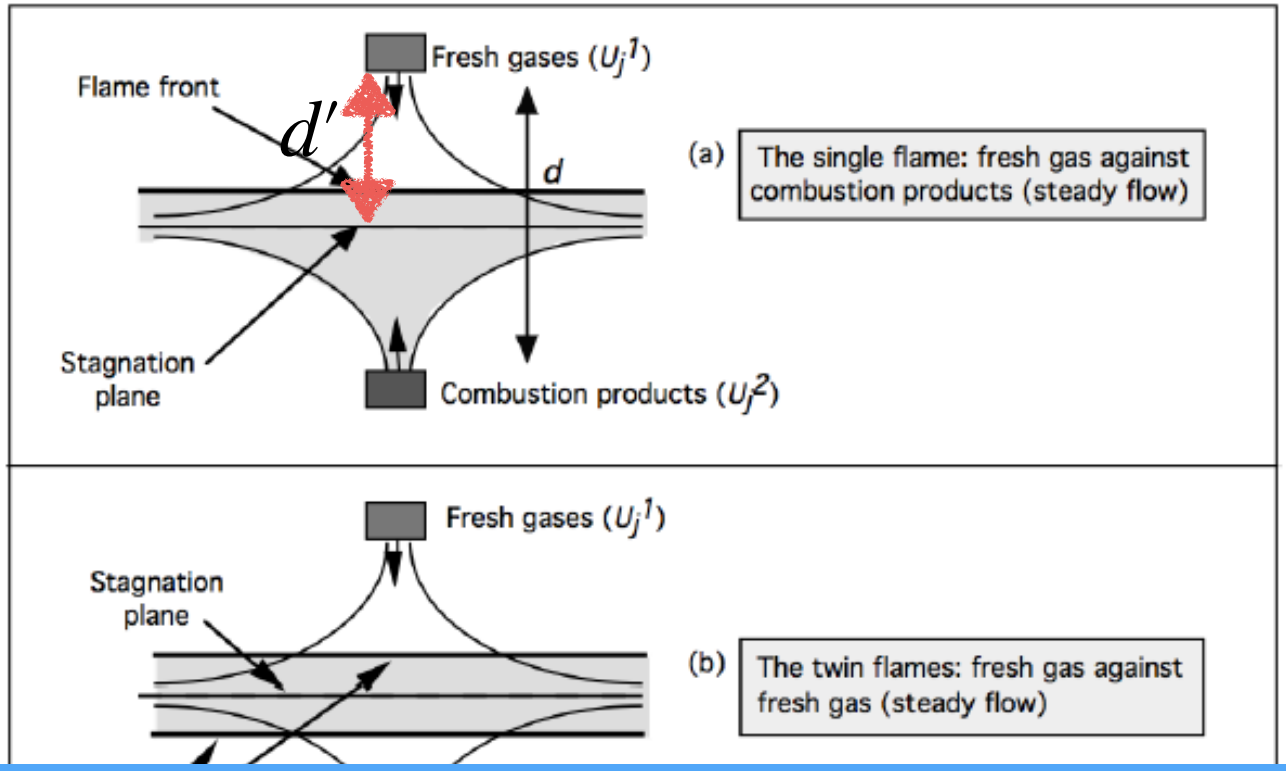






Examples of stretched premixed flames





$$\kappa = \frac{U_1 + U_2}{d}$$

$$\kappa = U_1 / d'$$

This is an average value: stretch is not constant along the flame

Combustion and Flame 162 (2015) 1540–1549

Contents lists available at ScienceDirect

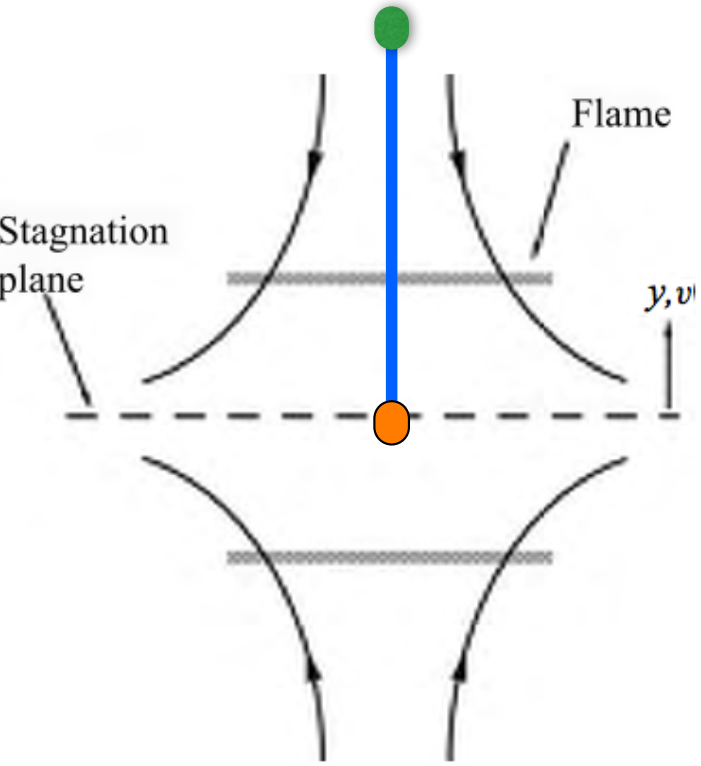
Combustion and Flame

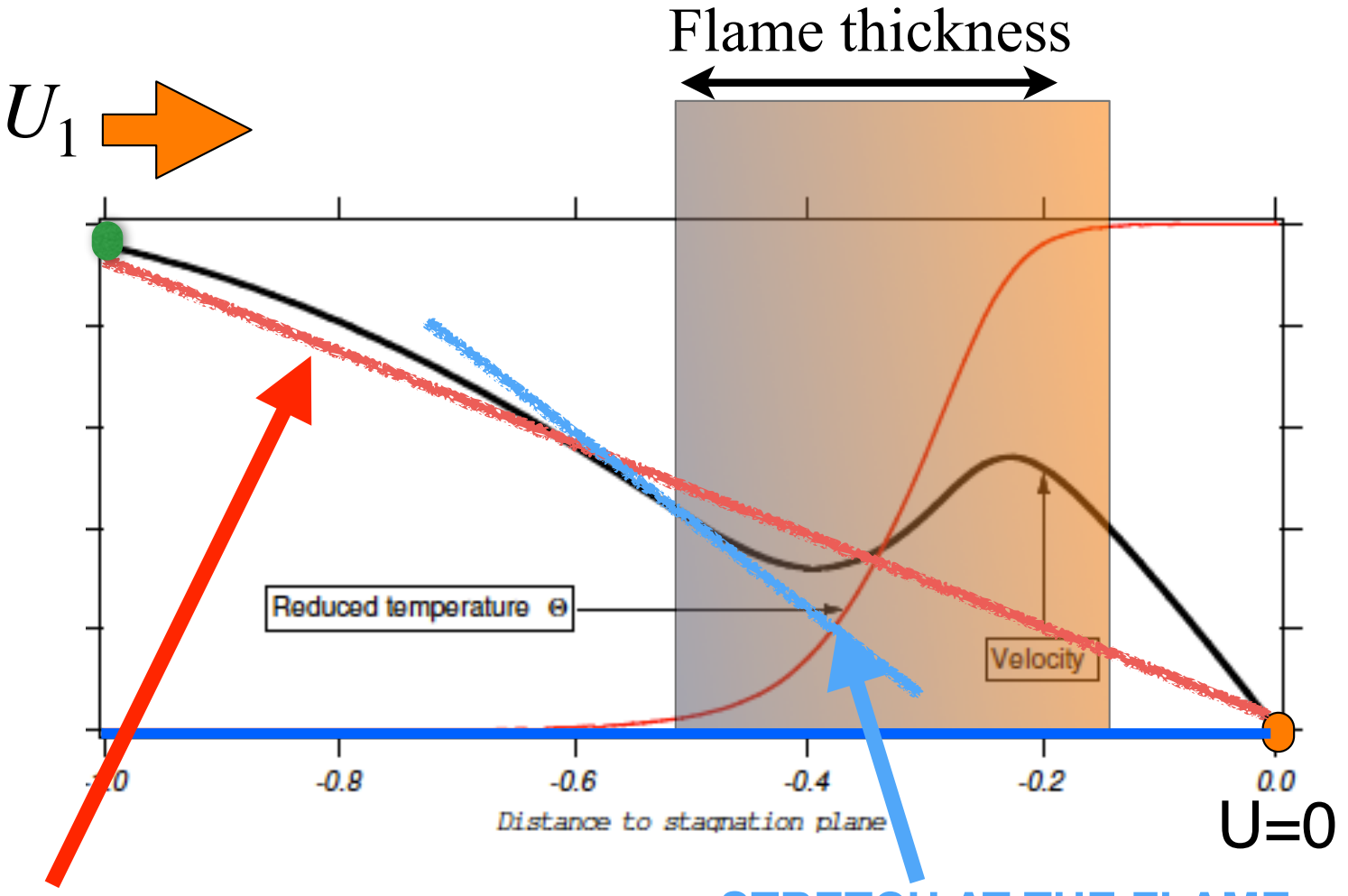
journal homepage: www.elsevier.com/locate/combustflame

Accuracies of laminar counterflow flame experiments

Ulrich Niemann *, Kalyanasundaram Seshadri, Forman A. Williams

Flame stretch in a stagnation point flow:

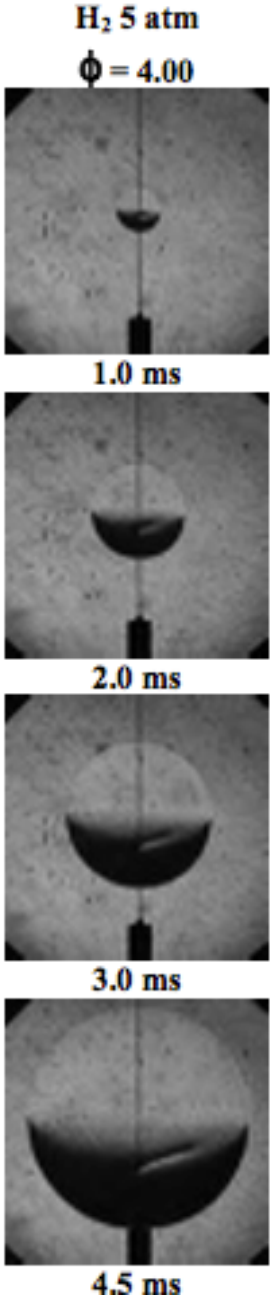


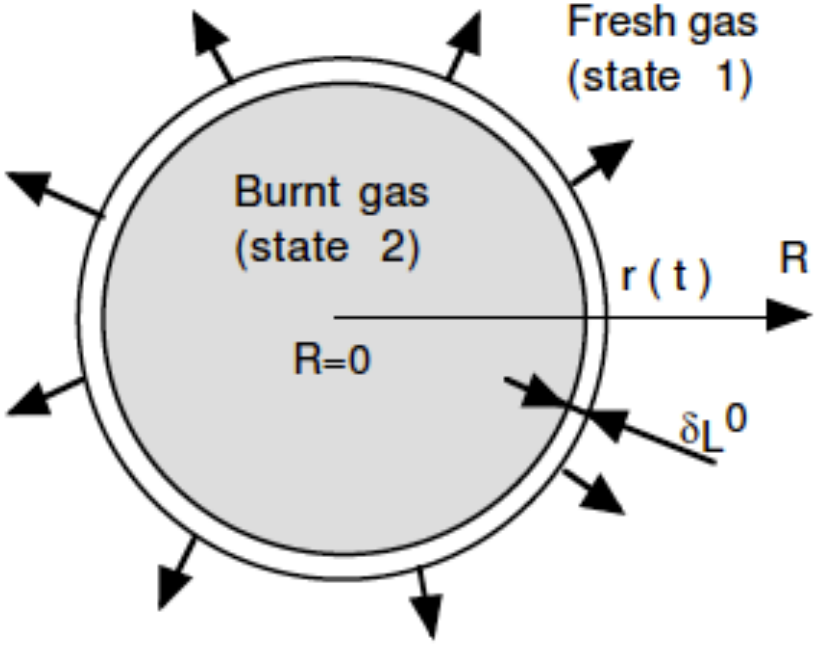


MEAN VALUE OF STRETCH

STRETCH AT THE FLAME FRONT

Evaluations of stretch: spherical flames





$$A = 4\pi r^2 \qquad \kappa = \frac{1}{A}\frac{dA}{dt} = \frac{2}{r}\frac{dr}{dt}$$

In a spherical flame:

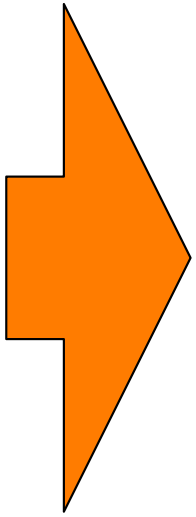
- **Stretch is constant on the flame front**
- **Knowing r(t) gives directly stretch**

Ch. 2 Sec 2.7

Spherical flames

$$\frac{dr}{dt} = \frac{\rho_1}{\rho_2} s_c$$

$$\kappa = \frac{1}{A}\frac{dA}{dt} = \frac{2}{r}\frac{dr}{dt}$$



$$\kappa = \frac{2}{t}$$

To first order, all spherical flames with the same age *t* are submitted to the same stretch ! (independent of the flame speed)

This stretch is very large at small times so that this first order approximation is usually wrong. The flame speed differs from the unstrained flame speed and this effect must be taken into account

Implication for measurements of flame speeds in spherical flames

To use the expression: $$\frac{dr}{dt} = \frac{\rho_1}{\rho_2} s_c$$

Corrections are needed on the consumption see to account for stretch effects.

$$\frac{dR}{dt} = \frac{\rho_2}{\rho_1} s_c(K) = \frac{\rho_2}{\rho_1} s_c(dR/dt)$$

where a model for $s_c(dR/dt)$ **is needed.**

Do we have one ?

Variations of flame speeds with stretch

Premixed flames are affected by stretch.

Theory can be used to derive the variations of speeds:

Markstein length

$$\frac{s_d(0)}{s_L^0} = 1 - \frac{L_a^d}{s_L^0}\kappa$$

Remember that this expression is obtained from theory only and only for simple chemistry. It does not really have to hold in real flames but we use it anyway. Read the papers by Matalon or Williams or Clavin

Markstein numbers

Markstein lengths are usually normalized by the flame thickness:

Markstein number ***Markstein length***

$$M_a^d = \frac{L_a^d}{\delta}$$

Flame thickness

$$\delta = \frac{D}{s_L^0}$$

$$\frac{s_d(0)}{s_L^0} = 1 - M_a^d \frac{\kappa\delta}{s_L^0}$$

Measuring Markstein numbers is extremely difficult...

But the dependence of premixed flame speeds on stretch is not very strong, compared to diffusion flames

Matalon's formula for the Markstein length of the displacement speed

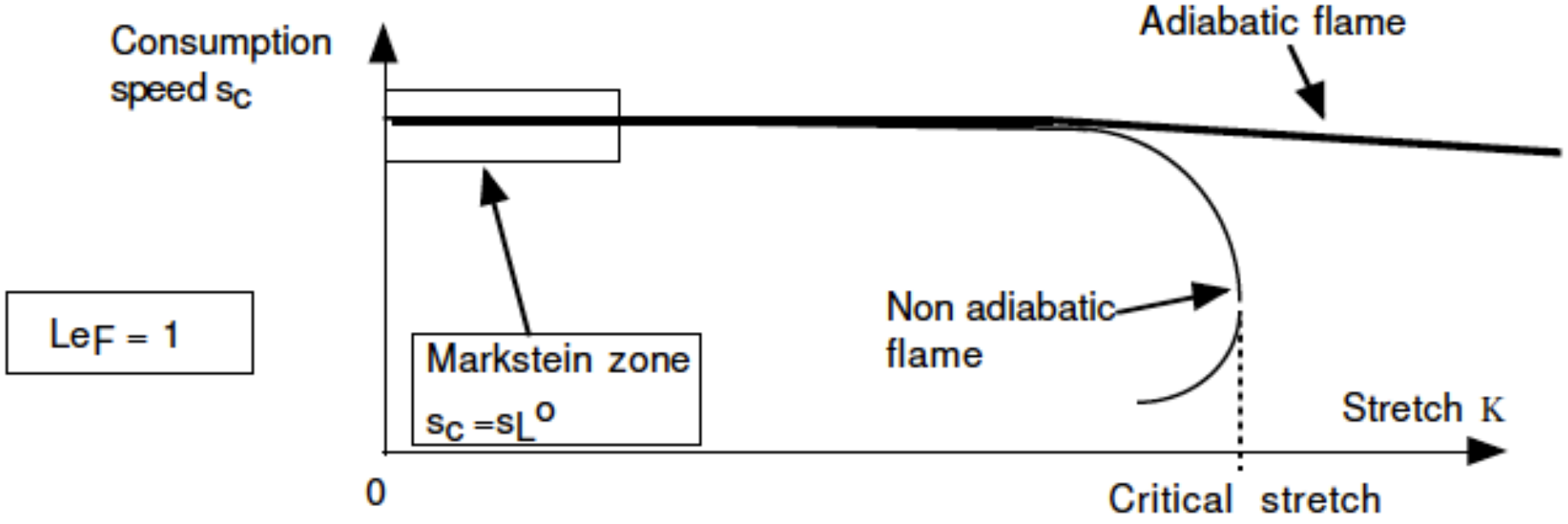
Assumption	Markstein number $(M_a^d(\theta=0) = L_a^d(\theta=0)/\delta)$
$\lambda = \text{cst}$	$\frac{T_2}{T_2-T_1}\ln(\frac{T_2}{T_1}) + \frac{1}{2}(Le_F-1)\beta\frac{T_1}{T_2-T_1}\int_0^{\frac{T_2-T_1}{T_1}}\frac{\ln(1+x)}{x}dx$
$\lambda = T^{1/2}$	$2\frac{T_2/T_1}{1+\sqrt{T_2/T_1}} + 2(Le_F-1)\beta\frac{1}{T_2/T_1-1}\left(\sqrt{\frac{T_2}{T_1}} - 1 - \ln(\frac{1}{2}(\frac{T_2}{T_1}+1))\right)$
$\lambda = T$	$\frac{T_2}{T_1} + \frac{1}{2}(Le_F-1)\beta$

Matalon's formula for the Markstein length of the consumption speed

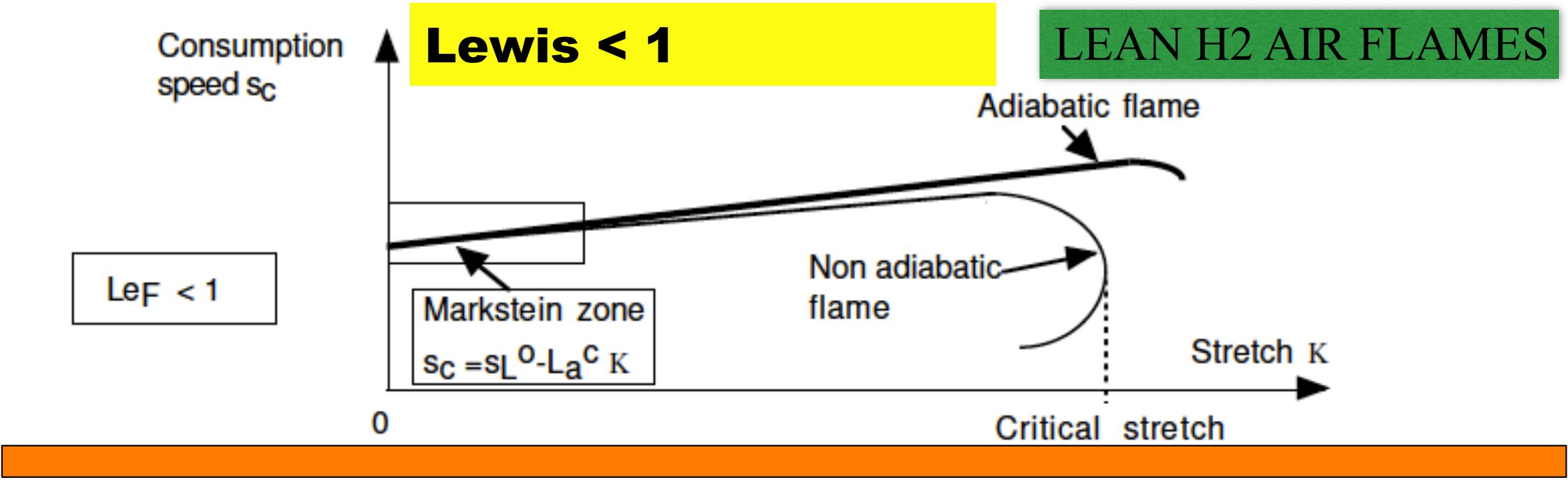
Assumption	Markstein number (M_a^c)
$\lambda = \text{cst}$	$\frac{1}{2}(Le_F - 1)\beta \frac{T_1}{T_2 - T_1} \int_0^{\frac{T_2 - T_1}{T_1}} \frac{\ln(1+x)}{x} dx$
$\lambda = T^{1/2}$	$2(Le_F - 1)\beta \frac{1}{T_2/T_1 - 1} \left(\sqrt{\frac{T_2}{T_1}} - 1 - \ln(\frac{1}{2}(\frac{T_2}{T_1} + 1)) \right)$
$\lambda = T$	$\frac{1}{2}(Le_F - 1)\beta$

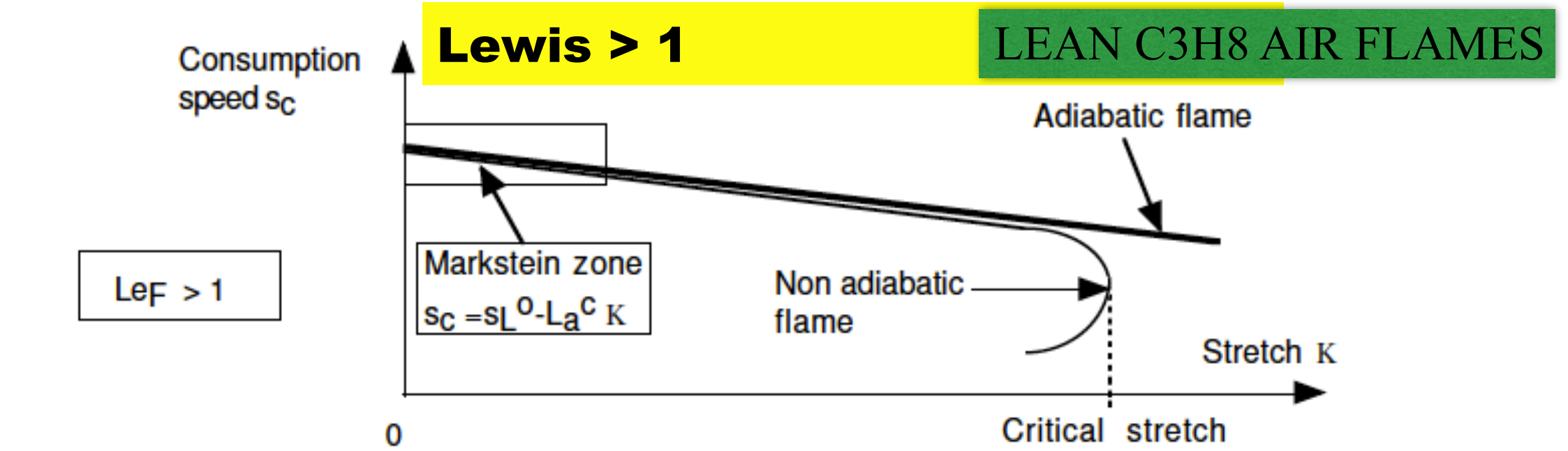
The Markstein length changes sign when Lewis is larger or smaller than unity

Flame speeds versus stretch: depend on the Lewis number of the deficient reactant AND on heat losses:



Lewis=1


Lewis < 1
LEAN H2 AIR FLAMES
Consumption speed s_c
Adiabatic flame
$Le_F < 1$
Markstein zone
$s_c = s_L^o - L_a^c \kappa$
Non adiabatic flame
Stretch κ
0
Critical stretch


Lewis > 1
LEAN C3H8 AIR FLAMES
Consumption speed s_c
Adiabatic flame
$Le_F > 1$
Markstein zone
$s_c = s_L^o - L_a^c \kappa$
Non adiabatic flame
Stretch κ
0
Critical stretch

OUTLINE

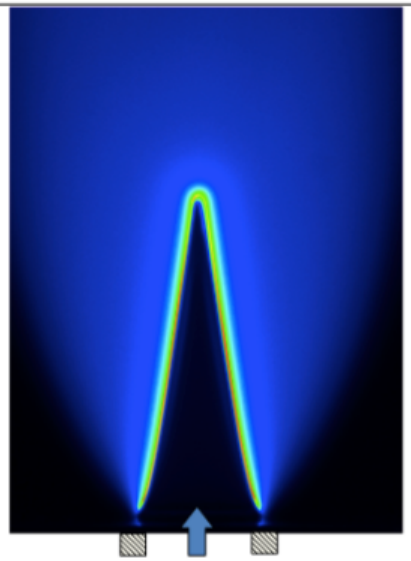
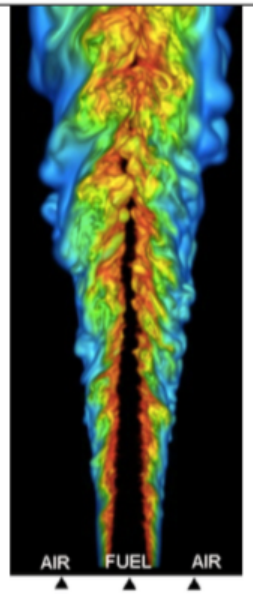
CONSERVATION EQUATIONS FOR REACTING FLOWS

PREMIXED FLAMES

DIFFUSION FLAMES

Ch. 3

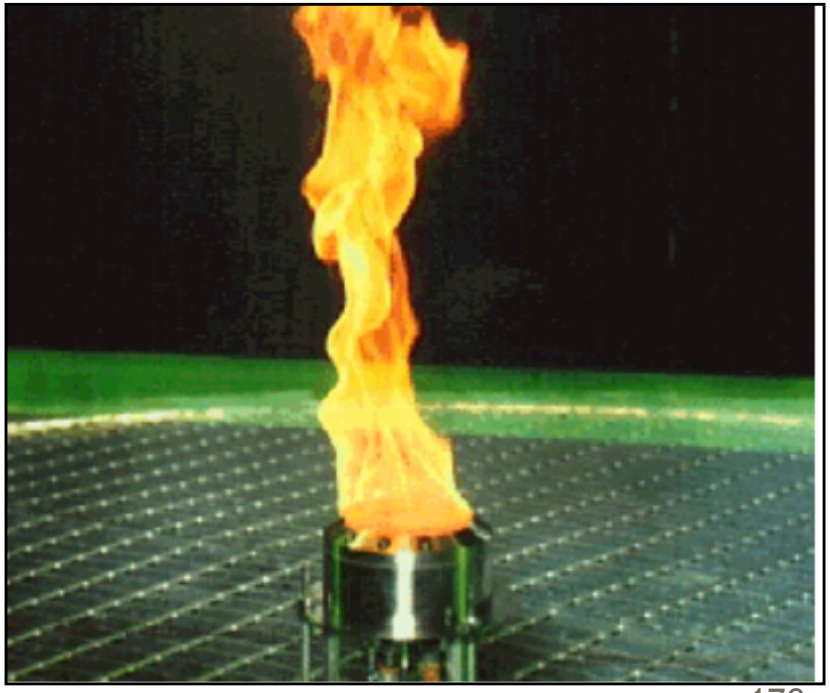
OTHER FLAMES: PARTIALLY PREMIXED, TRIPLE FLAMES

	LAMINAR FLAMES	***TURBULENT FLAMES***
PREMIXED FLAMES	 Chapter 2	 Chapters 4 and 5
NON-PREMIXED FLAMES (DIFFUSION)	 Chapter 3	 Chapters 4 and 6

Diffusion flames: very different from premixed flames...



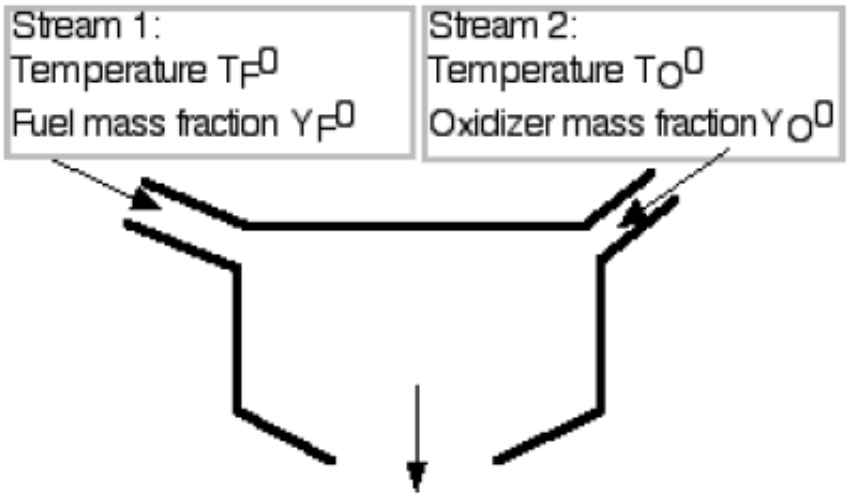


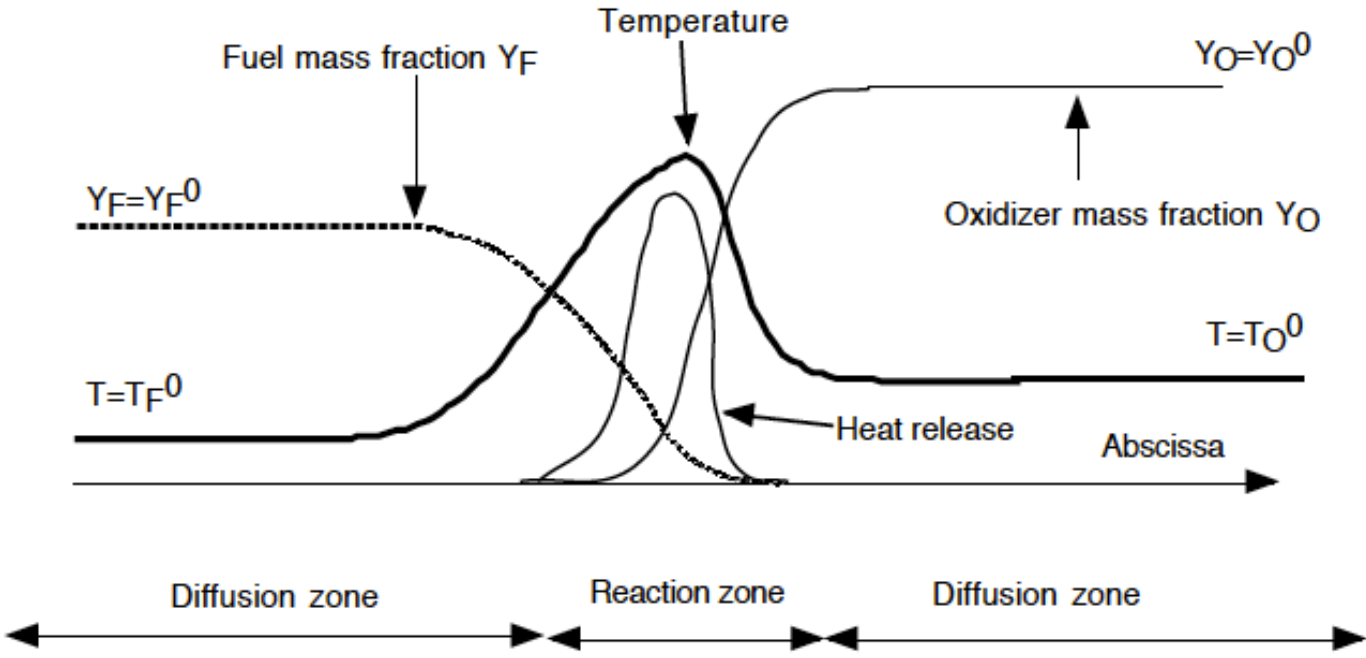


Models are also different

THE LAMINAR DIFFUSION FLAME

Ch. 3





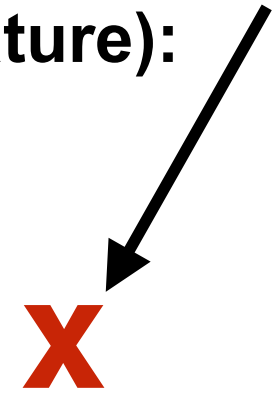
The other case where theory can be developed and is heavily used.

Most approaches rely on passive scalars and on the mixture fraction z.

WHAT IS A PASSIVE SCALAR ?

A passive scalar is a *scalar* quantity which does NOT have a source term (ie not a chemical species or temperature):

$$\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_i Z}{\partial x_i} = \frac{\partial}{\partial x_i}(\rho D \frac{\partial Z}{\partial x_i})$$



Avoiding to deal with a source term makes things MUCH easier…

But how do we build passive scalars ?

Ch. 2 Sec 3.2.1

A USEFUL PROPERTY OF PASSIVE SCALARS:

★IF TWO PASSIVE SCALARS Z1 and Z2 HAVE THE SAME BOUNDARY CONDITIONS:

- ➡ IF THEY ARE EQUAL AT $t = 0$, THEY WILL ALWAYS REMAIN EQUAL
- ➡ IF THEY DIFFER AT $t = 0$, THEY WILL CONVERGE TO THE SAME VALUE AFTER A FEW CHARACTERISTIC FLOW TIMES

★DEMO: by considering the norm of (Z2-Z1) OR by using intuition

INTUITIVE DEMO:

$$\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_i Z}{\partial x_i} = \frac{\partial}{\partial x_i}(\rho D \frac{\partial Z}{\partial x_i})$$

can also be written:

$$\rho \frac{DZ}{Dt} = \frac{\partial}{\partial x_i}(\rho D \frac{\partial Z}{\partial x_i})$$

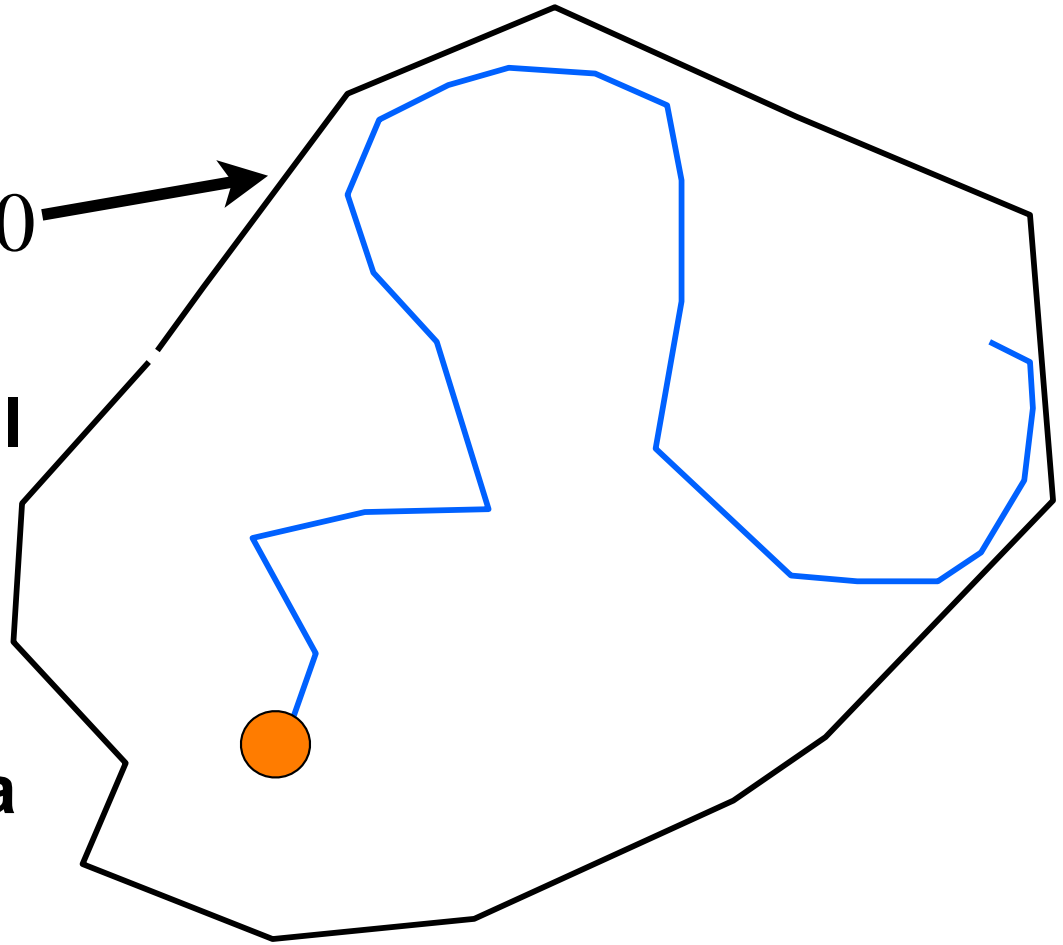
where D/Dt is the total derivative (the variation along the trajectories)

Consider two passive scalars Z1 and Z2.

Along trajectories, $Z = z_2 - z_1$ changes only because of diffusion:

$$\rho \frac{DZ}{Dt} = \frac{\partial}{\partial x_i}(\rho D \frac{\partial z}{\partial x_i})$$

- **with boundary condition: $Z = 0$**
- **If the initial condition is $Z = 0$, all gradients are zero and Z will remain 0**
- **If the initial condition is not $Z = 0$, any non-zero fluid element will go to $Z = 0$ after a few flow-through times.**

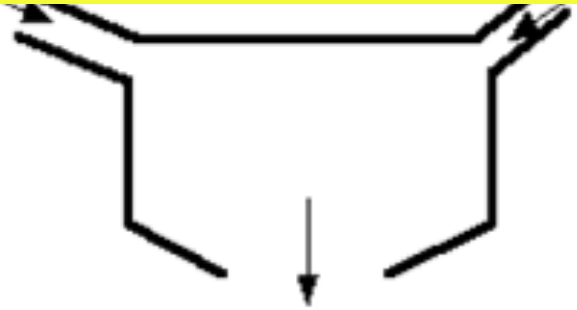


WHAT IS MIXTURE FRACTION ?

THE UNIQUE PASSIVE SCALAR WHICH GOES FROM 1 IN THE FUEL TO 0 IN THE OXIDIZER STREAM IS CALLED THE MIXTURE FRACTION z

$$\frac{\partial \rho z}{} + \frac{\partial \rho u_i z}{} = \frac{\partial}{}(\rho D \frac{\partial z}{})$$

ANY PASSIVE SCALAR GOING FROM 1 IN THE FUEL TO 0 IN THE OXIDIZER IS EQUAL TO THE MIXTURE FRACTION z



CAREFUL: IS THERE ONLY ONE MIXTURE FRACTION z ?

NO… There is ONE mixture fraction for each diffusivity D

$$\frac{\partial \rho z}{\partial t} + \frac{\partial \rho u_i z}{\partial x_i} = \frac{\partial}{\partial x_i}(\rho D \frac{\partial z}{\partial x_i})$$

The question is often: which value of D should we choose ?

WHAT DOES IT TAKE TO BE ABLE TO CONSTRUCT A MIXTURE FRACTION ?

Ch. 3 Sec 3.2

- ★ **H1: Constant pressure and equal C_{pk}'s**
- ★ **H2: All Lewis numbers equal to unity**
- ★ **H3: Global single step reaction**

$$\nu_F F + \nu_O O \rightleftharpoons \nu_P P$$

$$\dot{\omega}_O = s\dot{\omega}_F \qquad s = \frac{\nu_O W_O}{\nu_F W_F}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i Y_k\right) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_k}{\partial x_i}\right) + \dot{\omega}_k$$

So that we can track only *T*, Y_F and Y_O

IN THE ABSENCE OF COMBUSTION : PURE MIXING

$$\frac{\partial \rho Y_F}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_F) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_F}{\partial x_i}\right)$$

$$\frac{\partial \rho Y_O}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_O) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_O}{\partial x_i}\right)$$

$$\frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i T) = \frac{\partial}{\partial x_i}\left(\frac{\lambda}{C_p} \frac{\partial T}{\partial x_i}\right)$$

THREE PASSIVE SCALARS: IF WE CAN NORMALIZE THEM TO HAVE THE SAME BOUNDARY CONDITIONS (0 in air and 1 in fuel), THEY ARE ALL EQUAL TO z

NORMALIZE THE PASSIVE SCALARS:

$$\frac{\partial \rho Y_F}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_F) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_F}{\partial x_i}\right) \quad / Y_F^0$$

$$\frac{\partial \rho Y_O}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_O) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_O}{\partial x_i}\right) \quad / Y_0^0$$

$$\frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i T) = \frac{\partial}{\partial x_i}\left(\frac{\lambda}{C_p} \frac{\partial T}{\partial x_i}\right) \quad / (T_F^0 - T_O^0)$$

$$Z_1 = Y_F / Y_F^0$$

$$Z_2 = 1 - Y_O / Y_O^0$$

$$Z_3 = (T - T_O^0)/(T_F^0 - T_O^0)$$

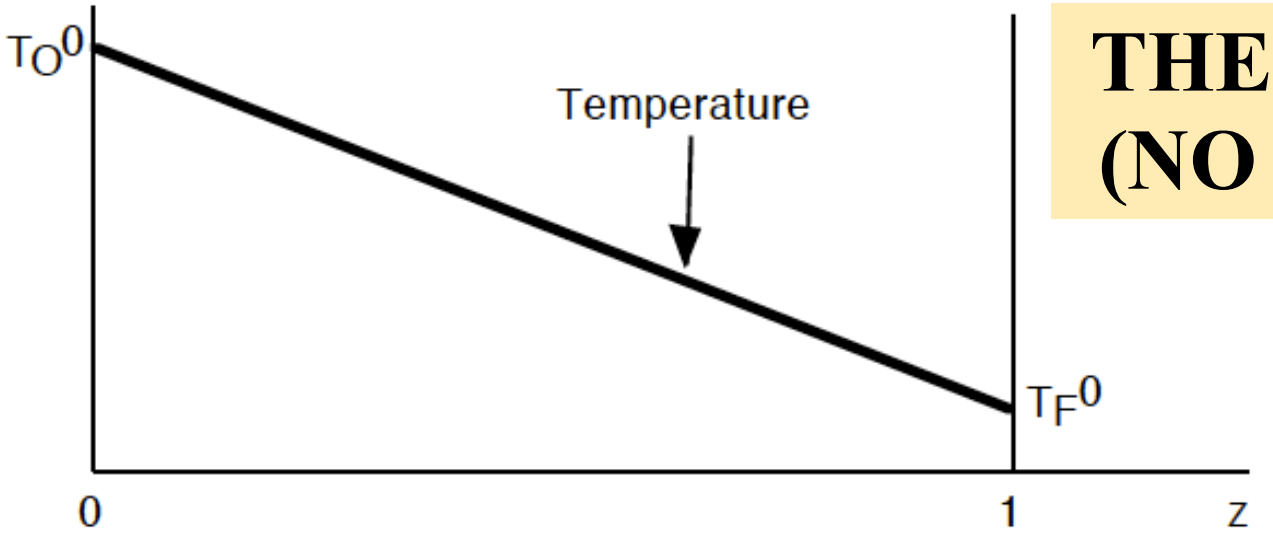
	FUEL	OXI
Z_1	1	0
Z_2	1	0
Z_3	1	0

THREE PASSIVE SCALARS WITH THE SAME BOUNDARY CONDITIONS: THEY ARE ALL EQUAL TO z

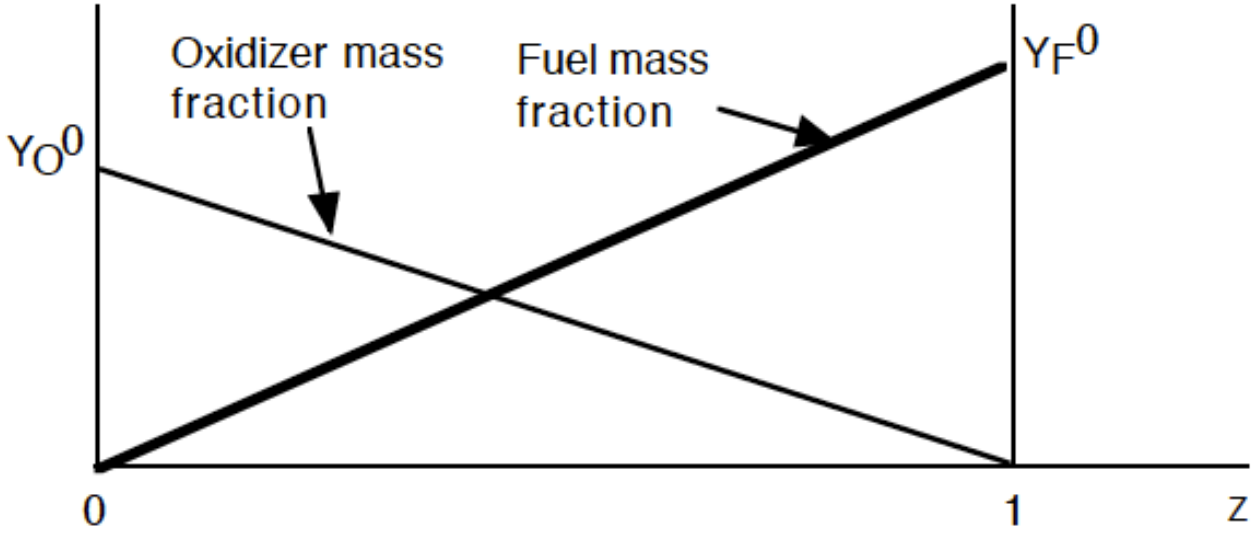
$$Z_1 = Z_2 = Z_3 = z$$

$$Y_F = Y_F^0 z \quad \text{and} \quad Y_O = Y_O^0 (1 - z)$$

$$T(z) = zT_F^0 + (1 - z)T_O^0$$

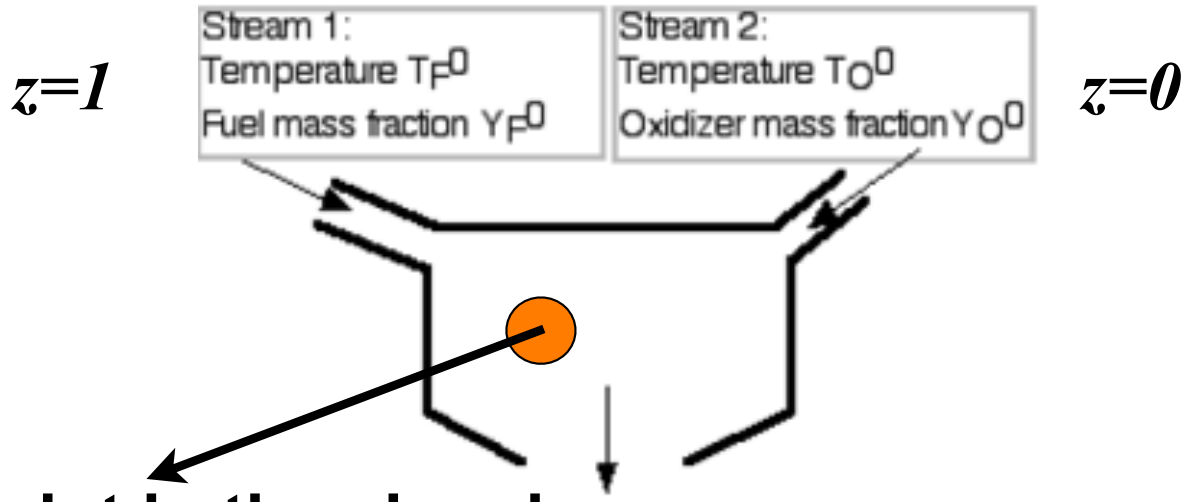


THE MIXING LINES (NO COMBUSTION)



Ch. 2 Sec 3.2.5

INTERPRETATION OF z : A MASS WEIGHTED MEASUREMENT OF MIXING

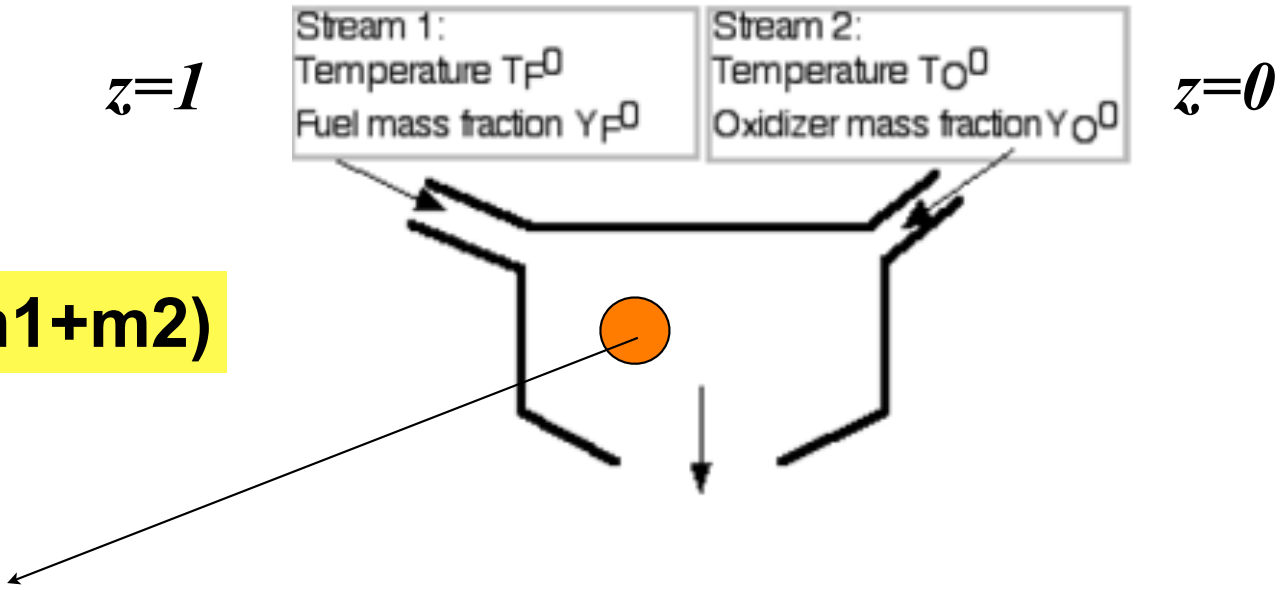


At a given point in the chamber:

- **mass coming from stream 1 = m1**
- **mass of fuel = m1 Y_F^0**
- **mass coming from stream 2 = m2**
- **total mass= m1+m2**
- **fuel mass fraction Y_F= m1 Y_F^0/ (m1+m2)**

- **mixture fraction $z = Y_F/Y_F^0 = m1/(m1+m2)$**

INTERPRETATION OF z :



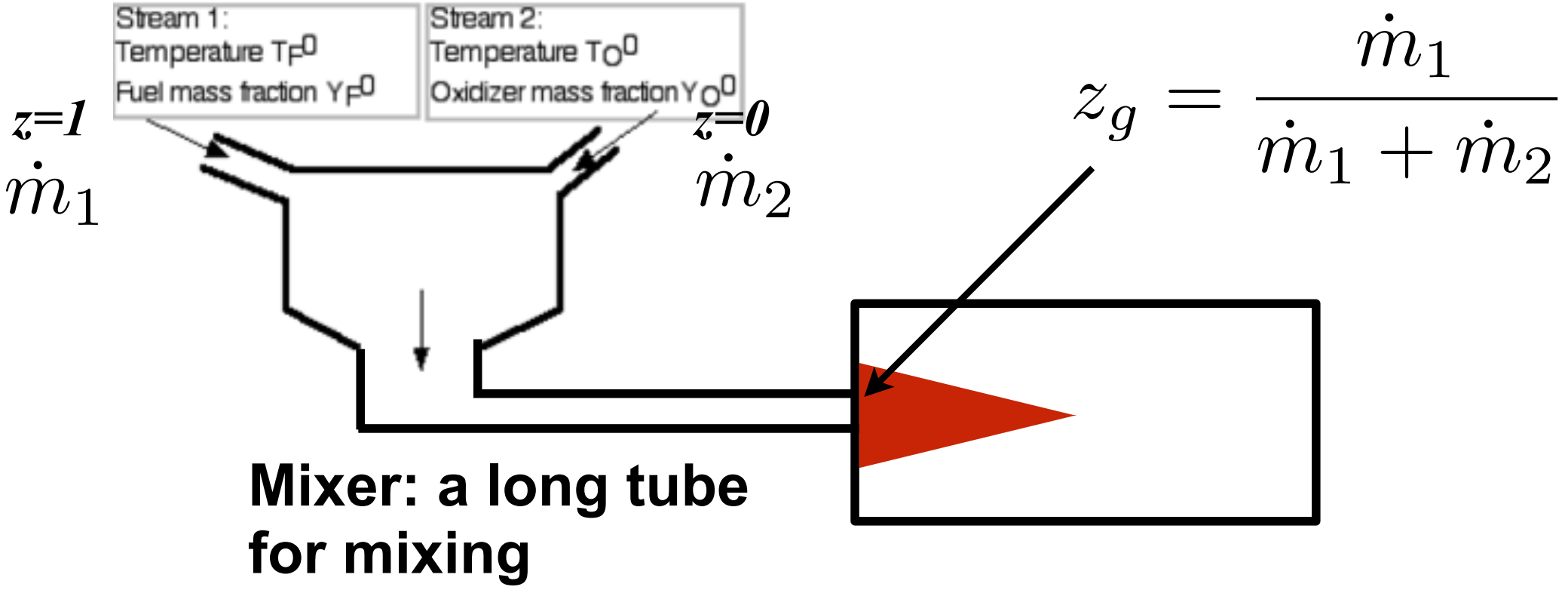
z = m1/(m1+m2)

If the mixture fraction at this point at time t is z, it means that at this point, in 1 kg of mixture:

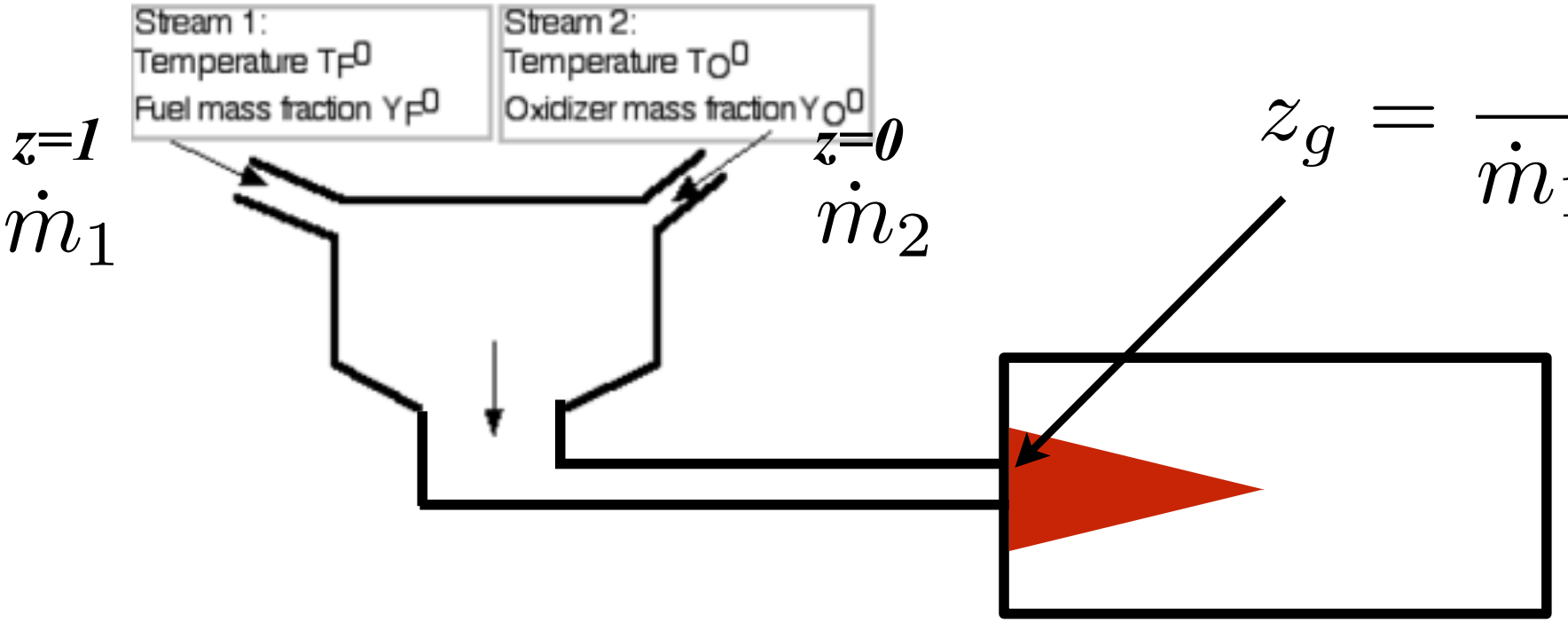
- **z kg come from stream 1**
- **(1-z) kg come from stream 2**

Careful: this works only if all Lewis numbers are equal

z can be local or global. For example, z is useful in a mixer for premixed flames:



This system, in the absence of combustion, acts like a premixer for a premixed flame which could come here.



$$z_g = \frac{\dot{m}_1}{\dot{m}_1 + \dot{m}_2}$$

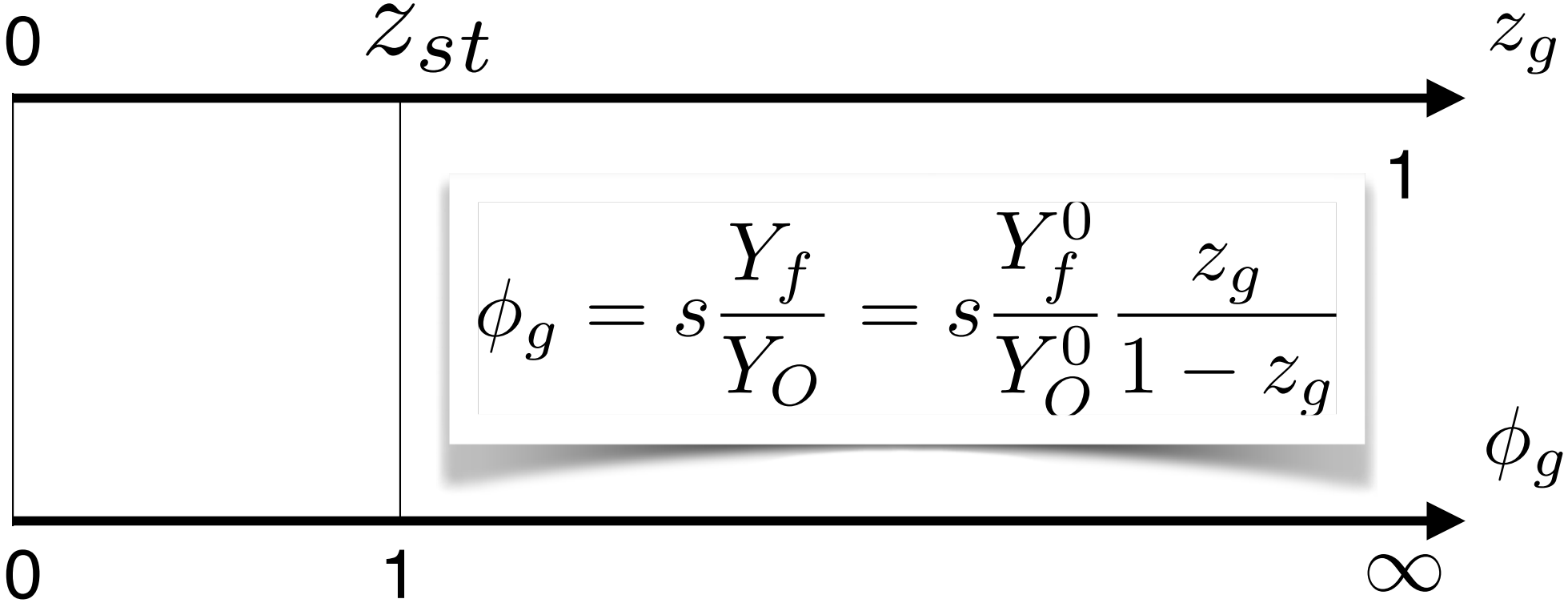
There is a link between global mixture fraction z_g and global equivalence ratio ϕ_g:

$$\boxed{Y_F = Y_F^0 z} \quad \text{and} \quad \boxed{Y_O = Y_O^0 (1 - z)}$$

$$\phi_g = s\frac{Y_f}{Y_O}$$

$$\phi_g = s\frac{Y_f}{Y_O} = s\frac{Y_f^0}{Y_O^0}\frac{z_g}{1 - z_g}$$

Equivalence ratio and mixture fraction:



$$\phi = 1 \quad \text{for} \quad z_g = z_{st} = \frac{1}{1 + sY_F^0/Y_O^0}$$

With combustion, z can also be introduced:

$$\frac{\partial \rho Y_F}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_F) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_F}{\partial x_i}\right) + \dot{\omega}_F$$

$$\frac{\partial \rho Y_O}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_O) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_O}{\partial x_i}\right) + s\dot{\omega}_F$$

$$\frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i T) = \frac{\partial}{\partial x_i}\left(\frac{\lambda}{C_p}\frac{\partial T}{\partial x_i}\right) - \frac{Q}{C_p}\dot{\omega}_F$$

Combining them two by two to eliminate source terms and normalizing to have the same boundary conditions leads to three passive scalars with identical bcs: they are all equal to the mixture fraction z

The mixture fraction z is now:

$$z = \frac{sY_F - Y_O + Y_O^0}{sY_F^0 + Y_O^0} = \frac{\frac{C_p}{Q}(T - T_O^0) + Y_F}{\frac{C_p}{Q}(T_F^0 - T_O^0) + Y_F^0} = \frac{\frac{sC_p}{Q}(T - T_O^0) + Y_O - Y_O^0}{\frac{sC_p}{Q}(T_F^0 - T_O^0) - Y_O^0}$$

In these expressions, only Y_F, Y_O and T are variable.

All other quantities are fixed:
- s is the stoichiometric ratio
- Y_F^0 and Y_O^0 are the fuel and oxidizer inlet mass fractions in stream 1 and 2 respectively
- Q is the heat of reaction per unit mass

How can we use the mixture fraction z ?:

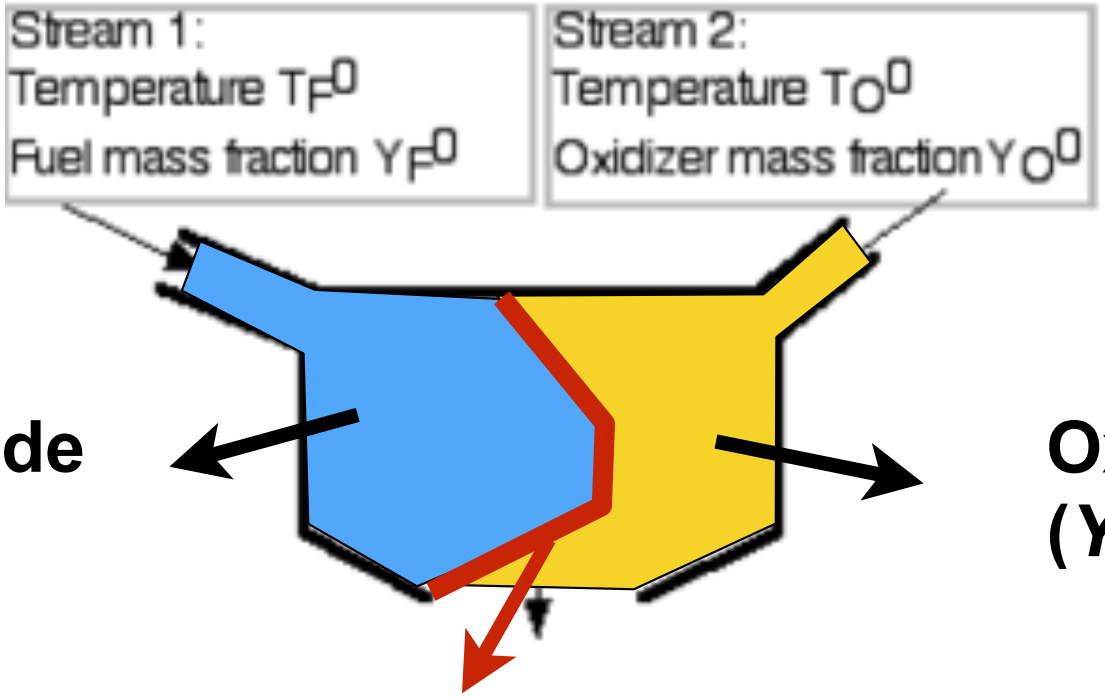
$$z = \frac{sY_F - Y_O + Y_O^0}{sY_F^0 + Y_O^0} = \frac{\frac{C_p}{Q}(T - T_O^0) + Y_F}{\frac{C_p}{Q}(T_F^0 - T_O^0) + Y_F^0} = \frac{\frac{sC_p}{Q}(T - T_O^0) + Y_O - Y_O^0}{\frac{sC_p}{Q}(T_F^0 - T_O^0) - Y_O^0}$$

Nice to have a quantity without source term but not sufficient. We can compute z in multiple flows but from z only, we cannot obtain T, Y_F and Y_O : in these expressions, we have relations for couples of variables (Y_F, Y_O) or (T, Y_O) or (Y_F, T) but not for individual variables Y_F, Y_O or T.

We need additional assumptions: the simplest one is the infinitely fast chemistry assumption

The infinitely fast chemistry assumption

- Suppose that kinetics are *faster* than all flow processes: fuel and oxidizer cannot co exist: so, either $Y_F=0$ or $Y_O=0$



Fuel side ($Y_O=0$)

Oxidizer side ($Y_F=0$)

Flame front ($Y_F=0$ and $Y_O=0$)

The infinitely fast chemistry assumption

- Suppose that kinetics are *faster* than all flow processes: fuel and oxidizer cannot co exist. There will be a 'oxidizer' side (Y_F=0) and a fuel side (Y_O=0)

$$z = \frac{sY_F - Y_O + Y_O^0}{sY_F^0 + Y_O^0} = \frac{\frac{C_p}{Q}(T - T_O^0) + Y_F}{\frac{C_p}{Q}(T_F^0 - T_O^0) + Y_F^0} = \frac{\frac{sC_p}{Q}(T - T_O^0) + Y_O - Y_O^0}{\frac{sC_p}{Q}(T_F^0 - T_O^0) - Y_O^0}$$

- The flame will be located on the surface where both Y_F and Y_O go to zero. This is the surface where z is equal to the value called the stoichiometric mixture fraction z_{st}:

$$z_{st} = \frac{1}{1 + \frac{sY_f^0}{Y_O^0}}$$

★**For pure CH4 (stream 1) and pure air (stream 2):**

$$z_{st} = \frac{1}{1 + \frac{sY_f^0}{Y_O^0}} = \frac{1}{1 + \frac{4*1}{0.23}} = 0.055$$

★**Now we can express Y_F, Y_O and T versus z.**

★**On the fuel side, there is no oxygen:**

$$z = \frac{sY_F - Y_O + Y_O^0}{sY_F^0 + Y_O^0} \qquad z = \frac{\frac{sC_p}{Q}(T - T_O^0) + Y_O - Y_O^0}{\frac{sC_p}{Q}(T_F^0 - T_O^0) - Y_O^0}$$

$$\begin{aligned} Y_F(z) &= zY_F^0 + (z-1)\frac{Y_O^0}{s} = Y_F^0 \frac{z - z_{st}}{1 - z_{st}} \\ Y_O(z) &= 0. \\ T(z) &= zT_F^0 + (1-z)T_O^0 + \frac{QY_F^0}{C_p} z_{st} \frac{1-z}{1-z_{st}} \end{aligned}$$

$$z = \frac{sY_F - Y_O + Y_O^0}{sY_F^0 + Y_O^0} = \frac{\frac{C_p}{Q}(T - T_O^0) + Y_F}{\frac{C_p}{Q}(T_F^0 - T_O^0) + Y_F^0} = \frac{\frac{sC_p}{Q}(T - T_O^0) + Y_O - Y_O^0}{\frac{sC_p}{Q}(T_F^0 - T_O^0) - Y_O^0}$$

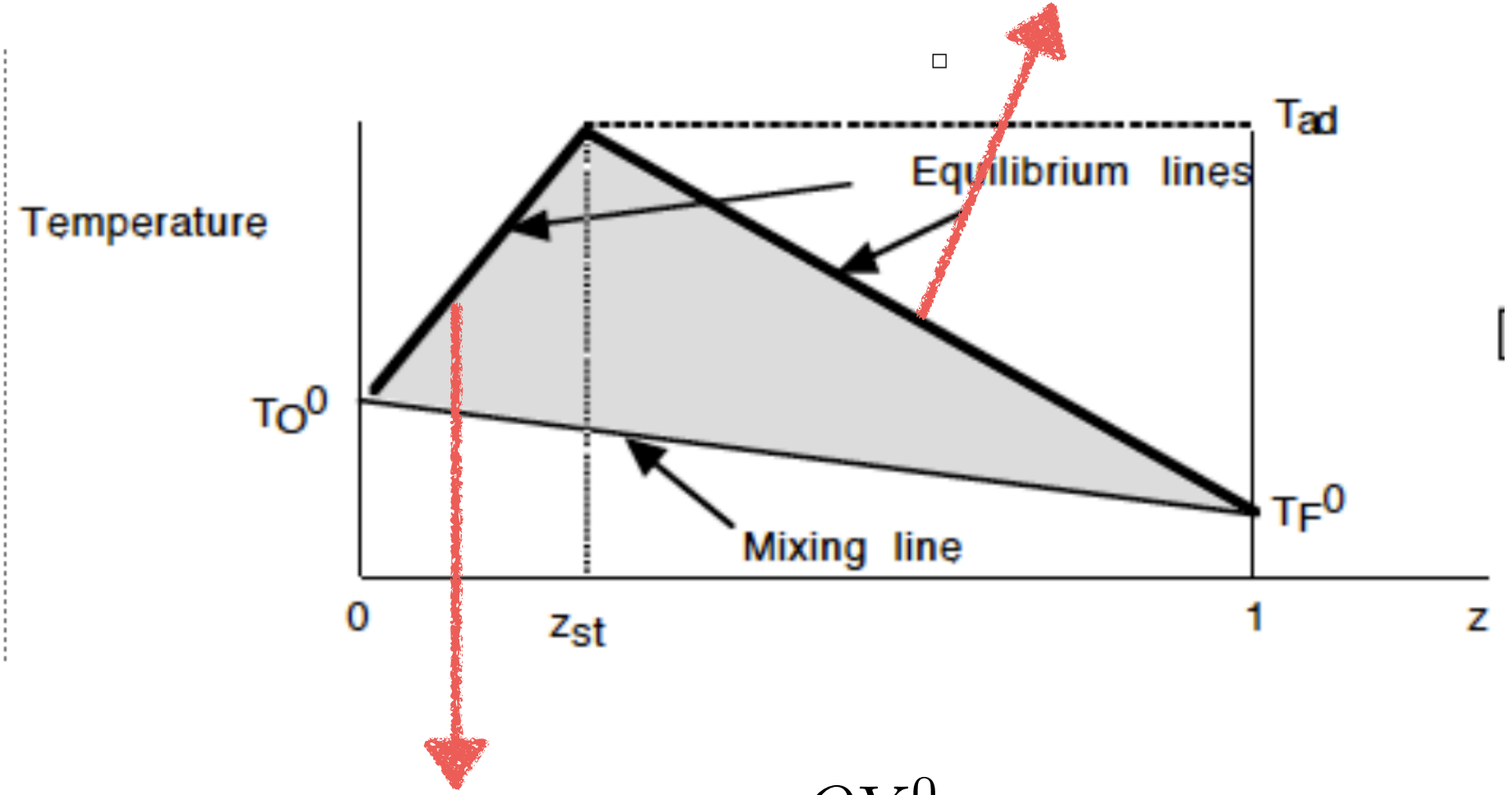
★**And on the oxidizer side, there is no fuel so that:**

$$Y_F(z) = 0$$

$$Y_O(z) = Y_O^0(1 - \frac{z}{z_{st}})$$

$$T(z) = zT_F^0 + (1 - z)T_O^0 + \frac{QY_F^0}{C_p}z$$

$$T(z) = zT_F^0 + (1-z)T_O^0 + \frac{QY_F^0}{C_p} z_{st} \frac{1-z}{1-z_{st}}$$



$$T(z) = zT_F^0 + (1-z)T_O^0 + \frac{QY_F^0}{C_p} z$$

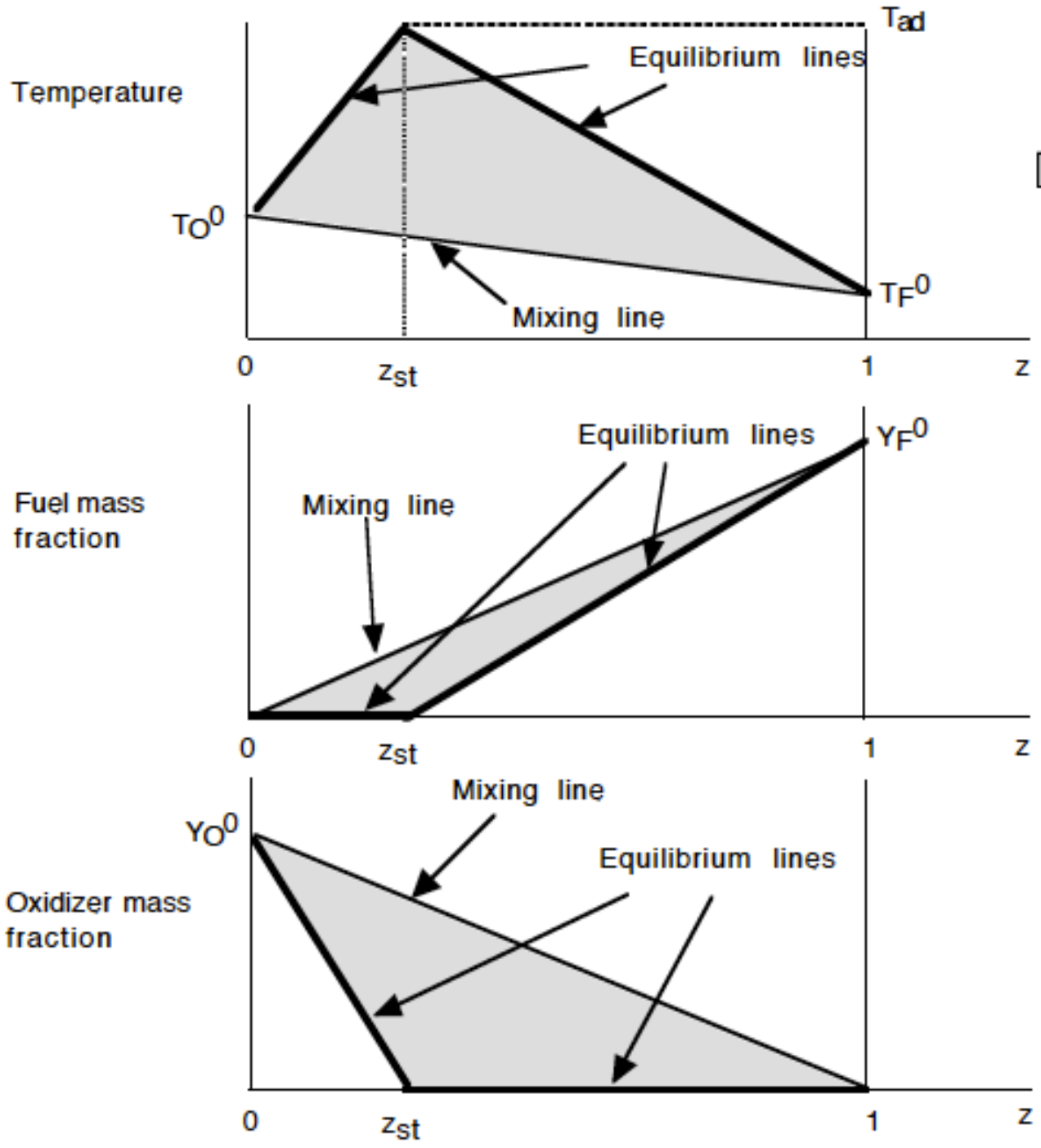
The z diagram.

Assumptions:

-infinitely fast chemistry

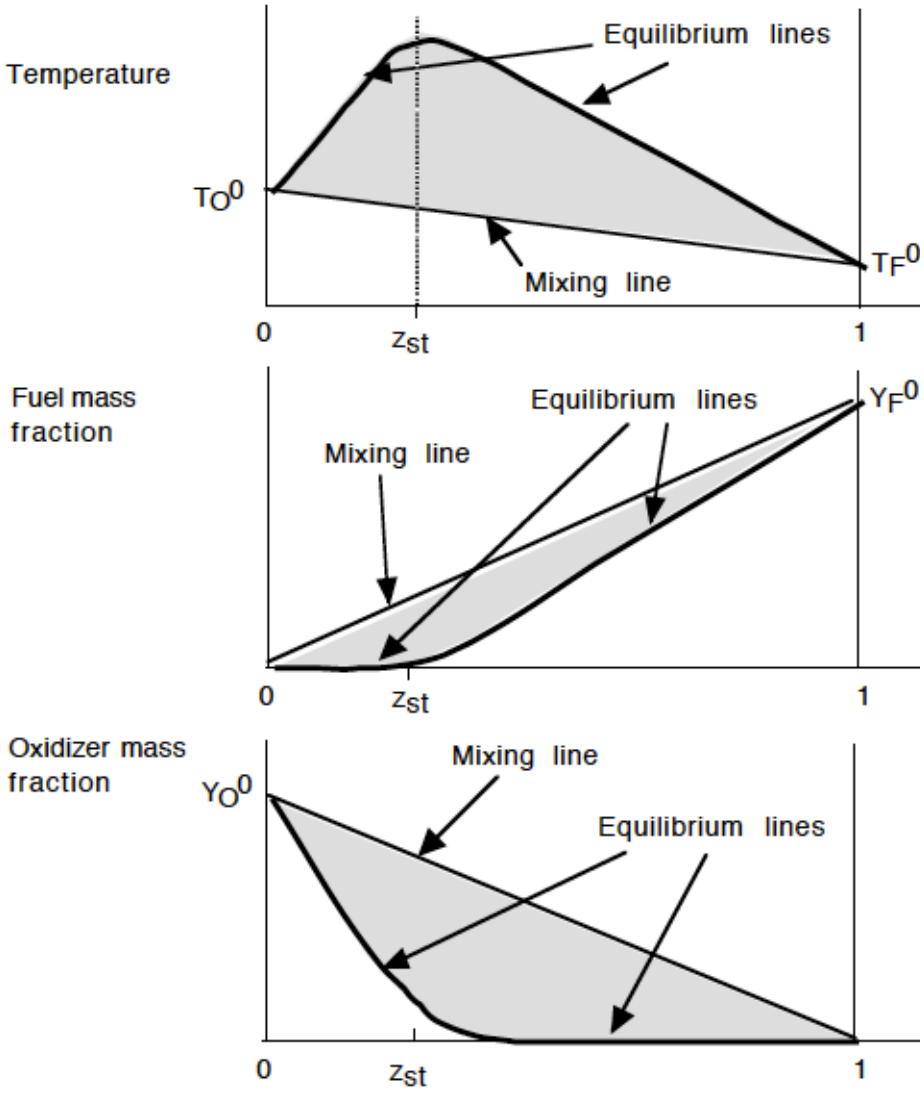
- unity Lewis numbers

- constant pressure

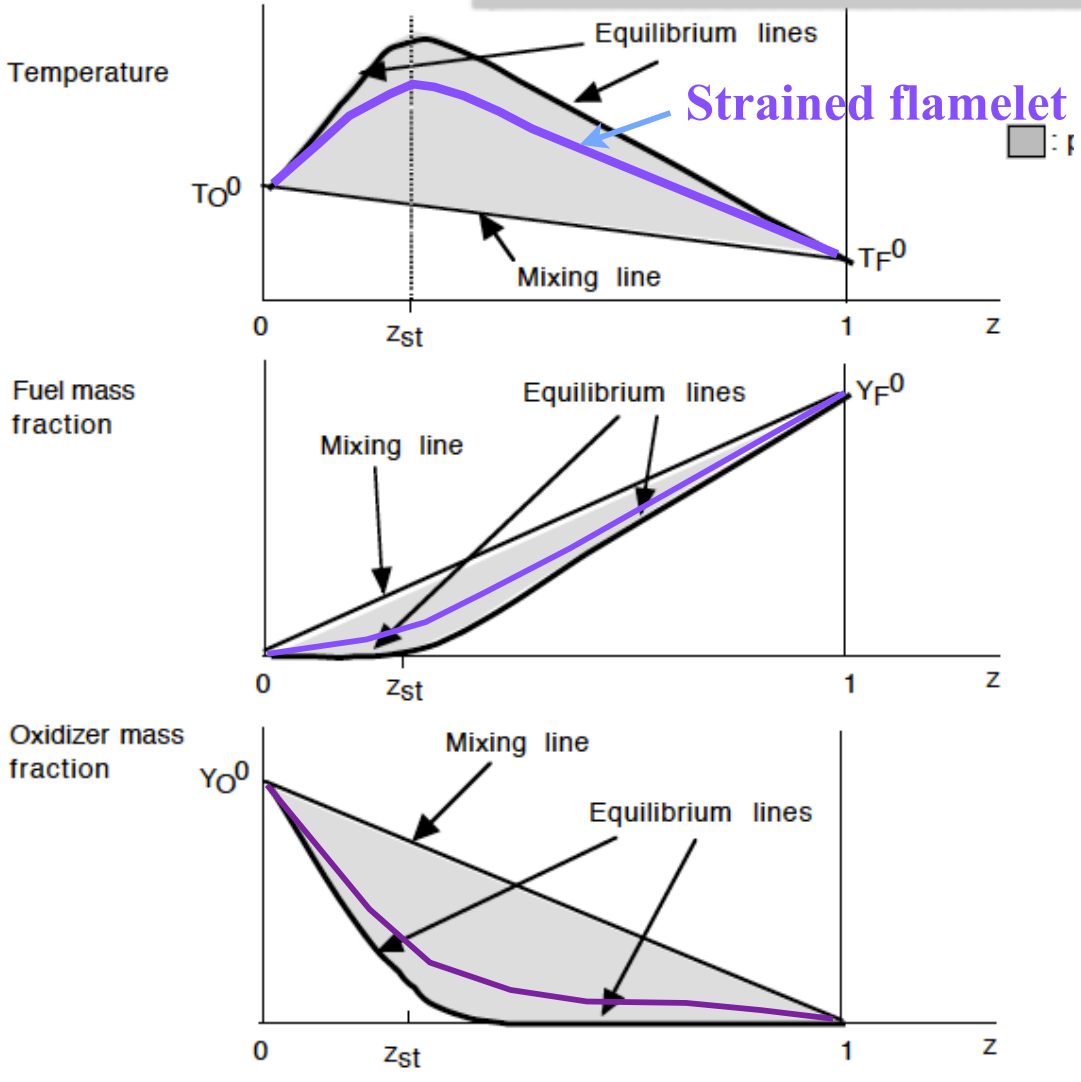


There are multiple other z diagrams of growing complexity

Ch. 3, Sect 3.5



Reversible single step



Flamelet strained assumption

OK we have T, Yk = f(z). So what ?

★ What we really want is to have T and all Yk's as functions of time and spatial positions.

★ Does z help us ?

➡ Yes: it helps us to analyze flames. For ex, the z diagram is often used in turbulent flames

➡ Yes, it also helps to compute flames: the introduction of z represents a significant simplification as described now:

Instead of solving:

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i Y_k\right) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_k}{\partial x_i}\right) + \dot{\omega}_k$$

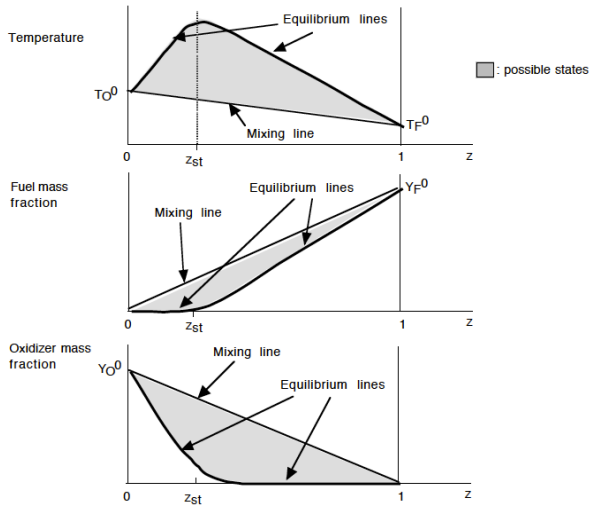
$$\rho C_p \frac{DT}{Dt} = \dot{\omega}'_T + \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) - \rho \frac{\partial T}{\partial x_i}\left(\sum_{k=1}^{N} C_{p,k} Y_k V_{k,i}\right)$$

Only solve the z equation:

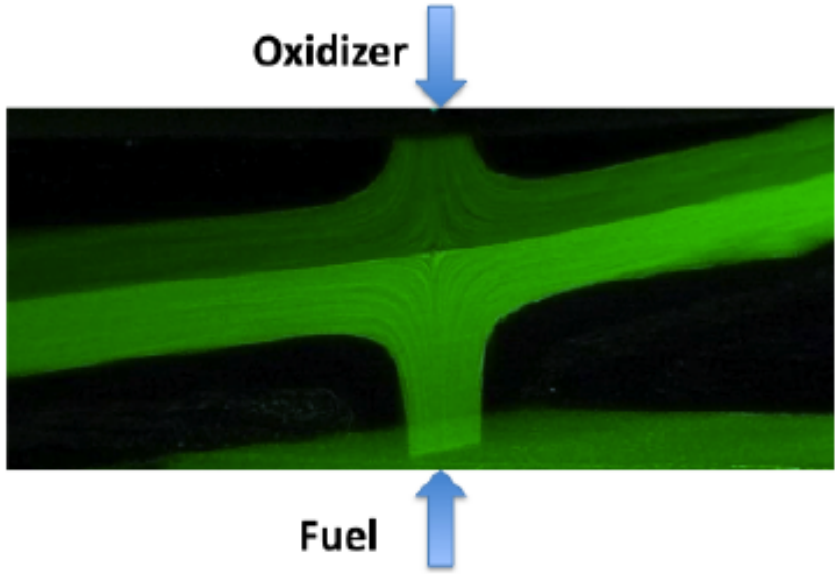
$$\frac{\partial \rho z}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i z\right) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial z}{\partial x_i}\right)$$

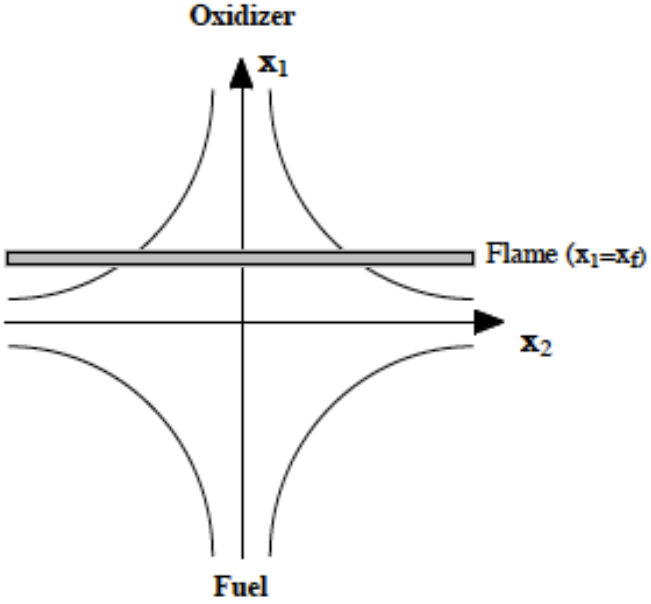
And read T and Yk in the z diagram. We'll use this in turbulent flames

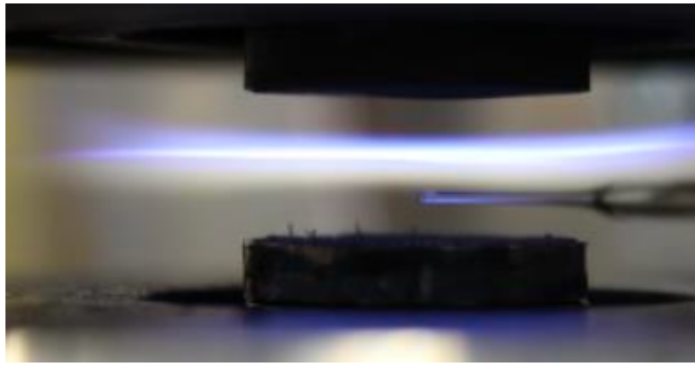
Z diagram structure:
T(z)
$Y_F(z)$
Yo(z)



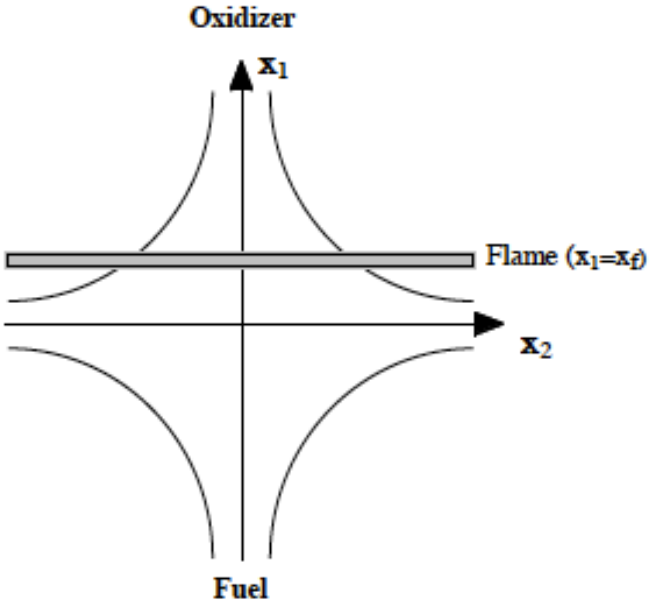
Let us begin by using the z diagram for a steady strained diffusion flame with negligible heat release (constant density):







$$\frac{\partial \rho Y_F}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_F) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_F}{\partial x_i}\right) + \dot{\omega}_F$$



We impose a stagnation point velocity field:

$$u_1 = -ax_1 \quad \text{and} \quad u_2 = ax_2$$

$$\frac{\partial \rho z}{\partial t} + \frac{\partial}{\partial x_1}(\rho u_1 z) + \frac{\partial}{\partial x_2}(\rho u_2 z) = \frac{\partial}{\partial x_1}\left(\rho \mathcal{D} \frac{\partial z}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\rho \mathcal{D} \frac{\partial z}{\partial x_2}\right)$$

$$\rho \frac{\partial z}{\partial t} + \rho u_1 \frac{\partial z}{\partial x_1} + \rho u_2 \frac{\partial z}{\partial x_2} = \frac{\partial}{\partial x_1}\left(\rho \mathcal{D} \frac{\partial z}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\rho \mathcal{D} \frac{\partial z}{\partial x_2}\right)$$

$$-ax_1 \frac{\partial z}{\partial x_1} = \mathcal{D} \frac{\partial^2 z}{\partial x_1^2}$$

$$-ax_1 \frac{\partial z}{\partial x_1} = \mathcal{D} \frac{\partial^2 z}{\partial x_1^2}$$

Usual change of variables: $\zeta = x_1 \sqrt{a/2\mathcal{D}}$

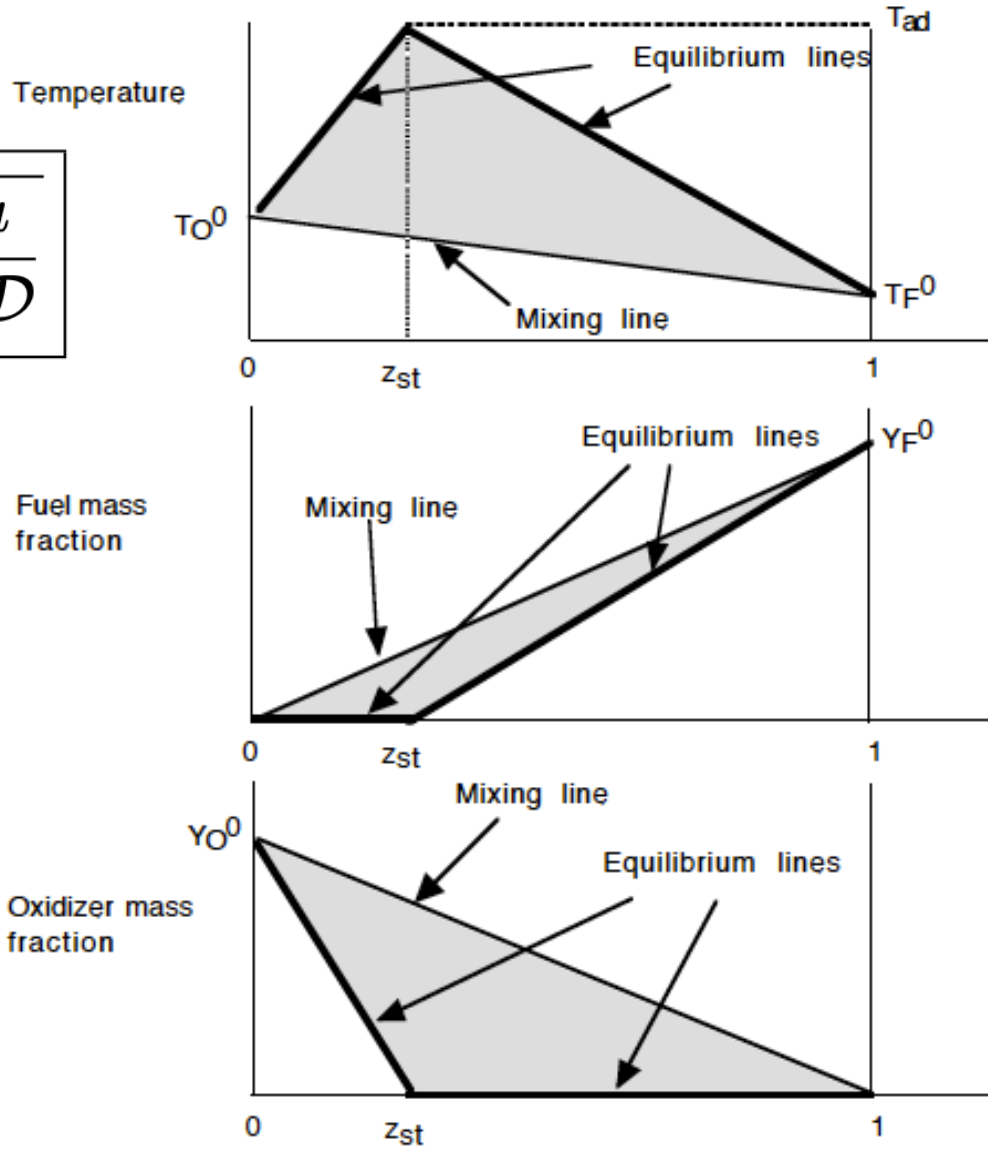
Gives:

$$\frac{\partial^2 z}{\partial \zeta^2} + 2\zeta \frac{\partial z}{\partial \zeta} = 0$$

$$\boxed{z = \frac{1}{2}\left[1 - \mathrm{erf}(\zeta)\right] \qquad \text{with} \qquad \zeta = x_1 \sqrt{\frac{a}{2\mathcal{D}}}}$$

FULL SOLUTION:

$$z = \frac{1}{2}\left[1 - \mathrm{erf}(\zeta)\right] \qquad \text{with} \qquad \zeta = x_1\sqrt{\frac{a}{2\mathcal{D}}}$$



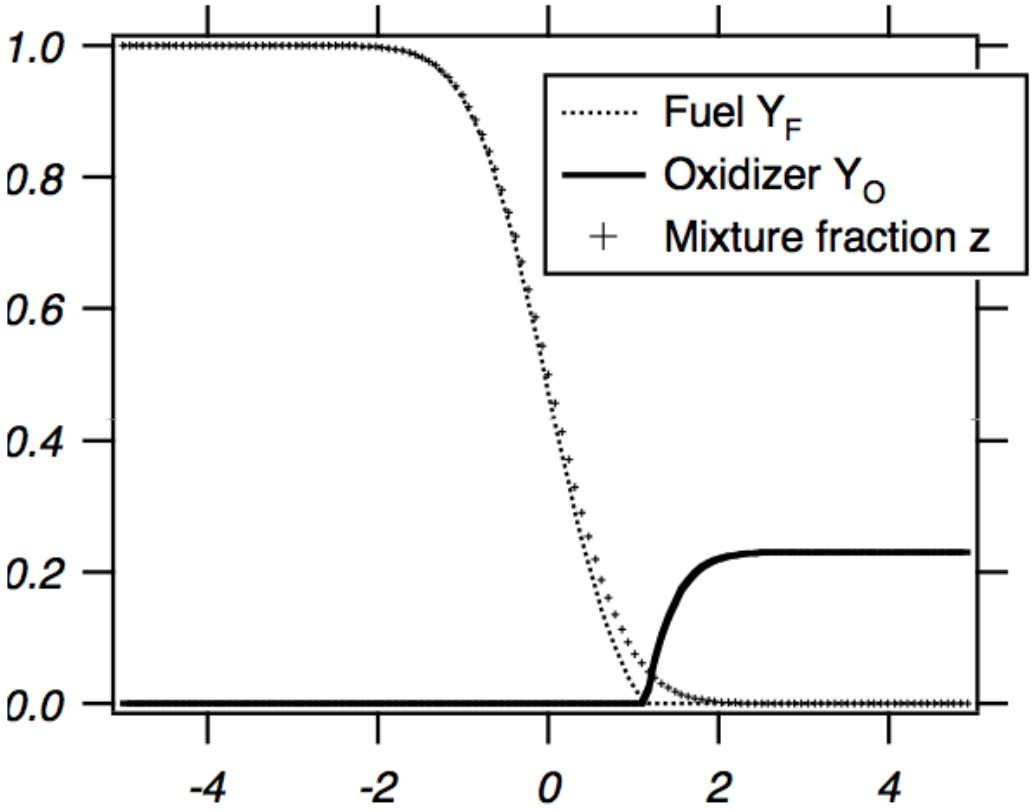
WE HAVE $z(x)$

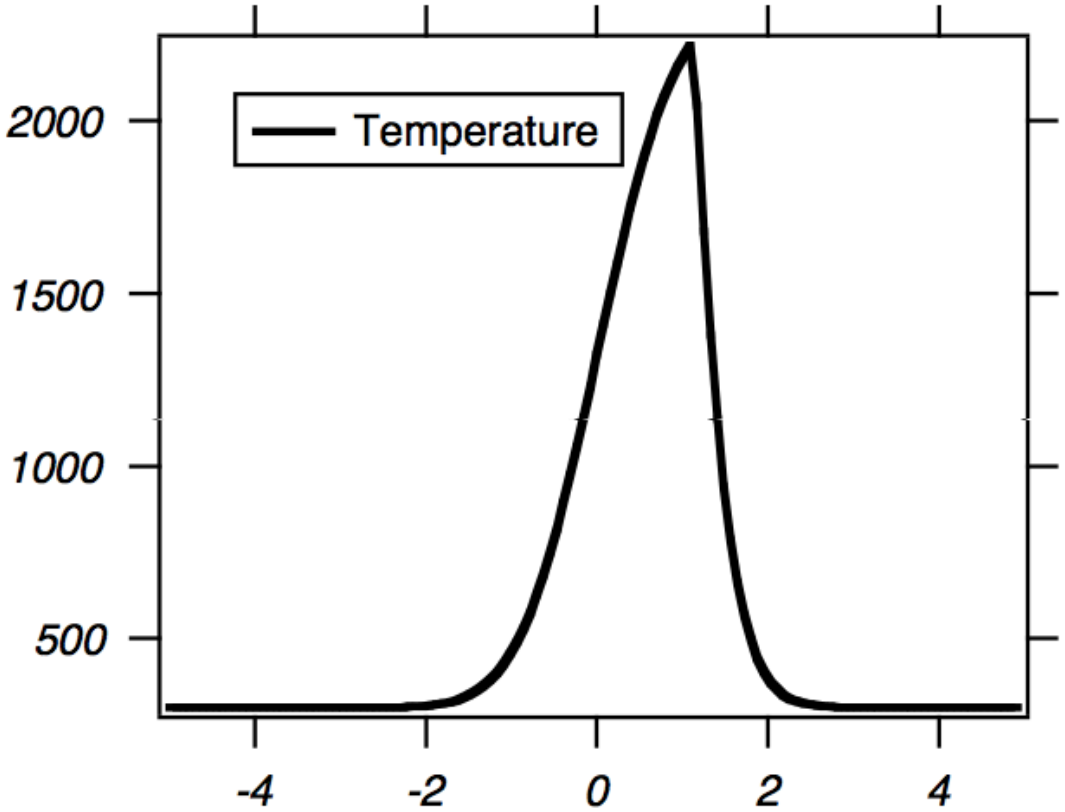
The z diagram gives us

$Y_F(z), Y_O(z), T(z)$

FINISHED...

SOLUTION FOR THE PLANAR DIFFUSION FLAME WITH INF FAST CHEMISTRY:





$$\zeta = x_1 \sqrt{\frac{a}{2\mathcal{D}}}$$

a: strain
D: diffusivity

$$\zeta = x_1 \sqrt{\frac{a}{2\mathcal{D}}}$$

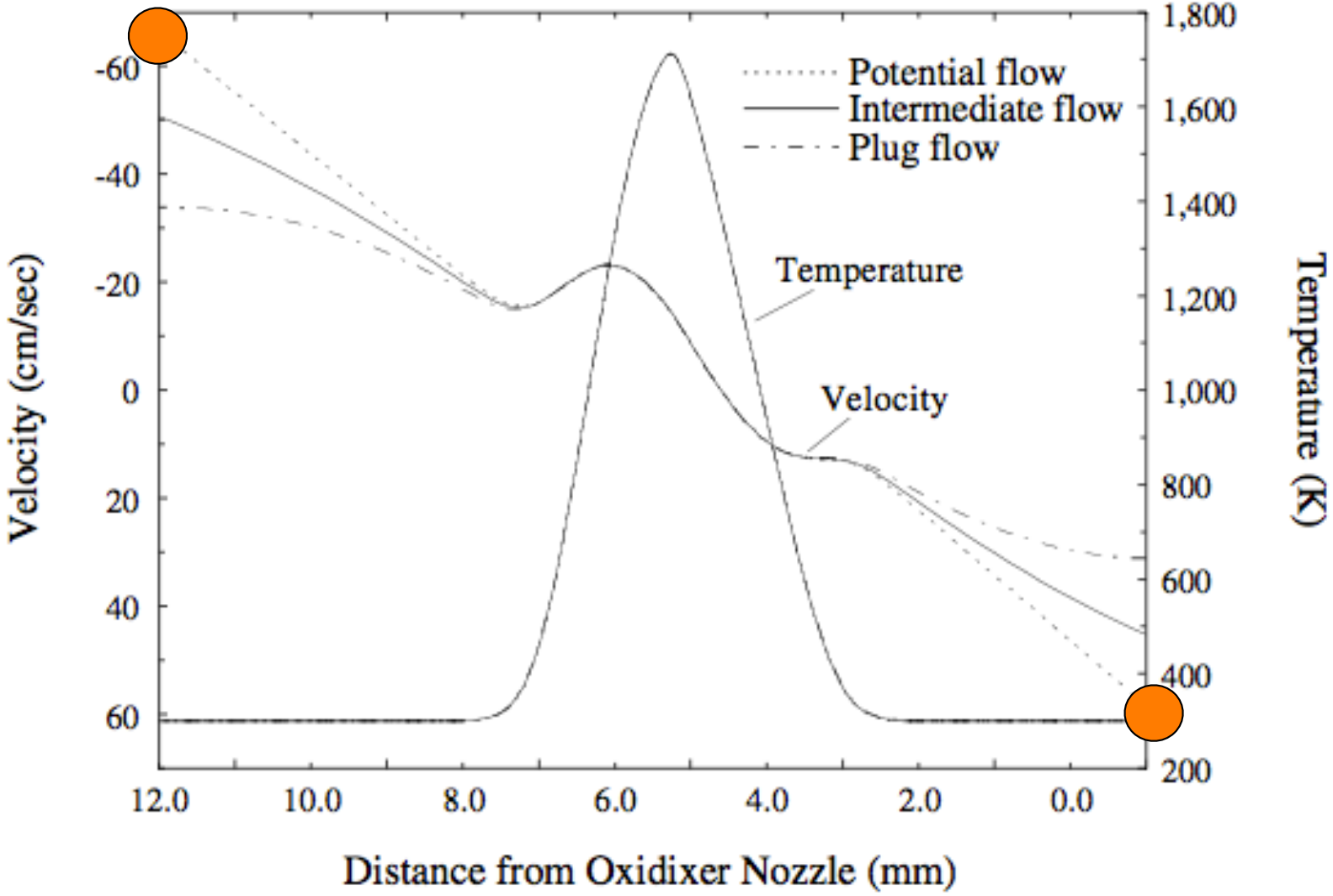


Figure 6.5.2. Calculated velocity and temperature profiles for a symmetric, nozzle-generated counterflow flame established by impinging a 23 percent methane-in-nitrogen stream against a 23 percent oxygen-in-nitrogen stream, for different descriptions of the flow (Sung, Liu & Law 1995).

Useful properties and interpretations of the mixture fraction z:

1 - z does not vary through a premixed flame front

2 - in a diffusion flame, there is always a surface $z = z_{st}$ on which the temperature is maximum and Nox formation very high

3 - the total amount of fuel burnt per unit surface is controlled by diffusion

1 - The mixture fraction z does not change through a premixed flame front

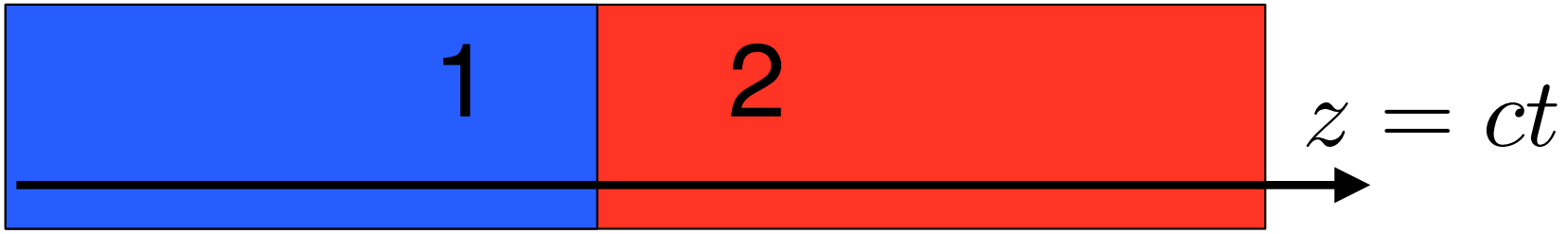
State 1: Y_F^1, Y_O^1

$$z_1 = \frac{sY_F^1 - Y_O^1 + Y_O^0}{sY_F^0 + Y_O^0}$$

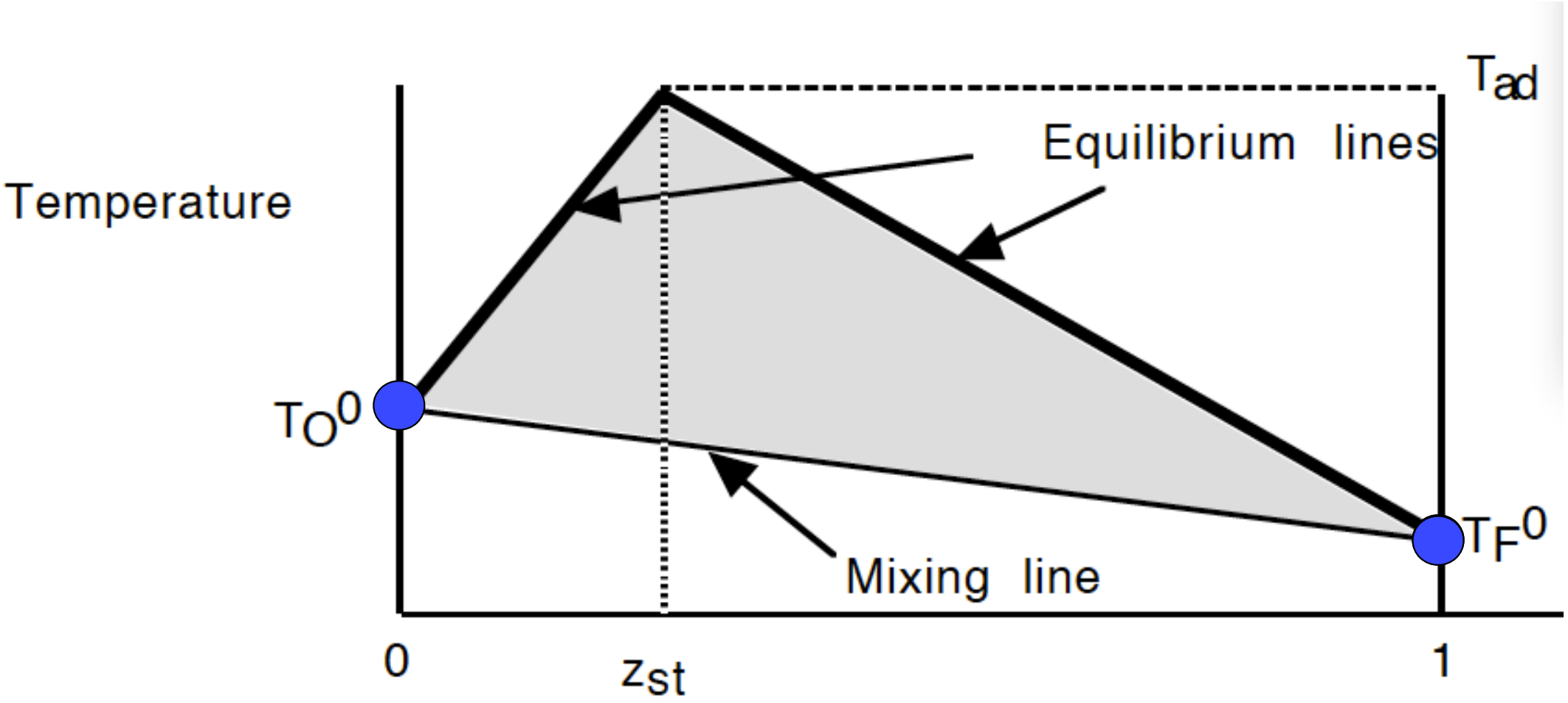
State 2: $Y_F^1 - \Delta Y_F^1, Y_O^1 - s\Delta Y_F^1$

By definition of s

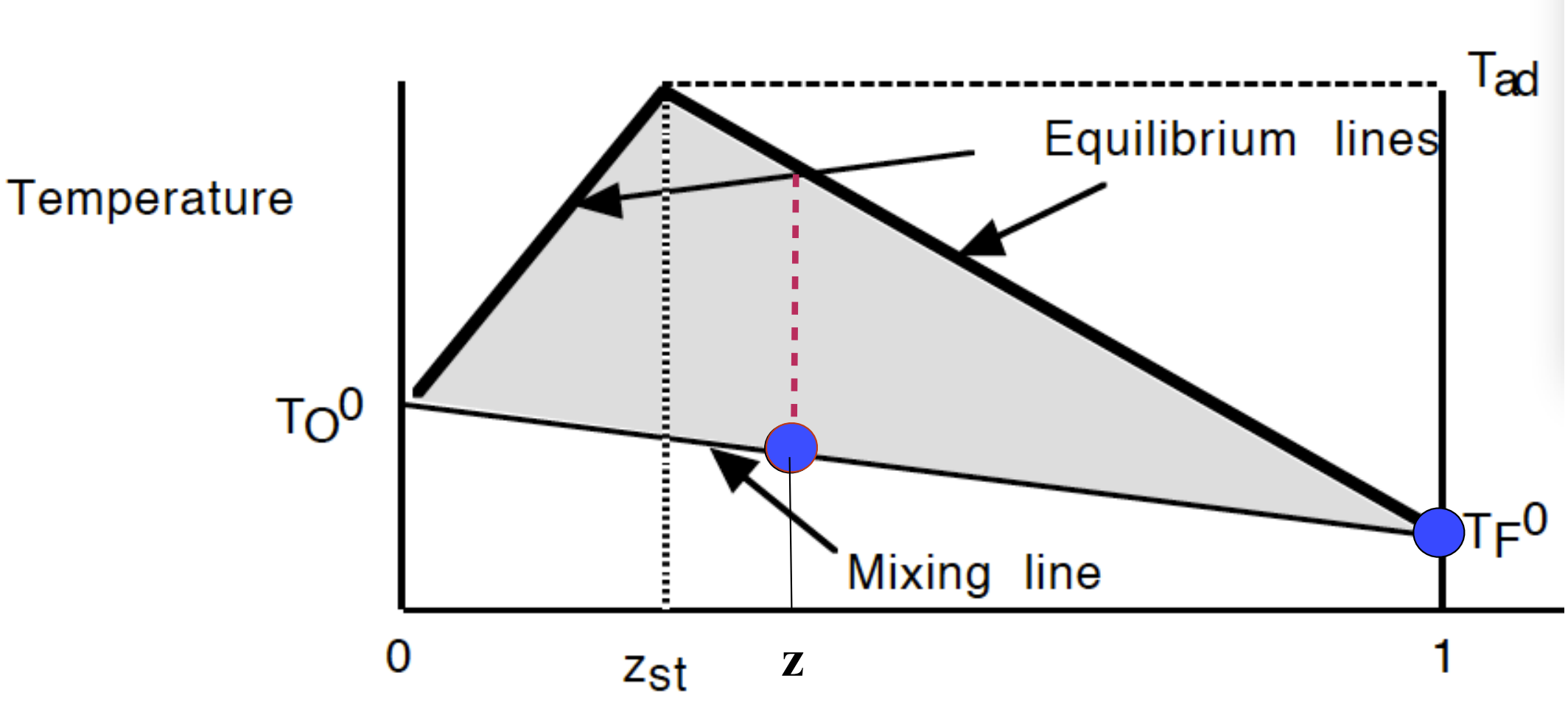
$$z_2 = \frac{s(Y_F^1 - \Delta Y_f^1) - (Y_O^1 - s\Delta Y_F^1) + Y_O^0}{sY_F^0 + Y_O^0} = z_1$$



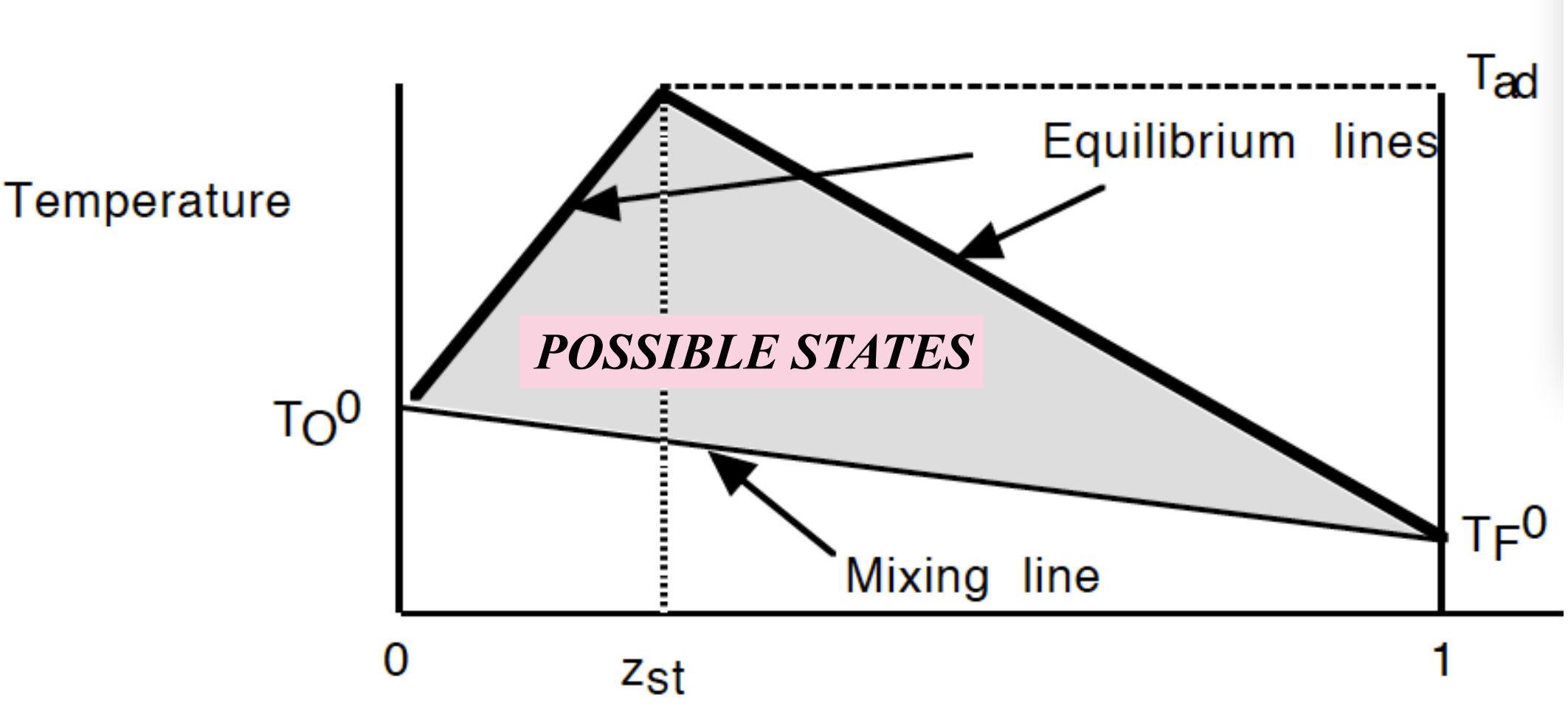
The z diagram helps to see trajectories: MIXING PHASE: you mix and reach a given z...



Combustion phase: after mixing, you burn. And you stop burning when you reach the equilibrium lines



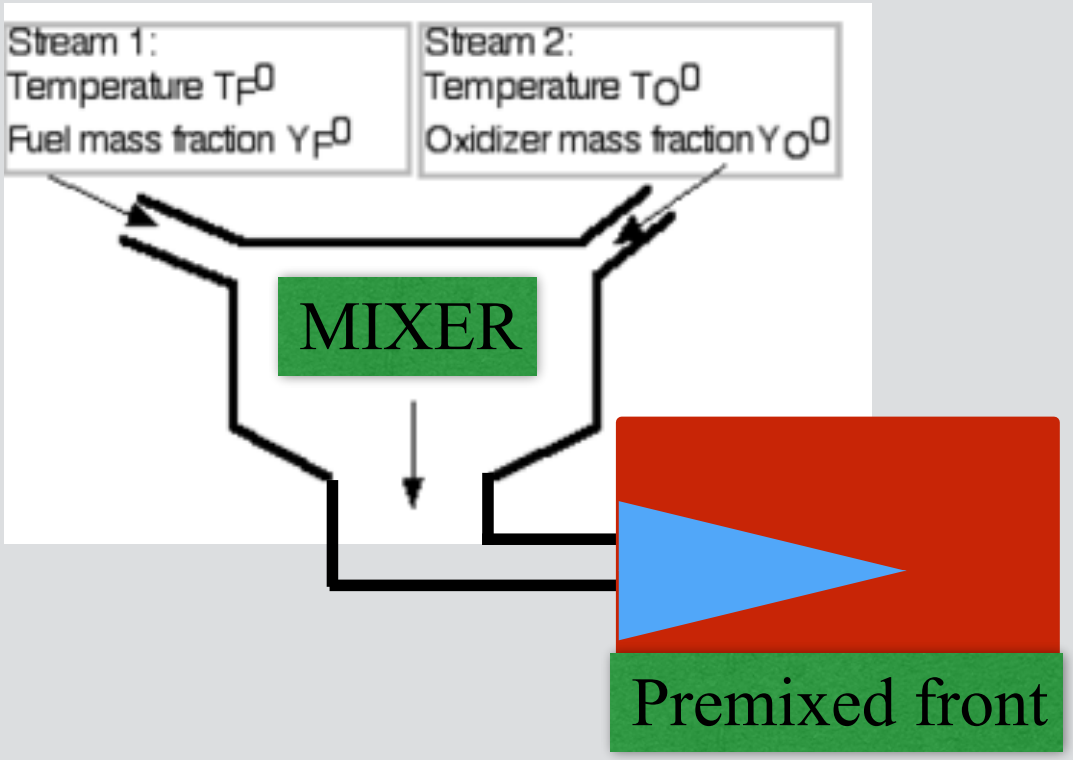
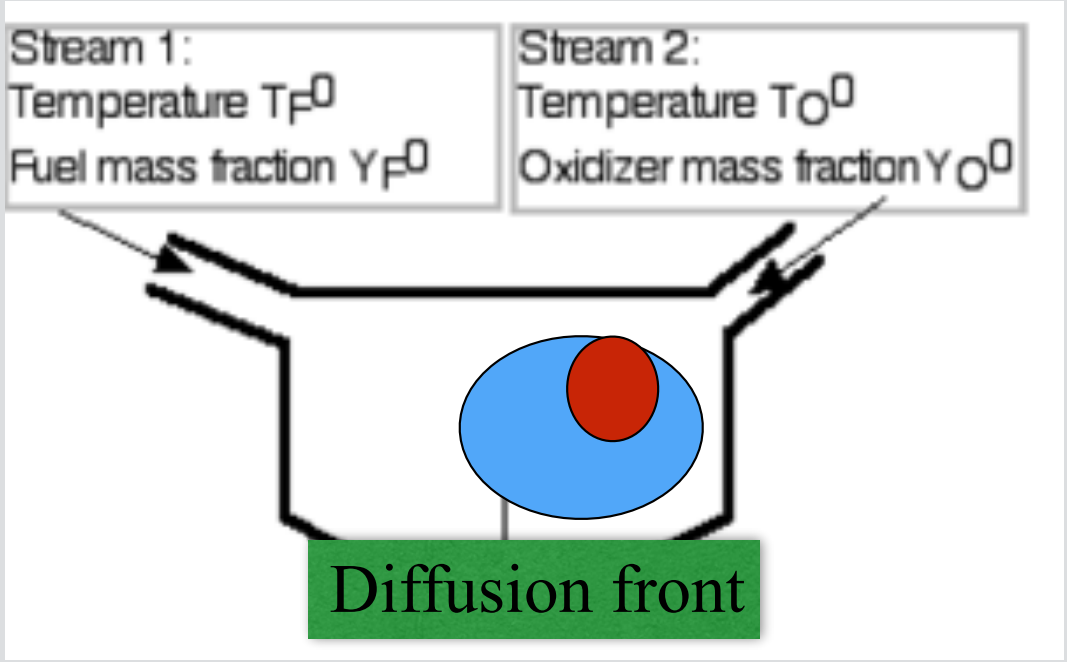
2 - Possible states: all states must be inside the triangle limited by equilibrium and mixing lines



Comparing diffusion and premixed flames:

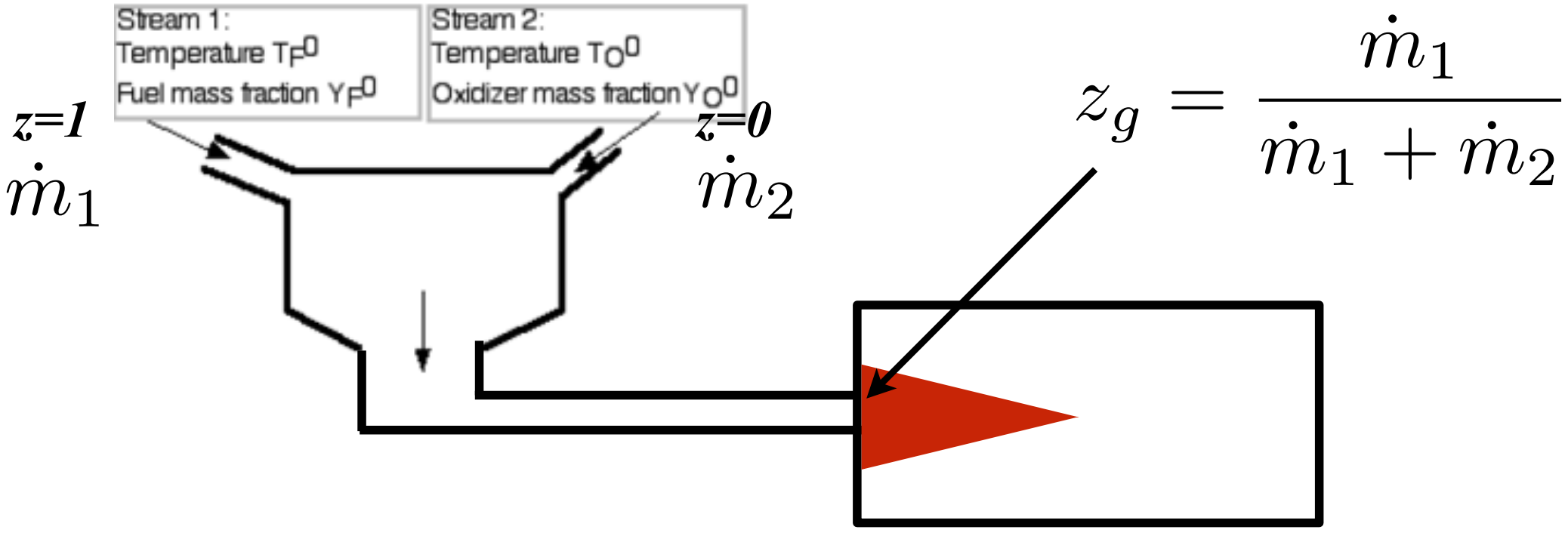
What is the maximum temperature reached in these two flames ?

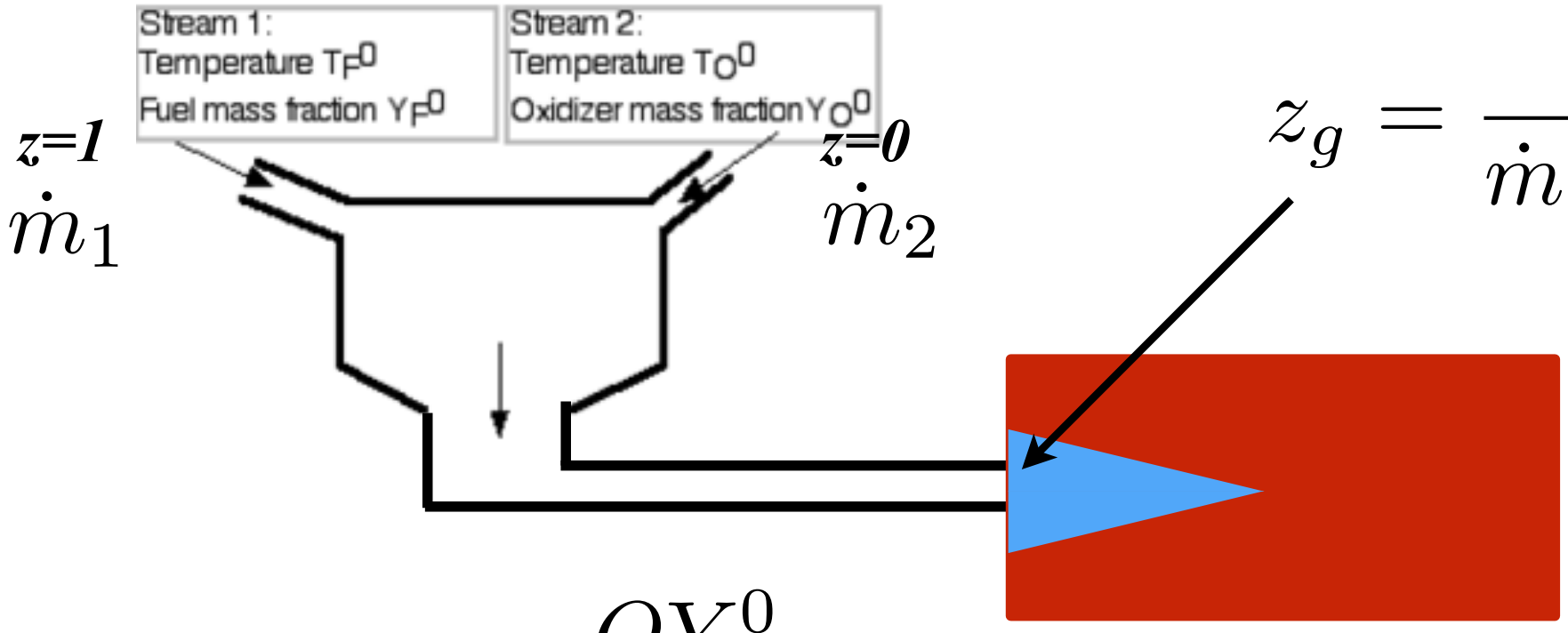
$$T_F^0 = T_O^0$$

PREMIXED	DIFFUSION
	

Comparing diffusion and premixed flames:

Begin by the PREMIXED flame:





$$z_g = \frac{\dot{m}_1}{\dot{m}_1 + \dot{m}_2}$$

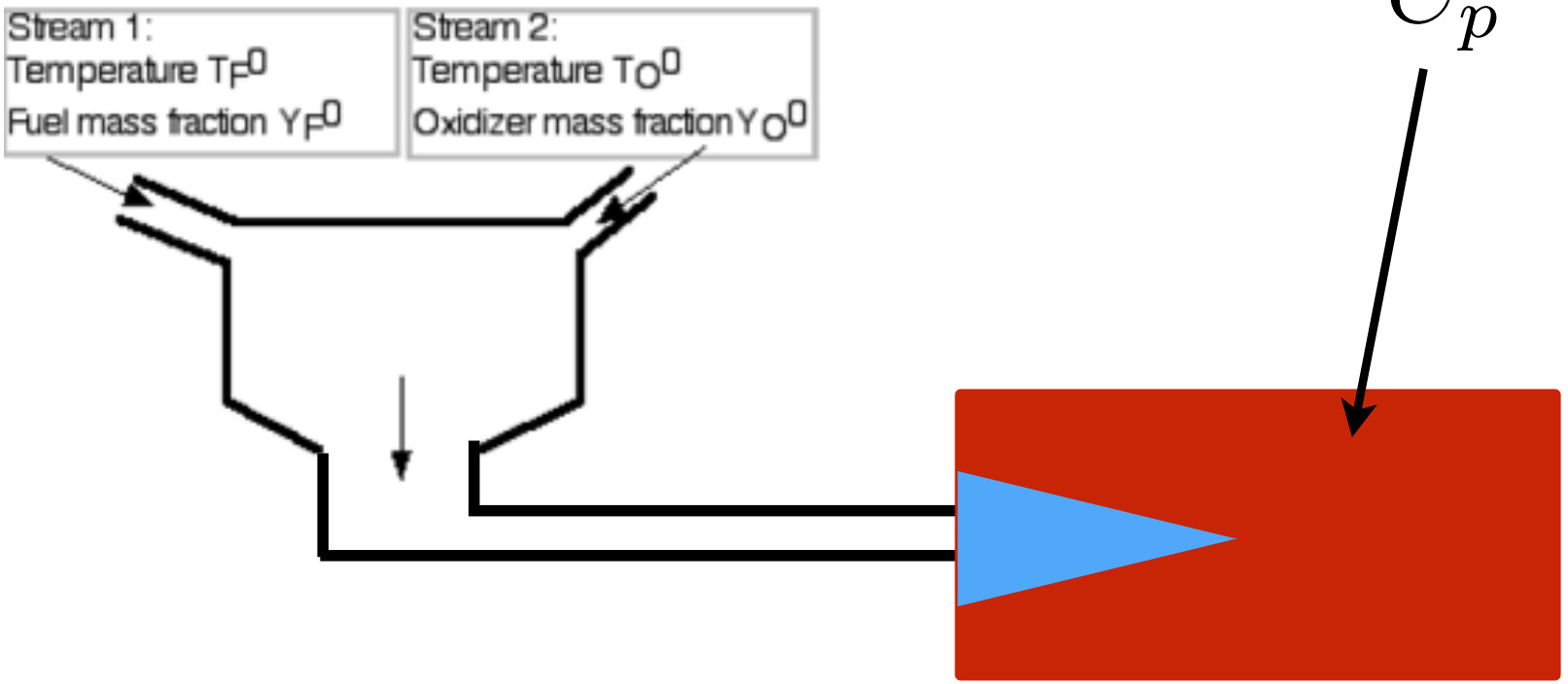
$$T(z) = T_F^0 + \frac{QY_F^0}{C_p} z_g$$

In this premixed flame, the temperature:

- **is homogeneous in the burnt gases**
- **varies with the flow rates of fuel and oxidizer because z_g changes**

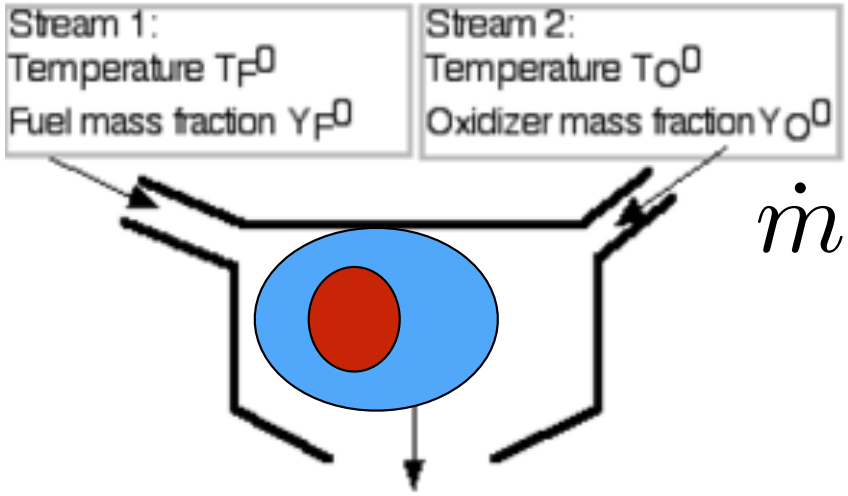
It reaches its maximum when the mixer provides a stoichiometric mixture:

$$z_g = z_{st} \qquad T(z) = T_F^0 + \frac{QY_F^0}{C_p} z_{st}$$



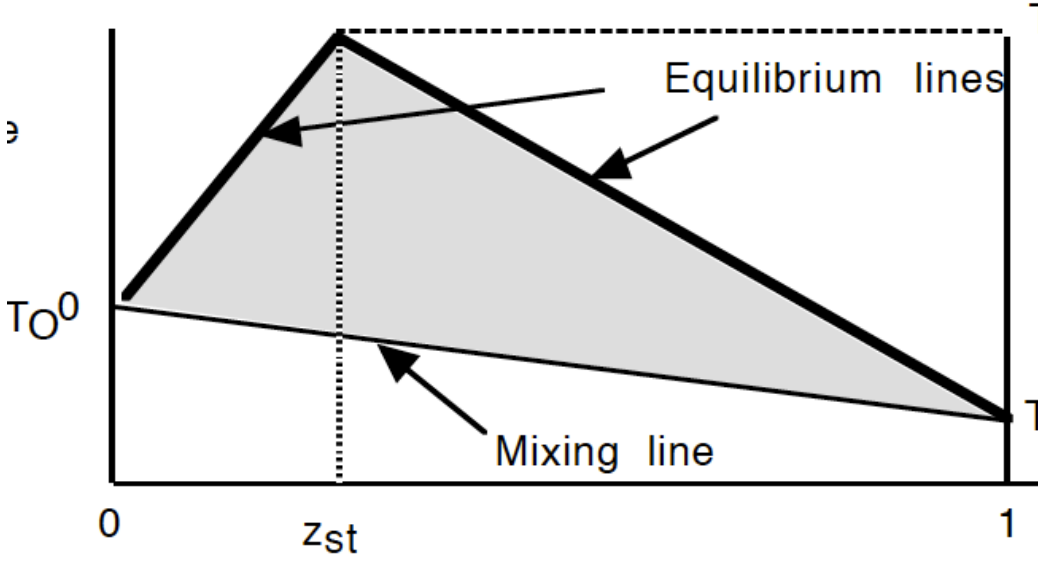
In this premixed flame, burnt gases all reach the maximum temperature (but not more). This temperature varies with the flow rates of fuel and oxidizer

What happens in the diffusion flame ?



$$T(z) = T_0^F + \frac{QY_F^0}{C_p} z$$

The temperature in the burnt gases is NOT homogeneous. It depends on z following the z diagram



It reaches its maximum on the stoechiometric surface $z = z_{st}$

$$T(z) = T_F^0 + \frac{QY_F^0}{C_p} z_{st}$$

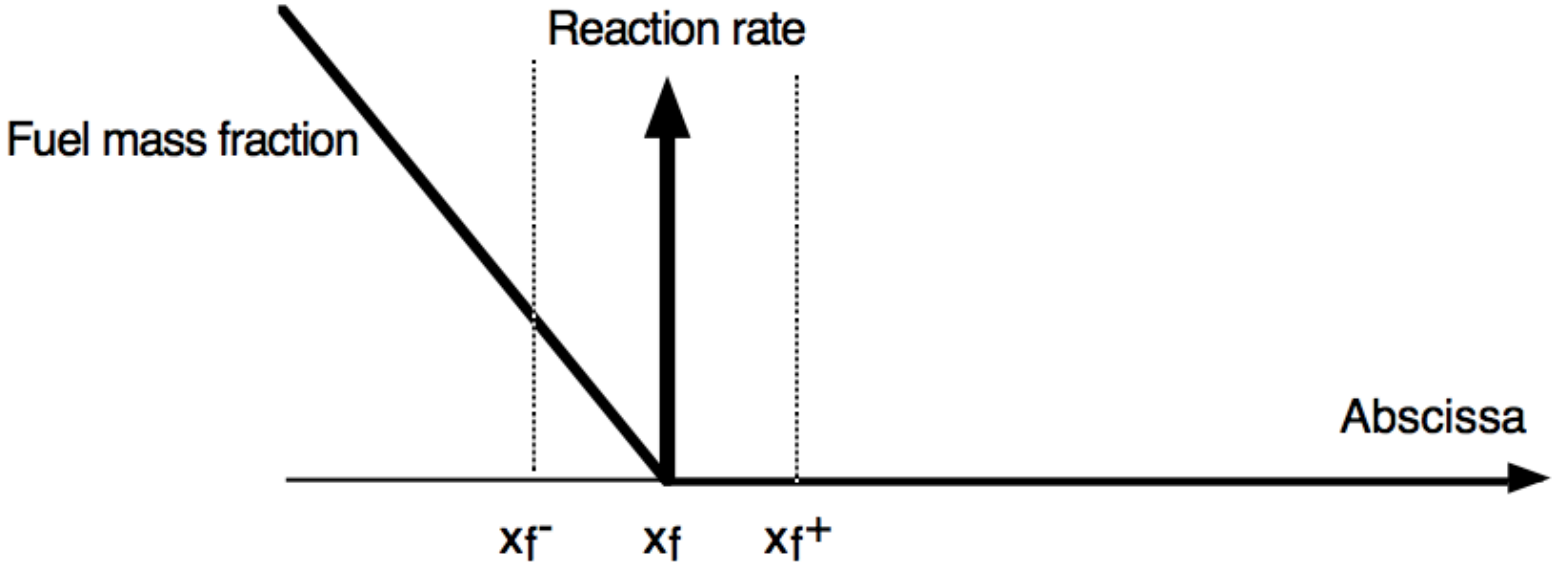
In a diffusion flame, the maximum temperature does not depend on the flow rates.

It is equal to the temperature reached in a stoichiometric premixed flame.

All other premixed flames are colder.

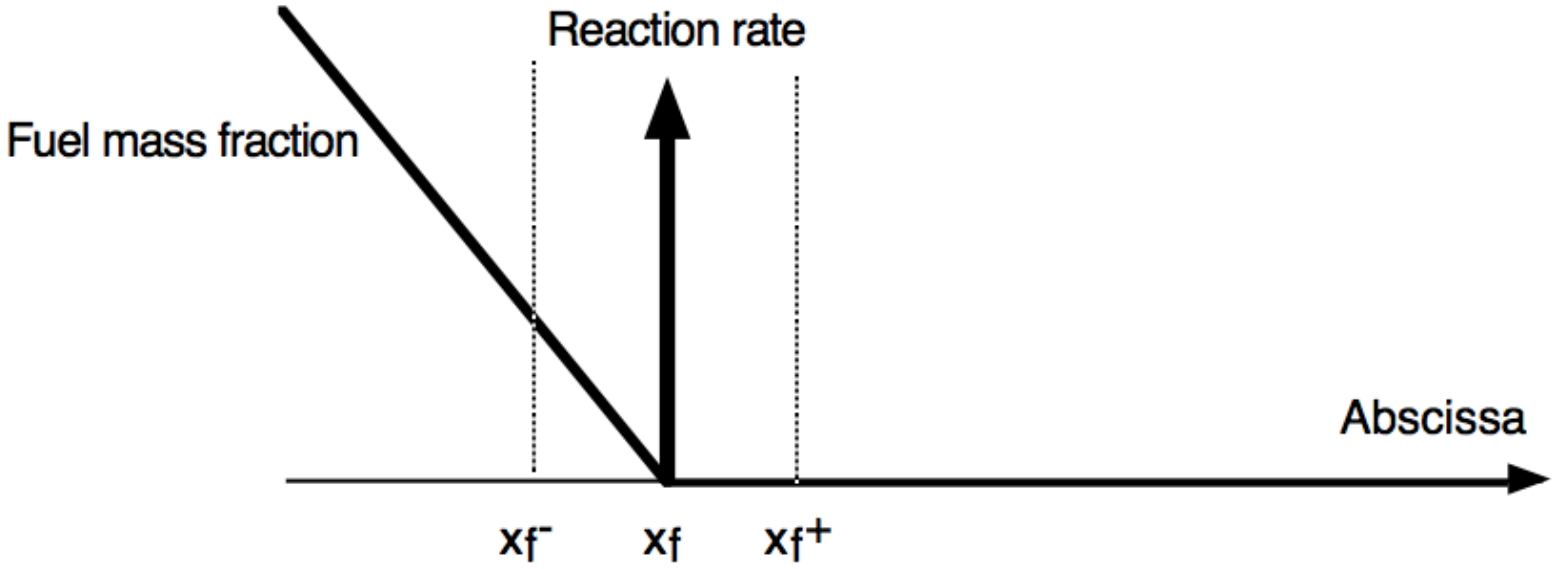
3 - How much does the diffusion flame burn ? (integral of the reaction rate)

- ★ Not an infinite number even if chemistry is infinitely fast !
- ★ Can be computed by integrating the fuel equation around the flame zone. Careful: profiles are not continuous for derivatives…



INTEGRATE THE FUEL EQUATION:

$$\frac{\partial \rho Y_F}{\partial t} + \boxed{\frac{\partial}{\partial x_i}(\rho u_i Y_F)} = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial Y_F}{\partial x_i}\right) + \boxed{\dot{\omega}_F}$$



AND MAKE x_f^- AND x_f^+ GO TO x_f

$$\dot{\Omega}_F = \int_{x_f^-}^{x_f^+} \dot{\omega}_F dx = -\left[\rho \mathcal{D} \frac{\partial Y_F}{\partial x}\right]_{x_f^-}^{x_f^+} = \left[\rho \mathcal{D} \frac{\partial Y_F}{\partial x}\right]_{x=x_f^-}$$

- ★ **The TOTAL mass of fuel burnt by unit time is NOT controlled by chemistry (which is fast) but by the rate at which the fuel can reach the flame front through diffusion. This is why we call them 'DIFFUSION FLAMES'**
- ★ **This does not make them very efficient because diffusion is slow**
- ★ **We can make a diffusion flame burn faster by increasing gradients: flame stretch**

The limits of the z diagram

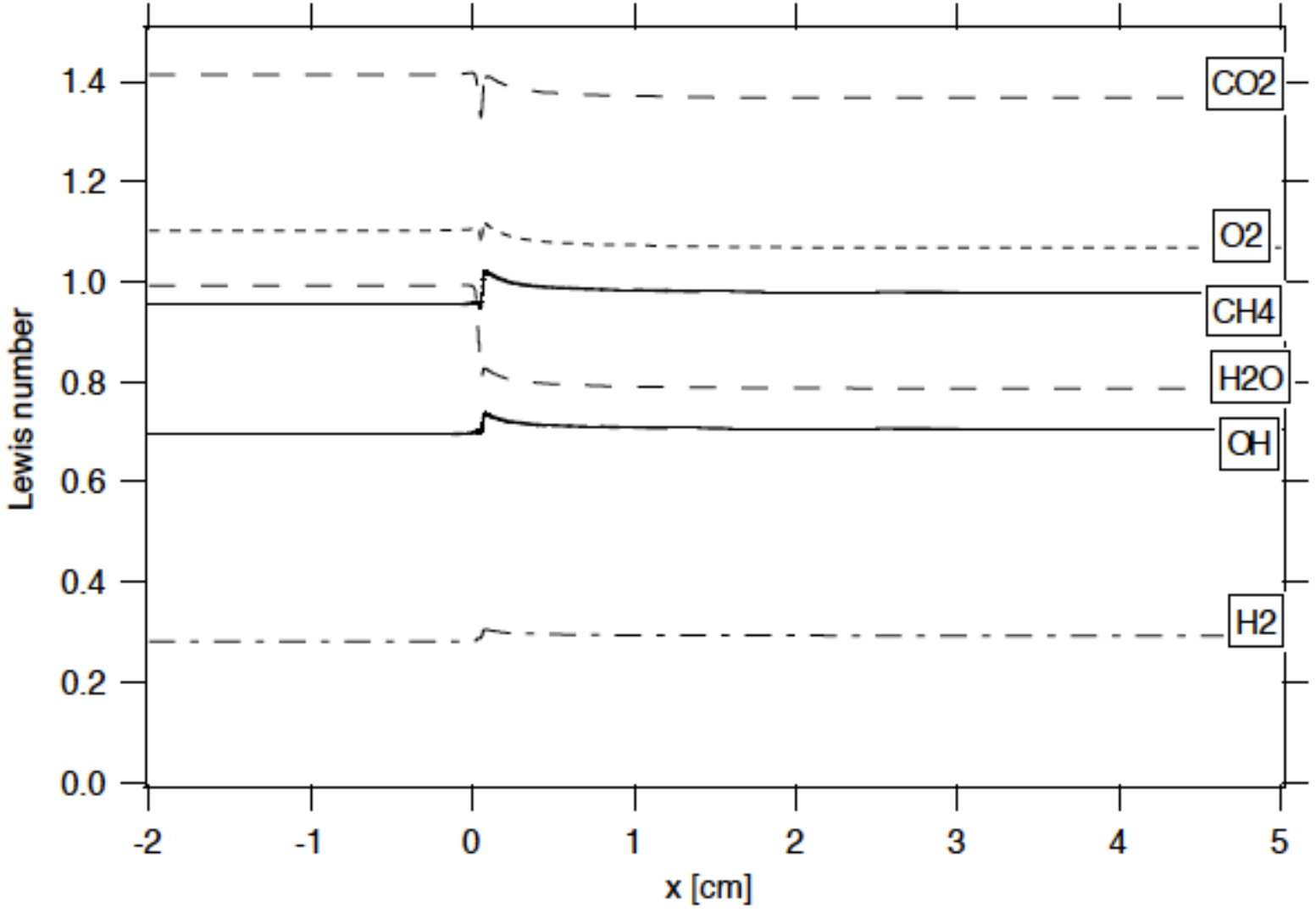
- The concept of splitting the resolution of diffusion flame structures in two parts (z diagram and mixing problem) is common in many codes, laminar or turbulent.

- We also use z for post processing

- But can we really do this ? can we base all our models on z ? let us come back to the assumptions required to define a mixture fraction z.

Equal Lewis numbers ??

Never happens. Lewis numbers are not equal and not equal to unity. Lewis numbers measured in a 1D premixed flame



Alternative definitions for z ?

Ch. 3 Sec 3.6.2

- The literature contains multiple 'improved' definitions of z (based on elements, or on combination of elements).
- The mixture fraction defined using a single step global reaction is of course limited. For H2+1/2O2 -> H2O, define a mixture fraction z_1:

$$z_1 = \frac{sY_{H_2} - Y_{O_2} + Y^0_{O_2}}{sY^0_{H_2} + Y^0_{O_2}} = \frac{sY_{H_2} - Y_{O_2} + 1}{9}$$

- We know that this is not a good definition in practice since in the real world, we have more than one reaction
- Solution: work on elements (C, H or O) because elements are always conserved. Generalized mixture fractions

Other mixture fractions:

★ For example, build a passive scalar on H atom:

$$Z_H = W_H \left(\frac{2Y_{H_2}}{W_{H_2}} + \frac{Y_H}{W_H} + \frac{2Y_{H_2O}}{W_{H_2O}} + \frac{Y_{OH}}{W_{OH}} + \frac{Y_{HO_2}}{W_{HO_2}} + \frac{2Y_{H_2O_2}}{W_{H_2O_2}} \right)$$

★ and a mixture fraction z_H from it:

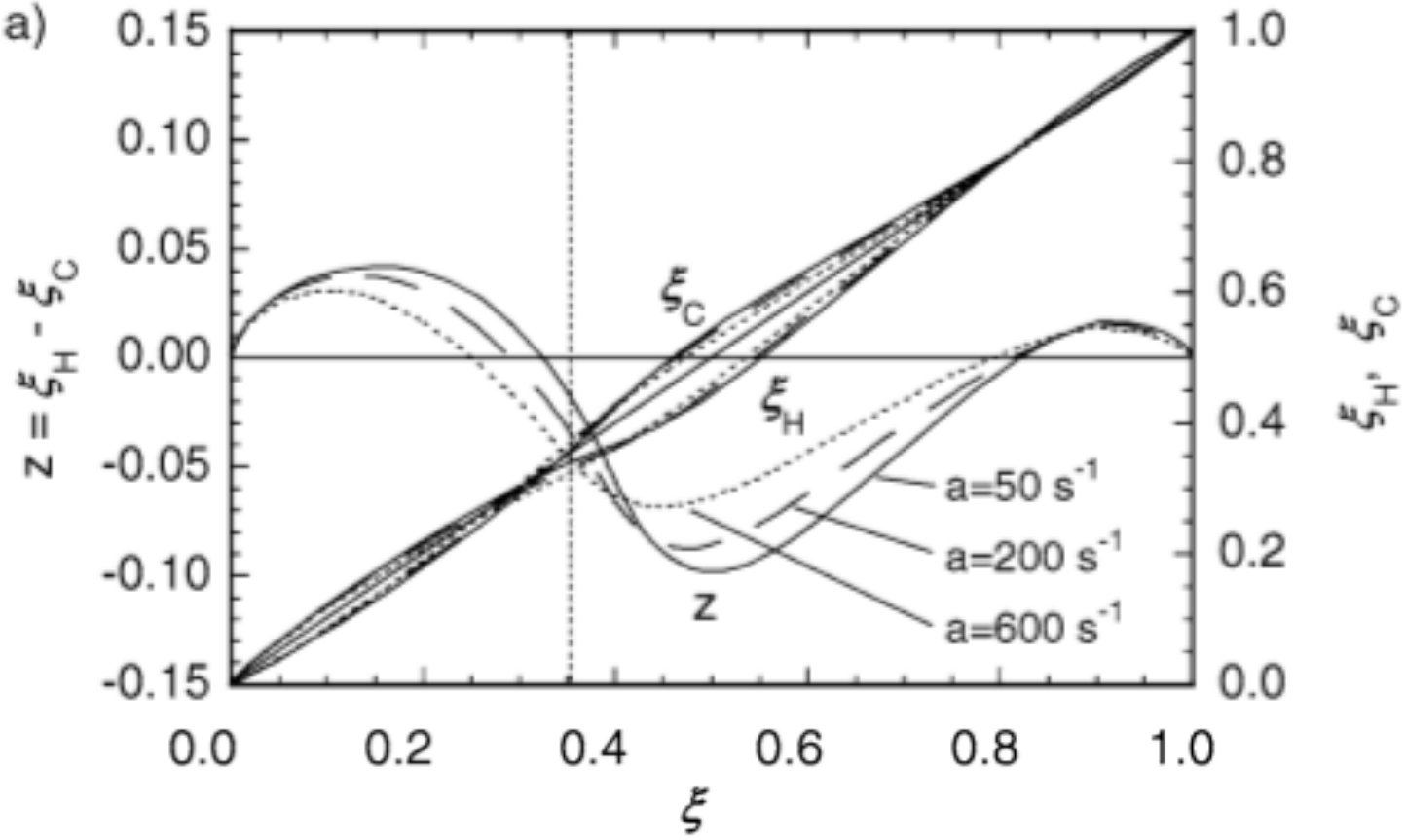
$$z_H = \frac{Z_H - 0}{2Y^0_{H_2} W_H / W_{H_2} - 0}$$

★ See Bilger, Barlow, Pope's papers for other extensions.
For example in the TNF workshop, Bilger's definition is:

$$z_B = \frac{2(Y_C - Y_{C,2})/w_C + (Y_H - Y_{H,2})/2w_H - (Y_O - Y_{O,2})/w_O}{2(Y_{C,1} - Y_{C,2})/w_C + (Y_{H,1} - Y_{H,2})/2w_H - (Y_{O,1} - Y_{O,2})/w_O}$$

But all mixture fractions are … different:

Measurements of various mixture fractions (based on C and H) in a piloted diffusion flame vs Bilger's *z*:



R.S. Barlow et al. / Combustion and Flame 143 (2005) 433–449

Alternative definitions for z ?

- **In the end, 'there is no such thing as a real mixture fraction' z because nothing (species or elements) diffuses at the same speed in a multispecies gas.**

- **This leads to multiple problems in practice since the multiple definitions of z lead to z's which are not equal...**

Last comment on Lewis numbers

- When we will discuss turbulent flames, we will see that many authors assume unity Lewis number.
- Why ?

➡ It seems to work better...

➡ It may be justified by the fact that small scale turbulence leads to turbulent transport which dominates transport and is the same for all species, thereby justifying the equal Lewis number assumption

Stretch and scalar dissipation

★For diffusion flames, stretch has the same definition as in premixed flames (except that the flame speed of a diffusion flame is zero) . It is also important:

$$\kappa = \frac{1}{A}\frac{dA}{dt}$$

★But the effects of stretch are very different in diffusion and premixed flames

Stretch and diffusion flames:

In diffusion flames, flame strain (or stretch) is often replaced by a quantity called 'scalar dissipation':

$$\chi = 2\mathcal{D}\left(\frac{\partial z}{\partial x_i}\frac{\partial z}{\partial x_i}\right)$$

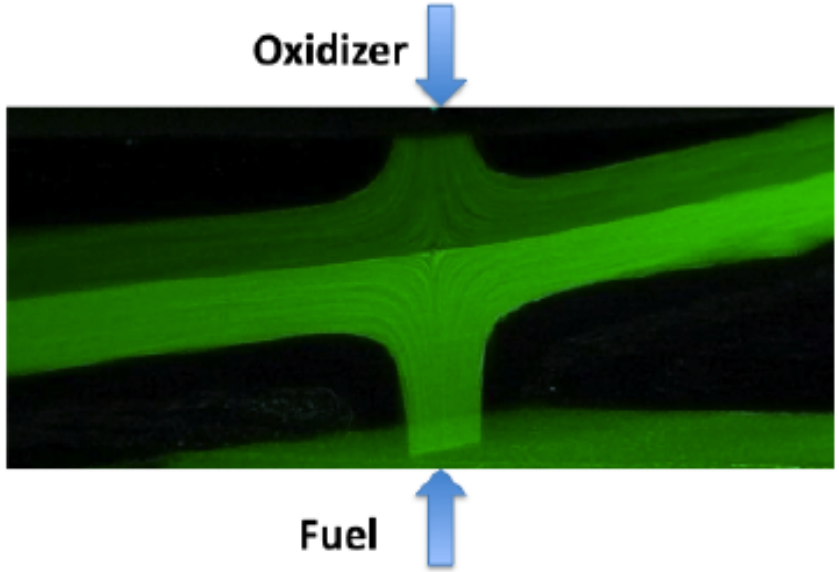
Why ?

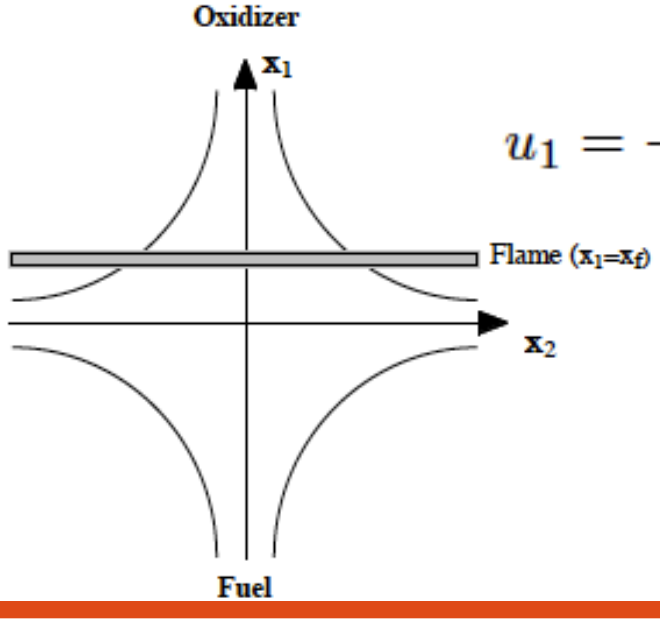
- Scalar dissipation does not depend on the flame orientation (as flame stretch does).

- For simple cases (stretched diffusion flame), stretch and scalar dissipation are simply proportional.

Ch. 3.2.2

The diffusion flame with infinitely fast chemistry:





$$u_1 = -ax_1 \quad \text{and} \quad u_2 = ax_2$$

Flame stretch

$$\chi_f = \frac{a}{\pi} \exp\left[-2\left(\text{erf}^{-1}\left(\frac{\phi - 1}{\phi + 1}\right)\right)^2\right]$$

$$\phi = s\frac{Y_F^0}{Y_O^0}$$

Scalar dissipation on the flame front

Ch. 3.2.2

We can work with stretch OR with scalar dissipation

Link between strain and total reaction rate:

$$\dot{\Omega}_F = \int_{x_f^-}^{x_f^+} \dot{\omega}_F dx = -\left[\rho \mathcal{D} \frac{\partial Y_F}{\partial x}\right]_{x_f^-}^{x_f^+} = \left[\rho \mathcal{D} \frac{\partial Y_F}{\partial x}\right]_{x=x_f^-}$$

★ **Since we know the link between Y_f and z,**

$$z = \frac{1}{2}\left[1 - \mathrm{erf}(\zeta)\right] \qquad \text{with} \qquad \zeta = x_1 \sqrt{\frac{a}{2\mathcal{D}}}$$

★ **we can compute the total reaction rate:**

$$\dot{\Omega}_F = -\rho \frac{Y_F^0}{1 - z_{st}} \sqrt{\frac{a\mathcal{D}}{2\pi}} e^{-\zeta_f^2}$$

Diffusion flames are VERY sensitive to stretch (or scalar dissipation)

$$\dot{\Omega}_F = -\rho \frac{Y_F^0}{1 - z_{st}} \sqrt{\frac{a\mathcal{D}}{2\pi}} e^{-\zeta_f^2}$$

Ch. 3.4.2

Total fuel consumption in a stretched diffusion flame

Flame stretch

When you stretch a diffusion flame, it burns more: we all know we must blow on wood fires to increase their combustion rate: we bring them more air by bringing more stretch (or more scalar dissipation). There is a limit to this: if you stretch it too much, you can quench it. You should not blow too much on a candle, otherwise you kill it...

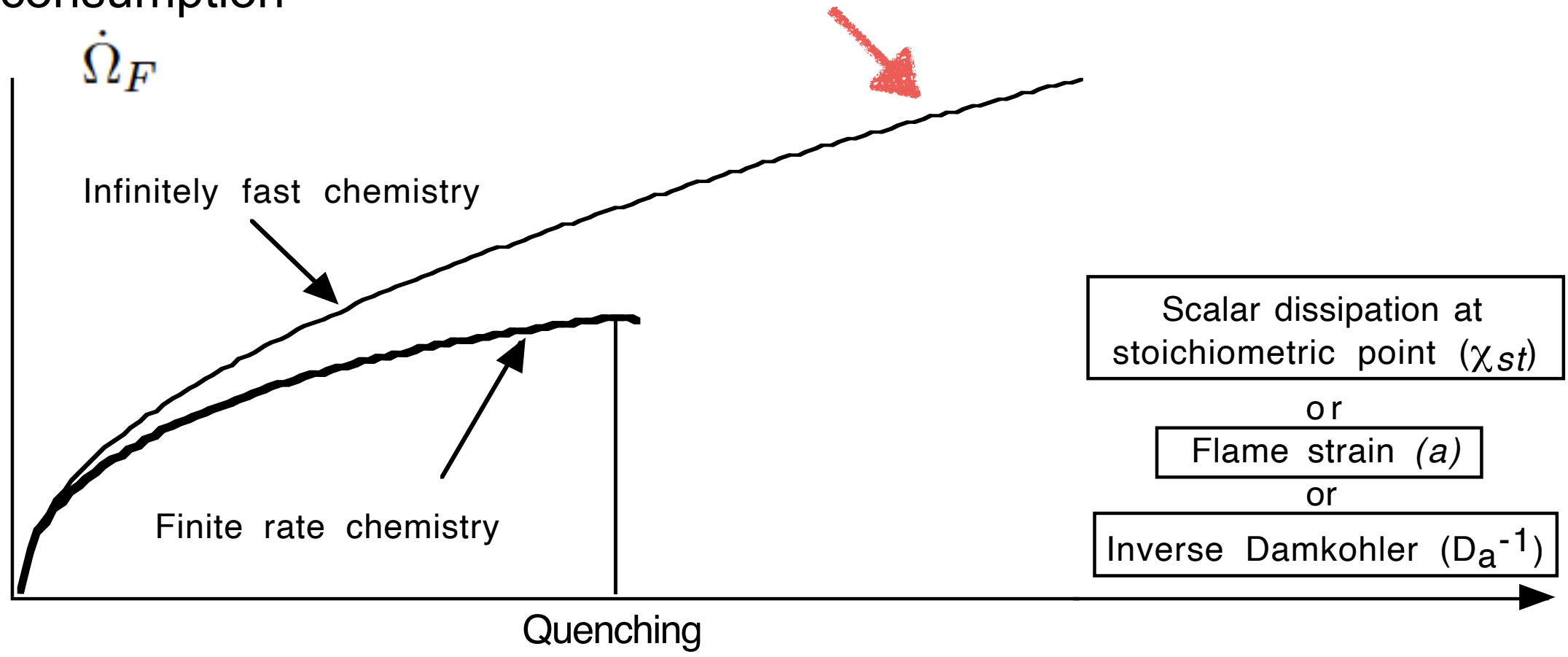
Stretching a diffusion flame:

Ch. 3.5.2

$$\dot{\Omega}_F = -\rho \frac{Y_F^0}{1 - z_{st}} \sqrt{\frac{a\mathcal{D}}{2\pi}} e^{-\zeta_f^2}$$

Total fuel consumption

$\dot{\Omega}_F$



Implications for turbulent flames:

In turbulent flames, the unsteady velocity field will induce strain and therefore stretch:

$$\kappa = \nabla_t \cdot \vec{\mathbf{u}} - s_d \left(\frac{1}{\mathcal{R}_1} + \frac{1}{\mathcal{R}_2} \right) = \nabla_t \cdot \vec{\mathbf{u}} + s_d \nabla_t \cdot \vec{\mathbf{n}}$$

Strain in the tangent plane to the flame

Strain due to flame propagation

In turbulent flames:

★We will need to establish a link between the velocity field (created by an ensemble of vortices) and flame stretch:

$$\kappa = \nabla_t \cdot \vec{\mathbf{u}} - s_d \left(\frac{1}{\mathcal{R}_1} + \frac{1}{\mathcal{R}_2} \right) = \nabla_t \cdot \vec{\mathbf{u}} + s_d \nabla_t \cdot \vec{\mathbf{n}}$$

★This will be the job of the turbulent combustion models

OUTLINE

CONSERVATION EQUATIONS FOR REACTING FLOWS

PREMIXED FLAMES

DIFFUSION FLAMES

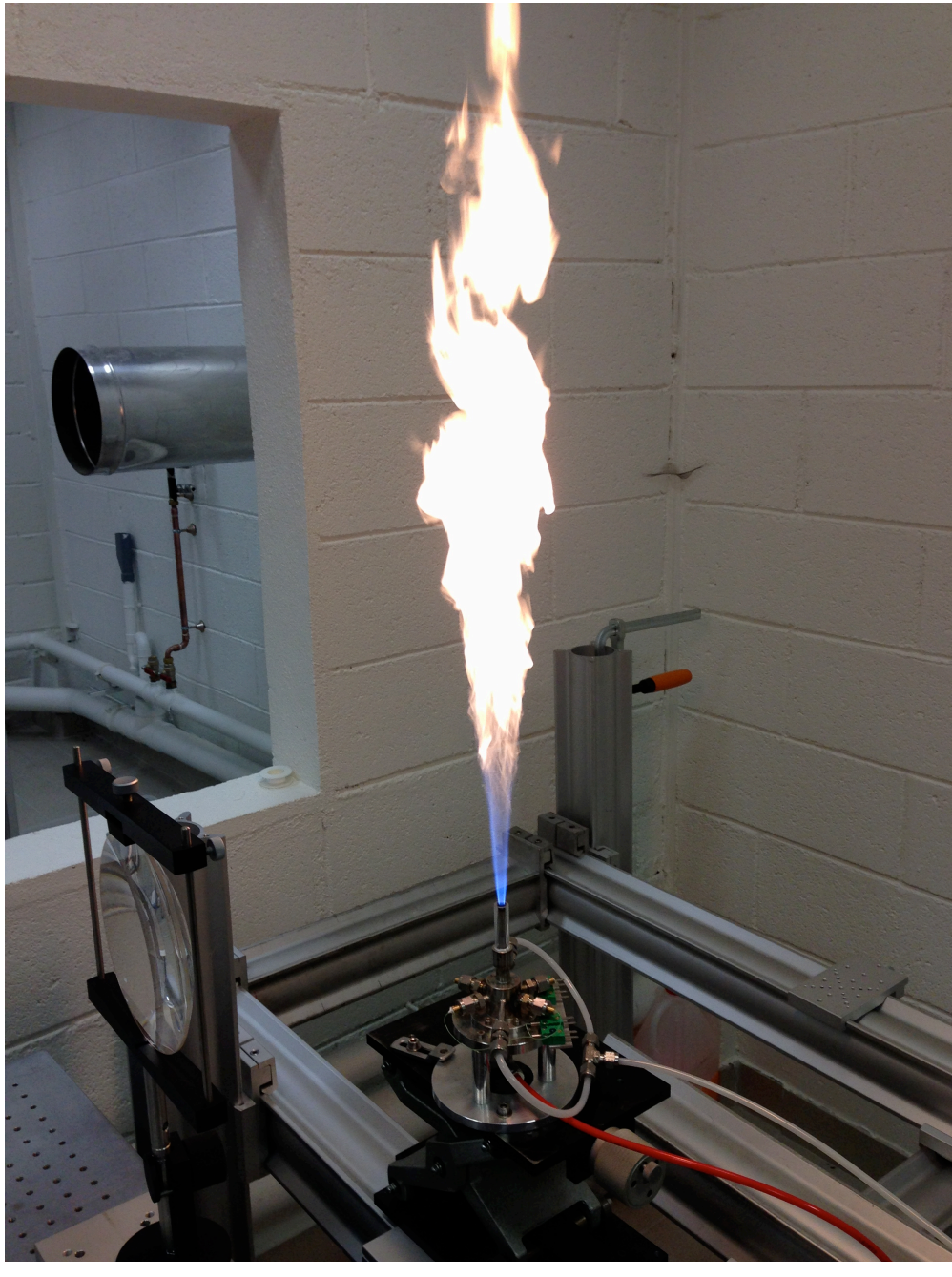
Ch. 6

OTHER FLAMES: PARTIALLY PREMIXED, TRIPLE FLAMES

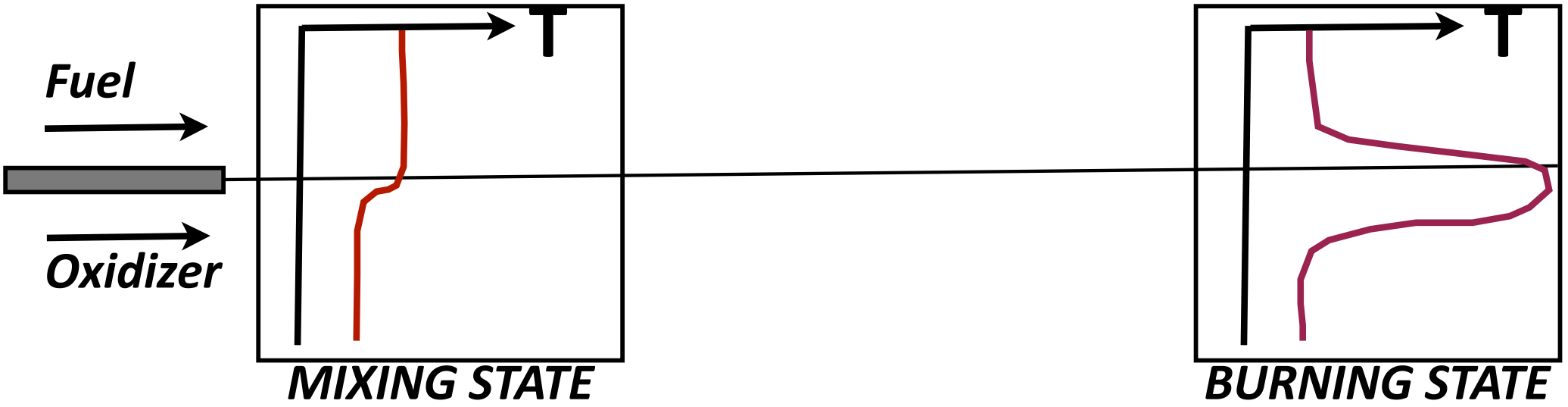
Are all flames premixed or non-premixed ?

★ No and two other cases must be mentioned:

- ➡ triple flames
- ➡ partially premixed flames

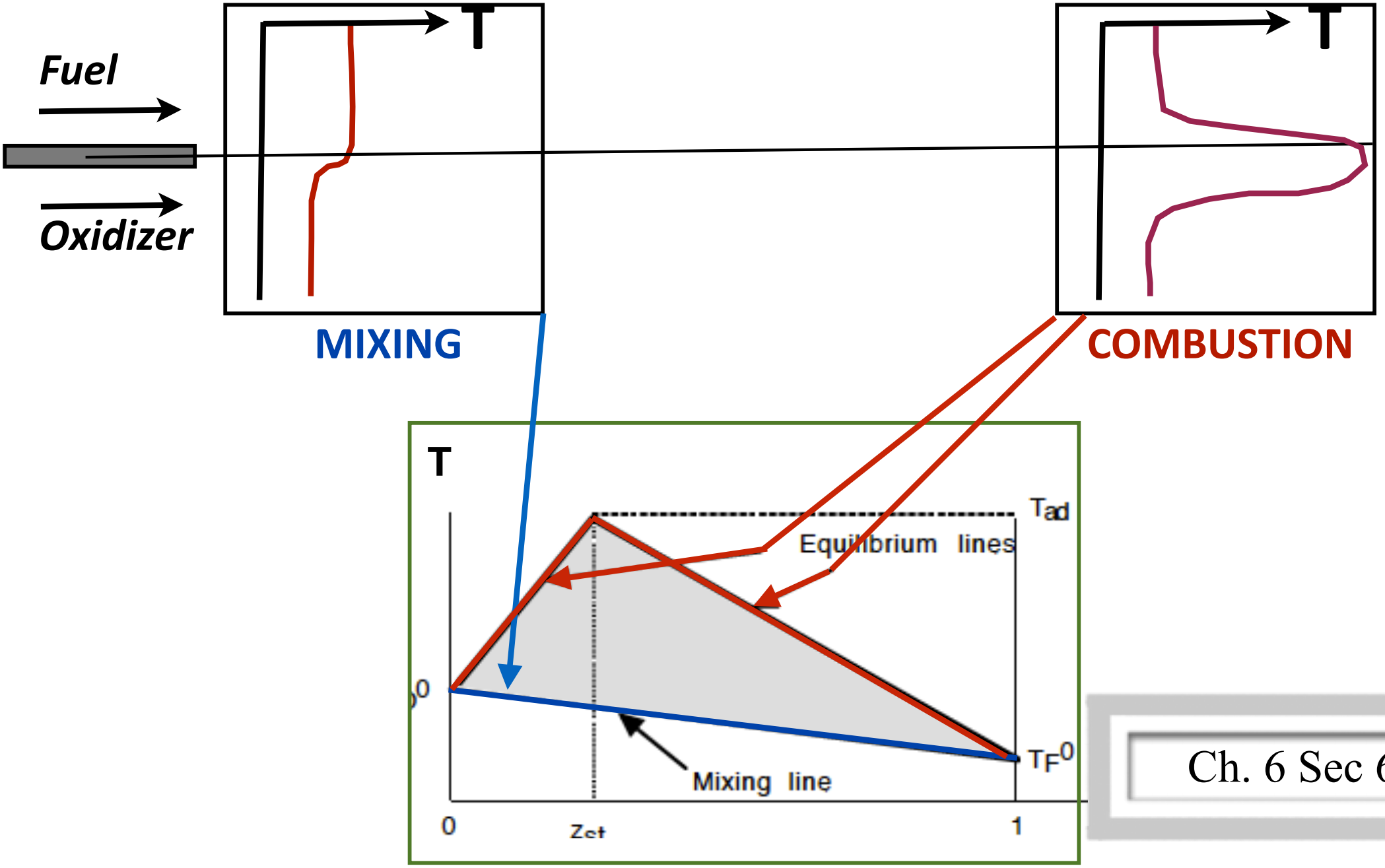


TRIPLE FLAMES: THE STRUCTURE WHICH SEPARATES IGNITED FROM NON IGNITED DIFFUSION LAYERS



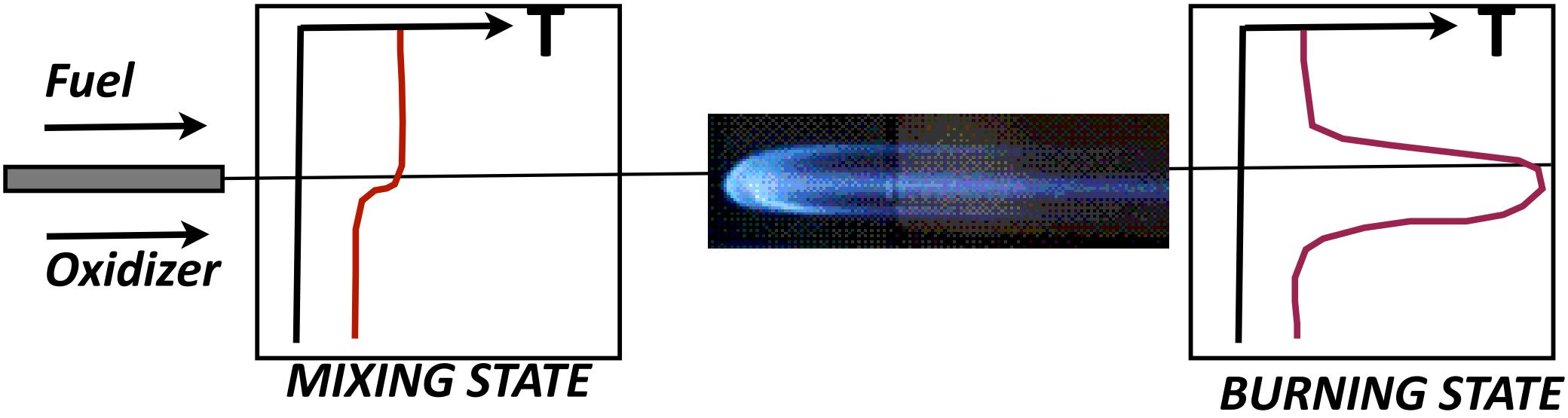
In any system, where you inject pure fuel and pure oxidizer, you start in a mixing state. Downstream, you are on the combustion state. How ?

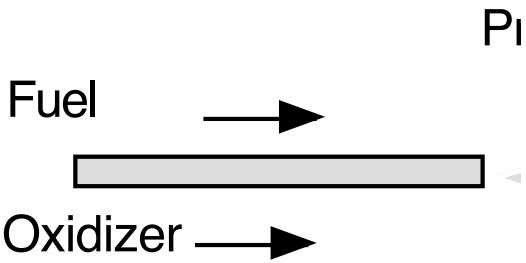
In other words: how do you *stabilize* a diffusion flame ?


Fuel
Oxidizer
T
MIXING
T
COMBUSTION
T
Tad
Equilibrium lines
Mixing line
TF0
0
Zst
1

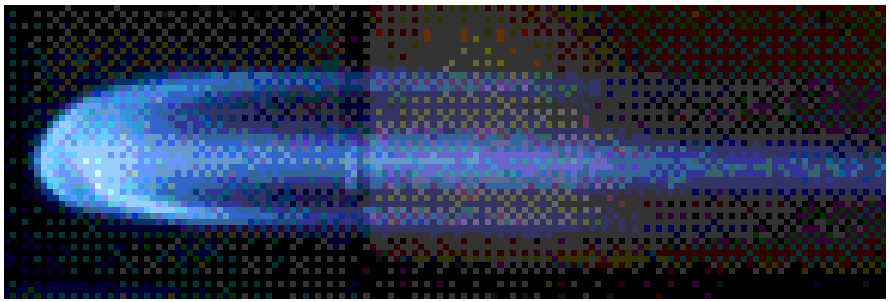
Ch. 6 Sec 6.2.3

TRIPLE FLAMES: THE STRUCTURE WHICH SEPARATES IGNITED FROM NON IGNITED DIFFUSION LAYERS

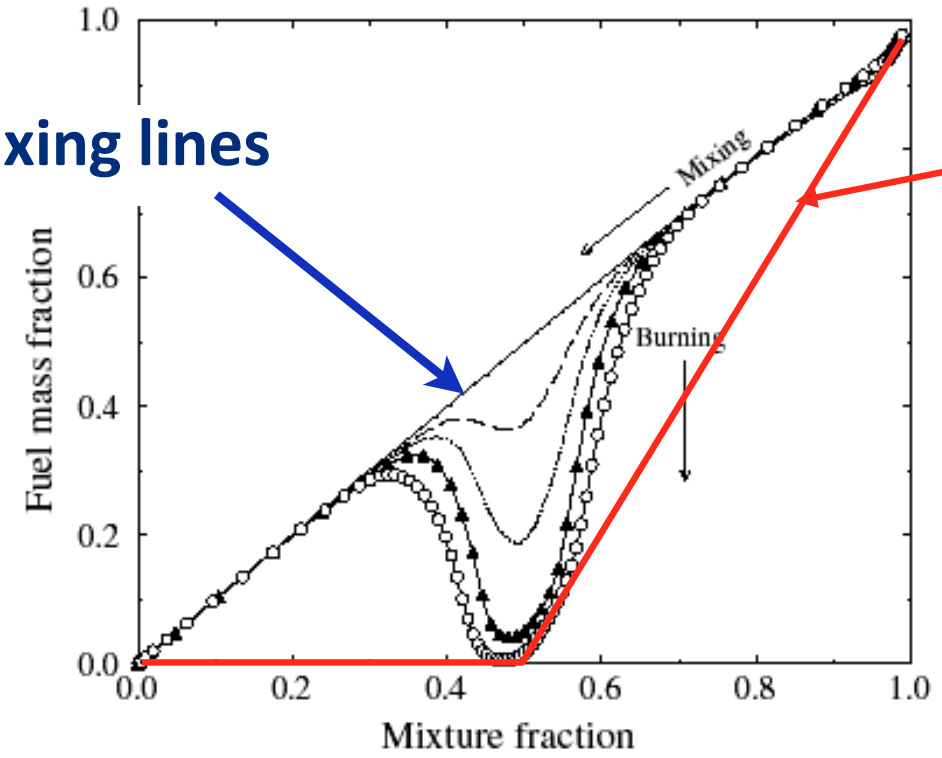


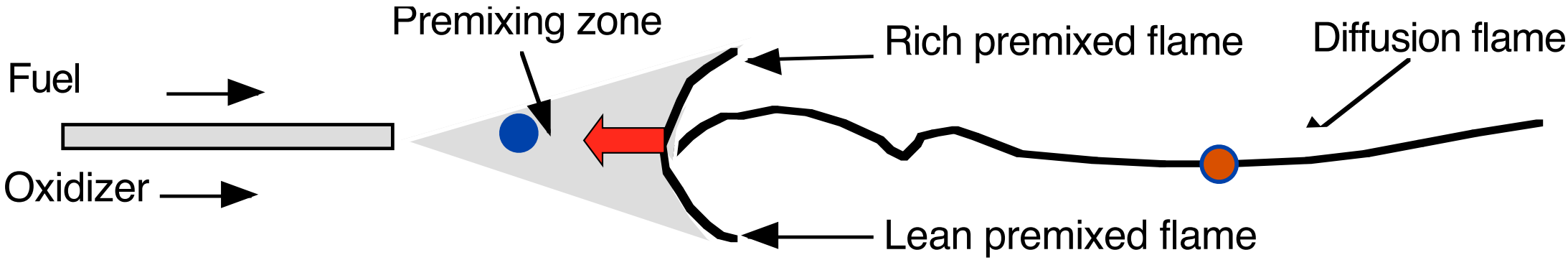


Kioni triple flame

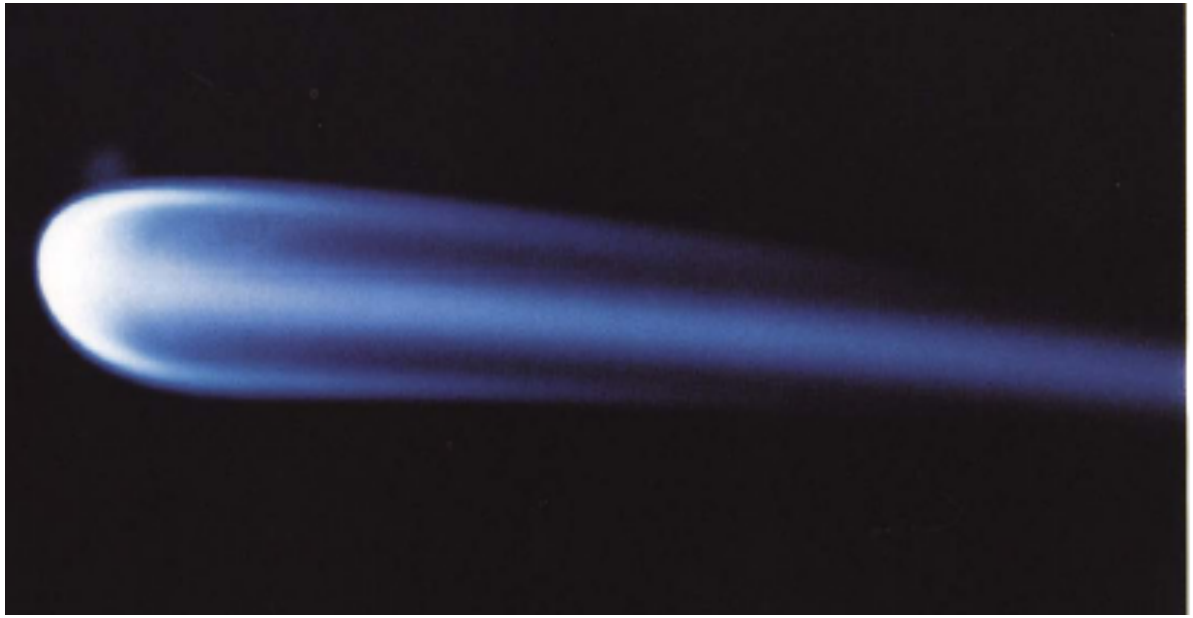


TRIPLE FLAME POINTS IN A z DIAGRAM:





1/ TRIPLE FLAMES PROPAGATE: THEY HAVE A SPEED
2/ THEY PROPAGATE FASTER THAN PREMIXED FLAMES



- **A TRIPLE FLAME SPEED SCALES LIKE:**

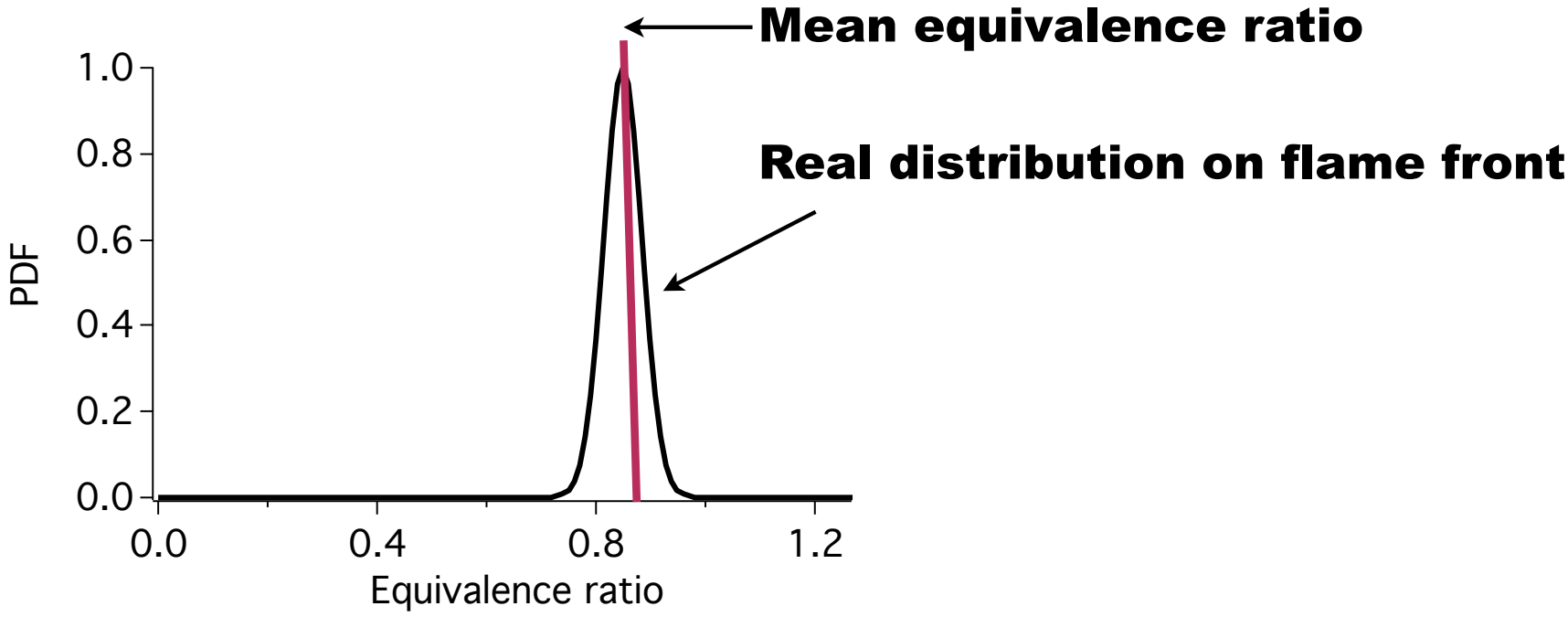
$$s_{Triple} = s_L^0 \sqrt{\frac{\rho_1}{\rho_2}}$$

Stoechiometric laminar flame speed

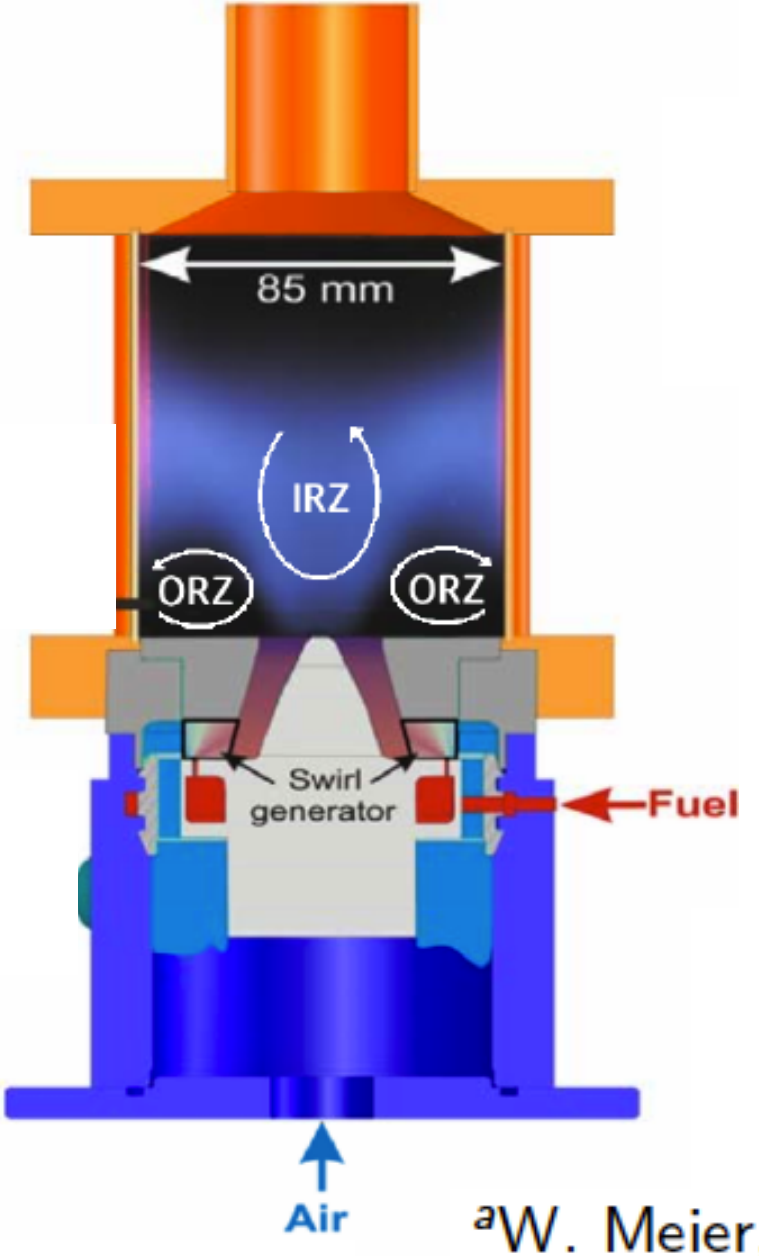
Density ratio

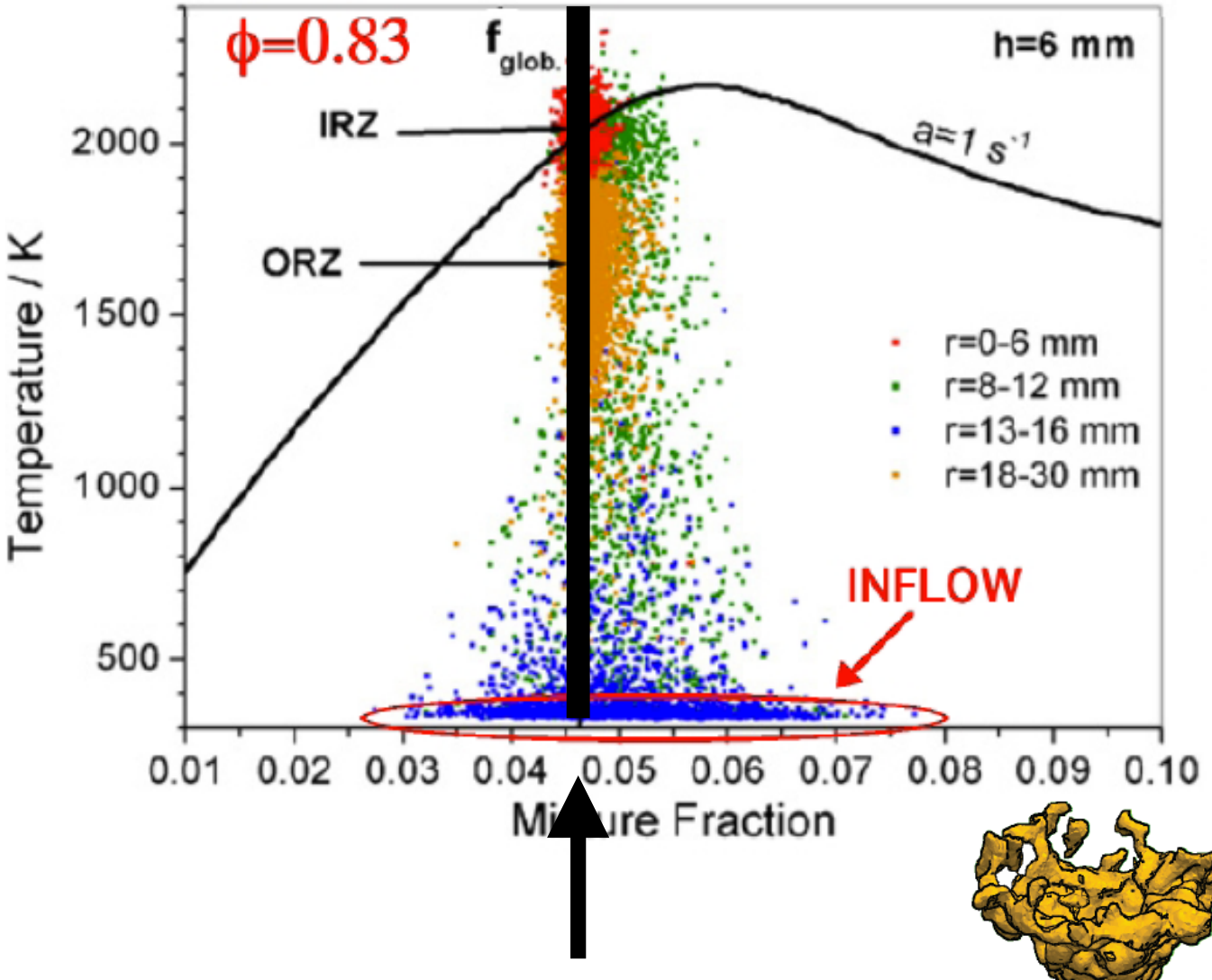
Partially premixed flames

- ★ **Perfectly premixed flames: too *dangerous***
- ★ **Pure diffusion flames: not *efficient***
- ★ **Most flames will be produced in devices where we TRY to mix at the last moment to reach premixed conditions but never really make it.... Partially premixed flames**

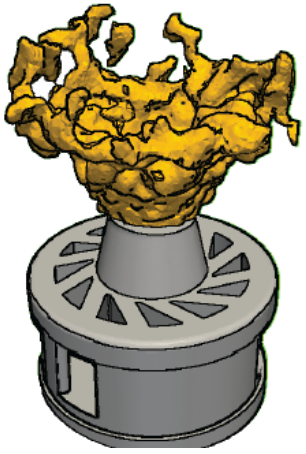


The PRECCINSTA burner





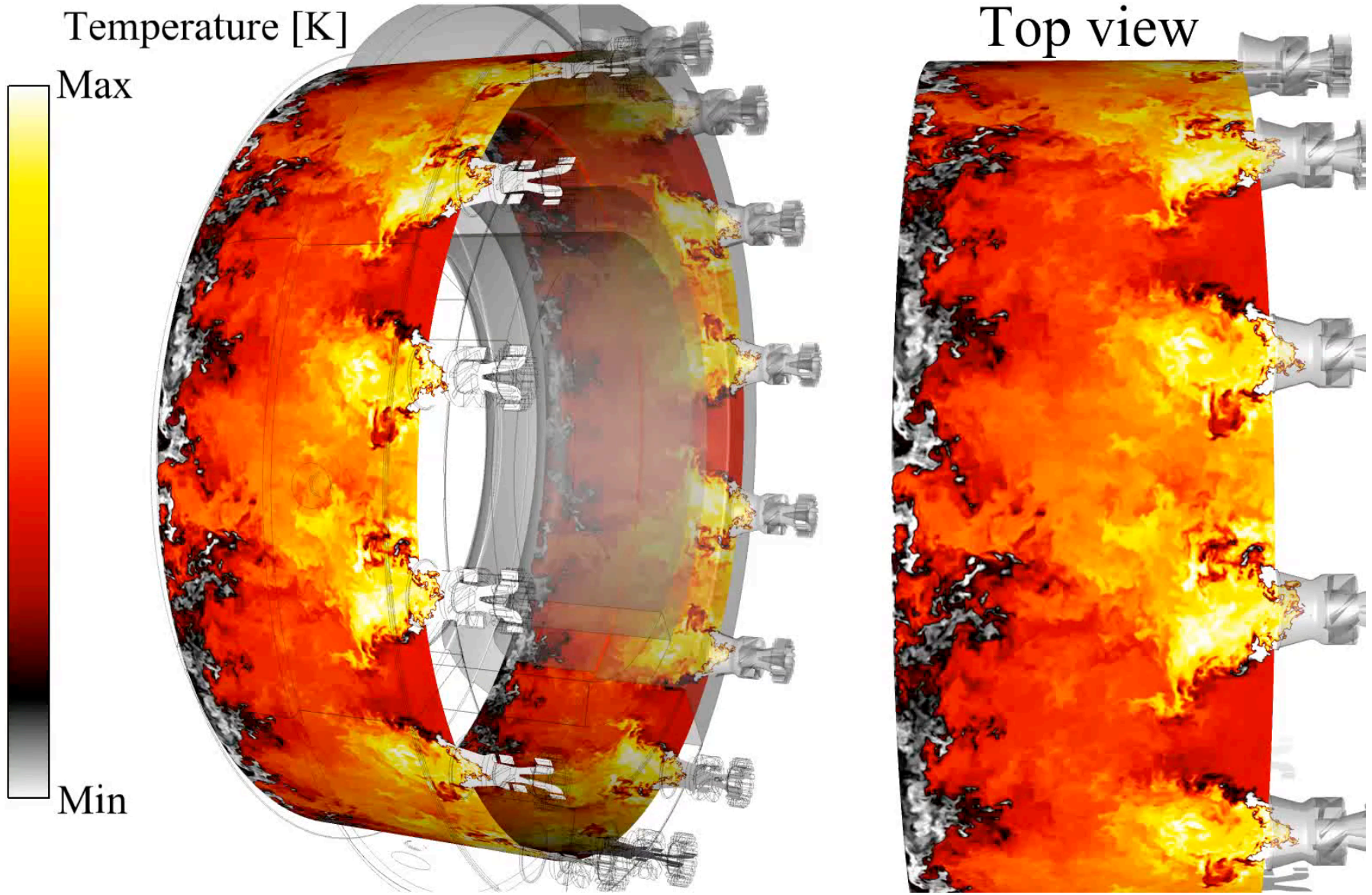
PERFECTLY PREMIXED LIMIT



[a]W. Meier, P. Weigand, X.R. Duan, and R. Giezendanner-Thoben. Combust. Flame, 150 (2007)

Turbulent combustion

Ch. 4, 5, 6



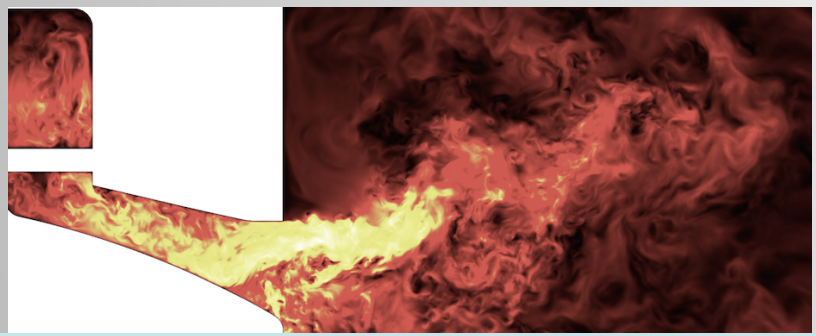
Questions:

RAISE YOUR HAND:

- If you have already had a course on turbulent combustion
- If you have already had a course on turbulence and know what $k^{-5/3}$ means and Kolmogorov theory is
- Know what the k-epsilon model is ?

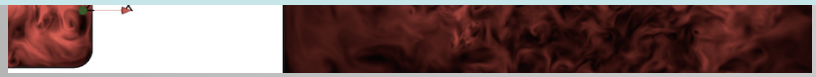
Turbulence and combustion

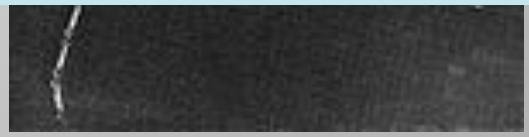
On turbulence alone:
Horace Lamb (famous british applied mathematician) said:
« ***I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the turbulent motion of fluids. And about the former I am rather optimistic*****. »**



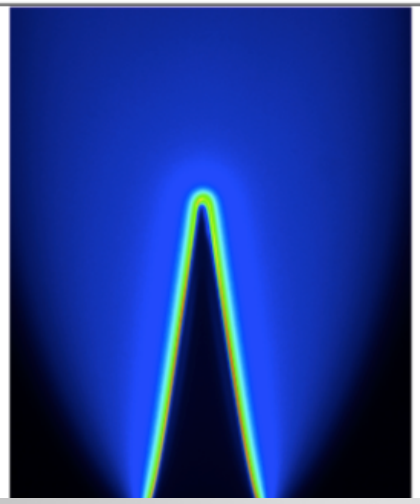
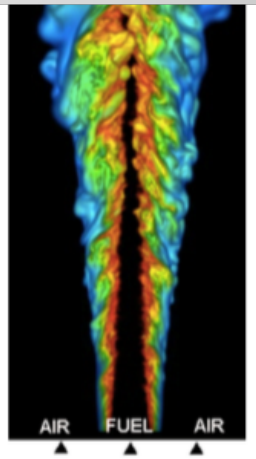


Which does not mean we should not do anything ! We can do a lot but the one thing we should not do, is to believe CFD codes blindly…





And we must add chemical kinetics to that…

	LAMINAR FLAMES	TURBULENT FLAMES
PREMIXED FLAMES		
NON-PREMIXED FLAMES (DIFFUSION)		
	Chapter 3	Chapters 4 and 6

FLOW RATES INCREASE
POWERS INCREASE
REYNOLDS INCREASES

OUTLINE

- Phenomenology of turbulent flames (Ch 4)
- Classical modeling approaches for turbulent flames
  - Premixed flames (Ch 5)
  - Diffusion flames (Ch 6)
- Requirements for most real turbulent flames and models

Ch. 4

OUTLINE

- Phenomenology of turbulent flames (Ch 4)
  - ➡ Differences between laminar and turbulent flames
  - ➡ The turbulent flame diagrams
  - ➡ The turbulent flame speed
  - ➡ Averaging

A TURBULENT FLAME IS THE RESULT OF THE INTERACTION BETWEEN:

- **A FLAME FRONT**
- **A TURBULENT FLOW**

BUT DO WE KNOW WHAT WE REALLY MEAN BY TURBULENCE ?

WHAT IS TURBULENCE ?

Entry #: 84174

Vortices within vortices: hierarchical nature of vortex tubes in turbulence

Kai Bürger[1], Marc Treib[1], Rüdiger Westermann[1],
Suzanne Werner[2], Cristian C Lalescu[3],
Alexander Szalay[2], Charles Meneveau[4], Gregory L Eyink[2,3,4]

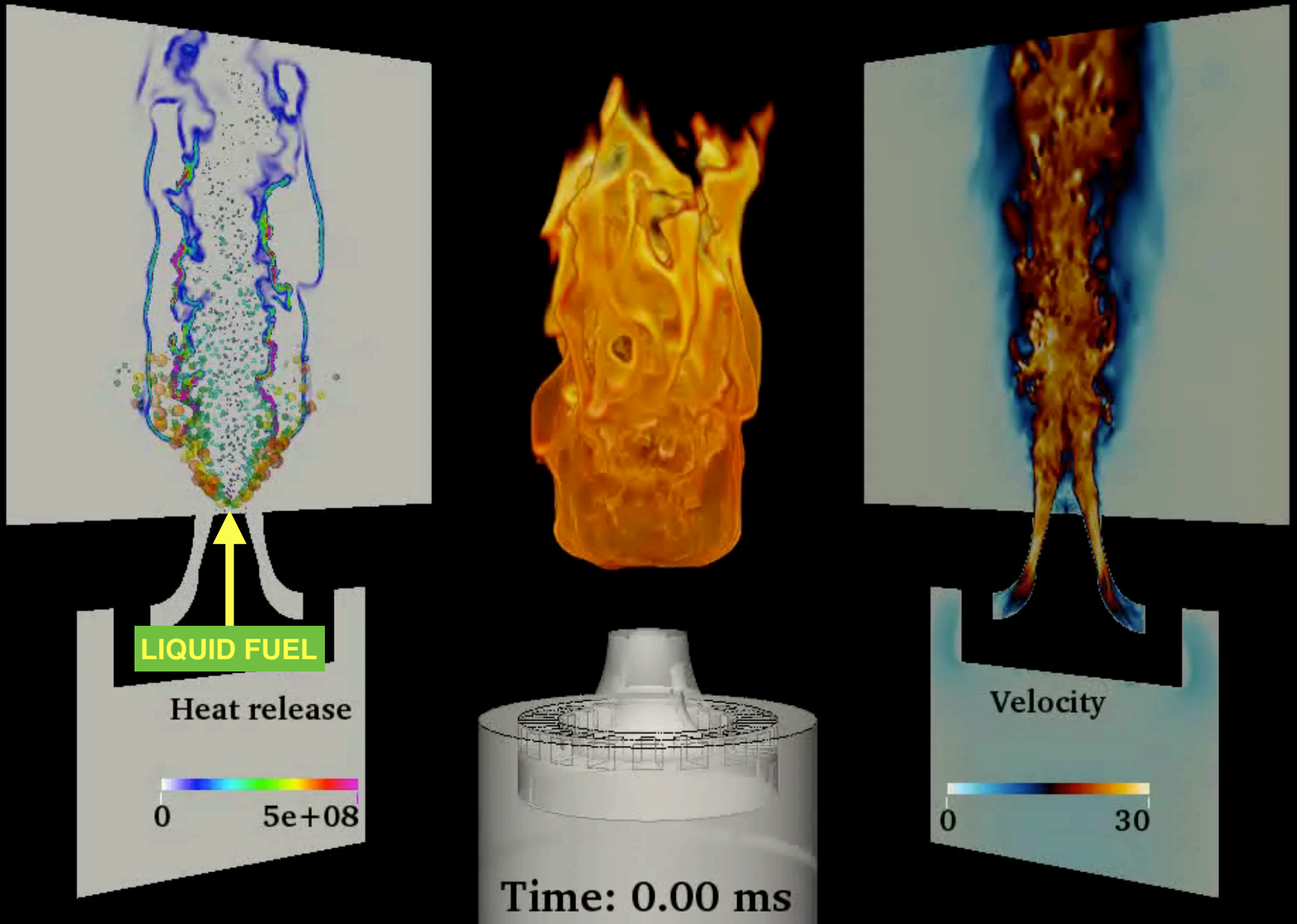
[1] Informatik 15 (Computer Graphik & Visualisierung), Technische Universität München
[2] Department of Physics & Astronomy, The Johns Hopkins University
[3] Department of Applied Mathematics & Statistics, The Johns Hopkins University
[4] Department of Mechanical Engineering, The Johns Hopkins University

Two - phase flow combustion

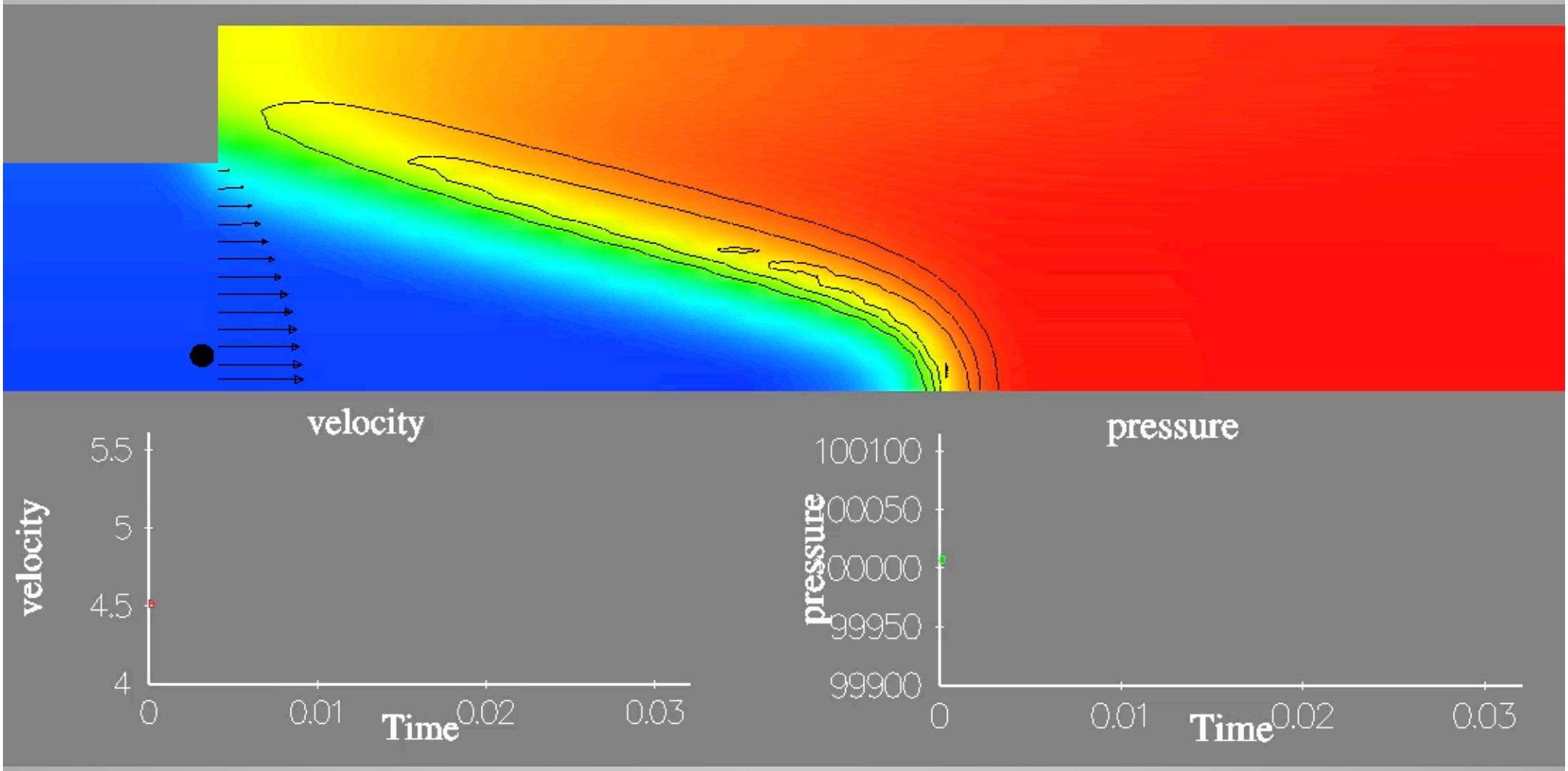
- Many fuels are injected as liquid
- Droplet injection, vaporization and combustion become additional problems in turbulent flows
- This is not discussed here

KIAI SPRAY BURNER CONFIG.

F. Shum-Kivan



Turbulent flames are not unsteady laminar flames



Turbulent flames appear when the flow is turbulent

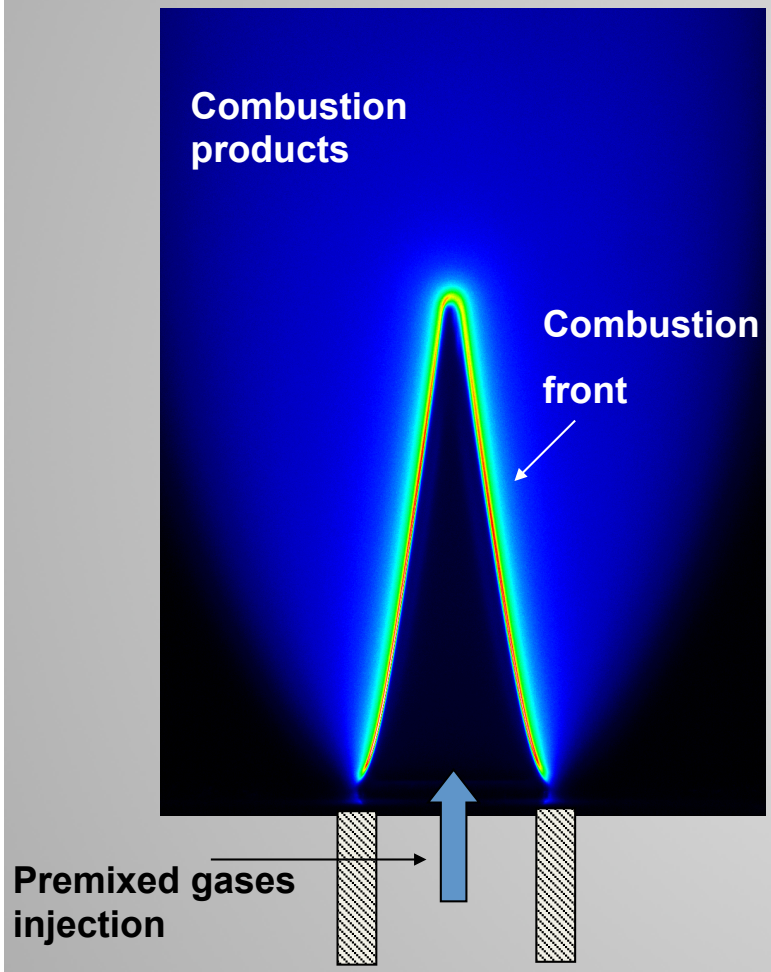
- When the flow feeding a flame is turbulent, the flame becomes turbulent too
- Difficult to avoid in real systems: most flows are turbulent. Only the candle and the lighter are laminar: we **must** study turbulent flames

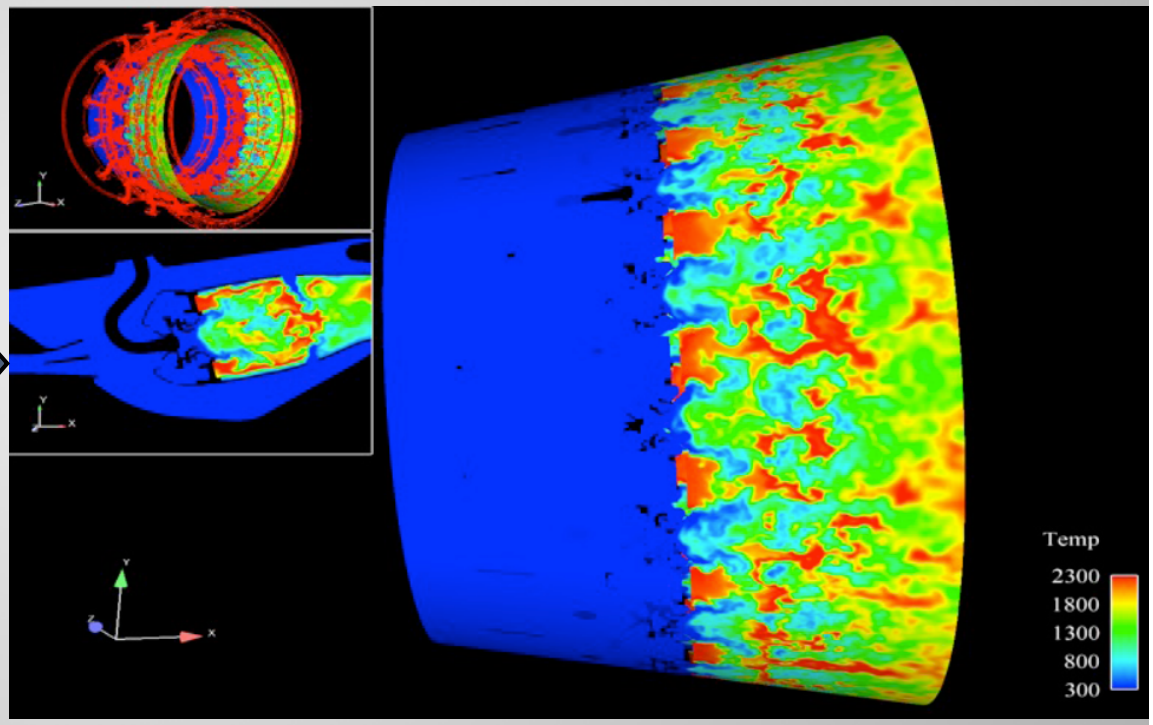
Ch. 4

It is MUCH MORE difficult to compute turbulent flames precisely

1cm

1m





Laminar flame speed:
Error < 3 % ?

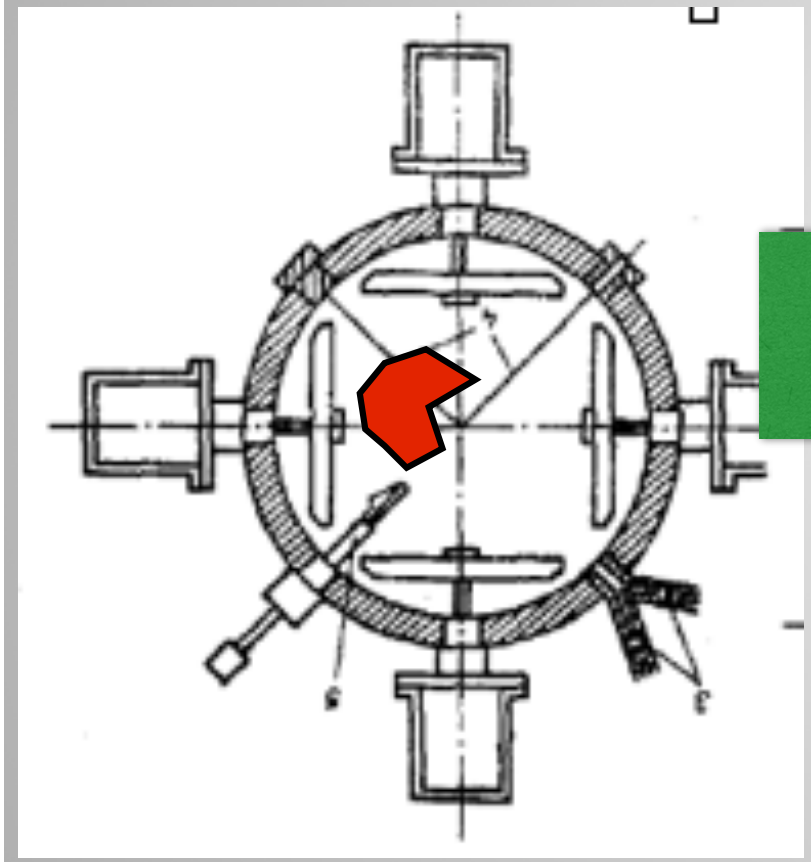
Turbulent combustor:
Error can be100 % ?

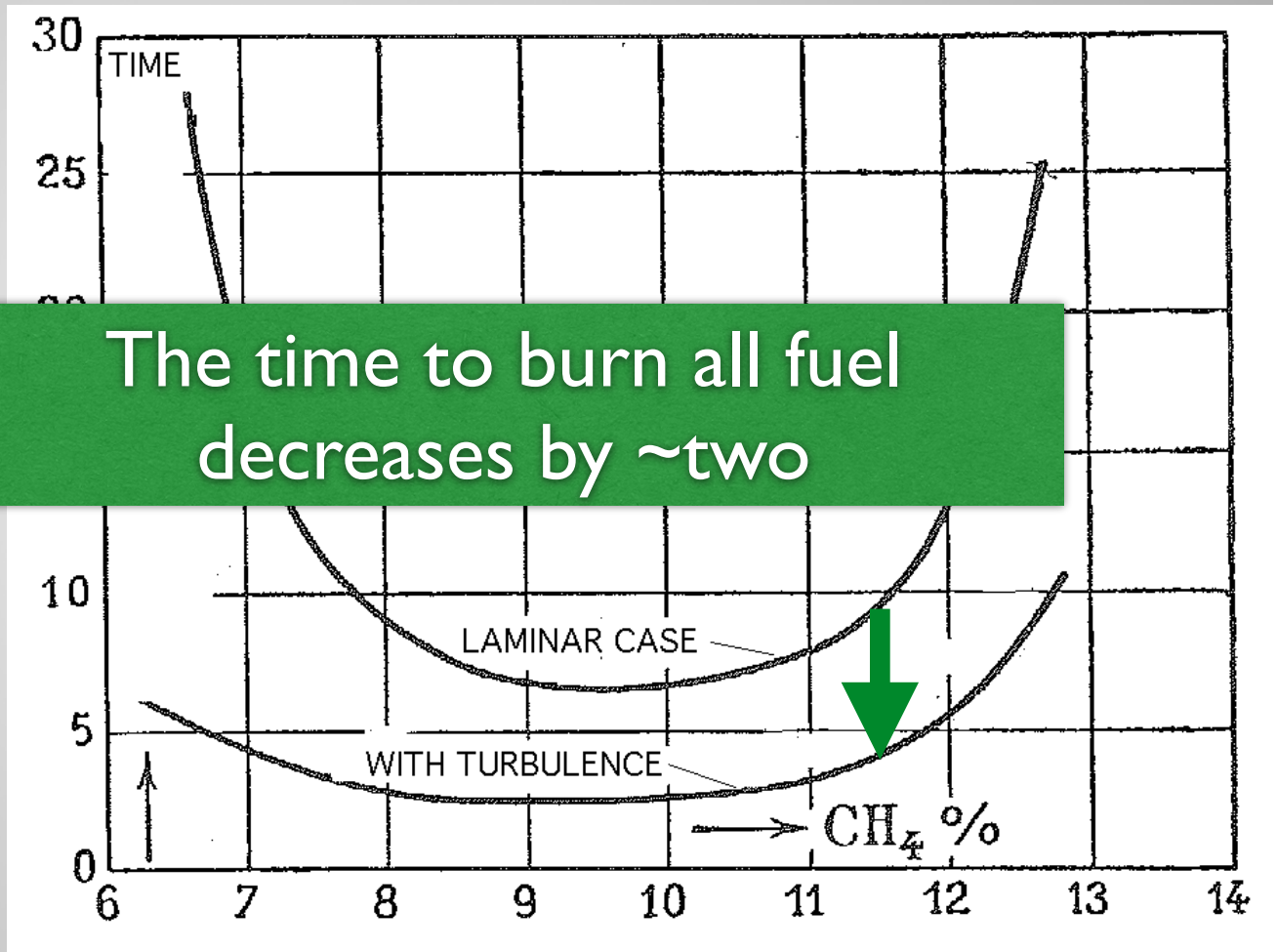
Turbulent combustion is also good for us !



- Without turbulent combustion, most systems would not work: the example of a piston engine working at idle (800 rpm) and full power (16000 rpm)...
- What provides an increase by a 20 factor in combustion speed ? The **turbulence/flame** interaction
- This has been known for a long time... but even today we have difficulties to master it

Combustion time in a stirred bomb (Laffite 1939, Mallard et le Chatelier 1907)

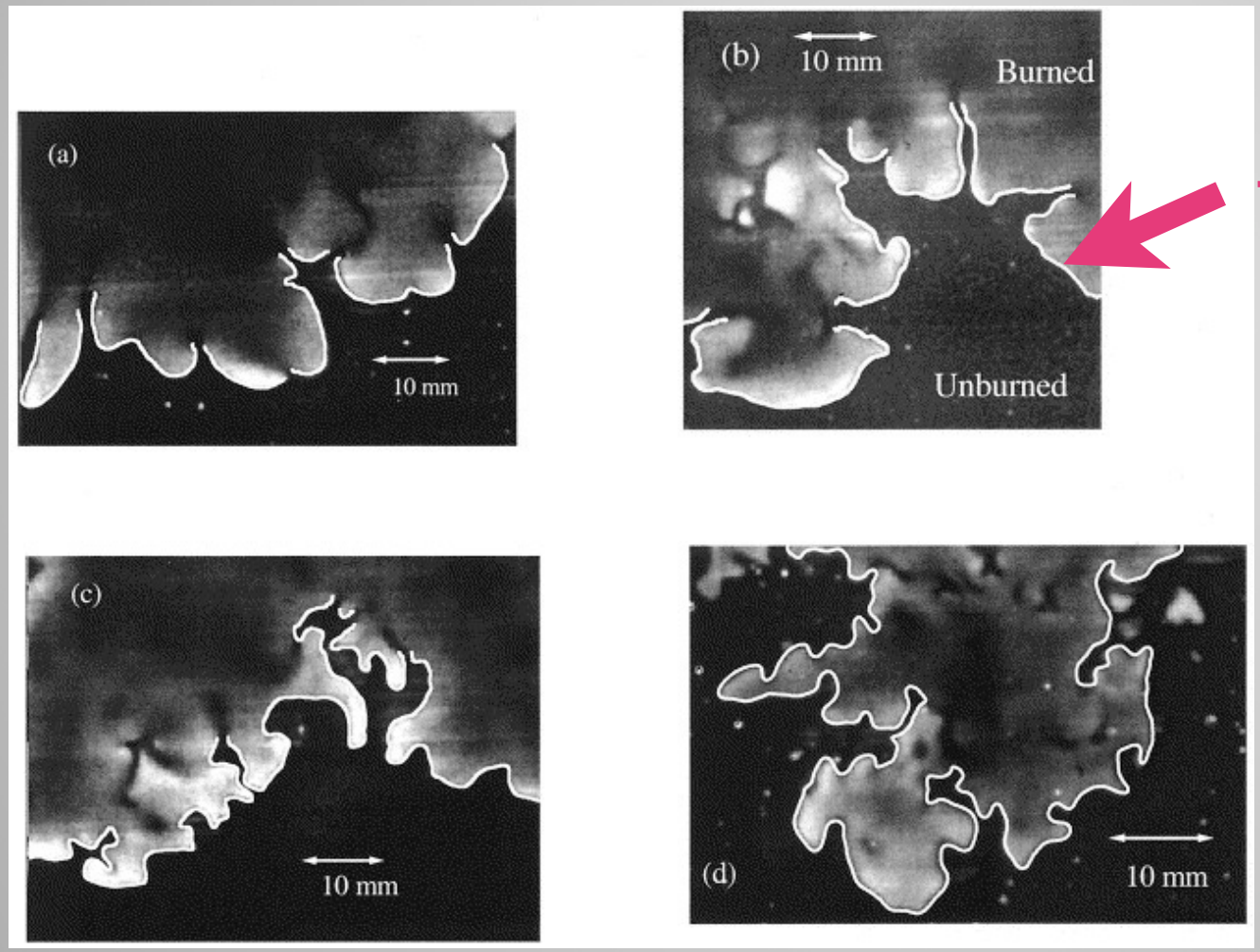




The time to burn all fuel decreases by ~two

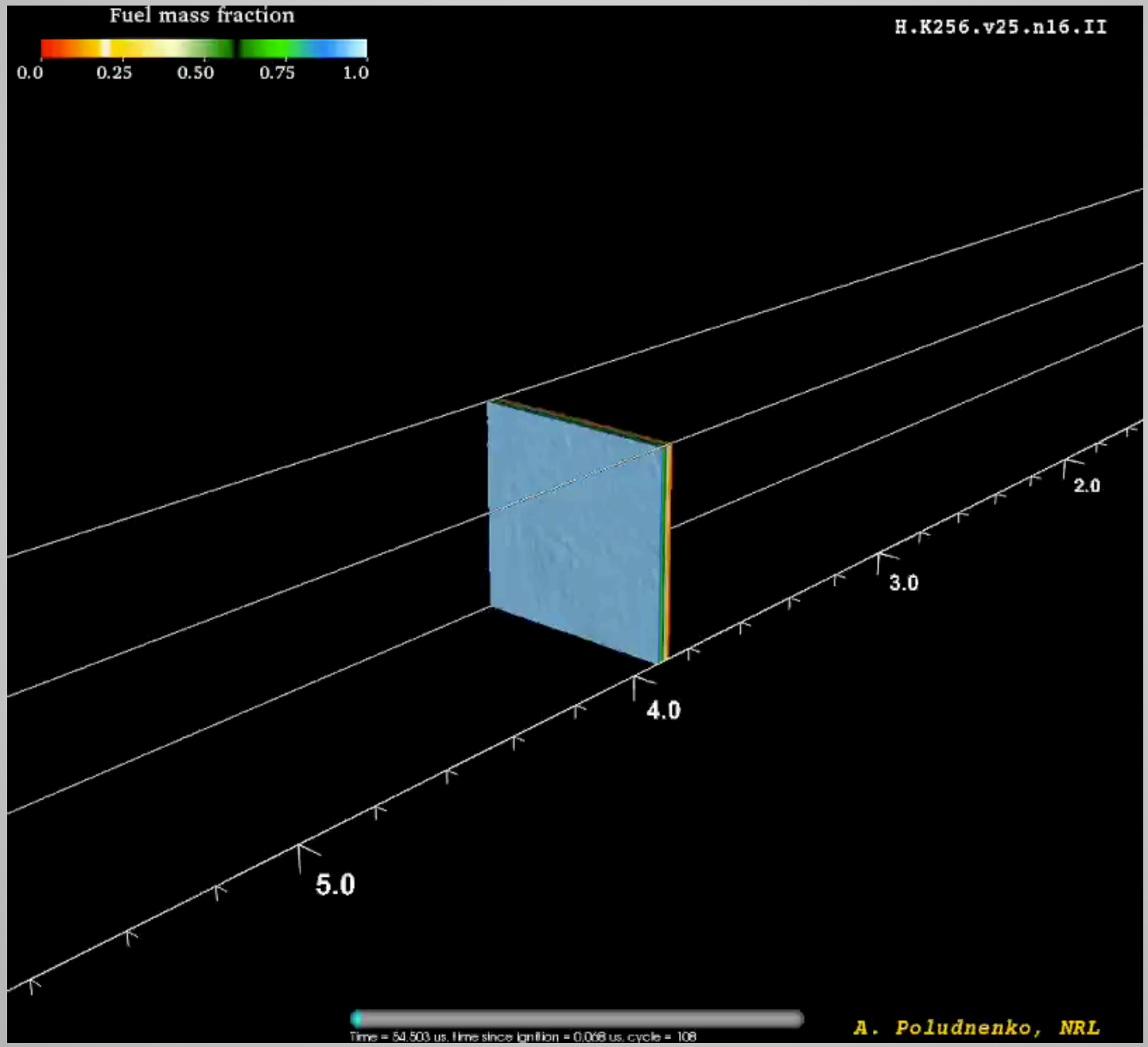
Laffite said, 100 years ago: « when the flow is turbulent, the flame speed is multiplied by... 'two' » -> the first turbulent combustion model

The main issue is to know the flame surface and the consumption speed



Is this a laminar flame element ? (a flamelet)

SIMULATION OF 3D PREMIXED TURBULENT FLAME

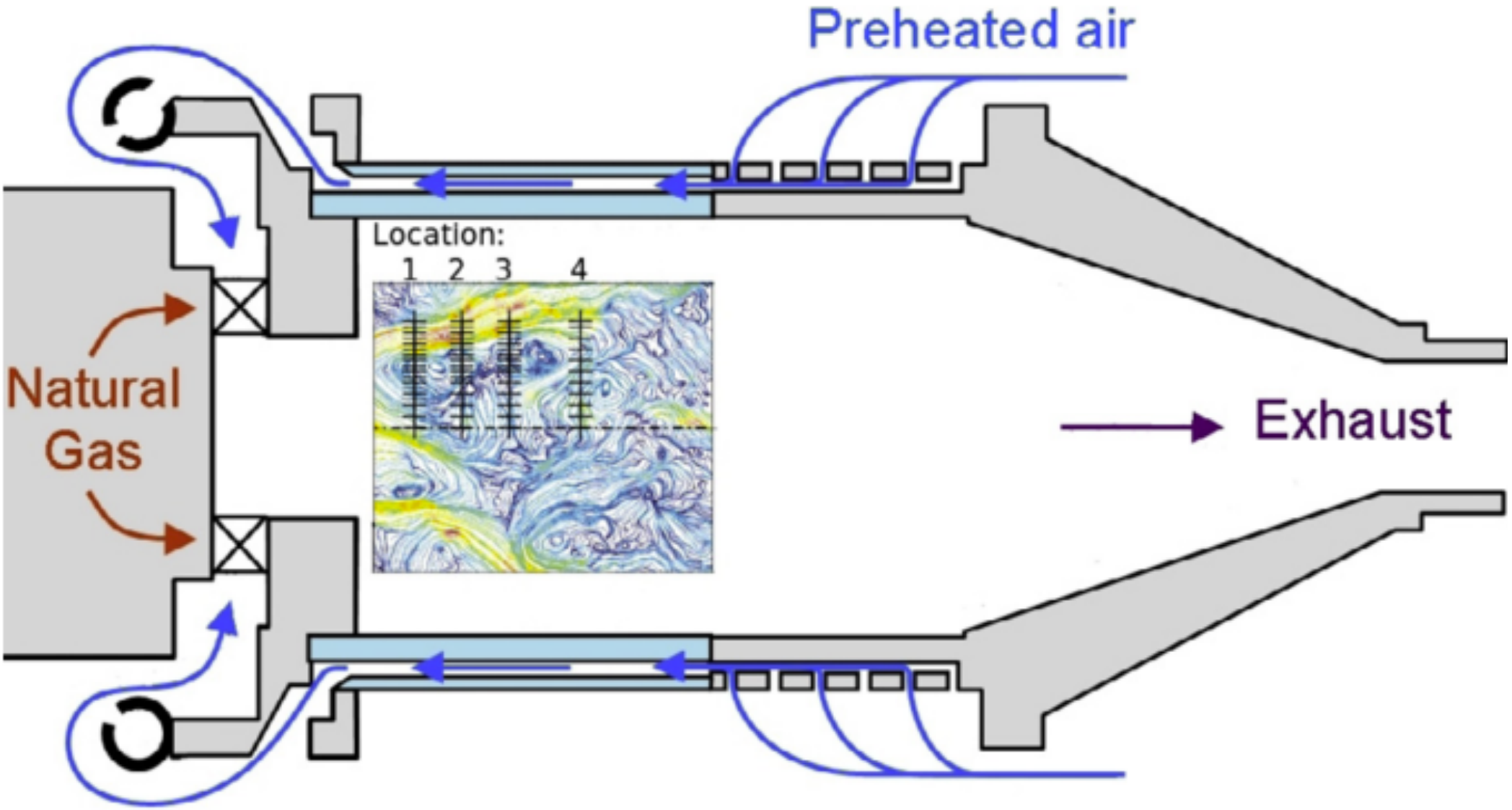


E. Oran's group

A basic assumption about most models for turbulence / flame interaction

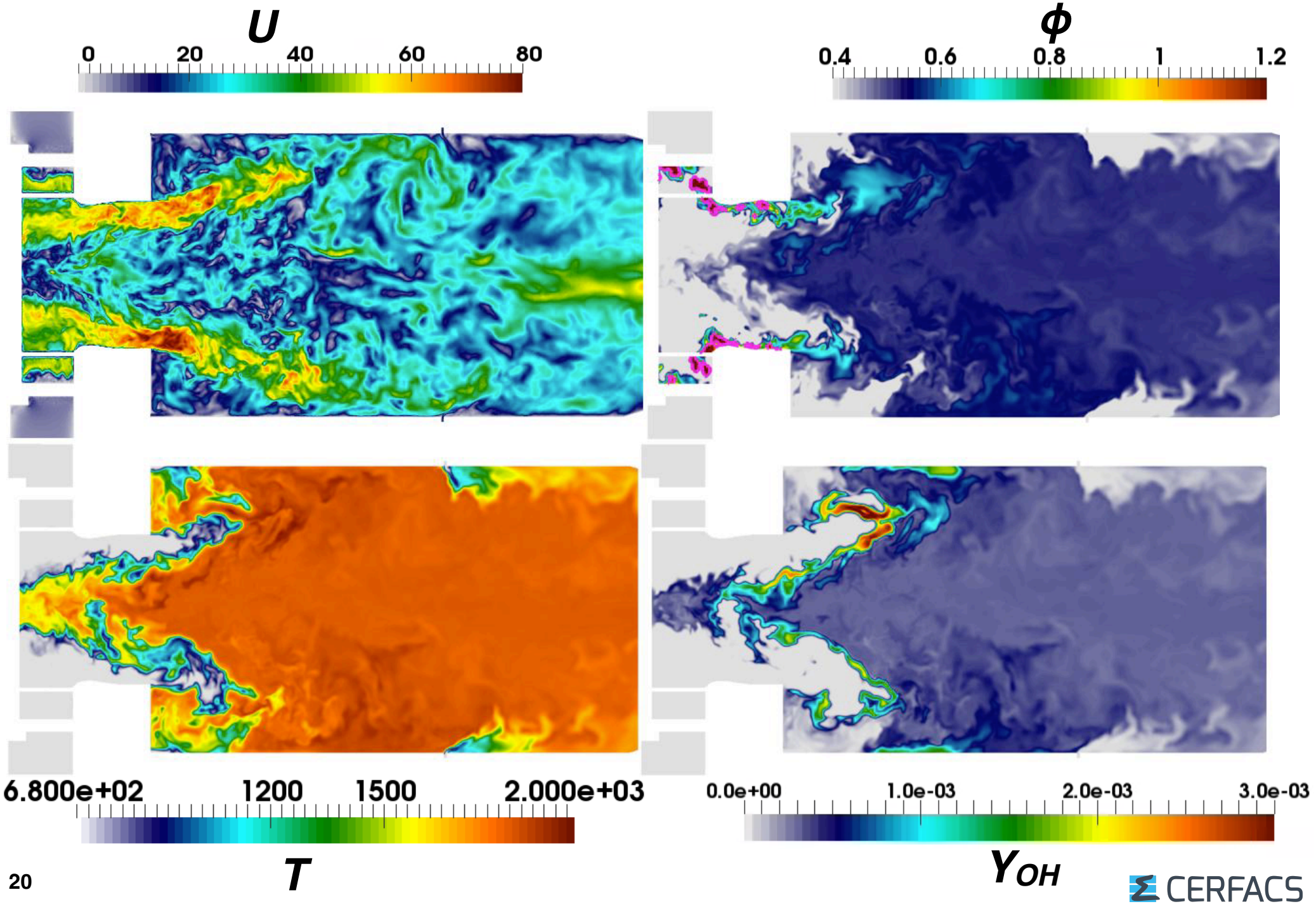
- Turbulence is not universal: every flow has its own turbulent field
- Theoretically, this means that we would need to have a model for each case of flame / turbulence interaction

A GAS TURBINE [1]



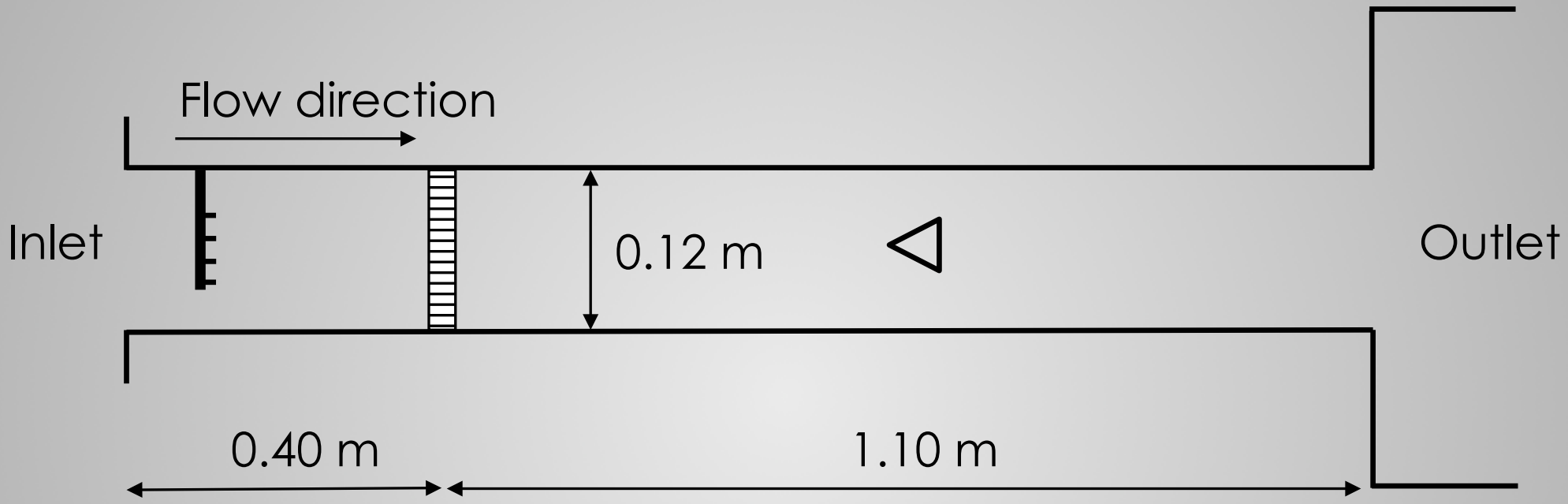
[1] Stopper et al, C&F, 2013

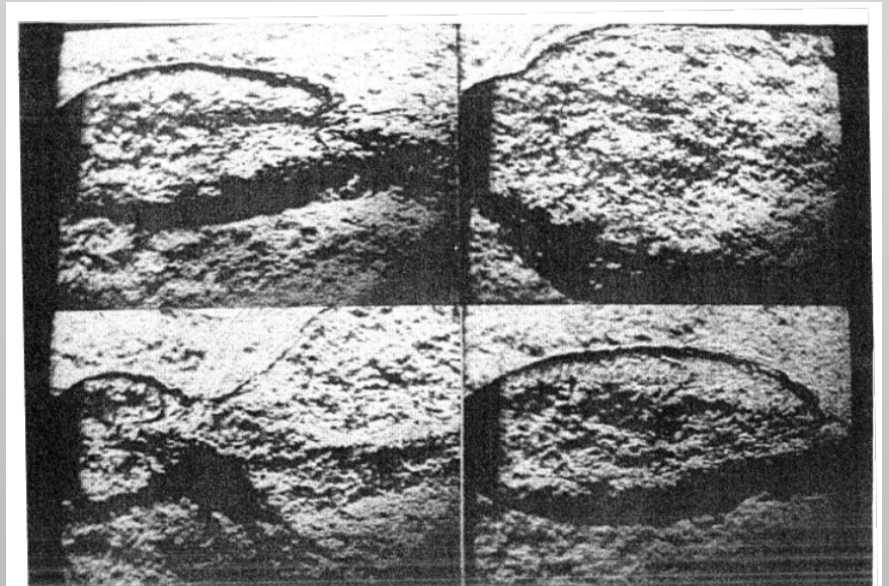
LES of a gas turbine flow:



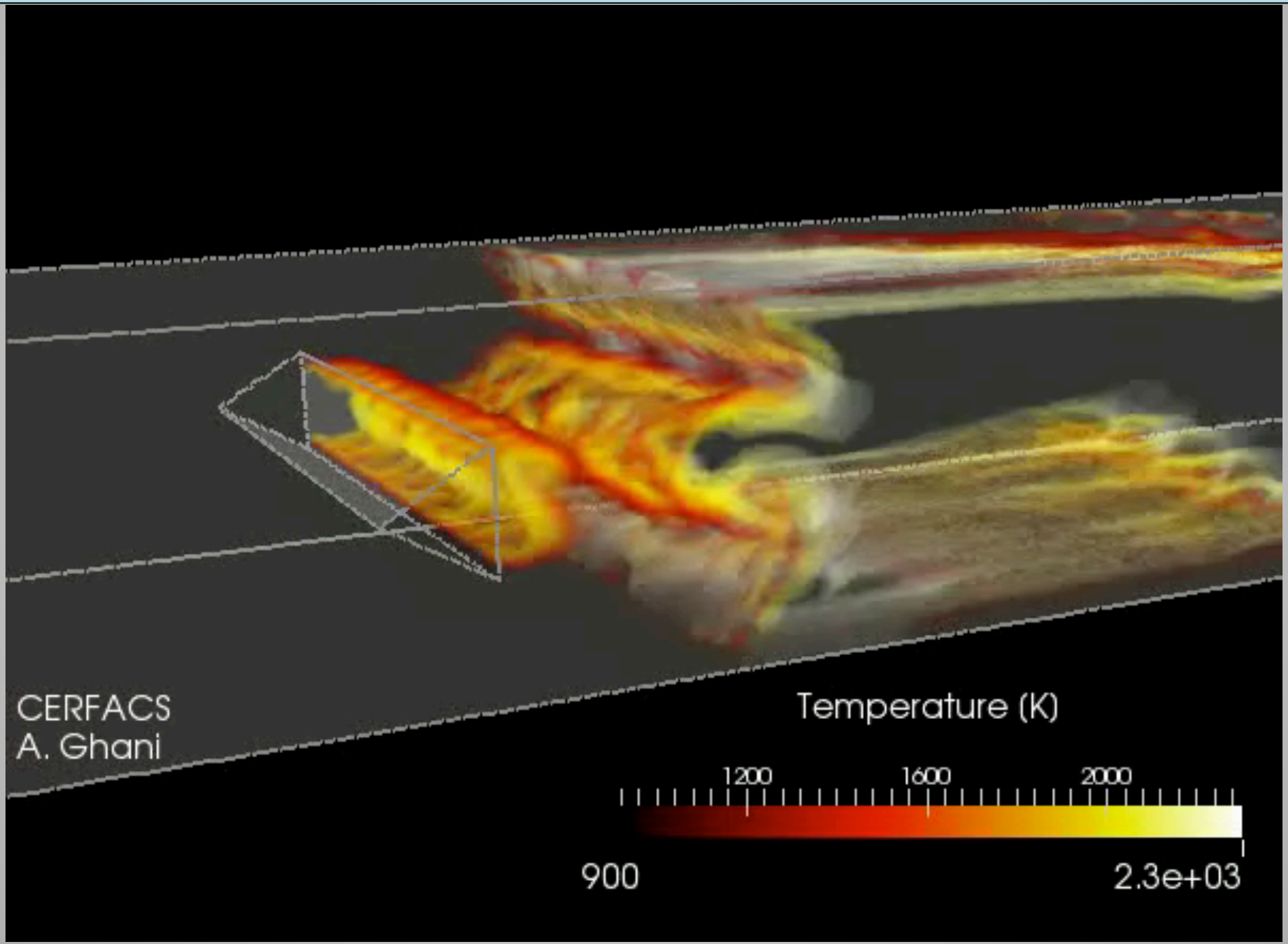
CERFACS

A V-FLAME (VOLVO - POST COMBUSTION)





LES OF THE VOLVO RIG

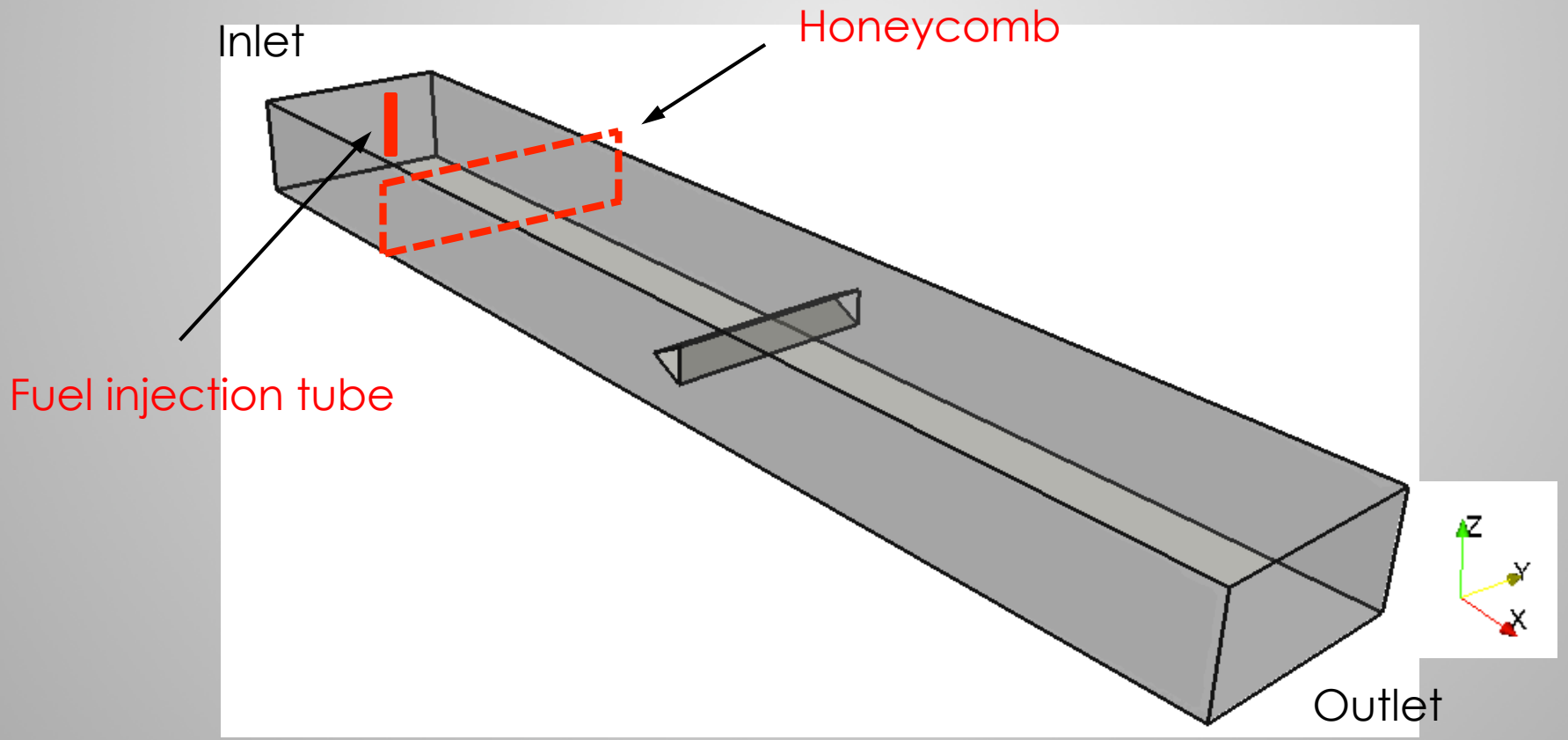


We must assume some type of universal behavior

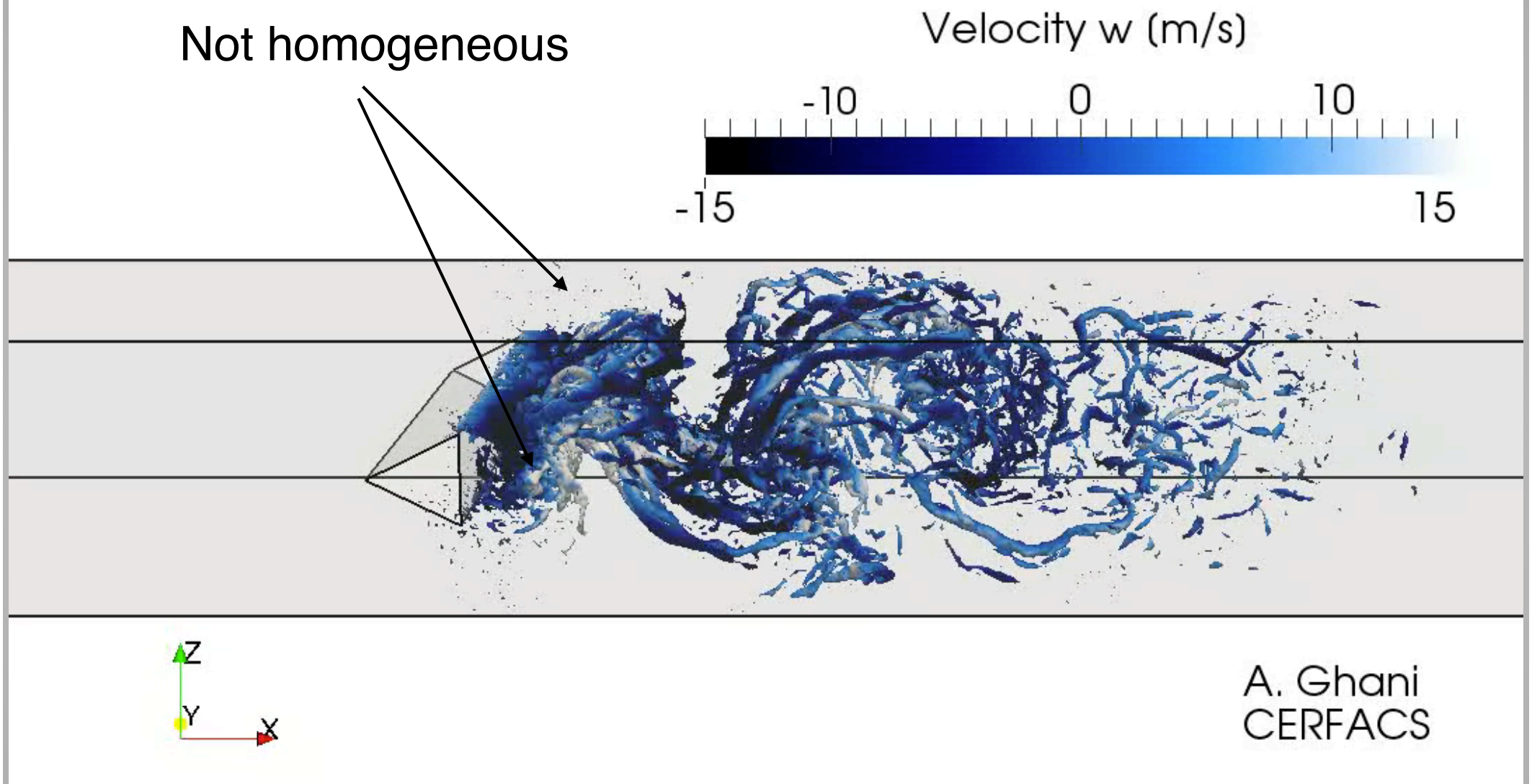
- So, we choose to say that the interaction between flame and turbulence in real flames is THE SAME AS the interaction between flame and homogeneous isotropic turbulence (HIT)
- Because HIT is a flow we understand and which depends on a limited number of parameters:
  - integral scale length L and RMS speed u'
  - better: the spectrum of the turbulent flow

This is a BIG assumption

- There is no reason to expect that turbulence is similar to HIT in all cases: in most flows, turbulent fluctuations are neither isotropic nor homogeneous



Not homogeneous



A. Ghani
CERFACS

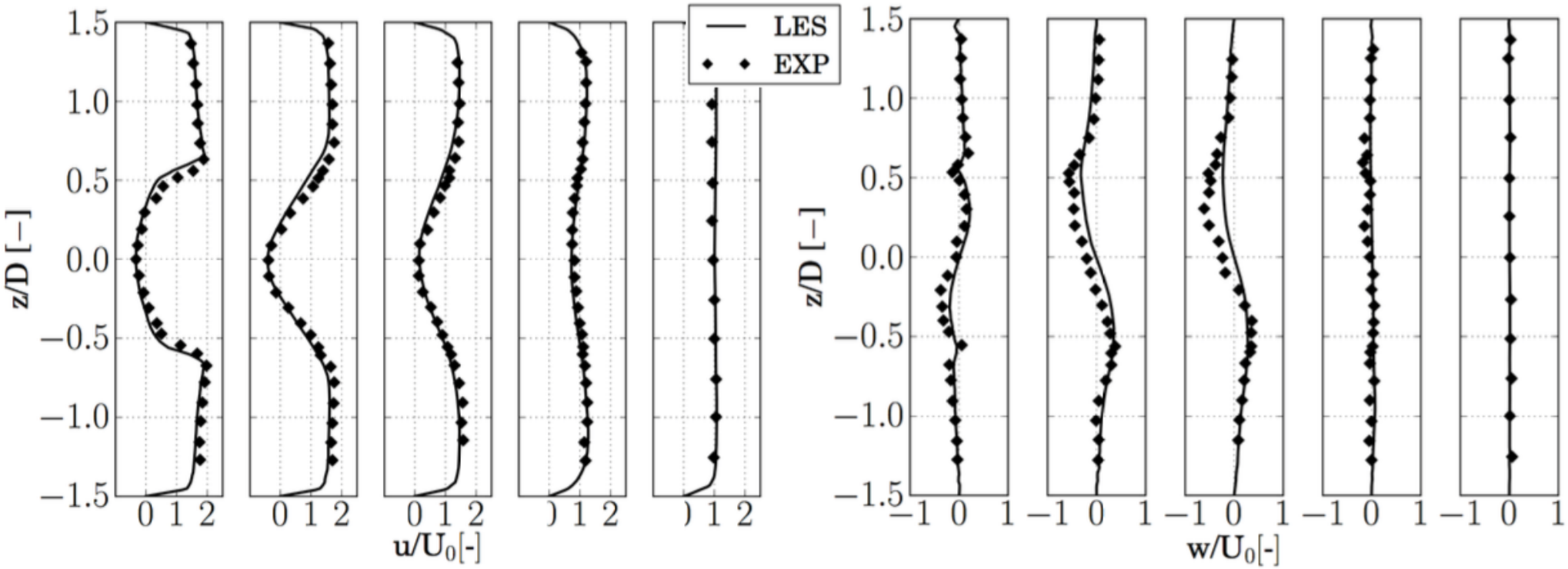


Figure 7: Non-reacting case velocities at measurement planes M_1 to M_5. Left: Normalized axial velocities. Right: Normalized transverse velocities.

RMS values are NOT equal in all directions: not HIT

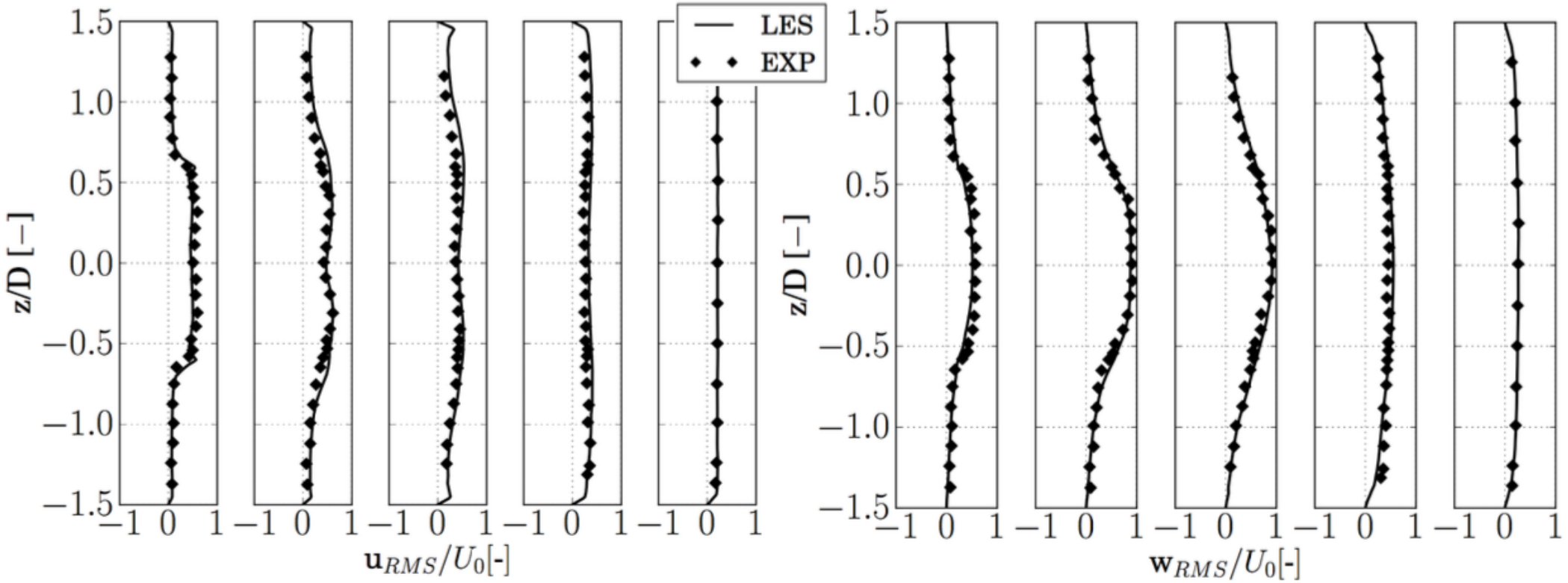


Figure 8: Non-reacting case velocities at measurement planes M_1 to M_5. Left: Normalized axial RMS velocities. Right: Normalized transverse RMS velocities.

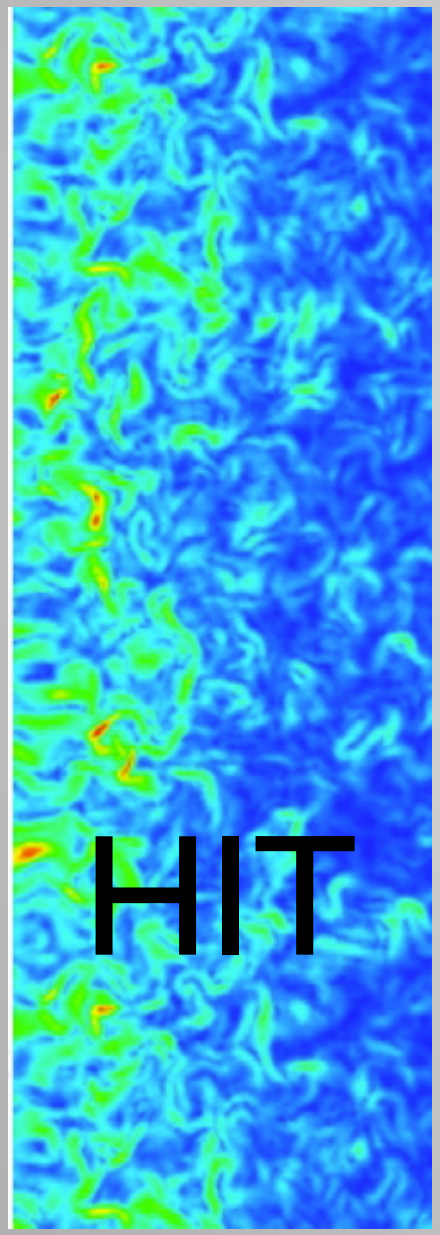
But we will do it anyway

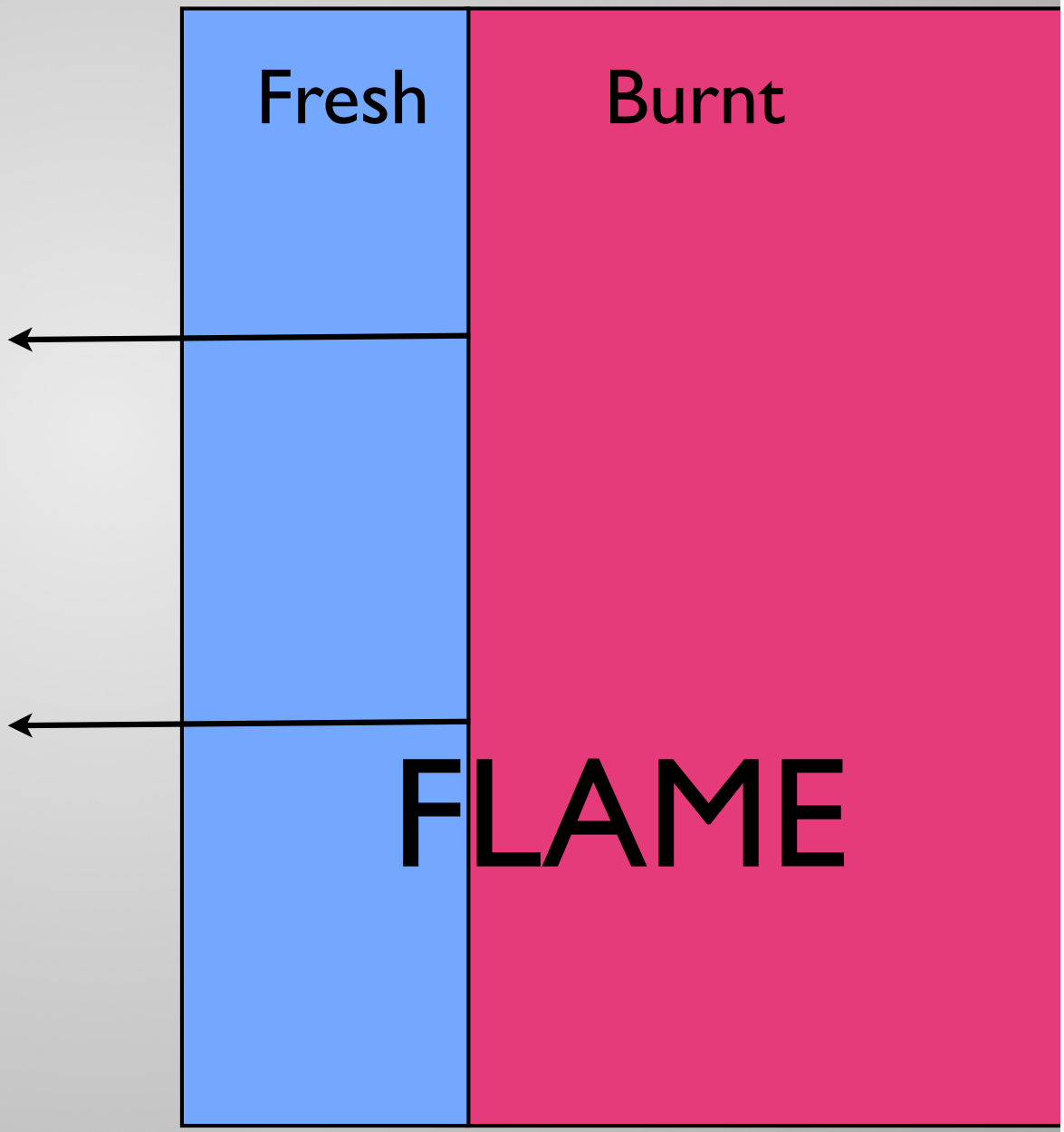
- Because this is already a huge task
- Because what may be true is to assume that the SMALLEST scales present in a turbulent flow are similar to HIT -> this is what LES does :

➡ resolve/compute the large scales

➡ model the small scales as if it was HIT.

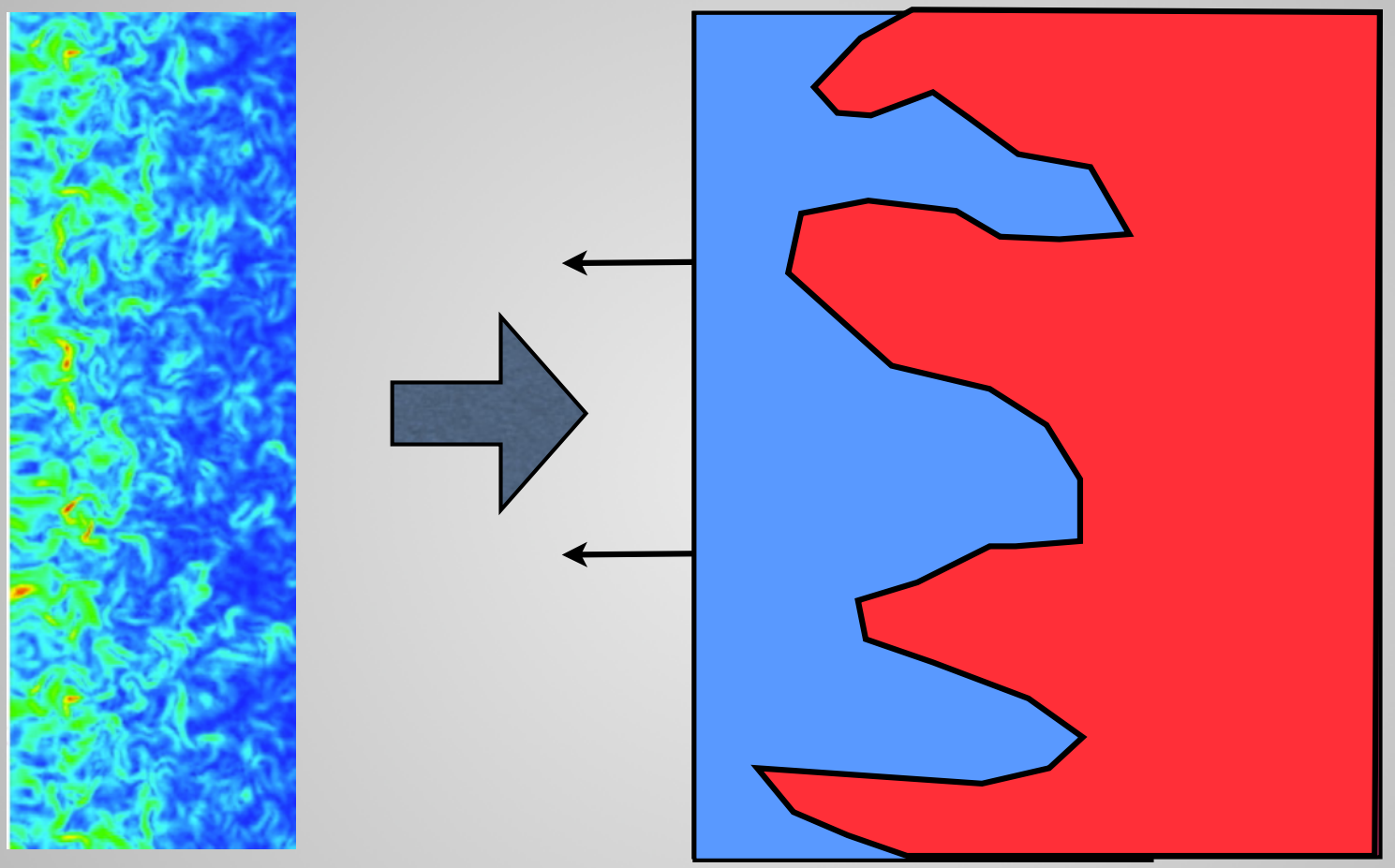
Flame / turbulence fight:





DIRECT COUPLING:

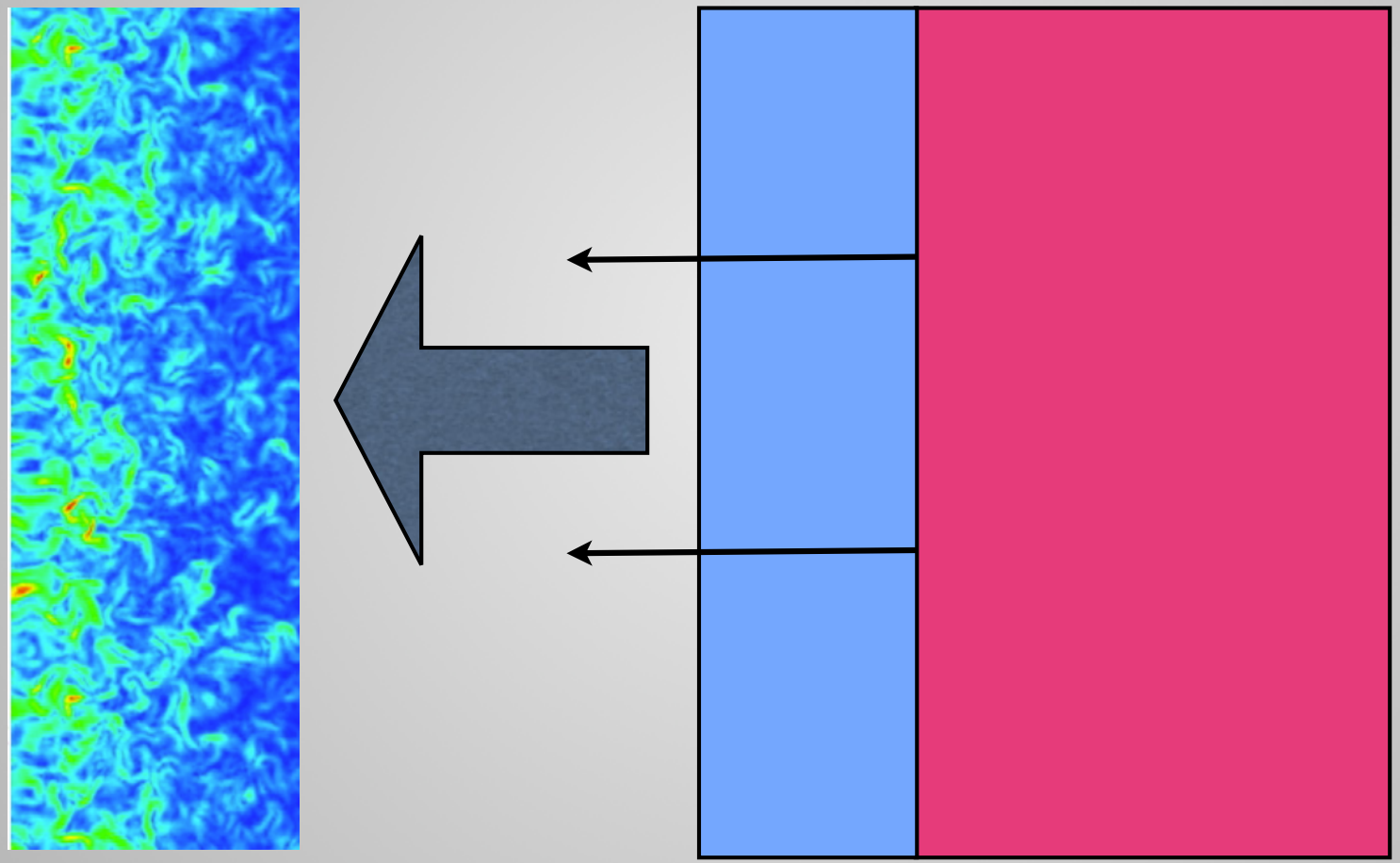
I - Turbulence wrinkles the flame:



More **flame surface** means **more power**: here comes our acceleration factor. Turbulence creates what we need: flame surface

TWO WAY COUPLING:

II - The flame also modifies turbulence



TWO WAY COUPLING:

II - But the flame also affects the flow in two ways:

I/ Kinematic viscosity increases: burnt gases are more viscous than fresh gases.

$$\nu = \nu_0 \left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)^2$$

*This will **damp turbulence***

This means for example that:

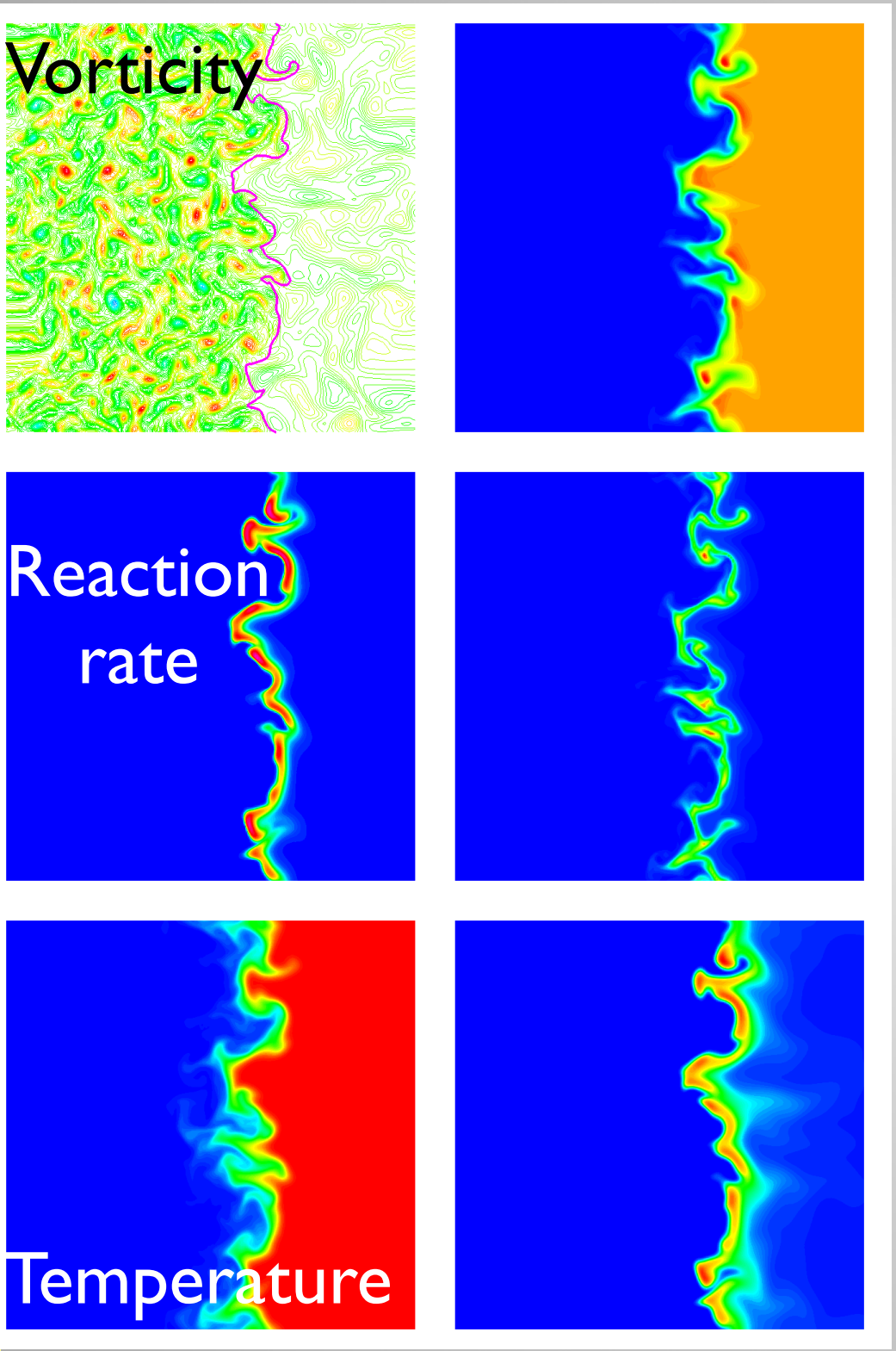
- when T goes from 300 to 2400 K, ν increases by $8^2 = 64$
- a turbulent cold jet can laminarize when it is ignited

II/ Velocities increase: the velocities in the burnt gases increase by a factor of the order of the density ratio.

*This will **increase turbulence***

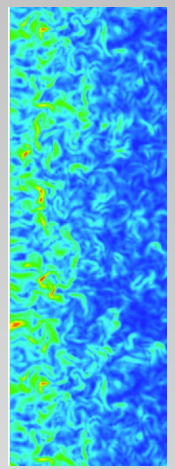
Turbulent combustion regimes

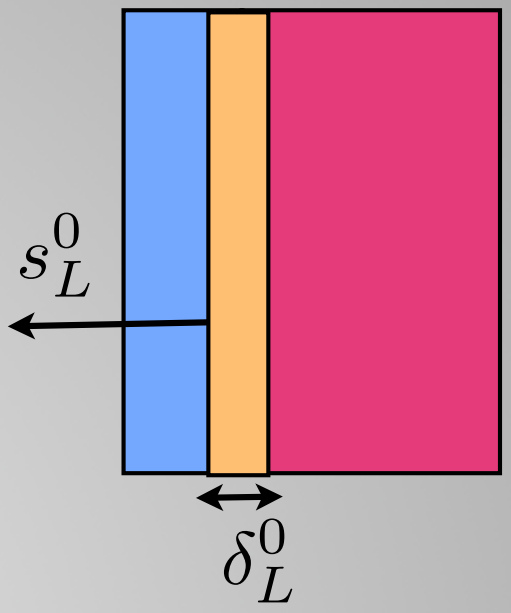
- One of the oldest games in the field of premixed turbulent combustion. Objective: knowing the characteristics of the turbulent flow and of the flames (usually speeds and sizes), guess what the interaction between the two will be…
- Reduced control parameters: usually, two:
  - Ratio of **speeds**: RMS speed u' / flame speed s_L^0
  - Ratio of **sizes** : integral scale l / flame thickness δ_L^0
- Since the turbulent flow has a wide range of scales, the reference quantity for the flow corresponds to the largest scale: the integral scale l .

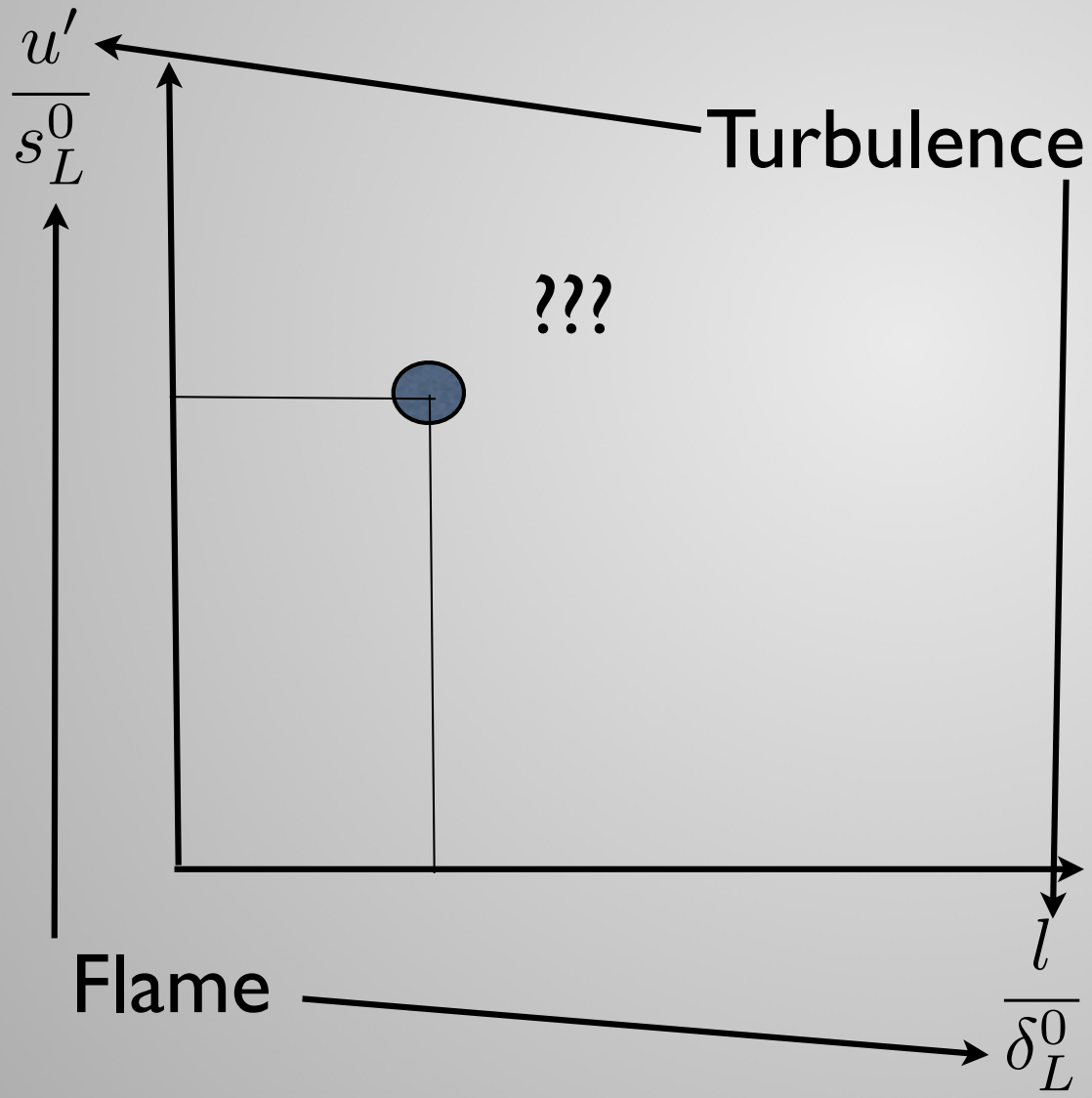


Baum M. , Poinsot T. et Haworth D. (1994) "Direct Numerical Simulation of H2/O2/N2 flames with complex chemistry in two dimensional turbulent flows", *J. Fluid Mechanics* 281, p1-32.

Turbulent combustion diagram



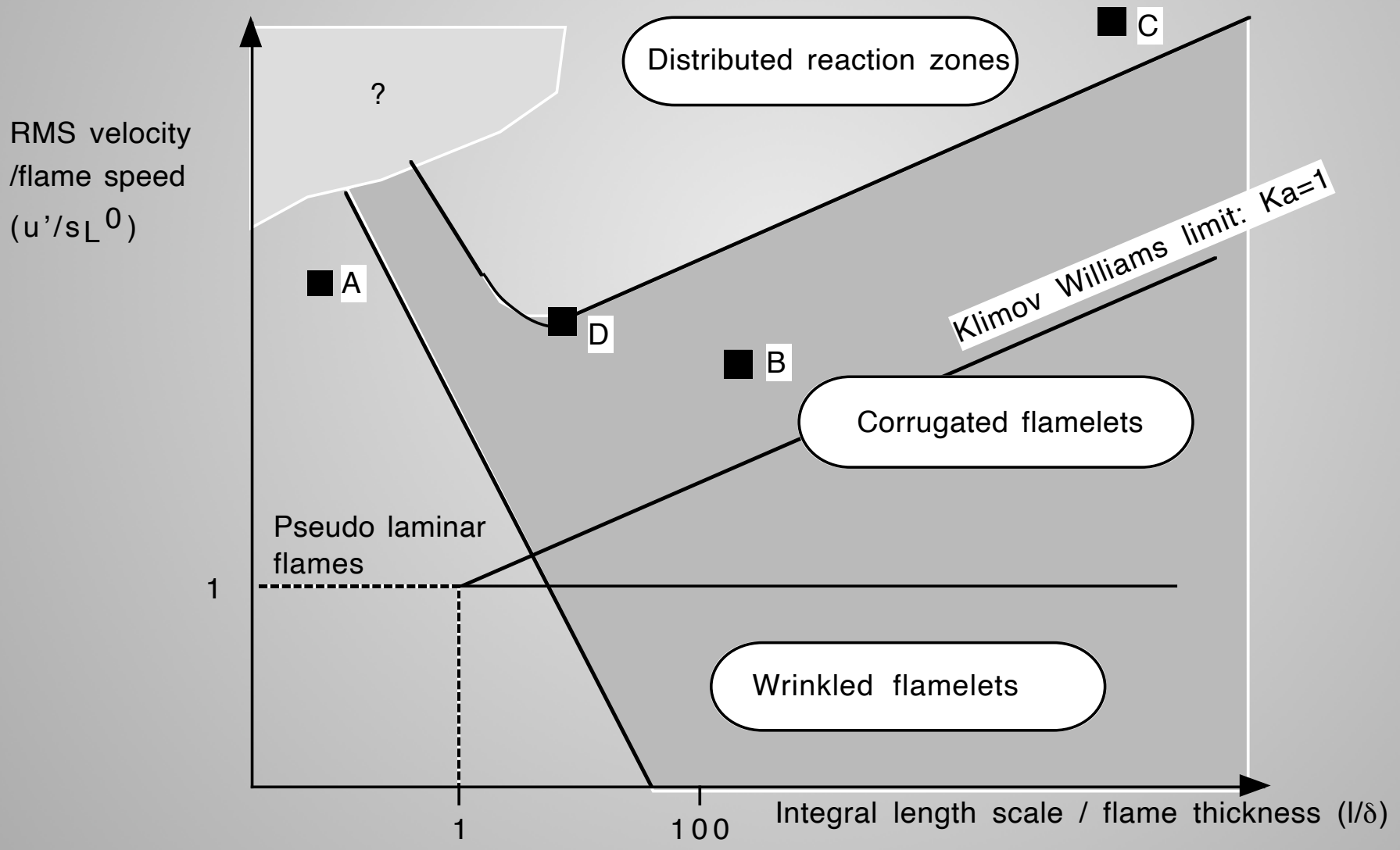




Borghi
Peters
Poinsot

Example of diagram

(Poinsot et al J. Fluid Mech.1992)

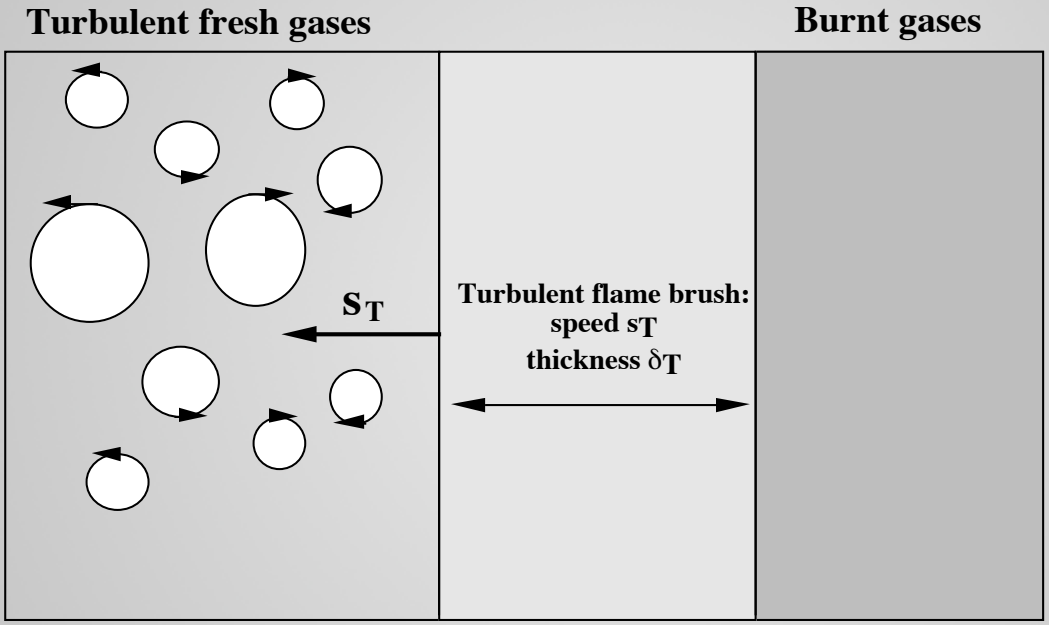


The turbulent flame speed

- Another popular but probably wrong notion
- Based on the idea that there is a turbulent speed for a turbulent front similar to the laminar speed for a laminar flame front
- Defined from simple conservation arguments

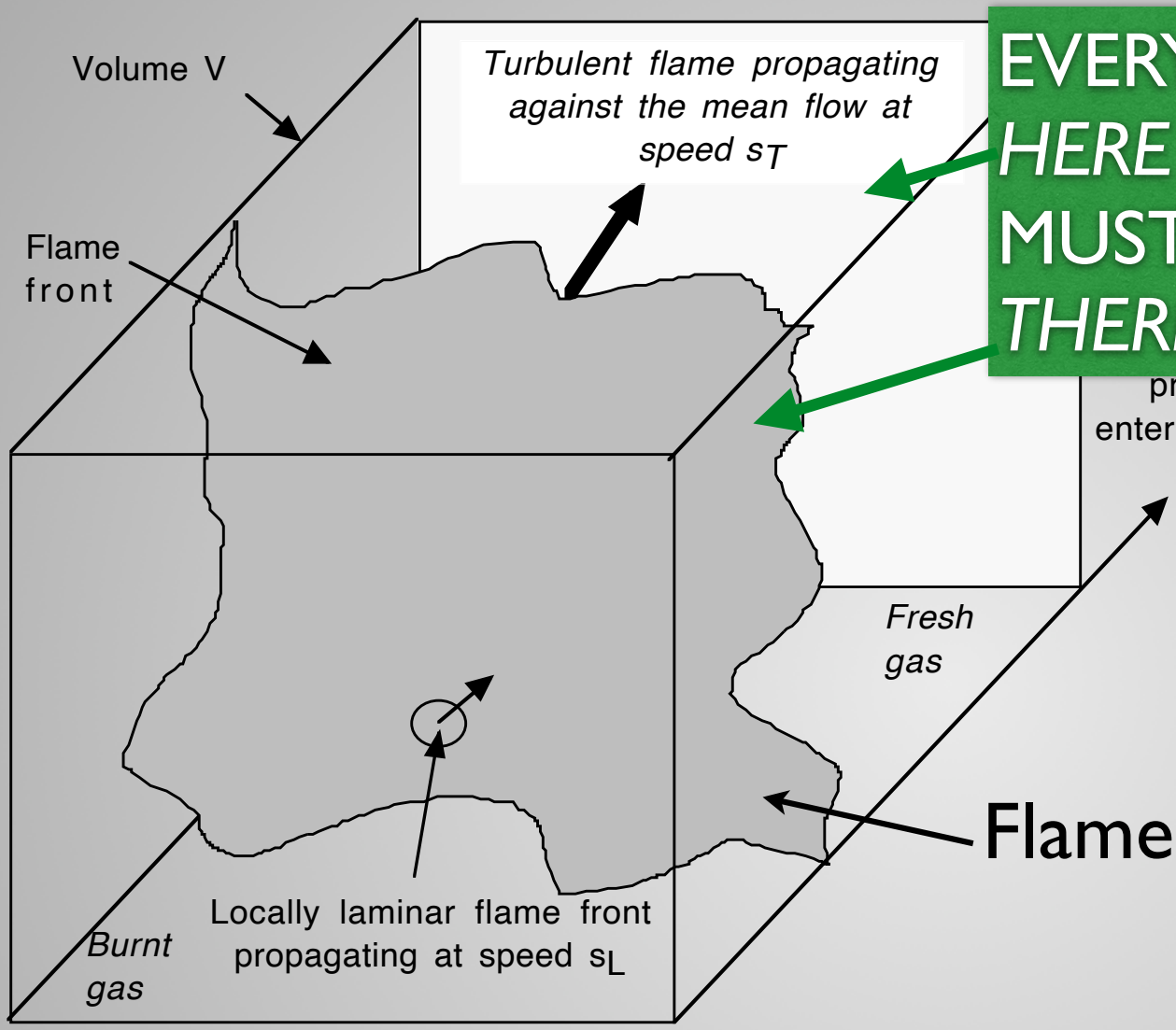
Defining the turbulent flame speed:

Ch. 5 Sec. 5.1.1



Assume:

- that the turbulent flame brush thickness does NOT grow
- that the local flame structure is 'flamelet' like



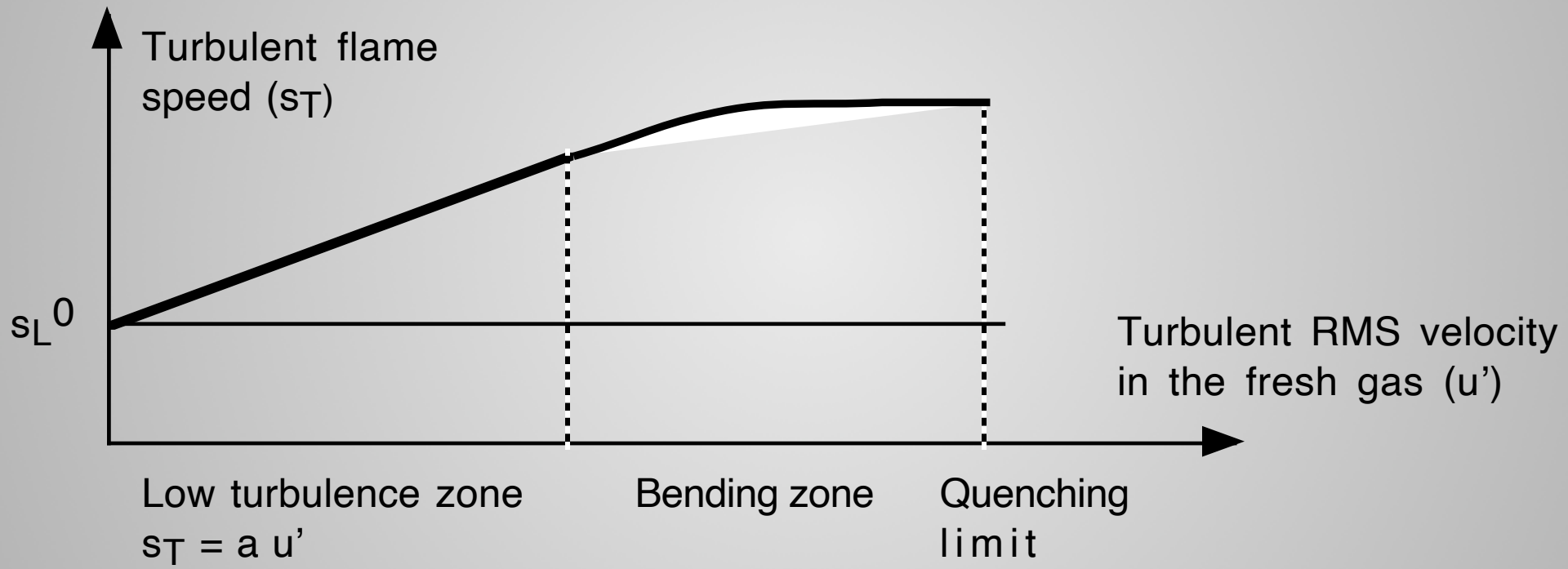
EVERYTHING ENTERING *HERE*
MUST GET OUT *THERE*

Flame area A_T

Volume (or mass since density is constant between inlet and flame) flow conservation between inlet and flame:

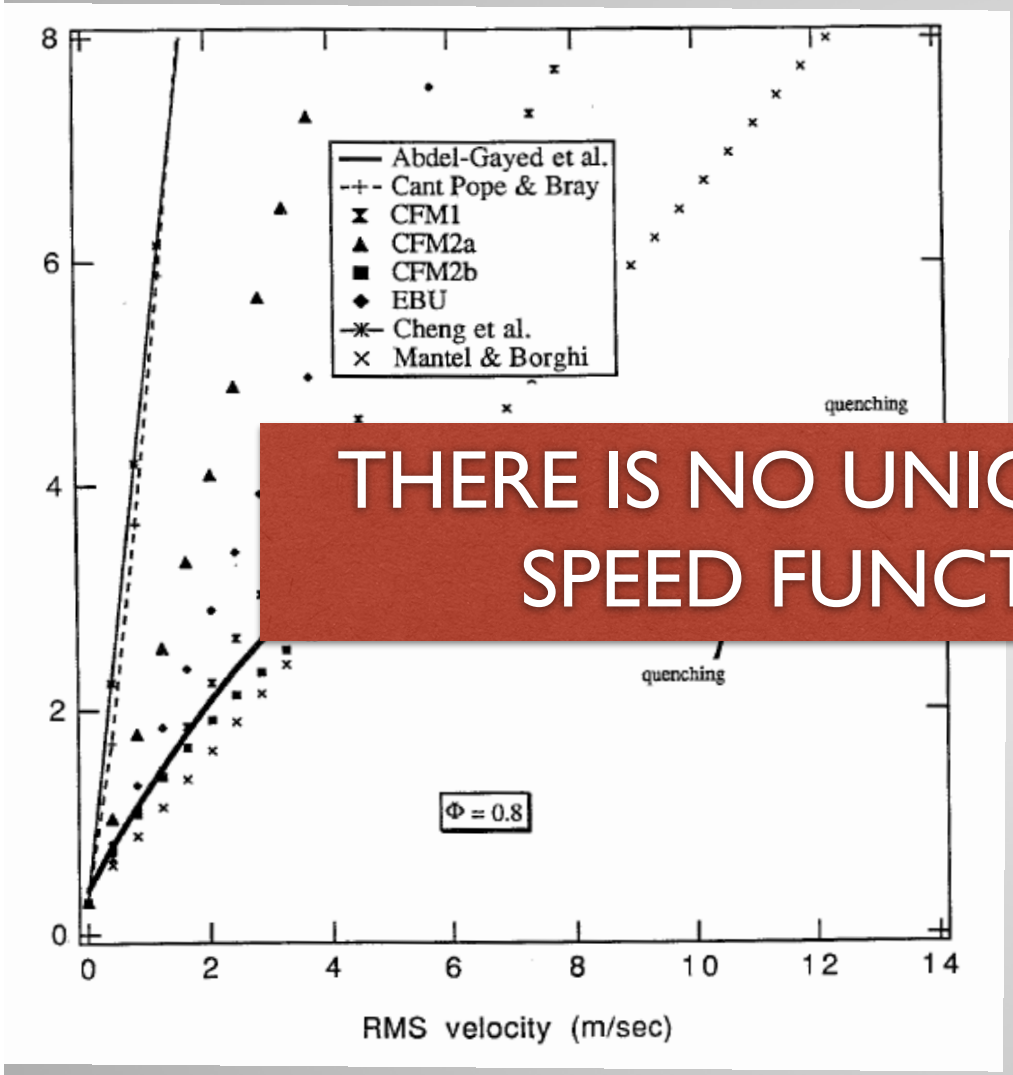
$$\mathbf{A s_T = A_T s_L} \qquad \mathbf{s_T = \frac{A_T}{A} s_L = \Theta s_L}$$

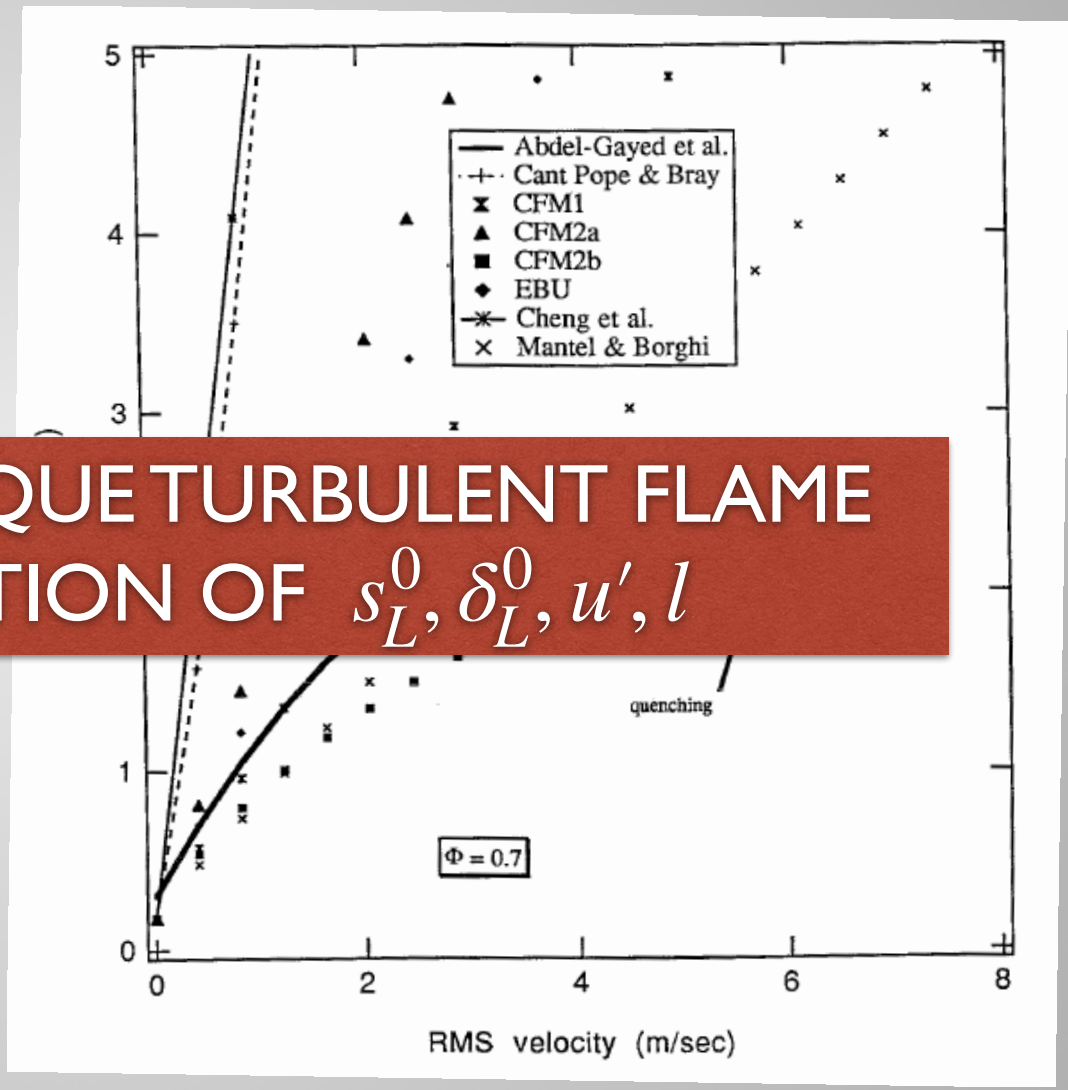
Turbulent flame speed variations vs turbulent velocity u': $s_T = f(u')$ (3 millions hits on Google):



Problem: these functions are configuration dependent, fuel dependent, time dependent, Lewis number dependent etc

Comparison of 7 turbulent flame speed models and of exptl data.
Turbulent flame speed versus RMS velocity:



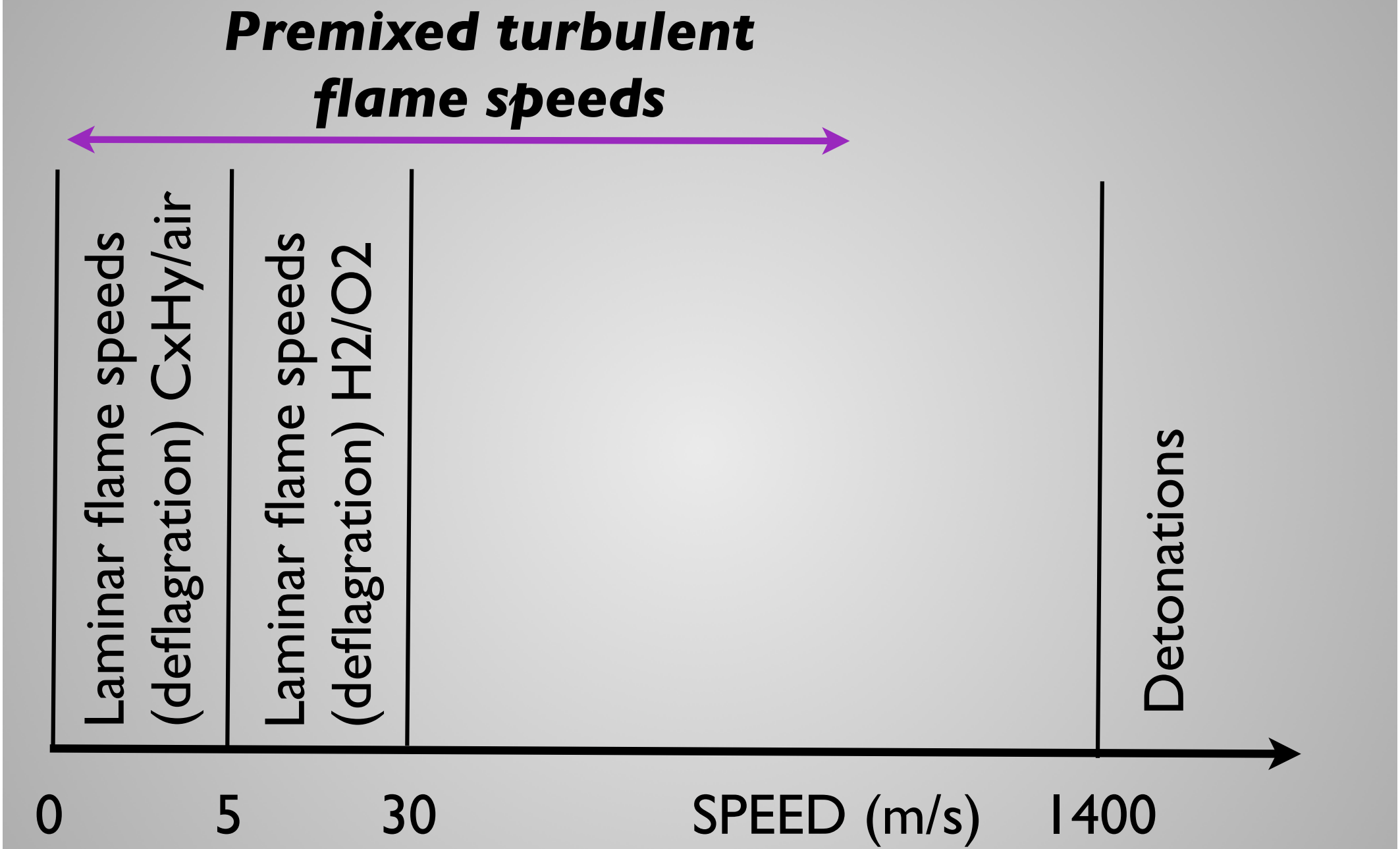


THERE IS NO UNIQUE TURBULENT FLAME SPEED FUNCTION OF s_L^0, δ_L^0, u', l

Duclos et al, *Comb Flame*, 95, 101-117, 1993

Final word on speeds:

- Even though there is no universal ‘turbulent flame speed’, turbulent flames do move at a variety of speeds, depending on geometries, pressures, time
- Let us compare these speeds to the other flame speeds we defined:


Premixed turbulent flame speeds
Laminar flame speeds (deflagration) CxHy/air
Laminar flame speeds (deflagration) H2/O2
Detonations
0
5
30
SPEED (m/s)
1400



This turbulent flame reaches speeds of the order of 200 m/s

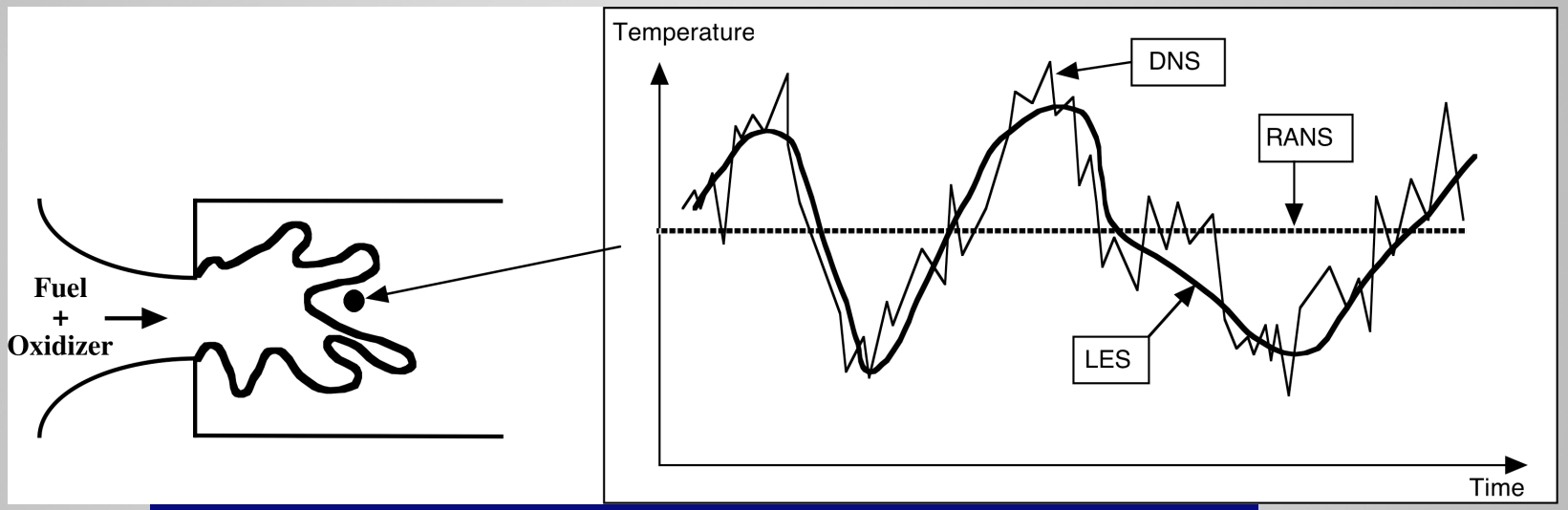
Modeling and CFD codes

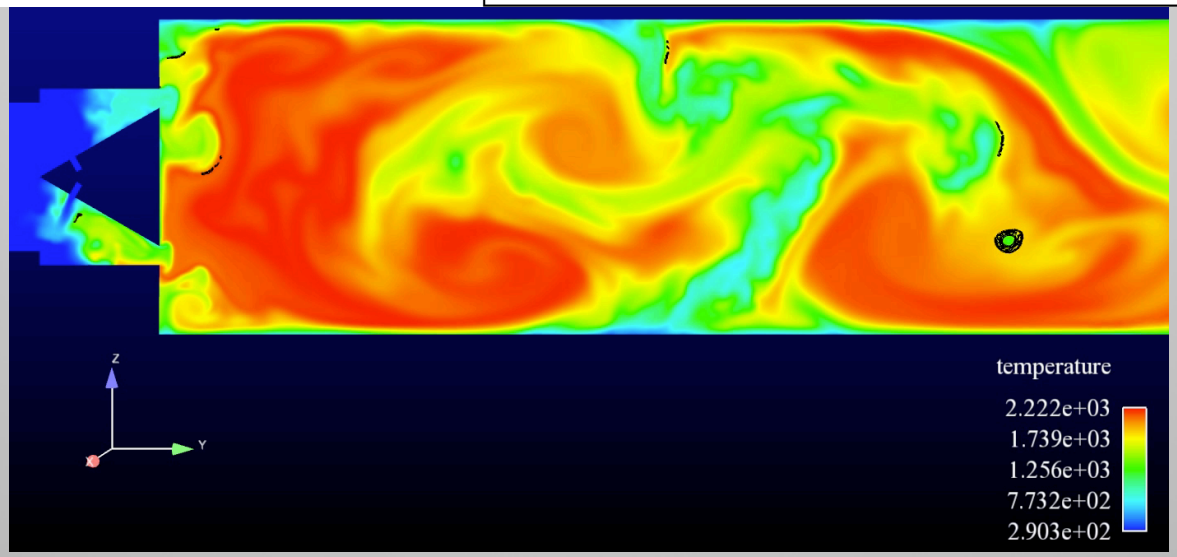
- Laminar flames were one-dimensional steady flows. You can compute them 'easily' (*more or less*...) and this has been done for 40 years
- Turbulent flames are 3D, time-dependent flows.
- 40 years ago, we could not use brute force to compute them. Even today DNS (Direct Numerical Simulation) is possible only for simple cases
- Giving up on the unsteady nature of the flow and looking for '**averages**' was the only reasonable path

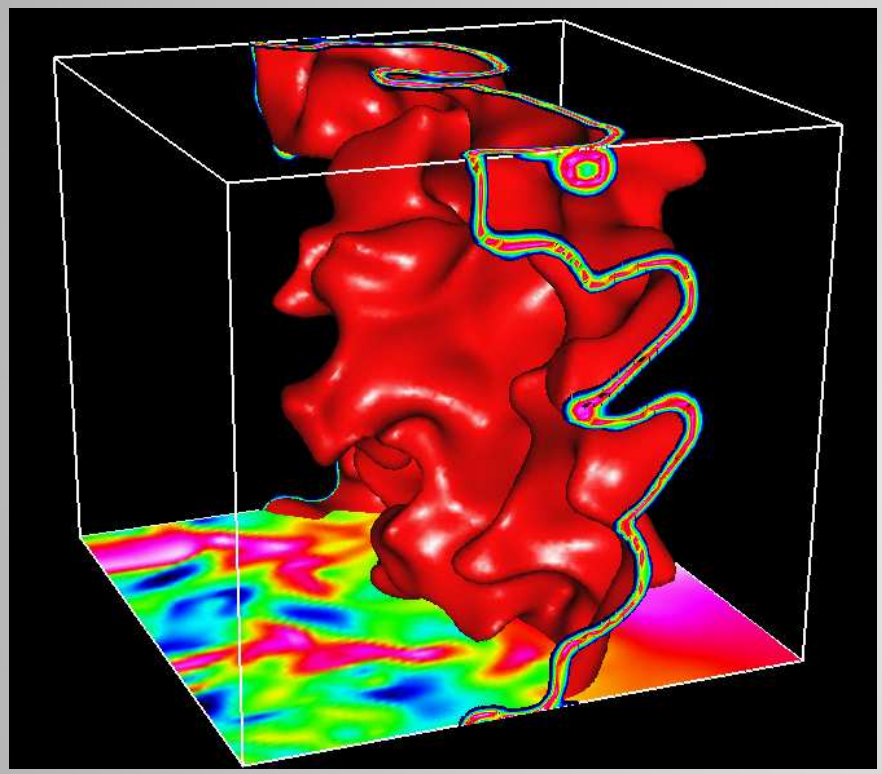
Averaging:

The simplest averaging approach was to look for **time averages** in flows which were statistically steady.

==>RANS methods



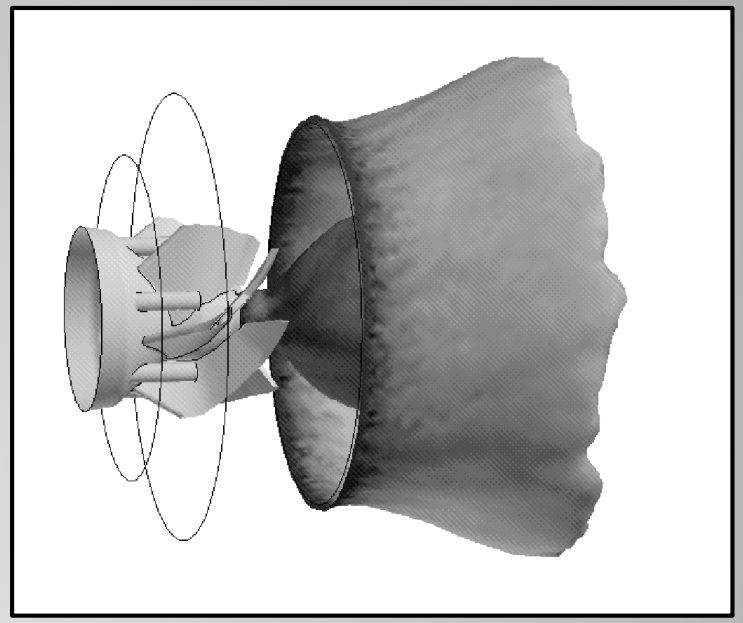




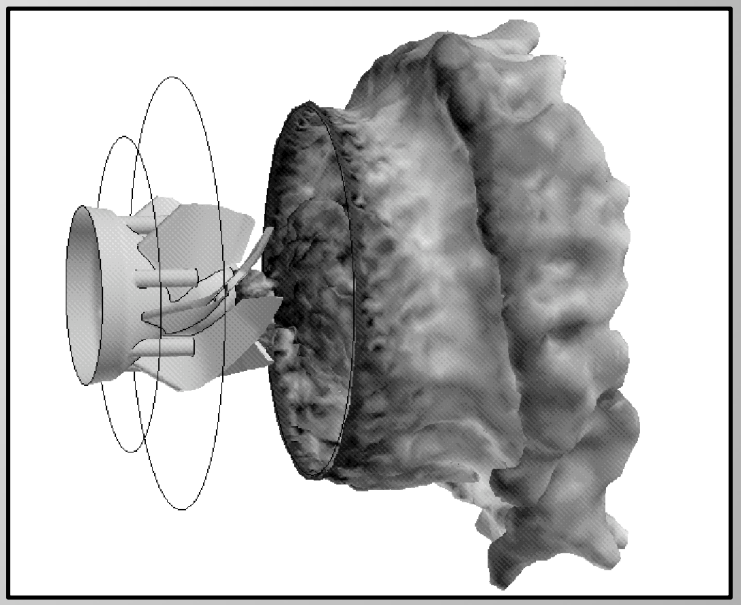
DNS

(Boger et al, 1998)

RANS
(mean flow)



LES
(instantaneous flow)



(Selle, 2004)

Time averaging has to be replaced by **cycle** averaging (averaging over realizations) for flows which are not steady in the mean (typically piston engines or explosions)

SGEmac project

Consecutive cycles by LES of a spark ignition engine

Unstable by dilution operating point

Compression ratio : 9.9
Engine speed : 1200 rpm
Fuel : C_3H_8
Equivalence ratio : 1
Dilution by N_2 : 32 % vol.
Mean IMEP : 3.2 bars
cov(IMEP) : 7.2 %

Granet et al., Combustion and Flame, in press, doi:10.1016/j.combustflame.2011.11.018
Enaux et al., Flow Turbulence and Combustion 86 (2), pp 153-177, 2011
Enaux et al., Proceedings of the Combustion Institute, 33 (2), pp 3115-3122, 2011

- Time (or cycle) averaging is used for RANS methods.

$$\bar{f} = \frac{1}{\tau}\int_0^{\tau} f dt$$

RANS

- When Large Eddy Simulations started, another averaging method was used: space filtering (local)

$$\bar{f}(x) = \int f(x')F(x - x')\,dx'$$

LES

- **Space filtering and time averaging** are different even though models seem very similar...

Ch. 5 Sec. 4.7

Now we need equations for MEAN quantities: mean temperature, mean density, etc

The only starting point we have is the instantaneous Navier Stokes equations we have seen before

The procedure is to average these equations and see if we can obtain equations for the mean quantities

Useful relations for averages:

$$\bar{f} = \frac{1}{\tau}\int_0^{\tau} f\,dt$$

Mean value of any function f

'REYNOLDS' Averaging

$$u_i = \bar{u}_i + u_i'$$

Constant **Time dependent**

$$\bar{\bar{u}}_i = \bar{u}_i$$

The average of a constant is the same constant

$$\bar{u}_i = \overline{\bar{u}_i + u_i'} \longrightarrow \bar{u}_i' = 0$$

The average of a perturbation is zero

Useful relations for averages:

$$\overline{f+g} = \bar{f} + \bar{g}$$

$$\overline{\lambda f} = \lambda \bar{f} \qquad \text{if } \lambda \text{ is constant}$$

$$\overline{fg} = \bar{f}\bar{g} + \bar{f}\bar{g'} + \bar{f'}\bar{g} + \overline{f'g'}$$

$$\overline{fg} = \bar{f}\bar{g} + \overline{f'g'}$$

All the averaging methodology is well known in the world of turbulence models for 'cold, constant density flows' where Reynolds averages are used everywhere for RANS and LES of aerodynamics. Many of you know the k-ϵ model for non reacting flows for ex.

Unfortunately, in combustion, density is NOT constant

The variable density problem in averaging:

- Averaging, in space (LES) or in time (RANS), is difficult in a **non-constant density** flow
- Why ? Let us take the example of RANS using Reynolds averaging:

$$\overline{\mathbf{f}} = \frac{\mathbf{1}}{\tau}\int_{\mathbf{0}}^{\tau} \mathbf{f}\mathbf{dt}$$

If density changes, using Reynolds averaging, mass conservation equation reads:

$$\frac{\partial \rho}{\partial \mathbf{t}} + \frac{\partial}{\partial \mathbf{x_i}}(\rho \mathbf{u_i}) = \mathbf{0}$$

$$\rho = \overline{\rho} + \rho' \qquad\qquad \mathbf{u_i} = \overline{\mathbf{u}}_\mathbf{i} + \mathbf{u}'_\mathbf{i}$$

To obtain an equation for averages, one averages the instantaneous equation:

$$\rho = \overline{\rho} + \rho' \qquad \mathbf{u_i} = \overline{\mathbf{u}}_\mathbf{i} + \mathbf{u}'_\mathbf{i}$$

$$\frac{\partial \rho}{\partial \mathbf{t}} + \frac{\partial}{\partial \mathbf{x_i}}(\rho \mathbf{u_i}) = \mathbf{0}$$

$$\frac{\partial \overline{\rho}}{\partial \mathbf{t}} + \frac{\partial}{\partial \mathbf{x_i}}(\overline{\rho \mathbf{u_i}}) = \mathbf{0}$$

$$\overline{\rho u} = \overline{(\overline{\rho} + \rho')(\overline{u} + u')} = \overline{\overline{\rho}\,\overline{u}} + \overline{\rho u'} + \overline{\rho' \overline{u}} + \overline{\rho' u'}$$

$$= \overline{\rho}\,\overline{u} + \overline{\rho}\,\overline{u'} + \overline{\rho'}\,\overline{u} + \overline{\rho' u'}$$

This leads to an averaged continuity equation:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\,\overline{u_i} + \overline{\rho' u_i'}) = 0$$

which does not conserve mass...

Having a combustor with an average inlet flow of 2 kg/s and and average outlet flow of 2.2 kg/s is unpleasant.

So, the community moved to Favre averaging:

$$\tilde{f} = \frac{\overline{\rho f}}{\overline{\rho}}$$

which is a **mass weighted** average where heavy samples contribute more to the average than light ones. Not quite democratic but ... it conserves mass as shown now:

Starting again from continuity and averaging it:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

'FAVRE' Averaging

Using the property of Favre averaging:

$$\overline{\rho f} = \overline{\rho}\tilde{f}$$

gives:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\ \tilde{u}_i) = 0$$

Now, mass (for averaged quantities) is conserved !

But is it that simple ?

What does Favre averaging mean ?

$$\overline{\rho}\tilde{\mathbf{f}} = \overline{\rho}\overline{\mathbf{f}} + \overline{\rho'\mathbf{f}'}$$

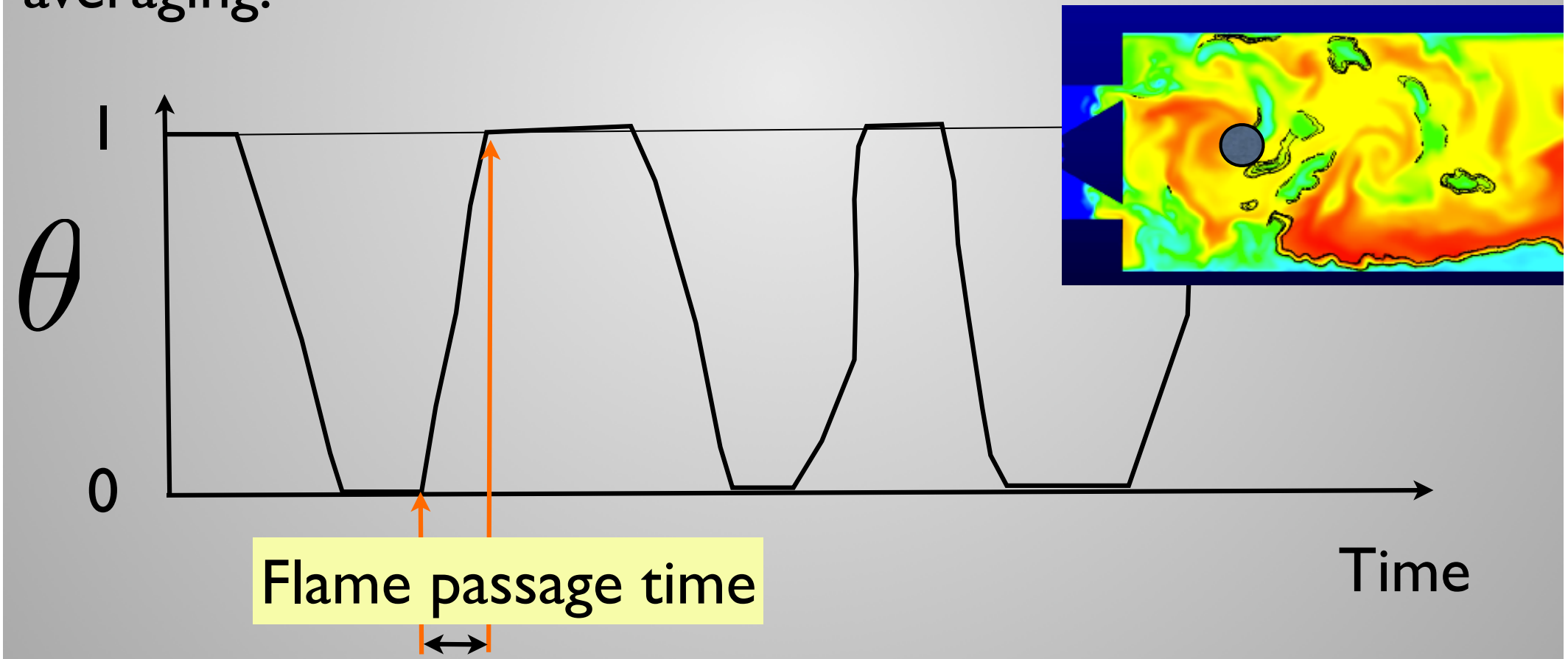
Unclosed terms are hidden in Favre averages

$$\overline{\rho}\tilde{\mathbf{f}} = \overline{\rho}\overline{\mathbf{f}} + \overline{\rho' \mathbf{f}'}$$

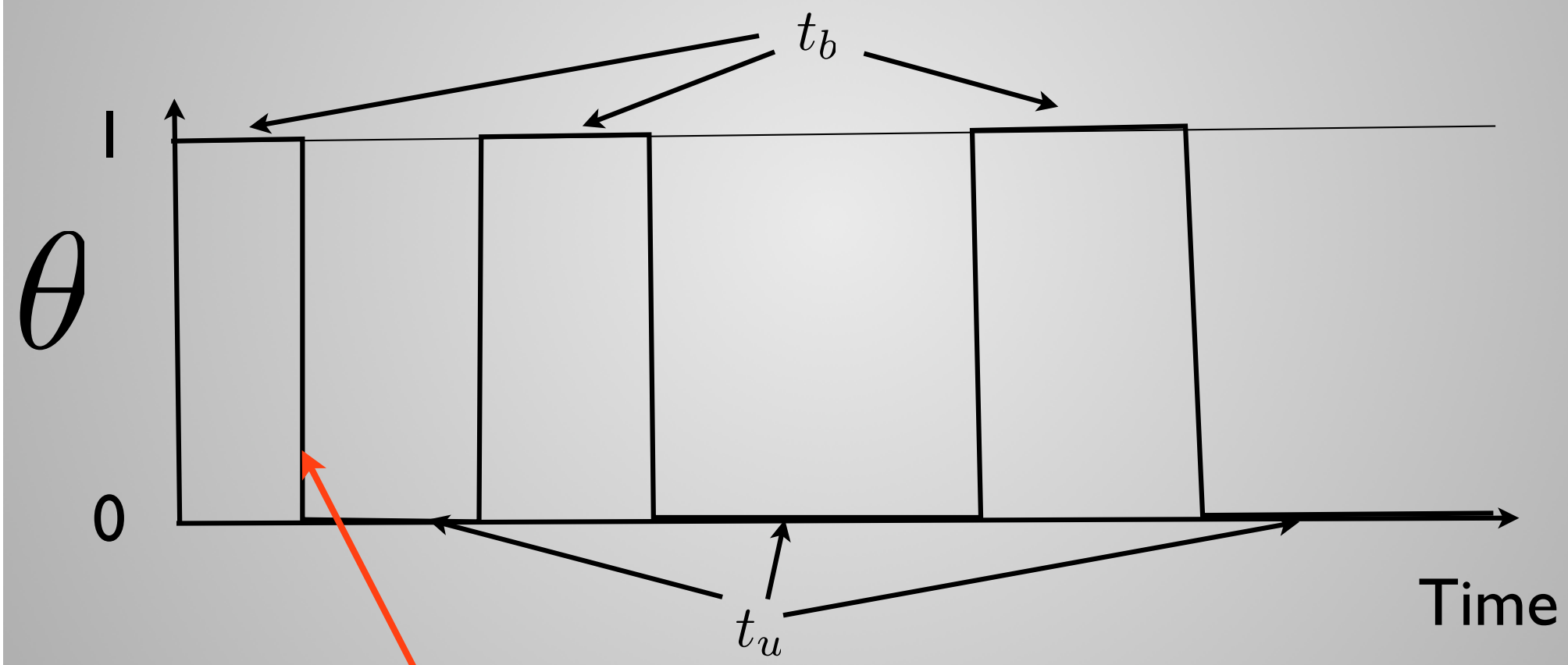
- Second, what do we measure in an experiment and how do we compare simulations with experiments if we do not know which averages are used ?
- Experimentally, averages depend on the method. But in general, it is quite difficult for experimentalists to say whether they are providing Favre or Reynolds averages.
- Is this a problem ? It would not be if Favre and Reynolds averages would be the same... But they are not ! Can we compare them ?

Favre vs Reynolds averages: we have a theory to compare them. the BML model.

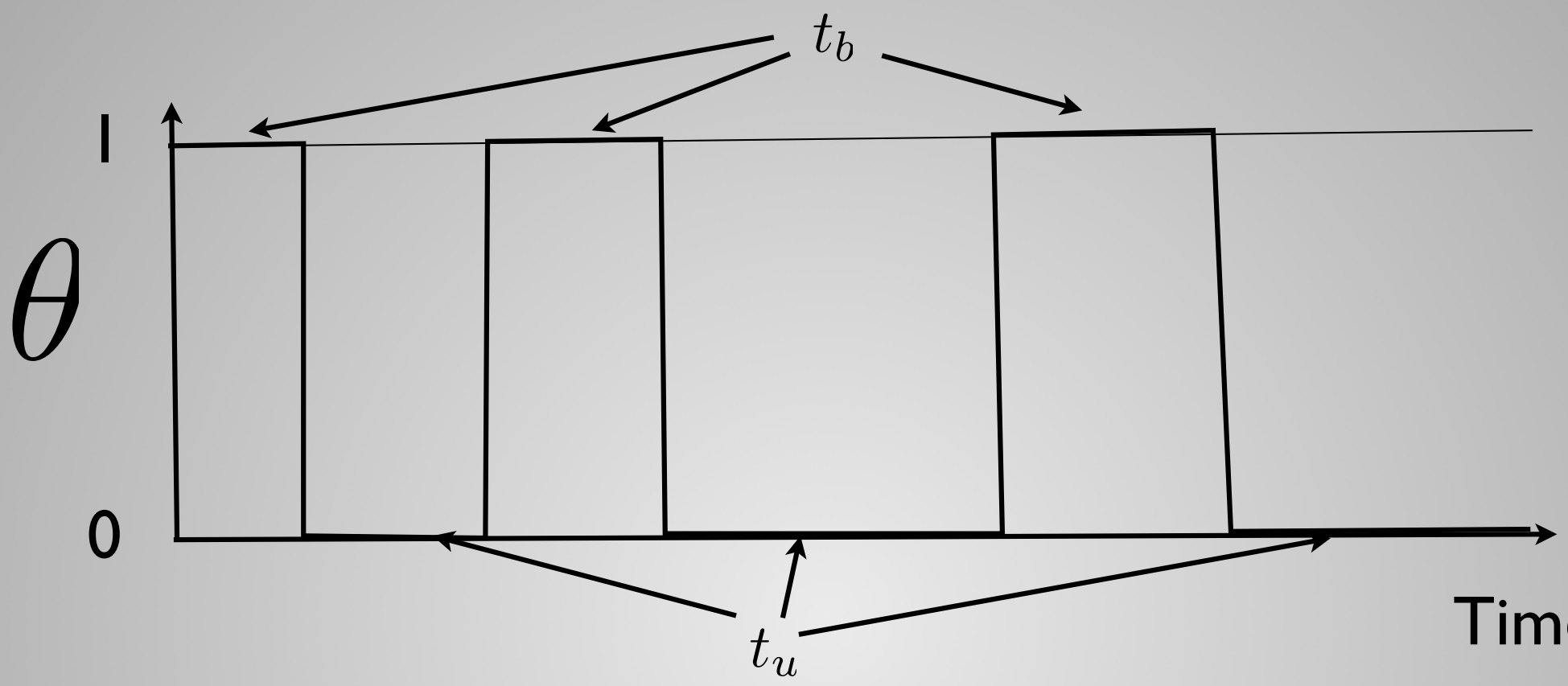
If the flame is infinitely thin, the Bray Moss Libby model (TNC p 201) can be used to compare Favre and Reynolds averaging.



Suppose that the flames are infinitely thin: the passage times are zero. The pdf of θ becomes bimodal: fresh (during a time t_u) or burnt (during a time t_b)



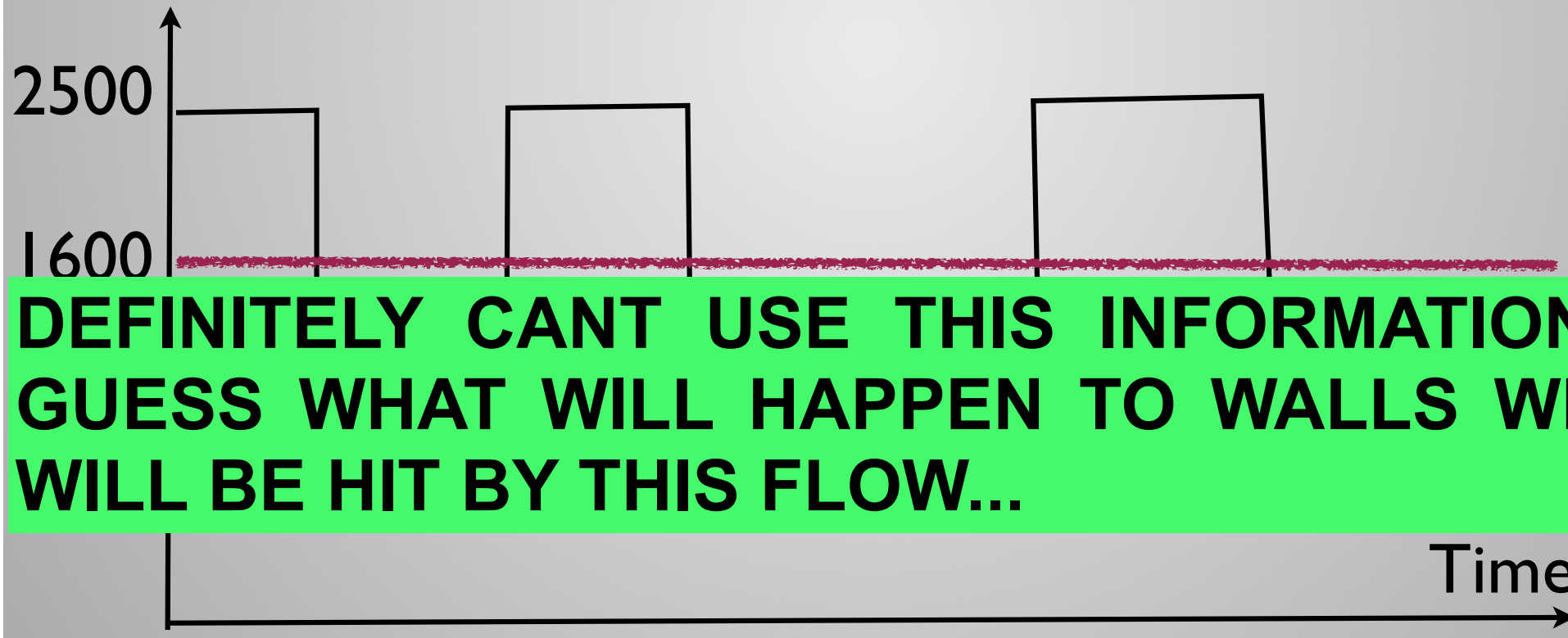
Thin flame=> flame passage times are zero



$$\overline{\theta} = \frac{t_u * 0 + t_b * 1}{t_u + t_b} = \frac{t_b}{t_u + t_b}$$

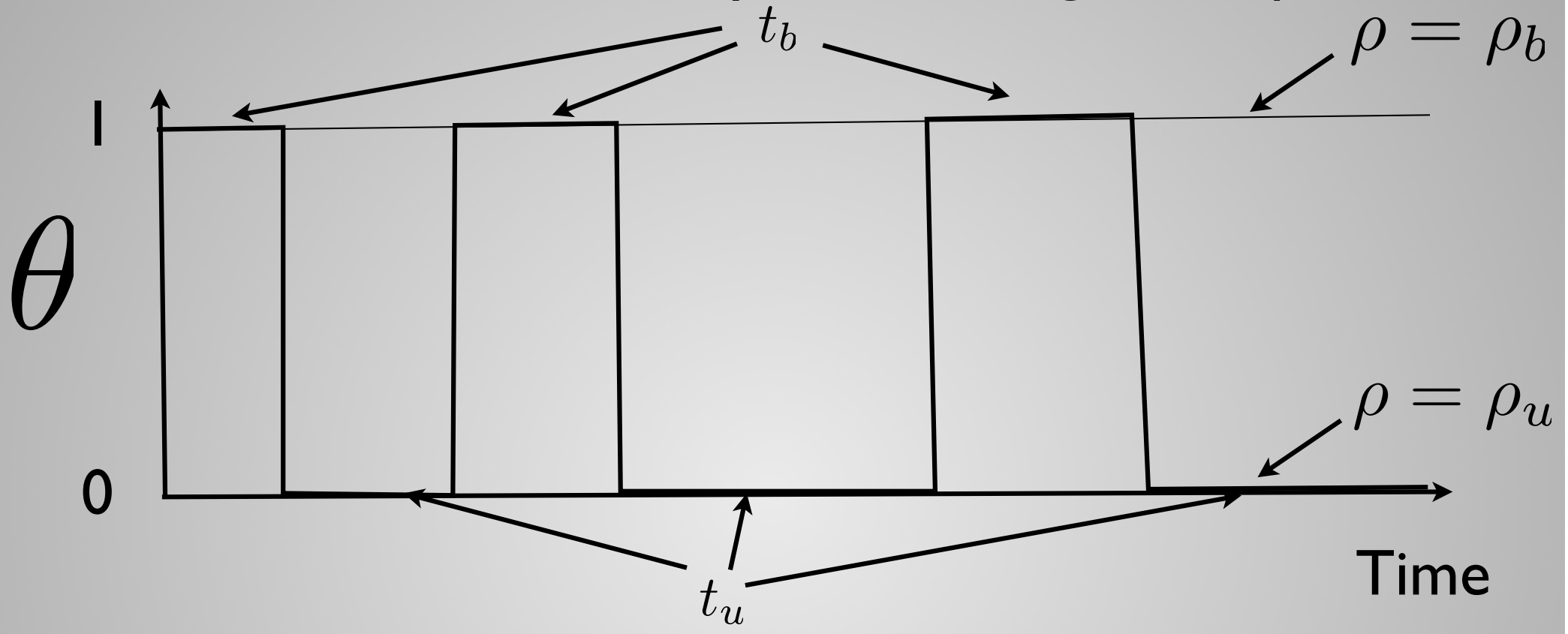
The Reynolds averaged temperature is not really a temperature. It could be called a probability to have burnt gases at one point

WHEN A RANS CODE TELLS THAT THE MEAN TEMPERATURE IS 1600 K IN A PREMIXED TURBULENT FLAME, IT ACTUALLY MEANS THAT THE PROBABILITY OF HAVING BURNT GASES AT THIS POINT IS (1600-300)/(2500-300)=59 %



DEFINITELY CANT USE THIS INFORMATION TO GUESS WHAT WILL HAPPEN TO WALLS WHICH WILL BE HIT BY THIS FLOW...

Link between Favre and Reynolds averaged temperatures:



$$\overline{\rho} = \frac{t_u * \rho_u + t_b * \rho_b}{t_u + t_b} = \rho_b \overline{\theta} + \rho_u (1 - \overline{\theta})$$

$$\overline{\rho\theta} = \frac{t_u * \rho_u * 0 + t_b * \rho_b * 1}{t_u + t_b} = \rho_b \overline{\theta}$$

$$\overline{\rho} = \frac{t_u * \rho_u + t_b * \rho_b}{t_u + t_b} = \rho_b \overline{\theta} + \rho_u (1 - \overline{\theta})$$

$$\overline{\rho\theta} = \frac{t_u * \rho_u * 0 + t_b * \rho_b * 1}{t_u + t_b} = \rho_b \overline{\theta}$$

$$\Rightarrow \quad \tilde{\theta} = \frac{\overline{\rho\theta}}{\overline{\theta}}$$

$$\boxed{\tilde{\theta} = \frac{\overline{\theta}}{\tau(1 - \overline{\theta}) + 1}}$$

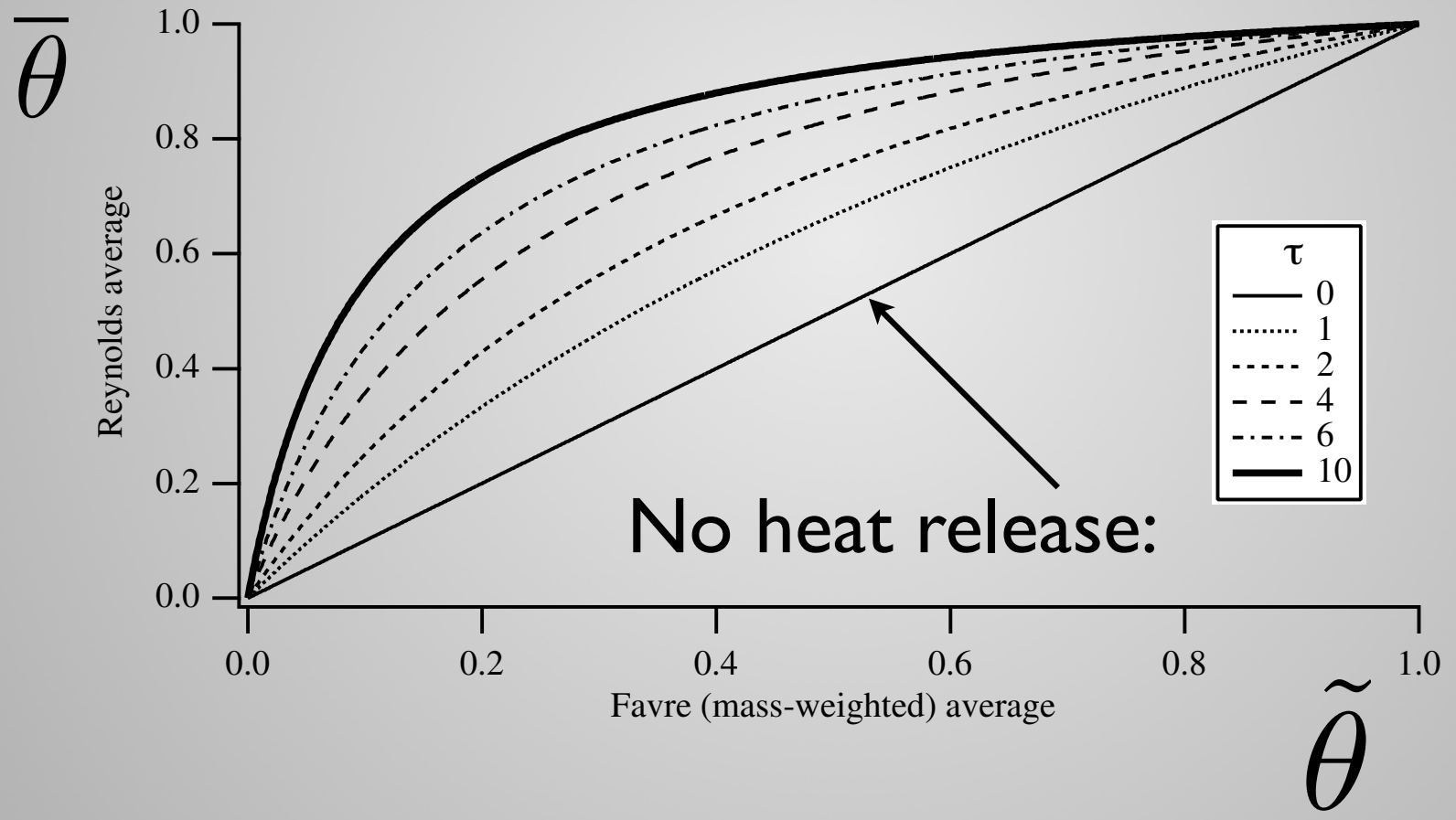
with $\quad \tau = \frac{\rho_u}{\rho_b} - 1$

or $\quad \boxed{\overline{\Theta} = \frac{(1 + \tau)\widetilde{\Theta}}{1 + \tau\widetilde{\Theta}}}$

If no heat release: $\quad \tau = 0 \quad$ and $\quad \overline{\theta} = \tilde{\theta}$

With heat release:

In a non-constant density flow, using Reynolds or Favre-average leads to huge differences in results



OUTLINE

- Phenomenology of turbulent flames
- Classical modeling approaches for turbulent flames
  - Premixed flames
  - Diffusion flames
- Requirements for most real turbulent flames and models

Averaging

- In RANS like LES, the procedure is the same.
- We want equations for averaged quantities (in space for LES, in time or in realizations for RANS)
- To build these equations, we average (in RANS) or filter (in LES) the instantaneous Navier Stokes equations.

Averaging

- If N-S equations were linear, life would be easy ! For a constant α

$$\overline{\alpha\theta} = \alpha\overline{\theta}$$

- But they are definitely not. Reaction and convection are the most non-linear terms:

$$\overline{\dot{\omega}_T(\theta)} \neq \dot{\omega}(\overline{\theta}) \qquad \overline{u\theta} \neq \overline{u}\overline{\theta}$$

- The difference between the average of products and the product of averages is what we must model:

$$\overline{u\theta} - \overline{u}\overline{\theta}$$

PROCEDURE: to have an equation for **averaged values**, we need to **average** the instantaneous conservation equations

- Take the Navier Stokes equations, use Favre averaging and express all terms as functions of the following quantities:

$$\overline{\rho} \qquad \tilde{\mathbf{u}}_\mathbf{i} \qquad \tilde{\mathbf{T}} \qquad \tilde{\mathbf{Y}}_\mathbf{k} \qquad \tilde{\mathbf{P}}$$

- In this process, non linearities will introduce unclosed terms: we will need 'closure' models

PREMIXED FLAMES

Similarly to laminar premixed flames, assume:

- Unity Lewis number
- Single step reaction limited by fuel
- Constant pressure
- Adiabatic conditions

The reduced temperature is: $\Theta = (T - T_1)/(T_2 - T_1)$

(also called *c* from time to time. Sorry about this...)

The reduced mass fraction is: $Y = Y_F/Y_F^0$

Under the previous assumptions: $\Theta + Y = 1$

Starting from the instantaneous Navier Stokes equations:

The instantaneous NS equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

$$\frac{\partial}{\partial t}\rho u_j + \frac{\partial}{\partial x_i}\rho u_i u_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i}$$

$$\frac{\partial(\rho\Theta)}{\partial t} + \frac{\partial}{\partial x_i}(\rho\Theta u_i) = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial \Theta}{\partial x_i}\right) + \dot{\omega}_\Theta$$

$\Theta = (T - T_1)/(T_2 - T_1)$ is the progress variable introduced for laminar premixed flames

And averaging: certain terms do NOT disappear and will need closure models

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i) = 0$$

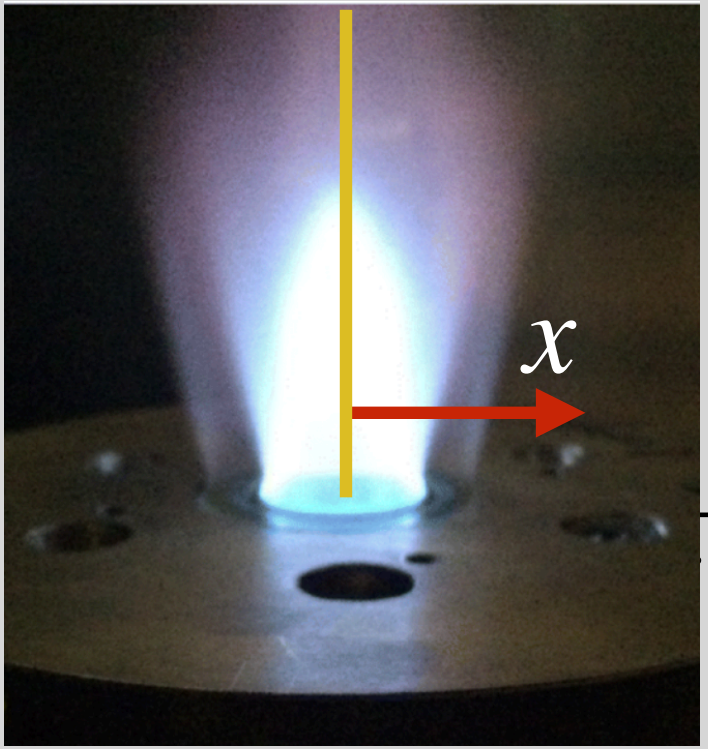
$$\frac{\partial \overline{\rho}\widetilde{u}_j}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left(\overline{\tau}_{ij} - \overline{\rho}\widetilde{u_i'' u_j''}\right)$$

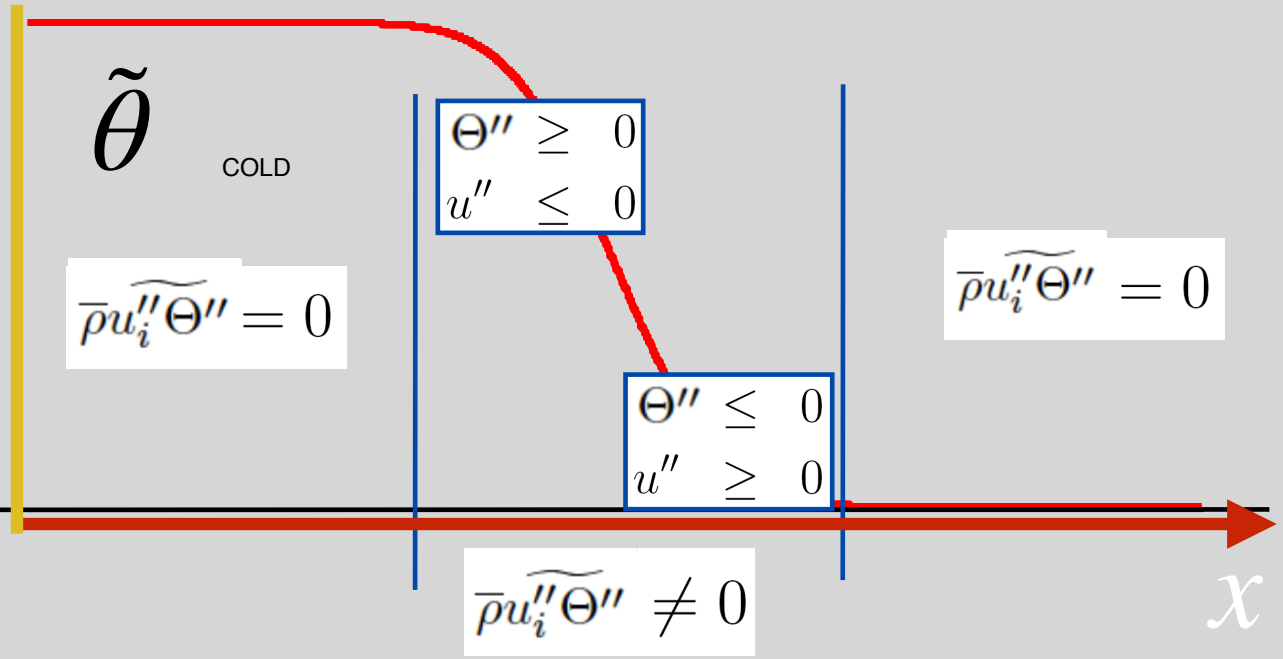
$$\frac{\partial(\overline{\rho}\widetilde{\Theta})}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{\Theta}\widetilde{u}_i) = \frac{\partial}{\partial x_i}\left(\overline{\rho}\overline{D}\frac{\partial \widetilde{\Theta}}{\partial x_i} - \overline{\rho}\widetilde{u_i''\Theta''}\right) + \overline{\dot{\omega}}_\Theta$$

Turbulent diffusion

Mean reaction rate

Turbulent transport term $\widetilde{\overline{\rho} u_i'' \Theta''}$

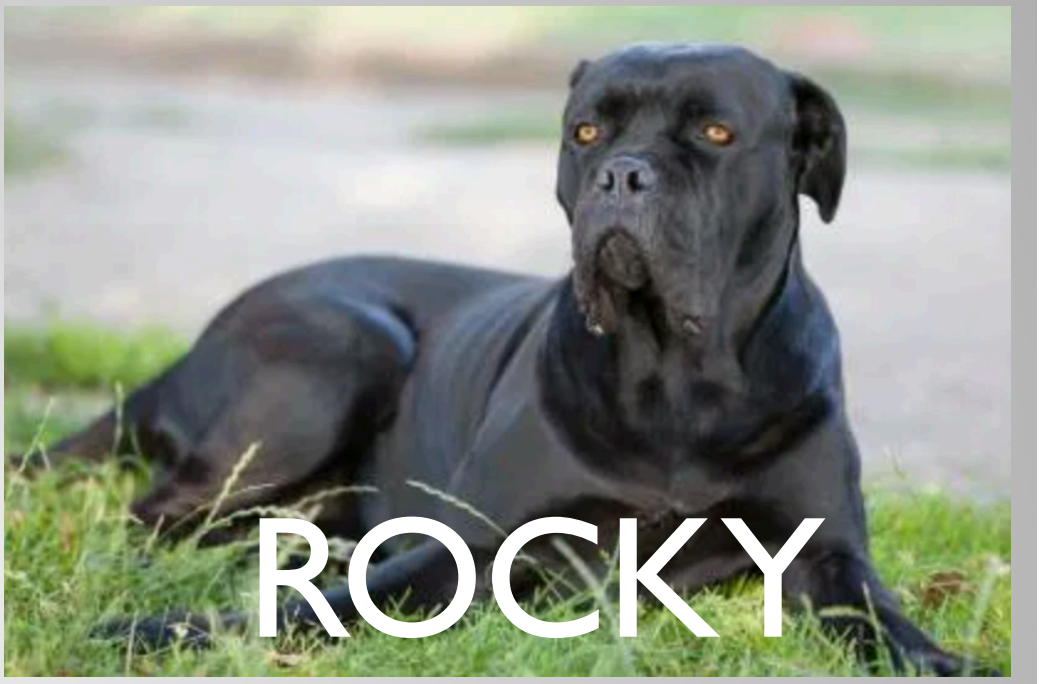




$$\overline{\rho} \widetilde{u_i'' \Theta''} = - \frac{\mu_t}{\sigma_t} \frac{d\tilde{\theta}}{dx}$$

You call this a model ?





- Medor is a black dog with four legs
- Rocky is a black dog for with four legs (too)
- SO ==> Medor = Rocky ! (or at least we believe that Medor is a good model of Rocky)

You call this a model ?

$\overline{\rho}\widetilde{u_i''\Theta''}$

- is zero in the fresh and the burnt gases
- has the dimension kg/ms^2

$-\overline{\rho}\dfrac{\nu_t}{Sc_\Theta}\dfrac{\partial\widetilde{\Theta}}{\partial x_i}$

- is zero in the fresh and the burnt gases
- has the dimension kg/ms^2

So they are equal ?

$$\overline{\rho}\widetilde{u_i''\Theta''} = -\overline{\rho}\frac{\nu_t}{Sc_\Theta}\frac{\partial\widetilde{\Theta}}{\partial x_i}$$

Turbulent diffusion:

$$\overline{\rho u_i'' \Theta''} = \overline{\rho} \widetilde{u_i'' \Theta''}$$

Usual gradient model: $$\overline{\rho} \widetilde{u_i'' \Theta''} = -\overline{\rho} \frac{\nu_t}{Sc_\Theta} \frac{\partial \widetilde{\Theta}}{\partial x_i}$$

Why it is convenient: because the turbulent viscosity is simply added to the laminar viscosity. The temperature equation becomes:

$$\frac{\partial(\overline{\rho}\widetilde{\Theta})}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{\Theta}) = \frac{\partial}{\partial x_i}\left(\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_\Theta}\right)\frac{\partial \widetilde{\Theta}}{\partial x_i}\right) + \overline{\dot{\omega}}_\Theta$$



Only need to add this term

Different levels of precision:

$$\frac{\partial(\overline{\rho}\widetilde{\Theta})}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{\Theta}) = \frac{\partial}{\partial x_i}\left(\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_\Theta}\right)\frac{\partial\widetilde{\Theta}}{\partial x_i}\right) + \overline{\dot{\omega}}_\Theta$$

Laminar diffusion term D: comes from kinetic theory of gases.
-> VERY precise

Turbulent diffusion term ν_t : comes from simplistic arguments.
-> VERY unprecise
-> BUT VERY large !
ν_t/D can vary between 10 and 1000

Why it is not a nice idea: the turbulent diffusion term was a LHS term initially: it was **non linear and CREATING turbulence**: $\rho \mathbf{u_i} \Theta$

We have first linearized it by splitting variables into mean and fluctuating parts: $\overline{\rho} \widetilde{\mathbf{u_i''} \Theta''}$

Then we moved it to the RHS of the averaged equation:

$$\frac{\partial(\overline{\rho}\widetilde{\Theta})}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{\Theta}\widetilde{u}_i) = \frac{\partial}{\partial x_i}\left(\overline{\rho}\overline{D}\frac{\partial \widetilde{\Theta}}{\partial x_i} - \overline{\rho}\widetilde{u_i''\Theta''}\right) + \overline{\dot{\omega}}_\Theta$$

And we have transformed it into a **viscous term which damps turbulence**:

$$\overline{\rho}\widetilde{\mathbf{u_i''}\Theta''} = -\overline{\rho}\frac{\nu_\mathbf{t}}{\mathbf{Sc_\Theta}}\frac{\partial \widetilde{\mathbf{\Theta}}}{\partial \mathbf{x_i}}$$

Conclusion on turbulent diffusion models

- The classical gradient model: $\widetilde{u''\theta''} = -\frac{\nu_t}{Sc_\theta}\nabla\tilde{\theta}$

- is used everywhere today.

But there are good reasons to believe that it is wrong at low turbulence intensity.
On the other hand who would want to have a negative diffusivity in his code ?

Averaging the instantaneous reaction rate:

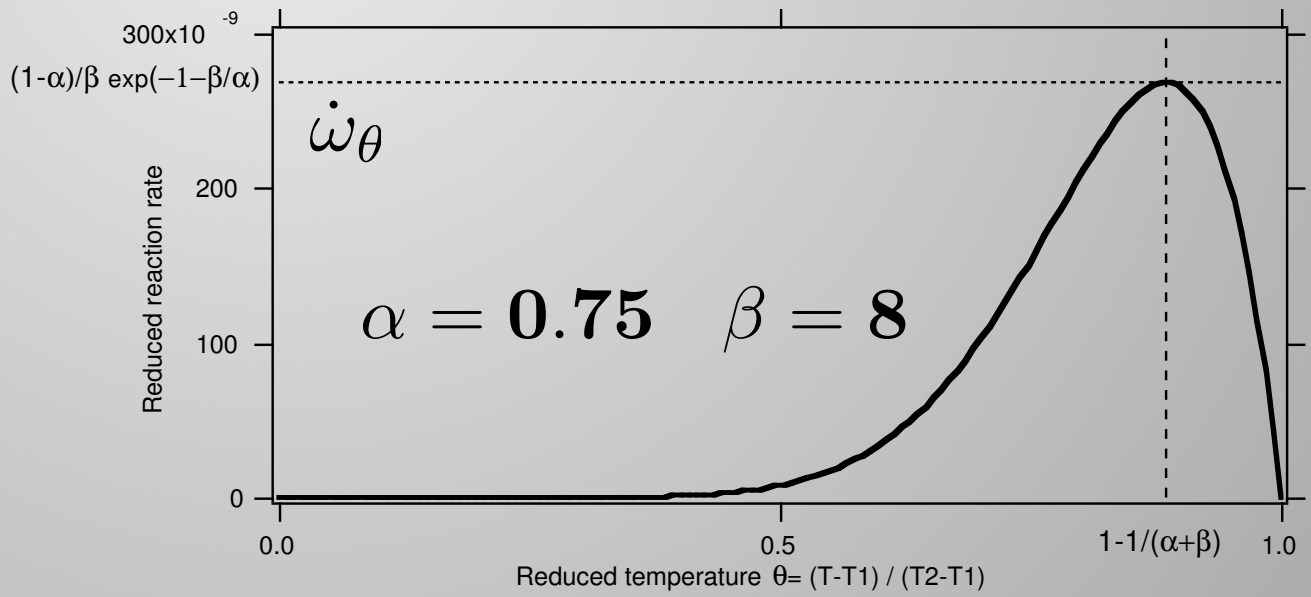
$$\dot{\omega}_\theta = \mathbf{B_1 e^{-\beta/\alpha}} \rho(1-\Theta)\exp\left(-\frac{\beta(1-\Theta)}{1-\alpha(1-\Theta)}\right)$$

With:

$$\alpha = (\mathbf{T_2 - T_1})/\mathbf{T_2} = \mathbf{Q Y_F^1}/(\mathbf{C_p T_2}) \longleftarrow \text{O(1)}$$

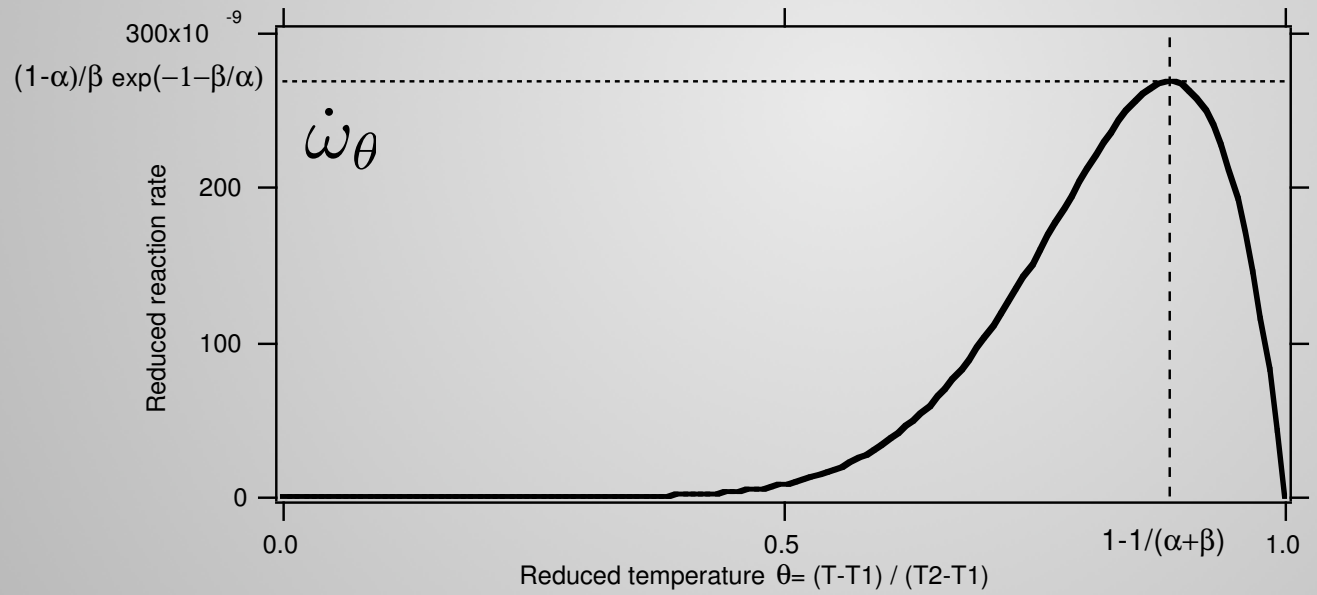
$$\beta = \alpha \mathbf{T_{a1}}/\mathbf{T_2}$$

O(10)



How do we model the average reaction rate?:

$$\dot{\omega}_\theta = \mathbf{B_1} \mathbf{e}^{-\beta/\alpha} \rho (1 - \mathbf{\Theta}) \exp\left(- \frac{\beta (1 - \mathbf{\Theta})}{1 - \alpha (1 - \mathbf{\Theta})} \right)$$



Non linear: ---> trouble ahead

Models for the mean reaction rate:

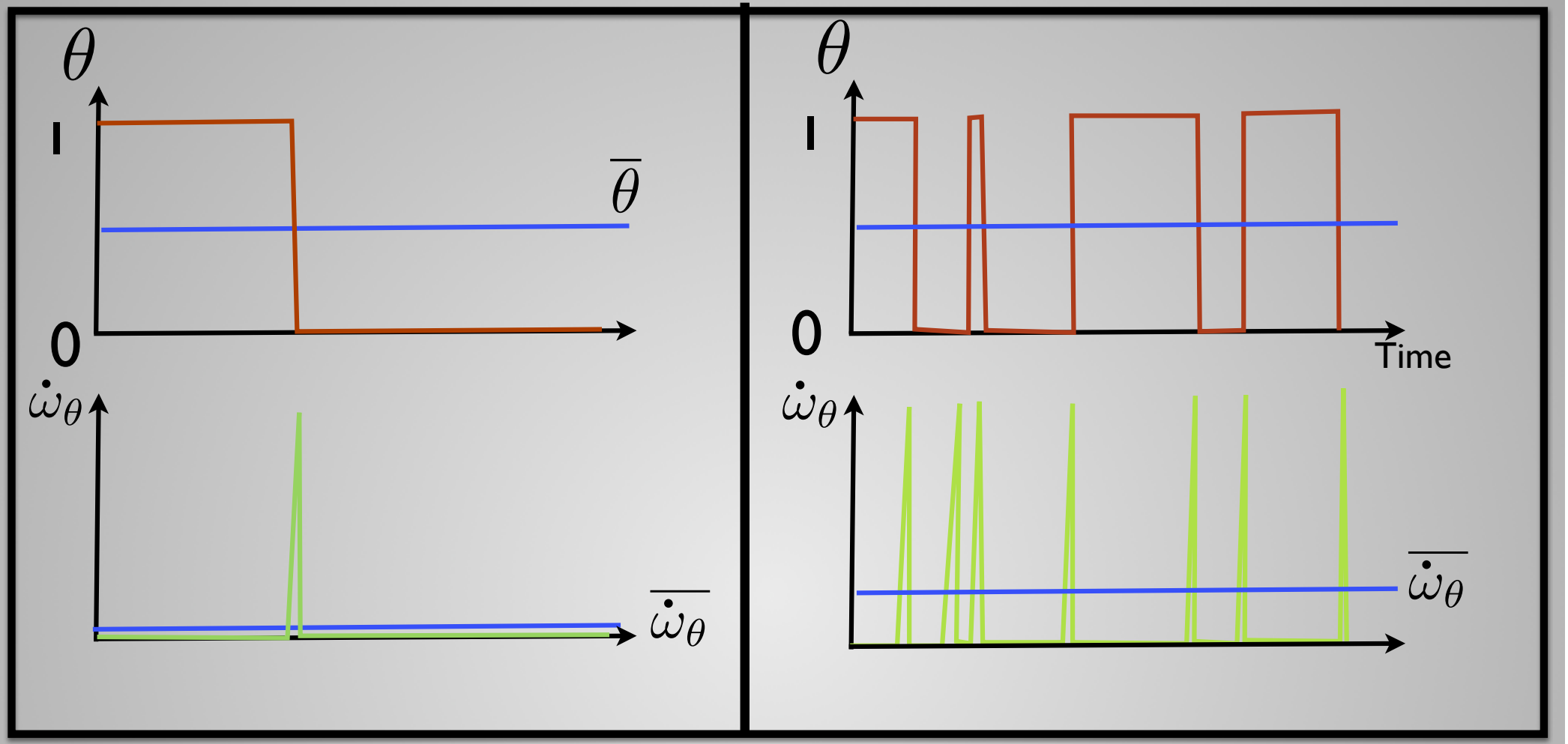
1. The models which never work: (a) zeroth order and (b) Taylor expansion
2. The EBU model
3. Pdfs models
4. Flame surface models and G equation
5. Thickened flame models
6. Deep learning models

(I) The model which never works: (a) zeroth order

Simply replacing instantaneous values by mean values everywhere does not work:

$$\overline{\dot{\omega}}_\Theta = \dot{\omega}_\Theta(\widetilde{\Theta}) = -B\overline{\rho}(1-\widetilde{\Theta})\exp\left(-\frac{T_a}{T_1+(T_2-T_1)\widetilde{\Theta}}\right)$$

This is what codes using finite rate chemistry and no model for flame / turbulence interaction do



These two temperature signals have the same mean temperature but different mean reaction rates

$\overline{\dot{\omega}_\theta}$ is never equal to $\dot{\omega}_\theta(\tilde{\theta})$

(b) Taylor expansion

$$\overline{\dot{\omega}_F} = \overline{-A_1 \rho^2 T^{\beta_1} Y_F Y_O \exp\left(-\frac{T_A}{T}\right)}$$

$$\exp\left(-\frac{T_A}{T}\right) = \exp\left(-\frac{T_A}{\widetilde{T}}\right)\left(1 + \sum_{n=1}^{+\infty} P_n \frac{T''^n}{\widetilde{T}^n}\right) \quad ; \quad T^{b-1} = \widetilde{T}^{b-1}\left(1 + \sum_{n=1}^{+\infty} Q_n \frac{T''^n}{\widetilde{T}^n}\right)$$

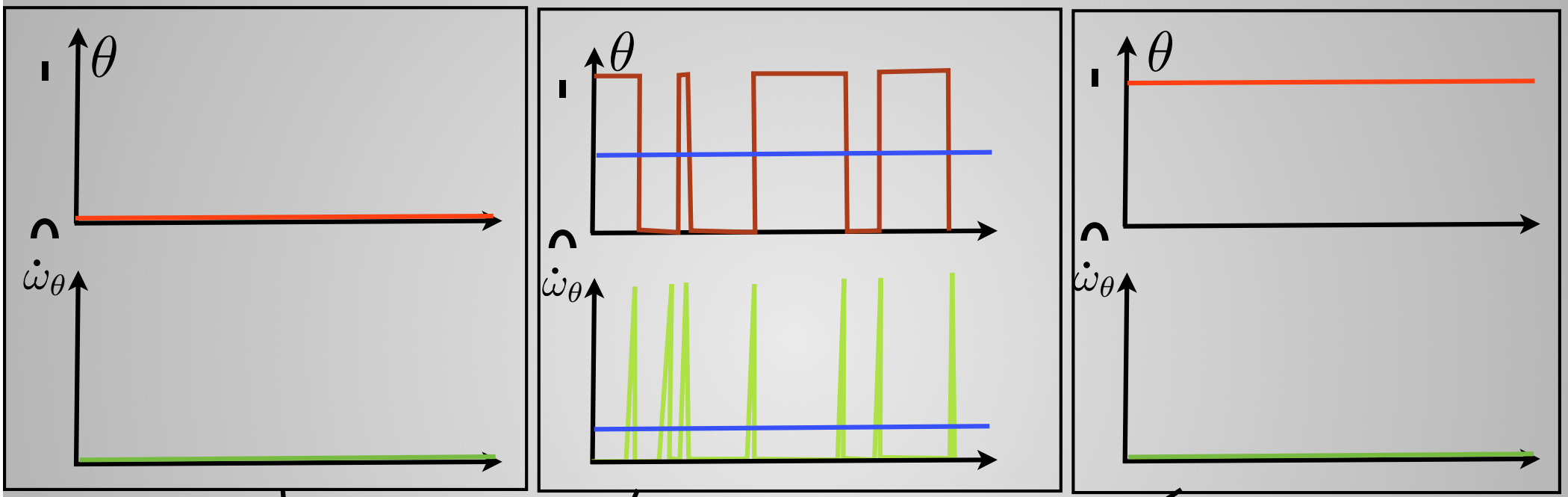
$$P_n = \sum_{k=1}^{n} (-1)^{n-k} \frac{(n-1)!}{(n-k)!\left[(k-1)!\right]^2 k}\left(\frac{T_A}{\widetilde{T}}\right)^k \quad ; \quad Q_n = \frac{(b-1)(b-2)...(b-n)}{n!}$$

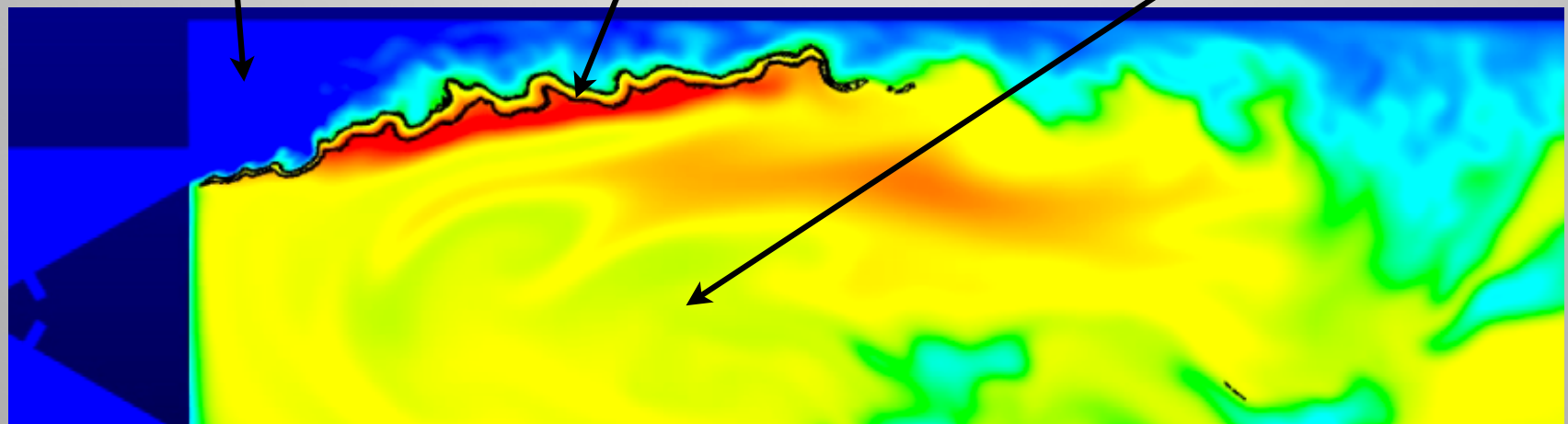
This is the 'no model' contribution

$$\overline{\dot{\omega}_F} = -A_1 \overline{\rho}^2 \widetilde{T}^{\beta_1} \widetilde{Y}_F \widetilde{Y}_O \exp\left(-\frac{T_A}{\widetilde{T}}\right)\left[1 + \frac{\widetilde{Y''_F Y''_O}}{\widetilde{Y}_F \widetilde{Y}_O} + (P_1 + Q_1)\left(\frac{\widetilde{Y''_F T''}}{\widetilde{Y}_F \widetilde{T}} + \frac{\widetilde{Y''_O T''}}{\widetilde{Y}_O \widetilde{T}}\right)\right.$$
$$\left. + (P_2 + Q_2 + P_1 Q_1)\left(\frac{\widetilde{T''^2}}{\widetilde{T}^2} + \frac{\widetilde{Y''_F T''^2}}{\widetilde{Y}_F \widetilde{T}^2} + \frac{\widetilde{Y''_O T''^2}}{\widetilde{Y}_O \widetilde{T}^2}\right) + \ldots\right]$$

(2) The EBU model

Ch. 5 - Sect. 5.3.3





The EBU model

« Physically » based (Spalding 70s):

- Chemistry has no role (!)
- The important thing is '**how many times a flamelet crosses a given location**': this is proportional to the variance of the temperature and inversely proportional to a 'turbulent flame' time:

$$\overline{\dot{\omega}}_{\Theta} = C_{EBU}\,\overline{\rho}\,\frac{\sqrt{\widetilde{\Theta''^2}}}{\tau_{EBU}}$$

The EBU model

The flame time is usually supposed to be equal to the large structure time:

$$\tau_{EBU} = k/\varepsilon$$

so that:

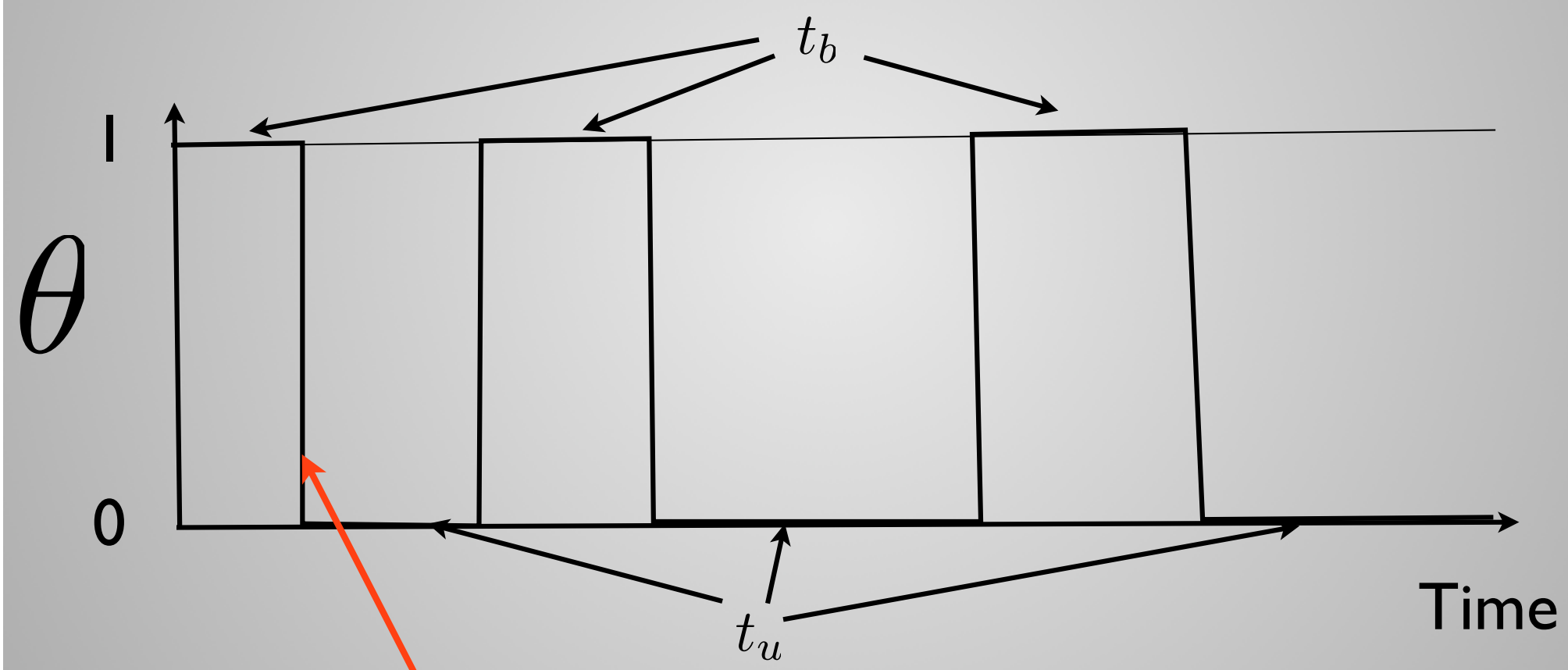
$$\overline{\dot{\omega}}_{\Theta} = C_{EBU}\,\overline{\rho}\,\frac{\sqrt{\widetilde{\Theta''^2}}}{\tau_{EBU}}$$

We still do not know the temperature variance $\widetilde{\theta''^2}$

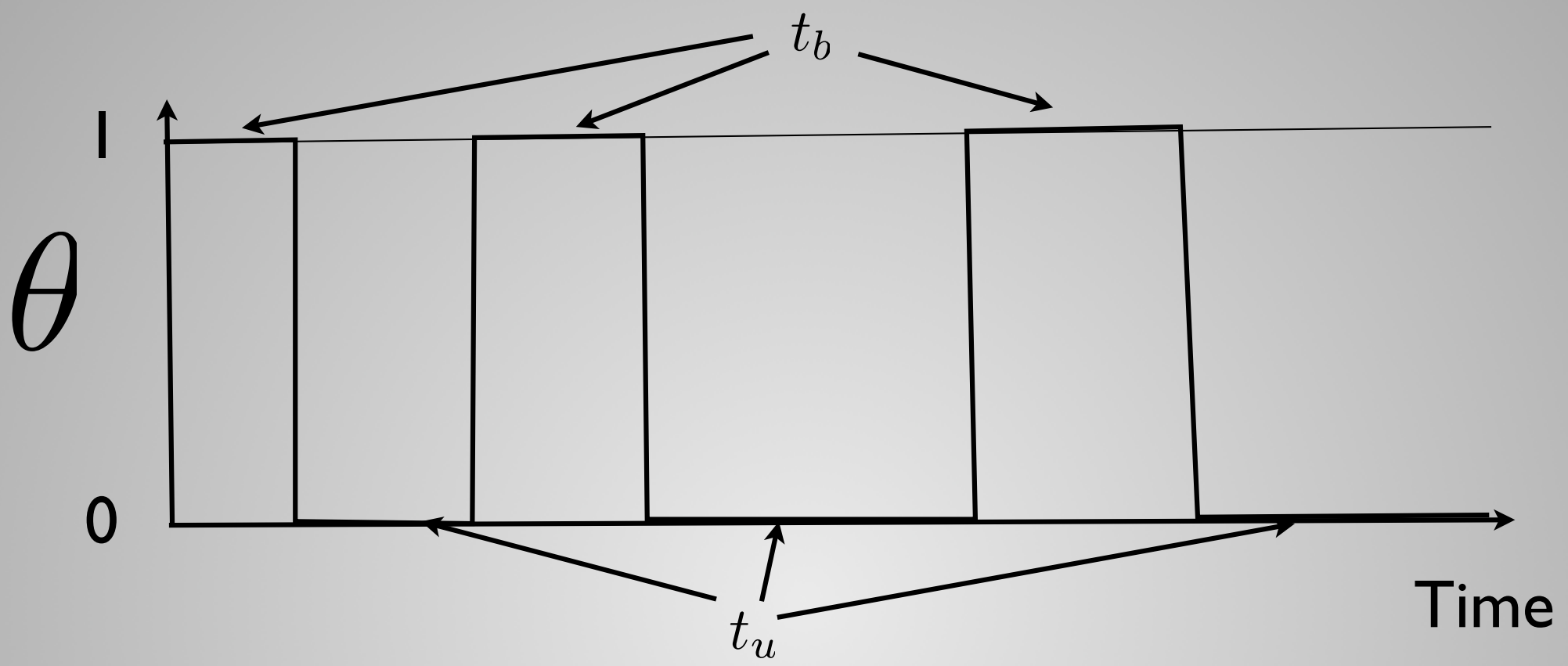
But if the flame is infinitely thin, BML again gives a simple evaluation of the variance $\widetilde{\theta''^2}$:

$$\overline{\rho}\widetilde{\Theta''^2} = \overline{\rho\left(\Theta - \widetilde{\Theta}\right)^2} = \overline{\rho}\left(\widetilde{\Theta^2} - \widetilde{\Theta}^2\right) = \overline{\rho}\,\widetilde{\Theta}\left(1 - \widetilde{\Theta}\right)$$

If the pdf of theta becomes bimodal: fresh (during a time t_u) or burnt (during a time t_b)

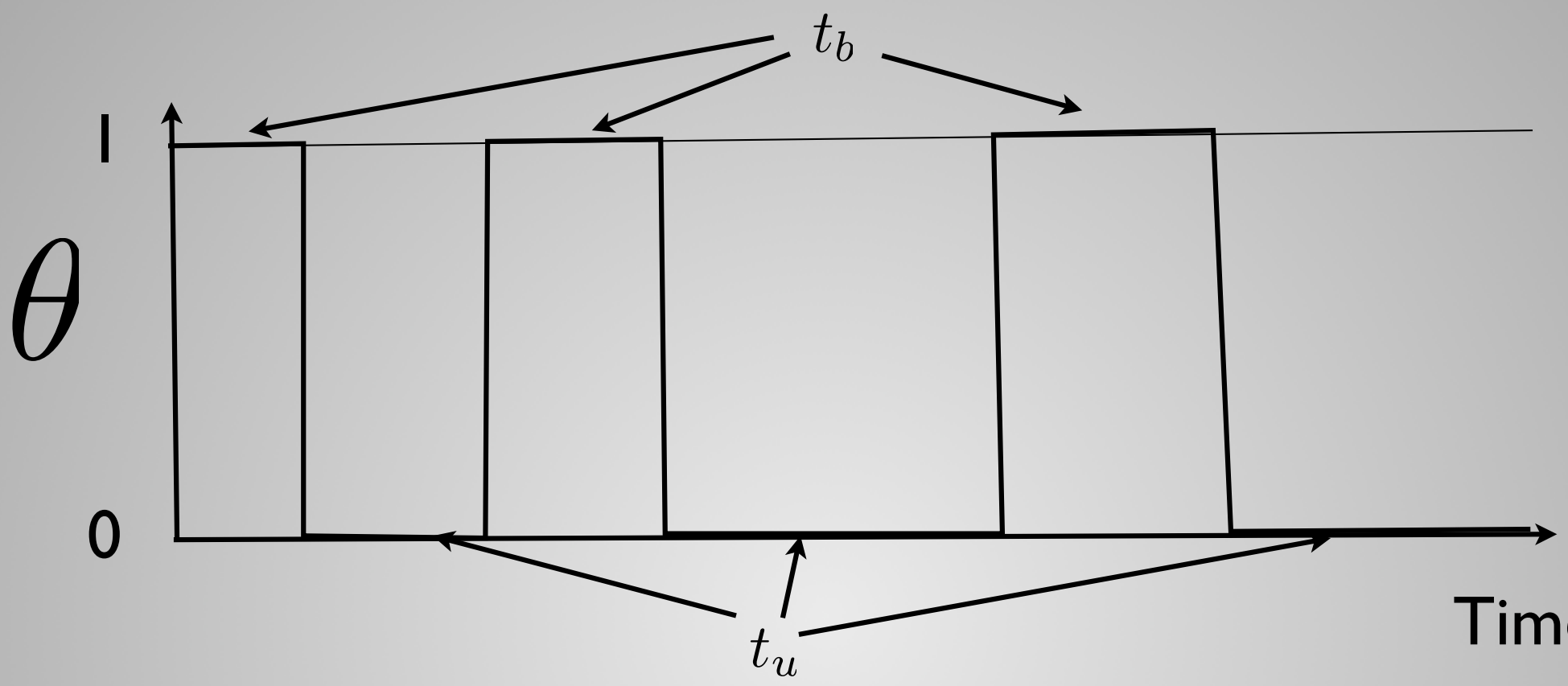


Thin flame=> flame passage times are zero



Neglect influence of density: Favre and Reynolds averages are the same

$$\overline{\theta} = \tilde{\theta} = \frac{t_u * 0 + t_b * 1}{t_u + t_b} = \frac{t_b}{t_u + t_b}$$



Compute the variance:

$$\widetilde{\theta''^2} = \frac{1}{T}\int_0^T (\theta - \tilde{\theta})^2 dt = \frac{1}{t_u + t_b}(t_u(0-\tilde{\theta})^2 + t_b(1-\tilde{\theta})^2)$$

Since $\tilde{\theta} = \dfrac{t_b}{t_u + t_b}$

$$\widetilde{\theta''^2} = (1-\widetilde{\theta})\tilde{\theta}^2 + \widetilde{\theta}(1-\tilde{\theta})^2 = \widetilde{\theta}(1-\tilde{\theta})$$

The final EBU model:

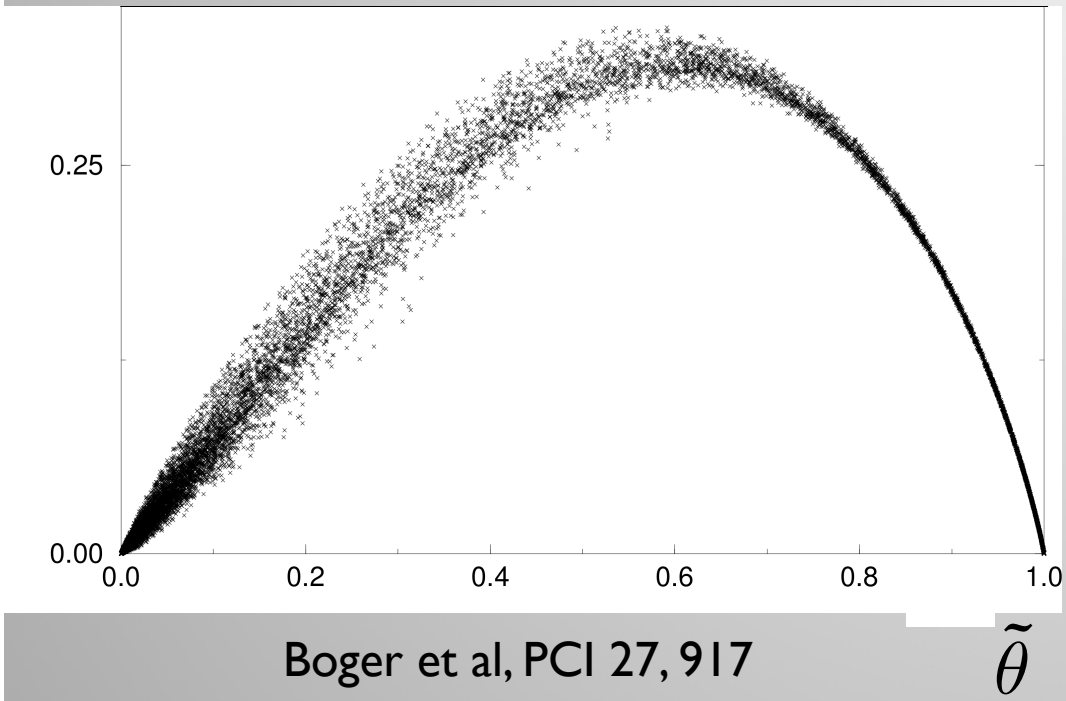
$$\overline{\dot{\omega}}_{\Theta} = C_{EBU}\,\overline{\rho}\,\frac{\varepsilon}{k}\widetilde{\Theta}\left(1-\widetilde{\Theta}\right)$$

The mean reaction rate varies like a parabolic function of the mean temperature (for a laminar flame, remember that the reaction rate was an exponential function of temperature)

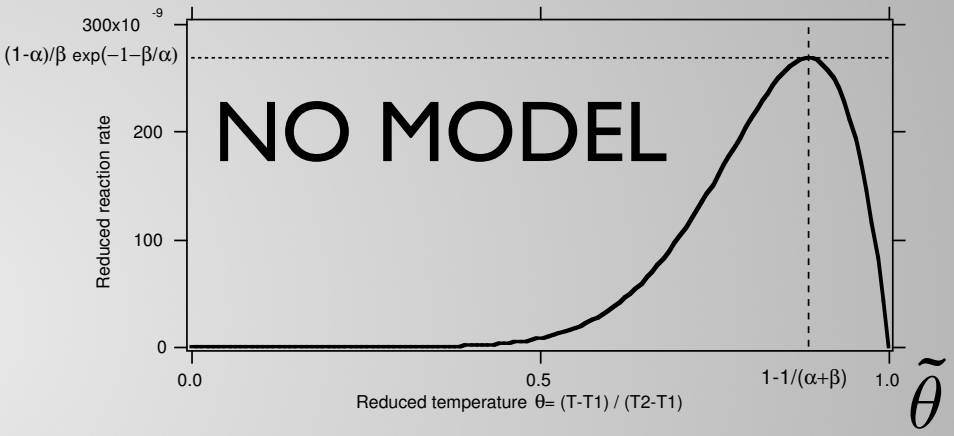
Experiments, no model and EBU model:

$\overline{\dot{\omega}_\theta}$

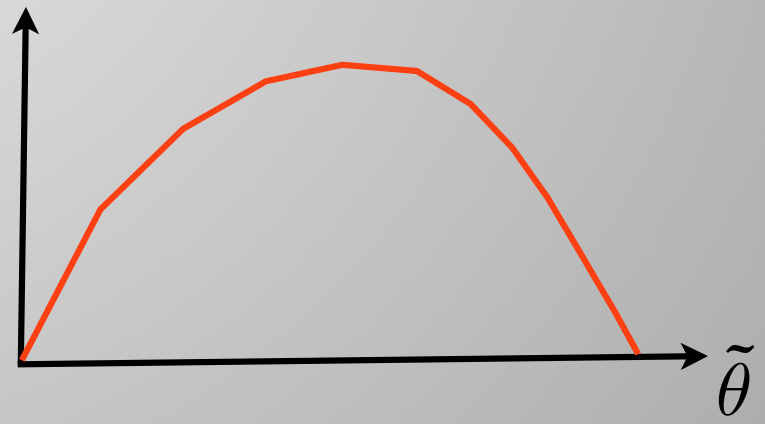
EXPERIMENTS



Boger et al, PCI 27, 917



EBU MODEL



EBU is good... ?

$$\overline{\dot{\omega}}_{\Theta} = C_{EBU}\,\overline{\rho}\,\frac{\varepsilon}{k}\widetilde{\Theta}\left(1-\widetilde{\Theta}\right)$$

$$C_{EBU}(\alpha, \beta, T_a, B_1, \ldots)$$

Wait a second. The laminar reaction rate was:

$$\dot{\omega}_{\theta} = \mathbf{B_1 e}^{-\beta/\alpha}\rho(1-\mathbf{\Theta})\exp\left(-\frac{\beta(1-\mathbf{\Theta})}{1-\alpha(1-\mathbf{\Theta})}\right)$$

But where did chemistry go in the EBU model ?? where is the preexponential constant B_1 ? the

ONCE MORE WE SEE THAT IN THE TURBULENT COMBUSTION WORLD, MANY PHENOMENA GET HIDDEN IN MODEL CONSTANTS

(3) The ultimate model: pdfs

Ch. 5 - Sect. 5.3.7

- WHAT IS A PDF (Probability Density Function) ?
- Mathematical definition:

$$\mathbf{p}(\Theta^*)\,\mathbf{d}\Theta^* = \mathbf{Probability}\,(\Theta^* \leq \Theta < \Theta^* + \mathbf{d}\Theta^*)$$

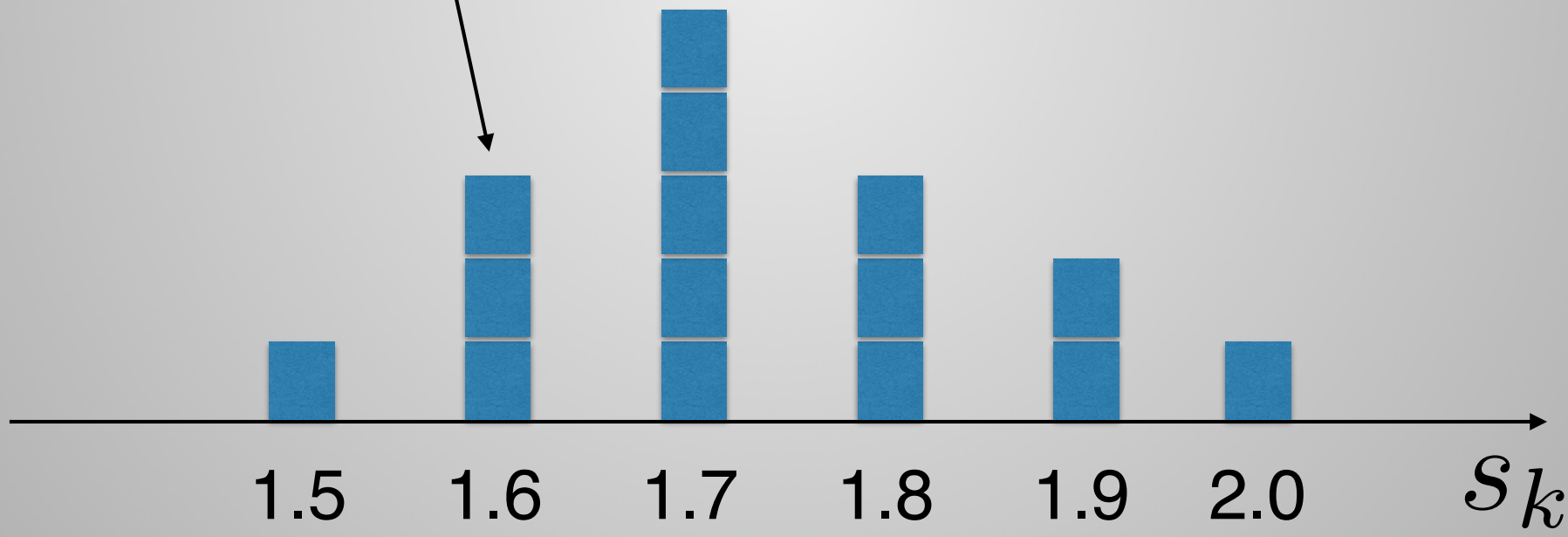
- Simpler definition: this is an histogram. Let us try to build the pdf of size of people in this room.

Histogram of size s

N = total nbr of people = $\Sigma_k N_k$

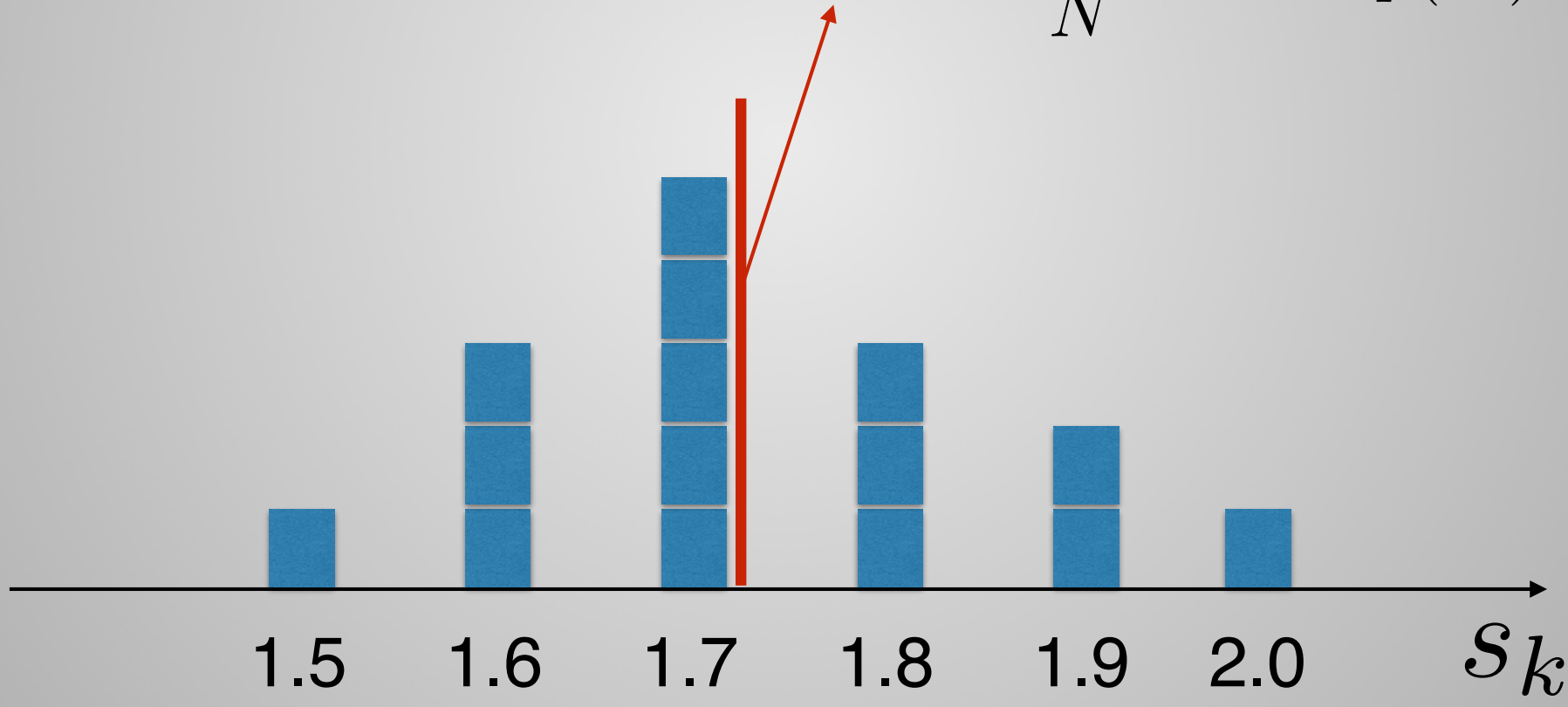
N_k = nbr of people with size s_k

$p(s_k) = N_k/N$



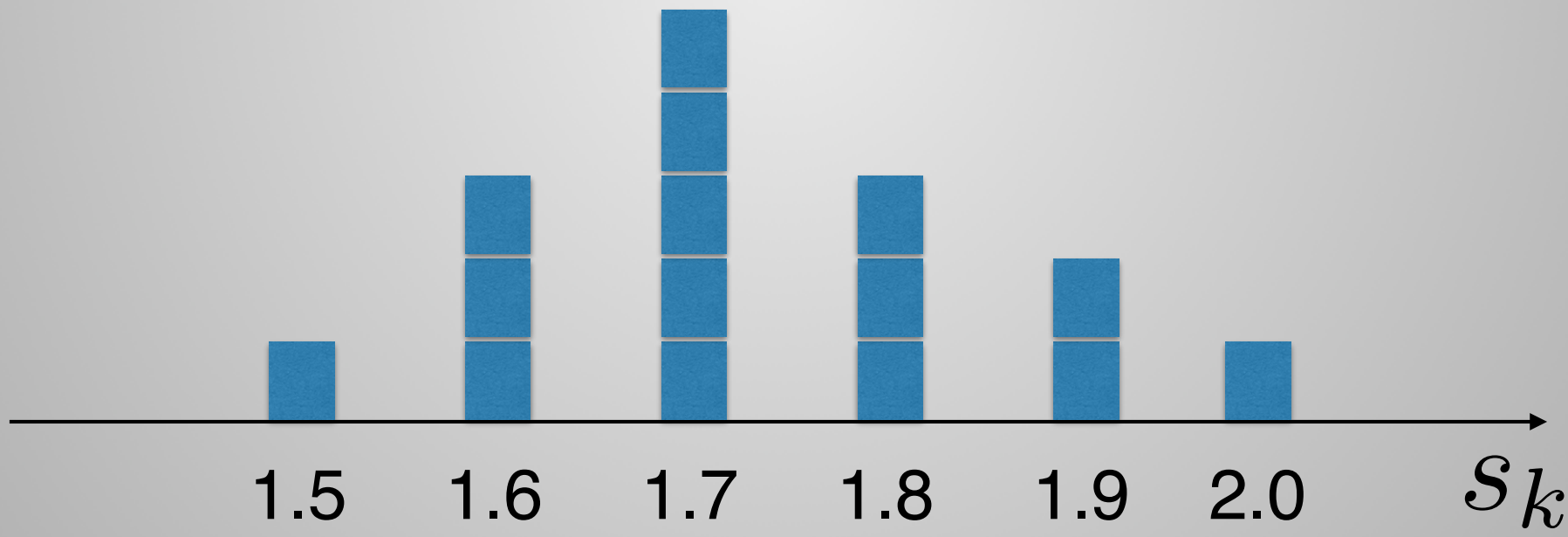
If I know p (the pdf), I can compute all means:

The mean value of s: $\bar{s} = \Sigma_k \frac{N_k}{N} s_k = \Sigma_k p(s_k) s_k$



And the mean value of any function of s:

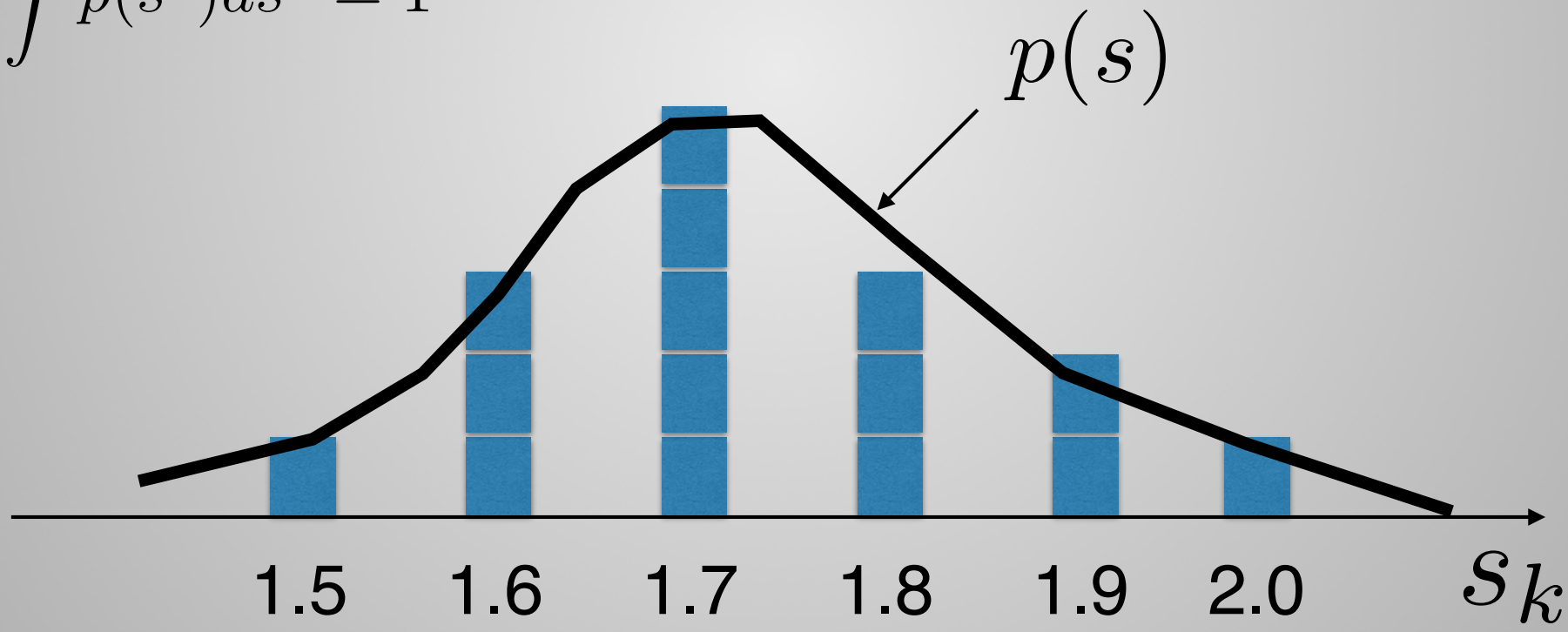
$$\bar{f}(s) = \Sigma_k \frac{N_k}{N} f(s_k) = \Sigma_k p(s_k) f(s_k)$$



In the continuous world: we replace the discrete p by its continuous pdf:

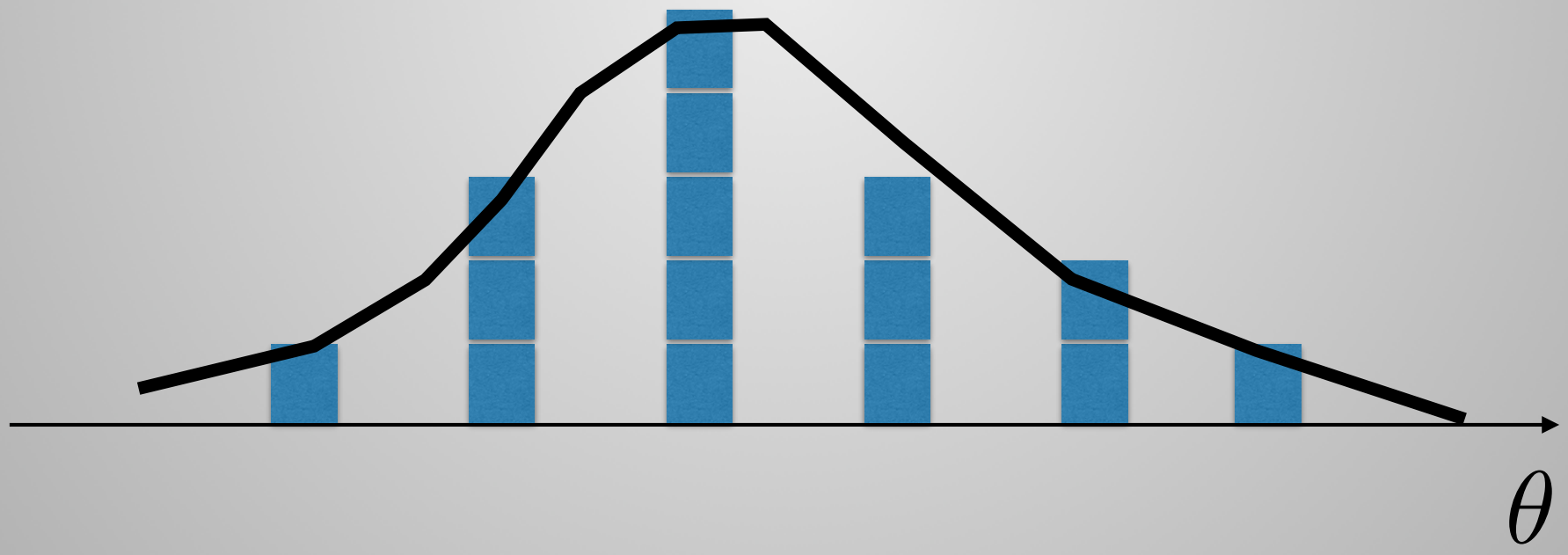
$$p(s^*)ds^* = \text{prob}(s^* < s < s^* + ds^*)$$

$$\int p(s^*)ds^* = 1$$



Suppose we have the pdf of temperature, the mean reaction rate will be:

$$\bar{\dot{\omega}} = \int p(\theta)\dot{\omega}(\theta)d\theta$$

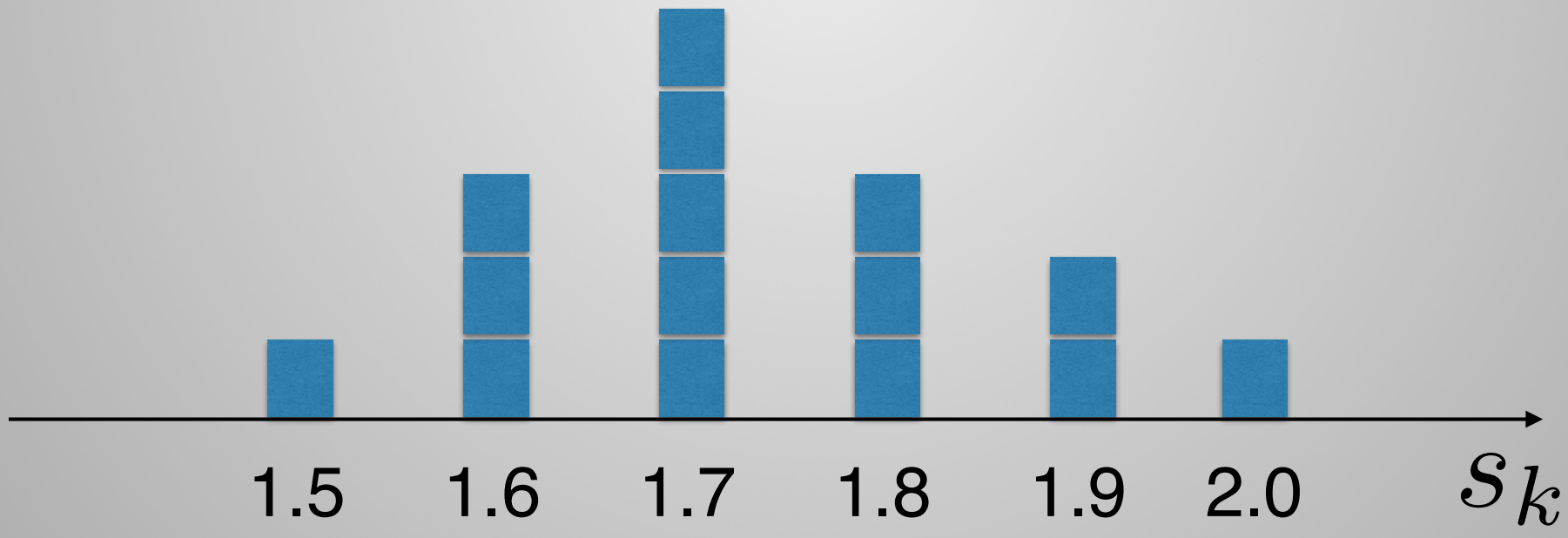


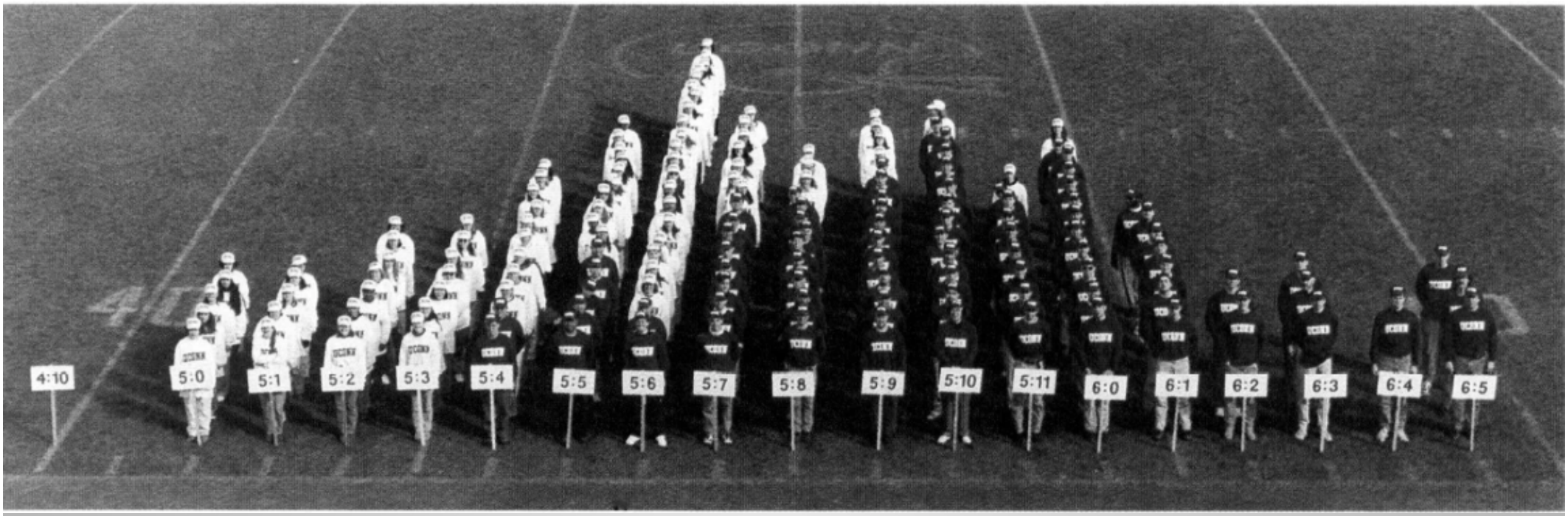
So… if we know the pdf of temperature we have everything to close the equations of combustion for averaged temperature

But how do we find the pdf ?

Pdfs are difficult to find

- Let us go back to the pdf of the sizes of people in this course
- How does it look like ? Can you guess its shape?





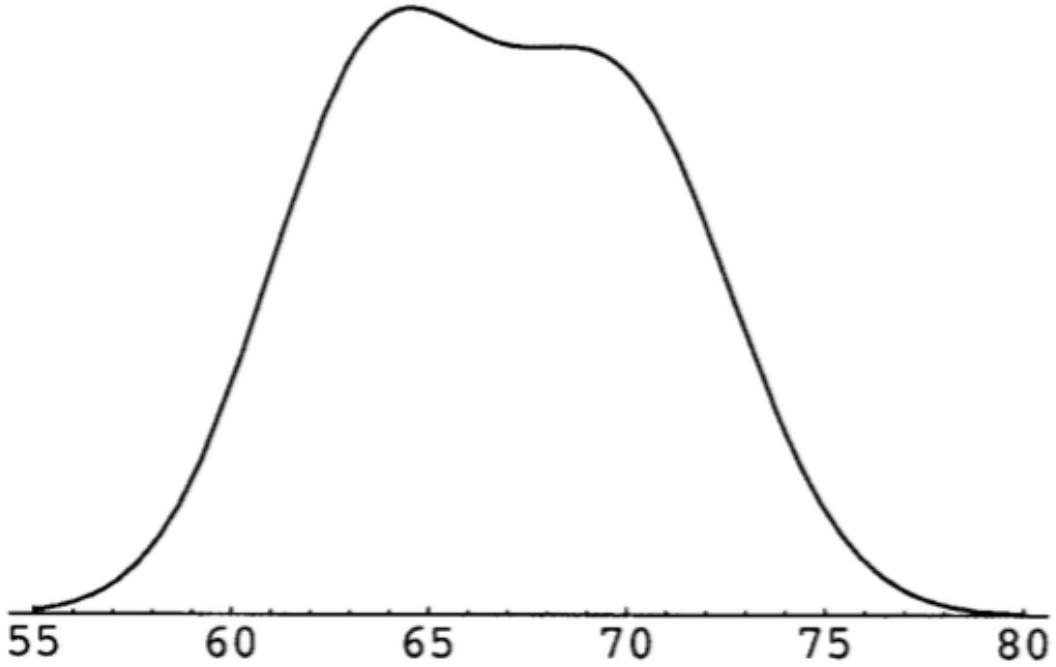
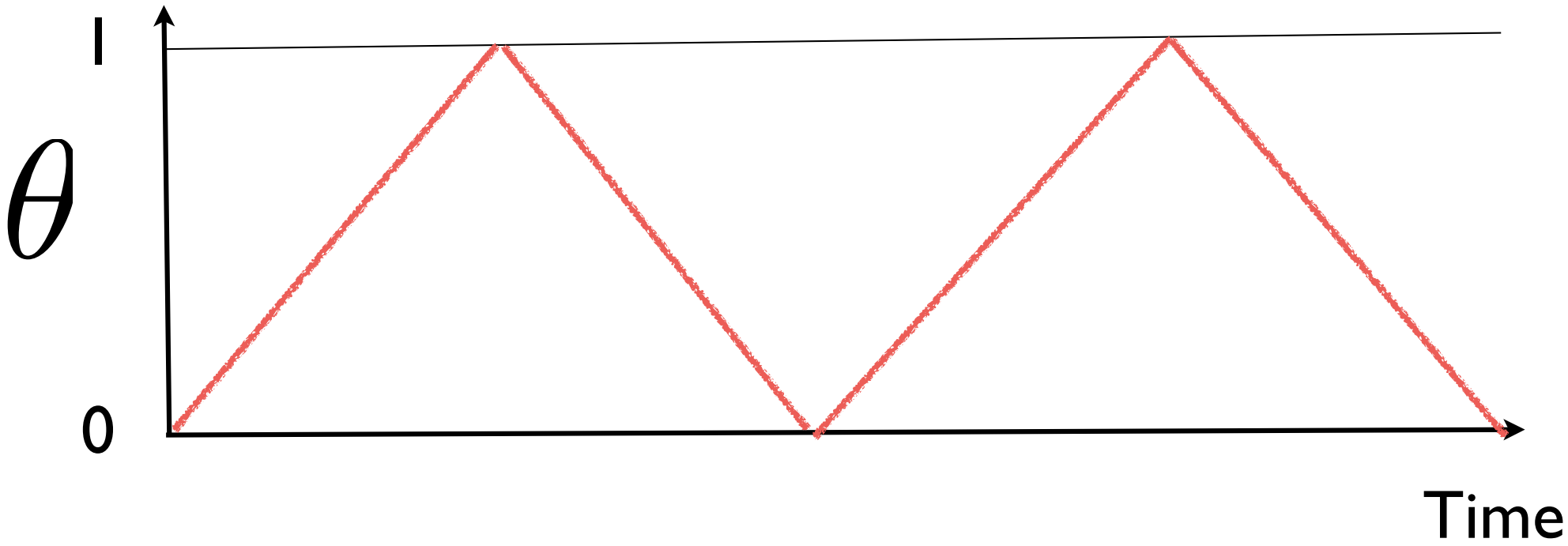


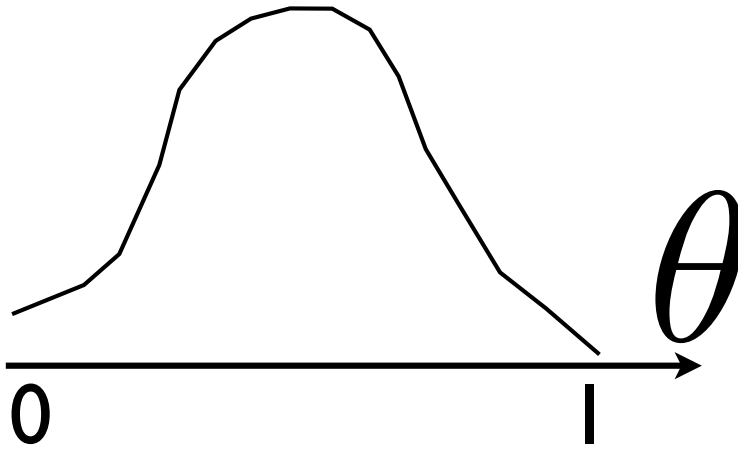
Figure 11. Theoretical distribution of U.S. young adult human height, if males round up to the next inch and females round down.

Small tests: how good are you at guessing pdfs…

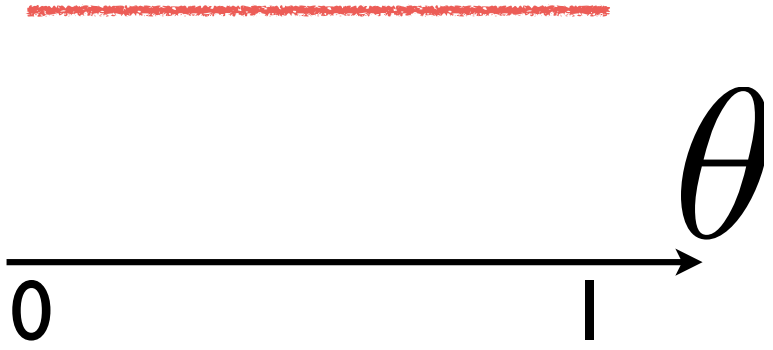


Answers:

1/ A Gaussian shape:

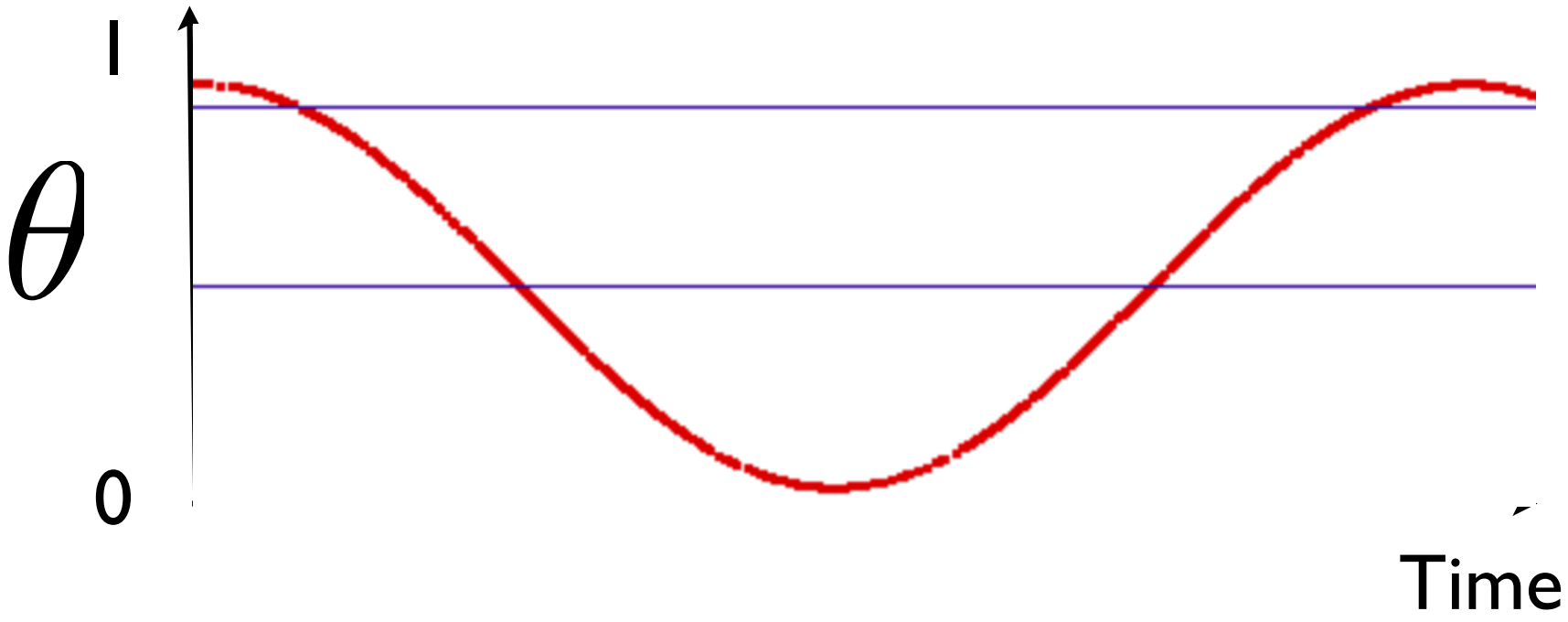


2/ A flat function:



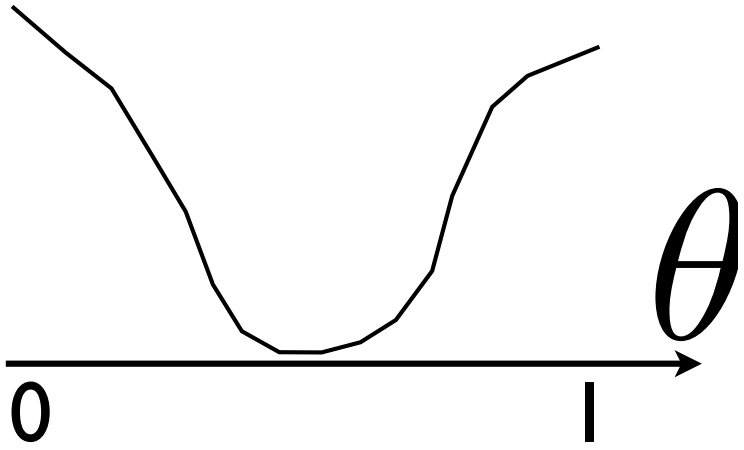
3/ Other

Small tests: how good are you at guessing pdfs…

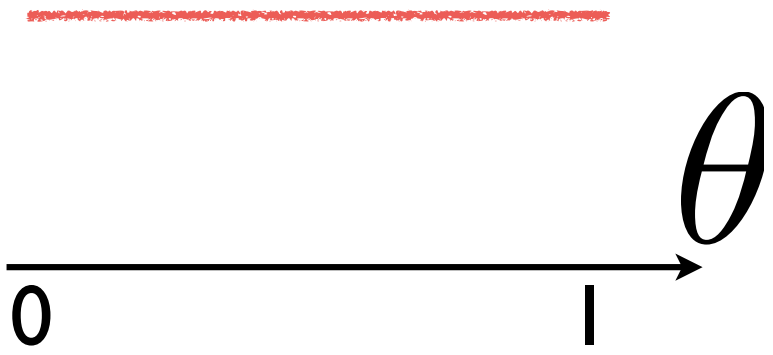


Answers:

1/ A inverted bell shape:

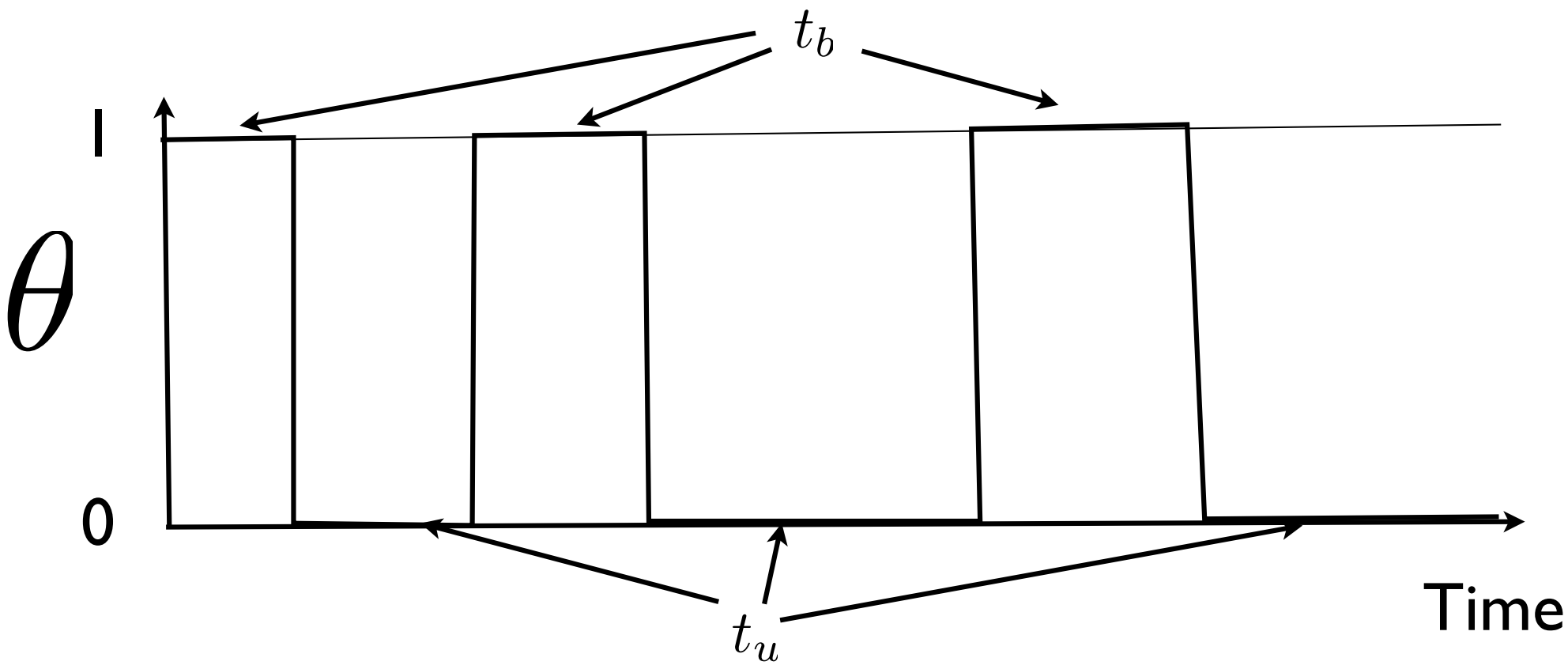


2/ A flat function:



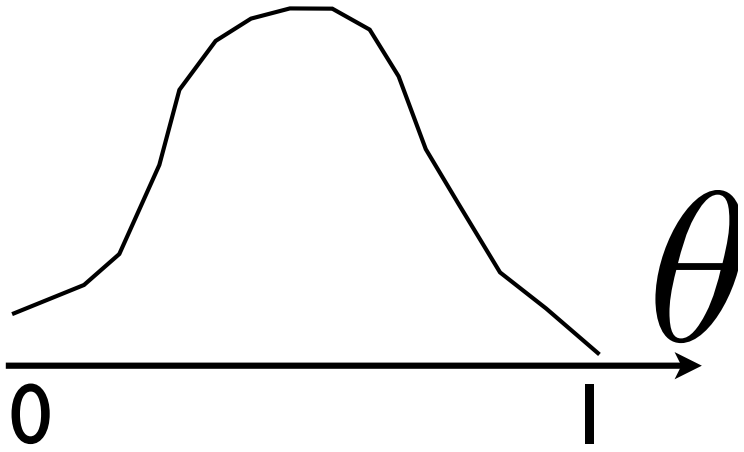
3/ Other

Let us go to flames: what is the pdf of temperature at a point where the temperature signal is the following ? (assume the flame is infinitely thin):

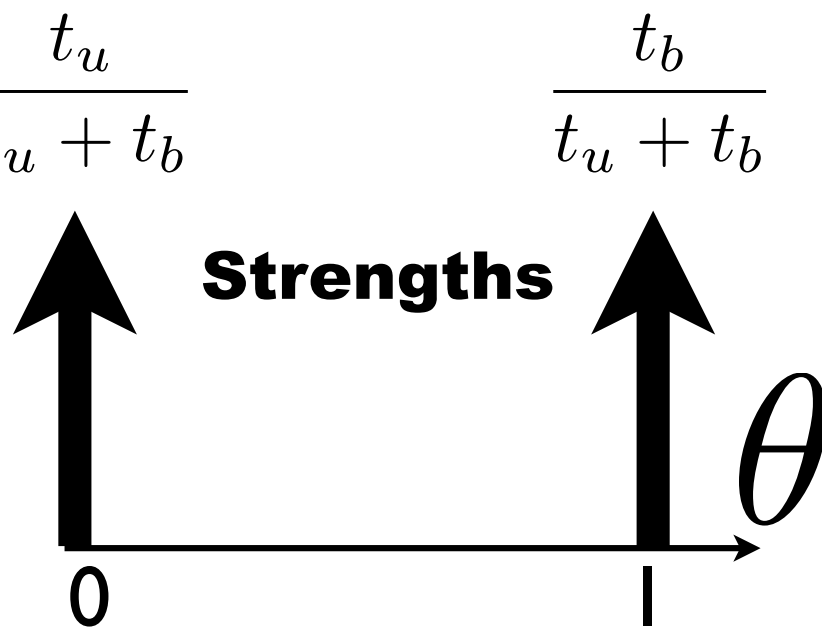


Answers:

1/ A Gaussian shape:

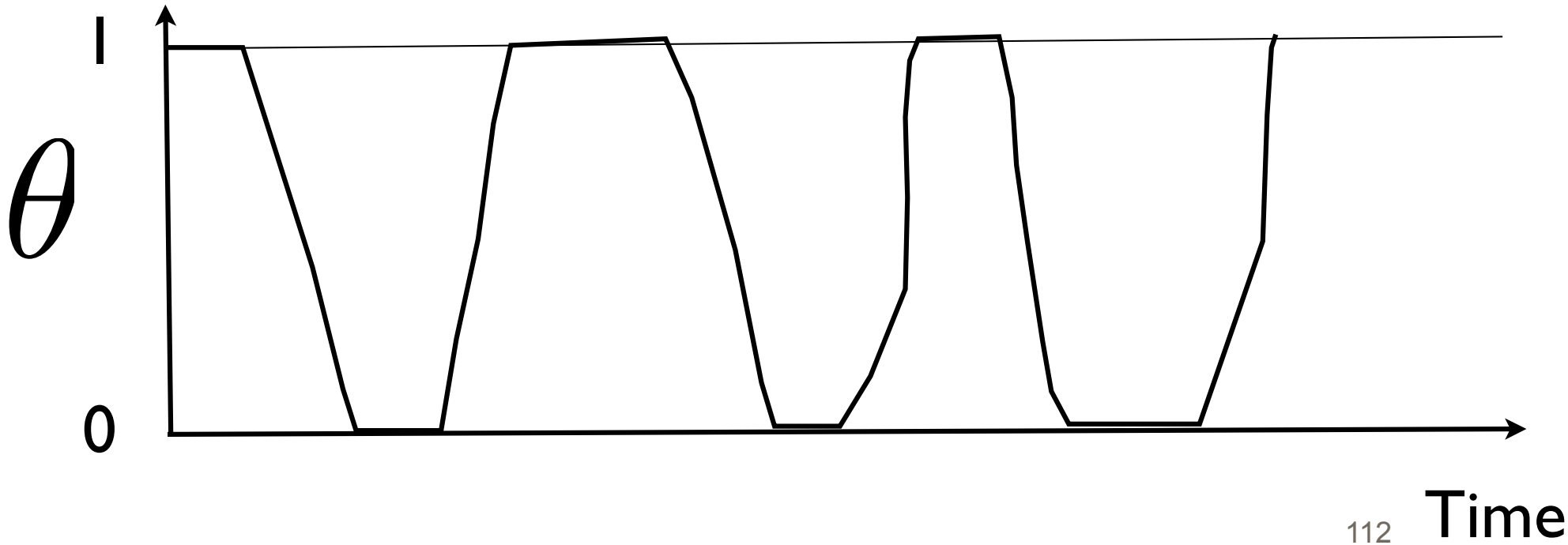


2/ Two Dirac functions:



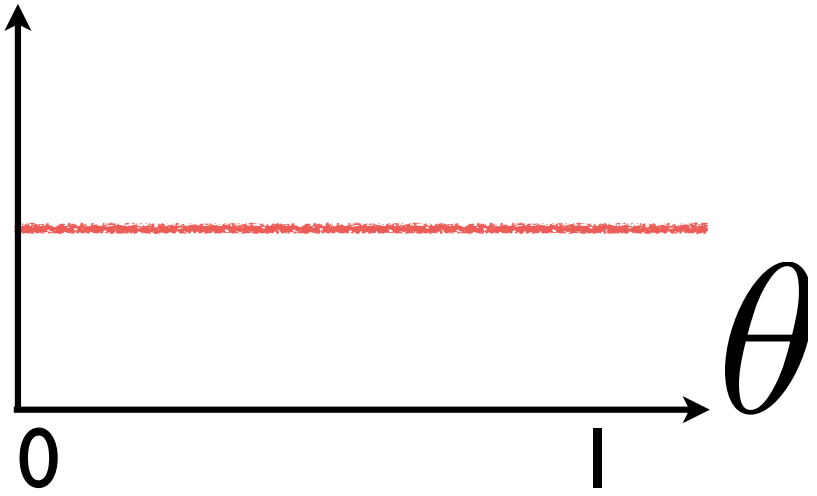
3/ Other

Same question if we do not neglect the flame thickness:

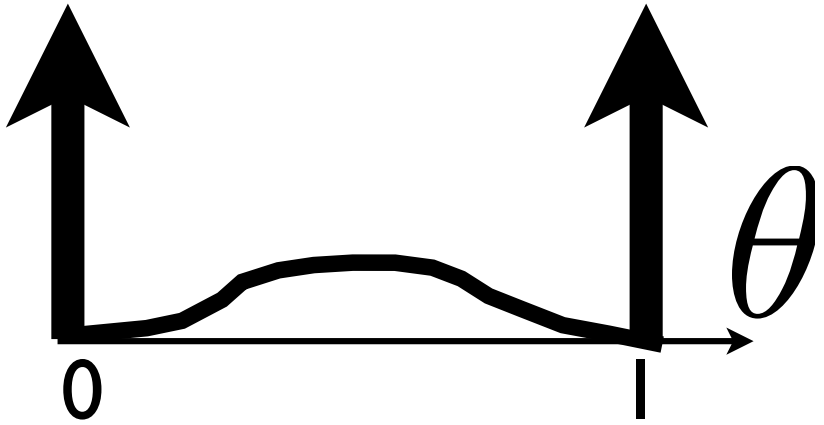


Answers:

1/ A flat shape:

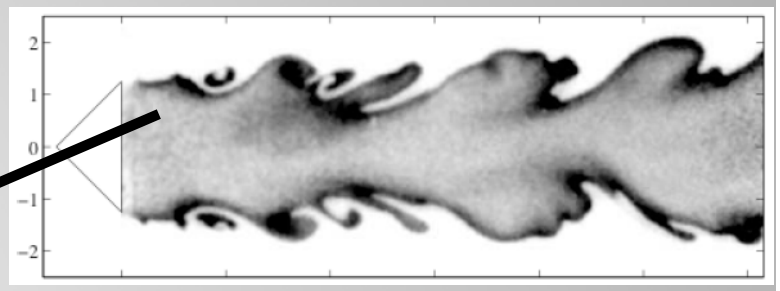


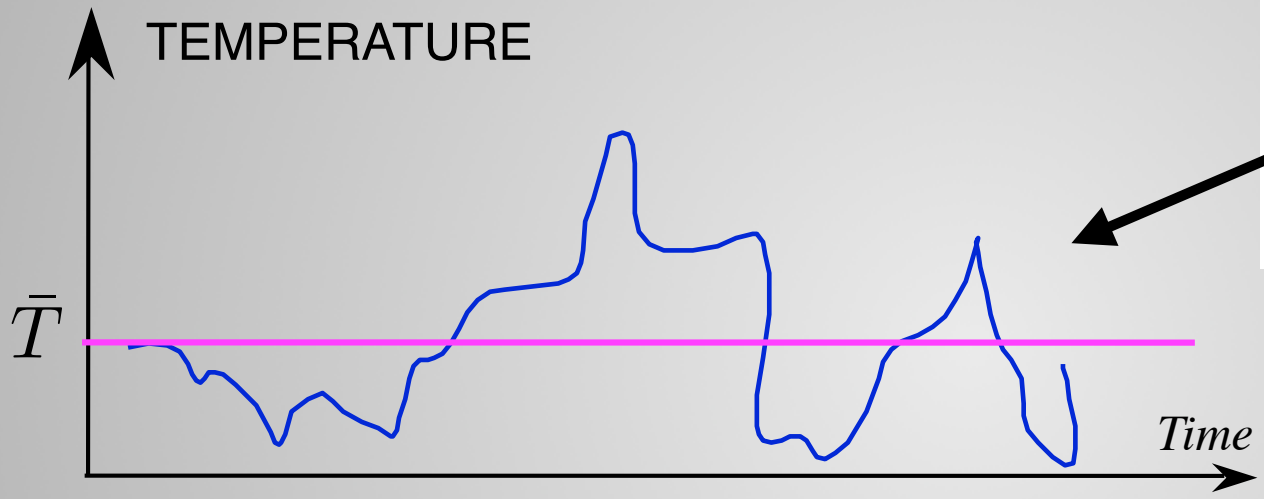
2/ Two Dirac functions + something in between:

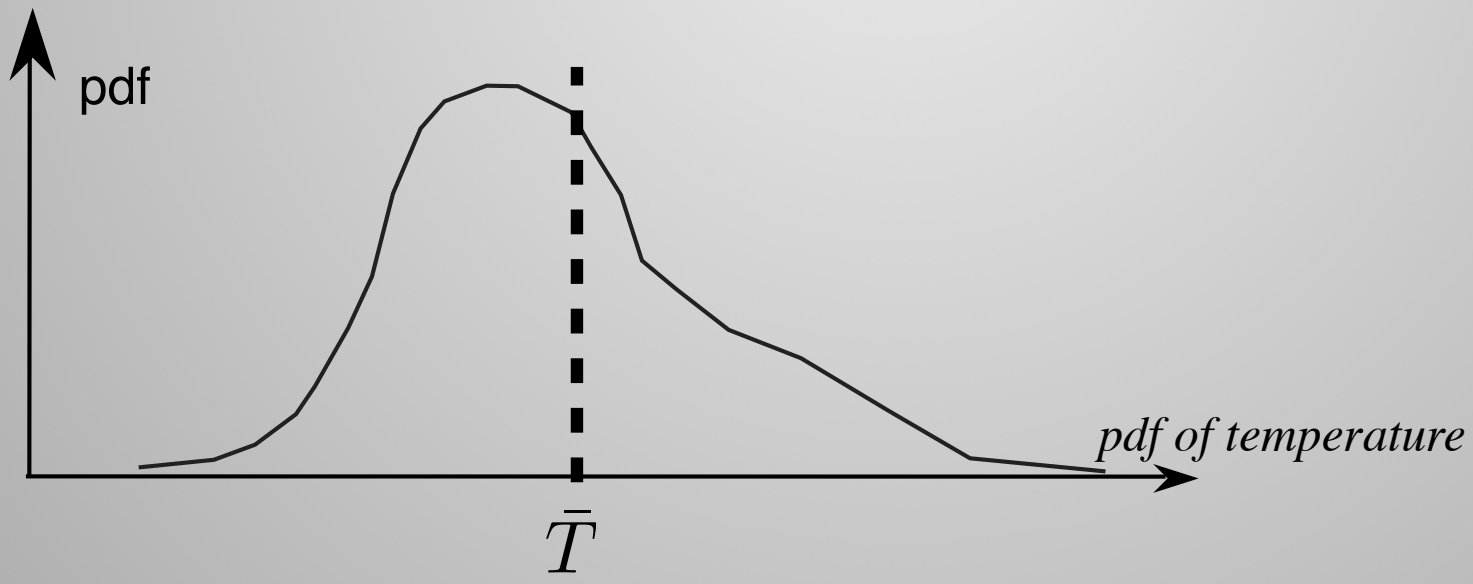


3/ Other

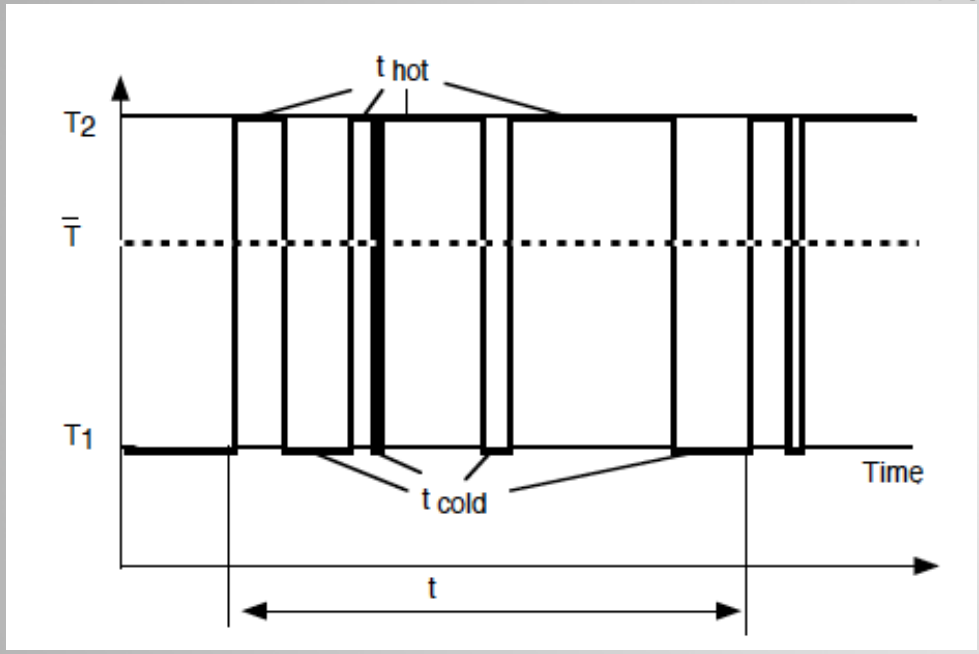
For the turbulent variables needed in combustion, knowing their pdf is as good as knowing all the details of the time signal because pdfs' allow us to compute all non linear correlation terms we need to close our models.

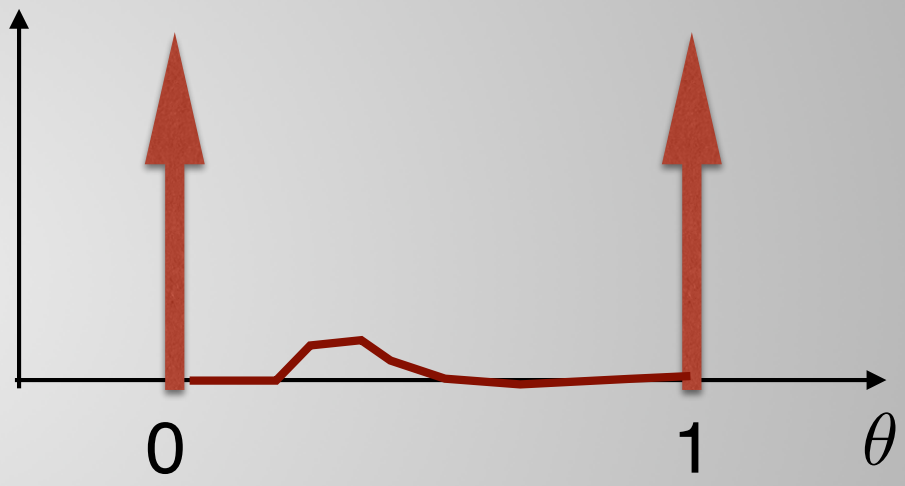


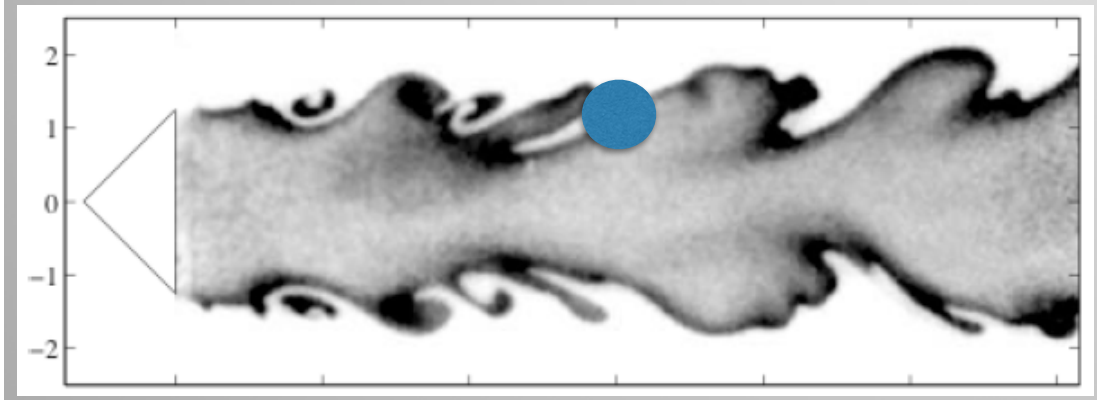




Typical pdfs in premixed flames:

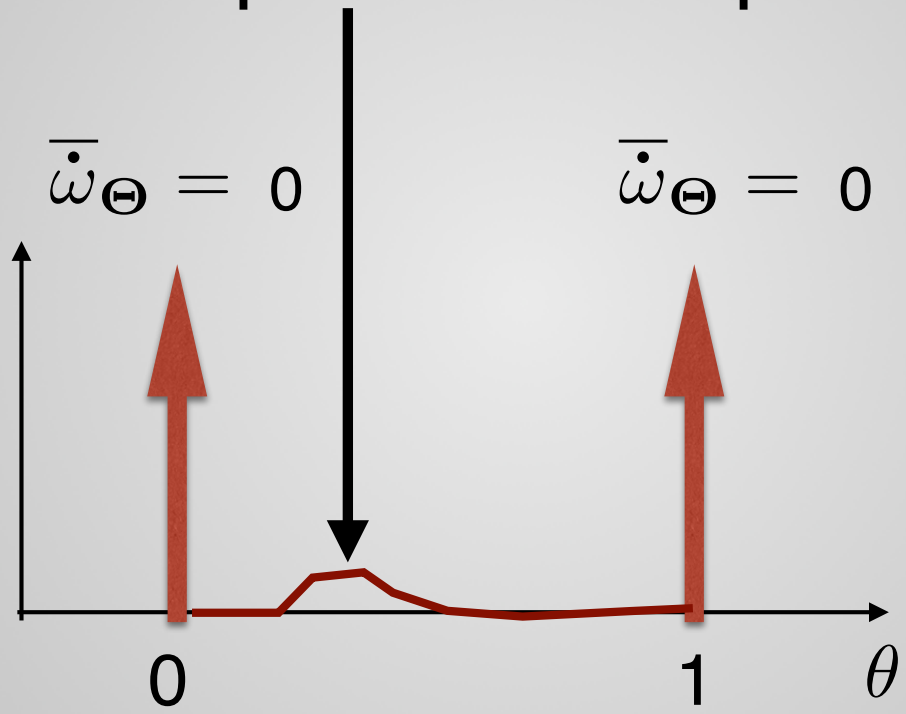






$$\overline{\dot{\omega}}_{\Theta} = \int_0^1 \dot{\omega}_{\theta}(\Theta^*)\mathrm{p}(\Theta^*)\,\mathrm{d}\Theta^*$$

- Only this zone contributes to the mean reaction rate and it is a very small one. It corresponds to instants where the flame passes on the probe



$$\overline{\dot{\omega}}_{\Theta} = \int_0^1 \dot{\omega}_{\theta}(\Theta^*)\mathrm{p}(\Theta^*)\,\mathrm{d}\Theta^*$$

- Knowing the pdf gives all other moments:

$$\overline{\Theta} = \int_0^1 \Theta^* \mathbf{p}(\Theta^*)\, \mathbf{d}\Theta^* \quad \text{and} \quad \overline{\Theta'^2} = \int_0^1 \left(\Theta^* - \overline{\Theta}\right)^2 \mathbf{p}(\Theta^*)\, \mathbf{d}\Theta^*$$

- As well as the mean reaction rate:

$$\overline{\dot{\omega}}_\Theta = \int_0^1 \dot{\omega}_\theta(\Theta^*)\mathbf{p}(\Theta^*)\, \mathbf{d}\Theta^*$$

The ultimate model: pdfs?

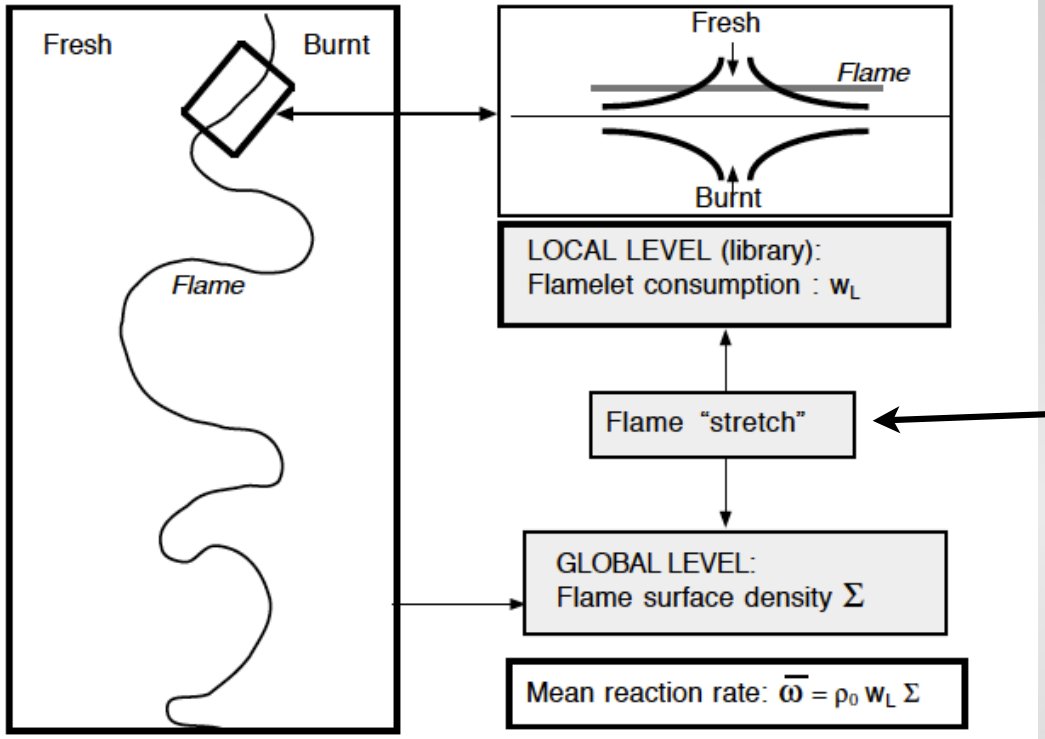
- The question is now how to find the local pdfs (see Steve Pope's contributions on this topic and multiple examples in the literature): they can be presumed or computed using Monte Carlo methods
- Not discussed here because not used often for premixed flames where pdfs (too) often have a bi modal shape
- We will see that they are more useful in diffusion flames

Additional issue in pdf models

- We have assumed a combustion model with only one variable θ
- In practice, we have N independent species: we will need a multidimensional pdf
- There are methods to handle this but it gets complicated

4. Flame surface models

Ch. 5 - Sect. 5.3.6



'Flamelet' models

Stretch

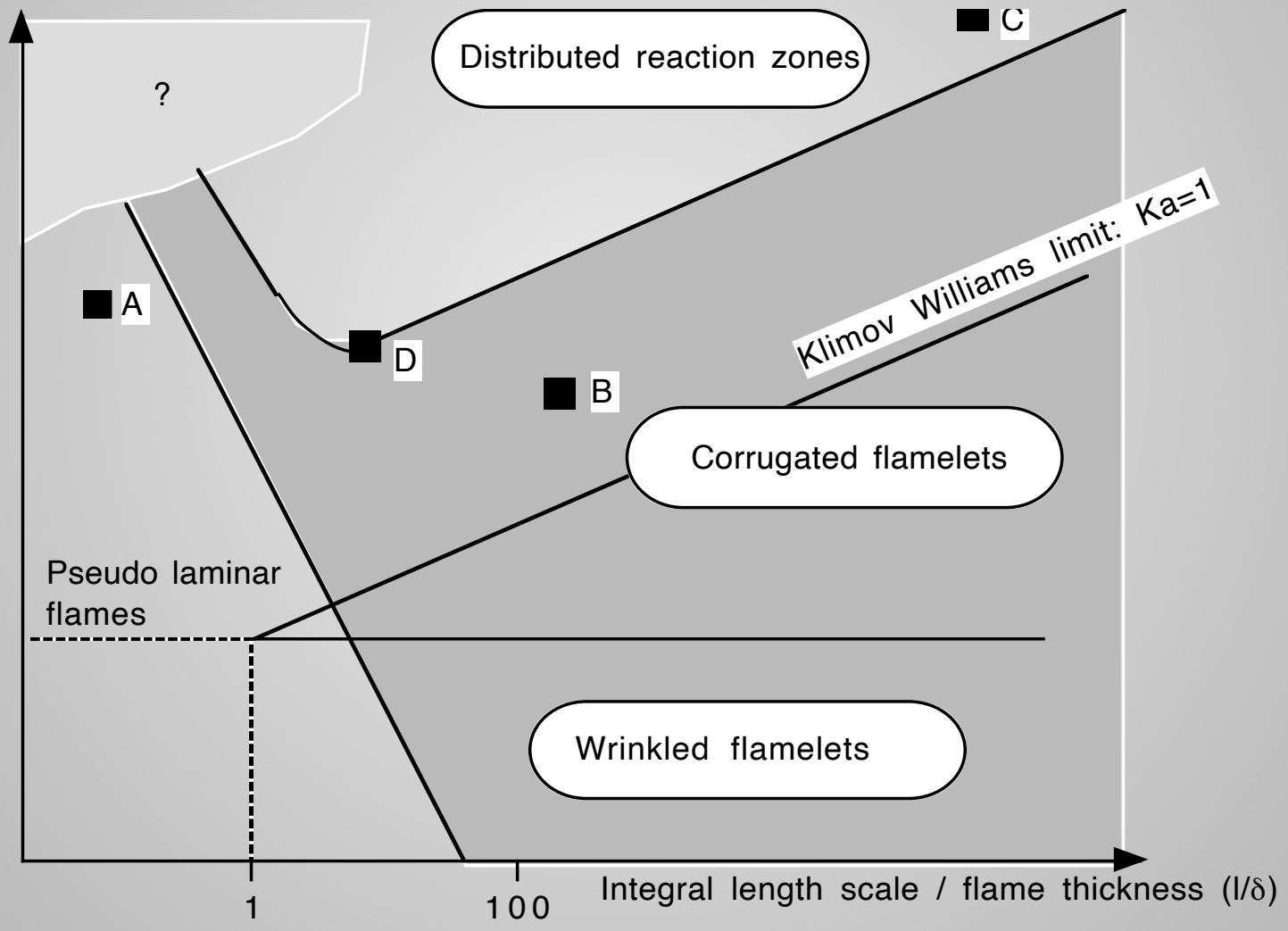
Flame surface density (m^2/m^3)

$$\overline{\dot{\omega}}_\Theta = \rho_0 \langle s_c \rangle_s \Sigma$$

Local consumption speed (contains kinetics)

Better than EBU: we can include kinetics

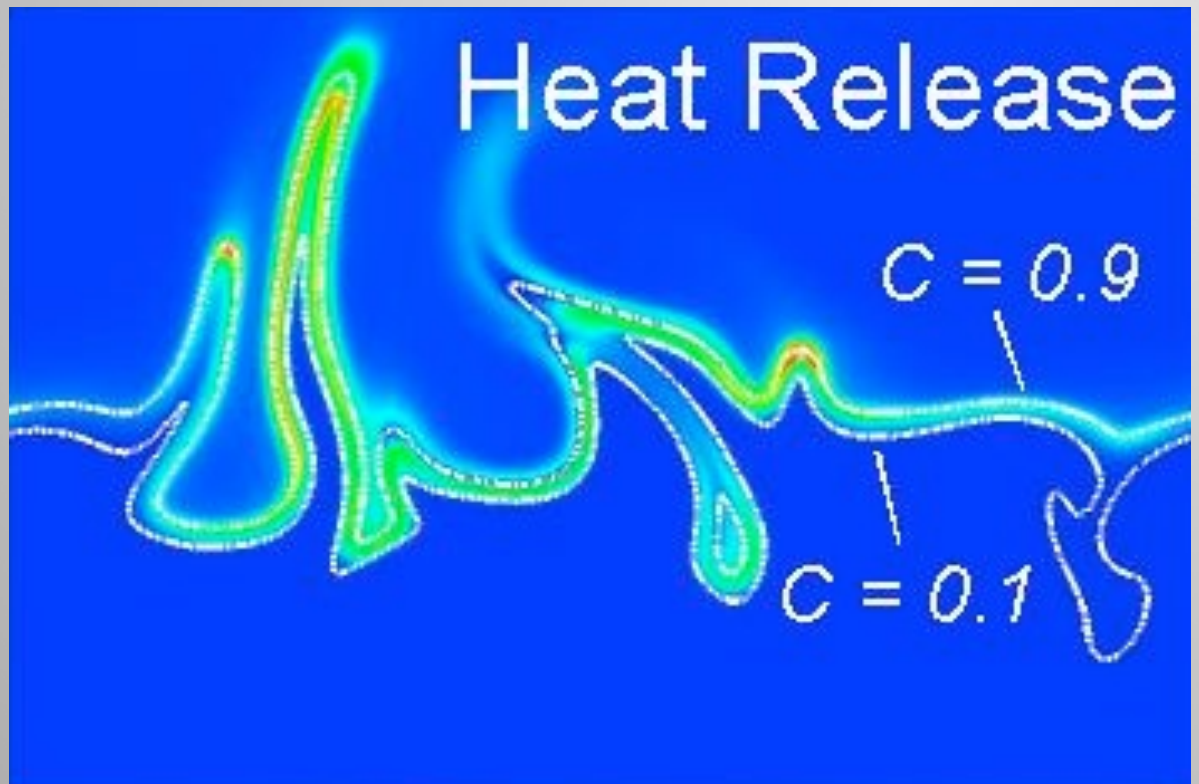
Only in the flamelet regime:



The mean reaction rate

$$\overline{\dot{\omega}}_\Theta = \rho_0 \langle s_c \rangle_s \Sigma$$

How do we obtain the **mean consumption speed** ?: hundreds of DNS devoted to this problem (TNC book, chapter 5). In the end, saying that it is equal to the unstretched laminar flame speed is usually a good choice.



$$< s_c > \approx s_L^0$$

The mean reaction rate

$$\overline{\dot{\omega}}_\Theta = \rho_0 \langle s_c \rangle_s \Sigma$$

How do we obtain the **flame surface density** Σ ?
This is the real question ! The flame surface density is created by flame/turbulence interactions.

Writing an equation for it requires to rederive equations for an interface in turbulence (Pope Int. J. Engng Sci. 1988, Poinsot and Candel CST 1987, Trouve and Poinsot JFM 1991).

$$\overline{\dot{\omega}}_\Theta = \rho_0 \langle s_c \rangle_s \Sigma$$

$$\Sigma = \overline{|\nabla\Theta|\,\delta(\Theta-\Theta^*)} = \left(\overline{|\nabla\Theta|\,|\Theta=\Theta^*}\right) p(\Theta^*)$$

The unclosed flame surface density equation is:

(TNC book, Trouvé and Poinsot 1994):

$$\frac{\partial\Sigma}{\partial t} + \frac{\partial}{\partial x_i}\left(\langle u_i\rangle_s \Sigma\right) + \frac{\partial}{\partial x_i}\left[\langle s_d n_i\rangle_s \Sigma\right] = \underbrace{\left\langle (\delta_{ij}-n_i n_j)\frac{\partial u_i}{\partial x_j}\right\rangle_s \Sigma + \left\langle s_d \frac{\partial n_i}{\partial x_i}\right\rangle_s \Sigma}_{\langle\kappa\rangle_s \Sigma}$$

where the <> operator is defined by:

$$\langle Q\rangle_s = \frac{\overline{Q\,|\nabla\Theta|\,\delta(\Theta-\Theta^*)}}{\overline{|\nabla\Theta|\,\delta(\Theta-\Theta^*)}}$$

Closed flame surface models:

Ch. 5 - Sect. 5.4.5

- Generally written as:

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \widetilde{u}_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_c}\frac{\partial \Sigma}{\partial x_i}\right) + \kappa_m \Sigma + \kappa_t \Sigma - D$$

Source terms Sink

- The source terms are due to stretch:

$$\left\langle (\delta_{ij} - n_i n_j)\frac{\partial u_i}{\partial x_j}\right\rangle_s = \underbrace{(\delta_{ij} - \langle n_i n_j\rangle_s)\frac{\partial \widetilde{u}_i}{\partial x_j}}_{\kappa_m} + \underbrace{\left\langle (\delta_{ij} - n_i n_j)\frac{\partial u_i''}{\partial x_j}\right\rangle_s}_{\kappa_t}$$

Resolved part Turbulent part

- Example: the Coherent Flame model:

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \widetilde{u}_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_c}\frac{\partial \Sigma}{\partial x_i}\right) + \kappa_m \Sigma + \kappa_t \Sigma - D$$

becomes:

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \widetilde{u}_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_c}\frac{\partial \Sigma}{\partial x_i}\right) + \alpha_0 \frac{\varepsilon}{k}\Sigma - \beta_0 \langle s_c \rangle_s \frac{\Sigma^2}{1-\widetilde{\Theta}}$$

- At equilibrium, source terms annihilate:

$$\overline{\dot{\omega}}_\Theta = \rho_0 \frac{\alpha_0}{\beta_0}\frac{\varepsilon}{k}\left(1-\widetilde{\Theta}\right)$$

The CFM model reduces to EBU at equilibrium

- You can choose among a variety of models...

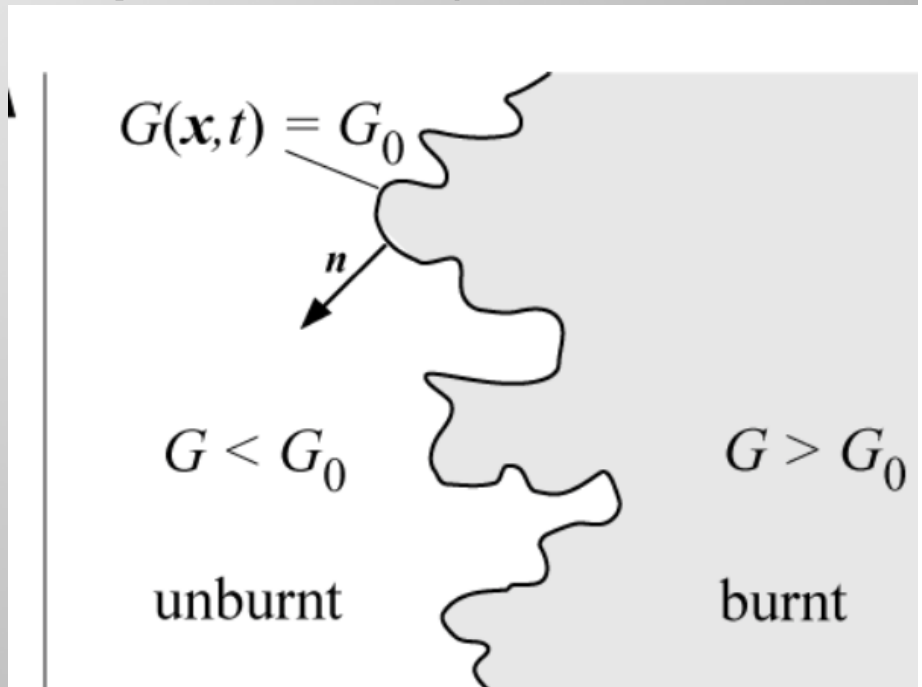
MODEL	$\kappa_m\Sigma$	$\kappa_t\Sigma$	D
CPB [112]	$A_{ik}\frac{\partial\widetilde{u}_k}{\partial x_i}\Sigma$	$\alpha_0 C_A\sqrt{\frac{\varepsilon}{\nu}}\Sigma$	$\beta_0\langle s_c\rangle_s\frac{2+e^{-aR}}{3(1-\widetilde{\Theta})}\Sigma^2$ $R=\frac{(1-\widetilde{\Theta})\varepsilon}{\Sigma\langle s_c\rangle_s k}$
CFM1 [189]	$A_{ik}\frac{\partial\widetilde{u}_k}{\partial x_i}\Sigma$	$\alpha_0\frac{\varepsilon}{k}\Sigma$	$\beta_0\frac{\langle s_c\rangle_s+C\sqrt{k}}{1-\widetilde{\Theta}}\Sigma^2$
CFM2-a [189]	$A_{ik}\frac{\partial\widetilde{u}_k}{\partial x_i}\Sigma$	$\alpha_0\Gamma_K\frac{\varepsilon}{k}\Sigma$	$\beta_0\frac{\langle s_c\rangle_s+C\sqrt{k}}{1-\widetilde{\Theta}}\Sigma^2$
CFM2-b [189]	$A_{ik}\frac{\partial\widetilde{u}_k}{\partial x_i}\Sigma$	$\alpha_0\Gamma_K\frac{\varepsilon}{k}\Sigma$	$\beta_0\frac{\langle s_c\rangle_s+C\sqrt{k}}{\widetilde{\Theta}\left(1-\widetilde{\Theta}\right)}\Sigma^2$
CFM3 [682]	$A_{ik}\frac{\partial\widetilde{u}_k}{\partial x_i}\Sigma$	$\alpha_0\Gamma_K\frac{\varepsilon}{k}\Sigma$	$\beta_0\langle s_c\rangle_s\frac{\Theta^*-\widetilde{\Theta}}{\widetilde{\Theta}\left(1-\widetilde{\Theta}\right)}\Sigma^2$
MB [417]	$E\frac{\widetilde{u_i''u_k''}}{k}\frac{\partial\widetilde{u}_k}{\partial x_i}\Sigma$	$\alpha_0\sqrt{Re_t}\frac{\varepsilon}{k}\Sigma$ $+\frac{F}{\langle s_c\rangle_s}\frac{\varepsilon}{k}\widetilde{u_i''\Theta''}\frac{\partial\widetilde{\Theta}}{\partial x_i}$	$\frac{\beta_0\langle s_c\rangle_s\sqrt{Re_t}\Sigma^2}{\widetilde{\Theta}\left(1-\widetilde{\Theta}\right)\left(1+c\frac{\langle s_c\rangle_s}{\sqrt{k}}\right)^{2\gamma}}$
CD [128]		$\alpha_0\lambda\frac{\varepsilon}{k}\Sigma$ if $\kappa_t\leq\alpha_0 K\frac{\langle s_c\rangle_s}{\delta_L}$	$\beta_0\frac{\langle s_c\rangle_s}{1-\widetilde{\Theta}}\Sigma^2$
CH1 [131]		$\alpha_0\sqrt{\frac{\varepsilon}{15\nu}}\Sigma$	$\beta_0\frac{\langle s_c\rangle_s}{\widetilde{\Theta}\left(1-\widetilde{\Theta}\right)}\Sigma^2$

The G equation

Ch. 5 - Sect. 5.3.6

- Idea: go one more step in the idea of flamelet. If the flame is just an interface, compute it as a zero-thickness interface and do not resolve its inner structure
- The flame becomes a thin surface moving at a local speed s_d (careful: this is the displacement speed and not the consumption speed. TNC Chap 2 Sc 2.7)

$$\frac{\partial G}{\partial t} + \vec{u}.\nabla G = s_d \left|\nabla G\right|$$



The G equation

Ch. 5 - Sect. 5.3.6

$$\frac{\partial G}{\partial t} + \vec{u}.\nabla G = s_d \left|\nabla G\right|$$

- See Norbert Peters book
- Not easy to implement numerically when density changes: propagating a front with ZERO thickness is quite difficult in practice because of density changes
- The displacement speed s_d is needed and this is another difficult quantity to model

5. Thickened flame model

The property derived for laminar flame holds for turbulent flames too: a premixed flame front can be thickened and still travel at the same speed.

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right) + \dot{\omega}_k \qquad \delta = \frac{D_{th}^1}{s_L}$$

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left(\rho \mathbf{F} D_k \frac{\partial Y_k}{\partial x_i}\right) + \frac{1}{\mathbf{F}}\dot{\omega}_k \qquad \delta = \frac{\mathbf{F} D_{th}^1}{s_L}$$

Multiply diffusivity by F

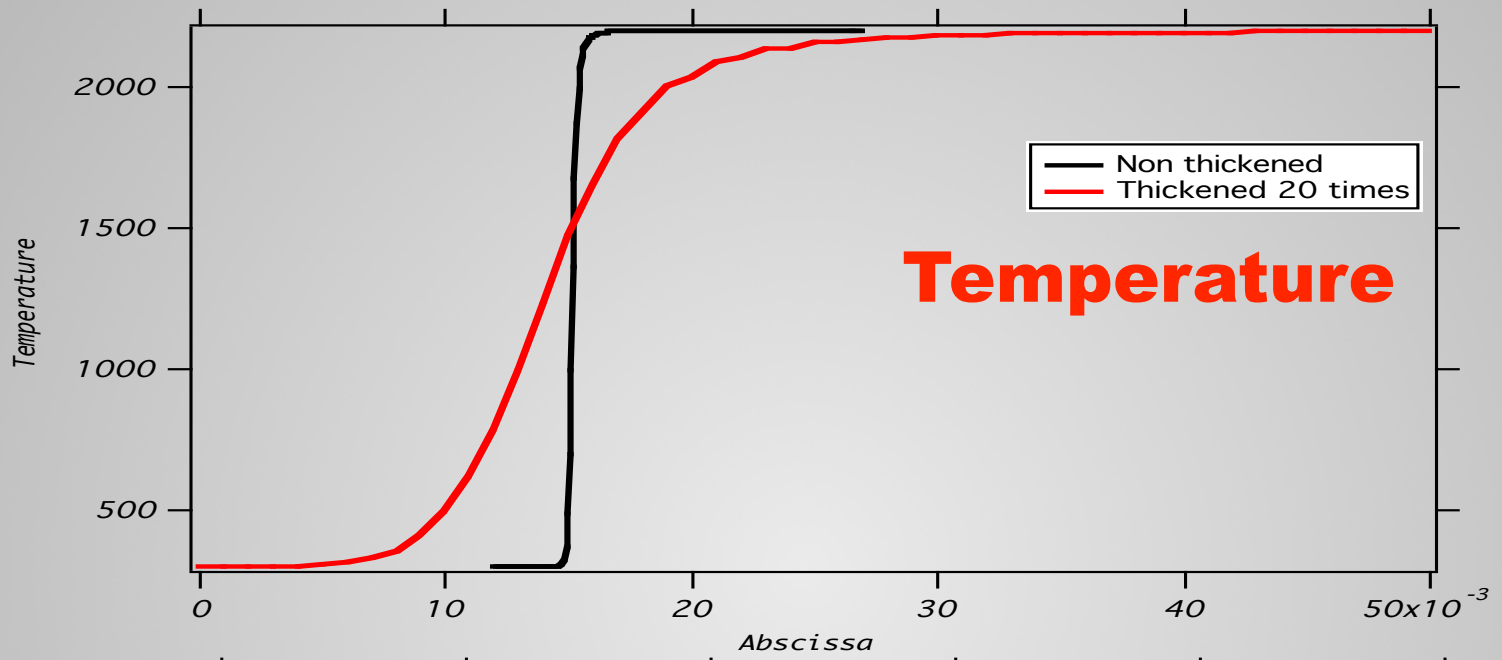
Divide reaction by F

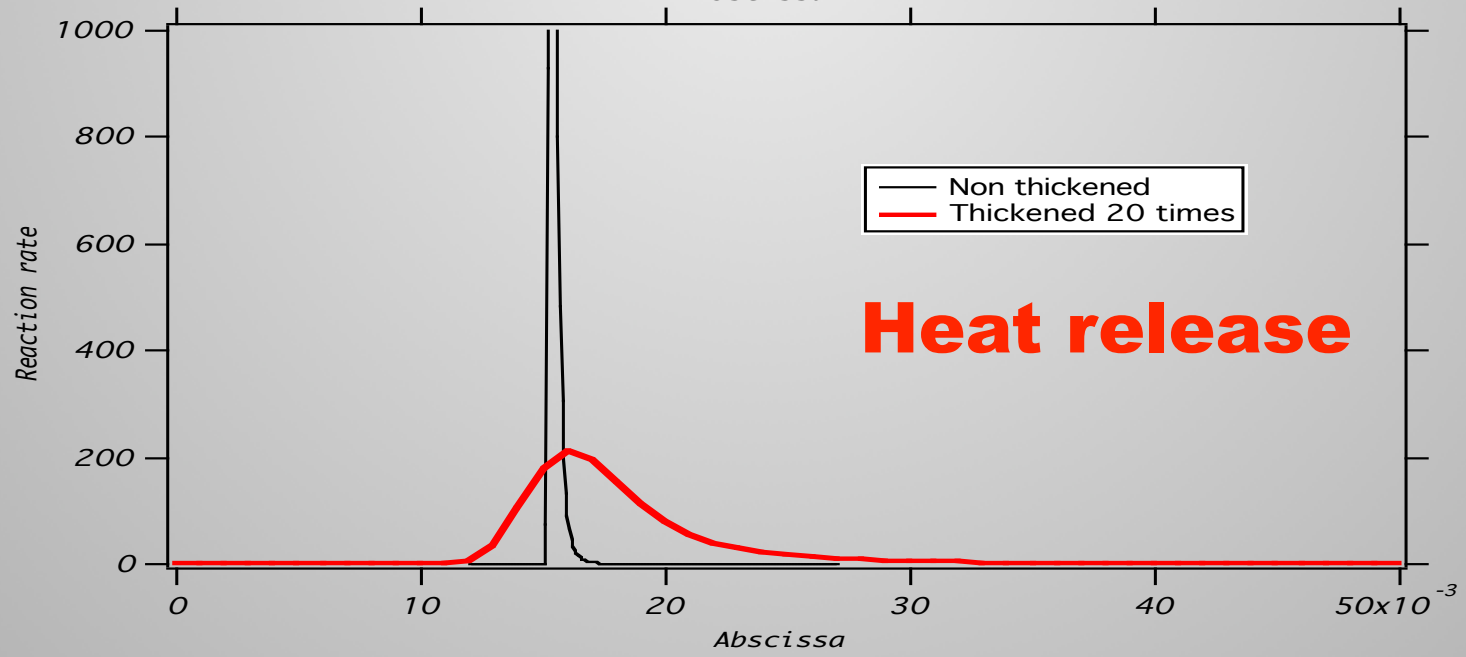
Both equations propagate laminar premixed flames at the same speed s_L.

But the flame thickness is increased by a factor F in the second case ==> the flame front can be adjusted to any thickness we want.

Since our main problem seems to be spatial resolution, why not use this property to make flames thick enough to be resolved on the available grids ?

Thickened and non-thickened flames (methane - air simple chemistry): F=20





TFLES MODELING: EFFECTS OF TURBULENCE ON THE PREMIXED FLAME FRONT

The thickened flame does not respond to turbulence like the initial unthickened flame. This can be parametrized (subgrid scale wrinkling) and included using an efficiency function **E** (*Colin et al, Phys. Fluids 2000*) derived from DNS of flame vortex interactions:

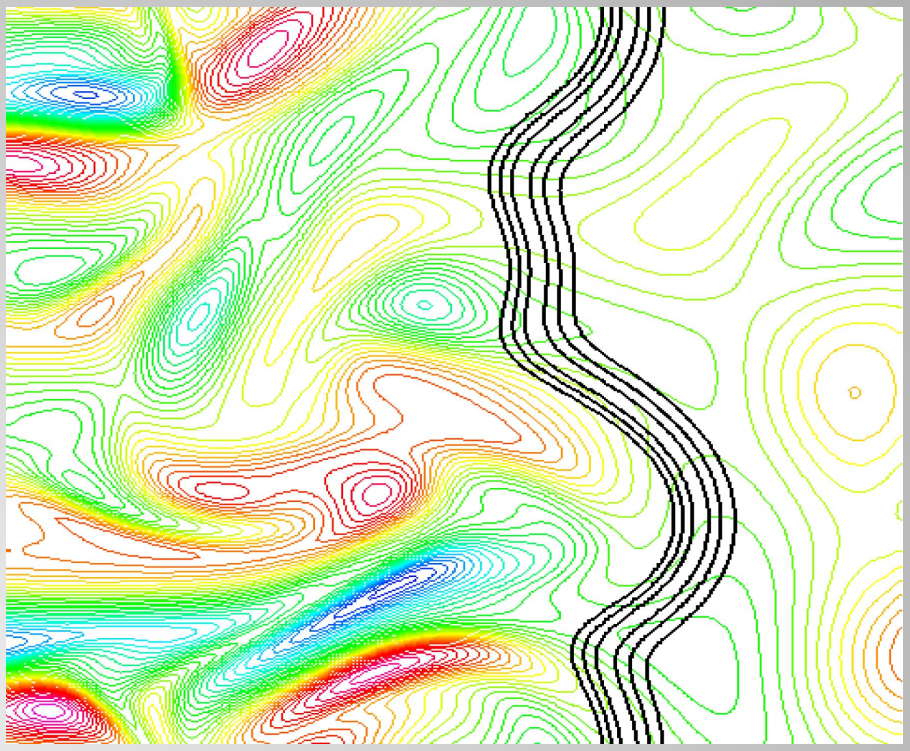
$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left(\rho \mathbf{F} D_k \frac{\partial Y_k}{\partial x_i}\right) + \frac{\mathbf{E}}{\mathbf{F}}\dot{\omega}_k$$

where **E** is a function of the local turbulence and of the premixed flame characteristics (speed and thickness).

E measures the subgrid scale wrinkling: can be characterized from specific DNS



F = 1



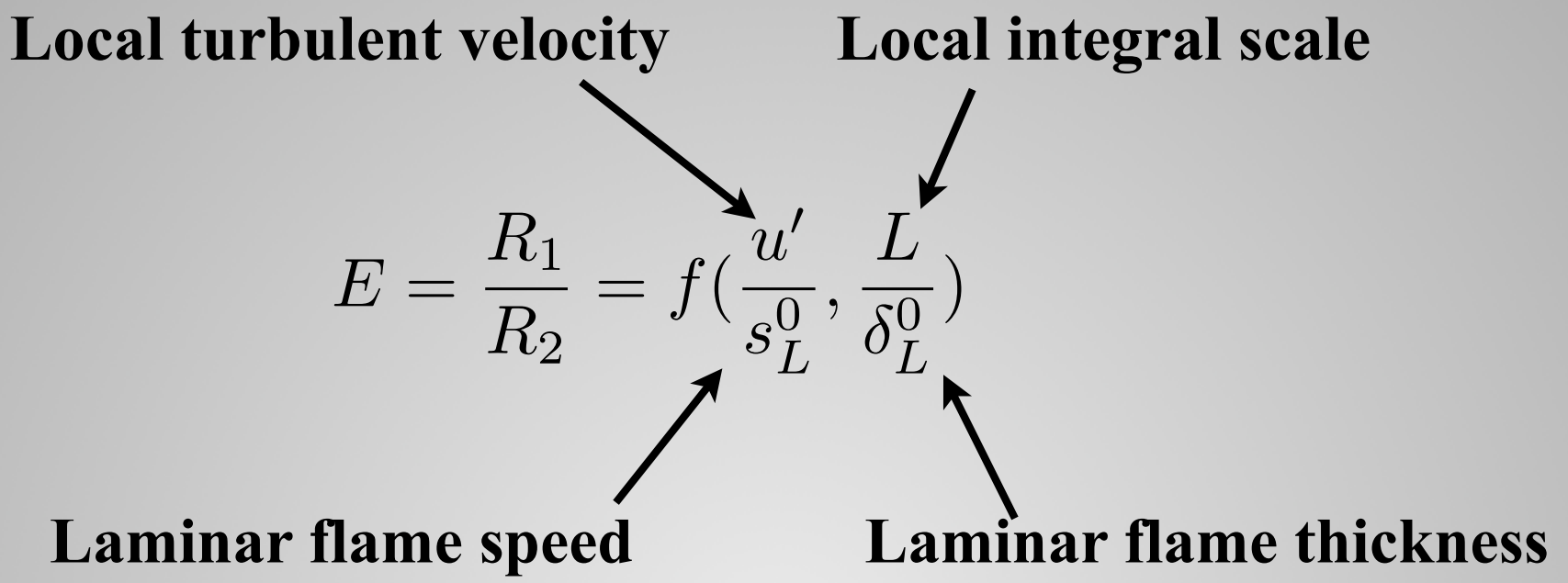
F = 5

Non thickened DNS:
Total reaction rate R1

Thickened DNS:
Total reaction rate R2

$$E = \frac{R_1}{R_2} = f(\frac{u'}{s_L^0}, \frac{L}{\delta_L^0})$$

Colin et al, Phys Fluids 2000, Poinsot Veynante, Chapter 5



Simple to implement: algebraic expressions given in the initial paper of Colin et al (Phys Fluids 2000).

Extensions in papers by Charlette et al, Comb Flame 2002

Dynamic versions by Wang et al Comb. Flame 2012, Volpiani et al Comb. Flame 2017

The whole question of flame / turbulence interactions is hidden in the E function. Careful...

Colin's model (Phys. Fluids 2000)

$$E\left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}, \mathrm{Re}_t\right) = 1 + \beta \frac{2\ln(2)}{3c_{ms}(\mathrm{Re}_t^{1/2} - 1)} \Gamma\left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}\right) \frac{u'_\Delta}{s_l^0}$$

with $$\Gamma\left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}\right) = 0.75 \exp\left[-\frac{1.2}{(u'_\Delta / s_l^0)^{0.3}}\right] \left(\frac{\Delta}{\delta_l^0}\right)^{2/3}$$

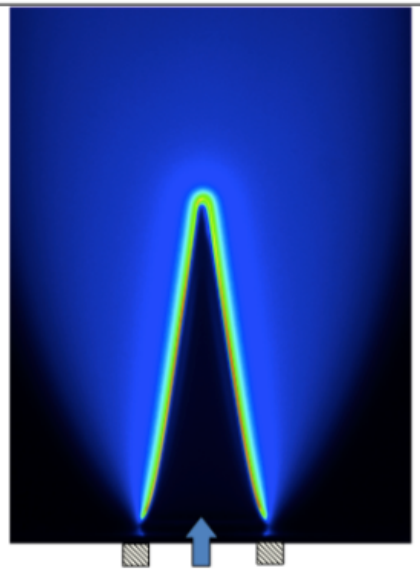
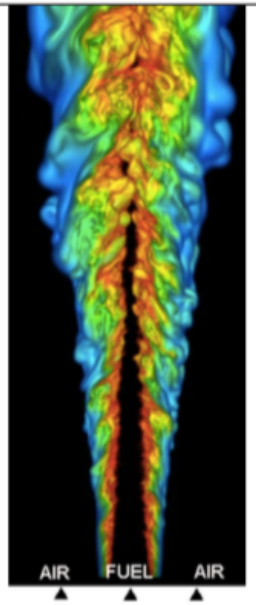
Charlette / Meneveau model (Comb Flame 2002)

$$E\left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}, \mathrm{Re}_\Delta\right) = \left(1 + \min\left(\frac{\Delta}{\delta_l^0}, \Gamma\left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}, \mathrm{Re}_\Delta\right) \frac{u'_\Delta}{s_l^0}\right)\right)^\beta$$

with $$\Gamma\left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}, \mathrm{Re}_\Delta\right) = fit\left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}, \mathrm{Re}_\Delta\right)$$

OUTLINE

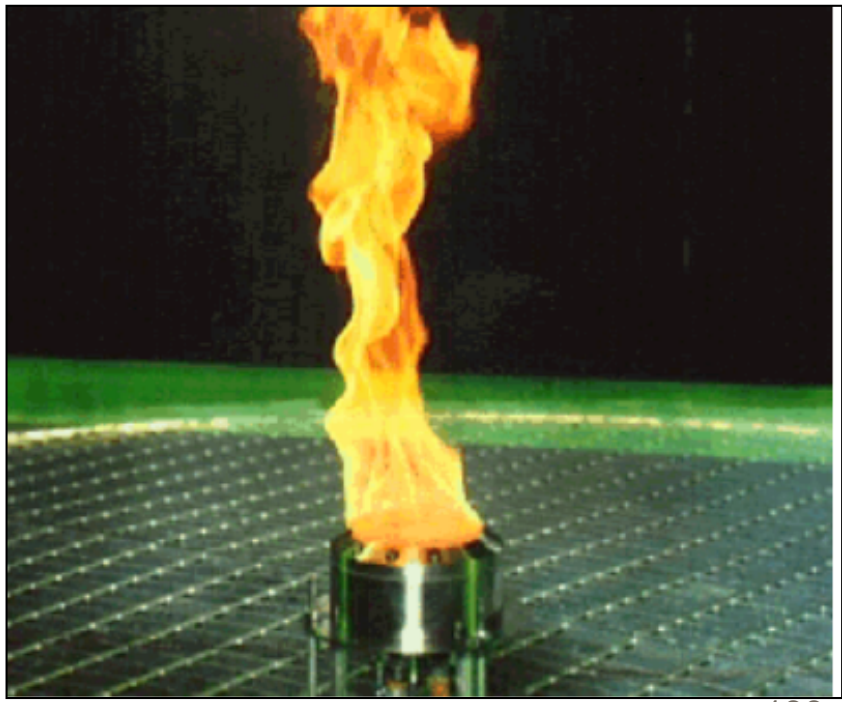
- Phenomenology of turbulent flames
- Classical modeling approaches for turbulent flames
  - Premixed flames
  - Diffusion flames
- Requirements for most real turbulent flames and models

	LAMINAR FLAMES	***TURBULENT FLAMES***
PREMIXED FLAMES	 Chapter 2	 Chapters 4 and 5
NON-PREMIXED FLAMES (DIFFUSION)	 Chapter 3	 Chapters 4 and 6

Very different from turbulent premixed flames.







Models are also different

Premixed versus diffusion ?

For premixed flames, we were looking at thin propagating fronts where having the flame surface was sufficient and mixing played no role.

In a turbulent diffusion flame, mixing is crucial and we must model it. To do so, we will use the same machinery developed for laminar diffusion flames: models based on mixture fraction

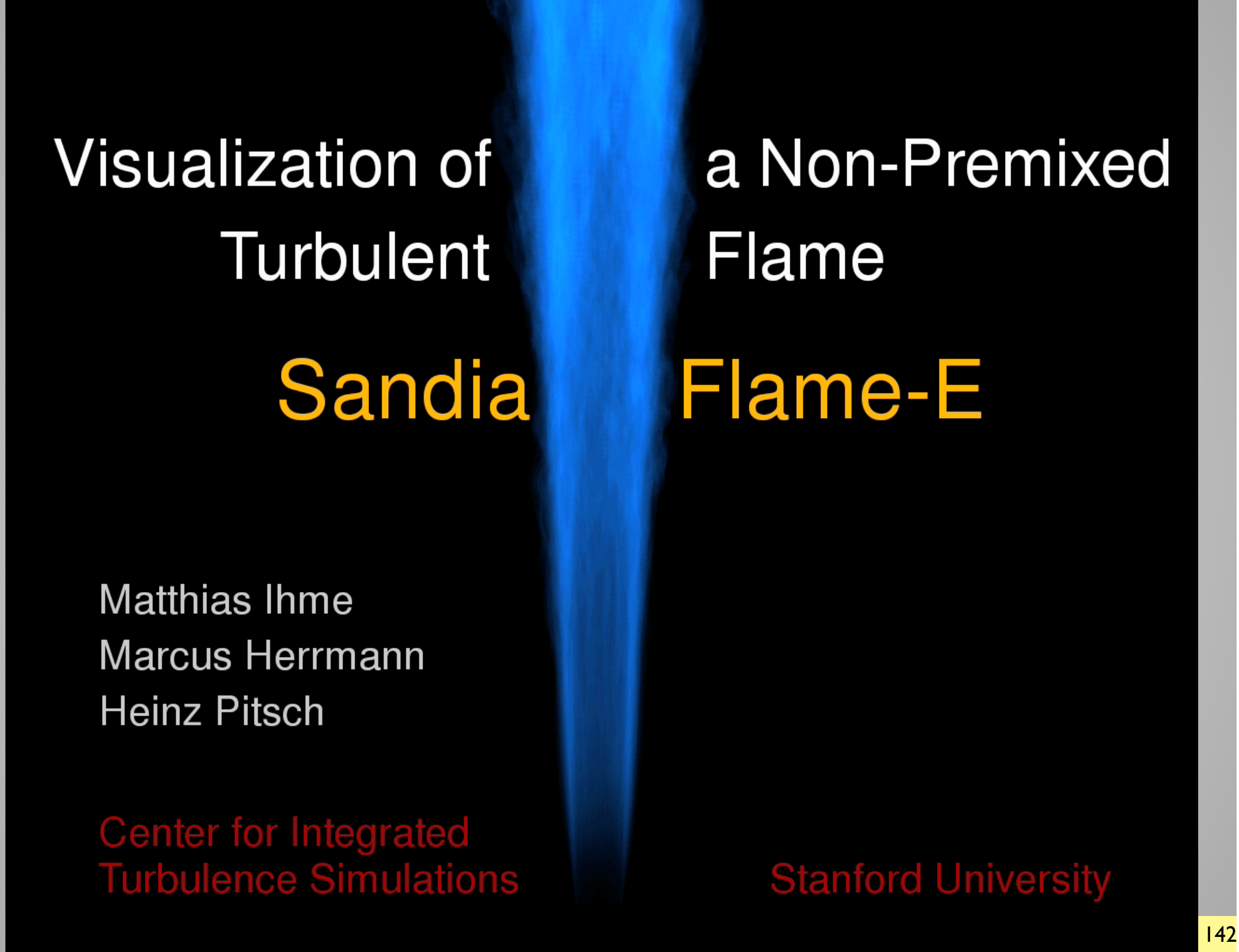
DIFFUSION FLAMES

- Models mostly based on mixture fraction and z diagram as described in the 'Basics' course

- Multiple tests for turbulent diffusion flames in the TNF workshop of Sandia (https://tnfworkshop.org/)



Ihme and Pitsch


Visualization of Turbulent
a Non-Premixed Flame
Sandia
Flame-E
Matthias Ihme
Marcus Herrmann
Heinz Pitsch
Center for Integrated Turbulence Simulations
Stanford University

Turbulent diffusion models

- pdf models with infinitely fast chemistry
  models with z diagram and primitive variables
- pdf models with finite rate chemistry and
  reaction rate

Ch. 6 - Sect. 6.4

- flame surface models
- CMC models

Ch. 6 - Sect. 6.5.1

- Linear eddy models
- Thickened flame model

Ch. 6 - Sect. 6.5.3

The z diagram with infinitely fast chemistry:

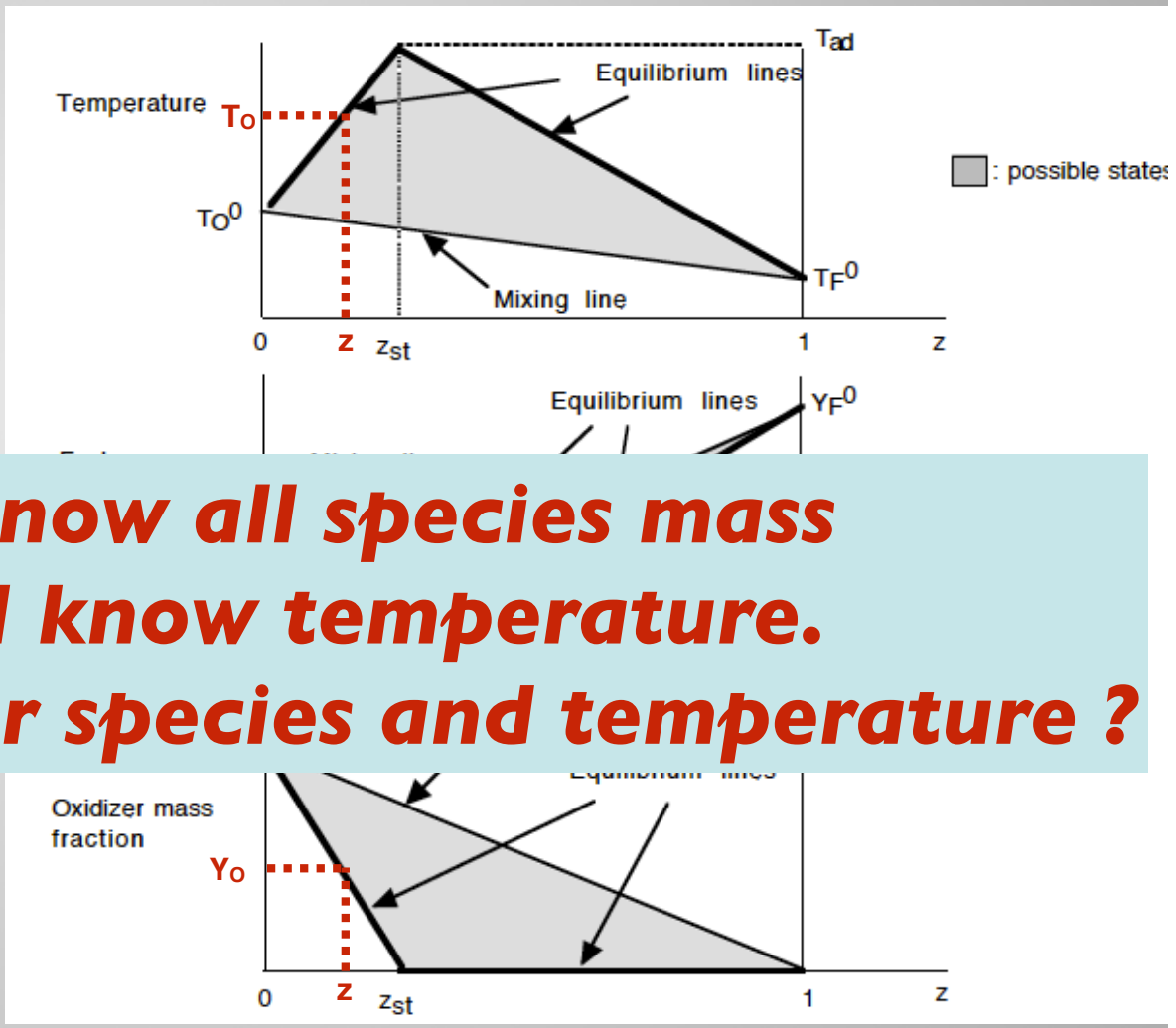
Assumptions:

Lewis numbers=1

Pressure is constant

Flow is adiabatic

T(z)



If I know z, I know all species mass fractions and I know temperature.

Why bother solving for species and temperature ?

Yo(z)

Main idea: no need to solve for species and temperature. Solve only for $\tilde{z}$:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i) = 0$$

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left(\overline{\tau}_{ij} - \overline{\rho}\widetilde{u_i''u_j''}\right)$$

$$\frac{\partial \overline{\rho}\tilde{z}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\tilde{z}) = \frac{\partial}{\partial x_i}\left(\overline{\rho}\mathcal{D}\frac{\partial \tilde{z}}{\partial x_i} - \overline{\rho}\widetilde{u_i''z''}\right) \quad \text{NEW}$$

Now, we need to solve this averaged or filtered equation for z:

$$\frac{\partial \overline{\rho}\tilde{z}}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{u}_i\widetilde{z}\right) = \frac{\partial}{\partial x_i}\left(\overline{\rho}\mathcal{D}\frac{\partial \tilde{z}}{\partial x_i} - \overline{\rho}\widetilde{u_i'' z''}\right)$$

Usually modeled with a turbulent viscosity:

$$\frac{\partial \overline{\rho}\tilde{z}}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{u}_i\widetilde{z}\right) = \frac{\partial}{\partial x_i}\left(\overline{\rho}(\mathcal{D} + \mathcal{D}_t)\frac{\partial \tilde{z}}{\partial x_i}\right)$$

An easy equation to solve in RANS or LES…

In RANS the turbulent viscosity is obtained by:

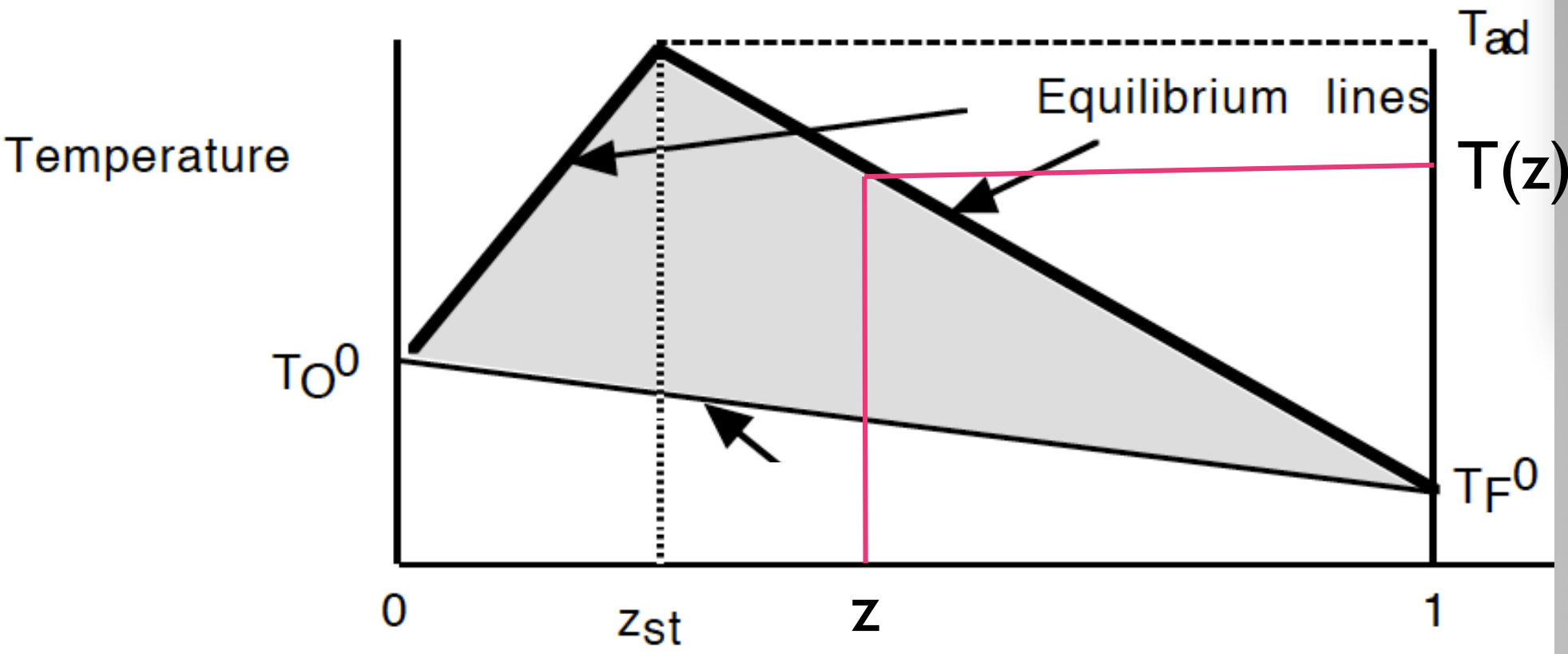
$$D_t = C_\mu \frac{k^2}{\epsilon}$$

$$\frac{\partial \overline{\rho}\tilde{z}}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{u}_i\widetilde{z}\right) = \frac{\partial}{\partial x_i}\left(\overline{\rho}(\mathcal{D}+\mathcal{D}_t)\frac{\partial \tilde{z}}{\partial x_i}\right)$$

We can compute $\tilde{z}$ from this equation but this is not enough to obtain $\tilde{T}$ or the mean species mass fractions $\tilde{Y}_k$

$$\tilde{T}(z) \neq T(\tilde{z}) \qquad \tilde{Y}_k(z) \neq Y_k(\tilde{z})$$

Having the mean mixture fraction $\tilde{z}$ is not enough to have the mean species $\tilde{Y}_k$ and temperature $\tilde{T}$.



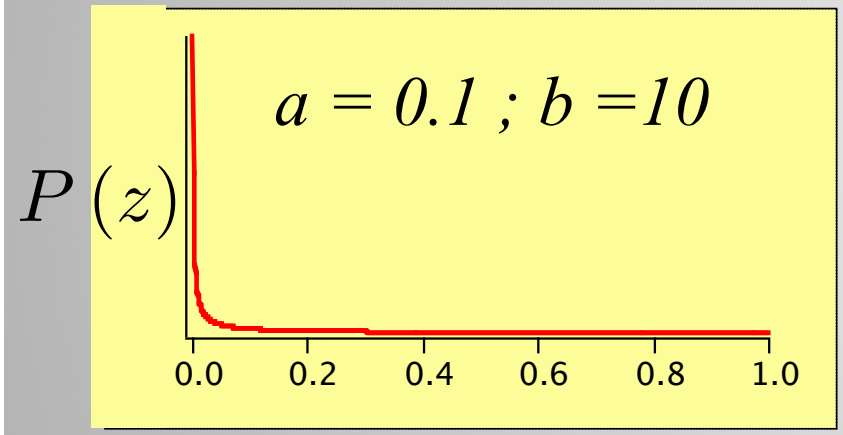
The link between z and $Y_k(z)$ or $T(z)$ holds only for instantaneous values.

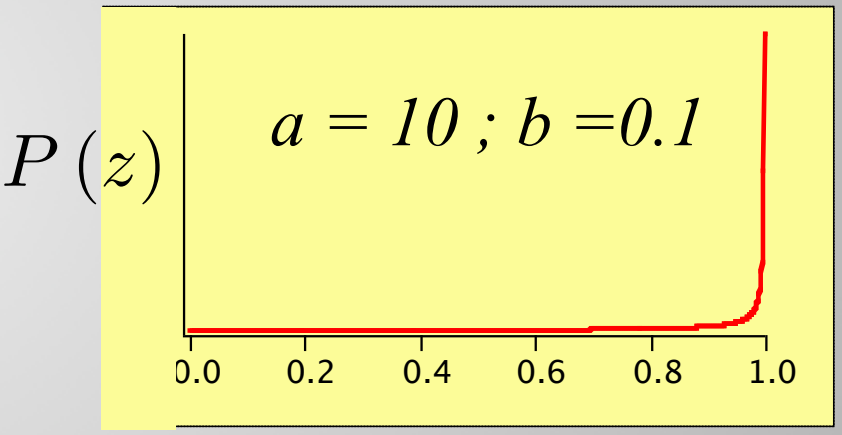
For mean quantities, the pdf z of is needed:

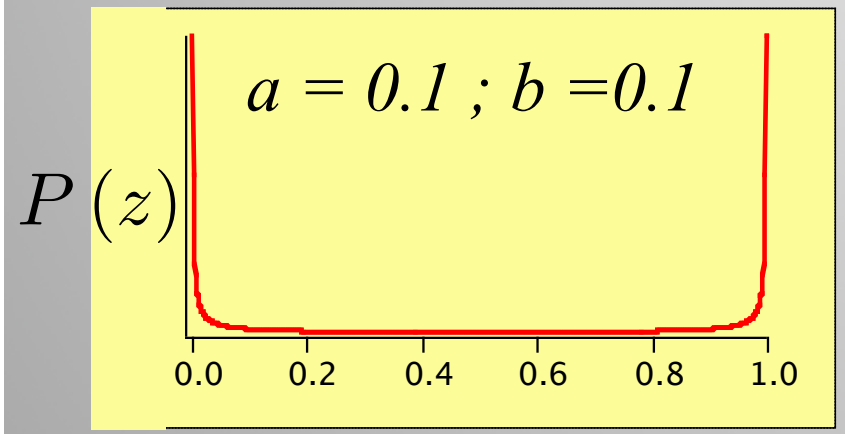
$$\overline{\rho}\widetilde{Y}_k = \int_0^1 \left(\overline{\rho Y_k | z^*}\right) p(z^*)\, dz^* \qquad \overline{\rho}\widetilde{T} = \int_0^1 \left(\overline{\rho T | z^*}\right) p(z^*)\, dz^*$$

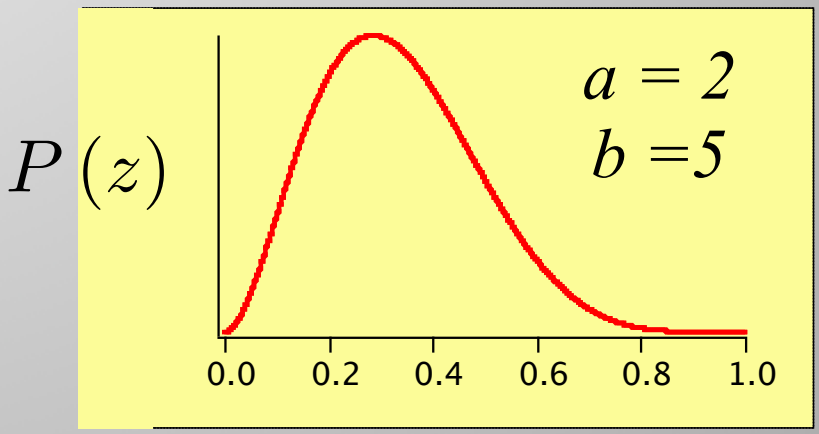
Beta pdf: widely used as the most convenient expression for the pdf of z:

β ***functions:*** $$P(z) = \frac{z^{a-1}(1-z)^{b-1}}{\int_0^1 z^{a-1}(1-z)^{b-1}\,dz}$$









In practice, we find a and b from two variables: the mean and its variance

β ***functions*** $$P(z) = \frac{z^{a-1}(1-z)^{b-1}}{\int_0^1 z^{a-1}(1-z)^{b-1}\,dz}$$

$$\tilde{z} = \int_0^1 z^* P(z^*)\,dz^*$$

$$\widetilde{z''^2} = \int_0^1 (z^* - \tilde{z})^2 P(z^*)\,dz^*$$

$$a = \tilde{z}\left(\frac{\tilde{z}(1-\tilde{z})}{\widetilde{z''^2}} - 1\right) \geq 0$$

$$b = a\left(\frac{1}{\tilde{z}} - 1\right) \geq 0$$

Ch. 5 - Sect. 5.3.7

If you know the mean and the variance of z you can have a and b such that the beta pdf of z will have these mean and variance values

$$a = \tilde{z}\left(\frac{\tilde{z}(1-\tilde{z})}{\widetilde{z''^2}} - 1\right) \geq 0$$

$$b = a\left(\frac{1}{\tilde{z}} - 1\right) \geq 0$$

But now we need balance equations for the mean value of z (we have it) but also for its variance $\widetilde{z''^2}$!!

A code for DNS of diffusion flames using the z diagram

Momentum give the 3 velocities:

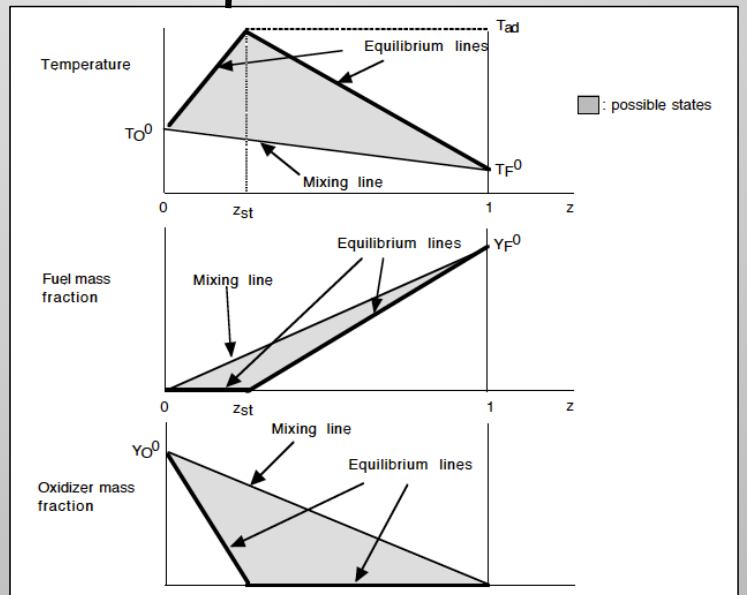
~~Density~~ In a low Mach number code where p=ct

~~Energy~~

Mixture fraction

z(**x**,t) Field + z diagram = all Yks + T

$$\frac{\partial \rho z_j}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i z_j) = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial z_j}{\partial x_i}\right)$$



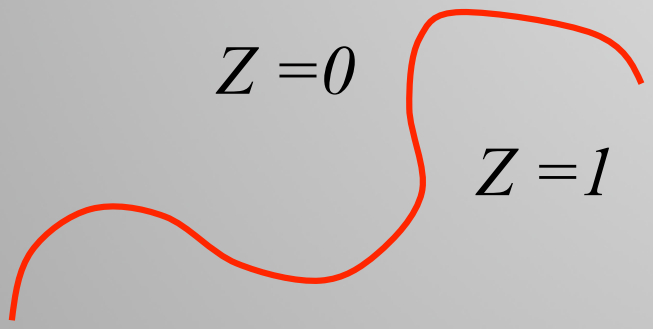
With the pdf of z and the z diagram, we can compute mean quantities:

➢ *assuming infinitely fast chemistry*

$$\widetilde{Y}_k = \int_0^1 Y_k(Z)\,\widetilde{P}(Z)\,dZ$$

Infinitely fast chemistry solution

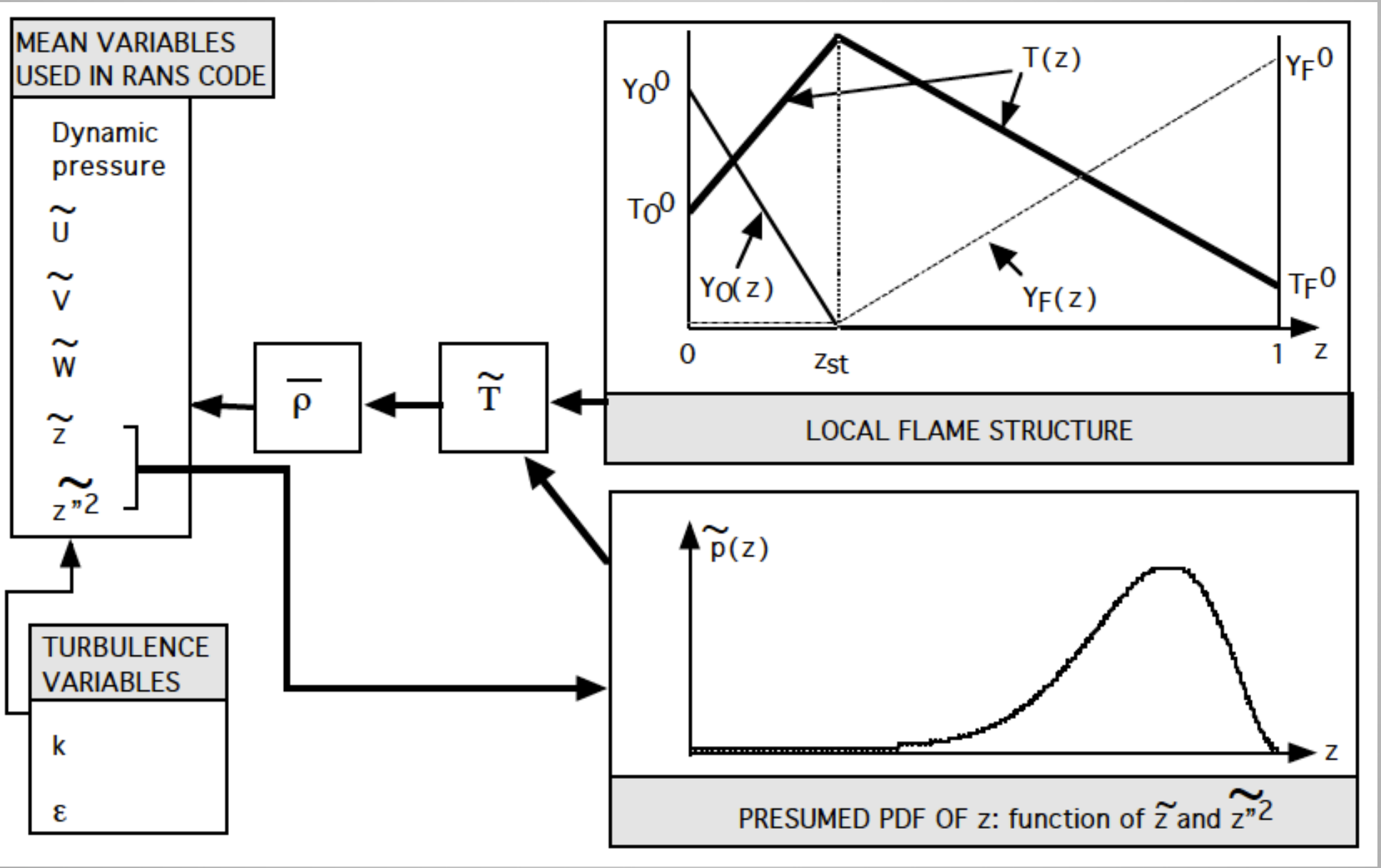
Presumed pdf (β functions)



Note that:

- Only the mixture fraction is needed
- Chemical reaction rates not required

Organization of a code for turbulent diffusion flames using infinitely fast chemistry:



OUTLINE

- Phenomenology of turbulent flames
- Classical modeling approaches for turbulent flames
  - Premixed flames
  - Diffusion flames
- Requirements for most real turbulent flames and models

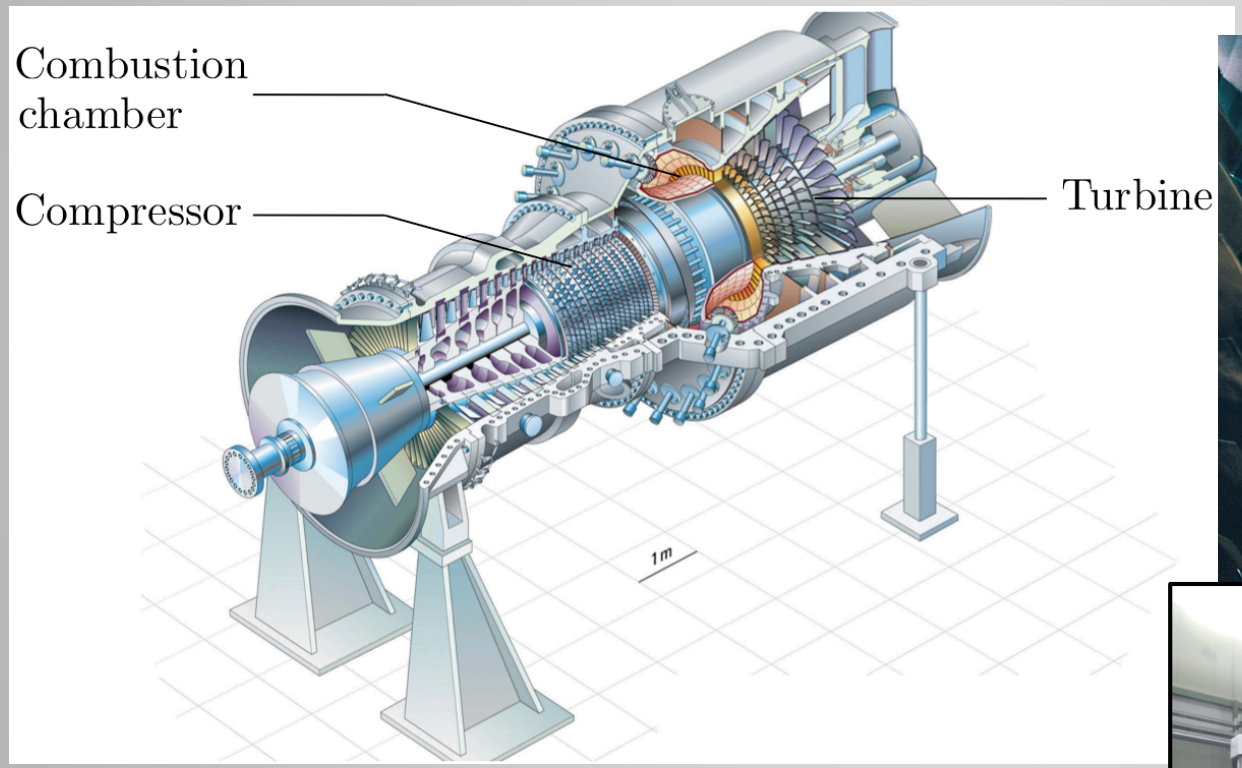
Requirements for most real turbulent flames and models

- In real combustors, most models derived for academic flames reach the limits of the assumptions used to build them
- The whole modeling strategy may have to be revisited

Real combustors

- Regime is unknown: not premixed, not diffusion. Present technological requirements usually lead to partially premixed flames. Critical issue today for hydrogen flames
- Flames are not adiabatic
- Mixture fractions are difficult to define: Lewis numbers are not equal and many flames are not fed by only two streams

Example: an industrial gas turbine



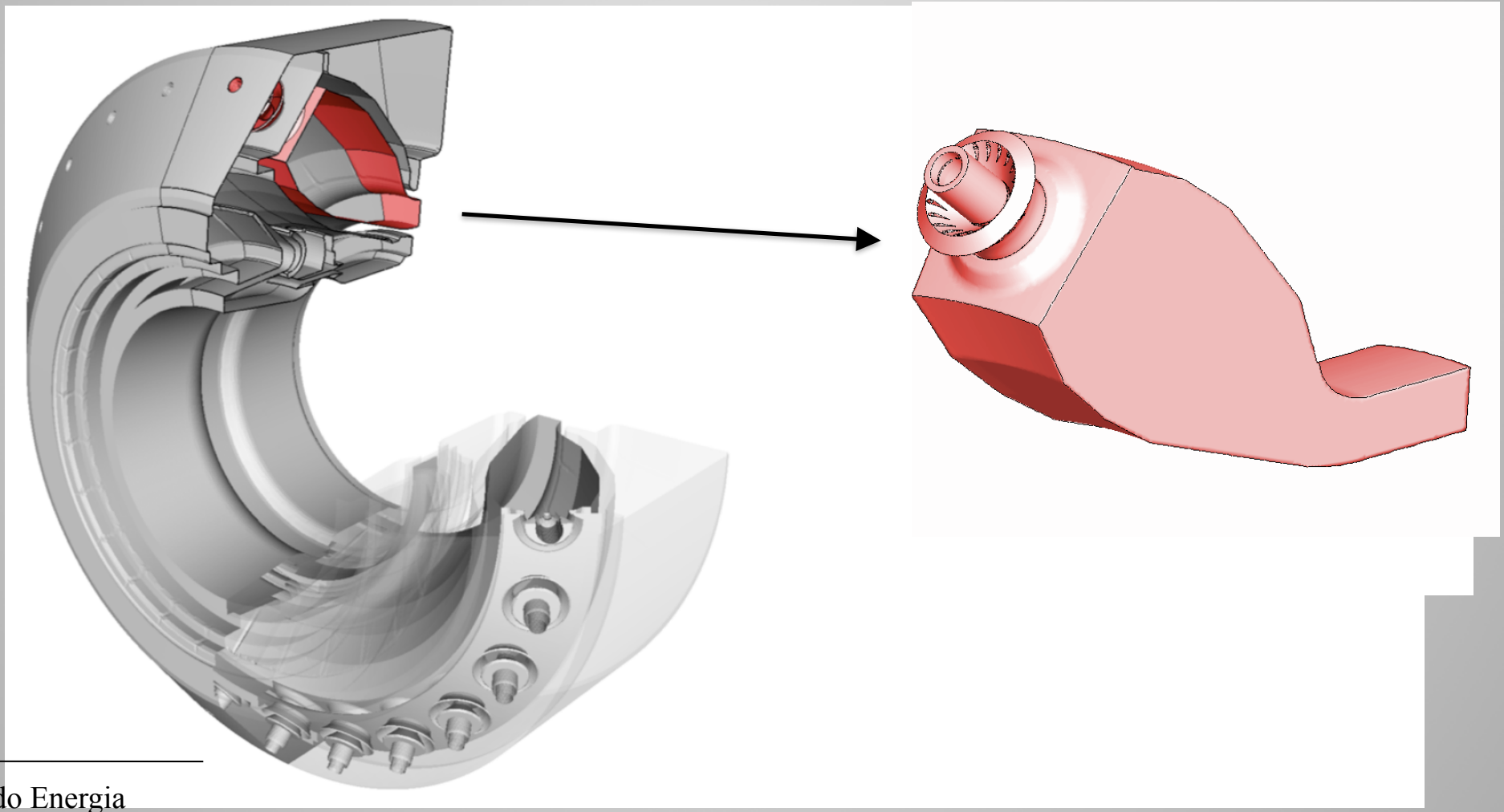




Target configuration

Annular combustion chamber [35]

LES of one sector

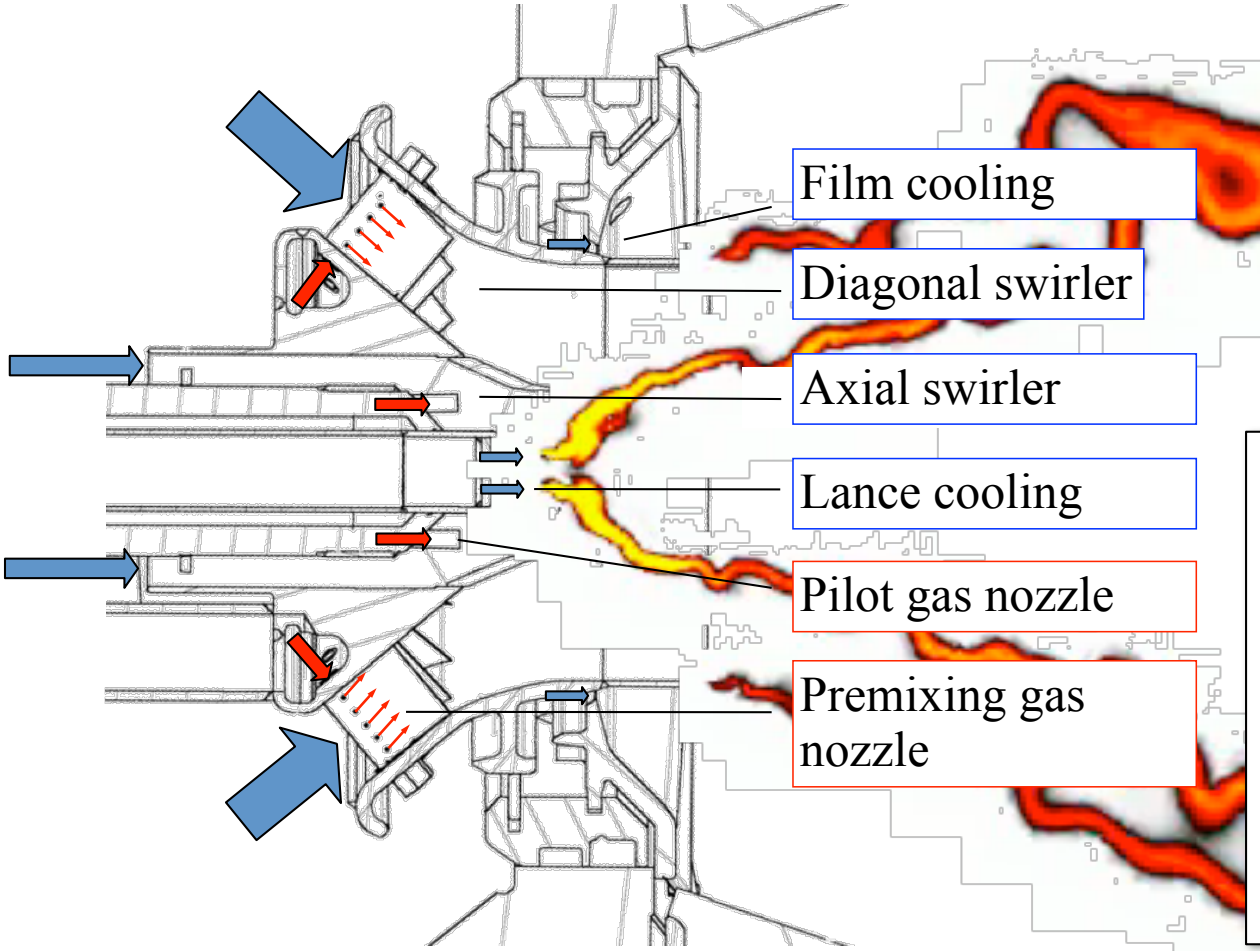


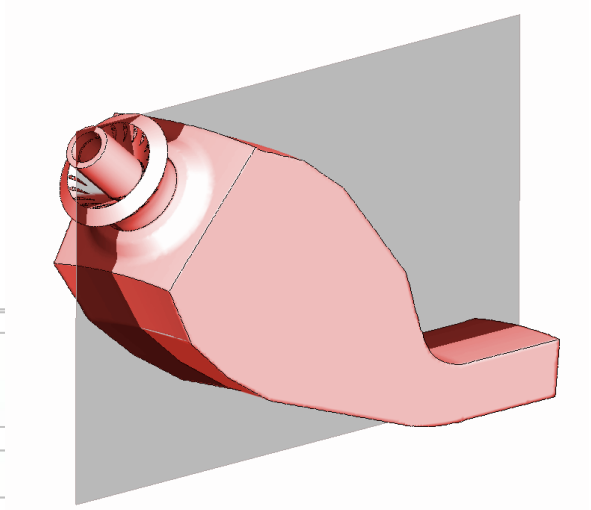
[35] Ansaldo Energia

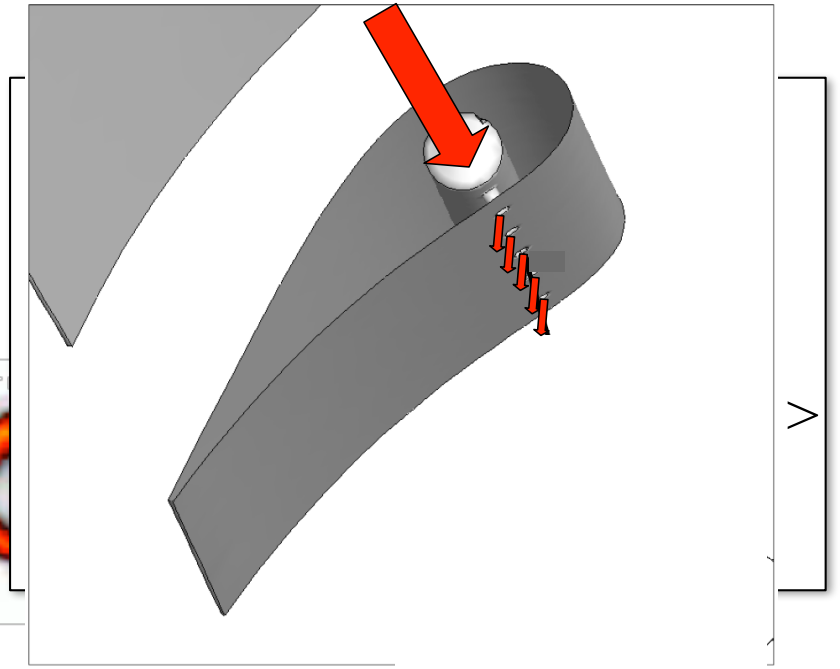
Target configuration

Burner

4 air inlets 2 CH_4 inlets

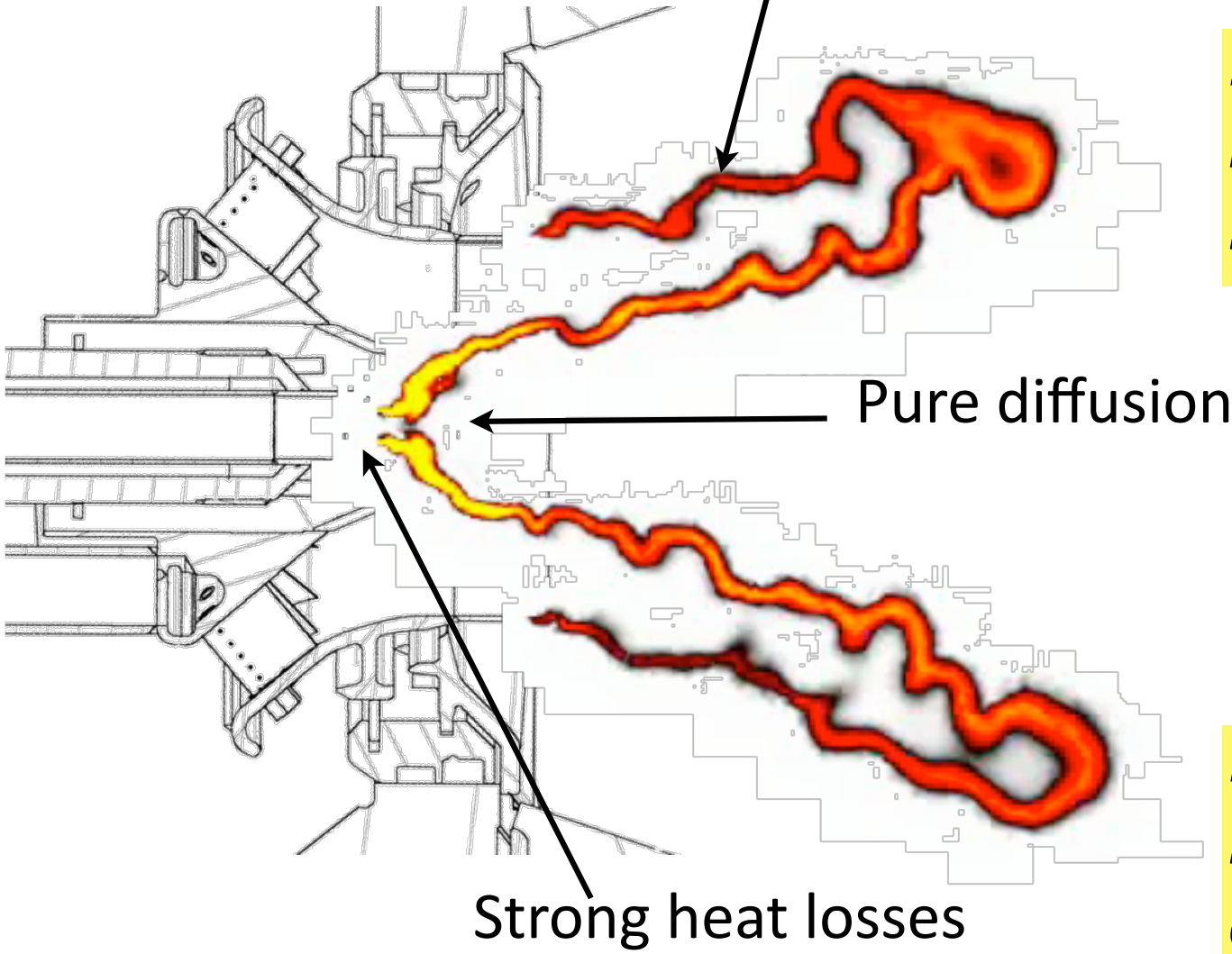






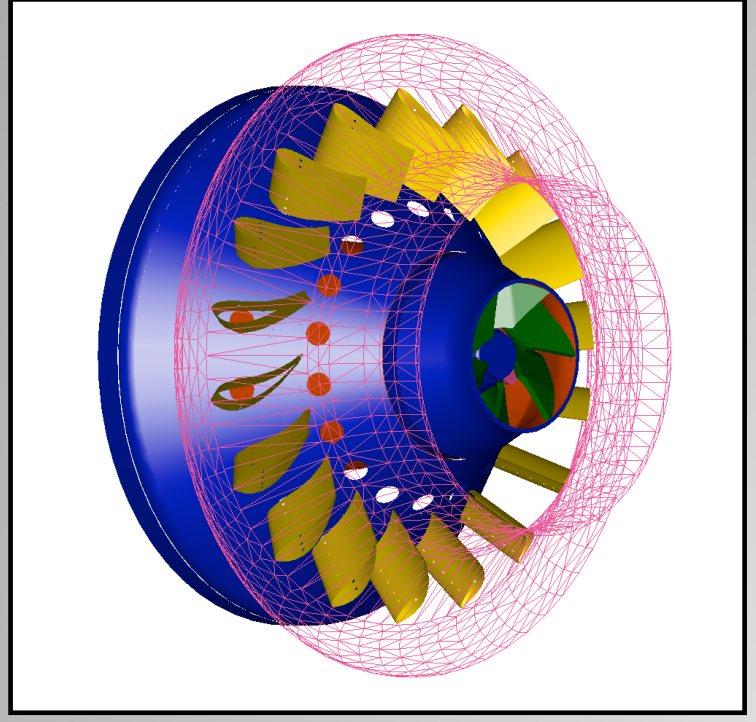
IMPLICATIONS FOR MODELING:

Six inlets ! Difficult to define a mixture fraction *z !*



Model must handle both regimes

Model must handle non adiabatic flames



LES Computations of the
Burner Fuel Injection

20°axisymmeric mesh, axial swirler closed

GEOMETRY

CERFACS, Toulouse

J. U. Schluter, T. Schonfeld, T. Poinsot

JANUARY 2000

All calculations made with AVBP

Not fully premixed
but not far

LES Computations of the
Burner Fuel Injection

20°axisymmeric mesh, axial swirler closed

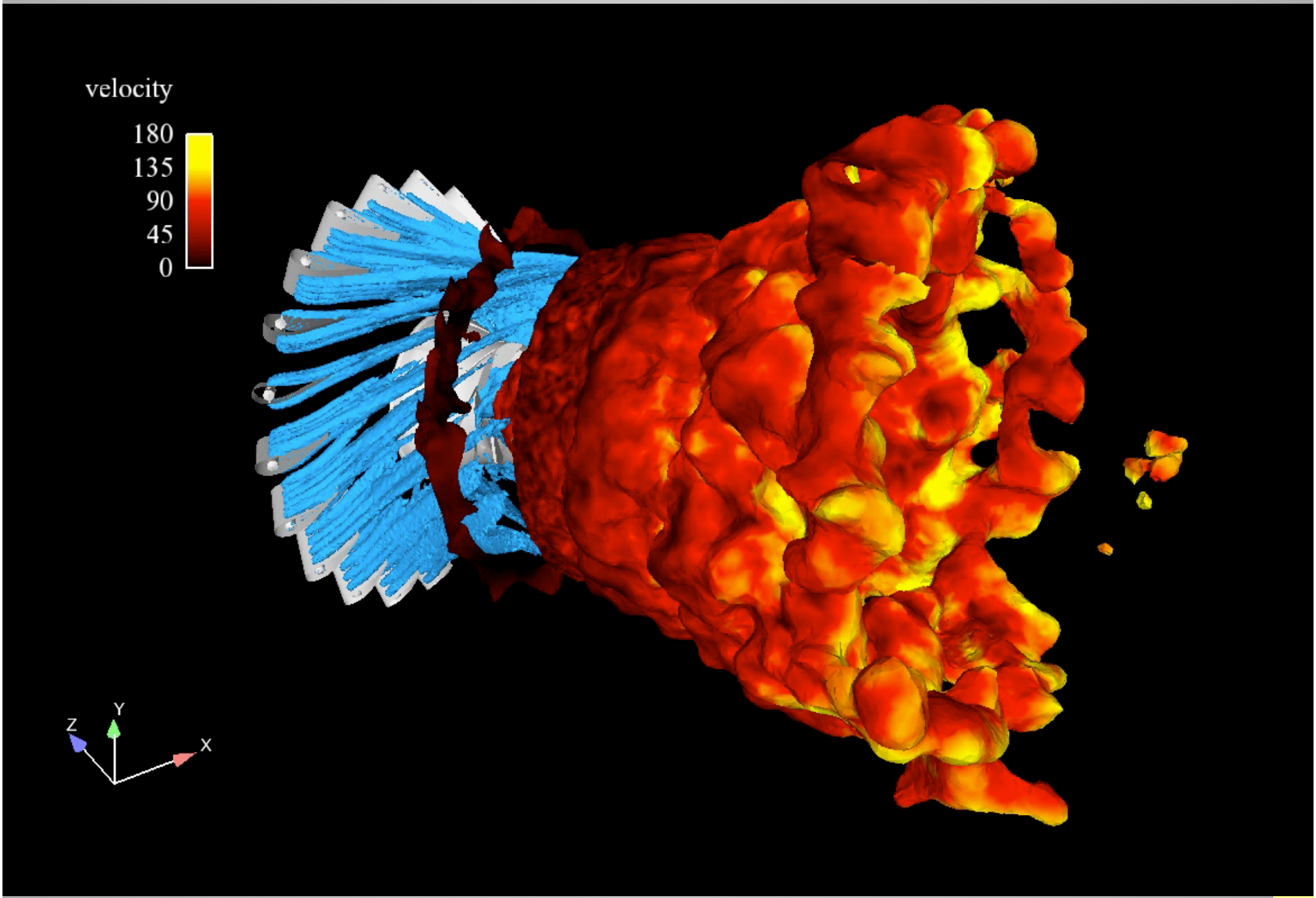
SMOKE VISUALIZATION (I)

CERFACS, Toulouse

J. U. Schluter, T. Schonfeld, T. Poinsot

JANUARY 2000

All calculations made with AVBP


velocity
180
135
90
45
0
Z
Y
X

Simulation tools for 3D flows

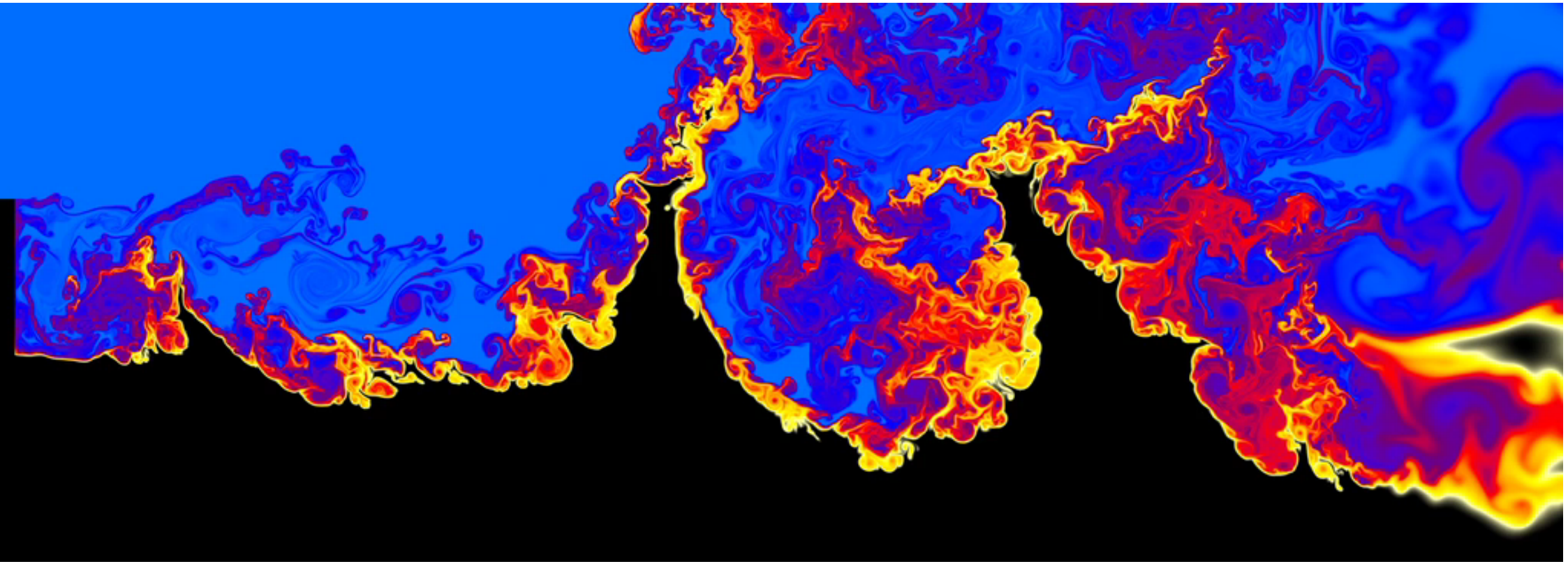
T. Poinsot

[1]*IMFT, CNRS, Toulouse France*

[2]*CERFACS, Toulouse France*

[3]*CTR, Stanford*

TNC book: Ch. 8, 9, 10



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OUTLINE:

RANS / LES / DNS: WHY LES WILL REPLACE RANS

WHAT IS NEEDED FOR LES - PHYSICAL MODELS:

- INTRODUCTION OF TURBULENCE AT INLETS
- CHARACTERISTIC BOUNDARY CONDITIONS
- TURBULENCE SUB GRID MODELS

WHAT IS NEEDED FOR LES - NUMERICS:

- DISPERSION AND DISSIPATION OF LES CODES
- GHOST WAVES AND BOUNDARY CONDITIONS
- ACOUSTIC ENERGY BALANCES
- MASSIVELY PARALLEL CODES

	LAMINAR	TURBULENT
0D codes: **T=f(t) Yk=gk(t)**	**CHEMKIN, COSILAB** **CANTERA**	**PSR: everything mixes infinitely fast. Only chemistry is going on**
PREMIXED	**CHEMKIN, COSILAB** **CANTERA: ‘premix’**	***TURBULENT CODES***
DIFFUSION	**CHEMKIN, COSILAB** **CANTERA: ‘oppdiff’**	

Will talk only about the compressible reacting Navier Stokes equations.

Arrhenius reaction rates (CHEMKIN based)

No simplifications using special models (infinitely fast chemistry, flamelet model etc).

Acoustics included

Full multispecies formulation, no simplification for the state equation, variable heat capacities

WE DO HAVE THE EQUATIONS: Navier Stokes (NS)

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0$$

$$\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial}{\partial x_i} \left(\rho \left(u_i + V_{k,i} \right) Y_k \right) = \dot{\omega}_k$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

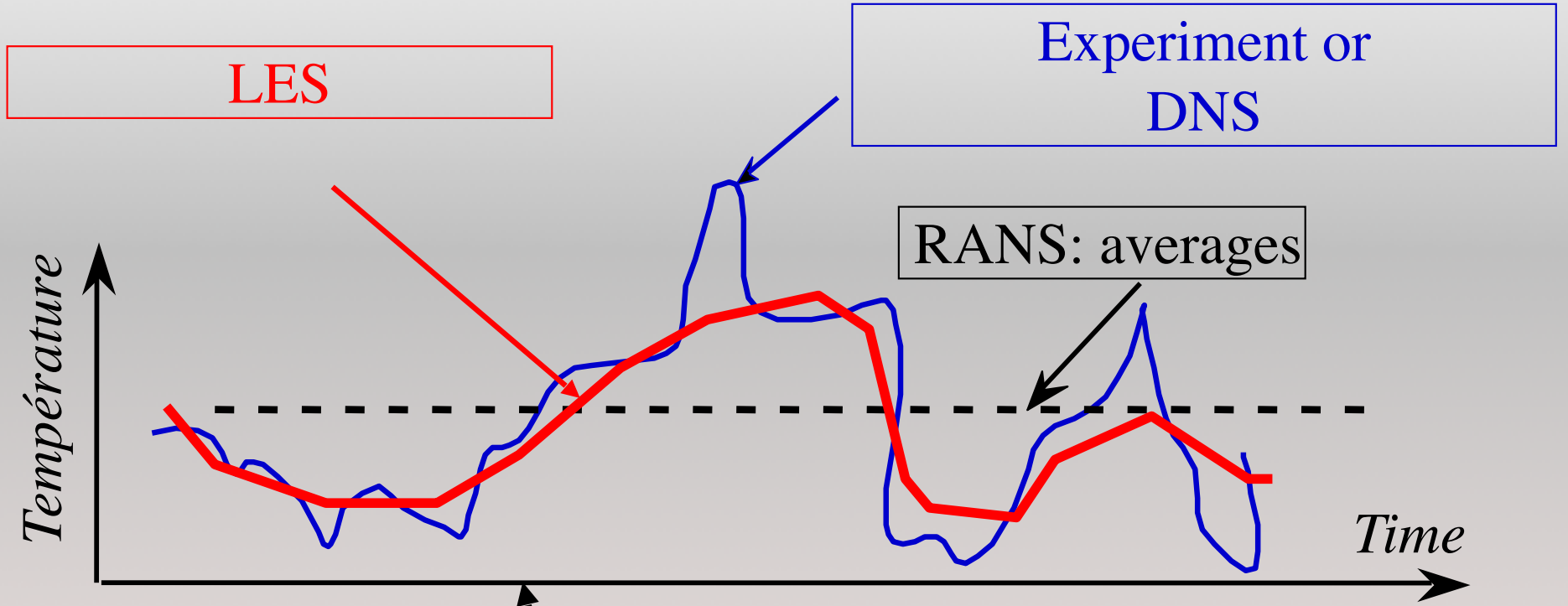
$$\rho \frac{DE}{Dt} = -\frac{\partial q_i^*}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij} u_i) - \frac{\partial}{\partial x_i}(p u_i) + \dot{\omega}_T$$

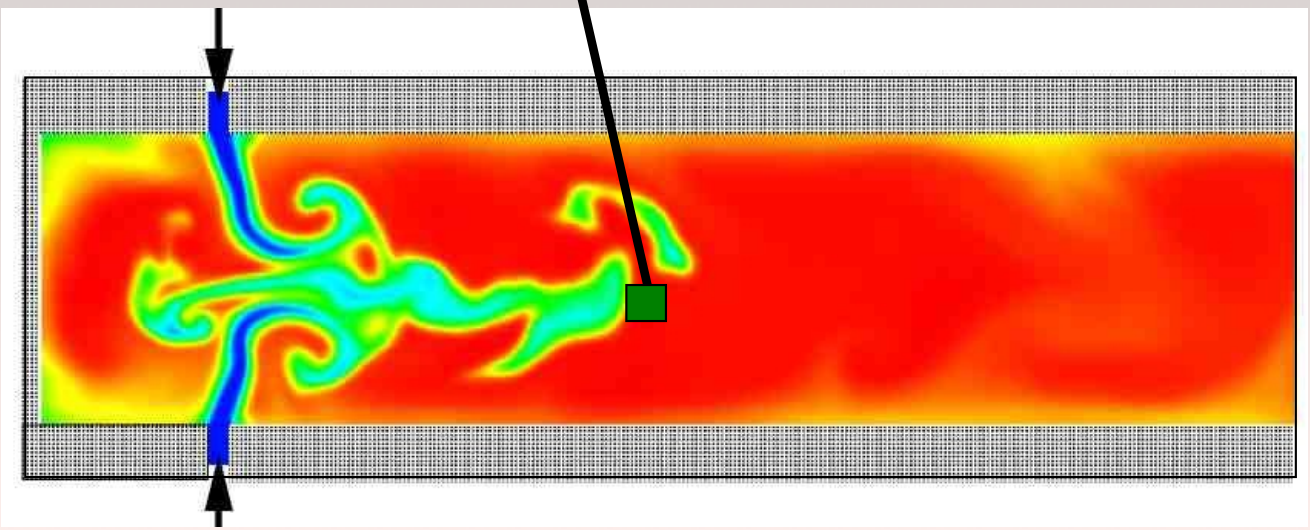
$$\frac{p}{\rho} = r\, T$$

1/ THE NS EQUATIONS ARE EXACT
2/ THE NS EQUATIONS CONTAIN TURBULENCE

THE MAIN ISSUE IS HOW TO HANDLE TURBULENCE !

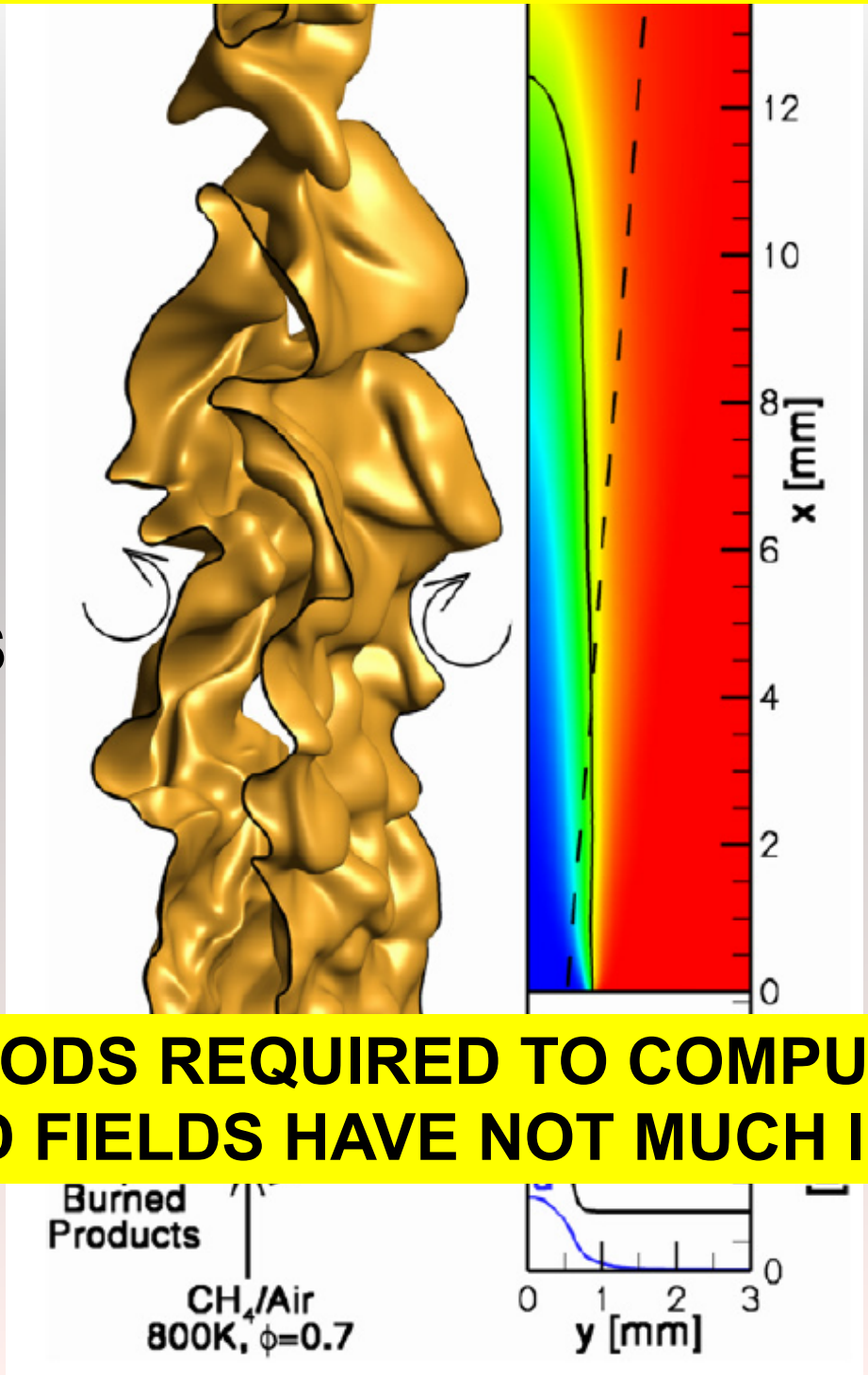
Methods for turbulent flows:





Ch. 4 Section 4.2

Instantaneous and averaged flows have not much in common



Chen et al
31st Symp.

INSTANTANEOUS

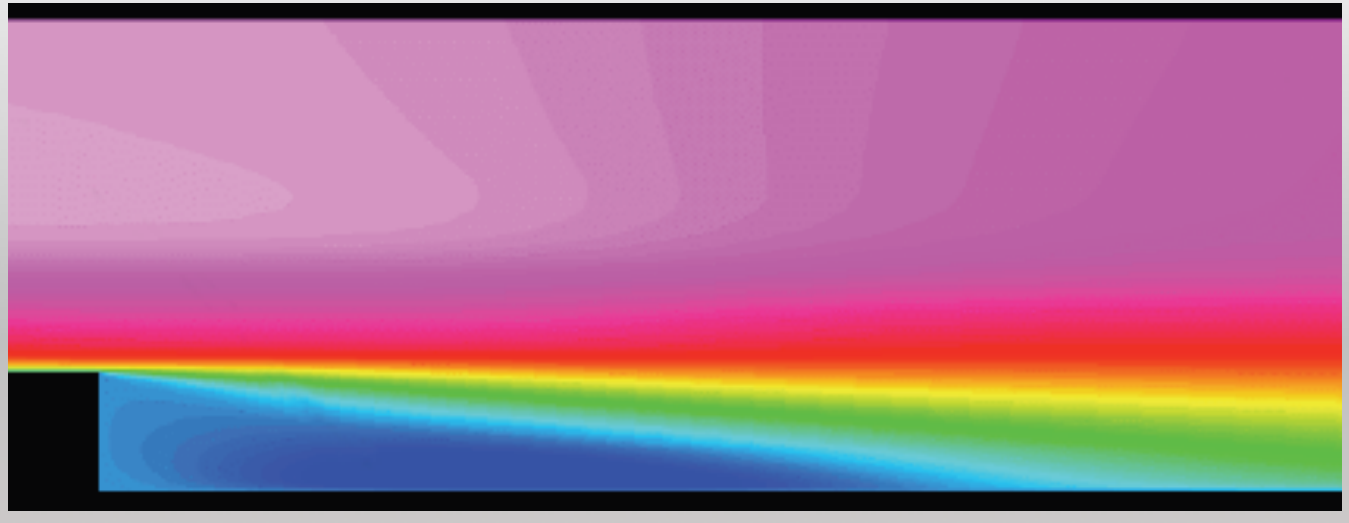
AVERAGED

AND THE METHODS REQUIRED TO COMPUTE INSTANTANEOUS OR AVERAGED FIELDS HAVE NOT MUCH IN COMMON EITHER

A big difference between RANS and LES averaging:

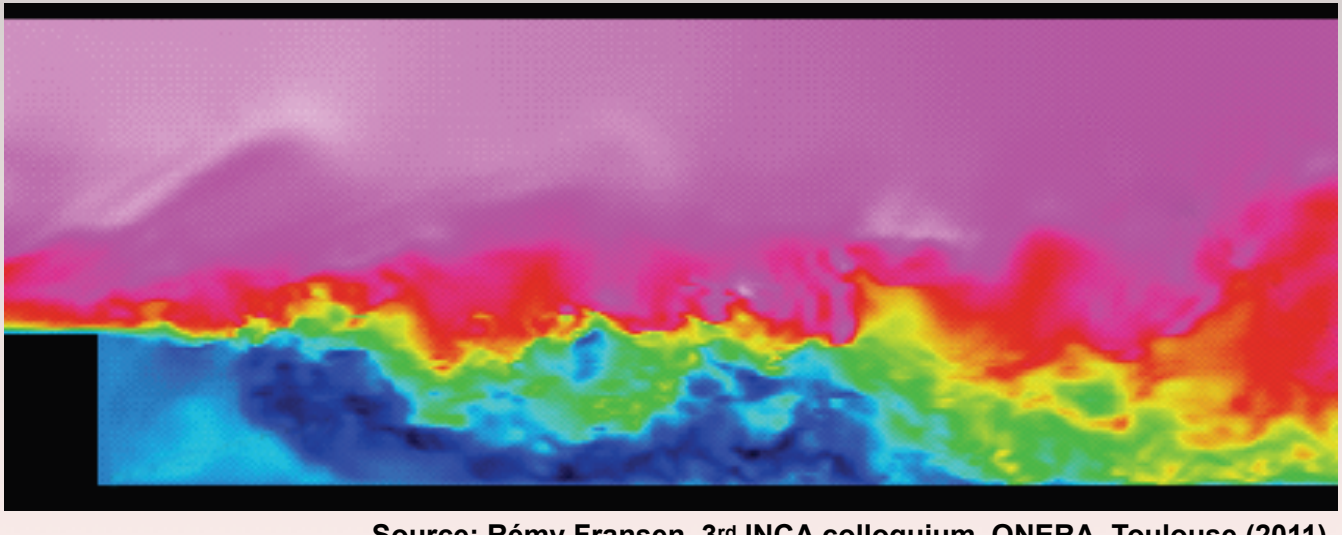
-In RANS, averaging is performed over time (or realizations). By definition, RANS variables do not depend on time (even if certain groups try to develop U-RANS methods)

- In LES averaging is performed locally over space (a small zone around each point). LES variables are time-dependent quantities



Source: Rémy Fransen, 3rd INCA colloquium, ONERA, Toulouse (2011)

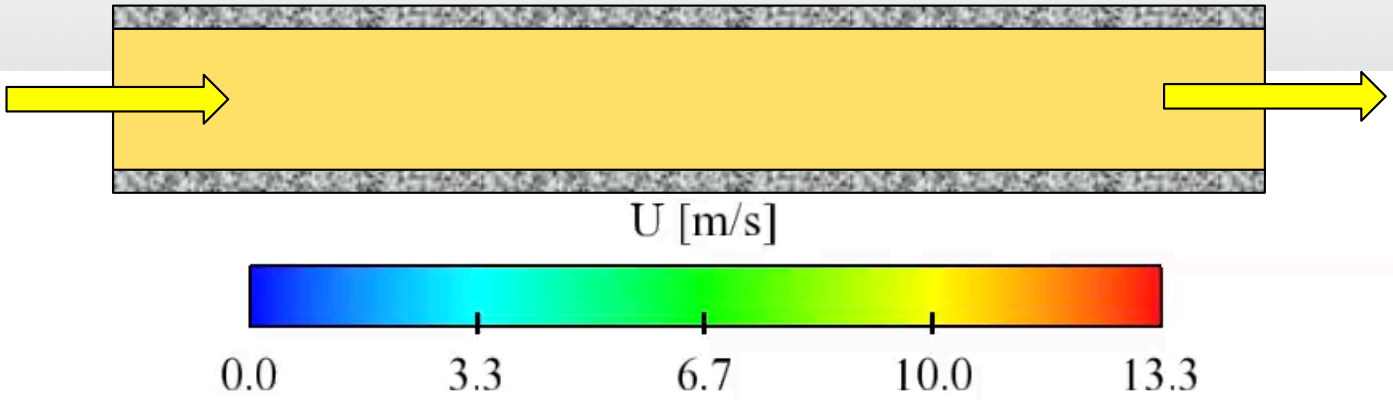
RANS



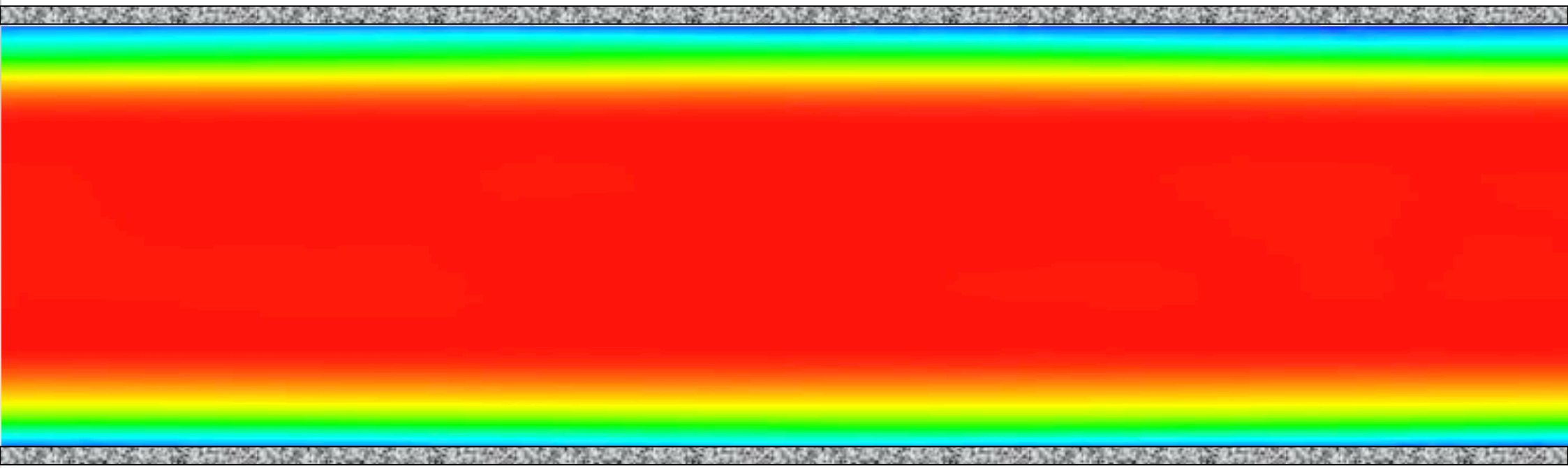
Source: Rémy Fransen, 3rd INCA colloquium, ONERA, Toulouse (2011)

LES

Same duct computed first with RANS and then with LES:



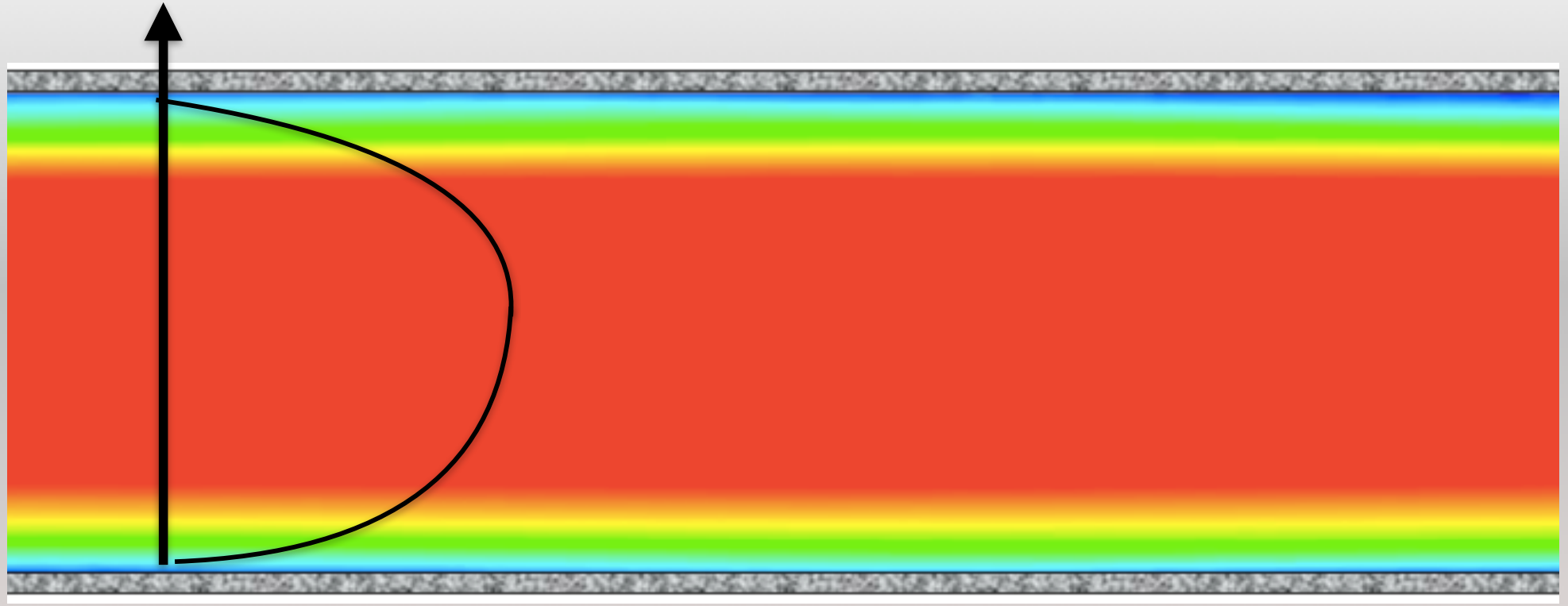
At t=0.5 s we switch from RANS to LES:



$t = 0.440$ s

NON REACTING

RANS

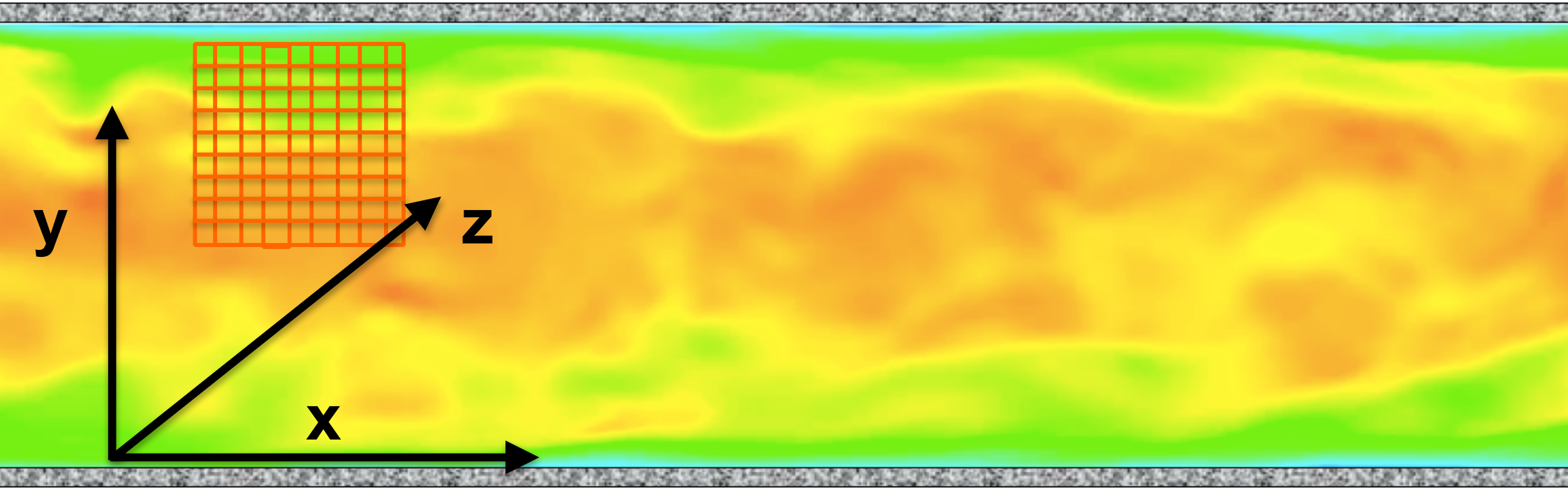


To resolve this velocity profile, we need:

- **10 points in the transverse direction**
- **2 in the longitudinal direction (there is no gradient)**

This is a very cheap RANS computation which can be done with only 20 points

LES



To resolve this velocity profile, we need:
- points in y direction because gradients are stronger
- points in z direction too because turbulence is … 3D !
- a resolution in time because all velocities fluctuate
This LES will require many points and many time iterations

RANS has other problems:

- Certain phenomena can simply not be averaged: ignition, quenching, instabilities

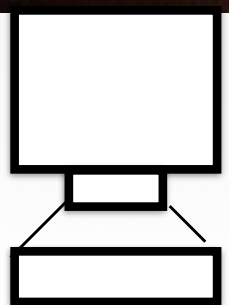
- Acoustic waves are not handled correctly by RANS formulations:

- **they are intrinsically unsteady mechanisms which can not be ‘averaged’**
- **the solvers used in RANS utilize large turbulent and numerical viscosities which kill acoustic waves**

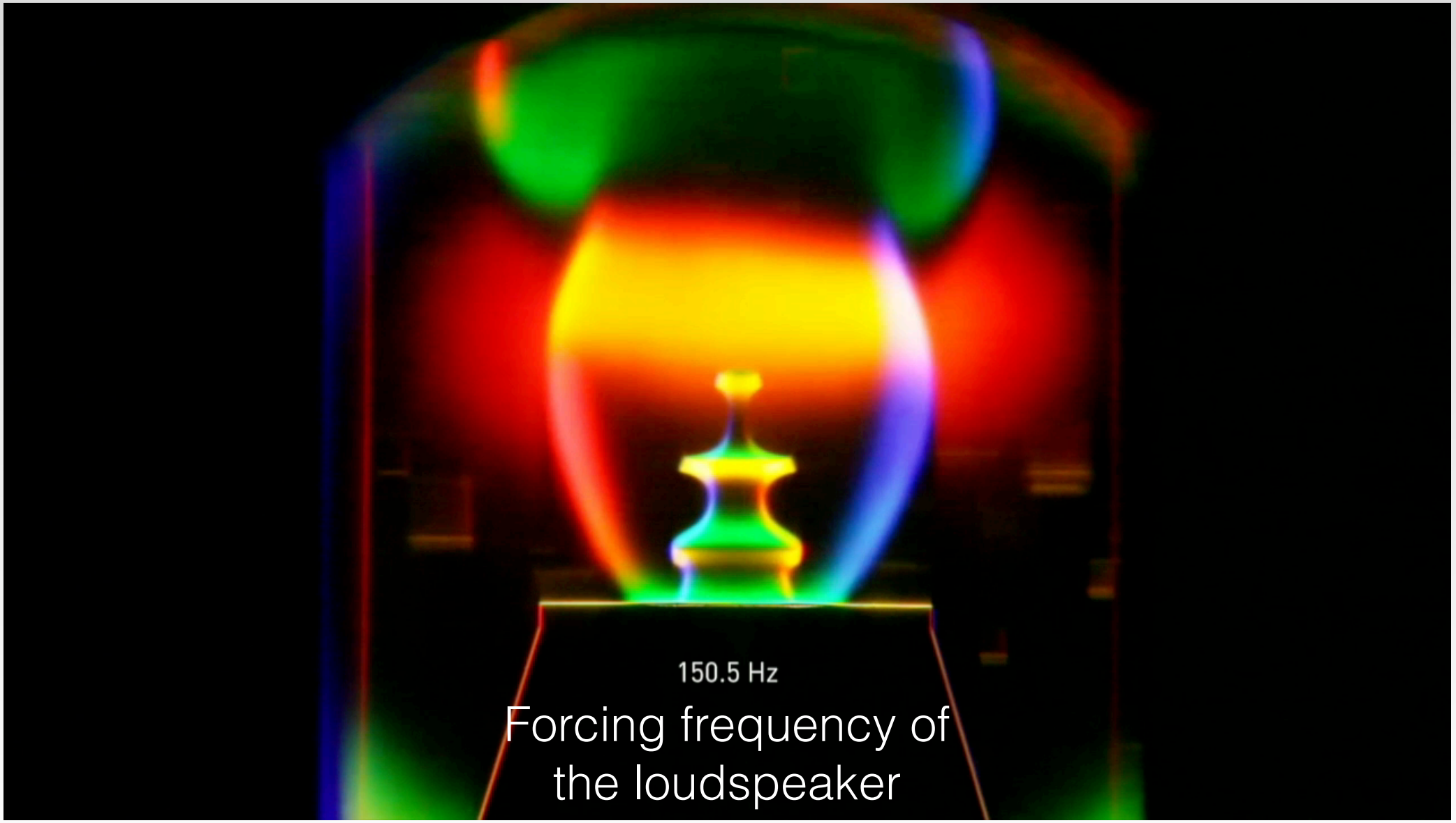
- Impossible to compute with RANS: **flames** excited by **acoustics**





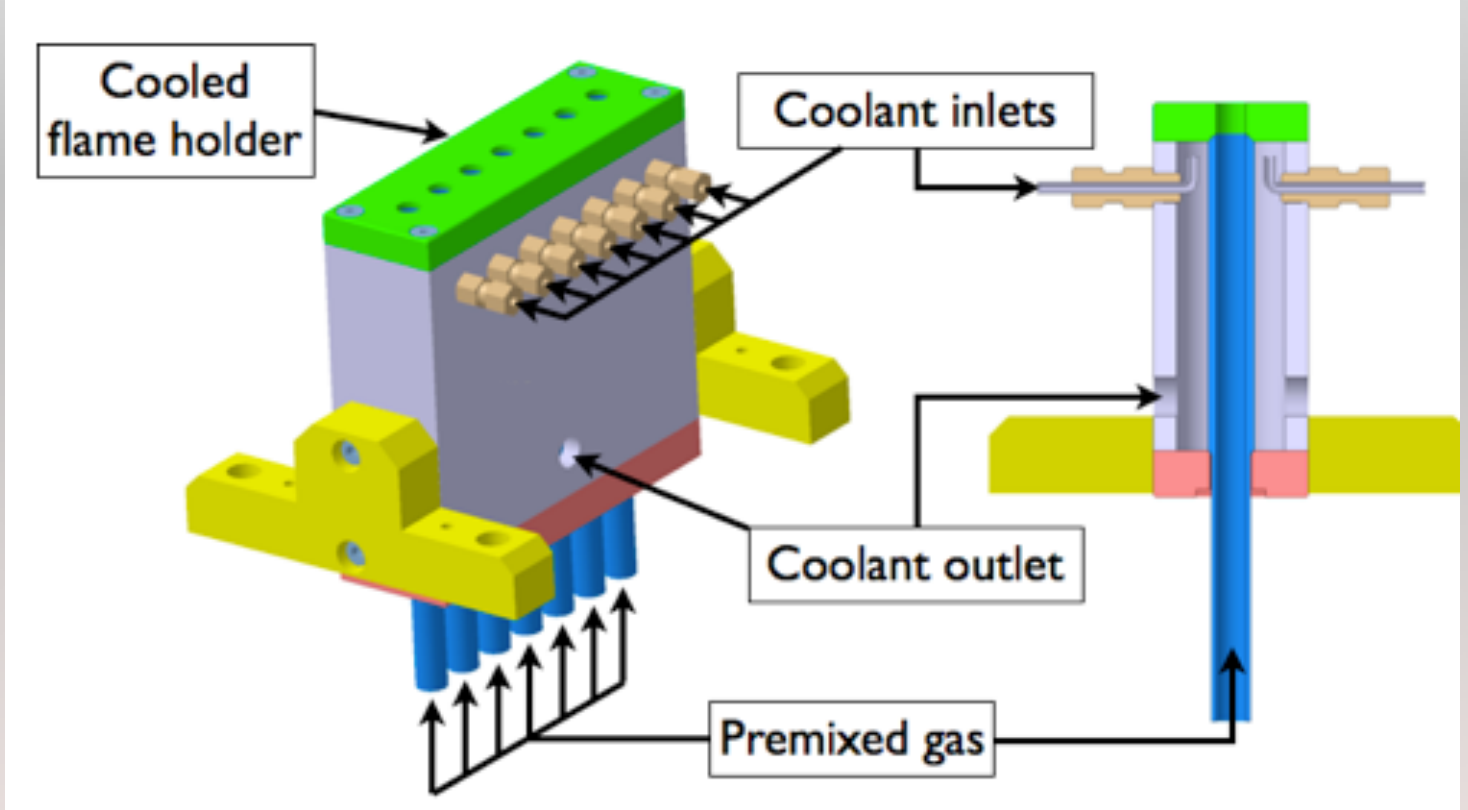


Loudpeaker


150.5 Hz
Forcing frequency of
the loudspeaker



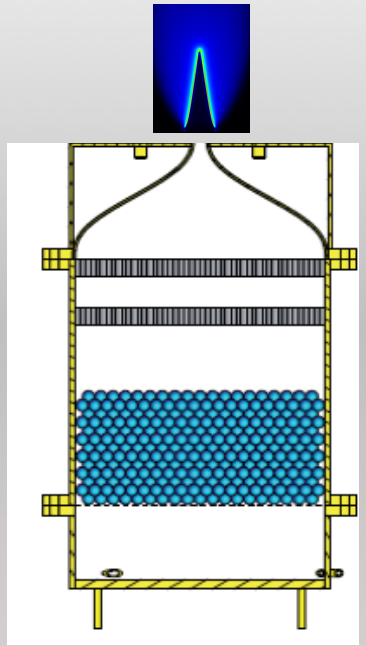
Example of experiment which cannot be computed with RANS:

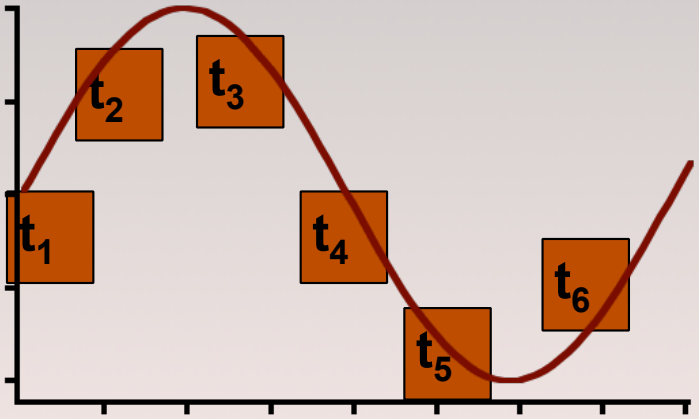


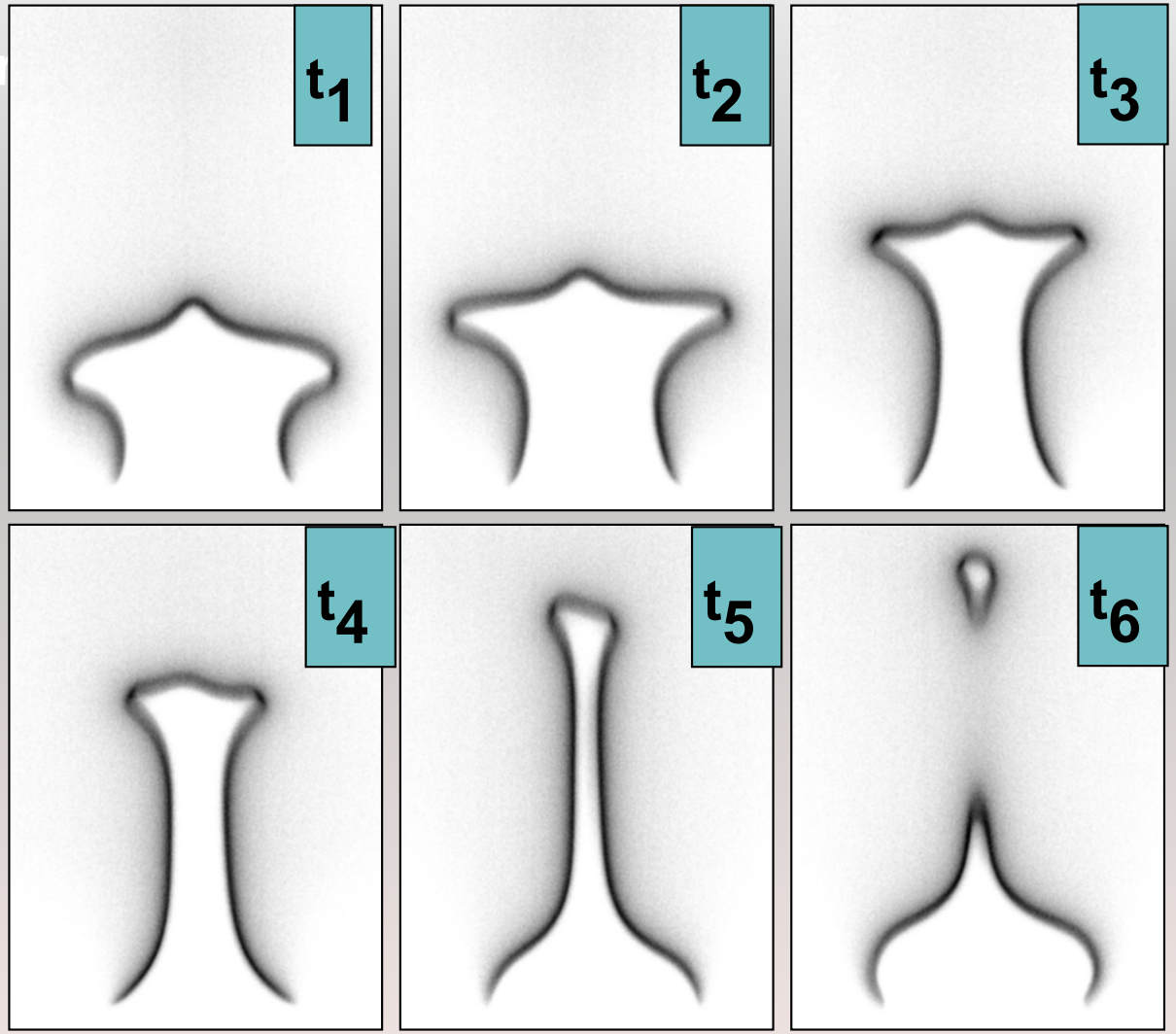


D. Mejia PhD IMFT

Response to harmonic forcing by a loud speaker:







Y. Dhue PhD IMFT

Response to music:

Columbian movie: image by D. Mejia (PhD),
music by Shakira



LeConte, J. On the influence of musical sounds on the flame of a jet of coal gas. American Journal of Science and Arts 23(2) (1858), 62–67.

RANS has other problems:

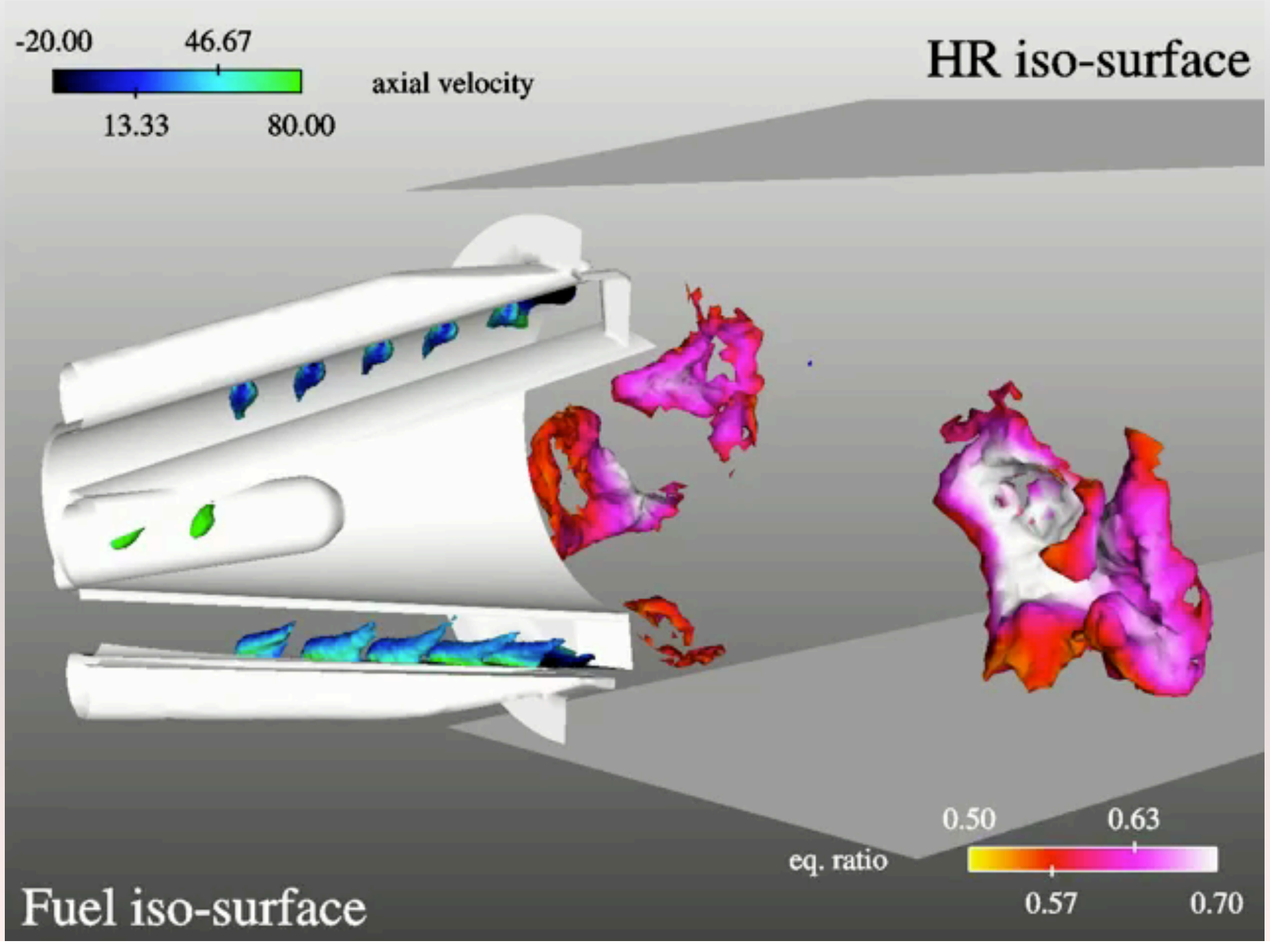
- Certain phenomena can simply not be averaged: ignition, quenching, instabilities

- Acoustic waves are not handled correctly by RANS formulations:
  - they are intrinsically unsteady mechanisms which can not be ‘averaged’
  - the solvers used in RANS utilize large turbulent and numerical viscosities which kill acoustic waves

- Thermoacoustics (combustion instabilities) is by nature unsteady and cant be computed with RANS

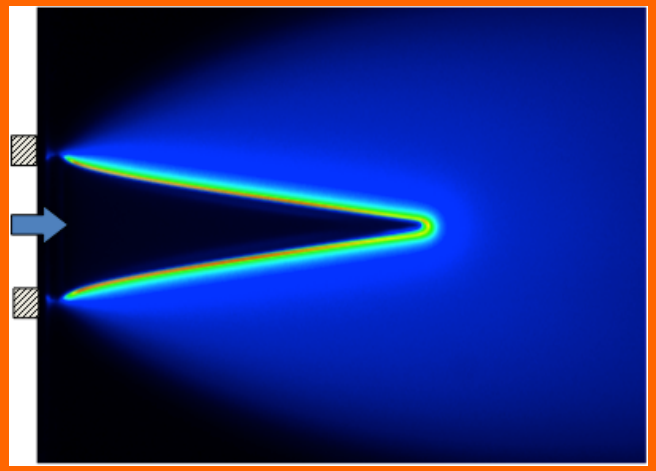
Ch. 8

WHAT WOULD THE MEAN OF THIS FLOW MEAN ?



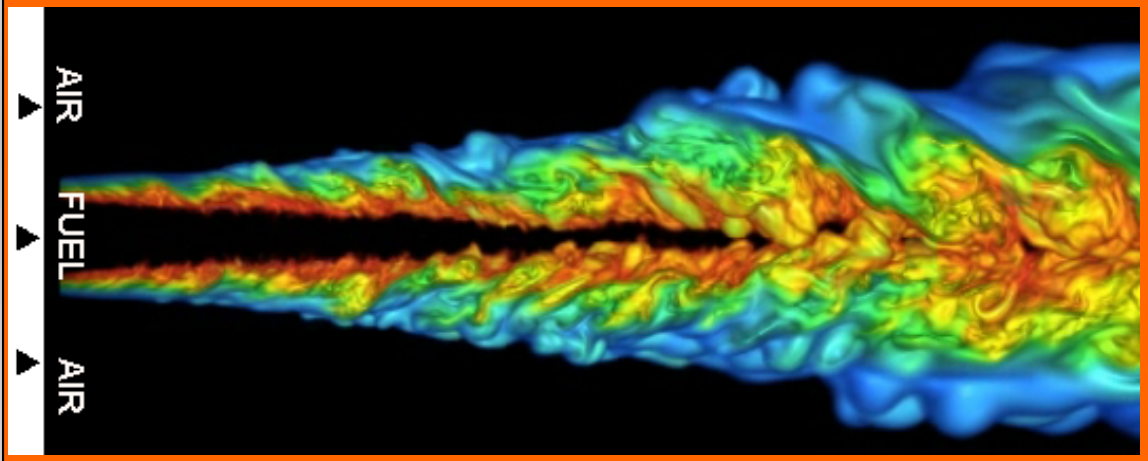
We classify flames as :

LAMINAR



IMFT group

OR TURBULENT

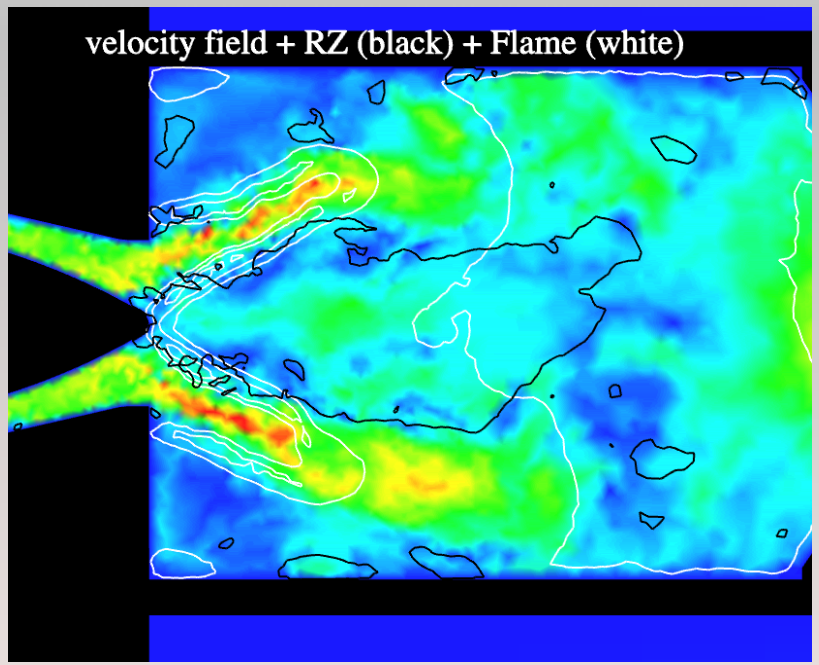


Sandia group

But flames can be LAMINAR AND TURBULENT:

- In space
- In time

LAMINAR AND TURBULENT IN SPACE: Some parts of a combustor may actually be laminar. Turbulence/flame models should degenerate to laminar flame models when the flow becomes laminar.

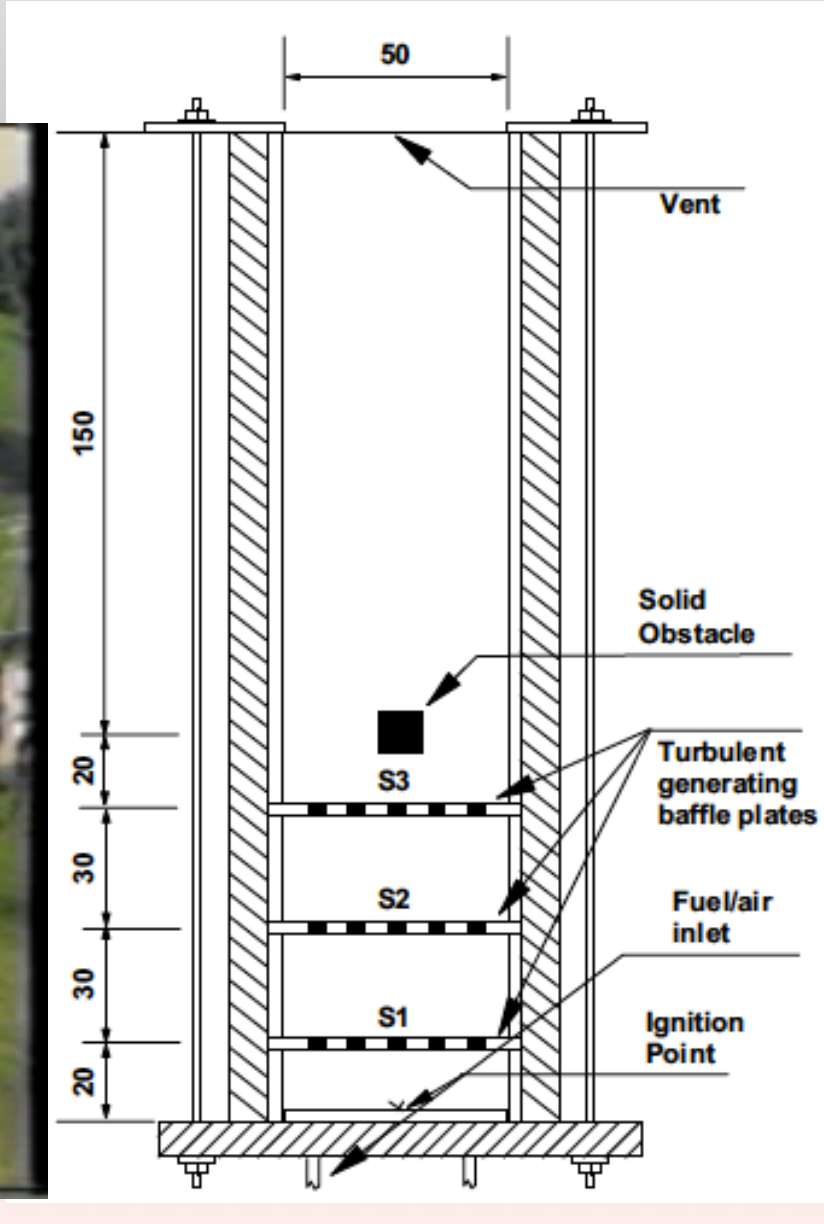


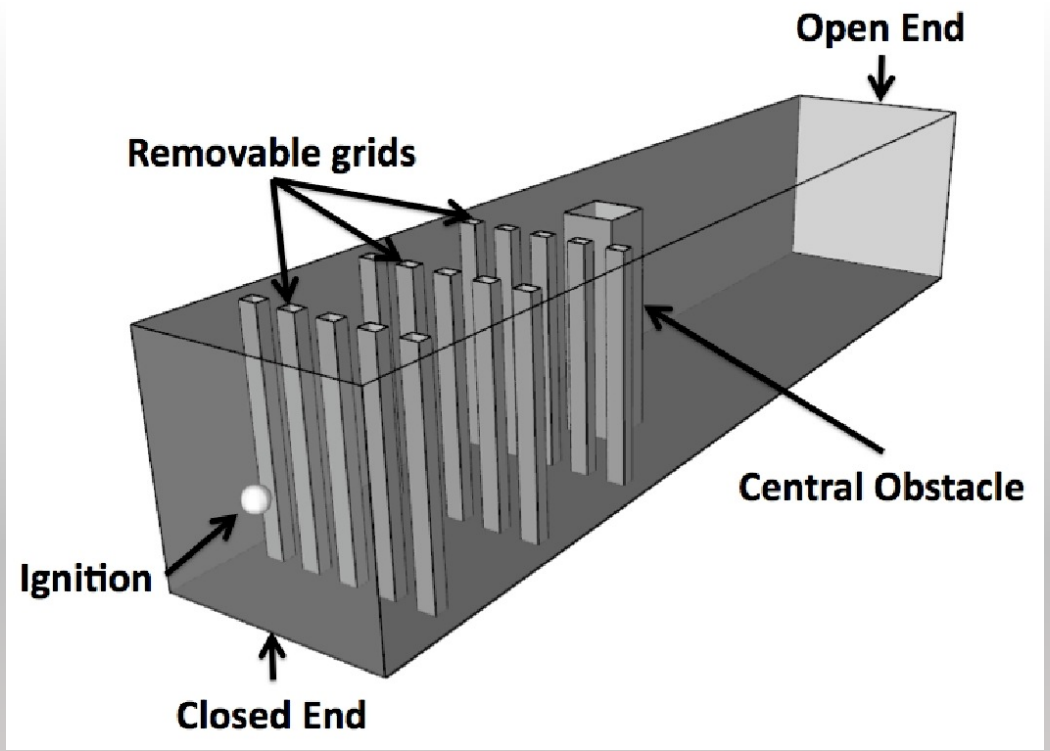
- Most RANS models don't… (EBU or Magnussen for example). Actually no turbulent combustion model can handle full chemistry with precision

LAMINAR AND TURBULENT IN TIME: flames can begin as laminar and become turbulent:

- Explosions
- Piston engines

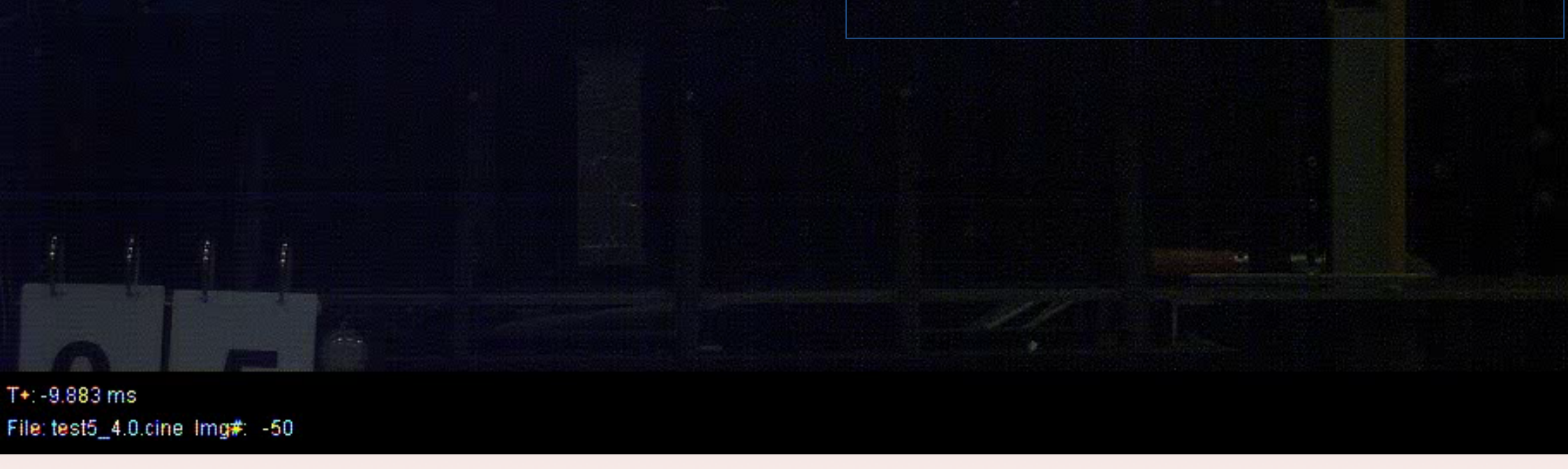


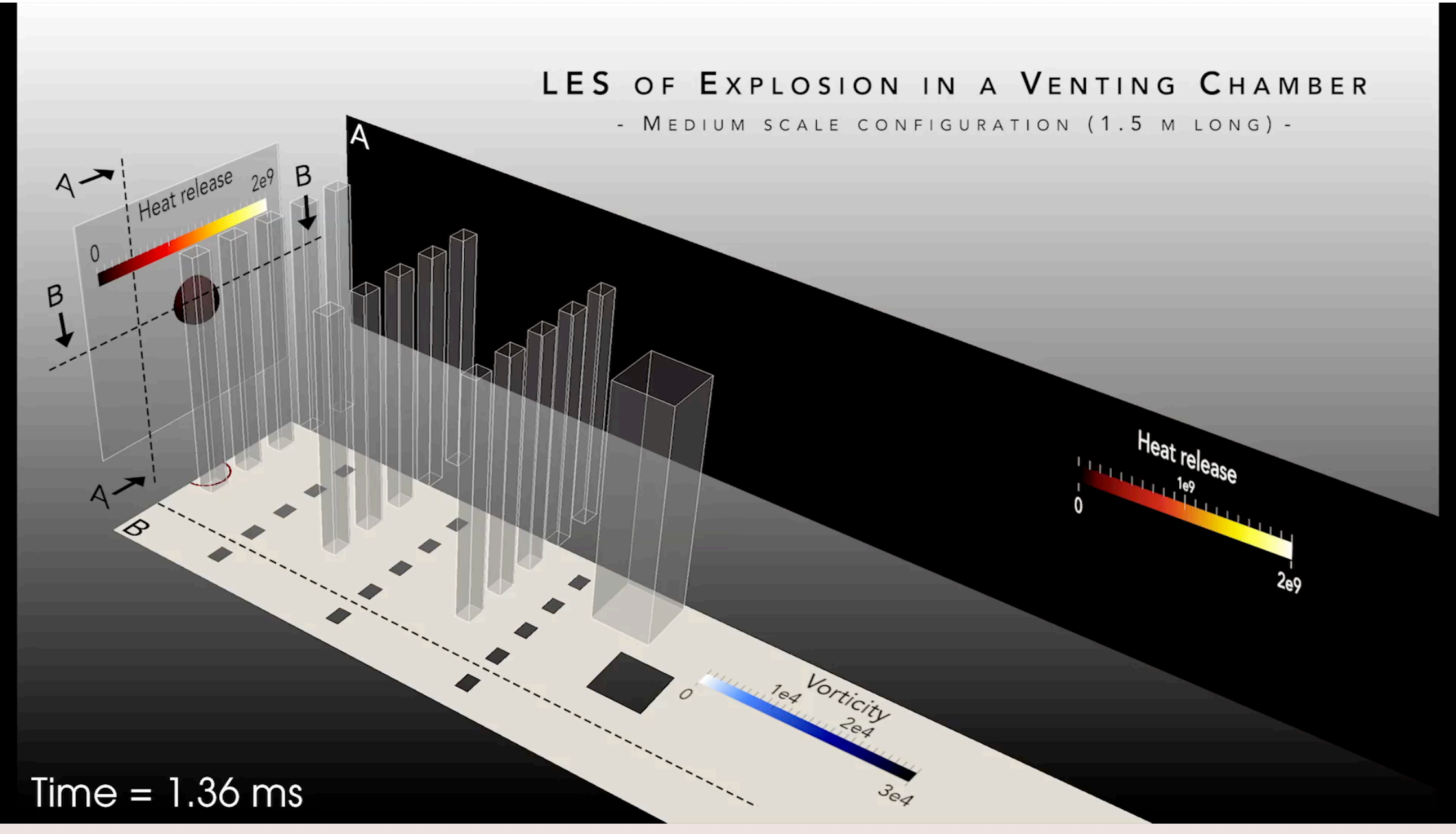




Sydney or Gexcon experiments

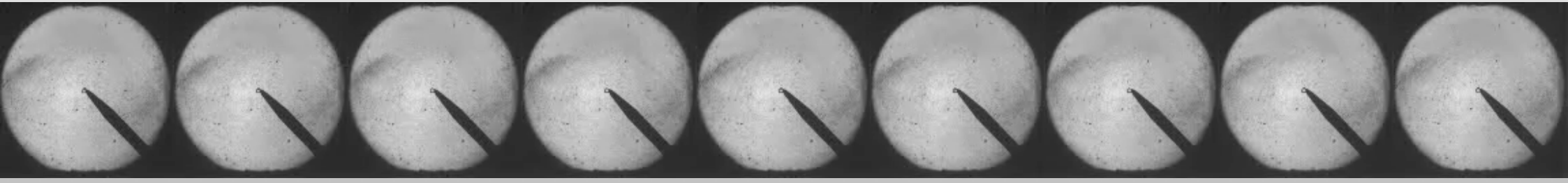
- Box : 5x5x25 cm
- Fuel/Air mixture at Φ=1
- Fuel :
  - LPG (95% C_3H_8)
  - CNG (90% CH_4)
  - H2
- One central square obstruction
- 3 turbulence generating grids





Initially laminar, fully unsteady, what would be the mean of this flow ?

Piston engines: flames begin as laminar kernels and become turbulent later.



A model for ignition in a piston engine must account for the initial laminar phase.

This initial phase lasts longer when the flow is less turbulent.

So:

RANS codes do turbulent flames
but can NOT do laminar flames:

- **RANS models do not resolve flame fronts**
- **RANS models resolve only the mean position of flames: the laminar structure is fully modelled**
- **RANS codes are usually very dissipative and cannot track flame dynamics: a RANS flame front has a thickness of the order of 1 cm**
- **Molecular transport is usually not modelled in many RANS formulations (needed for laminar flames)**

OK, we should not do RANS.

So, what do we do ?

LES.... or even DNS !

Problem: going from RANS to LES is a big step:
- Introduction of turbulence at inlets ?
- Characteristic boundary conditions
- Turbulence models ?
- Introduction of chemistry ?

TNC Ch. 4 Section 4.8

OUTLINE:

RANS / LES / DNS: WHY LES WILL REPLACE RANS

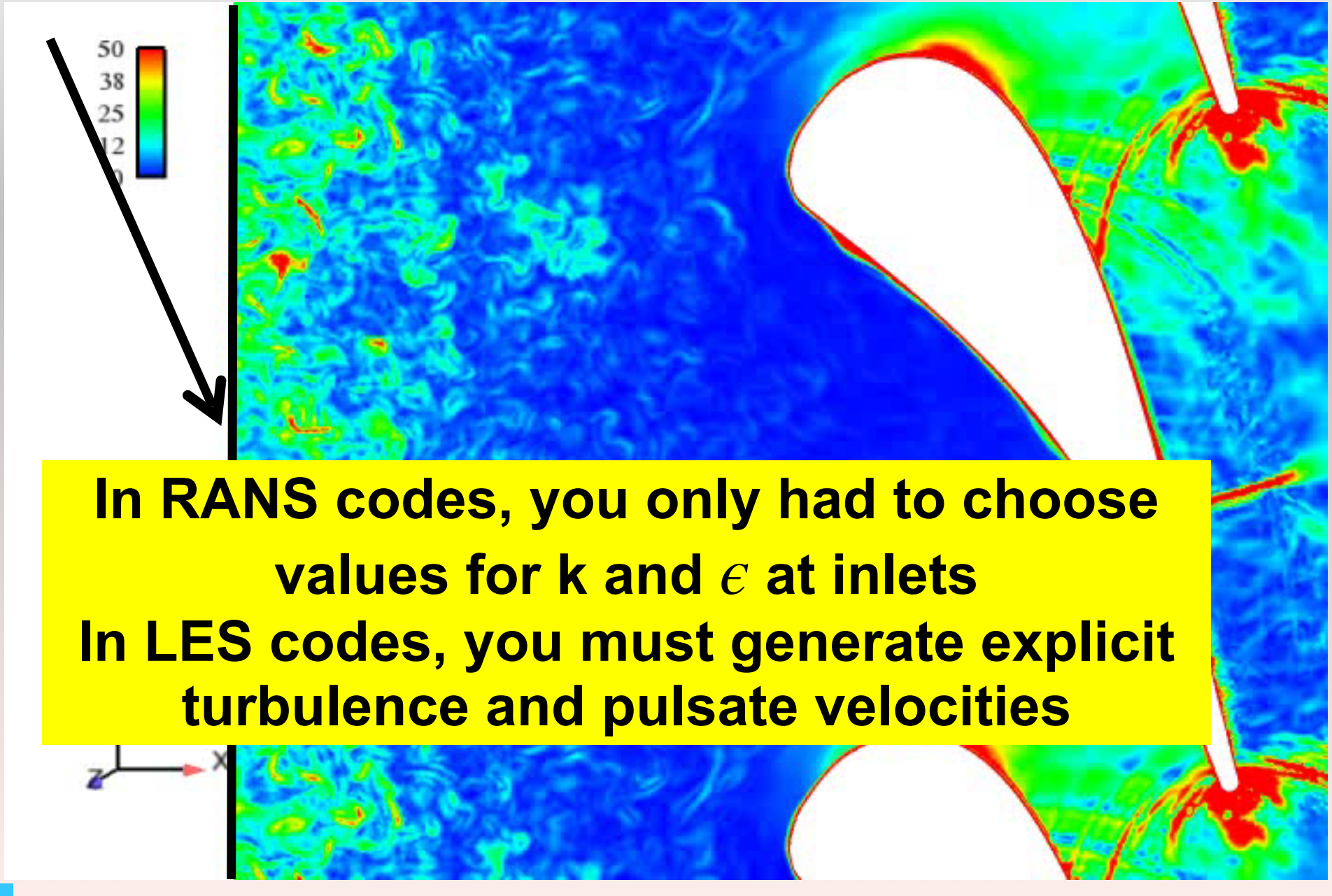
WHAT IS NEEDED FOR LES - PHYSICAL MODELS:

- INTRODUCTION OF TURBULENCE AT INLETS
- CHARACTERISTIC BOUNDARY CONDITIONS
- TURBULENCE SUB GRID MODELS

WHAT IS NEEDED FOR LES - NUMERICS:

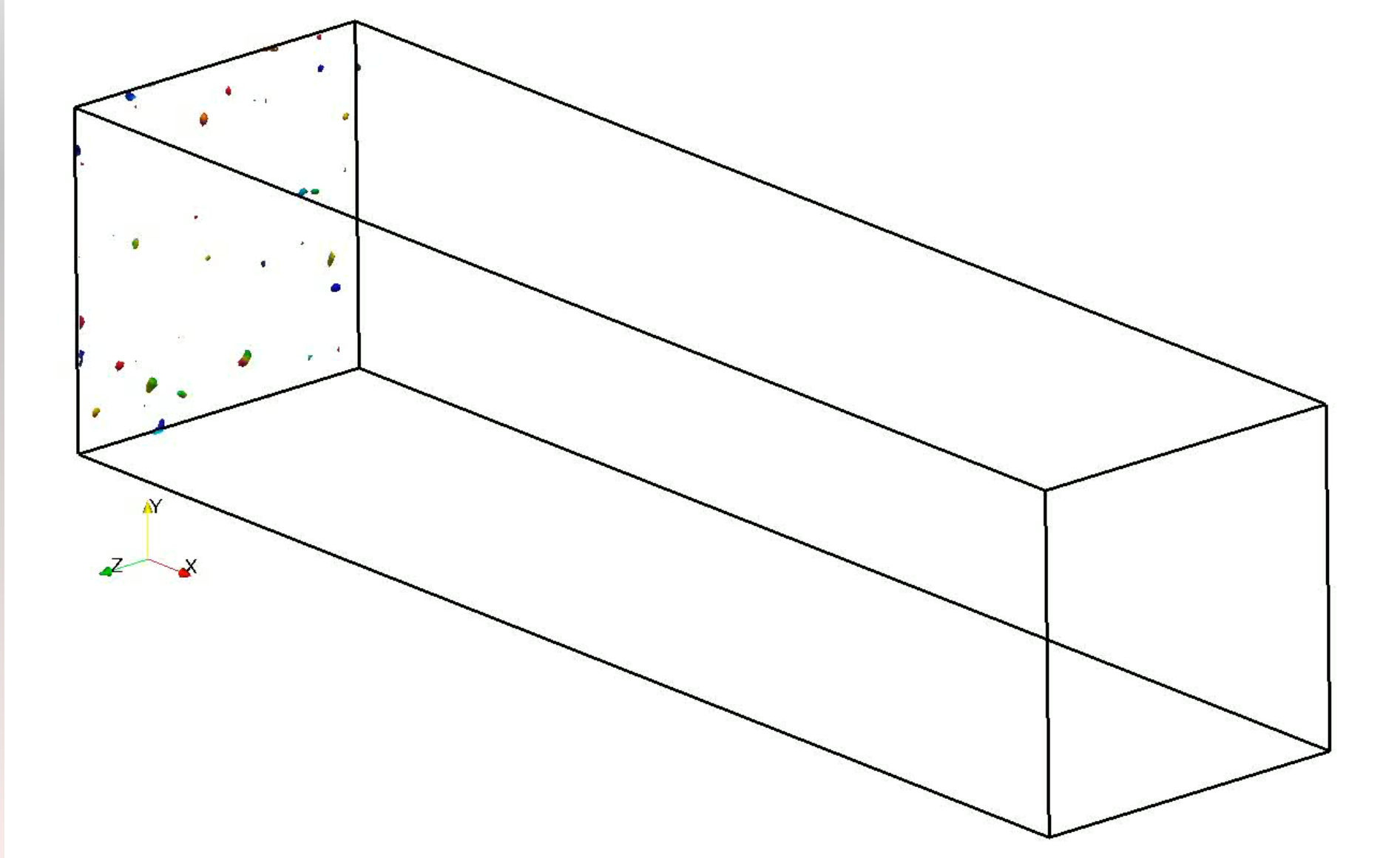
- DISPERSION AND DISSIPATION OF LES CODES
- GHOST WAVES AND BOUNDARY CONDITIONS
- ACOUSTIC ENERGY BALANCES
- MASSIVELY PARALLEL CODES

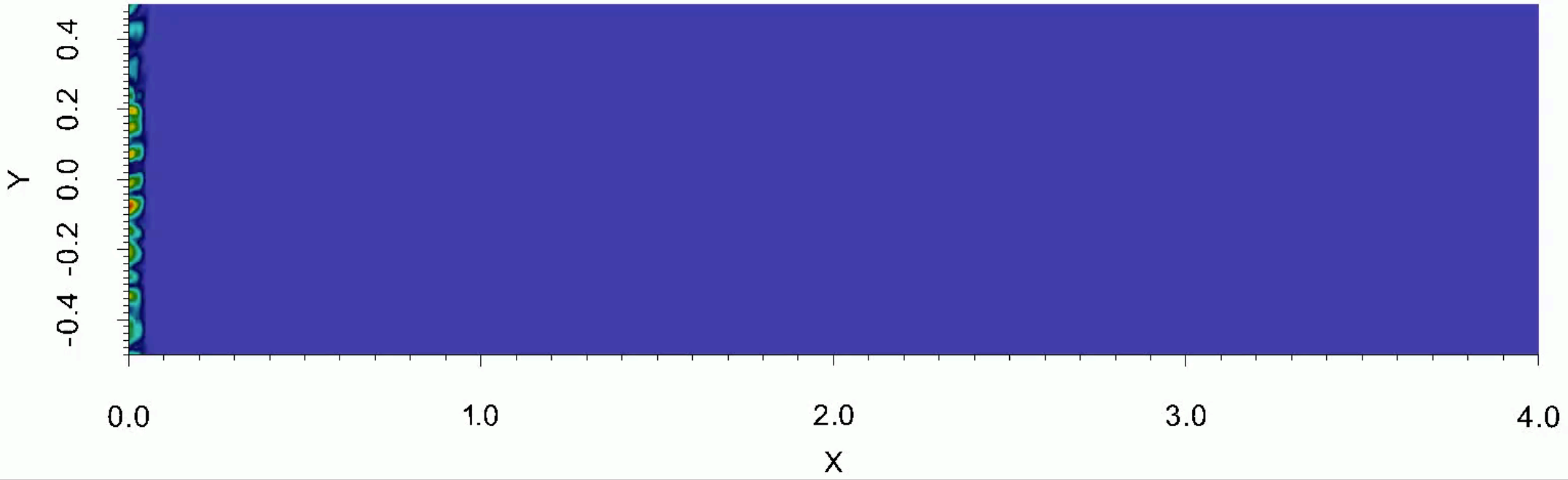
- # INTRODUCTION OF TURBULENCE AT INLETS



In RANS codes, you only had to choose values for k and ϵ at inlets

In LES codes, you must generate explicit turbulence and pulsate velocities


Y
Z
X



Injecting turbulence in a CFD code requires:

- to generate an unsteady turbulent flow

- and impose it at the inlet.

Injection of turbulence at inlets:

Ch. 9 Section 9.4.2

Two different issues:
- A turbulence spectrum must be chosen to construct a turbulent signal u,v,w (x,y,z=zo,t).
- This signal must then be imposed at the inlet of the LES. If this is a compressible flow, this must be done without introducing noise. In a subsonic flow this is difficult: we need to discuss boundary conditions treatments. Which means we need to talk about acoustics now…

Poinsot T. and Lele S. (1992). "Boundary conditions for direct simulations of compressible reacting flows", *Journal of Computational Physics 101, 1, 104-129.*
Guezennec and Poinsot. Acoustically Nonreflecting and Reflecting Boundary Conditions for Vorticity Injection in Compressible Solvers. *AIAA J.* 47, 7, 2009.
Yoo, C., and Im, H., "Characteristic Boundary Conditions for Simulations of Compressible Reacting Flows with Multidimensional, Viscous, and Reaction Effects," *Combustion Theory and Modeling*, Vol. 11, No. 2, 2007, pp. 259–286

ACOUSTICS:

Acoustic waves exist in all fluids and in all good compressible solvers… even if this flow has a small velocity. Start from :

$$\frac{\partial \rho}{\partial t} + \nabla(\rho u) = 0$$

$$\frac{\partial u}{\partial t} + u\nabla u + \frac{1}{\rho}\nabla p = 0$$

Consider a mean state in which there is no flow:

u=0 and p=po

Assume perturbations around this state and write

u= u' and p=po+p'

Assume isentropic flow:

$p = k\,\rho^{\gamma} \Rightarrow p'/p = \gamma\,\rho'/\rho \Rightarrow p' = c_o^2\,\rho'$

Linearize equations to obtain:

$$\frac{1}{c_o^2}\frac{\partial p'}{\partial t} + \rho_0 \nabla(u') = 0$$

$$\frac{\partial u'}{\partial t} + \frac{1}{\rho_0}\nabla p' = 0$$

For one-dimensional flow, combine these two equations to obtain the wave equation:

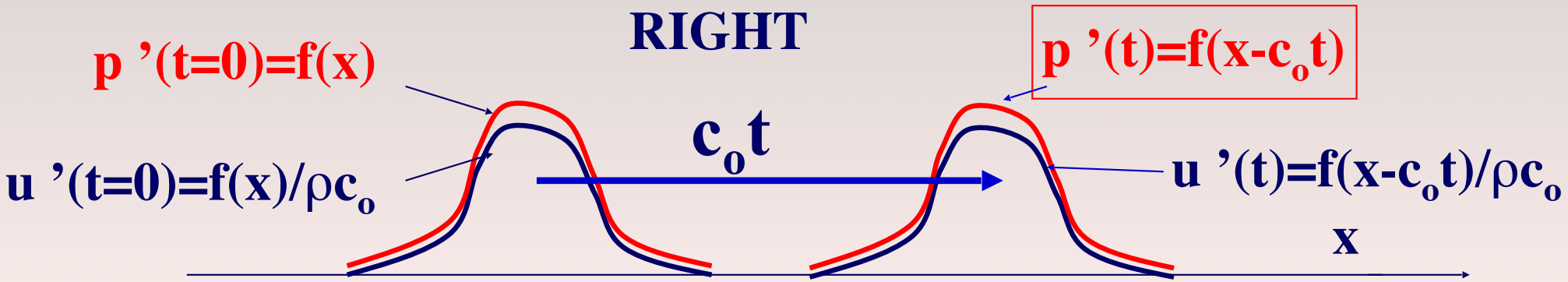
$$\frac{1}{c_o^2}\frac{\partial^2 p'}{\partial t^2} - \frac{\partial^2 p'}{\partial x^2} = 0$$

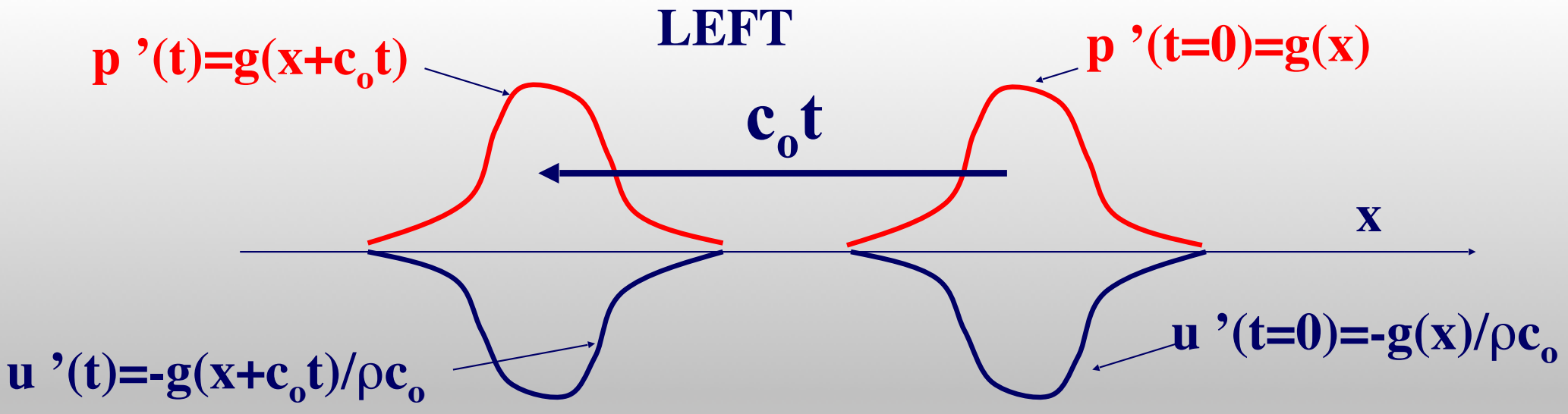
Two types of waves:

- right traveling: $p' = f(x - c_o t)$ *and* $u' = \frac{1}{\rho c_o} f(x - c_o t)$

- left traveling: $p' = g(x + c_o t)$ *and* $u' = -\frac{1}{\rho c_o} g(x + c_o t)$

where f and g are functions given by initial conditions.





General solution: $p'(t) = f(x - c_o t) + g(x + c_o t)$

$u'(t) = (f(x - c_o t) - g(x + c_o t))/\rho c_o$

Such waves exist:

- everywhere in real fluids

- but also (of course !) in all compressible codes

A useful tool : the acoustic energy

Start again from:

$$\frac{1}{c_o^2}\frac{\partial p'}{\partial t} + \rho_0 \nabla(u') = 0 \qquad p'/\rho_o$$

$$\frac{\partial u'}{\partial t} + \frac{1}{\rho_0}\nabla p' = 0 \qquad u'\rho_o$$

Summing:

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho_o u'^2 + \frac{1}{2}p'^2/(\rho_o c_o^2)\right] + \nabla(p'u') = 0$$

$$\frac{\partial}{\partial t}E + \nabla F = 0$$

E: local acoustic energy
F: acoustic flux = p' u'

Integrate over the whole domain V:

$$\frac{\partial}{\partial t}\mathcal{E} + \nabla \mathcal{F} = 0$$

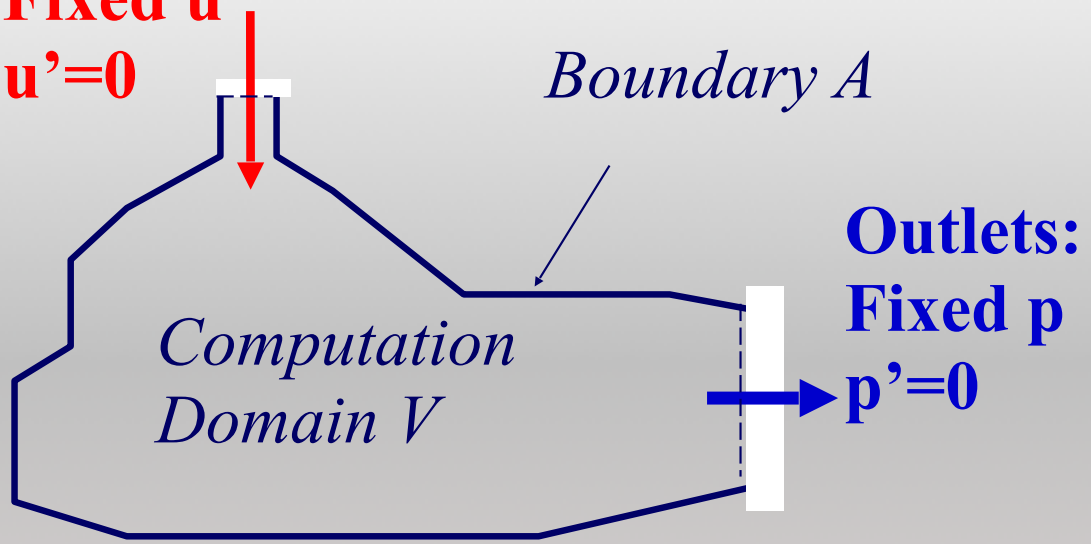
where :

$$\mathcal{E} = \iiint E dV$$

$$\mathcal{F} = \iiint F dA$$

$\mathcal{E}$: Total acoustic energy in the domain

$\mathcal{F}$: Total acoustic flux through the boundaries of the domain



A typical computation:
Domain V bounded by surface A

$$\frac{\partial}{\partial t}\mathcal{E}+\nabla\mathcal{F}=0$$

where :

$$\mathcal{E}=\iiint E\,dV$$

$$\mathcal{F}=\iiint F\,dA$$

with F=p'u'

What is the acoustic flux $\mathcal{F}$ on boundaries ?:

Walls: F= 0 since u=0
Inlets: F=0 since u'=0
Outlets: F=0 since p'=0

→ $\mathcal{F}$ **=0 !!**

→ **No acoustic flux leaving the domain…**

$\mathcal{E}$ **is constant !**

The acoustic energy present in the box at t=0 will never leave !

This derivation is true for non viscous, non reacting flows.

In the real world:

$$\frac{\partial}{\partial t}\mathcal{E}+\nabla\mathcal{F}=-\mu A$$

Viscous dissipation

In the CFD world:

$$\frac{\partial}{\partial t}\mathcal{E}+\nabla\mathcal{F}=-(\mu+\mu_t+\mu_a)A$$

Laminar viscosity

Turbulent viscosity

Artificial viscosity

In the real world, energy is dissipated through these two terms: the flux of acoustic energy through inlet and outlet and the laminar dissipation

$$\frac{\partial}{\partial t}\mathcal{E}+\nabla\mathcal{F}=-(\mu+\mu_t+\mu_a)A$$

Turbulent viscosity

Artificial viscosity

In the numerical world, two additional terms create dissipation: turbulent and artificial viscosities. None of them should ! Let us not use these terms to obtain the same effect for the wrong reasons

Let us look at the acoustic flux *F = p'u':*



$$\frac{\partial}{\partial t}\mathcal{E}+\nabla\mathcal{F}=-(\mu+\mu_t+\mu_a)A$$

$$\mathcal{F}=\iint F\,dA$$

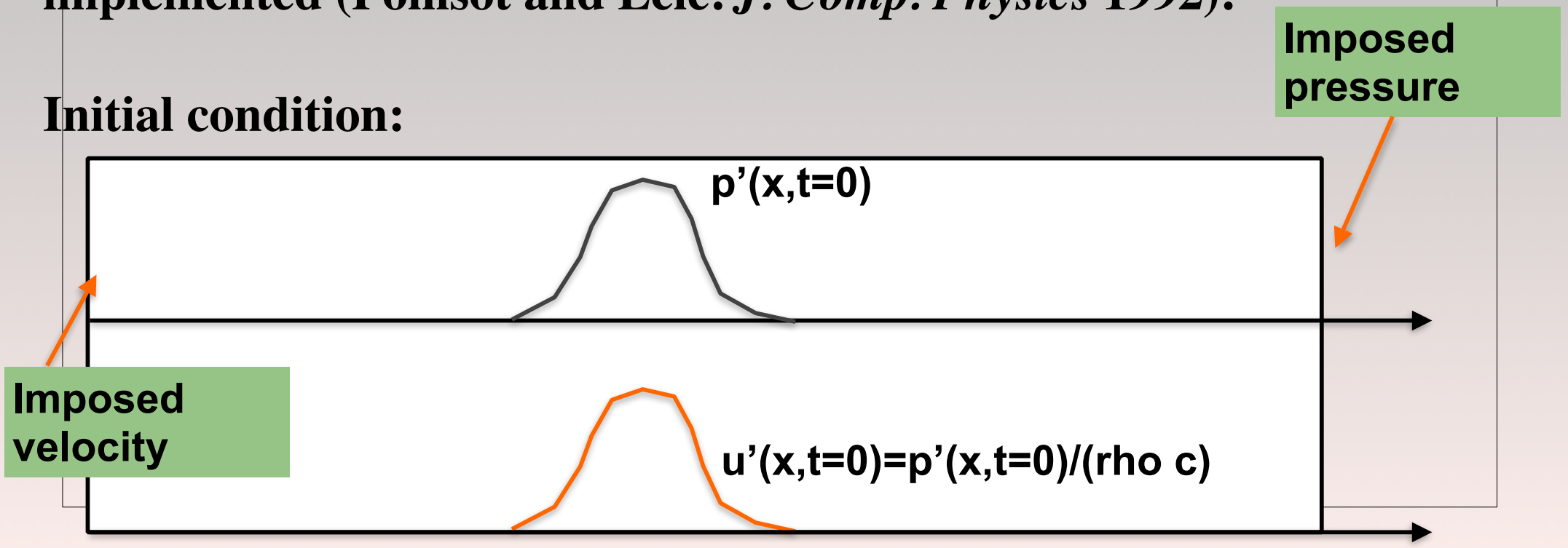
with F=p'u': acoustic flux on the boundaries of the domain.
How can we model F correctly ?: characteristic boundary condition
(Simple conditions such as u'=0 or p'=0 wont work)

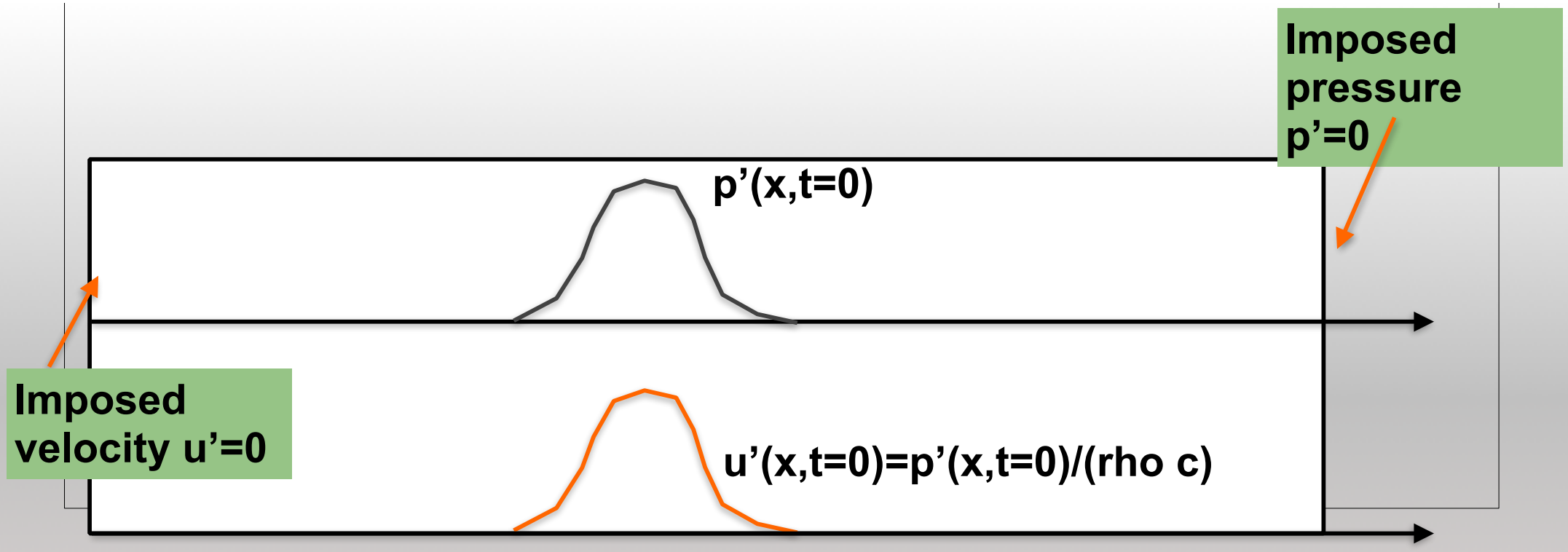
Controlling reflections on boundaries: the effects of p'u'

Why should we worry about reflections ? Because, in a GOOD CFD code, they control many things. We have already said that they control the decay of the acoustic energy.

Example: an acoustic wave hitting a boundary where NSCBC is implemented (Poinsot and Lele. *J. Comp. Physics* 1992):

Initial condition:





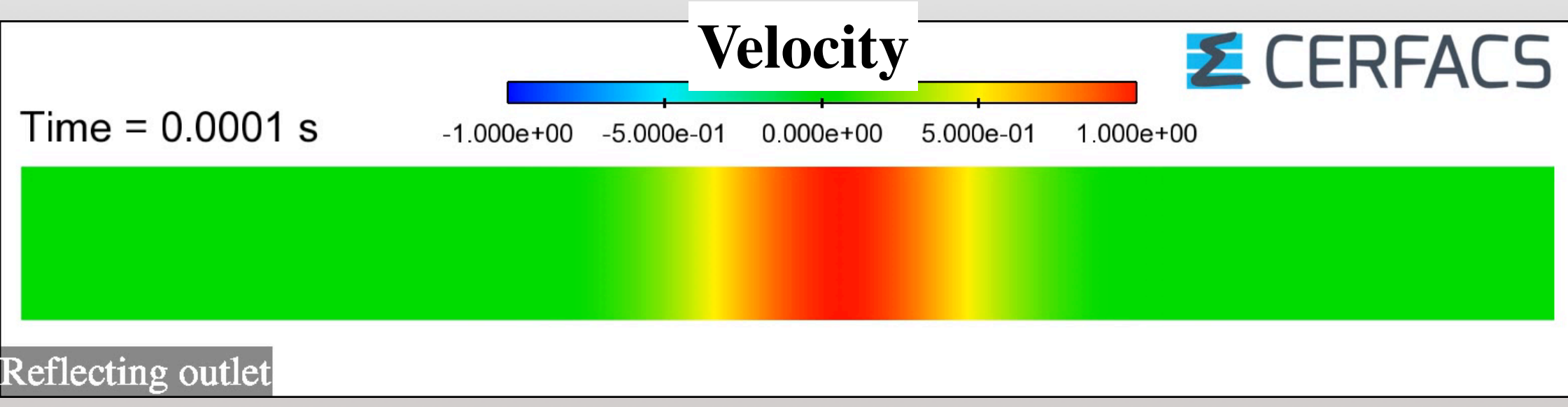
$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho_o u'^2+\frac{1}{2}p'^2/(\rho_o c_o^2)\right] + \nabla(p'u')=0$$

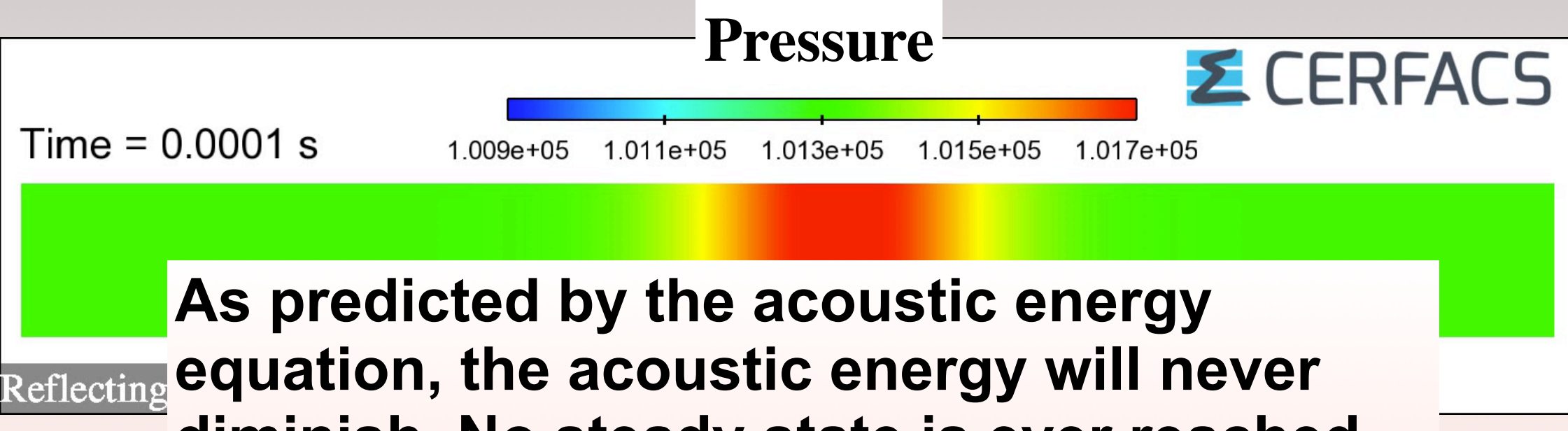
$$\frac{\partial}{\partial t}E + \nabla F=0$$

E: local acoustic energy
F: acoustic flux = p' u'

For this test case, the acoustic energy *E* contained in the box never goes to zero

Reflecting inlet (u'=0) and reflecting outlet (p'=0)

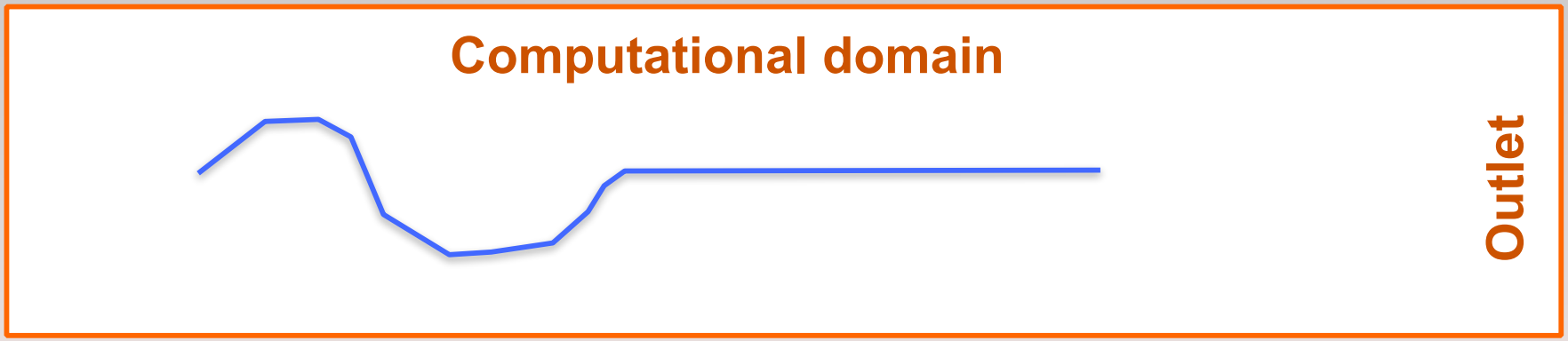




As predicted by the acoustic energy equation, the acoustic energy will never diminish. No steady state is ever reached

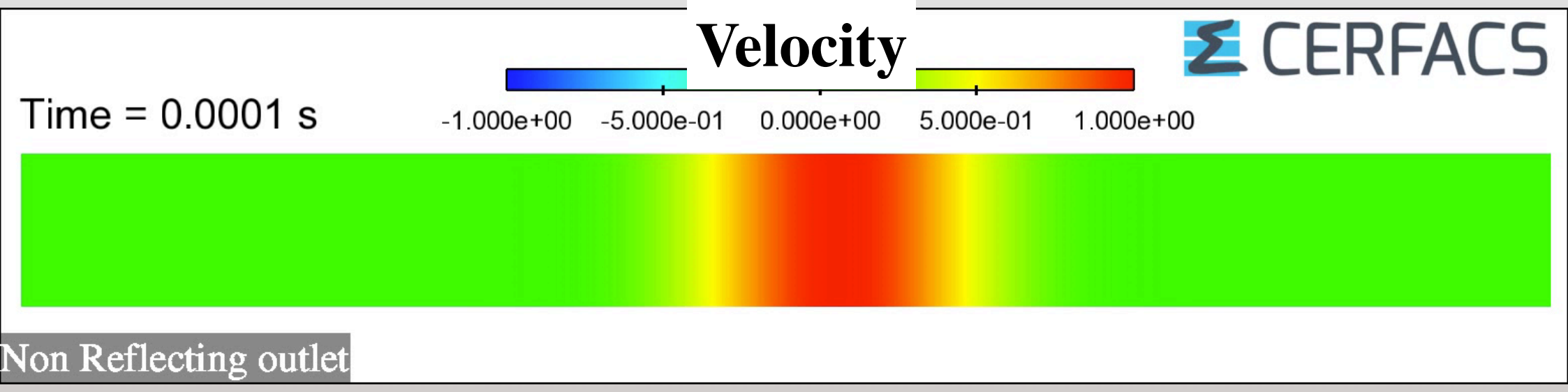
How do we avoid this ?

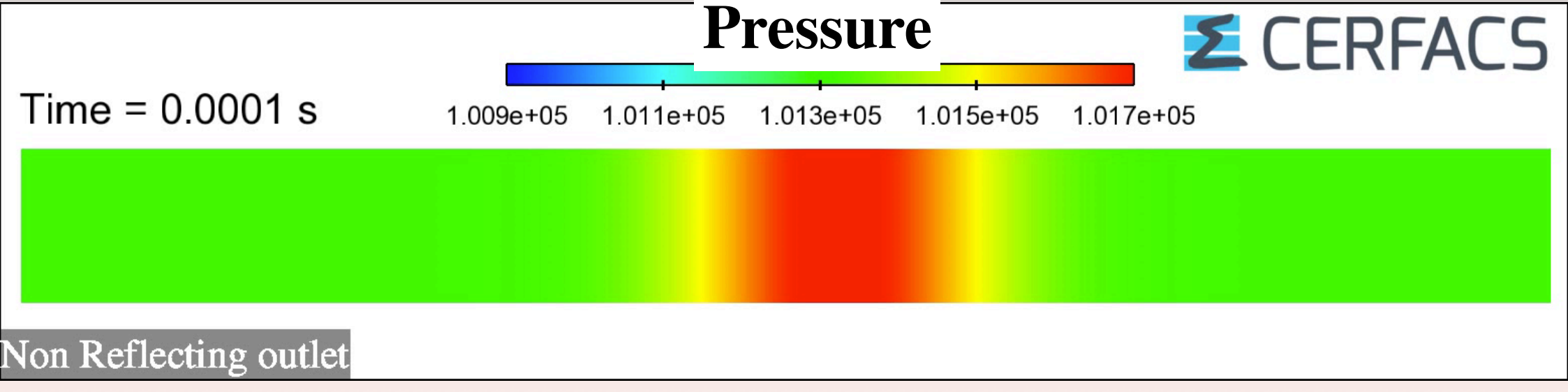
We must let the acoustic wave evacuate the domain through the boundaries by making them partially or totally ‘non reflecting’.
What does non reflecting mean ?
A perfectly non-reflecting boundary is a boundary where no wave is reflected from a wave going out:



Can we do this in a code ? Yes: with characteristics boundary conditions (TNC book chap 9)

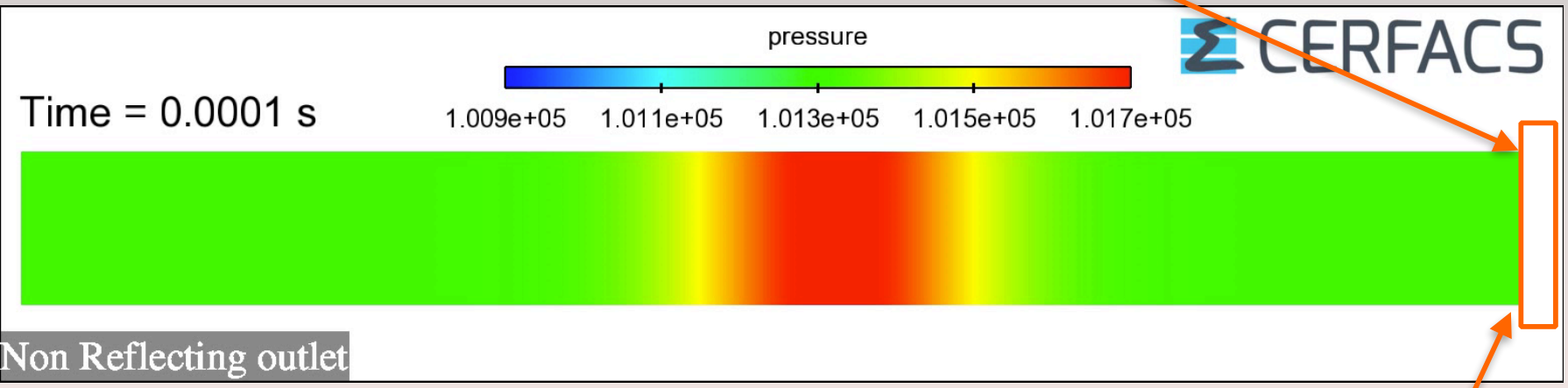
Non-reflecting outlet in AVBP





$$\frac{\partial}{\partial t}\mathcal{E}+\nabla\mathcal{F}=-(\mu+\mu_t+\mu_a)A$$

We have used the boundary flux here to evacuate the waves as it should be.
We did not use artificial dissipation or turbulent viscosity to dissipate waves



The acoustic energy has left from this face

TURBULENCE SUB GRID MODELS

Apparently, LES and RANS models for turbulent viscosity are not very different:

RANS, time averaged

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left[\overline{\tau}_{ij} - \overline{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j\right)\right]$$

$$\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j = -\nu_t\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \widetilde{u}_k}{\partial x_k}\right)$$

LES, space filtered

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left[\overline{\tau}_{ij} - \overline{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j\right)\right]$$

$$\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j = -\nu_t\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \widetilde{u}_k}{\partial x_k}\right)$$

$\nu_t = \mu_t / \rho$ **Turbulent viscosity**

Ch. 4

Seen from the Fortran lines, the only difference between LES and RANS is the turbulent viscosity

RANS, time averaged

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$$\nu_t = c_\mu \frac{k^2}{\epsilon}$$

LES, space filtered

Ch. 4 Section 4.7.3

$$\nu_t = (C_S \Delta)^2 \left|\overline{S}\right| = (C_S \Delta)^2 \left(2\overline{S}_{ij}\overline{S}_{ij}\right)^{1/2}$$

This could suggest that transforming a RANS code into a LES code can be achieved simply changing the k-epslion routine:

$$\nu_t = c_\mu \frac{k^2}{\epsilon}$$

into a Smagorinski routine:

$$\nu_t = (C_S \Delta)^2 \, |\overline{S}| = (C_S \Delta)^2 \, \left(2\overline{S}_{ij}\overline{S}_{ij}\right)^{1/2}$$

This would be a major mistake. LES is NOT ONLY in this routine. Actually, this is not the important part. The important part is the numerical scheme itself and its properties.

OUTLINE:

RANS / LES / DNS: WHY LES WILL REPLACE RANS

WHAT IS NEEDED FOR LES - PHYSICAL MODELS:

- INTRODUCTION OF TURBULENCE AT INLETS
- CHARACTERISTIC BOUNDARY CONDITIONS
- TURBULENCE SUB GRID MODELS

***WHAT IS NEEDED FOR LES* - NUMERICS:**

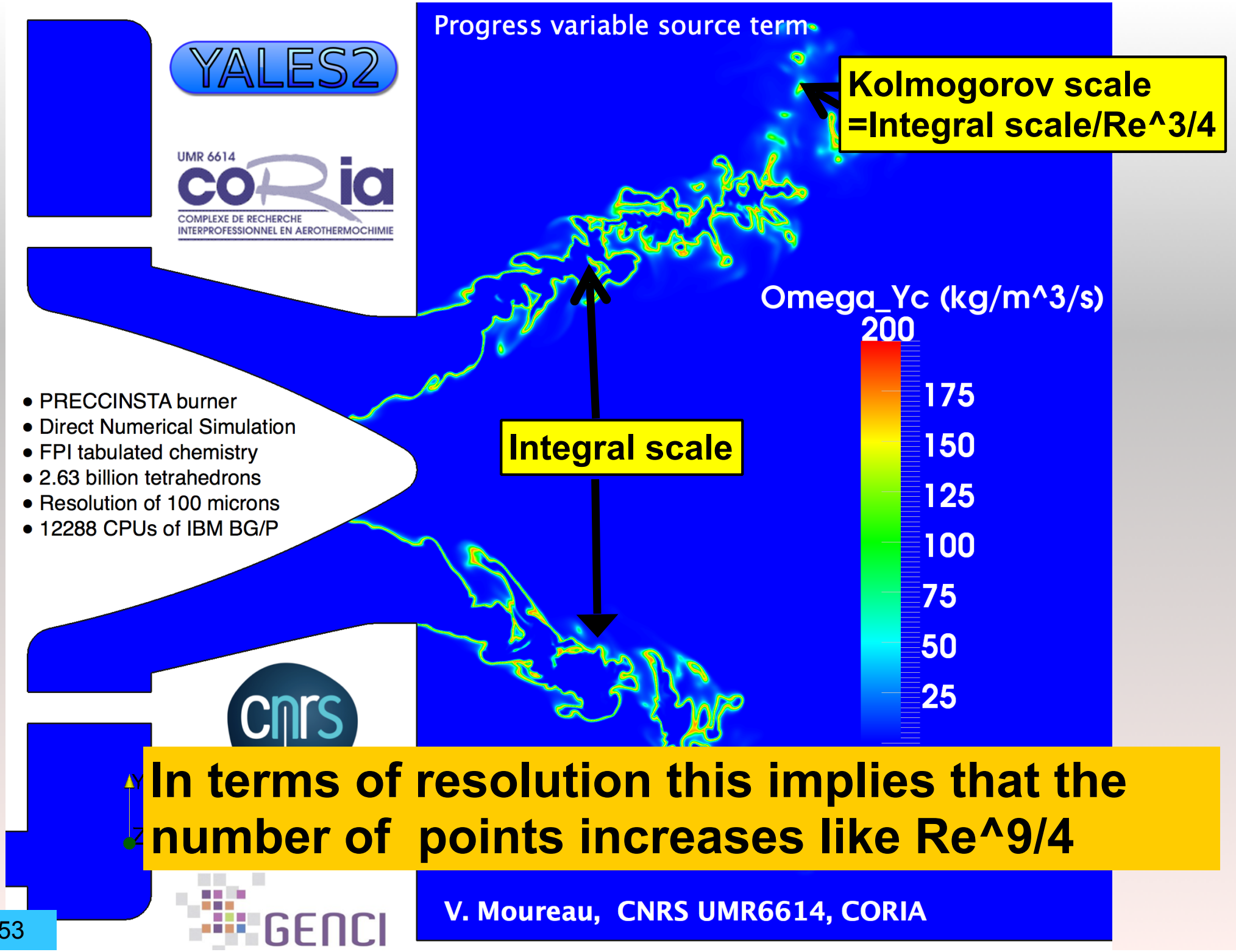
- **DISPERSION AND DISSIPATION OF LES CODES**
- **GHOST WAVES AND BOUNDARY CONDITIONS**
- **ACOUSTIC ENERGY BALANCES**
- **MASSIVELY PARALLEL CODES**

A cynical view at the true difference between codes doing LES, RANS and DNS ?

All applications of interest have large Reynolds numbers:

$$\mathrm{Re}(real) = UL/\nu$$

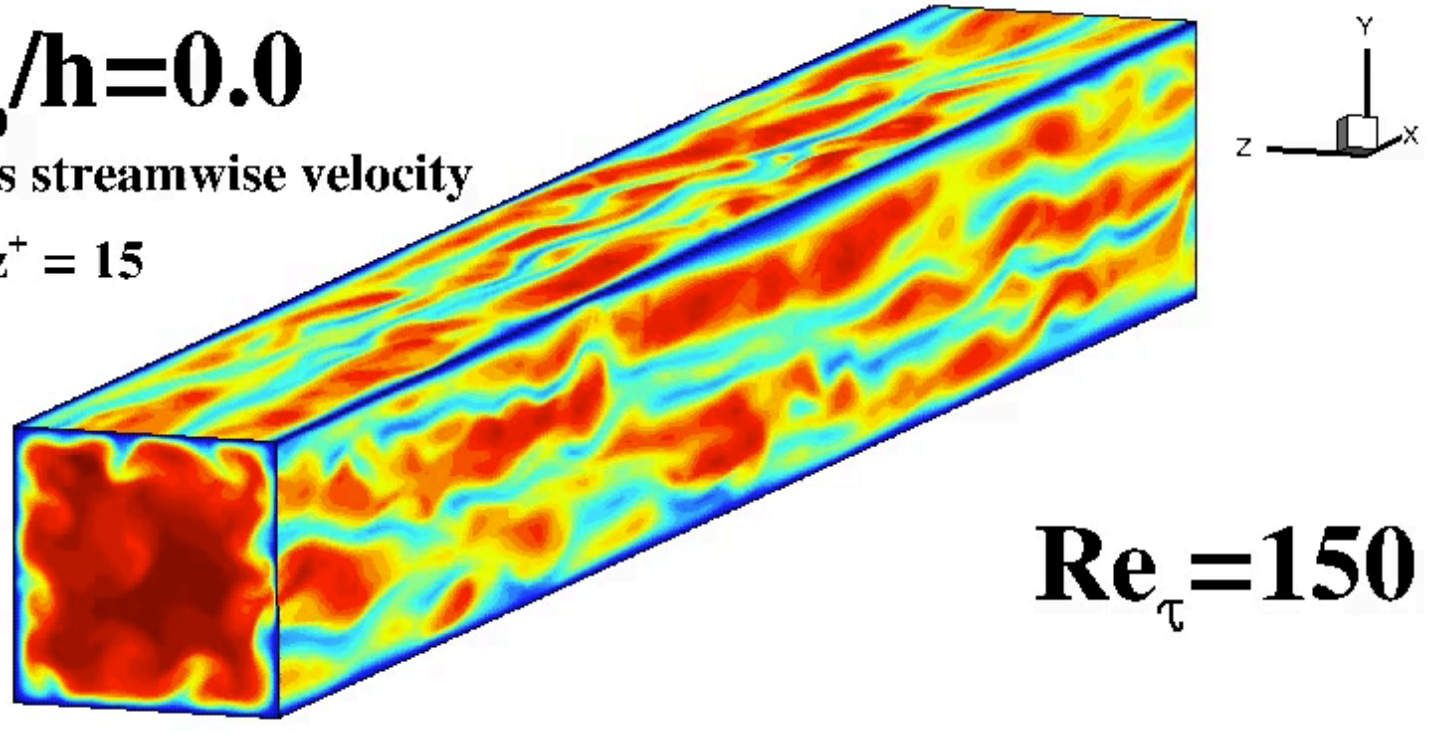
Large Reynolds numbers imply:
-> large difference between largest and smallest scales
-> large number of grid points which we simply dont have


YALES2
UMR 6614
CORIA
COMPLEXE DE RECHERCHE INTERPROFESSIONNEL EN AEROTHERMOCHIMIE
Progress variable source term
Kolmogorov scale
=Integral scale/Re^3/4
Omega_Yc (kg/m^3/s)
200
175
150
125
100
75
50
25
Integral scale
• PRECCINSTA burner
• Direct Numerical Simulation
• FPI tabulated chemistry
• 2.63 billion tetrahedrons
• Resolution of 100 microns
• 12288 CPUs of IBM BG/P
cnrs
In terms of resolution this implies that the number of points increases like Re^9/4
GENCI
V. Moureau, CNRS UMR6614, CORIA

$tu_b/h=0.0$

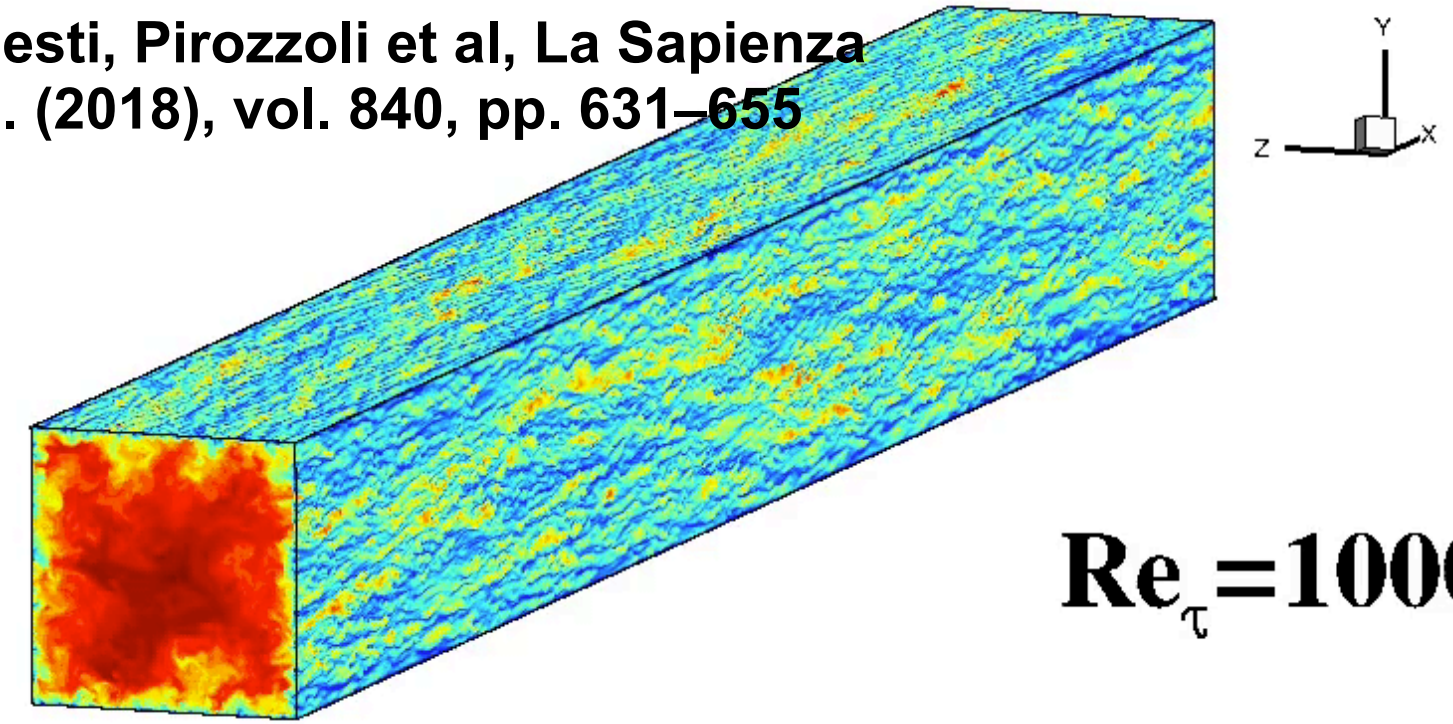
Instantaneous streamwise velocity

$y^+ = 15 \quad z^+ = 15$



$Re_\tau=150$

Source: Modesti, Pirozzoli et al, La Sapienza
J. Fluid Mech. (2018), vol. 840, pp. 631–655



$Re_\tau=1000$

So: we can not resolve all scales associated to large Reynolds numbers and real chambers... This was true in the 60s and it is still true today...

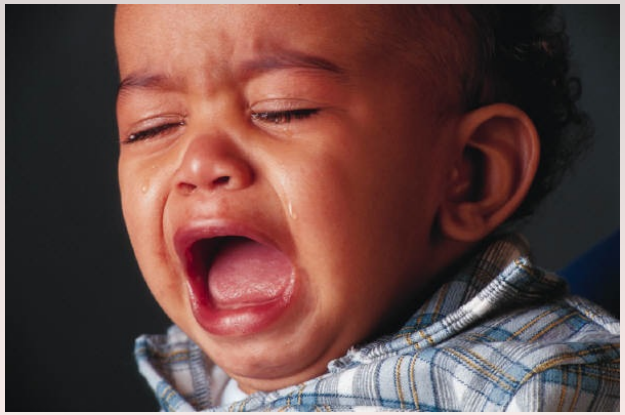
Had to find a solution !

We use two tricks (we call them 'models'):

- turbulence models: add turbulent viscosity ν_t
- dissipative schemes: add numerical viscosity ν_a

$$\frac{\partial}{\partial t}\rho u_j + \boxed{\frac{\partial}{\partial x_i}\rho u_i u_j} = -\frac{\partial p}{\partial x_j} \boxed{+ \frac{\partial \tau_{ij}}{\partial x_i}}$$

This is the :
- **non-linear term**
- **source of turbulence**
- **ennemy of all CFD codes**



This is the:
- **viscous term**
- **linear term**
- **damper of turbulence**
- **friend of all PhD students**



So... what is turbulent viscosity ?

It is the easiest (not the only one) solution when the Navier Stokes equations are averaged (in RANS) or filtered (in LES) to model the non linear terms due to the multiplications of correlations

$$\frac{\partial}{\partial t}\rho u_j + \frac{\partial}{\partial x_i}\rho u_i u_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i}$$

$$\tau_{ij} = -\frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

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Filter these equations in space (LES) or average them in time (RANS):

$$f = \tilde{f} + f''$$

Replace in momentum:

$$\frac{\partial \overline{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\tilde{u}_i\tilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left[\overline{\tau}_{ij} - \overline{\rho}\left(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j\right)\right]$$

$$T_{ij} = \widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j = \widetilde{u_i'' u_j''}$$

HOW CAN WE MODEL THIS TERM ?

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$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left[\overline{\tau}_{ij} - \overline{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j\right)\right]$$

WE WILL MODEL IT IN A FORM SIMILAR TO THE LAMINAR TERM

$$\bar{\tau}_{ij} = \mu\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right)$$

LAMINAR VISCOSITY

$$\overline{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j\right) = -\mu_t\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right)$$

TURBULENT VISCOSITY

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left[\overline{\tau}_{ij} - \overline{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j\right)\right]$$

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[(\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]$$

USING A TURBULENT VISCOSITY MODEL IS EQUIVALENT TO ADDING A (COMPLICATED) TURBULENT VISCOSITY TO THE LAMINAR ONE

Ch. 4 Section 4.7.3

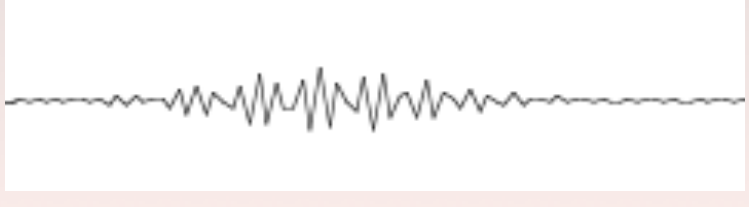
Careful: all diagonal terms have been hidden in the pressure

What is artificial viscosity ?: here, the viscous term is introduced through the numerical scheme

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0$$

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + u_i \frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} = o(\Delta x^2)$$

Numerical analysis 101: centered schemes have … problems: they generate wiggles as soon as the resolution is not sufficient



Introduce artificial viscosity:

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + u_i \frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} = \nu_a \frac{f_{i+1}^n + f_{i-1}^n - 2f_i^n}{\Delta x^2}$$

Makes the scheme more stable and able to handle gradients
However, in practice we are not solving:

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0$$

But:

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = \nu_a \frac{\partial^2 f}{\partial x^2}$$

Upwind schemes are NOT a solution:

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + u_i \frac{f_i^n - f_{i-1}^n}{\Delta x} = o(\Delta x)$$

Using:

$$f_{i-1}^n = f_i^n - \Delta x \frac{\partial f}{\partial x} + 1/2 \Delta x^2 \frac{\partial^2 f}{\partial x^2}$$

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 1/2 (u \Delta x) \frac{\partial^2 f}{\partial x^2} + o(\Delta x^2)$$

An upwind scheme is like a centered scheme with a numerical viscosity equal to *1/2 u* Δx

So… all turbulent flow solvers combine:

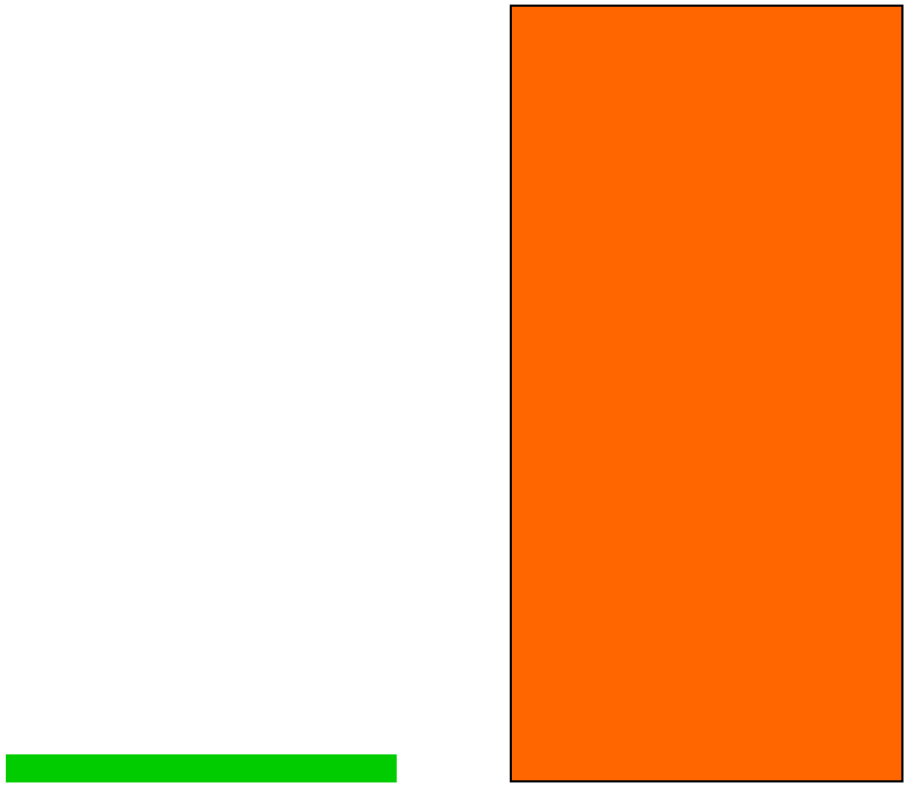
- turbulent viscosity ν_t
- numerical viscosity ν_a

to allow the code to run. But at which price ?
In practice, the Reynolds number seen by the code is :

$$\mathrm{Re}(num) = UL/(\upsilon + \upsilon_t + \upsilon_a)$$

which is much smaller than the Reynolds of the flow.
It can even be smaller than the critical Reynolds number to have turbulence in this flow.
==> We are not computing the same flow…: instead of a high Re turbulent flow, we are computing a laminar flow

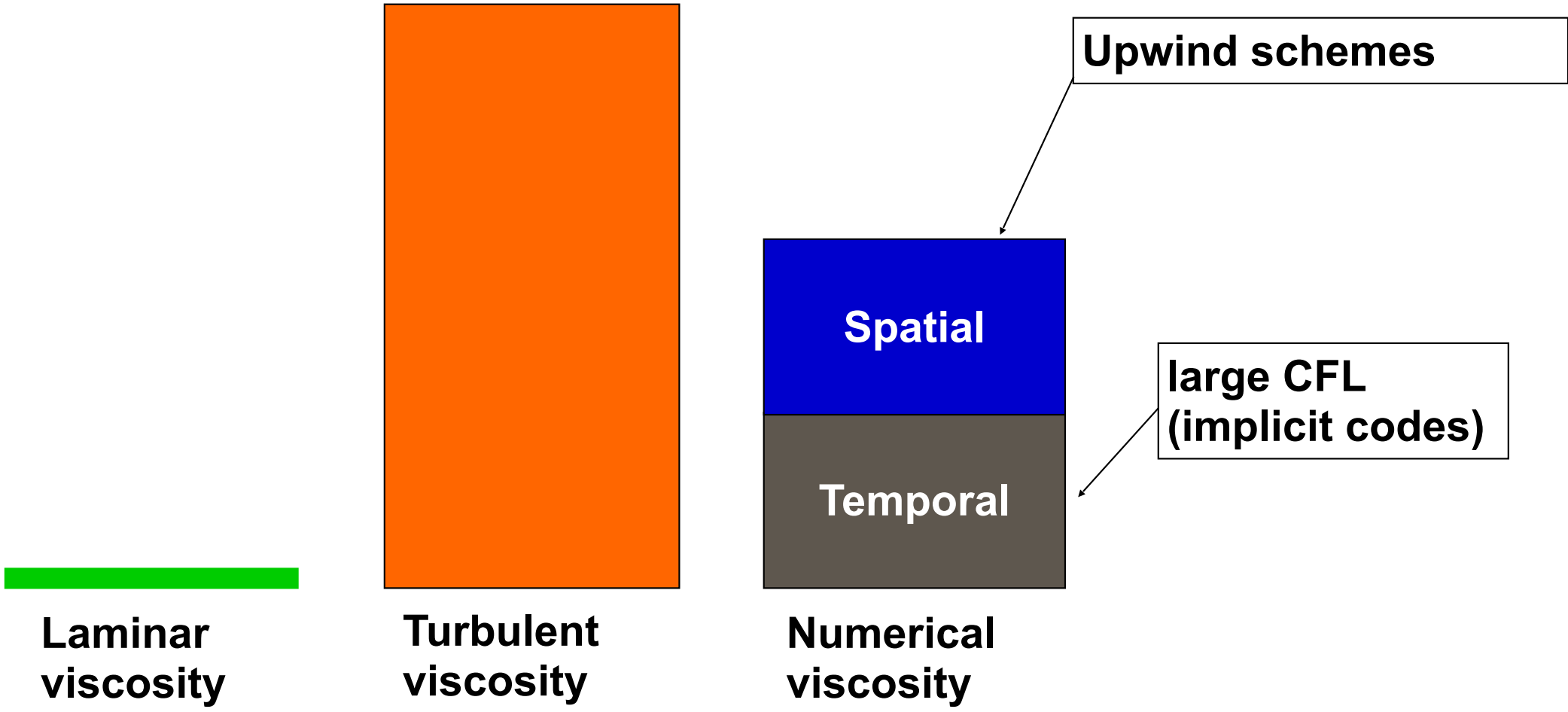
RANS: turbulent viscosity is very large ==> the Reynolds of the code is so small that the flow is steady (ie laminar)



Laminar viscosity

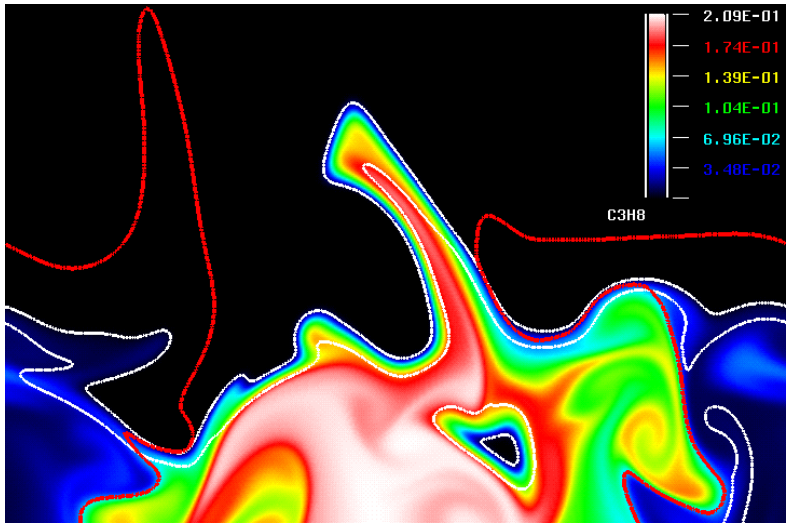
Turbulent viscosity

RANS: since the flow is so viscous, might as well use numerical viscosity



$$\mathrm{Re} = UL/(\upsilon + \upsilon_t + \upsilon_a) << \mathrm{Re}(real)$$

CODE DNS: nothing more than the laminar viscosity



High-order scheme
+
Small CFL

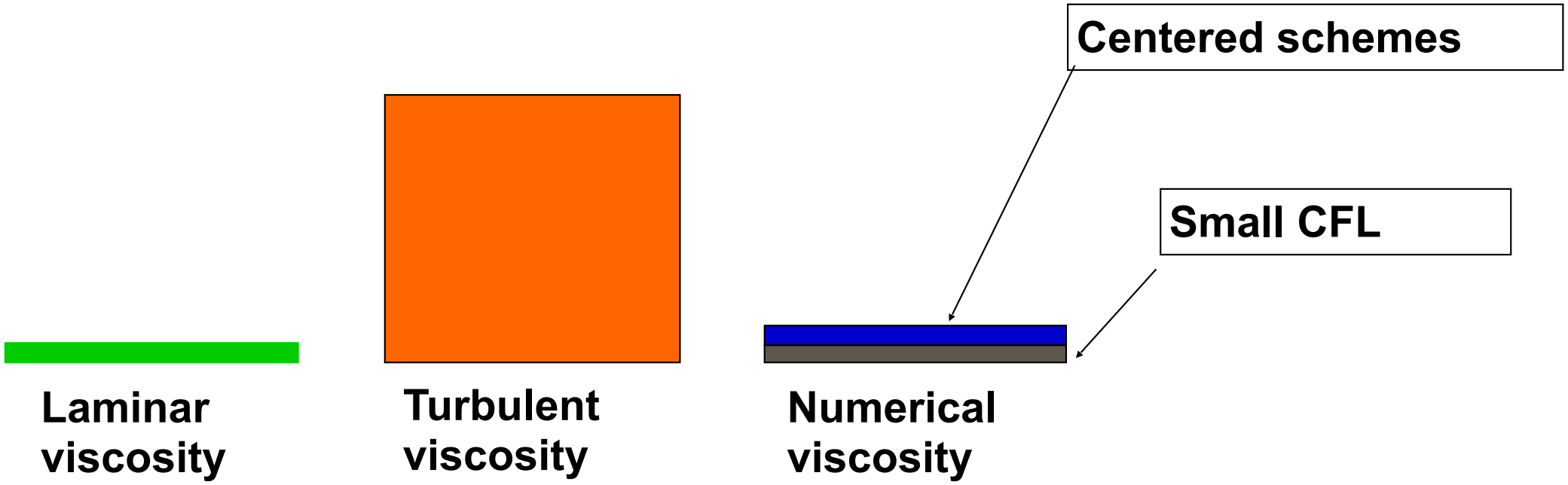
Laminar viscosity

Turbulent viscosity

Numerical viscosity

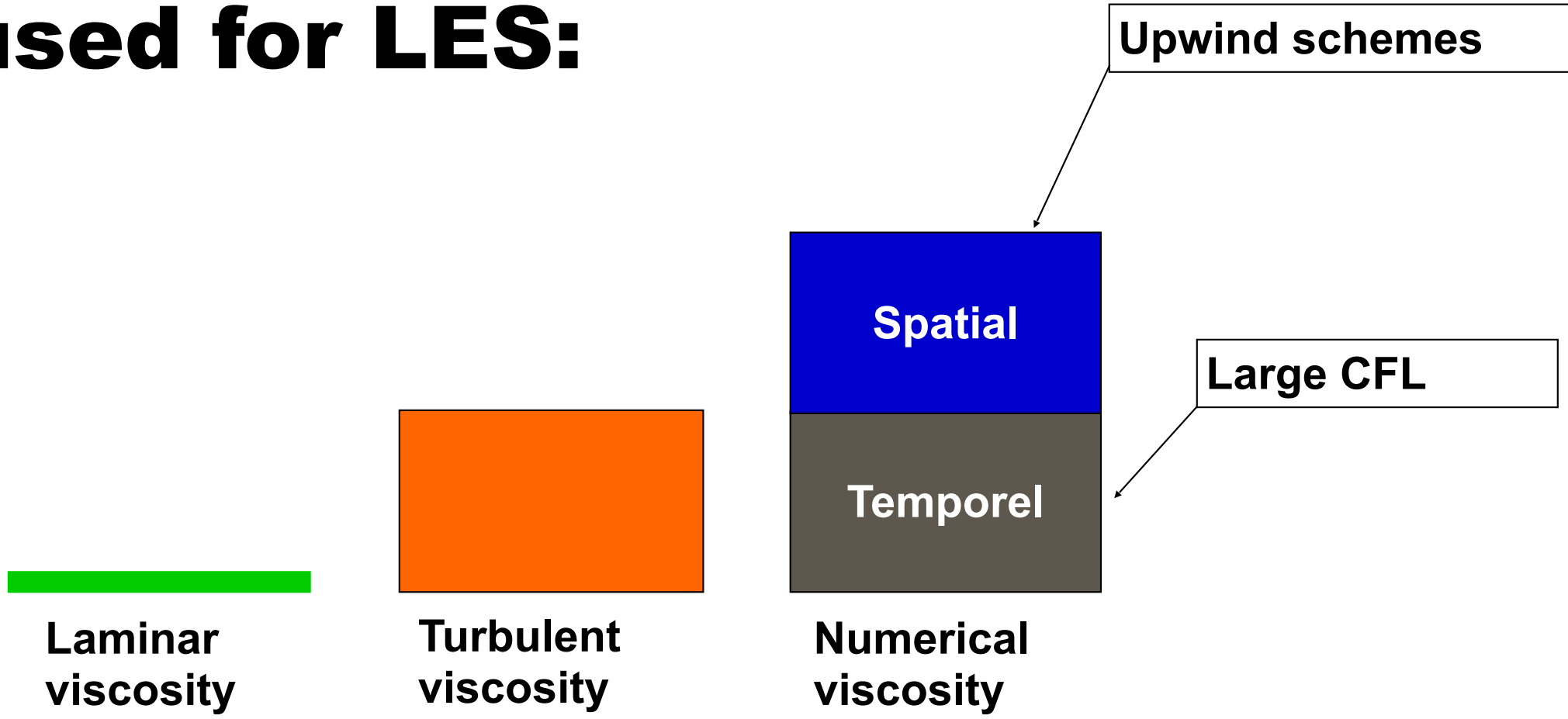
$$\mathrm{Re}(num) = UL/(\upsilon + \upsilon_t + \upsilon_a) = UL/\upsilon$$

A good LES code: turbulent viscosity reduced and limited numerical viscosity ==> Reynolds turbulent smaller than the true one but large enough for the flow



$$\mathrm{Re} = UL/(\upsilon + \upsilon_t + \upsilon_a) > \mathrm{Re}(crit)$$

DANGERS of RANS codes used for LES:



$$\mathrm{Re}(num) = UL/(\upsilon + \upsilon_t + \upsilon_a)\ too\ small$$

Good test: remove the turbulent viscosity



Laminar viscosity

Turbulent viscosity

Numerical viscosity

And see if something changes...
If nothing changes, this is not LES

CONCLUSION:

A good LES needs:

- **high order schemes**
- **small time steps**

(Otherwise it is LESWE: Large Eddy Simulation Without Eddy…)

- **This will require important CPU time**
- **THIS IS IMPOSSIBLE IF WE DO NOT USE MASSIVELY PARALLEL MACHINES**

Even if we have the CPU power, is it easy to do ? Actually NO ! Computing waves (vortices or acoustic waves or entropy waves) is tough.

LES must propagate vortices and acoustic waves.
This impacts our choices for numerical techniques:

- **How do codes propagate physical waves ? NOT SO WELL…**
- **Do codes propagate 'other' non-physical waves ? YES…**

NEED TO START DISCUSSING :

- **Dissipation: waves are attenuated by the numerical scheme**
- **Dispersion: the speed of waves is affected by the numerical scheme and depends on its wavelength**

TNC Ch. 9 Section 9.7.1

DISPERSION / DISSIPATION

IN THE REAL WORLD:

A medium is dispersive if the speed at which waves propagate depends on their frequency. A medium is dissipative if waves are dissipated when they propagate.

Example: Air is not dispersive for sound waves. But it is dissipative for high frequency waves.

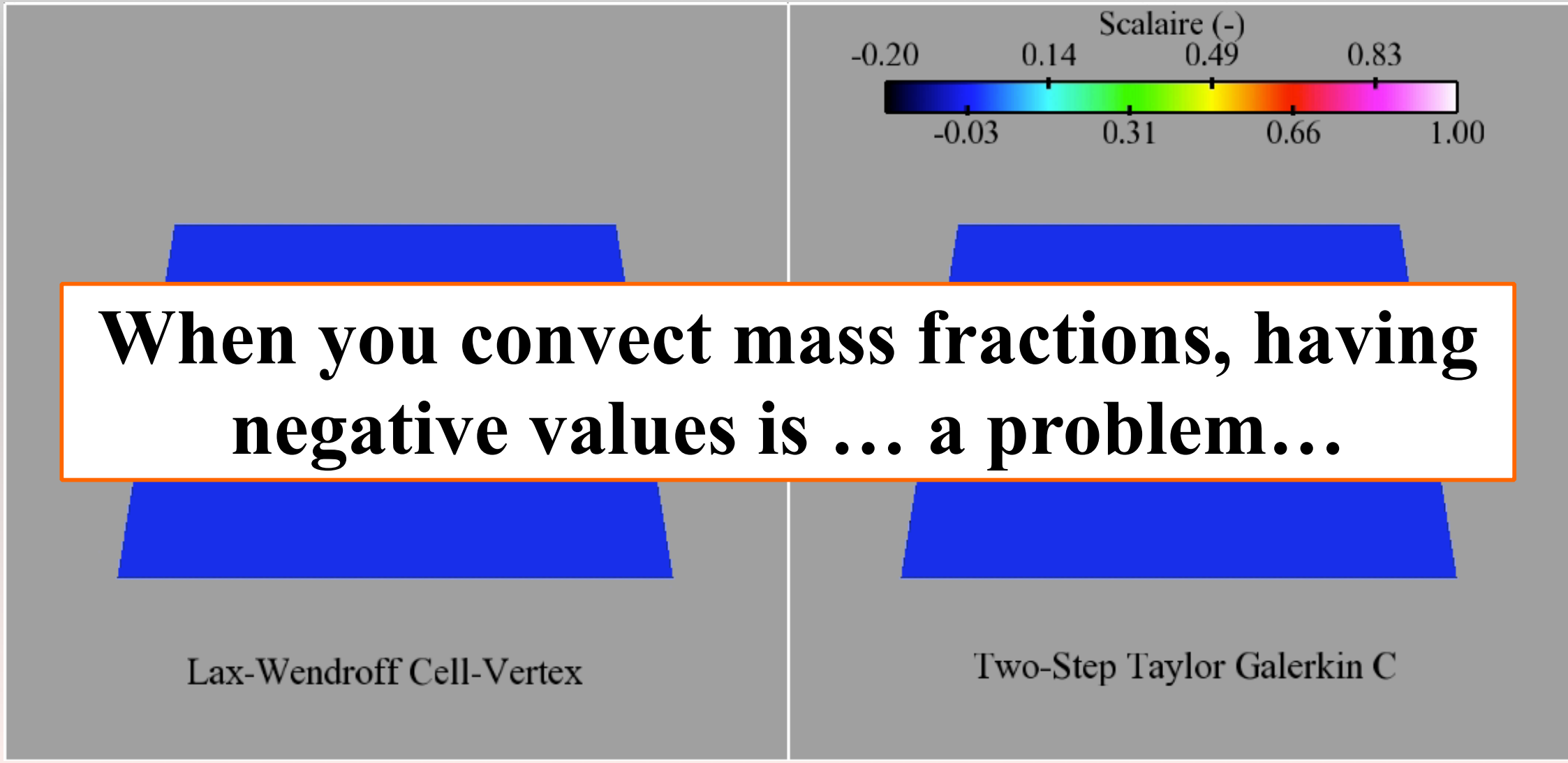
IN THE NUMERICAL WORLD:

Building a numerical technique which respects the dispersive and dissipative properties of gases is almost impossible.

For LES, this is bad news.

Example: convecting a scalar 'bump' in homogeneous flow with two methods:

- **Lax Wendroff (2nd order)**
- **TTGC (3rd/4th order)**



When you convect mass fractions, having negative values is … a problem…

Can we study these questions without writing a code ?

Yes !... consider the simplest case of one-dimensional convection equation at speed c:

$$\frac{\partial}{\partial t}u + c\frac{\partial}{\partial x}u = 0$$

For this equation, we can derive analytically what the results of a given scheme with perfect time advancement would be.
This equation is neither dispersive nor dissipative by nature: all signals are transported at speed *c* without any modification

Assumptions for the following slides:

$$\frac{\partial}{\partial t}u + c\frac{\partial}{\partial x}u = 0$$

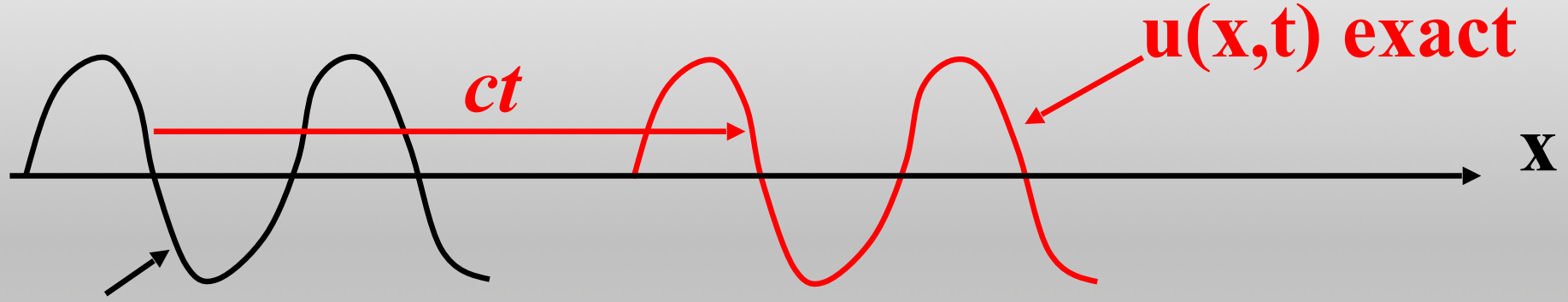
To make this derivation as simple as possible, assume that we use a code:

- with perfect time advancement
- one dimensional
- with second order centered scheme for spatial derivatives

$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

Generalizations: in text books on numerical analysis

The exact solution for this wave problem is a convection at speed c:



$$u(x,t=0) = v(0)\ \exp\left[2j\pi\omega x\right]$$

$$u(x,t) \quad = \quad u(x-ct,\ t=0) \ = \ v(0)\ \exp\left[2j\pi\omega(x-ct)\right]$$

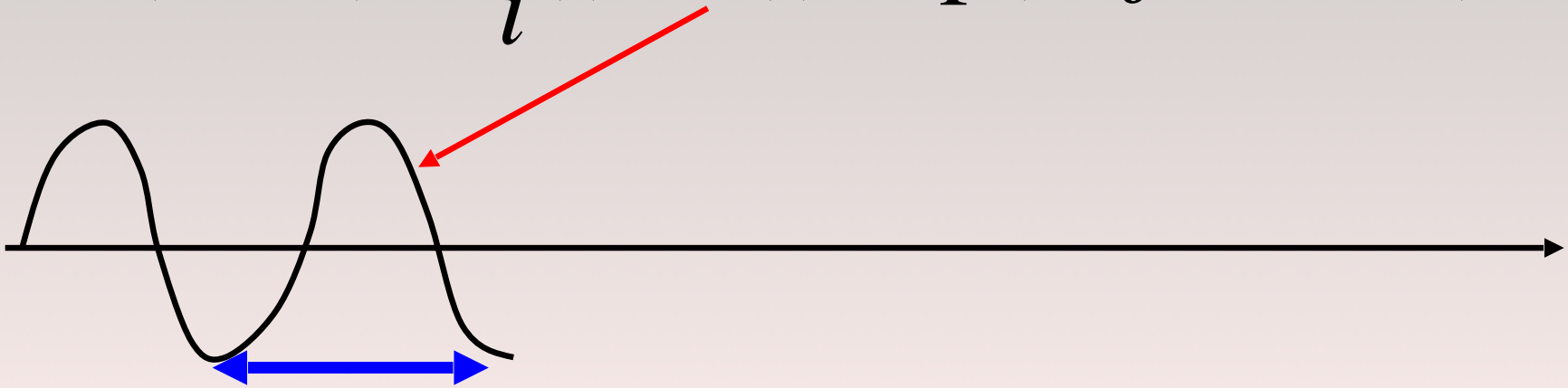
Being able to predict this convection speed is crucial for acoustics but also for turbulence (to convect vortices or entropy waves).

What happens in codes ? space is discretized…
Take the simplest finite difference example:

Discretize x axis: $x = i\Delta x$

Assume that u is a sinusoidal function of space (pulsation ω):

$$u(i\Delta x, t) = u_i(t) = v(t)\exp(2\pi j\ \omega\ i\Delta x) \qquad j^2 = -1$$



$$\lambda = 1/\omega$$

What does a second order code do ? Suppose we have perfect time advancement:

$$\frac{\partial}{\partial t}u_i + c\frac{u_{i+1}-u_{i-1}}{2\Delta x}=0 \qquad (1)$$

For sinusoidal wave propagation: $u_i = v(t)\exp(2\pi j\ \omega\ i\Delta x)$

Replacing *u* by *v(t)* in Eq. (1) leads to:

$$\frac{\partial}{\partial t}v = -cjv\ \sin(2\pi\omega\Delta x)/\Delta x$$

Or: $$v(t) = v(0)\exp(-cj\ \frac{\sin(2\pi\omega\Delta x)}{\Delta x}t)$$

The numerical solution for this problem will be:

$$u(x,t) = v(0)\exp\left[2j\pi\omega\left(x-c\frac{\sin(2\pi\omega\Delta x)}{2\pi\omega\Delta x}t\right)\right]$$

Comparing the exact and the numerical solution:

Exact: $u(x,t) = v(0)\exp\left[2j\pi\omega(x-ct)\right]$

Numerical: $u(x,t) = v(0)\exp\left[2j\pi\omega\left(x-c\frac{\sin(2\pi\omega\Delta x)}{2\pi\omega\Delta x}t\right)\right]$

The numerical scheme is dispersive: the speed is not right BUT the amplitude of the signal is right==> no damping is introduced by the centered scheme. Good for LES/DNS

This property is true of all centered schemes but not of upwind schemes. For the first order upwind scheme, for example, the numerical solution would be:

$$u(x,t) = v(0)\exp(-ct/\Delta x(1-\cos 2\pi\omega\Delta x))\exp\left[2j\pi\omega\left(x-c\frac{\sin(2\pi\omega\Delta x)}{2\pi\omega\Delta x}t\right)\right]$$

Numerical dissipation factor !

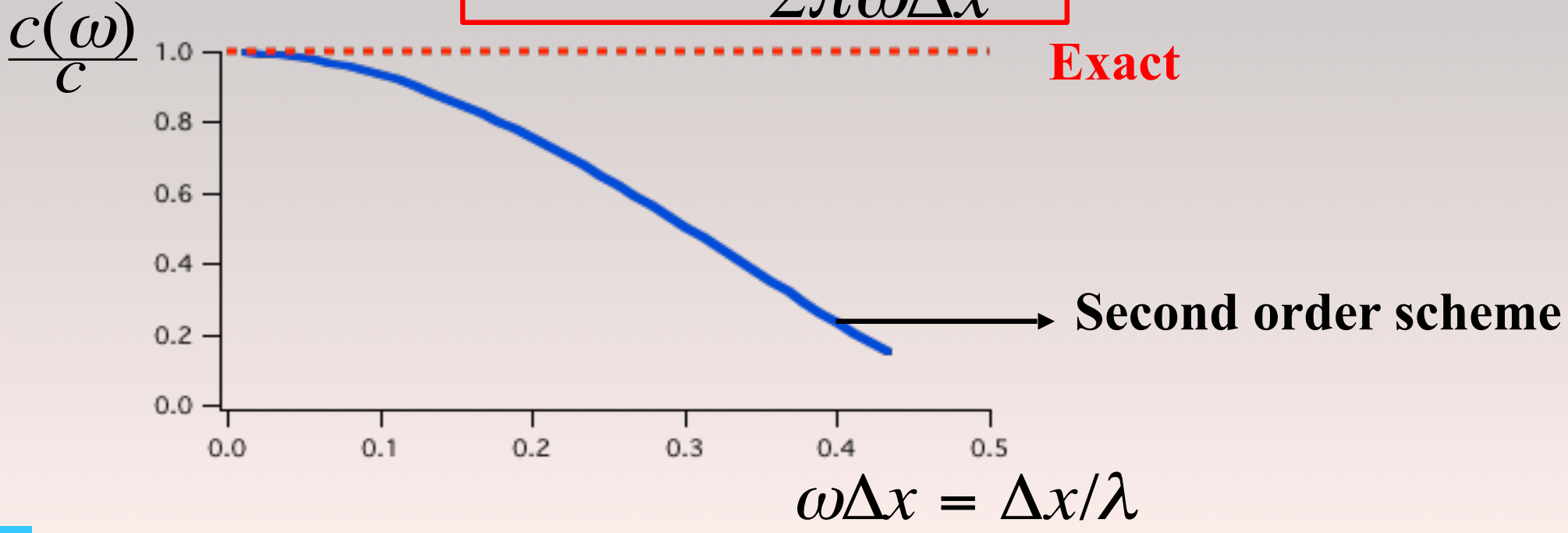
Moreover, for the centered scheme, comparing now the speeds:

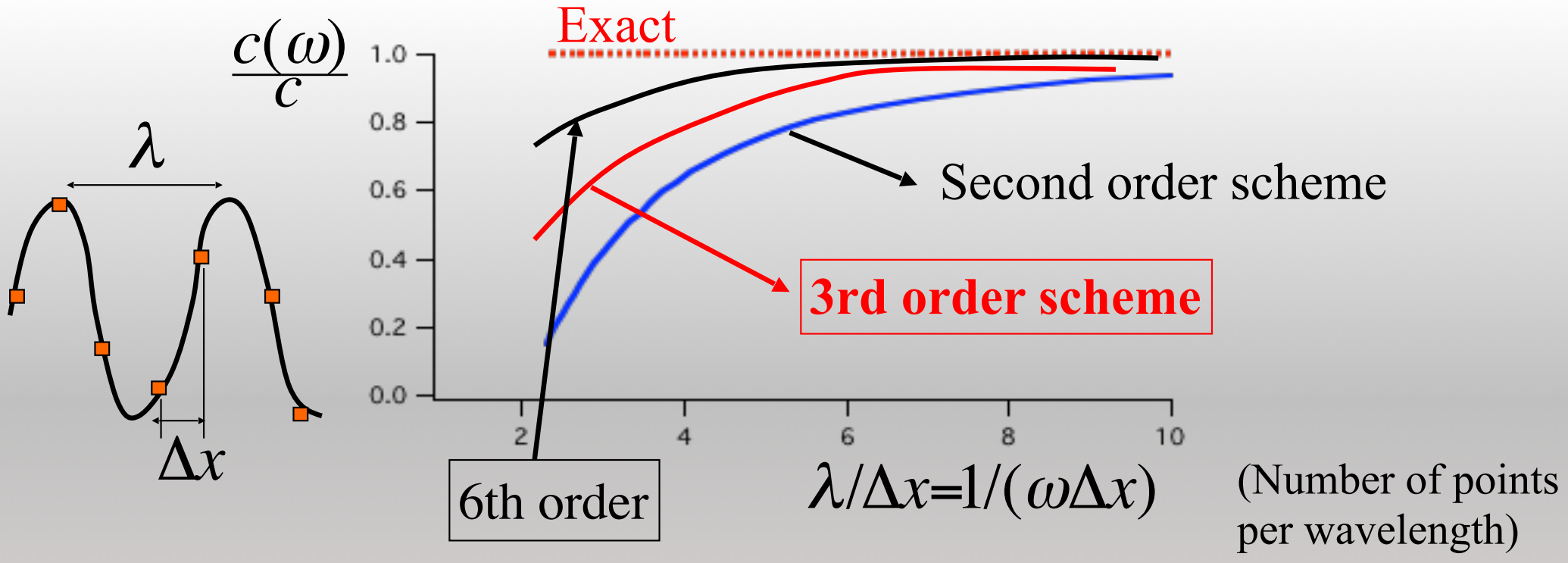
Exact: $u(x,t) = v(0)\exp\left[2j\pi\omega(x-ct)\right]$

Numerical: $u(x,t) = v(0)\exp\left[2j\pi\omega\left(x-c\frac{\sin(2\pi\omega\Delta x)}{2\pi\omega\Delta x}t\right)\right]$

The numerical scheme makes the flow 'dispersive'; different wavelengths ω are propagated at different speeds c(ω):

$$\frac{c(\omega)}{c} = \frac{\sin(2\pi\omega\Delta x)}{2\pi\omega\Delta x}$$





This is not good news for second-order schemes: they do not propagate waves at the right speed as soon as the resolution (ie the number of points per wavelength) is not very high.

$\lambda/\Delta x$

Higher order schemes do better.

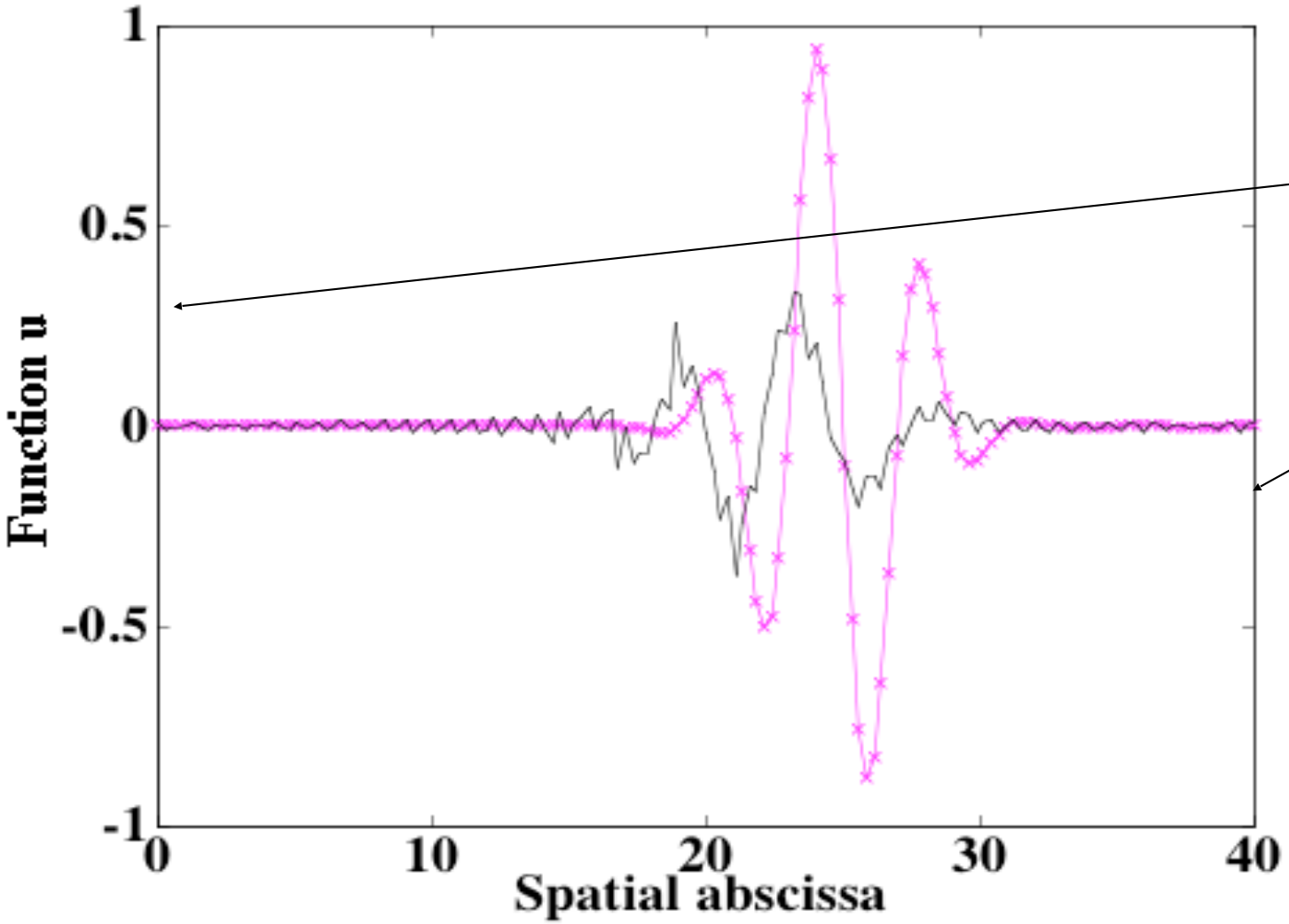
A simple example in one dimension

- Second order centered scheme
- Fourth order Runge Kutta time integration

$$\frac{\partial}{\partial t}u + c\frac{\partial}{\partial x}u = 0$$

Black:code

Cyan: exact



Periodic boundaries

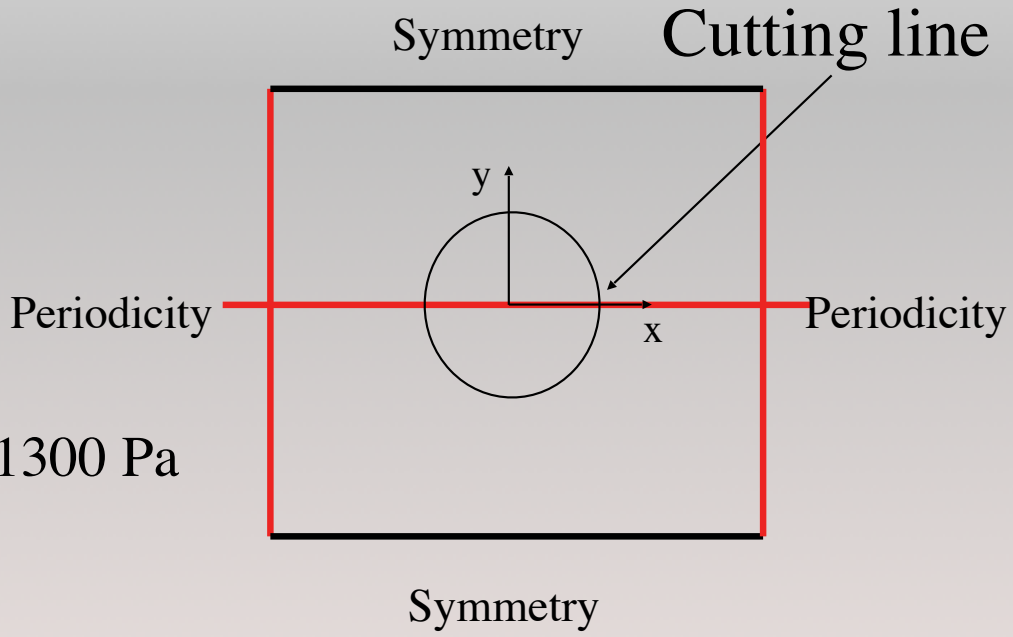
2D Vortex convection

Ch. 9 Section 9.7.3

Convecting vortices is the basic feature of LES

$$U_x = 100 m/s \qquad p - p_0 = -\frac{\rho \Gamma^2}{2R_c^2} e^{-\frac{x^2+y^2}{R_c^2}}$$

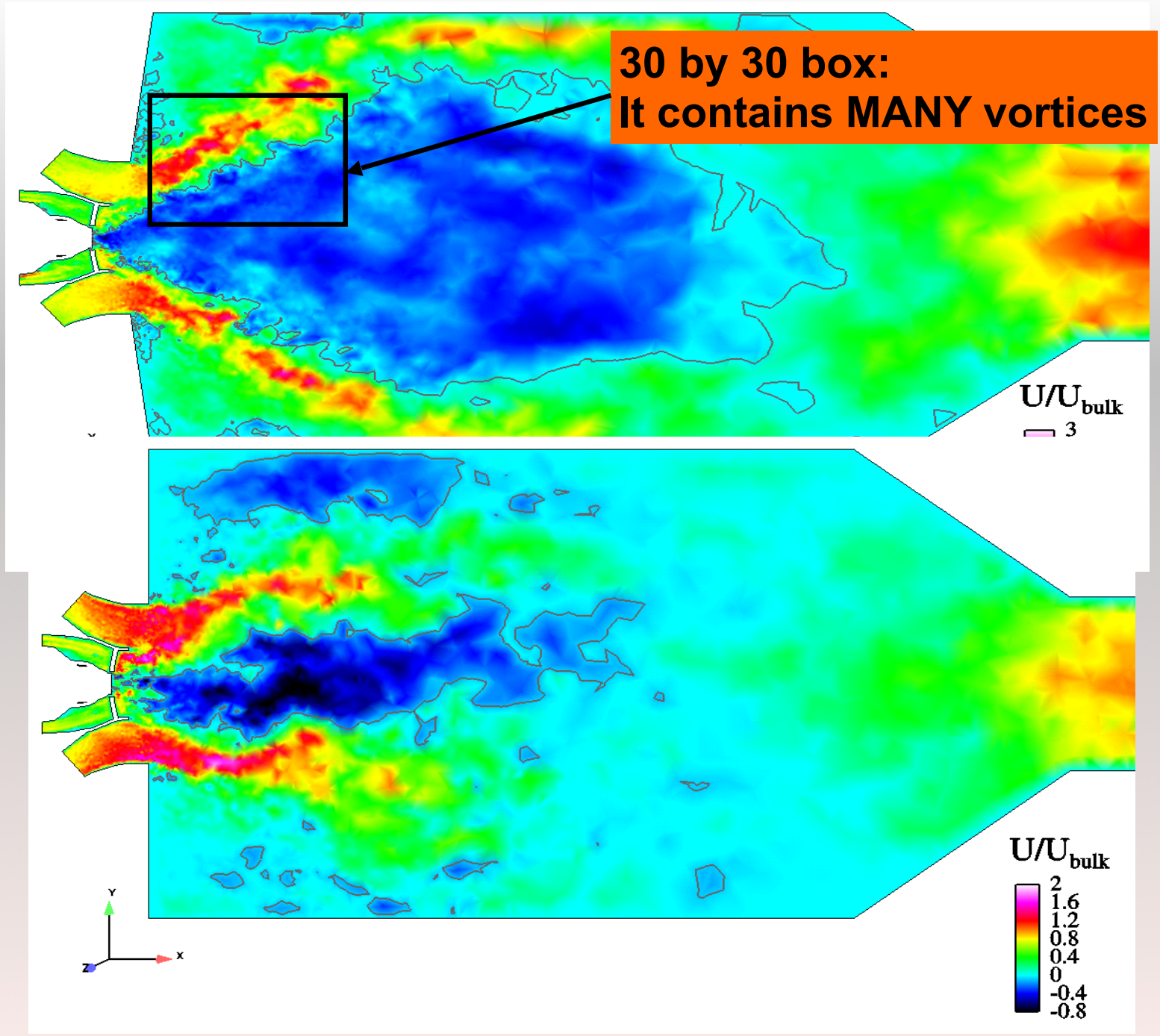
$$v = \frac{\Gamma}{R_c^2} x e^{-\frac{x^2+y^2}{2R_c^2}} \qquad u = -\frac{\Gamma}{R_c^2} y e^{-\frac{x^2+y^2}{2R_c^2}}$$



- Γ= 1 m/s^2 ; R_c = 19.45*10^{-3} m ; p_0 = 101300 Pa

- 2D structured mesh 30X30 elements.
- Analytical solution
- Tested LW (2nd order) and TTGC (3rd order) numerical scheme.
- Acoustic CFL = 0.7
- Tested also a commercial code. CFX 5.7 using a 2nd order centred finite volume scheme.

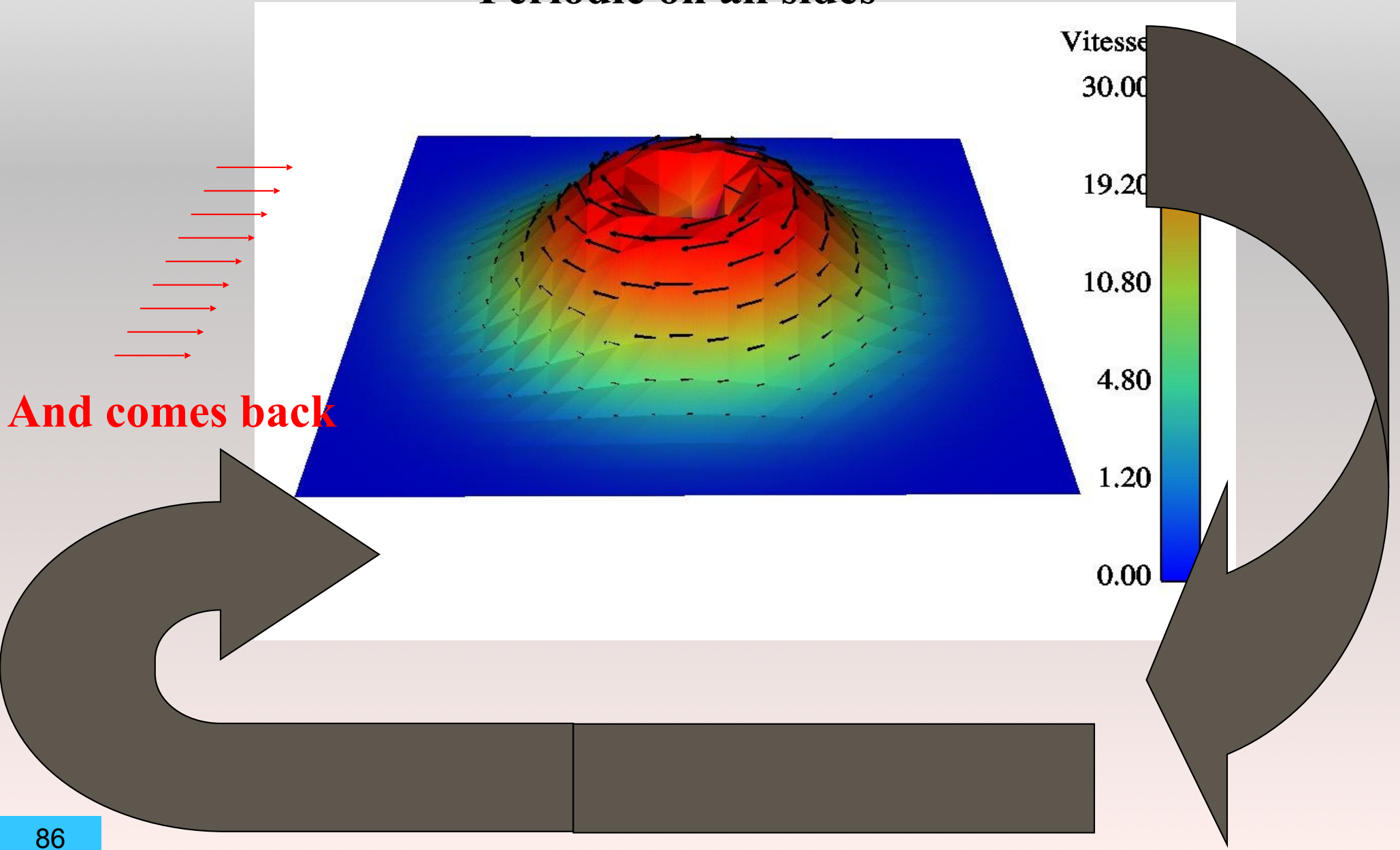
Moureau et al, JCP 2005



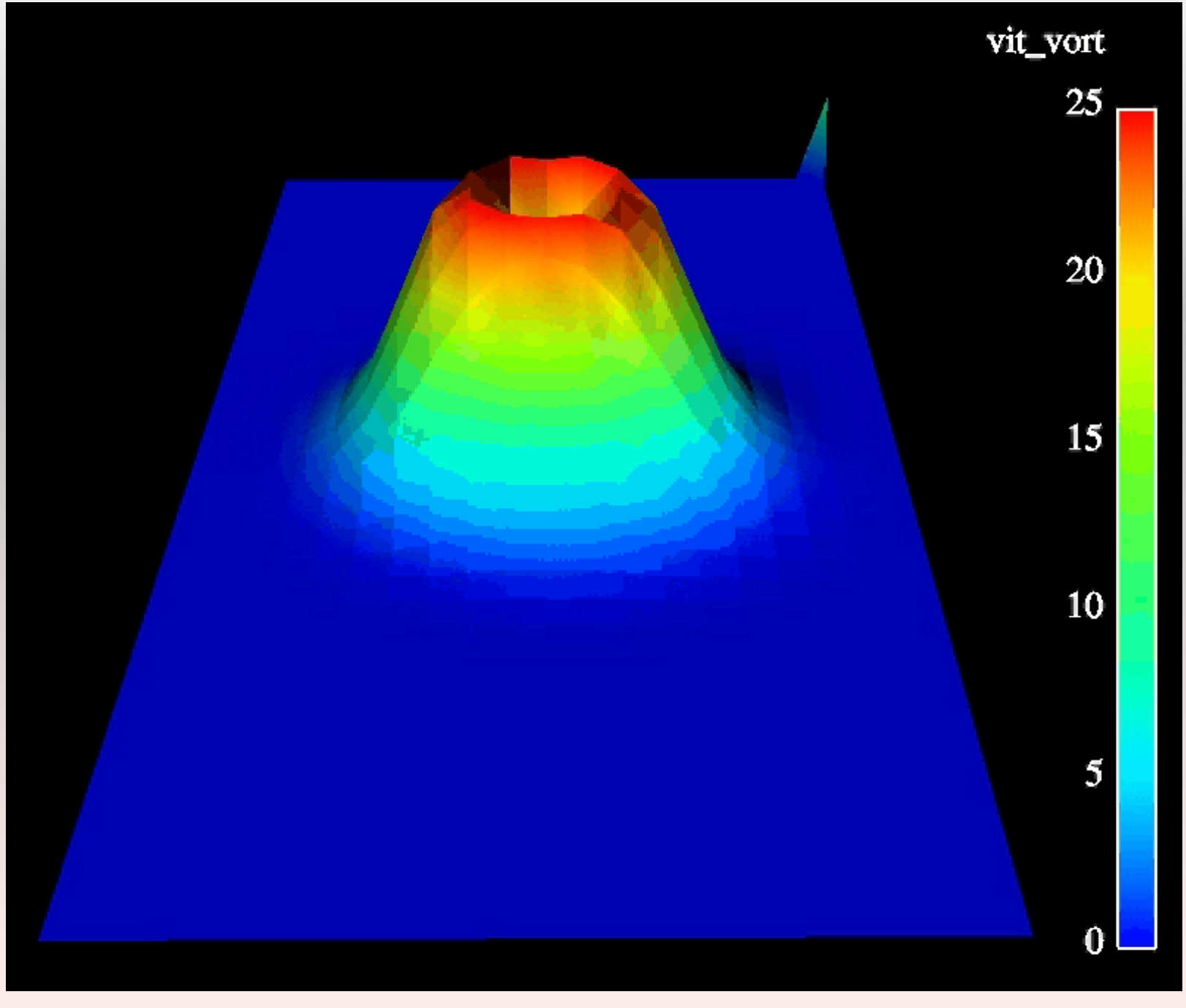
Siemens VR series: Selle et al Comb. Flame 2004.

Periodic on all sides

Vortex leaves



And comes back


vit_vort
25
20
15
10
5
0

Comparing three schemes:

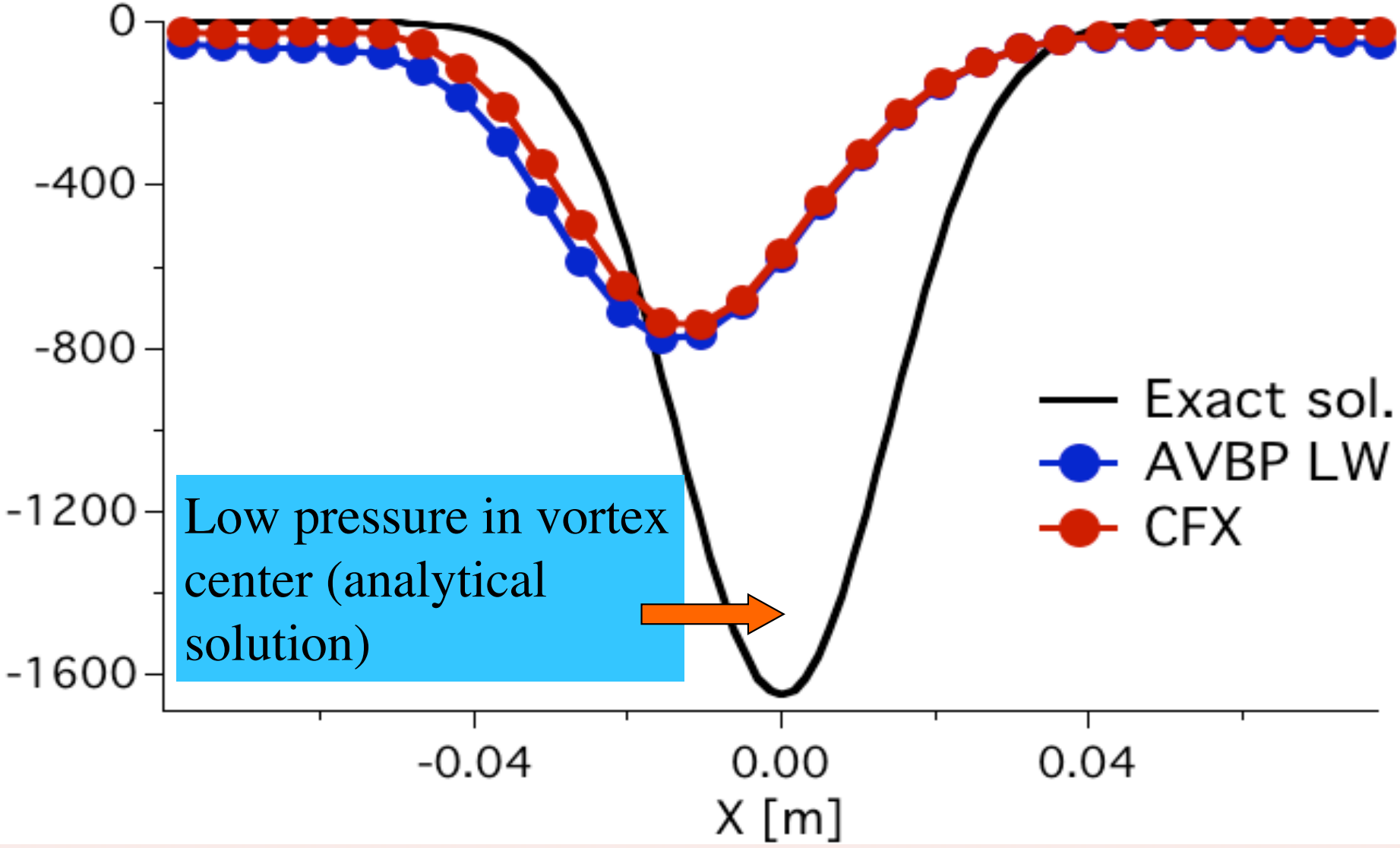
- 2nd order Lax Wendroff in AVBP (code CERFACS)
- 2nd order CFX
- 3rd order TTGC in AVBP (Oxford/CERFACS: Colin and Rudgyard, *J. Comp. Phys.* 162 (2000)).

Results after three turn over times

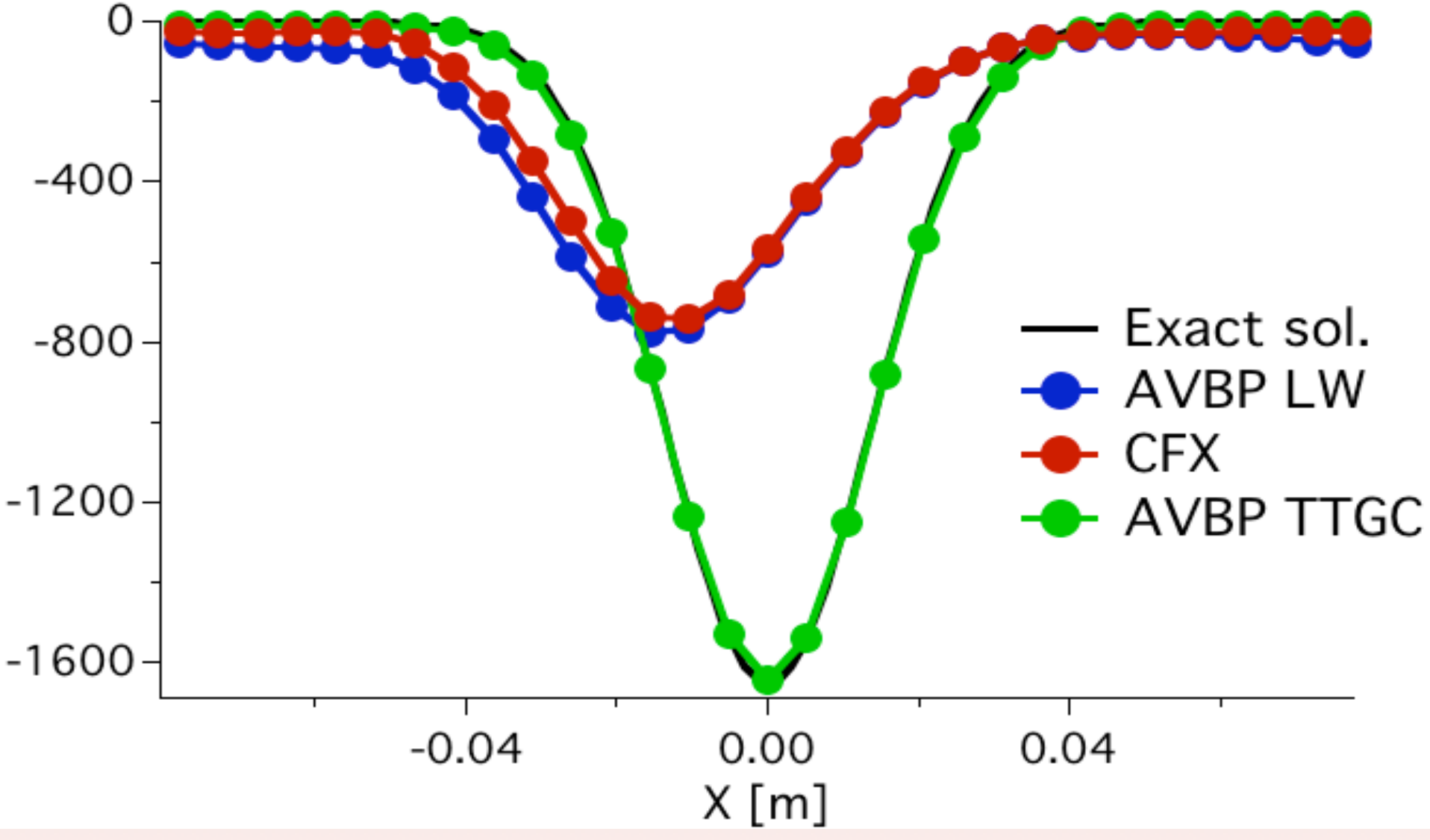
Time step is set by CFL = c $\Delta t/\Delta x$ = 0.7

http://elearning.cerfacs.fr/numerical/benchmarks/vortex2d/index.php

Relative pressure [Pa]



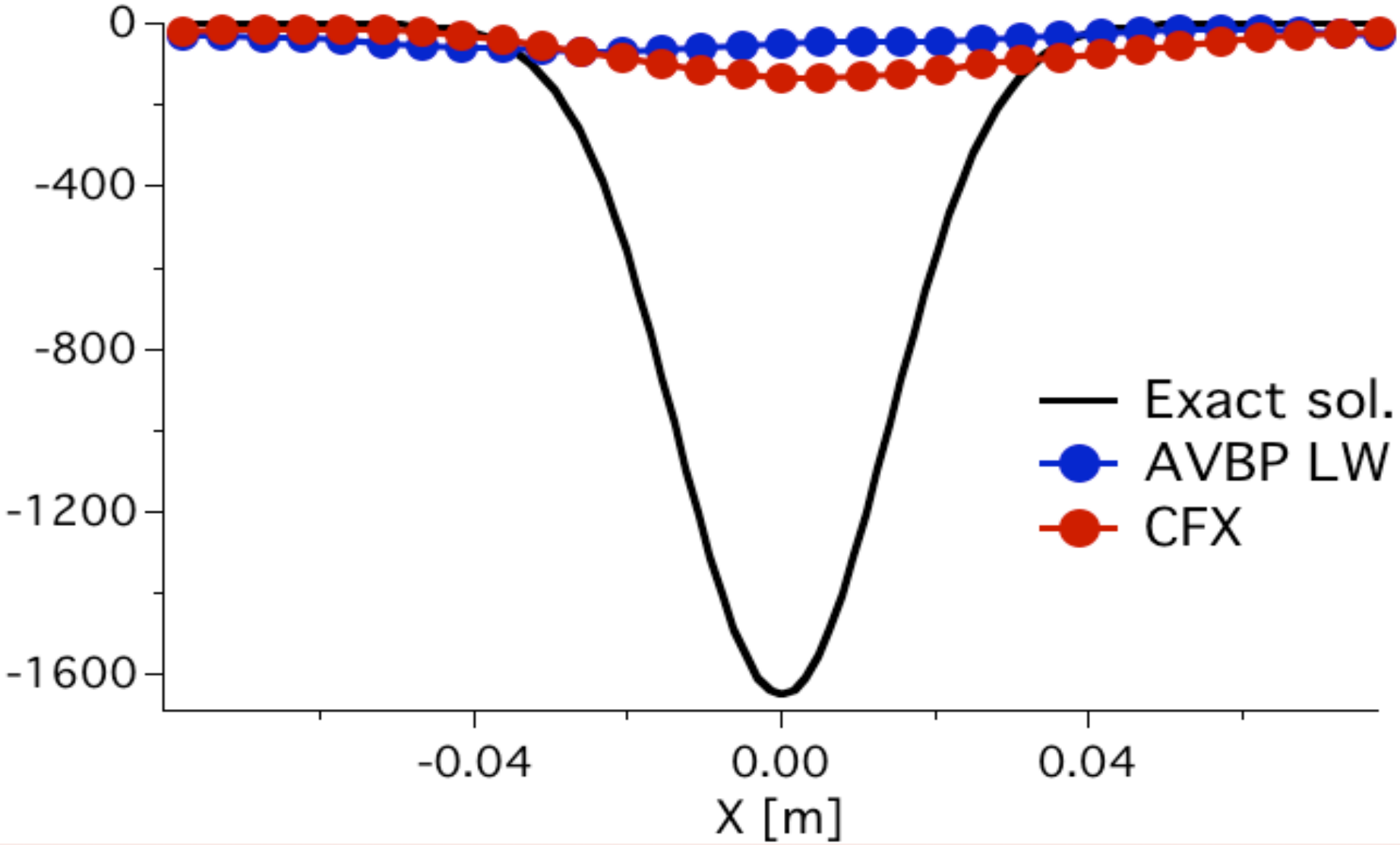
Relative pressure [Pa]



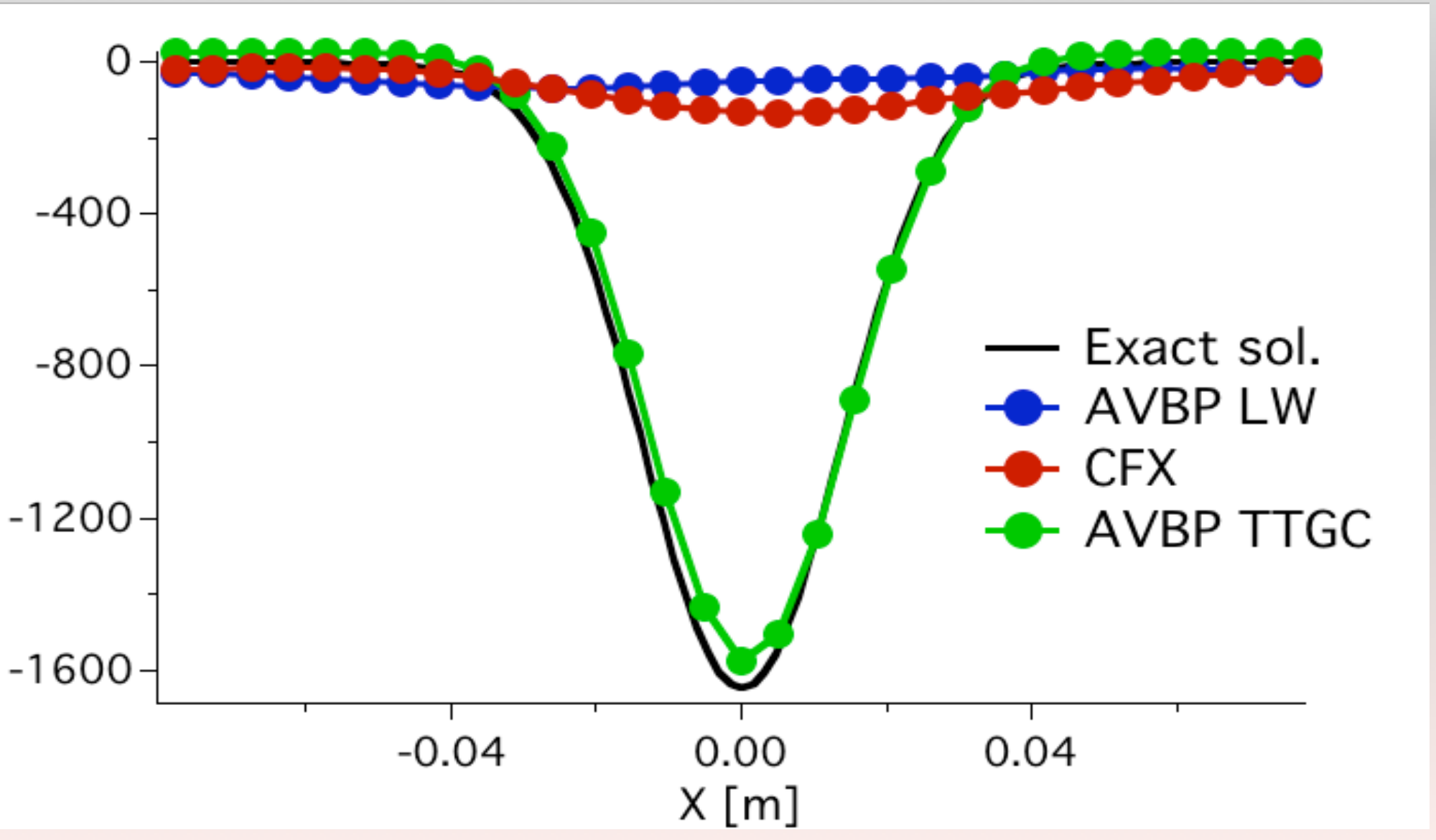
Results after ten turn over times

CFL = 0.7

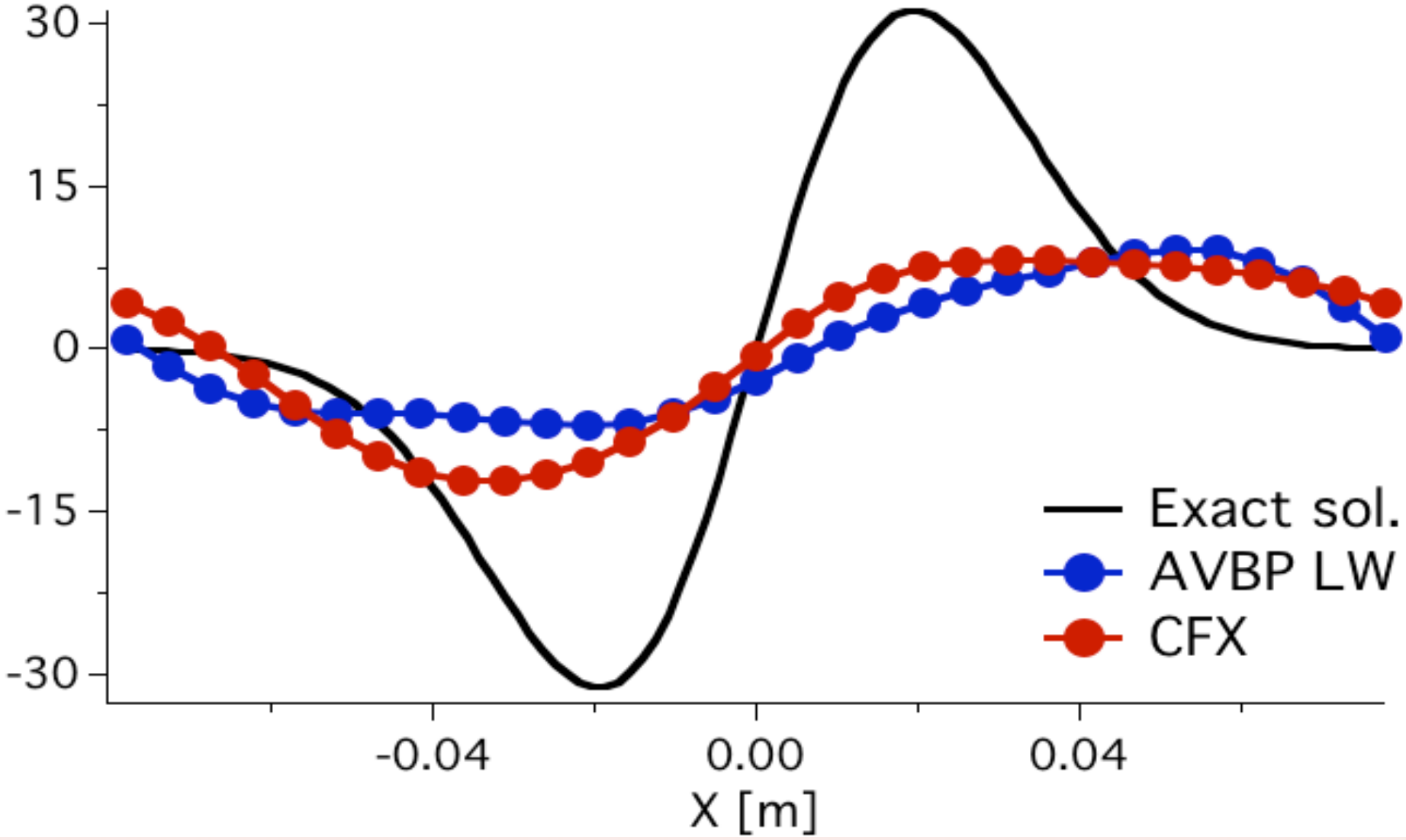
Relative pressure [Pa]



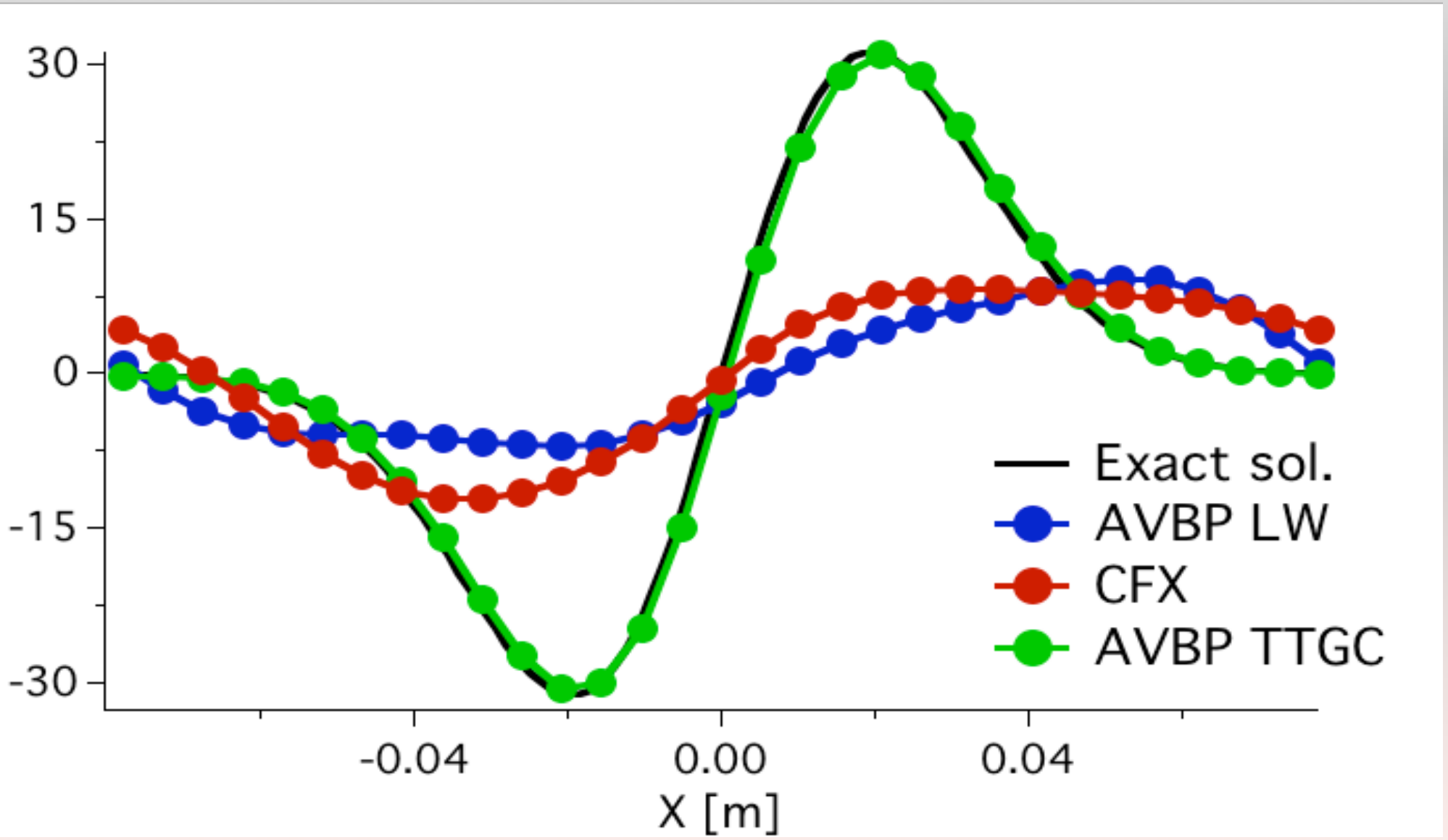
Relative pressure [Pa]



Velocity y [m/s]



Velocity y [m/s]



Influence of time step: the famous implicit/explicit controversy

Essential question for LES:

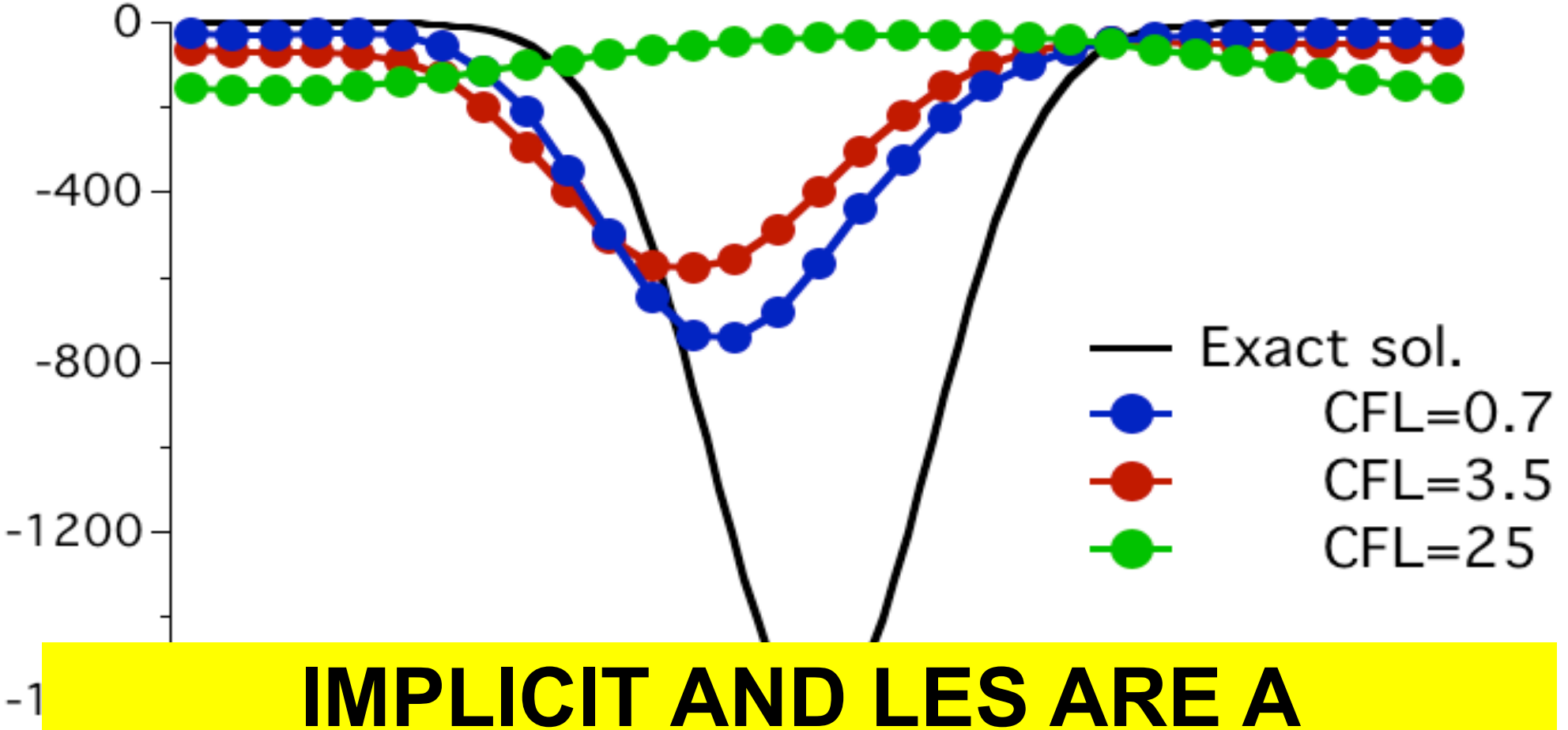
➢ explicit codes use a CFL-limited time step: no question on how to choose the time step, just take the max possible value for stability

➢ implicit codes can use any time step for stability. BUT for precision, the question is open ! The fact that the code can be run does not mean that the result is good ….

➢ In the present test case, an implicit code was used with various CFL up to 10 to 40 corresponding to convective CFL numbers from 1 to 5.

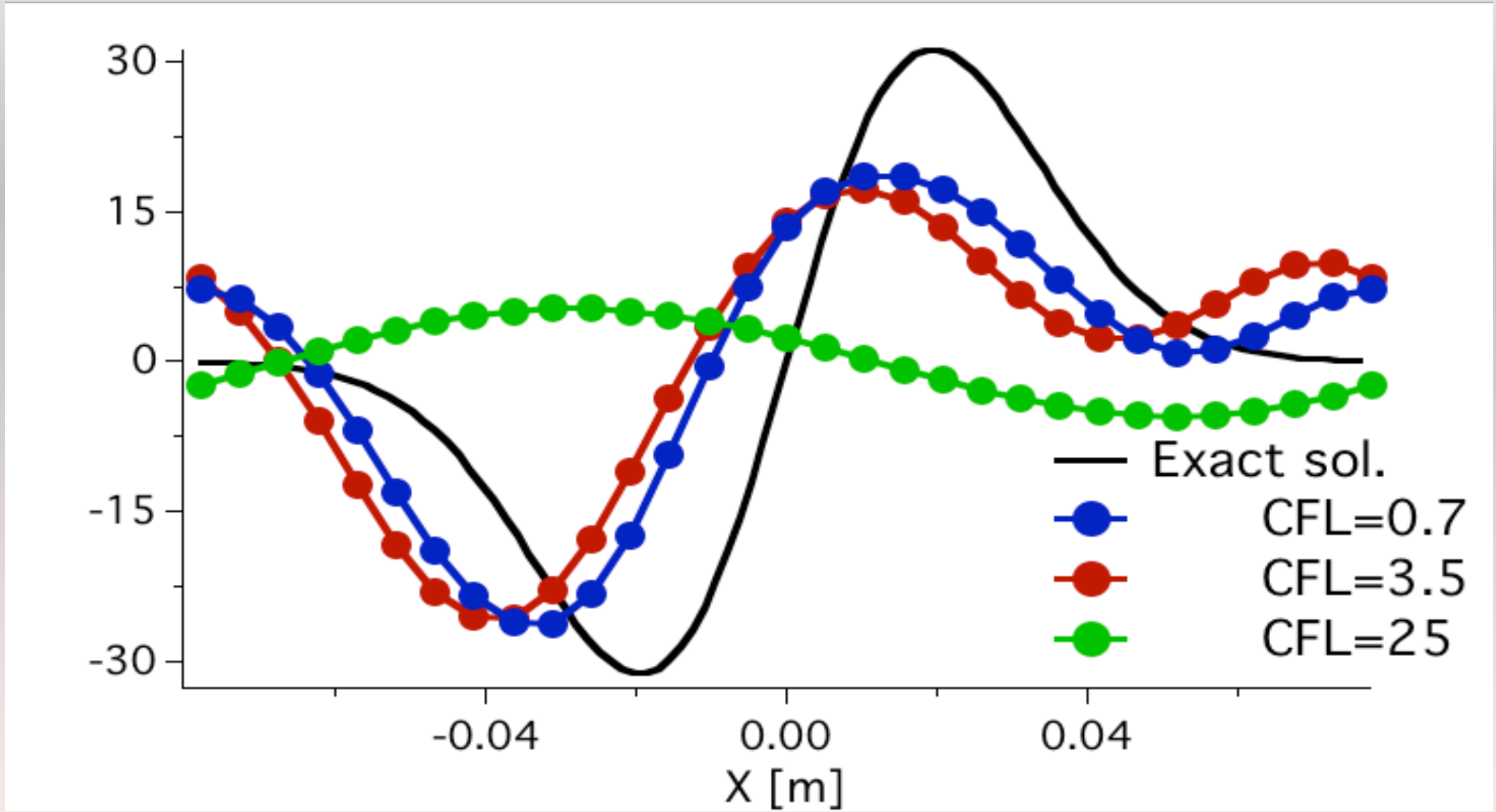
⟶ Results after 3 turn around times

Relative pressure [Pa]



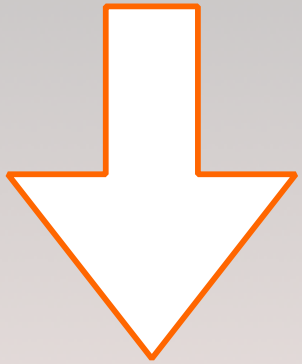
IMPLICIT AND LES ARE A COMBINATION WHICH STILL REQUIRE SOME WORK !

Velocity y [m/s]



What it we add viscosity and start computing species ?

$$\frac{\partial}{\partial t}u + c\frac{\partial}{\partial x}u = 0$$

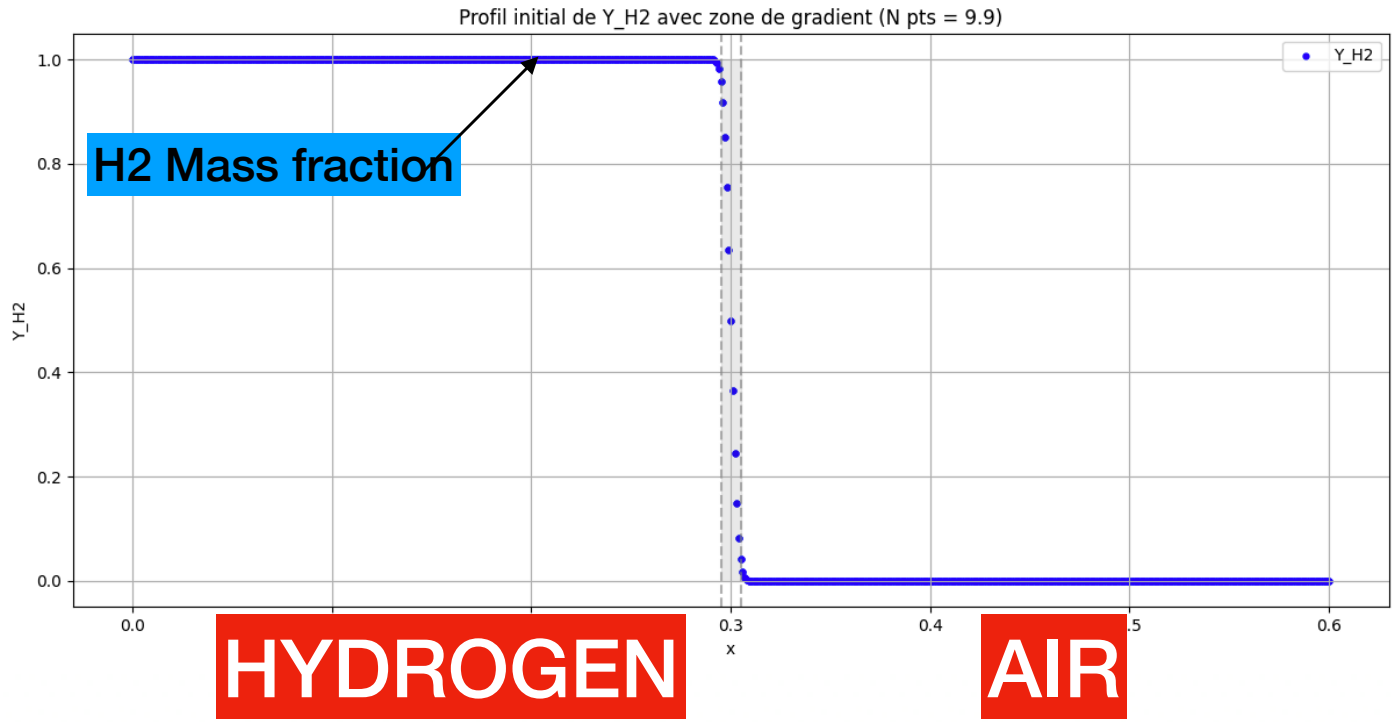


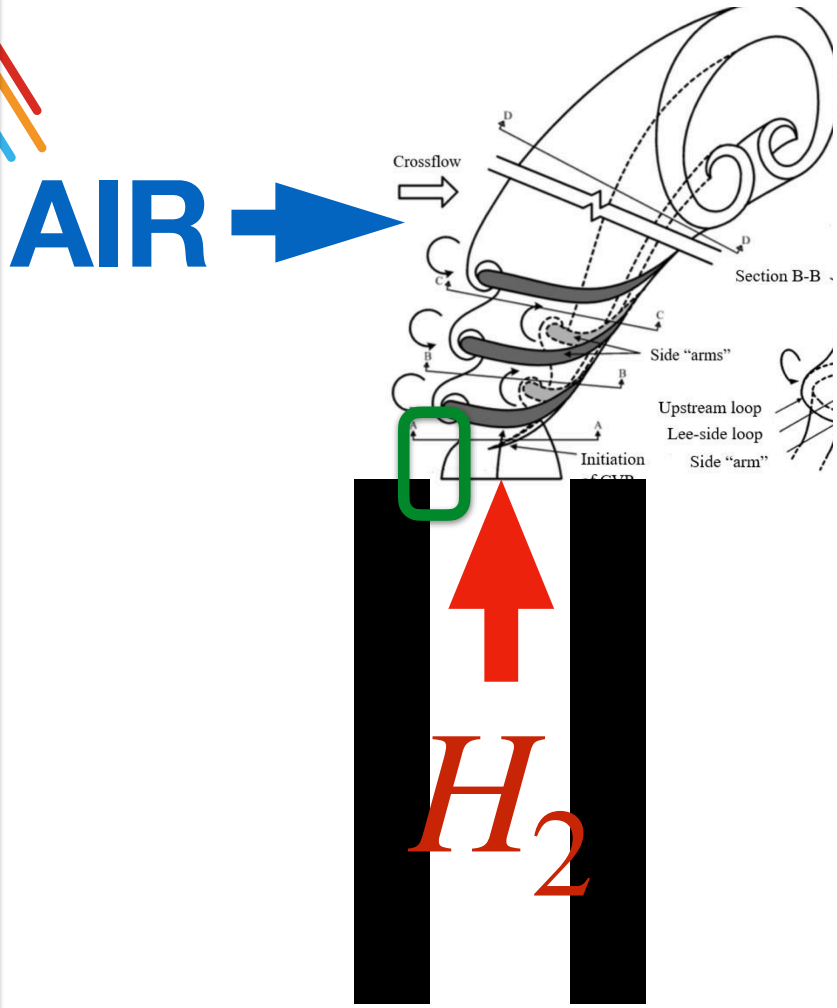
$$\frac{\partial F}{\partial t} + U\frac{\partial F}{\partial x} = \nu\frac{\partial^2 F}{\partial x^2}$$

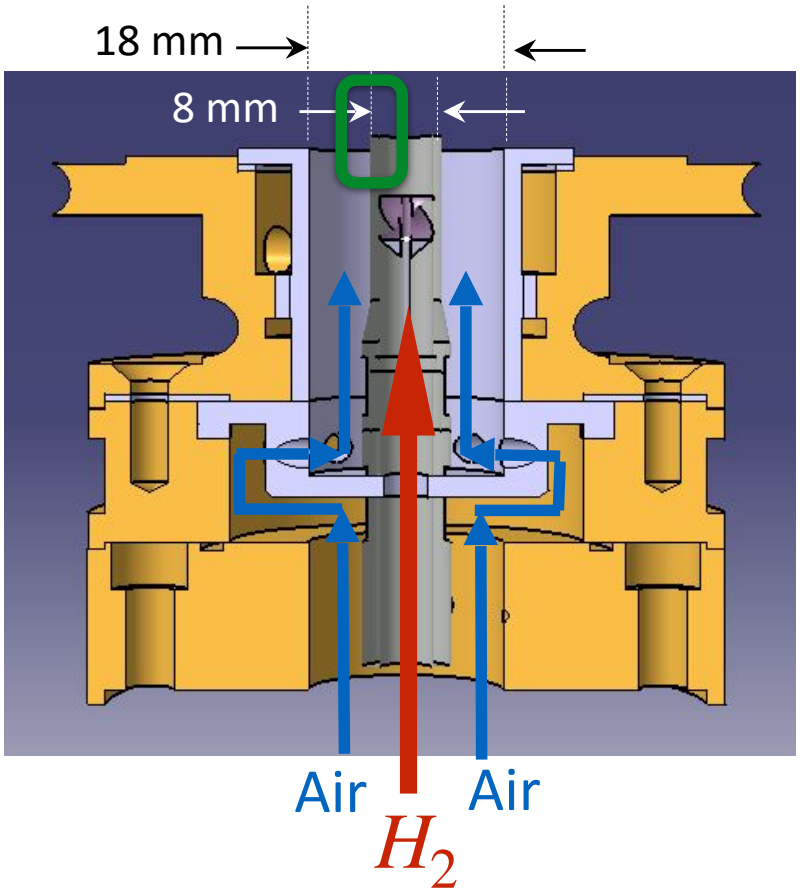
Suppose F is the fuel mass fraction:

Starting from the following equation:

- $$\frac{\partial F}{\partial t} + U\frac{\partial F}{\partial x} = \nu\frac{\partial^2 F}{\partial x^2}$$




AIR
Crossflow
Section B-B
Side "arms"
Upstream loop
Lee-side loop
Side "arm"
Initiation
H_2


18 mm
8 mm
Air
Air
H_2

Stability analysis

Starting from the following equation:

- $$\frac{\partial F}{\partial t} + U\frac{\partial F}{\partial x} = \nu\frac{\partial^2 F}{\partial x^2}$$

We use finite differencing:

- $$\frac{F_i^{n+1} - F_i^n}{\Delta t} = -U\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} + \nu\frac{F_{i+1}^n + F_{i-1}^n - 2F_i^n}{\Delta x^2}$$

-

Stability analysis

Starting from the following equation:

- $$\frac{\partial F}{\partial t} + U\frac{\partial F}{\partial x} = \nu\frac{\partial^2 F}{\partial x^2}$$

We use finite differencing:

- $$\frac{F_i^{n+1} - F_i^n}{\Delta t} = -U\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} + \nu\frac{F_{i+1}^n + F_{i-1}^n - 2F_i^n}{\Delta x^2}$$

We may now define:

- $\lambda = \frac{U\Delta t}{\Delta x}$ → CFL and $F = \frac{\nu\Delta t}{\Delta x^2}$ → Fourier which gives us :

$$Pe = \frac{\lambda}{F} = \frac{U\Delta x}{\nu}$$

Stability analysis

Starting from the following equation:

- $$\frac{\partial F}{\partial t} + U\frac{\partial F}{\partial x} = \nu\frac{\partial^2 F}{\partial x^2}$$

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We may now define:

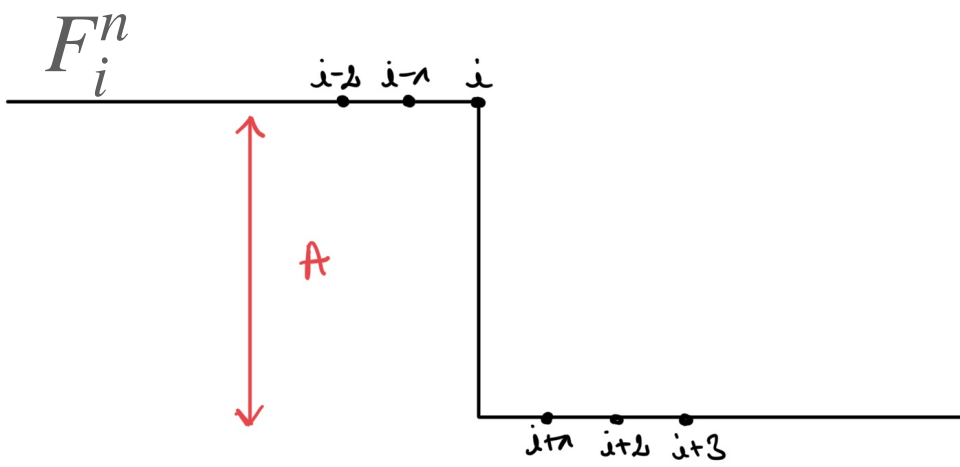
- $\lambda = \frac{U\Delta t}{\Delta x}$ → CFL and $F = \frac{\nu\Delta t}{\Delta x^2}$ → Fourier which gives us :

$$Pe = \frac{\lambda}{F} = \frac{U\Delta x}{\nu} \qquad (1)$$

Which gives F_{n+1} at iteration n+1:

- $$F_i^{n+1} = F_i^n(1-2F) + F_{i+1}^n\left(\frac{-\lambda}{2} + F\right) + F_{i-1}^n\left(\frac{\lambda}{2} + F\right)$$

Stability analysis for a step function in species mass fraction



Starting from the following equation:

- $\frac{\partial F}{\partial t} + U\frac{\partial F}{\partial x} = \nu\frac{\partial^2 F}{\partial x^2}$

We use finite differencing:

- $\frac{F_i^{n+1} - F_i^n}{\Delta t} = -U\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} + \nu\frac{F_{i+1}^n + F_{i-1}^n - 2F_i^n}{\Delta x^2}$

Given our profile, we have:

- $F_{i-1}^n = A,\ F_i^n = A$ and $F_{i+1}^n = 0$

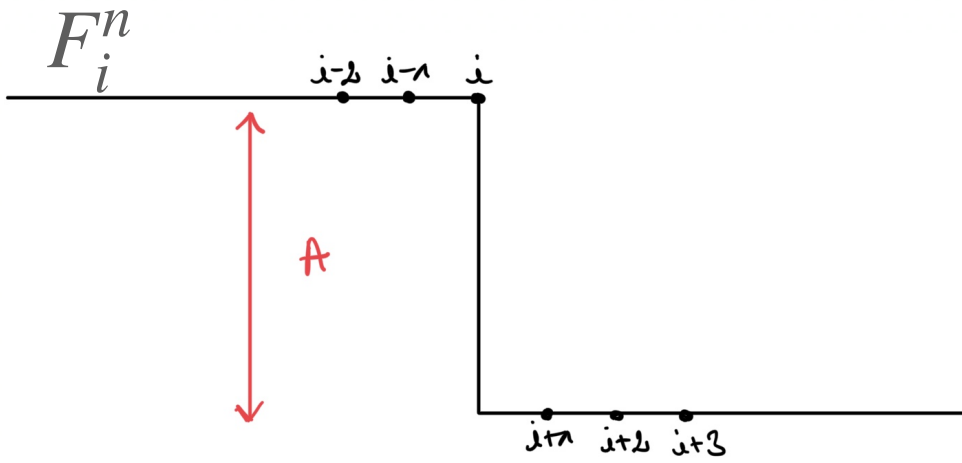
We may now define:

- $\lambda = \frac{U\Delta t}{\Delta x}$ → CFL and $F = \frac{\nu\Delta t}{\Delta x^2}$

  → Fourier which gives us :

$$Pe = \frac{\lambda}{F} = \frac{U\Delta x}{\nu} \quad (1)$$

Non linear stability analysis



Starting from the following equation:

- $\frac{\partial F}{\partial t} + U\frac{\partial F}{\partial x} = \nu\frac{\partial^2 F}{\partial x^2}$

We use finite differencing:

- $\frac{F_i^{n+1} - F_i^n}{\Delta t} = -U\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} + \nu\frac{F_{i+1}^n + F_{i-1}^n - 2F_i^n}{\Delta x^2}$

We may now define:

- $\lambda = \frac{U\Delta t}{\Delta x}$ →CFL and $F = \frac{\nu\Delta t}{\Delta x^2}$ →Fourier

  which gives us :

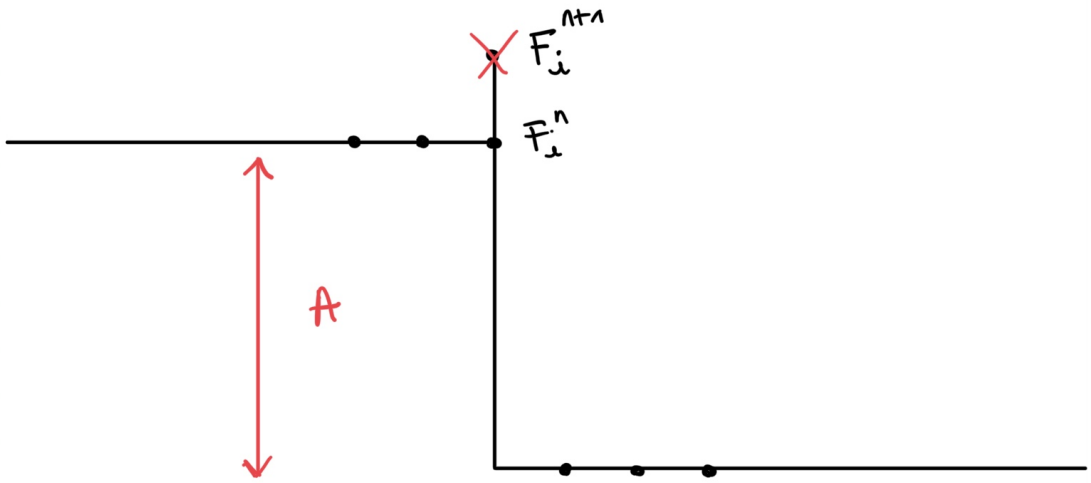
$$Pe = \frac{\lambda}{F} = \frac{U\Delta x}{\nu} \qquad (1)$$

Given our profile, we have:

- $F_{i-1}^n = A,\ F_i^n = A$ and $F_{i+1}^n = 0$

We can simplify (1):

- $F_i^{n+1} = A(1 - 2F + \frac{\lambda}{2} + F)$



Starting from the following equation:

- $\frac{\partial F}{\partial t} + U\frac{\partial F}{\partial x} = \nu\frac{\partial^2 F}{\partial x^2}$

We use finite differencing:

- $\frac{F_i^{n+1} - F_i^n}{\Delta t} = -U\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} + \nu\frac{F_{i+1}^n + F_{i-1}^n - 2F_i^n}{\Delta x^2}$

We may now define:

- $\lambda = \frac{U\Delta t}{\Delta x}$ →CFL and $F = \frac{\nu\Delta t}{\Delta x^2}$ →Fourier
  which gives us :

$$Pe = \frac{\lambda}{F} = \frac{U\Delta x}{\nu} \quad (1)$$

Given our profile, we have:

- $F_{i-1}^n = A,\ F_i^n = A$ and $F_{i+1}^n = 0$

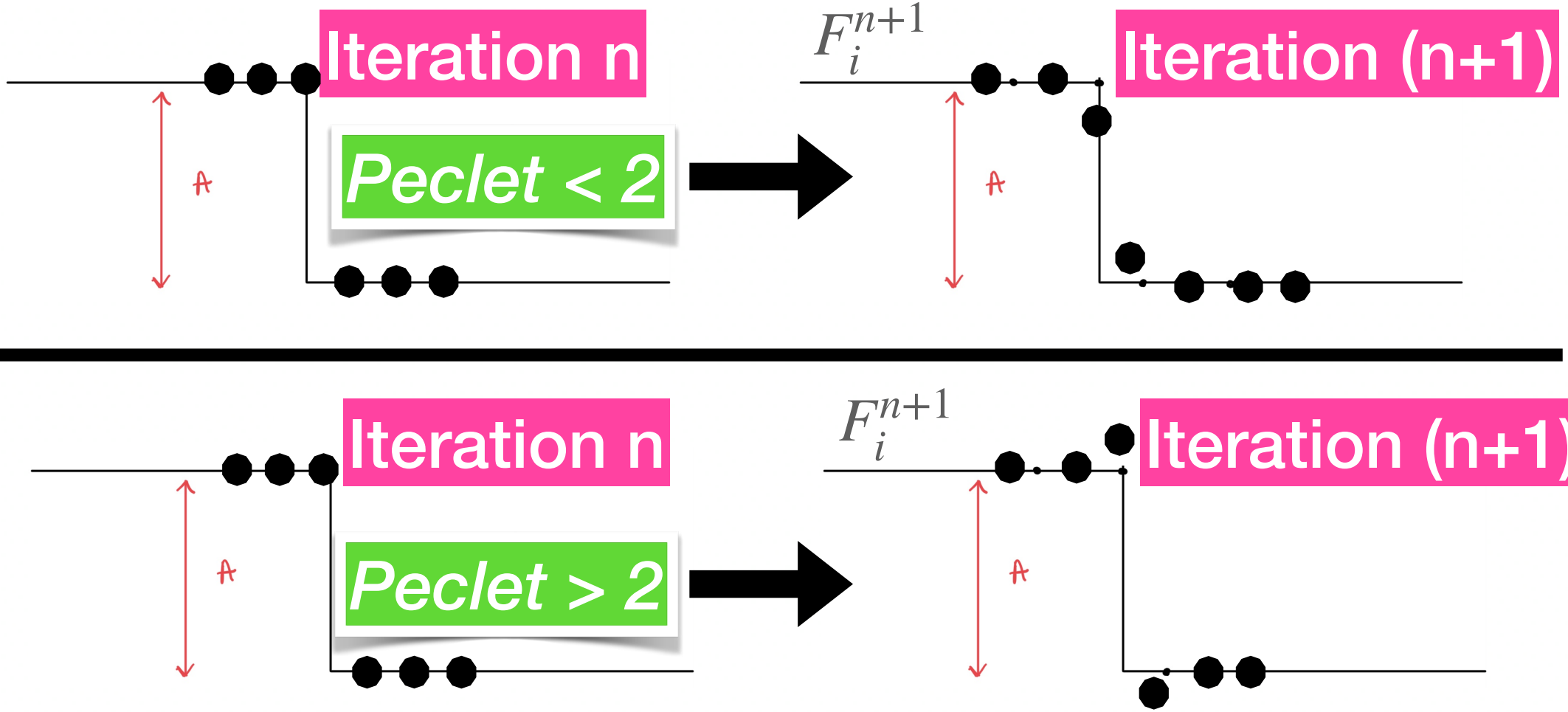
We can simplify (1):

- $F_i^{n+1} = A(1 - 2F + \frac{\lambda}{2} + F)$

Using the stability criterion $F_i^{n+1} \leq A$, we obtain: (2)

- $F - \frac{\lambda}{2} \geq 0$ and, as a consequence:

$$Pe \leq 2$$


Iteration n
Peclet < 2
F_i^{n+1}
Iteration (n+1)
A
Iteration n
Peclet > 2
F_i^{n+1}
Iteration (n+1)
A

Please help: give me artificial viscosity !

$$Pe = \frac{\lambda}{F} = \frac{U\Delta x}{\nu}$$

This Peclet can be larger than 2

$$Pe = \frac{\lambda}{F} = \frac{U\Delta x}{\nu + \nu_a}$$

But you can decrease this one to less than 2 by increasing ν_a

Introducing artificial viscosity will help.

It decreases Re= $UL/\nu \rightarrow UL/(\nu + \nu_a)$

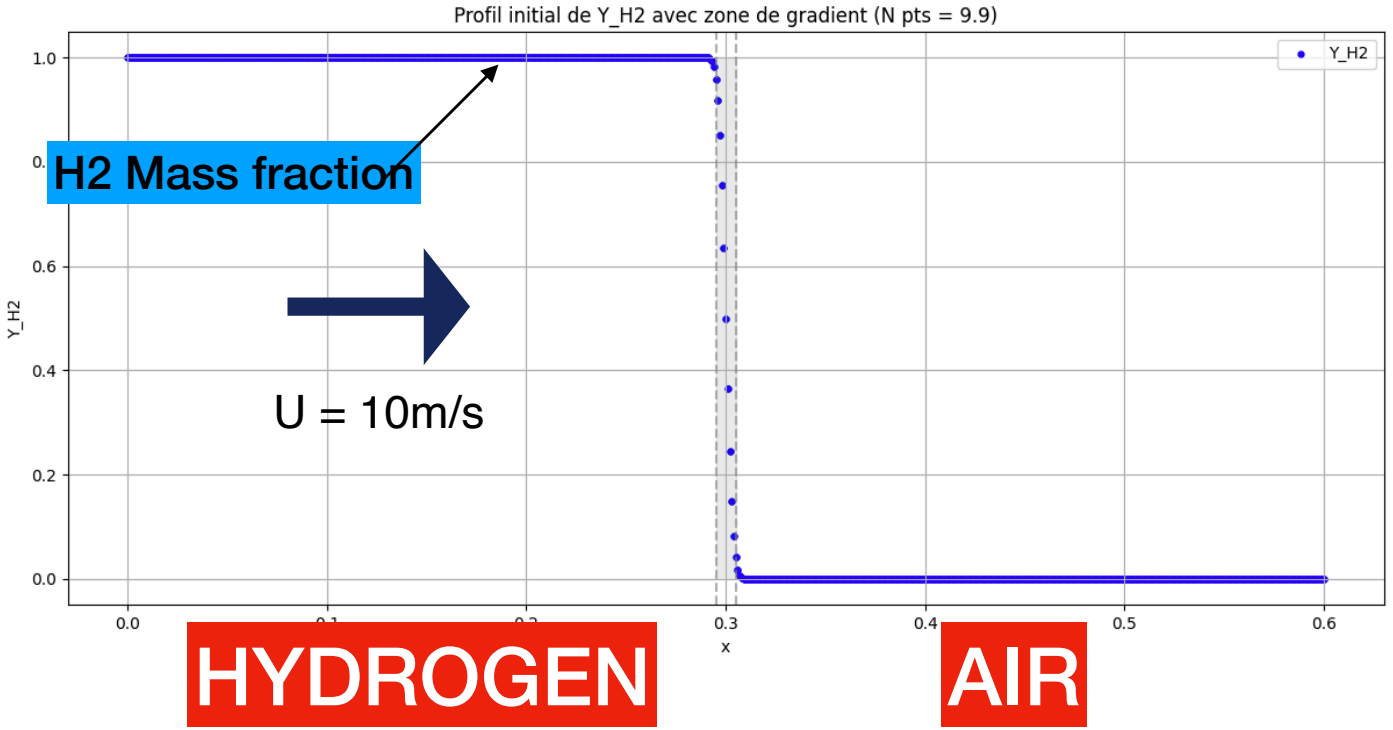
Like aspirin on a broken leg

1D test case: mixing between pure H2 (left) and air

Schmitt et al. [1] : test case in AVBP 1D

Initial solution: tanh function

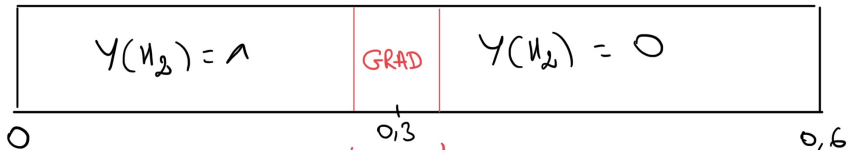
- **Setup numérique**:
  - No artificial viscosity
  - Euler
  - 1D domain, length 0.6m
  - Mean speed = 10 m/s everywhere

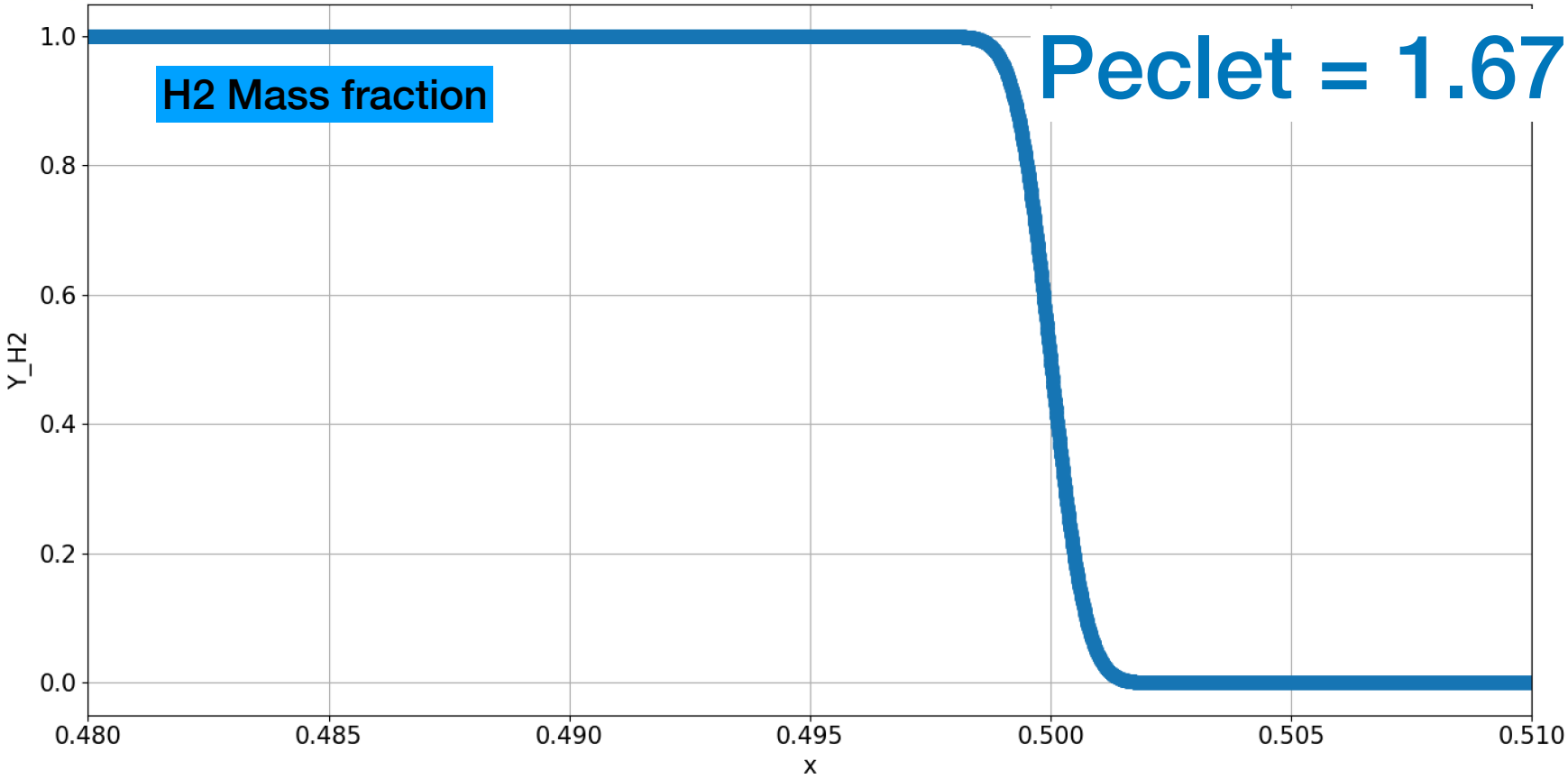


[1] Schmitt, T. Large-Eddy Simulations of the Mascotte Test Cases Operating at Supercritical Pressure. *Flow Turbulence Combust* 105, 159–189 (2020)..

Results

Init:

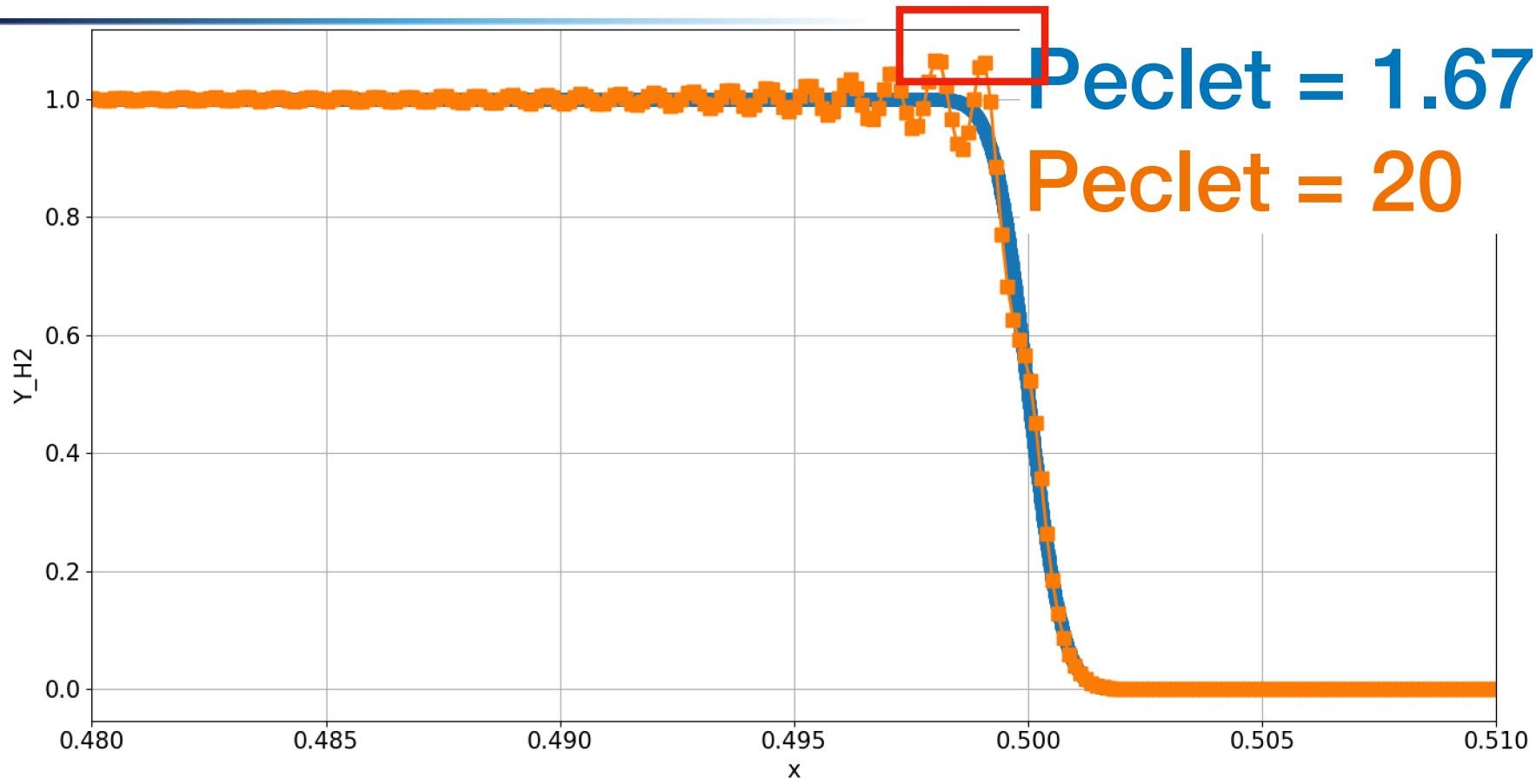




Reminders:

- Solver type : Euler
- Convection scheme : TTGC

$Y_{H_2} = 1.1$ Oups ?



Reminders:

- Solver type : Euler
- Convection scheme : TTGC

So, a perfect simulation (DNS typically) should have Peclet <2

This gives a simple resolution criterion in terms of number of mesh points Nx in each direction:

$$Pe = \frac{U\Delta x}{\nu} < 2$$

$$Pe = \frac{UL}{\nu} / (L/\Delta x) = Re/Nx$$

$$Nx > Re/2$$

In DNS maybe possible

In LES with Re= 100 000, would need *Nx* = 50 000 points … in each direction

Conclusions - for LES (or DNS):
(1) small time steps are needed
(2) high-order schemes are better:
==> well known for DNS codes

In the DNS community (which uses structured grids):
- Spectral schemes (not many in combustion)
- Pseudo spectral schemes
- Finite differences: 6th, 8th, 10th order in space

BUT IT IS NOT SIMPLE TO CONSTRUCT AN EXPLICIT HIGH-ORDER SCHEME ON UNSTRUCTURED MESHES !
1st order: easy
2nd order: OK
3rd order: much more difficult
4th order: ouch !

Structured meshes can not be a good approach for combustion chambers… PROBLEM FOR LES !

==> Care is needed to propagate physical waves (vortex and acoustic waves) at the right speed and amplitude.

But there are worse news: 'other' waves are created and propagated by codes. These waves travel in 'packets'.

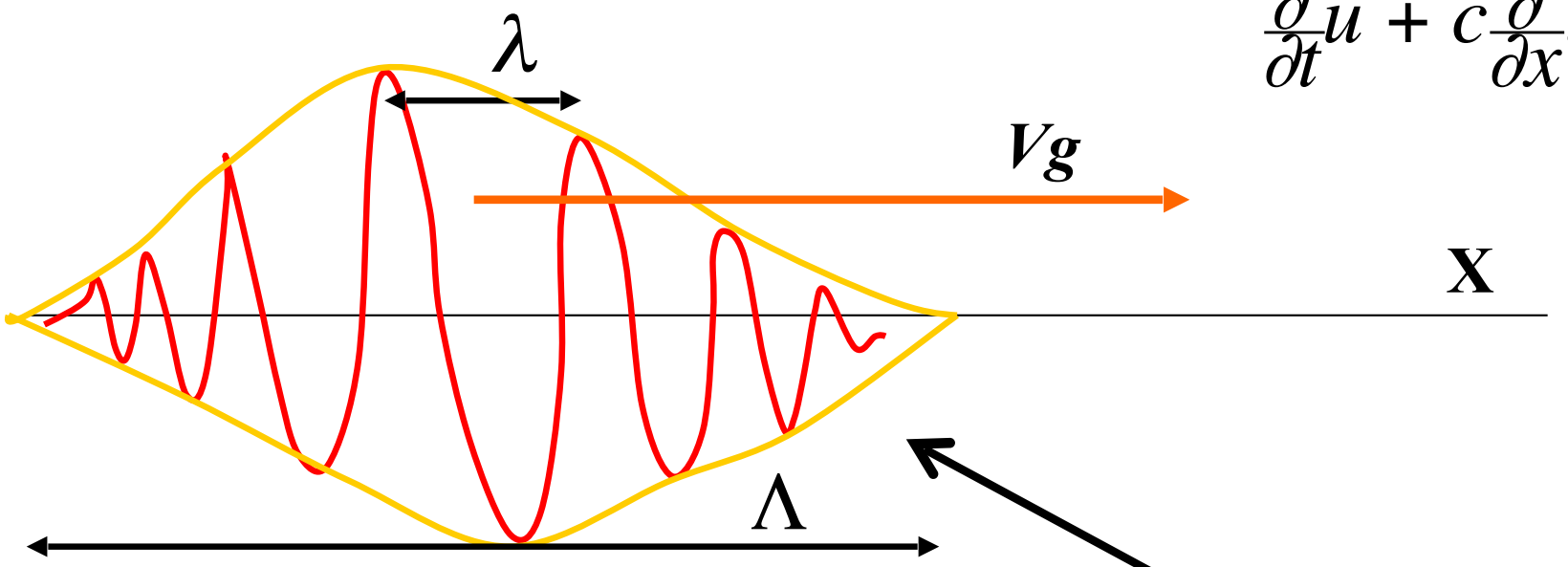
- ***Vichnevetski and Bowles 1982, SIAM studies in Applied Mechanics***
- ***Sengupta 2004 Fundamentals of Computational Fluid Dynamics***
- ***Poinsot Veynante TNC 2011***

Ch. 9 Section 9.7.1

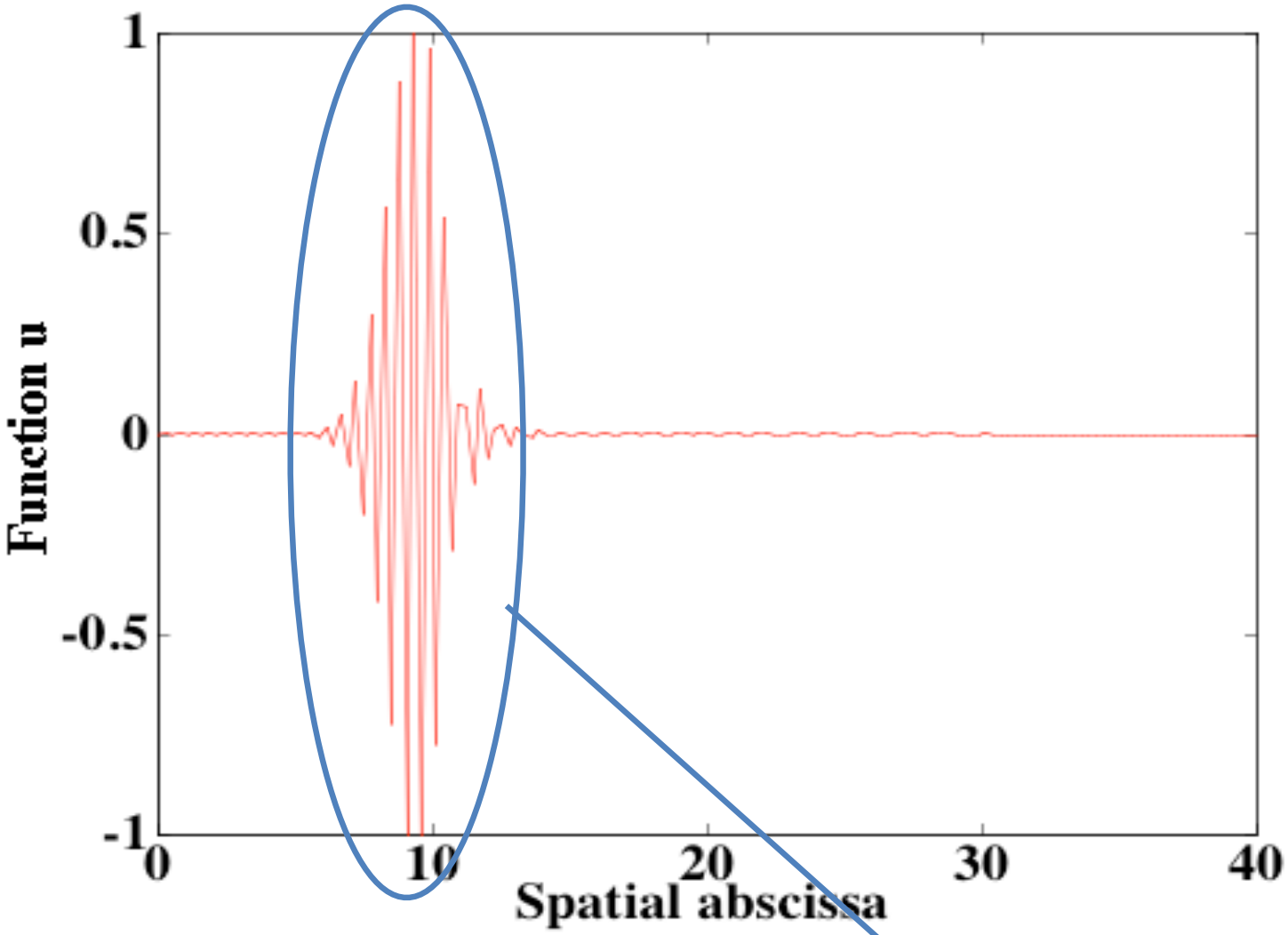
The group velocity of wiggles

In dispersive flows, the group velocity *Vg* (ω) of wave packets differ from *c(ω)*… Illustration for the advection equation:

$$\frac{\partial}{\partial t}u + c\frac{\partial}{\partial x}u = 0$$



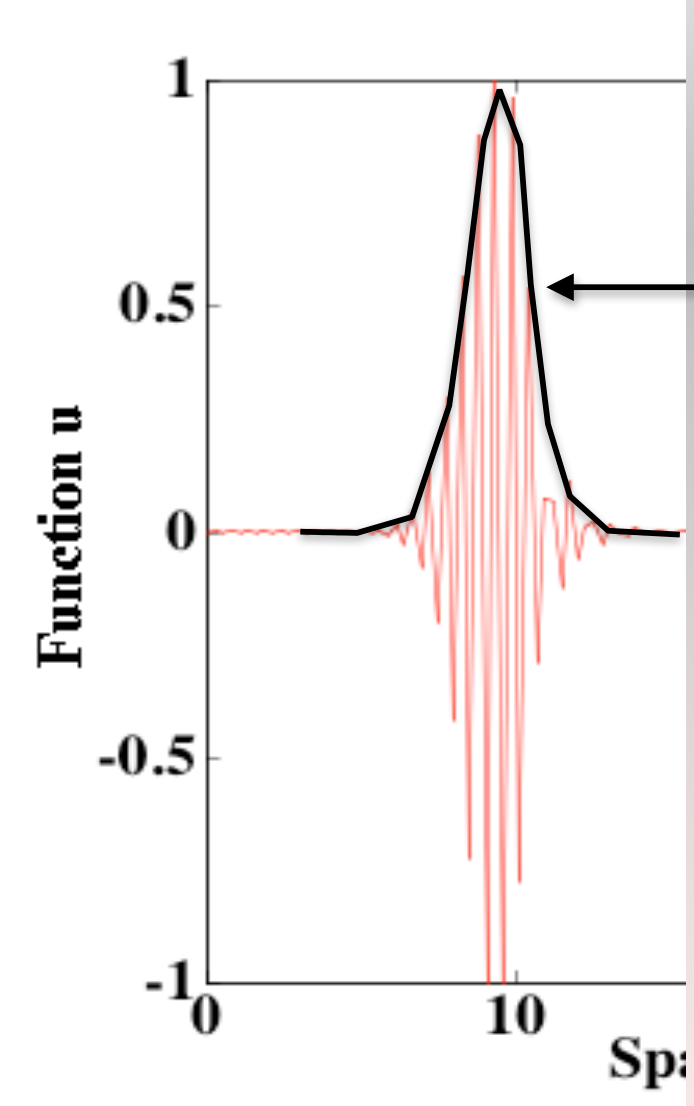
Typical wave packet:
envelope (long wave length Λ)
+
high frequency wave (short wave length λ)



Initial condition:
A typical wave packet

Numerical wave packet:
- **Wavelength=2 Δx**
- **Propagating in the wrong direction !**

Do we understand this ? Let us look at the speed at which a wave train of wavelength $\lambda = 2\Delta x$ and envelope *v(x)* moves:



$v(x)$

$$u(i\Delta x, t=0) = v(i) * (-1)^i$$

$$\frac{\partial}{\partial t}u + c\frac{\partial}{\partial x}u = 0$$

$$(-1)^i \frac{\partial v}{\partial t} + c\frac{(-1)^{(i+1)}v(x+\Delta x) - (-1)^{(i-1)}v(x-\Delta x)}{2\Delta x} = 0$$

$$\frac{\partial v}{\partial t} - c\frac{\partial v}{\partial x} = 0$$

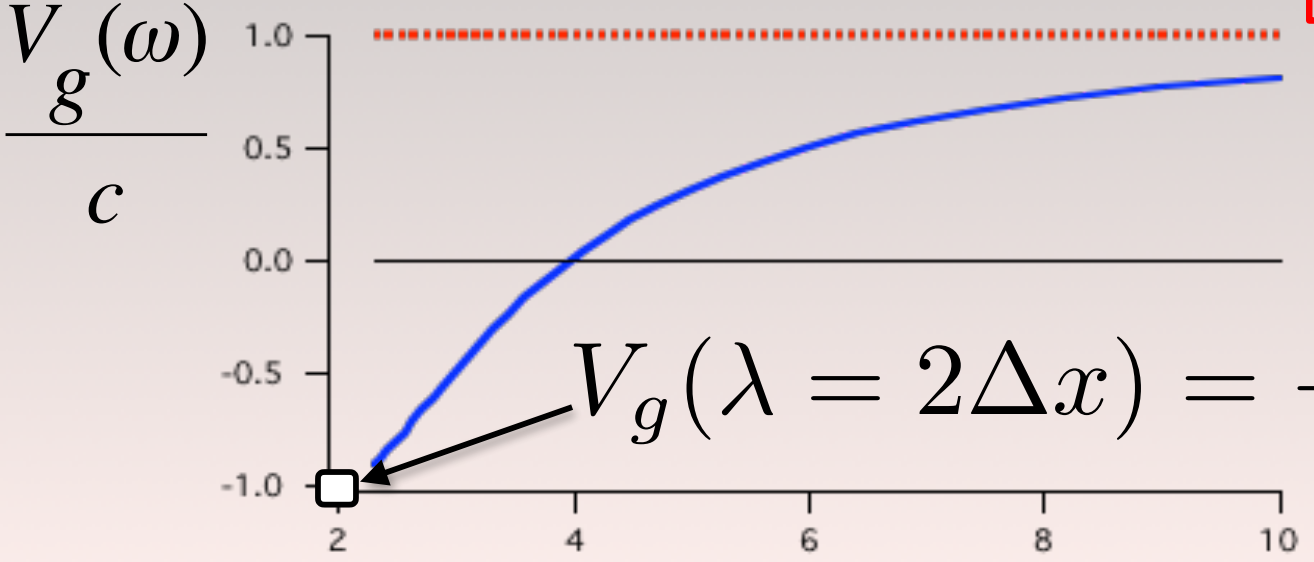
The *v* function travels LEFT at speed -c, as seen in the simulation…

Generalization to all wave lengths in waves books. For fluid flow and centered schemes, see *Vichnevetski and Bowles 1982, 1986* or *Sengupta 2004*. The main result is that the group velocity *Vg* of wave packets is given by:

$$\frac{V_g(\omega)}{c} = \frac{d}{d\omega}\left[\frac{\omega c(\omega)}{c}\right]$$

For the second-order scheme:

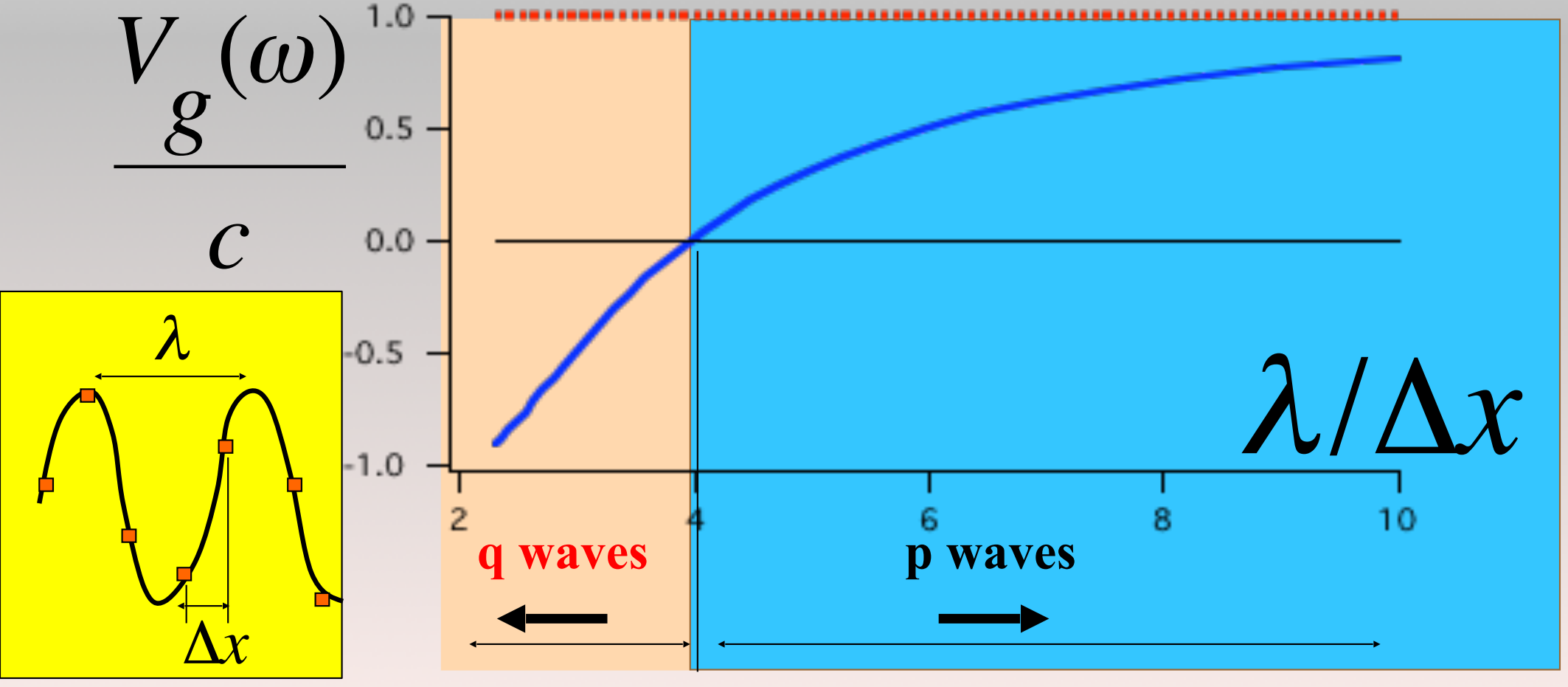
$$\frac{c(\omega)}{c} = \frac{\sin(2\pi\omega\Delta x)}{2\pi\omega\Delta x} \rightarrow \frac{V_g(\omega)}{c} = \cos(2\pi\omega\Delta x)$$



$\lambda/\Delta x = 1/(\omega\Delta x)$

Codes propagate two types of waves depending on the sign of Vg:

- **Physical waves called ‘p’ (long wave): they go with the flow**
- **Numerical waves (short wave): ’q’ going against the flow**



For the centered second order scheme, the group velocity of wiggles (waves with a wavelength equal to 2 Δx) is

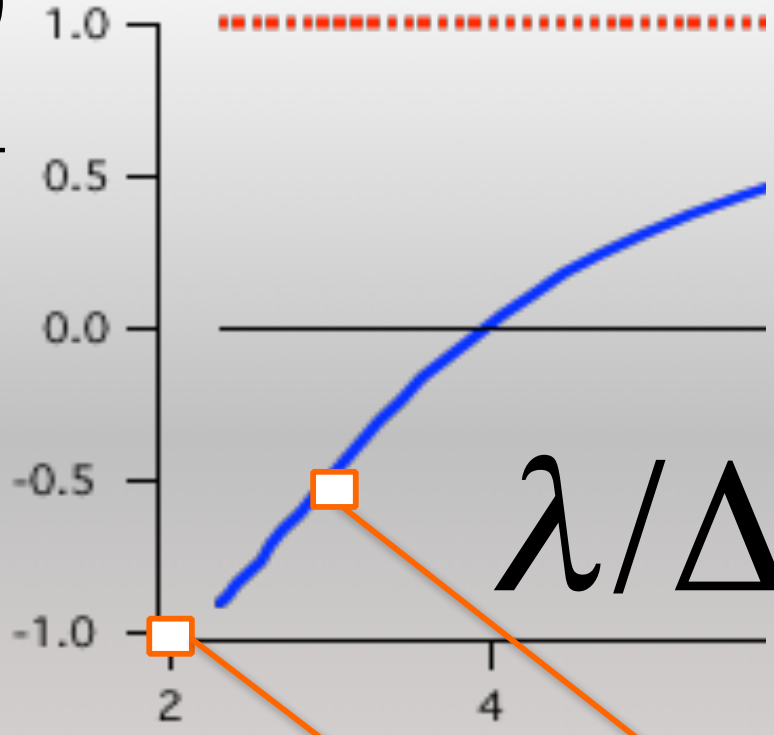
$$\frac{V_g(\omega)}{c} = -1$$

For higher order schemes, this velocity gets … worse. For example, a compact sixth-order scheme (Baum et al 1994):

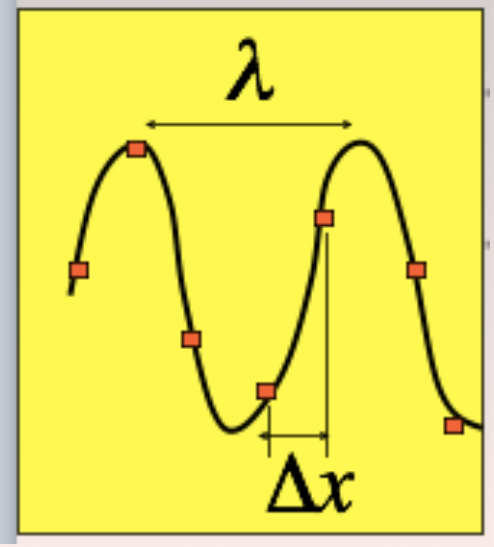
$$\frac{V_g(\omega)}{c} = -4.3$$

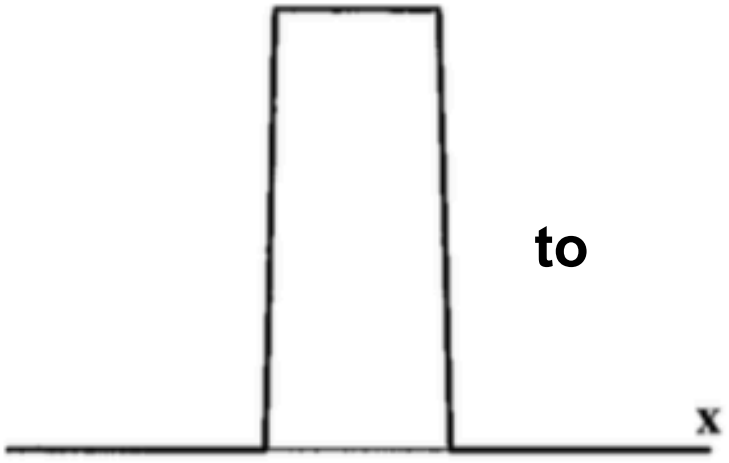
Here, wiggles propagate upstream at -4.3 times the sound speed.

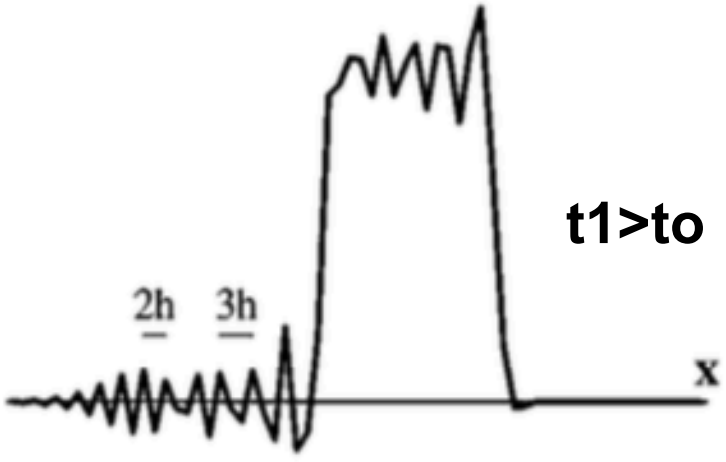
$$\frac{V_g(\omega)}{c}$$

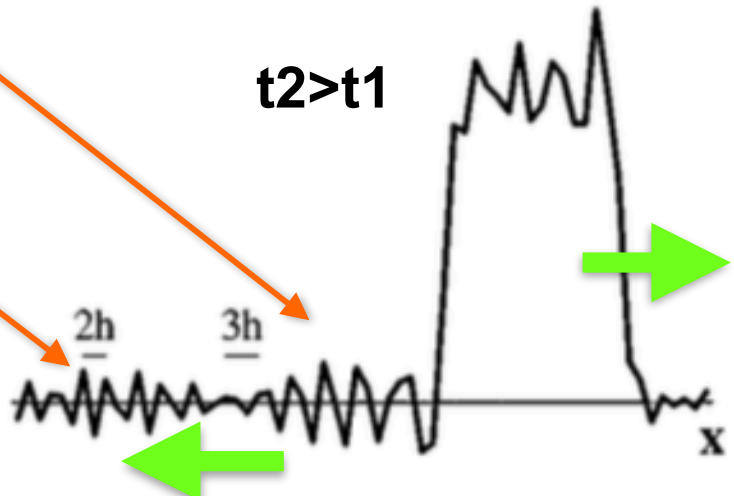


$\lambda/\Delta x$



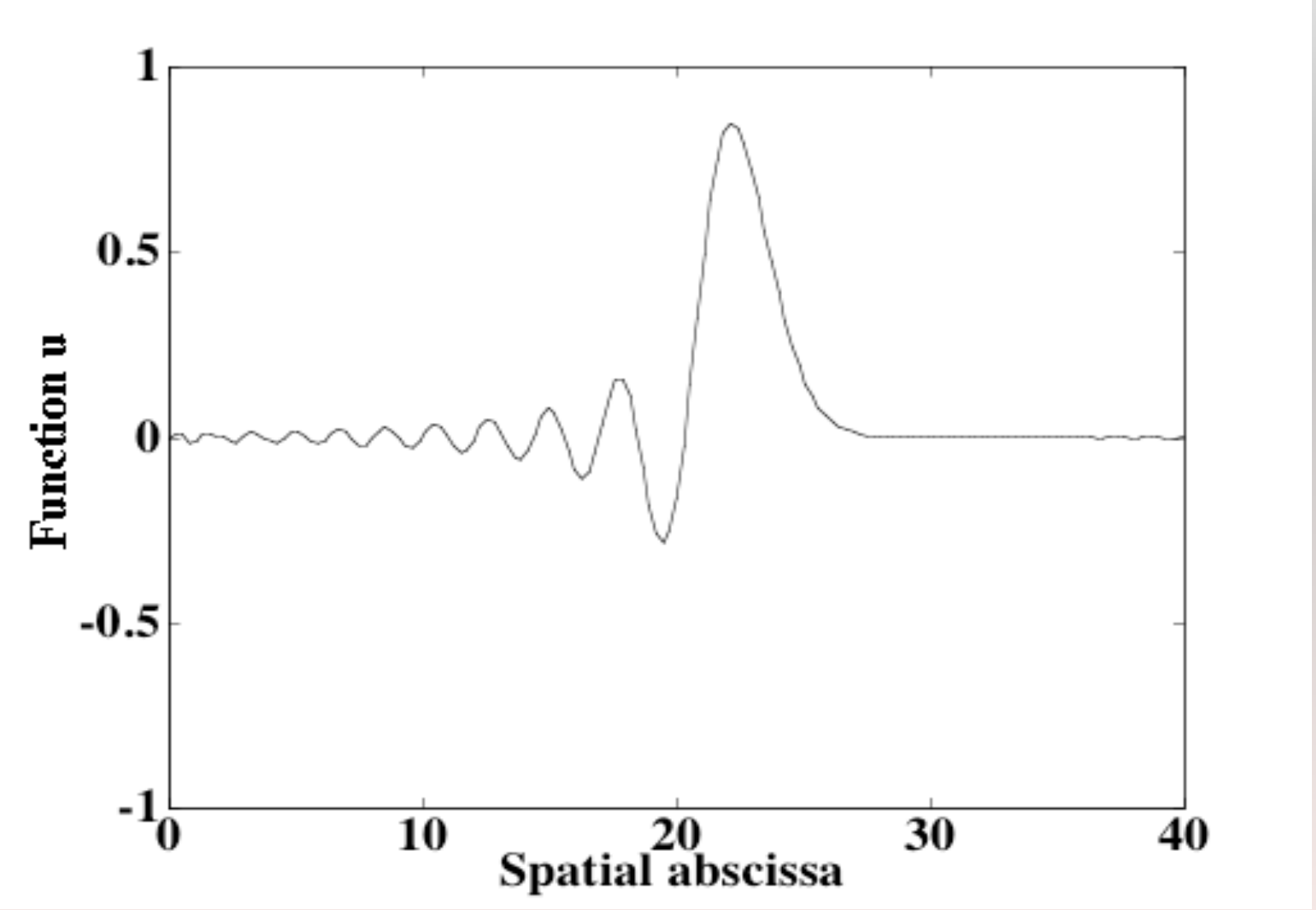




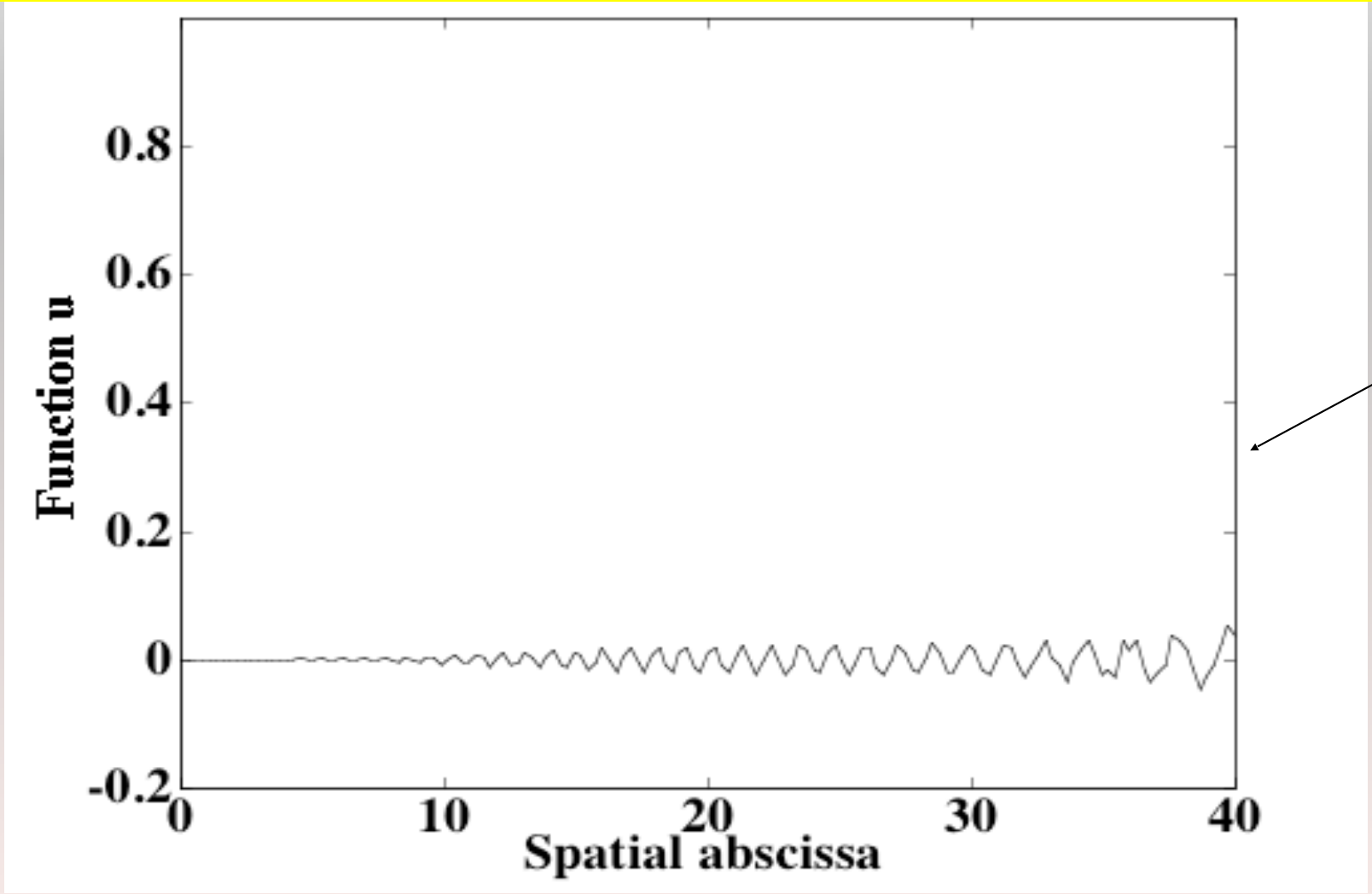


Kobayashi, JCP 156, 1999

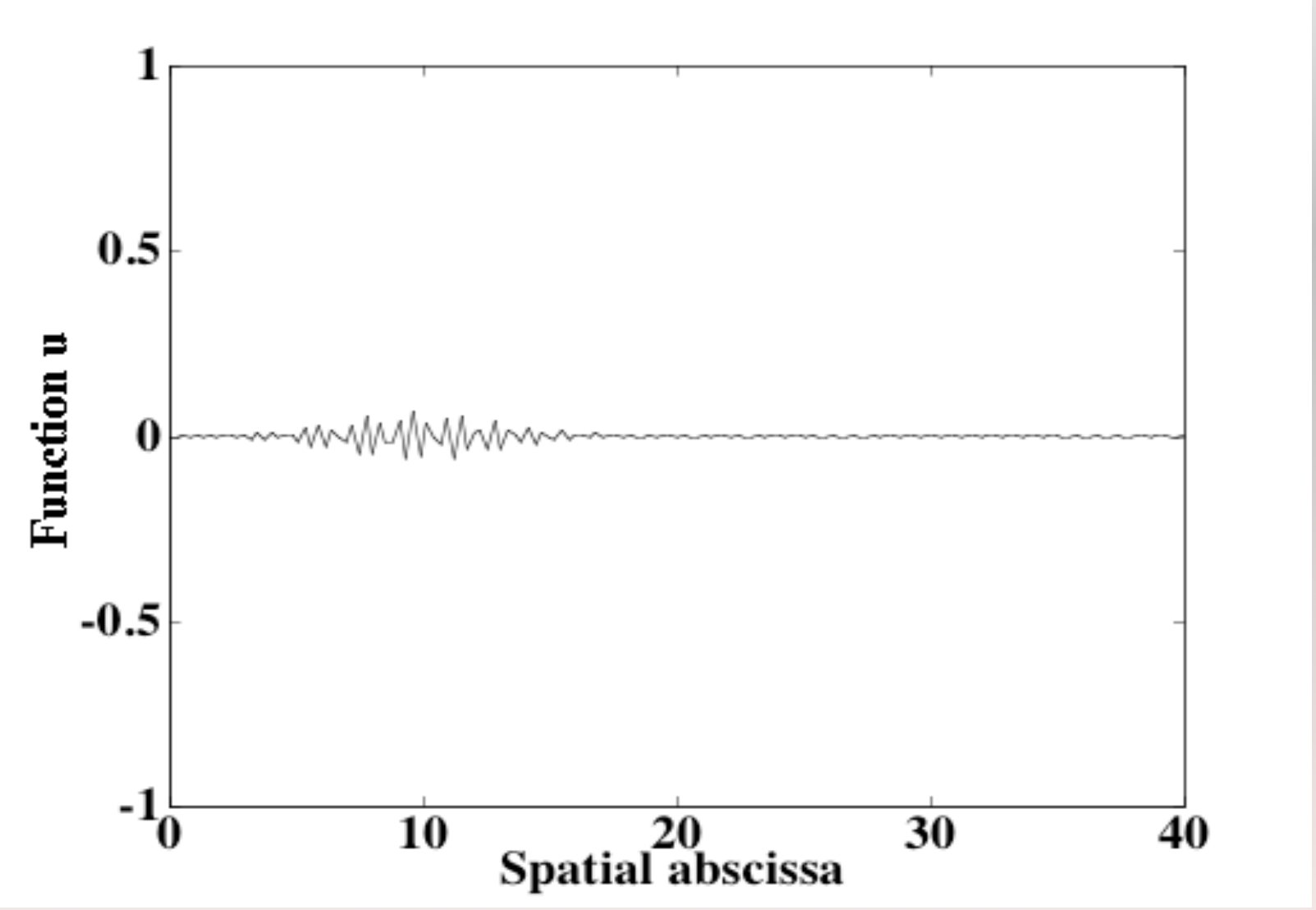
Why do we care about ‘q’ waves ? : they perturb the flow. They also reflect into ‘p’ waves at boundaries !



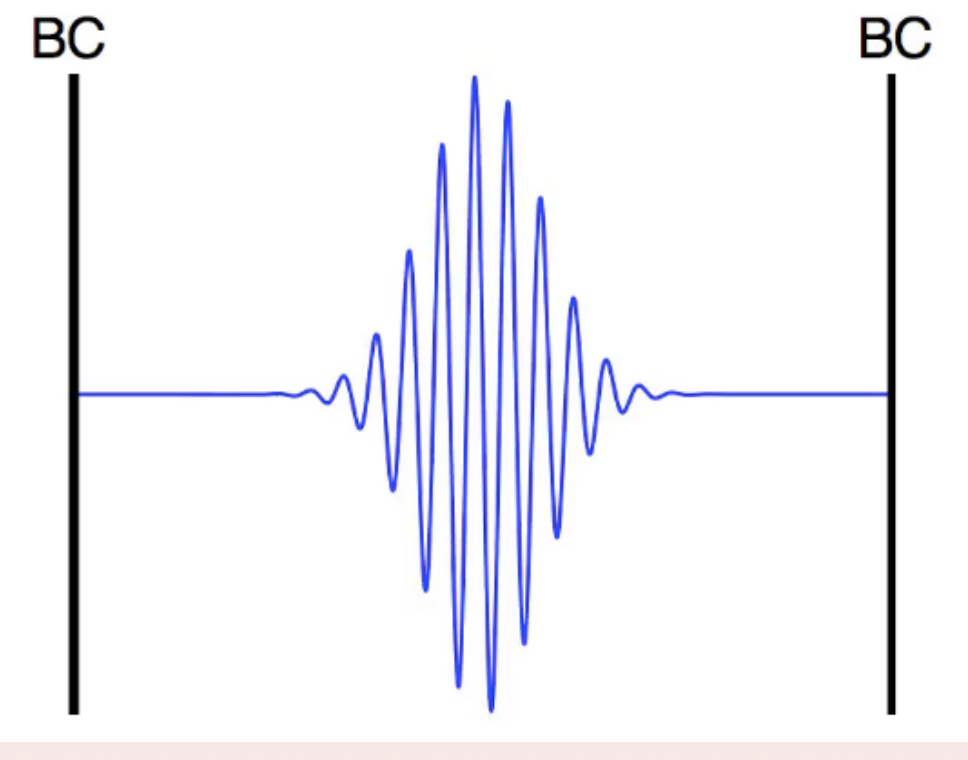
Numerical ‘q’ waves are difficult to avoid:
1/ They can be created by stiff initial conditions, even if the user does not see them



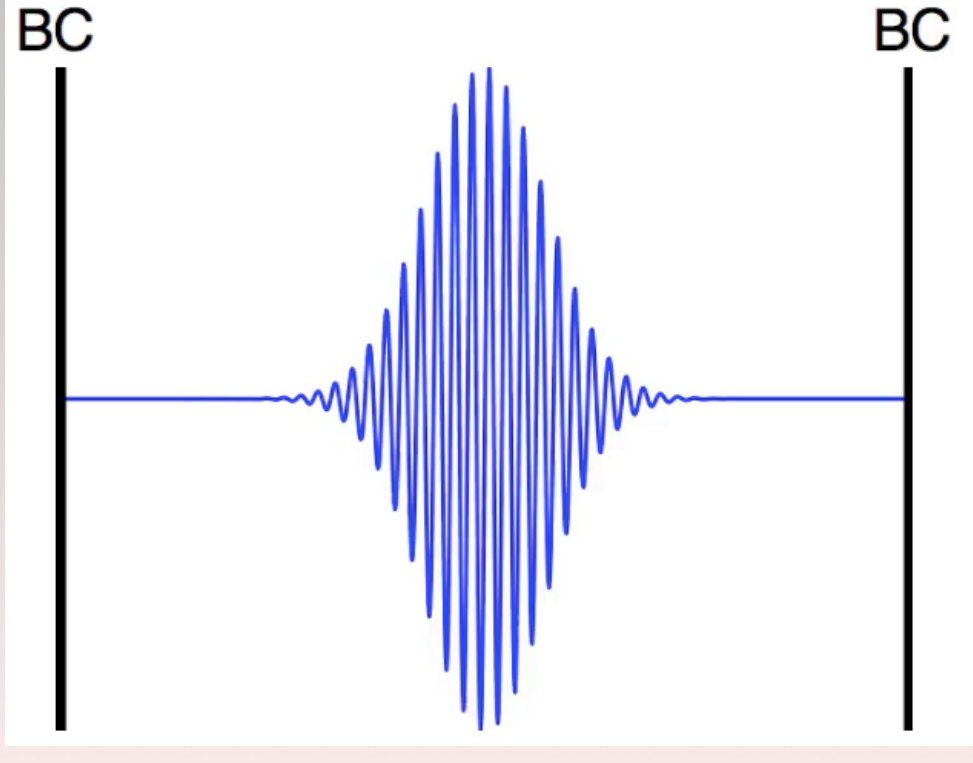
2/ Numerical ‘ q ’ waves are also generated when physical ‘ p ’waves interact with boundaries



The reflection coefficient of p-to-q waves at a boundary depends on boundary condition AND on the frequency of the incident wave:

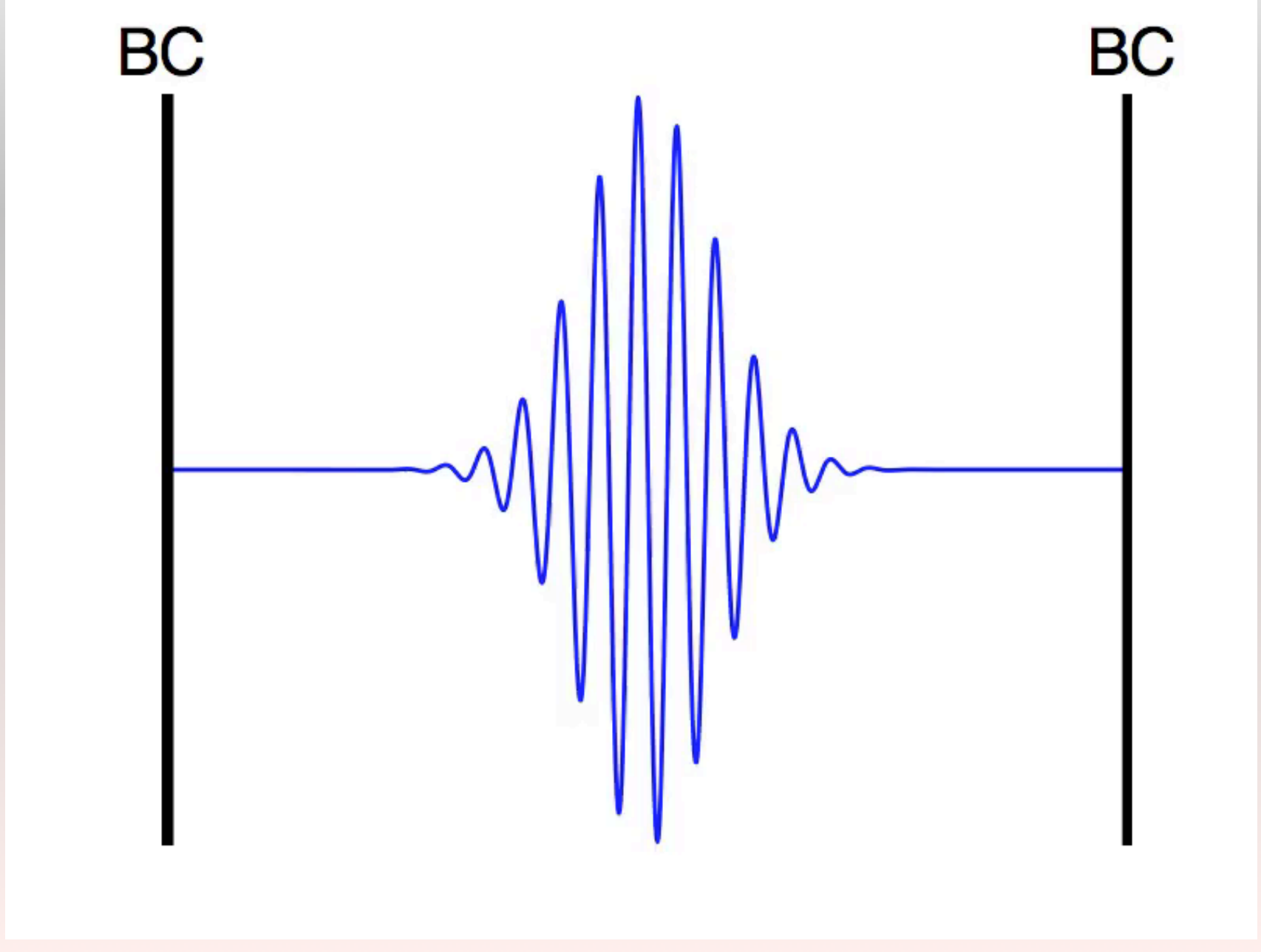


Low frequency

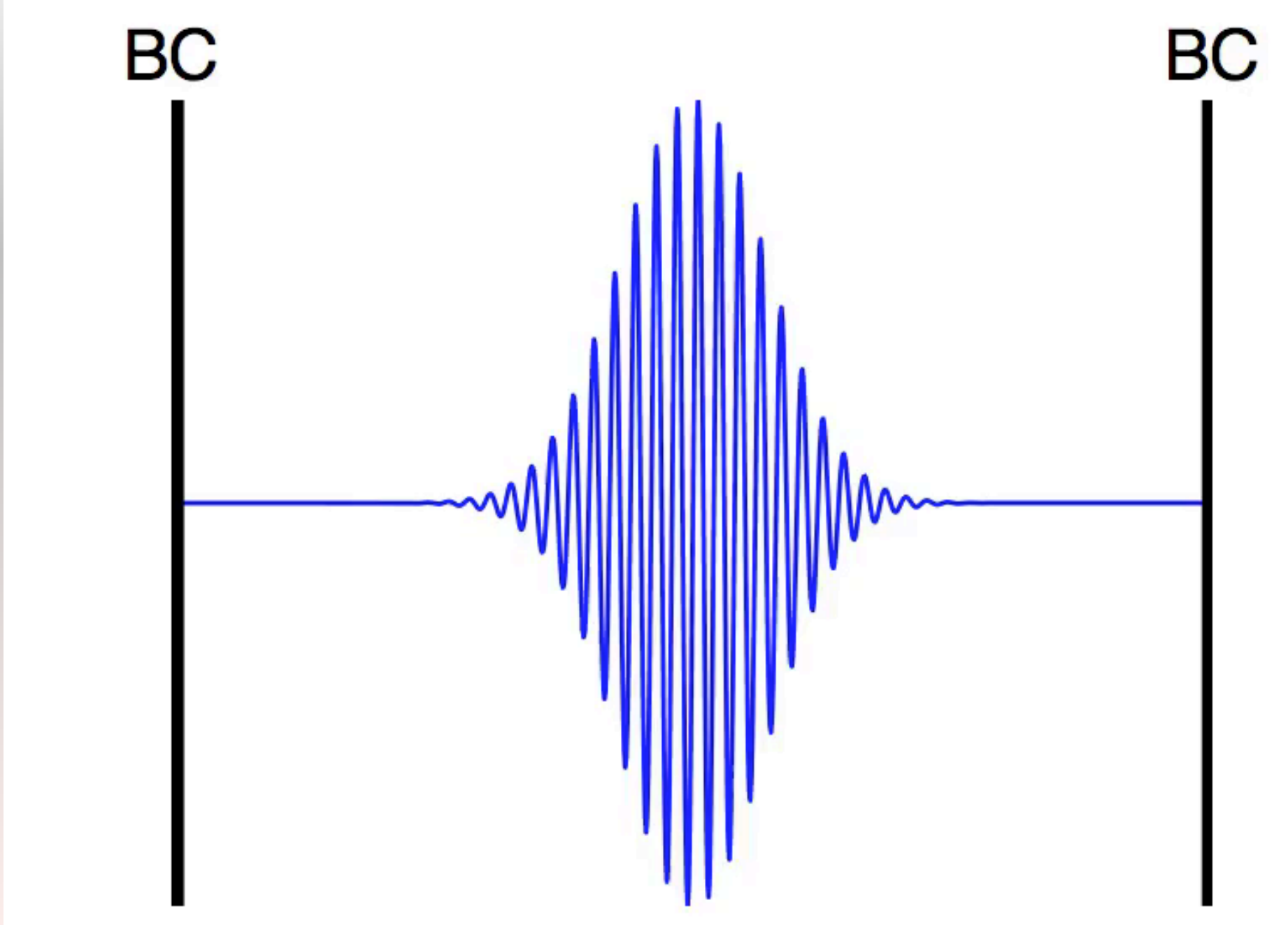


High frequency

Low frequency

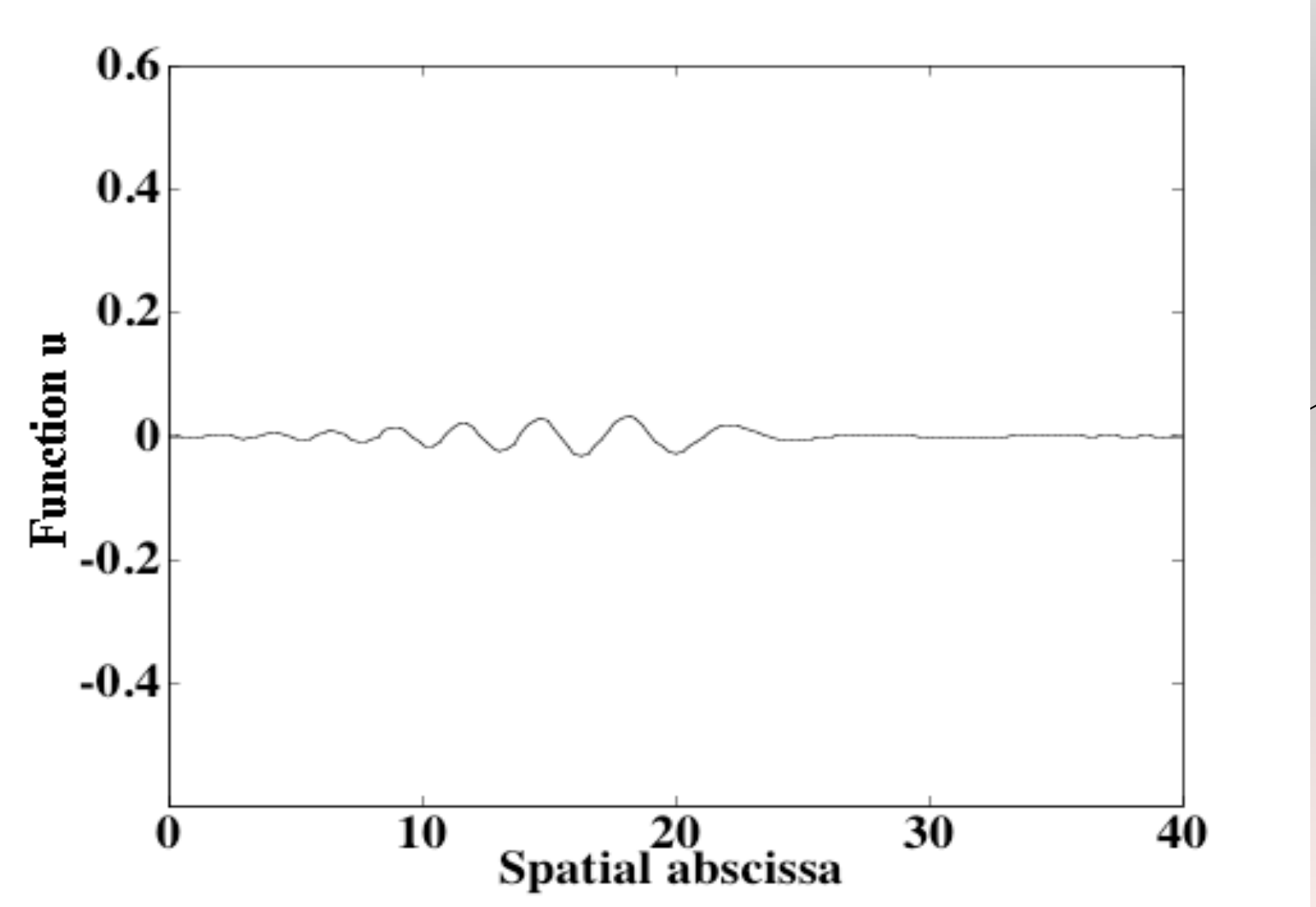


High frequency



As a consequence, numerical waves can induce false numerical resonances (see Buelle and Huerre CTR 1988, Poinsot and Lele 1992, Poinsot and Veynante 2005):

u=0



Non reflecting outlet

Will happen even in supersonic flows

Controlling q waves:

What we should not do:

- use dissipative schemes everywhere in the flow since they will decrease the Reynolds number of the flow
- use monotonic low-order schemes especially for species
- never ‘clip’: Yk=max(Yk,0)

What is done in practice:

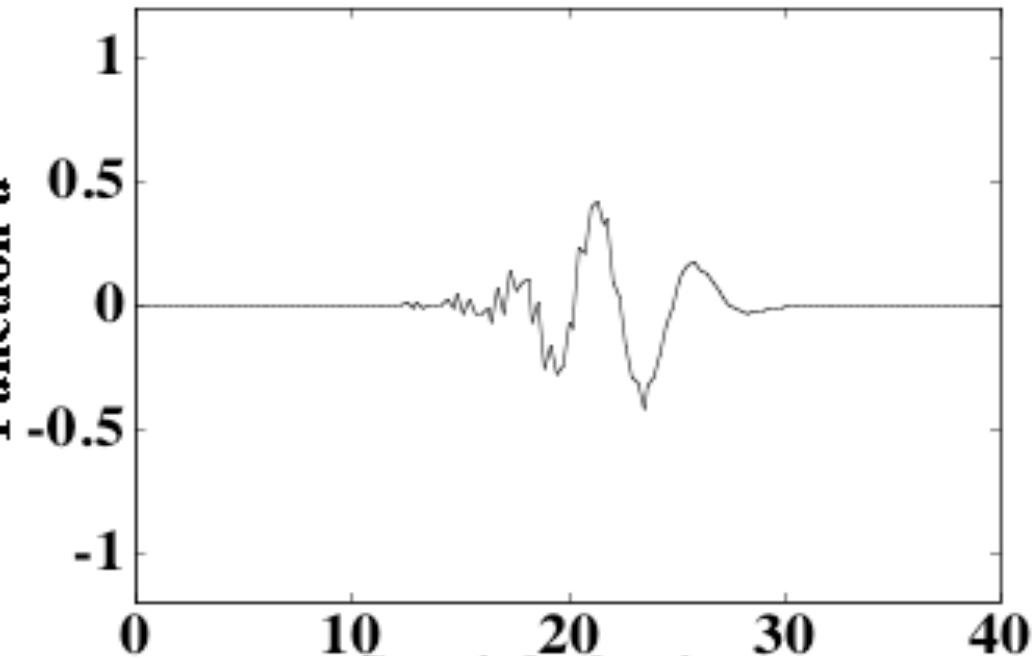
- add localized dissipation in places where wiggles appear and only there (« à la Jamieson »)
- upwind schemes locally

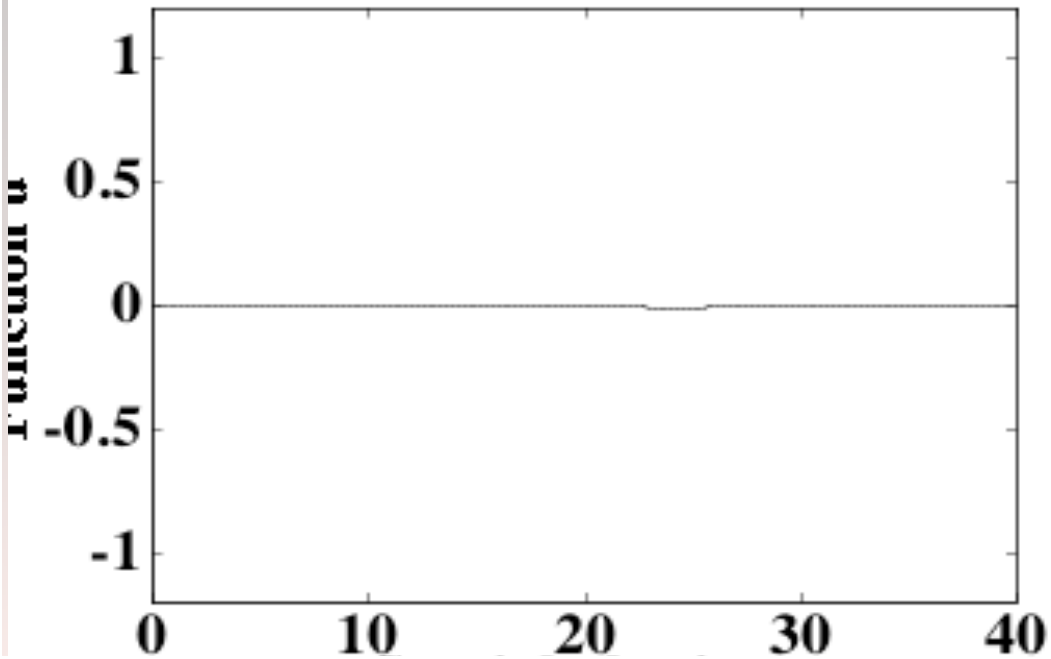
What it means: still an art ! Controlling wiggles ‘just enough' is difficult…

Some may wonder WHY we discuss this: they have never seen this problem in commercial codes !!
This is due to the viscosity of RANS codes. Example: non dissipative scheme (left) and typical RANS scheme (right)

NON DISSIPATIVE SCHEME (LES or DNS)

DISSIPATIVE SCHEME (RANS)





Conclusions:

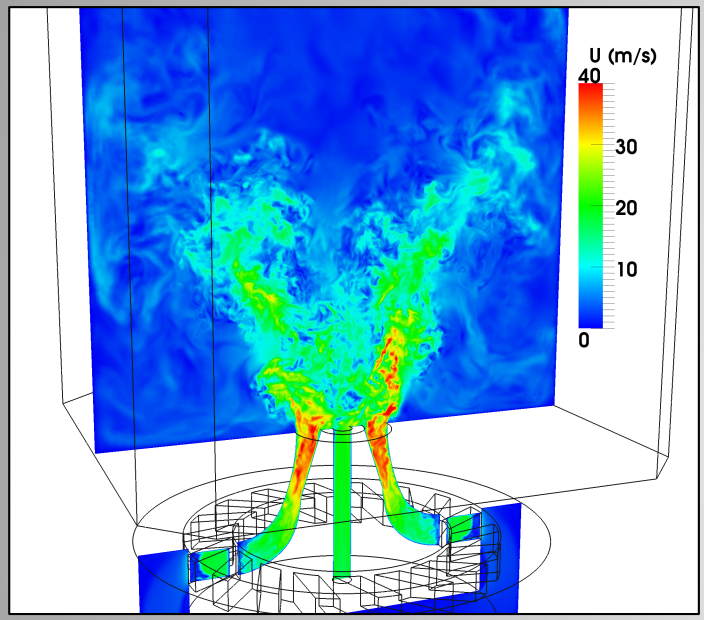
- LES is good

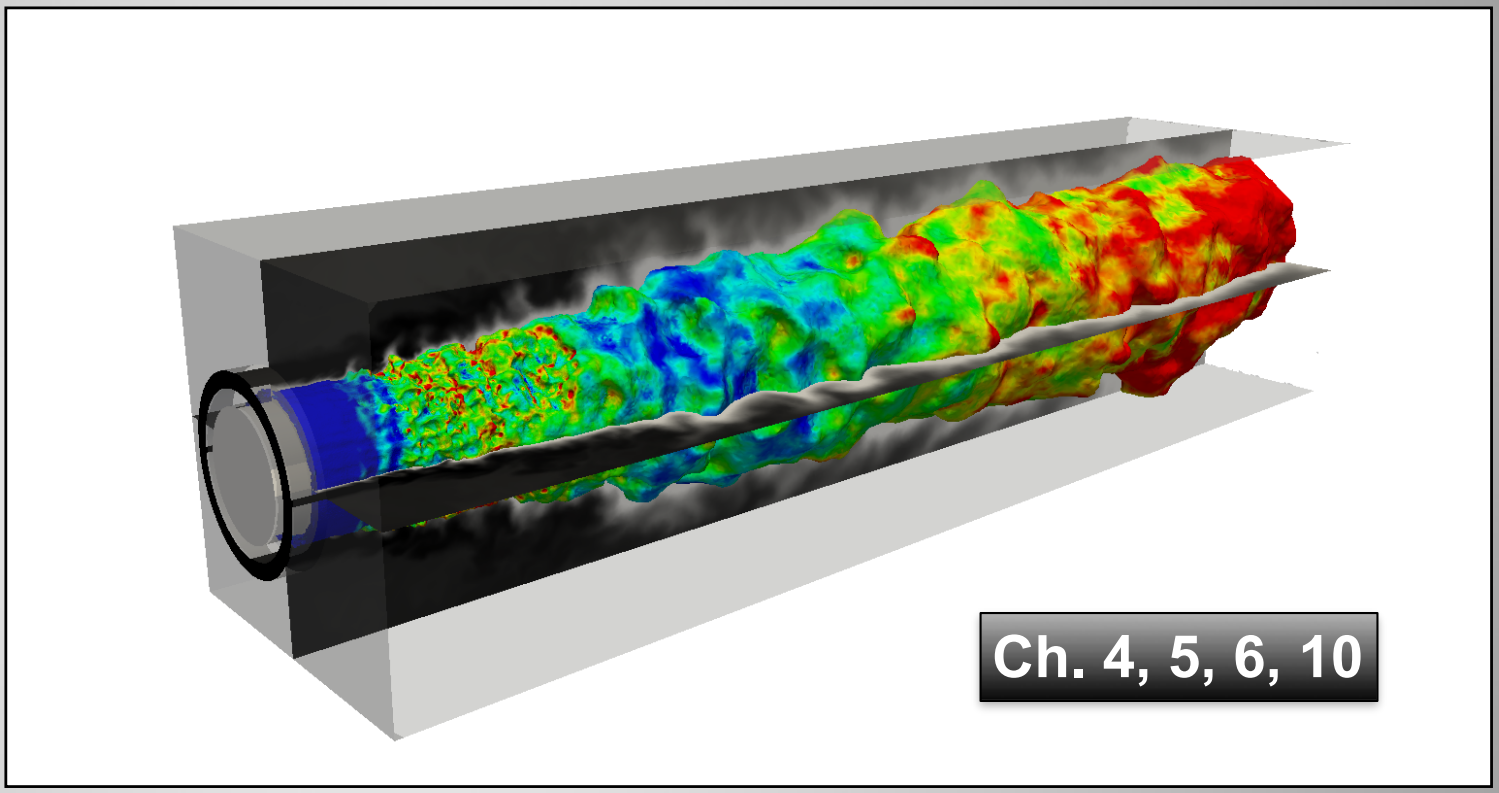
- LES is difficult and expensive

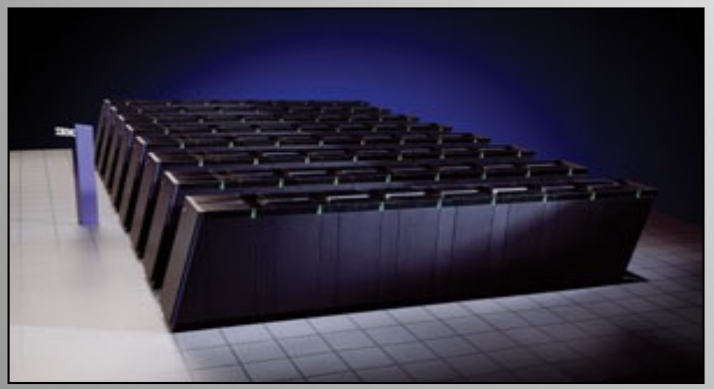
- Those who propose LES at the cost of RANS, with RANS codes and options (implicit, low order) are probably not saying the truth….

=> Massively parallel machines and GPUs are the only solution to make LES affordable

Chemistry description in 3D CFD codes for turbulent reacting flows.







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WE HAVE DESCRIBED NUMERICAL METHODS REQUIRED FOR LES OF TURBULENT FLOWS AND SHOWN THAT THEY WERE QUITE DIFFERENT FROM WHAT RANS CODES USE, WITH OR WITHOUT COMBUSTION.

NOW, FOCUS ON ONE ASPECT, SPECIFIC TO COMBUSTION:
THE DESCRIPTION OF CHEMISTRY IN 3D CFD CODES

COMBUSTION THEORY PLAYS AN ESSENTIEL ROLE HERE

I WANT TO DO H2 FLAMES

SO… SHOULD I USE A SINGLE STEP SCHEME:

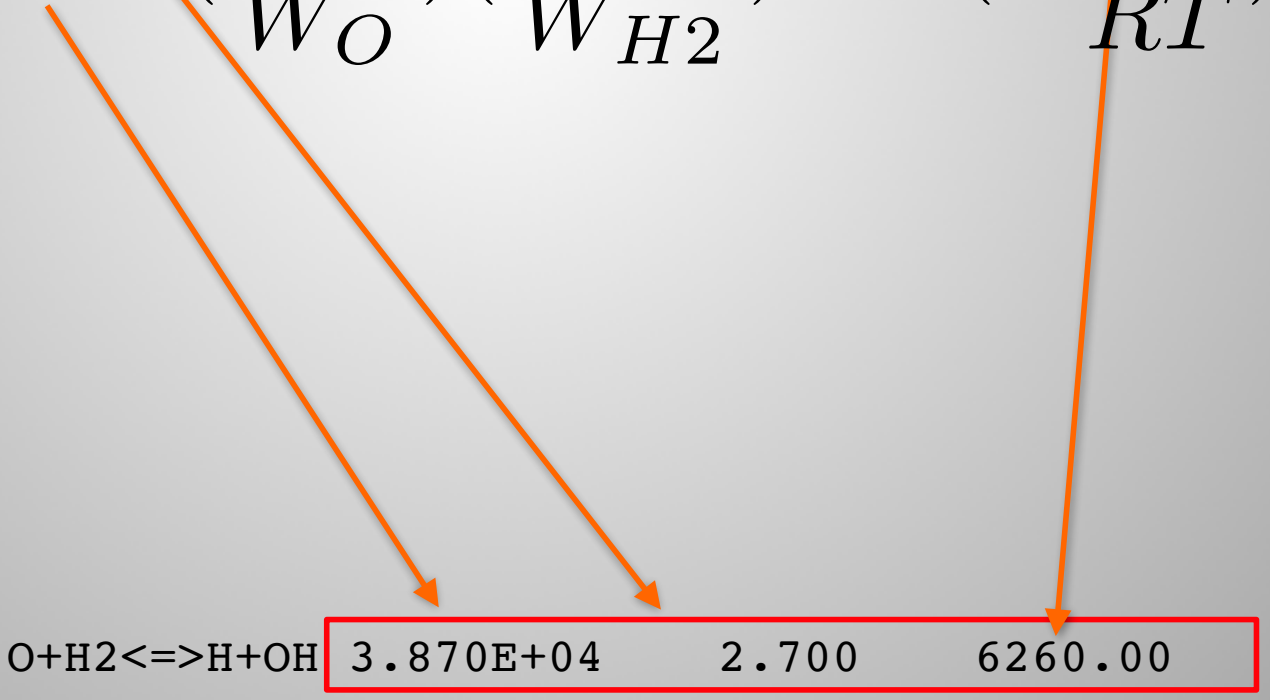
$$H_2 + 1/2O_2 -> H_2O$$

OR A FULL SCHEME :

```
H2+O2=OH+OH                          1.700E13   0.0     47780.
H2+OH=H2O+H                          1.170E09   1.30     3626.
H+O2=OH+O                           5.130E16  -0.816   16507.
O+H2=OH+H                           1.800E10   1.0      8826.
H+O2+M=HO2+M                          2.100E18  -1.0        0.
  H2/3.3/ O2/0./ N2/0./  H2O/21.0/
H+O2+O2=HO2+O2                        6.700E19  -1.42       0.
H+O2+N2=HO2+N2                        6.700E19  -1.42       0.
OH+HO2=H2O+O2                         5.000E13   0.0      1000.
H+HO2=OH+OH                          2.500E14   0.0      1900.
O+HO2=O2+OH                          4.800E13   0.0      1000.
OH+OH=O+H2O                          6.000E08   1.3         0.
H2+M=H+H+M                          2.230E12   0.5     92600.
  H2/3./ H/2./  H2O/6.0/
O2+M=O+O+M                           1.850E11   0.5     95560.
H+OH+M=H2O+M                          7.500E23  -2.6        0.
  H2O/20.0/
HO2+H=H2+O2                          2.500E13   0.0       700.
HO2+HO2=H2O2+O2                          2.000E12   0.0         0.
H2O2+M=OH+OH+M                           1.300E17   0.0     45500.
H2O2+H=H2+HO2                          1.600E12   0.0      3800.
H2O2+OH=H2O+HO2                          1.000E13   0.0      1800.
```

CHEMISTRY: WE MUST INCLUDE REALISTIC DESCRIPTIONS IN 3D SIMULATION CODES. TO DO THIS, WE NEED « CHEMICAL SCHEMES » CHEMKIN HAS DEFINED A COMMON STANDARD WHERE EACH ELEMENTARY REACTION IS SPECIFIED BY ITS CONSTANTS: A, β and E_a

$$q = AT^{\beta}\left(\frac{\rho Y_O}{W_O}\right)\left(\frac{\rho Y_{H2}}{W_{H2}}\right)\exp\left(-\frac{E_a}{RT}\right)$$



WHAT IS A CHEMICAL SCHEME ? : ONE EXAMPLE

H2 O2 CHEMISTRY:
the only simple one…

```
ELEMENTS
 H   O   N
END
SPECIES
H2 O2 OH O H H2O HO2 H2O2 N2
END
REACTIONS
H2+O2=OH+OH                      1.700E13   0.0    47780.
H2+OH=H2O+H                      1.170E09   1.30    3626.
H+O2=OH+O                        5.130E16  -0.816  16507.
O+H2=OH+H                        1.800E10   1.0     8826.
H+O2+M=HO2+M                      2.100E18  -1.0       0.
  H2/3.3/ O2/0./ N2/0./  H2O/21.0/
H+O2+O2=HO2+O2                    6.700E19  -1.42      0.
H+O2+N2=HO2+N2                    6.700E19  -1.42      0.
OH+HO2=H2O+O2                     5.000E13   0.0     1000.
H+HO2=OH+OH                      2.500E14   0.0     1900.
O+HO2=O2+OH                      4.800E13   0.0     1000.
OH+OH=O+H2O                      6.000E08   1.3        0.
H2+M=H+H+M                       2.230E12   0.5    92600.
  H2/3./ H/2./  H2O/6.0/
O2+M=O+O+M                       1.850E11   0.5    95560.
H+OH+M=H2O+M                      7.500E23  -2.6       0.
  H2O/20.0/
HO2+H=H2+O2                      2.500E13   0.0      700.
HO2+HO2=H2O2+O2                    2.000E12   0.0        0.
H2O2+M=OH+OH+M                     1.300E17   0.0    45500.
H2O2+H=H2+HO2                    1.600E12   0.0     3800.
H2O2+OH=H2O+HO2                    1.000E13   0.0     1800.
END
```

CH4/air CHEMISTRY: the famous GRI Mech scheme (the first page…)

```
! GRI-Mech Version 3.0 7/30/99  CHEMKIN-II format
! See README30 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page http://www.me.berkeley.edu/gri_mech/ or
! through http://www.gri.org , under 'Basic  Research',
! for additional information, contacts, and disclaimer
ELEMENTS
O  H  C  N  AR
END
SPECIES
H2      H       O       O2      OH      H2O     HO2     H2O2
C       CH      CH2     CH2(S)  CH3     CH4     CO      CO2
HCO     CH2O    CH2OH   CH3O    CH3OH   C2H     C2H2    C2H3
C2H4    C2H5    C2H6    HCCO    CH2CO   HCCOH   N       NH
NH2     NH3     NNH     NO      NO2     N2O     HNO     CN
HCN     H2CN    HCNN    HCNO    HOCN    HNCO    NCO     N2
AR      C3H7    C3H8    CH2CHO  CH3CHO
END
!THERMO
! Insert GRI-Mech thermodynamics here or use in default file
!END
REACTIONS
2O+M<=>O2+M                               1.200E+17   -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/  .83/
O+H+M<=>OH+M                              5.000E+17   -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+H2<=>H+OH                               3.870E+04    2.700    6260.00
O+HO2<=>OH+O2                             2.000E+13     .000        .00
O+H2O2<=>OH+HO2                           9.630E+06    2.000    4000.00
O+CH<=>H+CO                               5.700E+13     .000        .00
O+CH2<=>H+HCO                             8.000E+13     .000        .00
O+CH2(S)<=>H2+CO                          1.500E+13     .000        .00
O+CH2(S)<=>H+HCO                          1.500E+13     .000        .00
```

SO WHERE IS THE PROBLEM ?

We do have chemical schemes which are quite good for many fuels

BUT

we cannot use them in 3D codes: they are just too big

MAIN ISSUE: How do we include realistic chemistry in 3D codes ?

Look at kinetics from the point of view of the 3D code developers:

- **HOW MANY INDEPENDENT SPECIES ? -> more memory**
- **HOW MANY REACTIONS ? -> more CPU time**

We will describe FOUR ways to do this:

1/ BRUTE FORCE
2/ TABULATION METHODS OF FULL SCHEMES
3/ REDUCED SCHEMES
4/ ANALYTICALLY REDUCED SCHEMES

TERMINOLOGY:

We call ELEMENTARY REACTION a chemical reaction which really takes place in the flame.

Elementary reactions are usually included in a full kinetic scheme. Thousands of reactions and hundreds of species are needed for hydrocarbon flames

We call GLOBAL REACTION a reaction which does not really take place in the real world but which mimics the global effect of many elementary reactions

Global reactions characteristics are usually fitted to match certain flame characteristics (flame speed for ex). Using 1 to 4 global reactions is enough to have a crude description of chemistry

EXAMPLE FOR H2/O2:

WE NEED ONLY ONE GLOBAL REACTION for H2/O2 flames:

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$

BUT IF WE WANT TO BE PRECISE, WE NEED APPROX. 20 ELEMENTARY REACTIONS FOR H2/O2 FLAMES

OUTLINE

1/ BRUTE FORCE METHODS

2/ TABULATION TECHNIQUES

3/ REDUCED SCHEMES

4/ ANALYTICALLY REDUCED SCHEMES

BRUTE FORCE: solve for all species. VARIABLES: 5 (for flow) + N (for species)

We solve at each time step, at each point, for:

- Density
- Velocities
- Temperature
- *All species Yk, for k= 1 to N*

Ch. 1

And all equations are coupled: we keep the M elementary reactions taking place between the N species

In general, in a turbulent 3D code, it is difficult to use large values of N and M…. Today:

- In DNS codes, N=20 to 100; M= 10 to 40
- In LES codes, N= 6 to 20, M=1 to 4

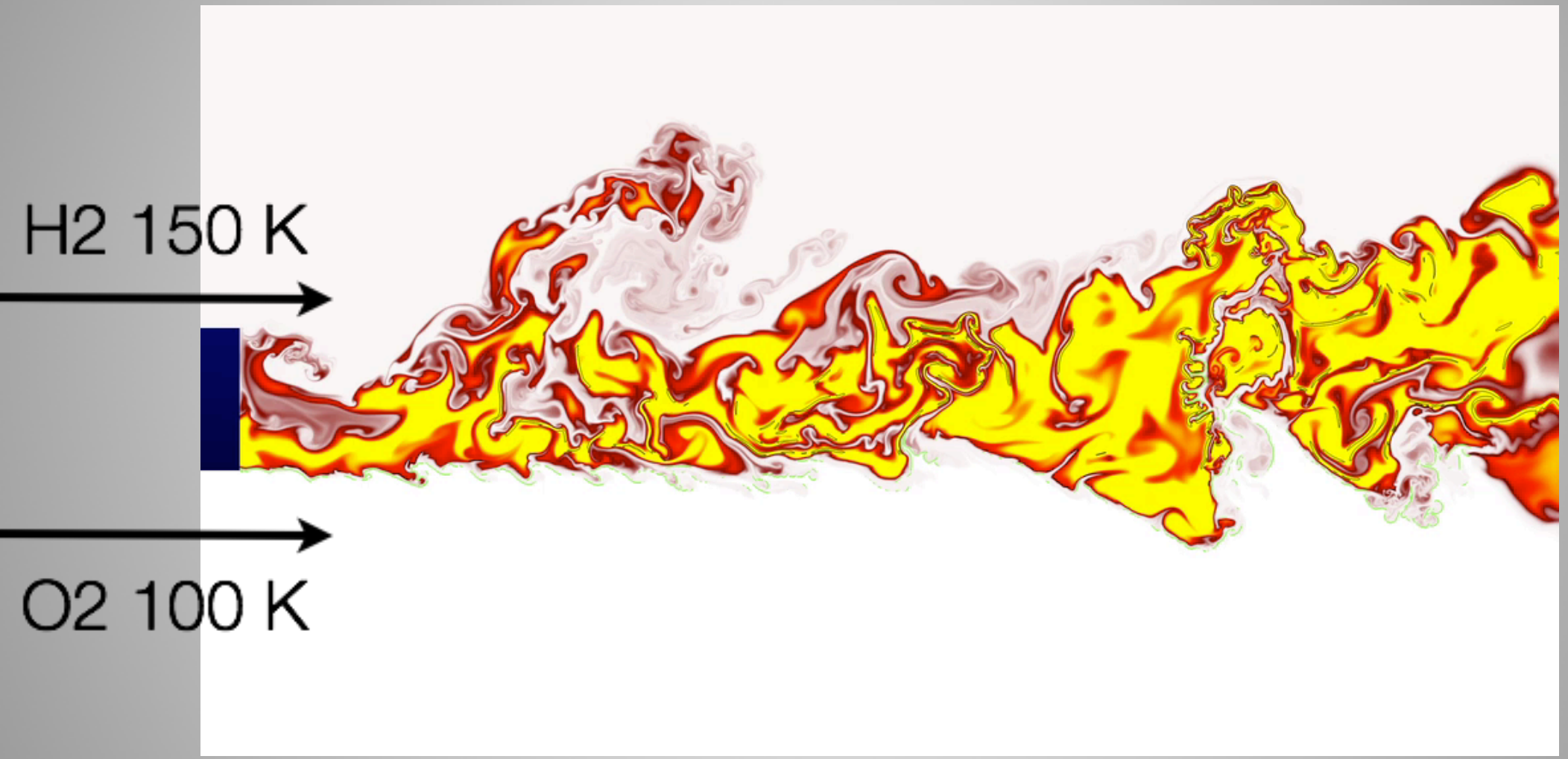
The brute force method: no compromise !

No assumption needed and no limitation except for the validity of the chemical scheme itself and the cost.

In practice, for 3D codes, this works only for:
- DNS and LES of H2 flames with full chemistry
- For small and simple configurations

FIRST MESSAGE: if you dont study H2 flames, you CAN NOT directly use full kinetic schemes in your 3D code

DNS of H2/O2 flame with 19 reactions and 9 species:



PhD A. Ruiz, 2012, CERFACS

Even full kinetic schemes are ... MODELS !

For a 10000 reaction scheme, we need 30000 constants: A_i, β_i ***and*** E_{ai} ***for all i=1 to 10000***

Chemists recognize that only 10 to 20 percent of these constants are 'reasonably' well known

Even to compute laminar flame speeds today, uncertainties due to chemical schemes are large → trying to mimic exactly what complex kinetic schemes predict has a limited interest.

OUTLINE

1/ BRUTE FORCE METHODS

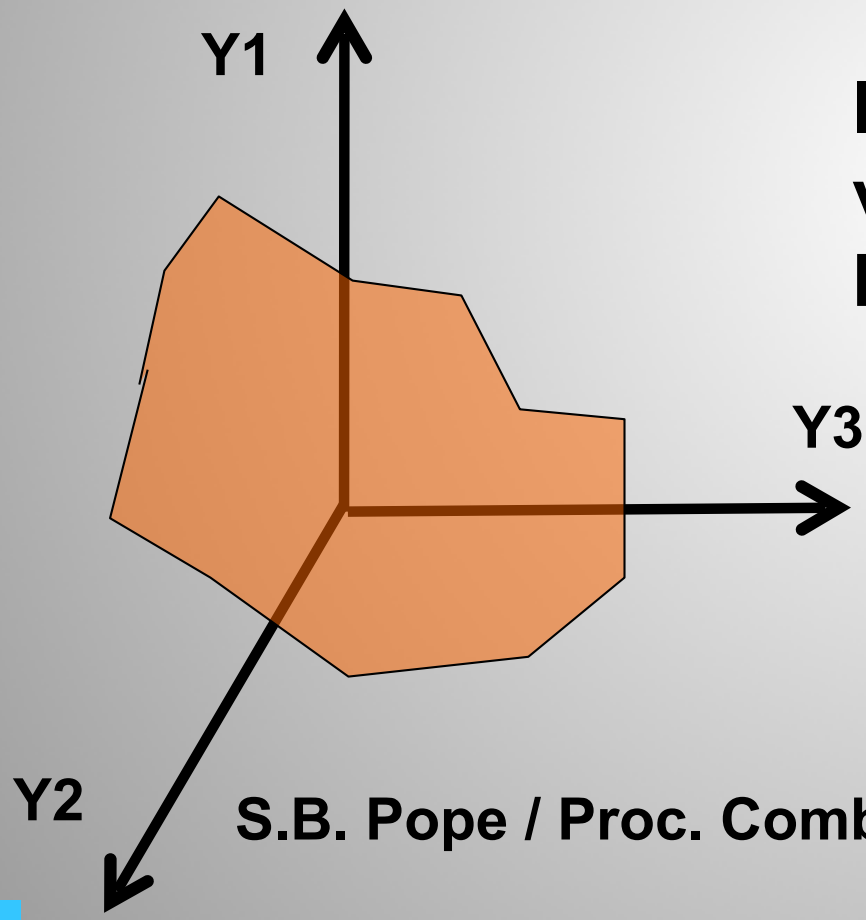
2/ TABULATION TECHNIQUES

3/ REDUCED SCHEMES

4/ ANALYTICALLY REDUCED SCHEMES

Manifolds in combustion (S. Pope)

Even though all species are 'independent' variables and should be computed separately, the examination of mass fraction trajectories in most flames shows that, in composition space, most points fall on a manifold of limited size.

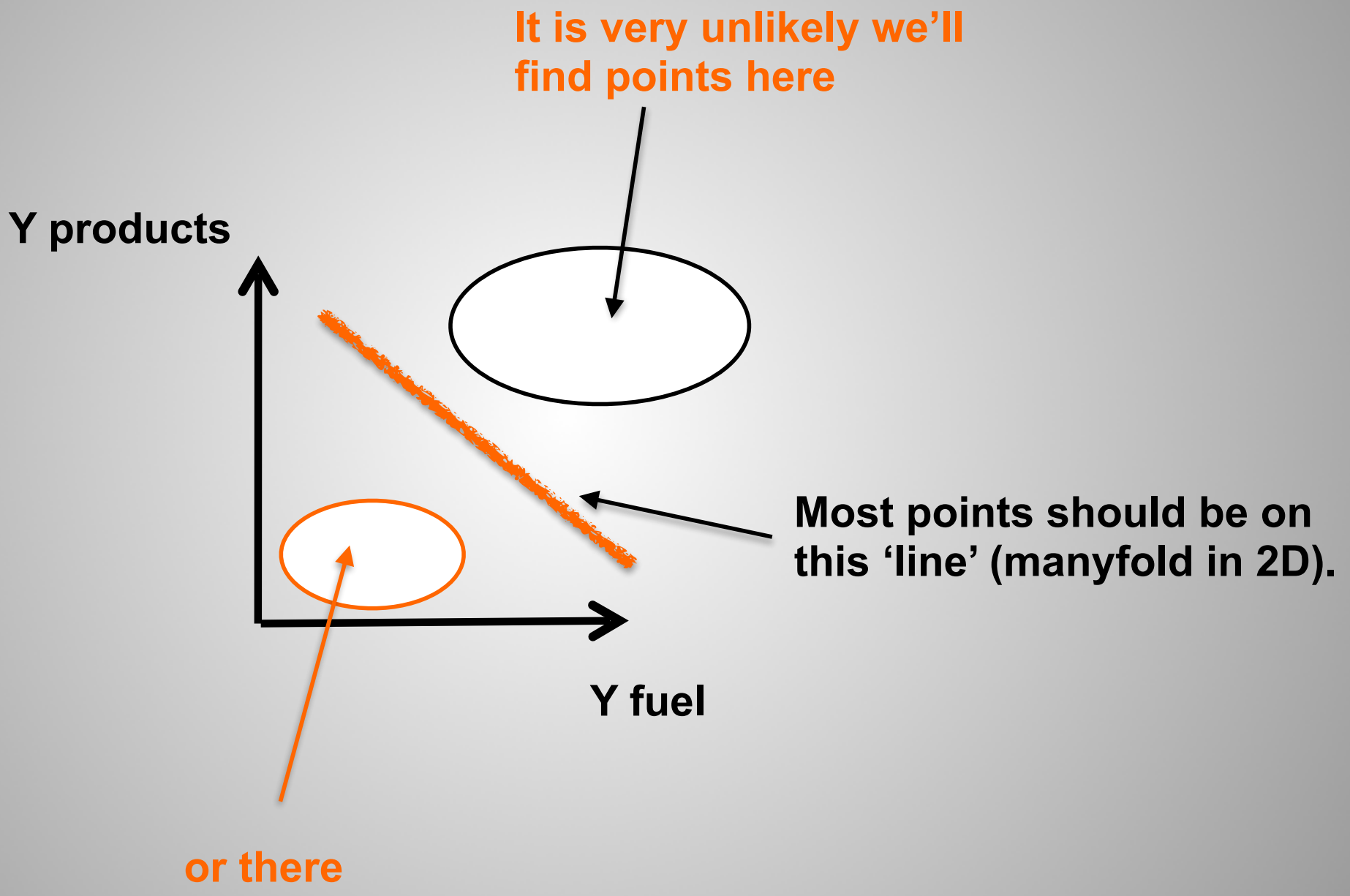


Instead of N independent variables, the whole system can be described with less variables.

S.B. Pope / Proc. Comb. Inst. 34 (2013) 1–31

Ch. 4 Section 4.8.3

Example of manyfold in a turbulent premixed flame:



Solve at each time step, at each point, the conservation equations for:

- Density

- Velocities

- Temperature

~~**- N independent chemical species**~~

- 1 or 2 *independent variables (usually c and z)*

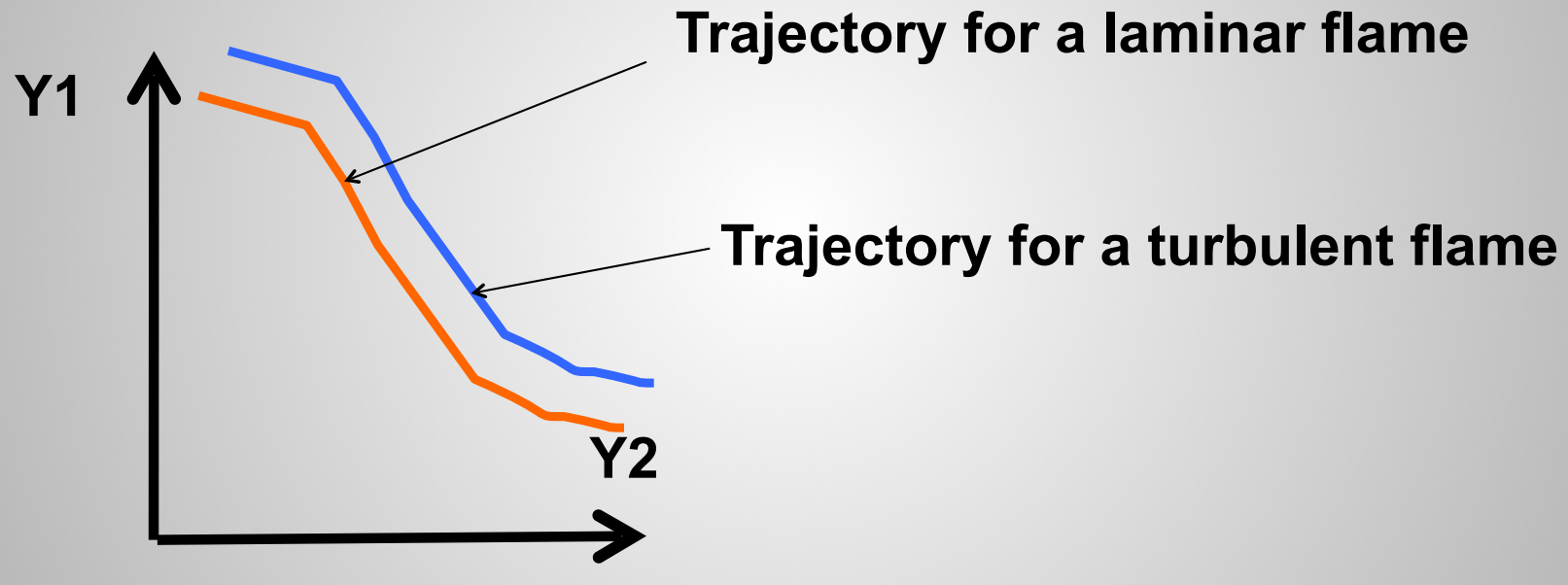
***All* other species Yk are functions of these two variables and are not solved for**

== > TABULATION !

Ch. 4 Section 4.8

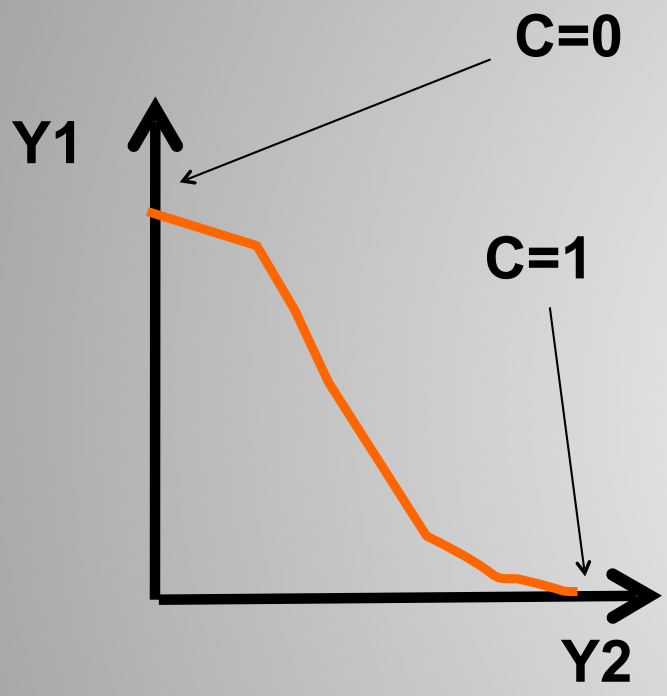
Assumption of universality of manifolds in combustion

Assume that ALL flames (laminar or turbulent) follow the same manifold:



Measure this manifold in laminar cases and then use if for all other flames

Which variables should be used to tabulate the manifold ?



The most intuitive ones are:

- progress variable c

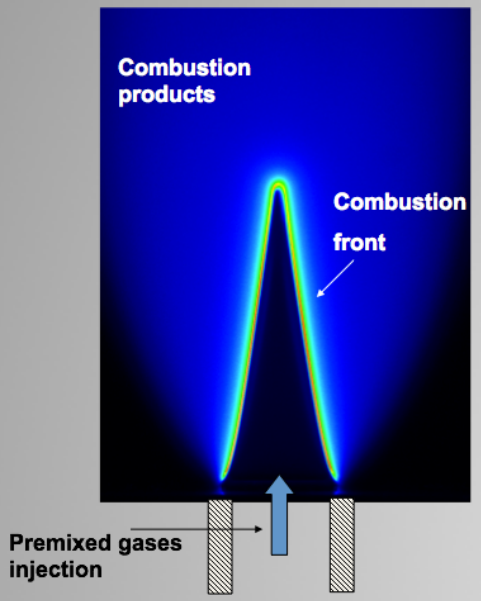
- mixture fraction z

Defining the progress variable can be difficult. In most hydrocarbon flames, use:

$$c = \frac{Y_C - Y_C^{fresh}}{Y_C^{burnt} - Y_C^{fresh}}$$

$$Y_c = Y_{CO} + Y_{CO2}$$

Example for the reaction rate:

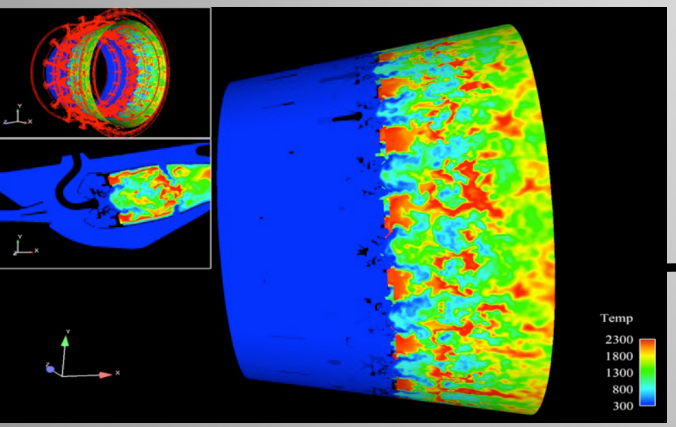


Manifold assumption

$$\dot{\omega}(Y_1, Y_2, Y_3 \ldots Y_k) = \dot{\omega}_1(c, z)$$

$$\dot{\omega}_1(c, z) = \dot{\omega}_2(c, z)$$

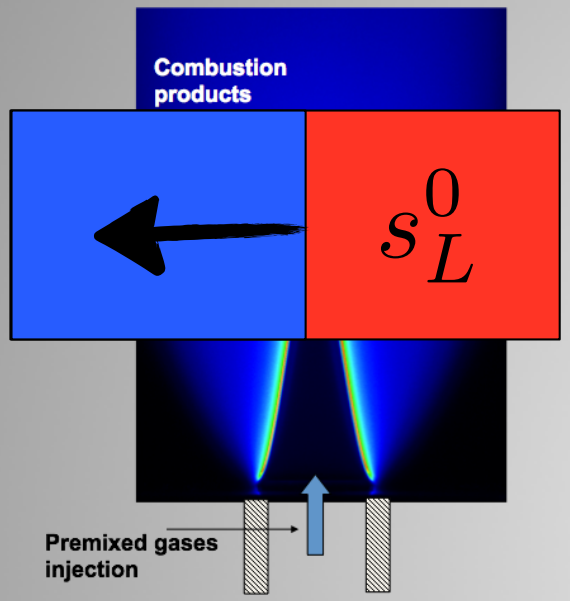
Manifold universality assumption



$$\dot{\omega}(Y_1, Y_2, Y_3 \ldots Y_k) = \dot{\omega}_2(c, z)$$

Manifold assumption

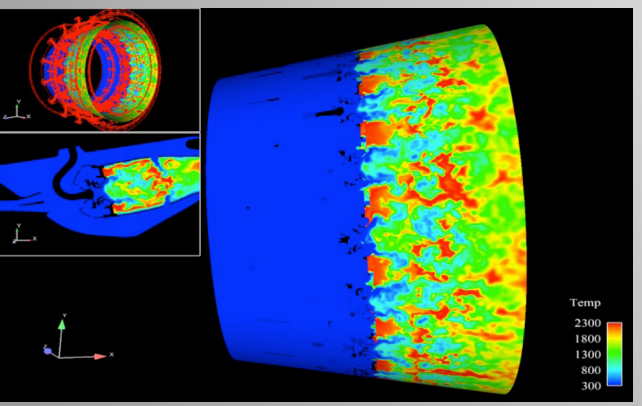
Tabulation procedure



Take a laminar flame. Build a table with c and z as entries and the reaction rate as output.

$$\dot{\omega} = f(c, z)$$

In the 3 D code, add two conservation equations: one for c and one for z. From c and z, read the reaction rate in the table and apply it in the 3D code



Universality of manifolds ?

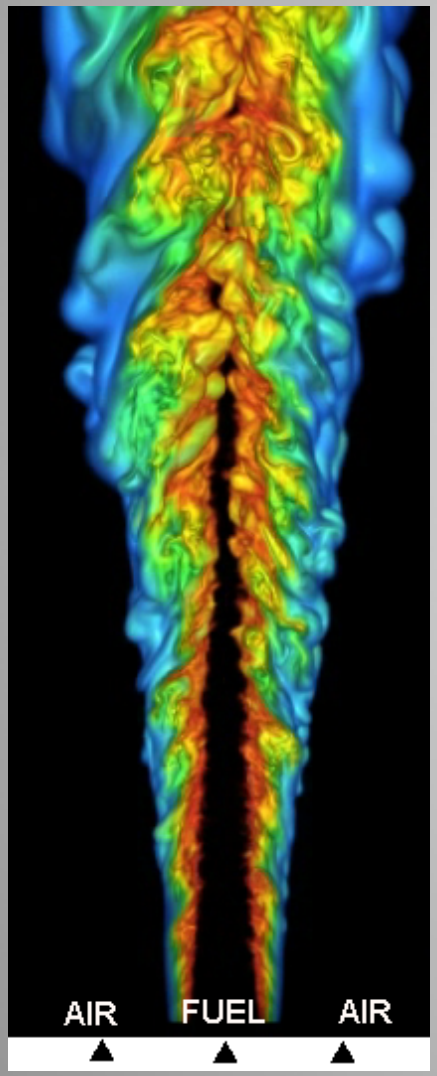
Can we use a tabulation written for a diffusion flame in a premixed flame ?

Which tabulation must be used in a partially premixed flame ?

Can we really assume that the same manifold holds in laminar AND turbulent flames ?

Example of tabulation based methods

Two cases where theory (again) proves that tabulation methods DO work with only ONE variable:



diffusion flame with infinitely fast chemistry (using mixture fraction *z*)

perfectly premixed flame (using progress variable c)

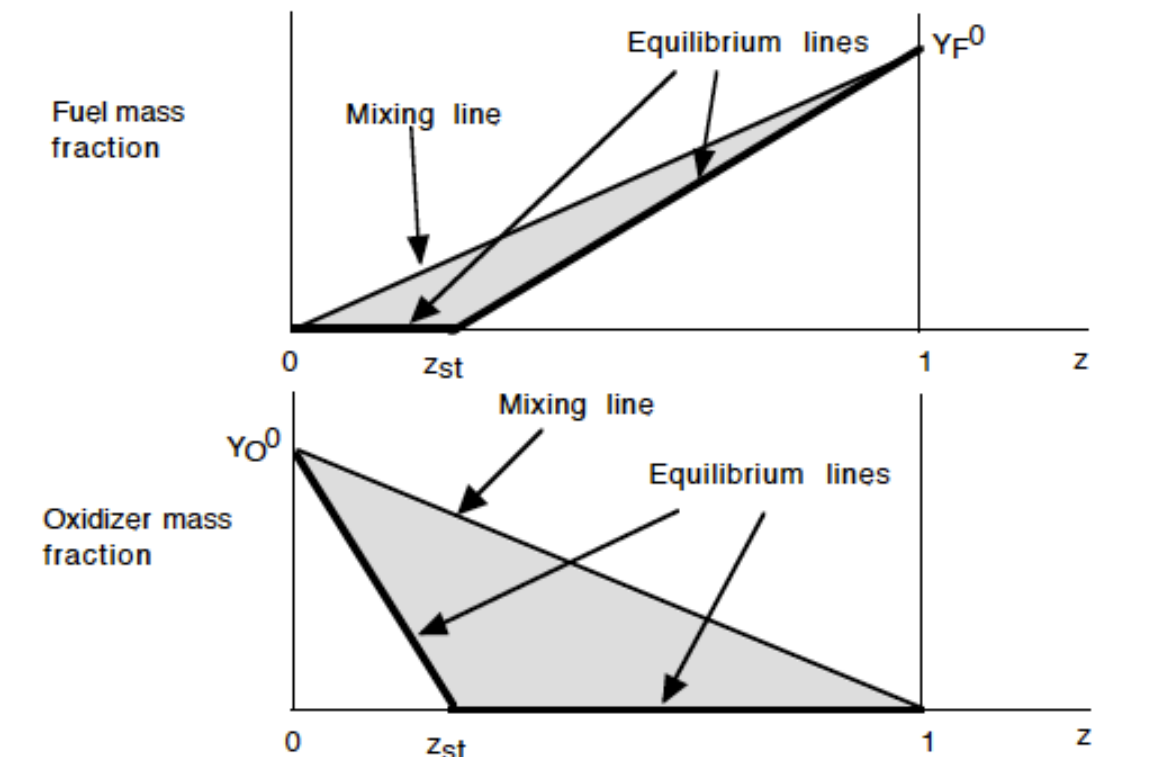


Fuel + air

THE SIMPLEST TABULATION: DIFFUSION FLAMES WITH INFINITELY FAST CHEMISTRY: 3 species (F, O, P), 0 reaction !

If all Lewis numbers are equal to unity, if pressure is constant, if only two streams feed the combustion chamber, if the flow is adiabatic and if chemistry is infinitely fast, we have already seen that all variables depend only on the mixture fraction z.

That is a lot of 'if's….



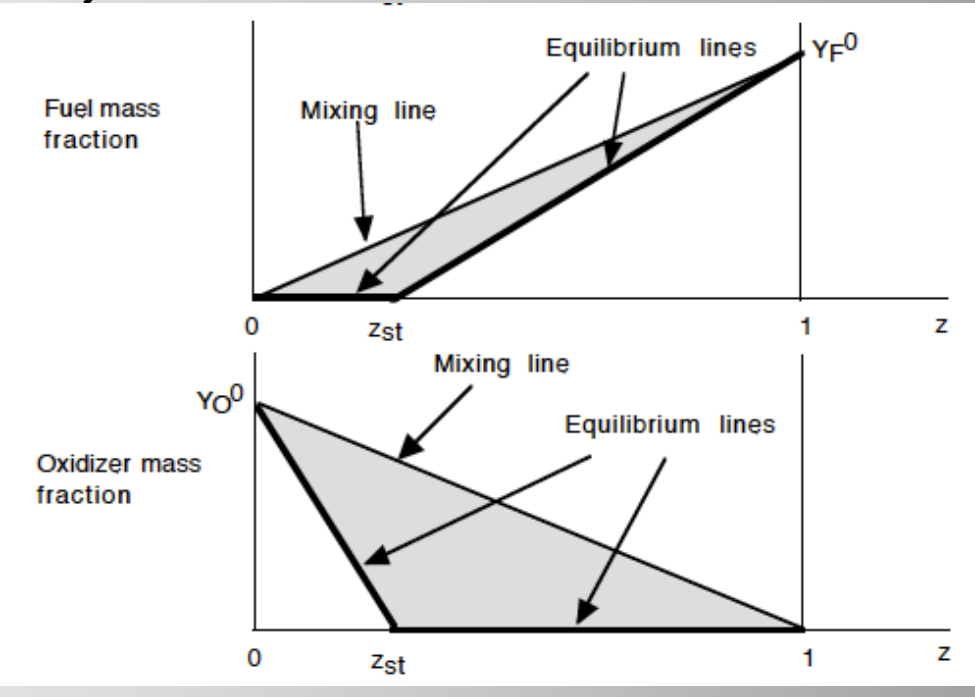
A 3D CODE FOR DIFFUSION FLAMES WITH INFINITELY FAST CHEMISTRY:

Solve at each time step, at each point, the conservation equations for:

- Density

- Velocities

- Mixture fraction z

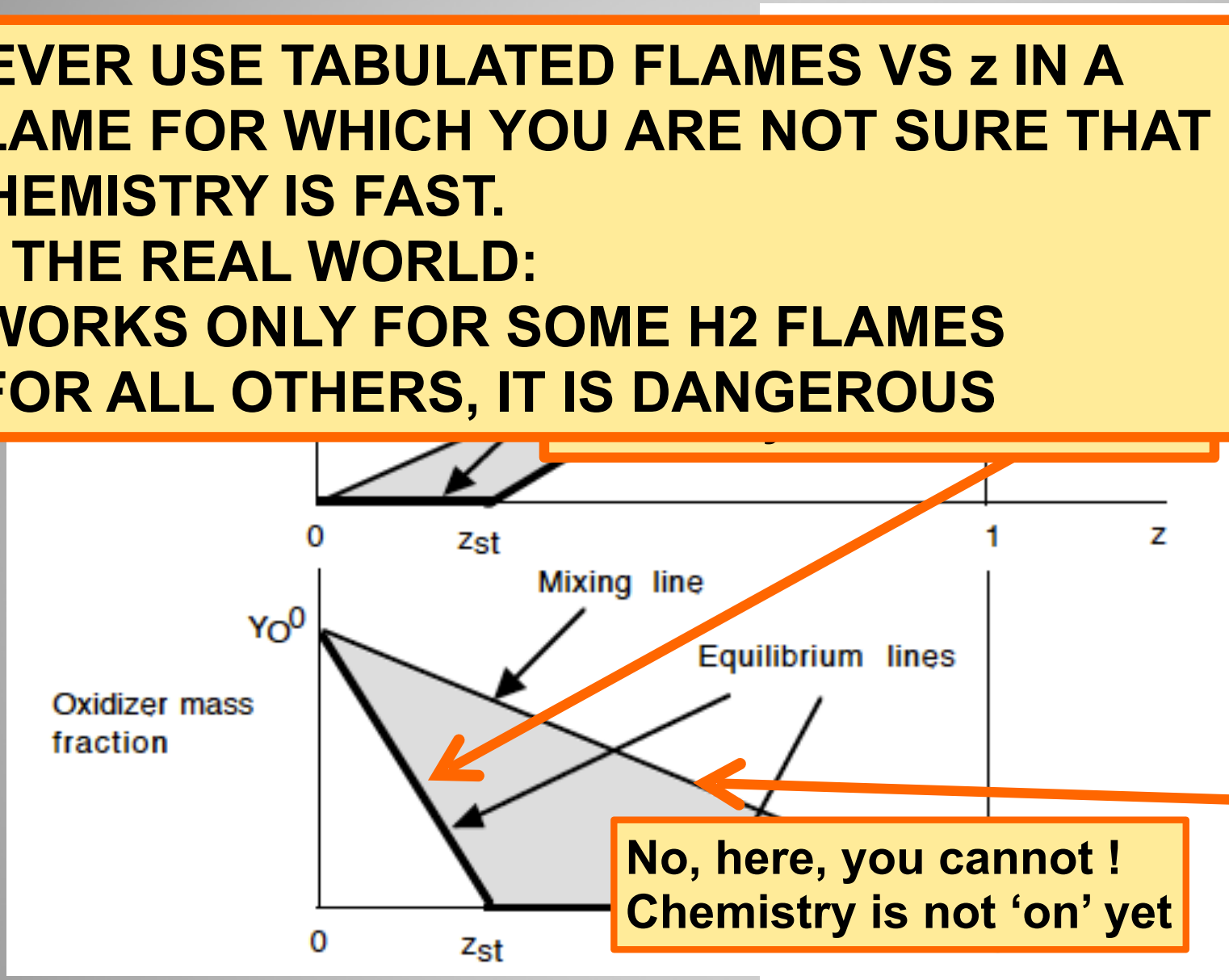


All other species are directly given by z using the z diagram.

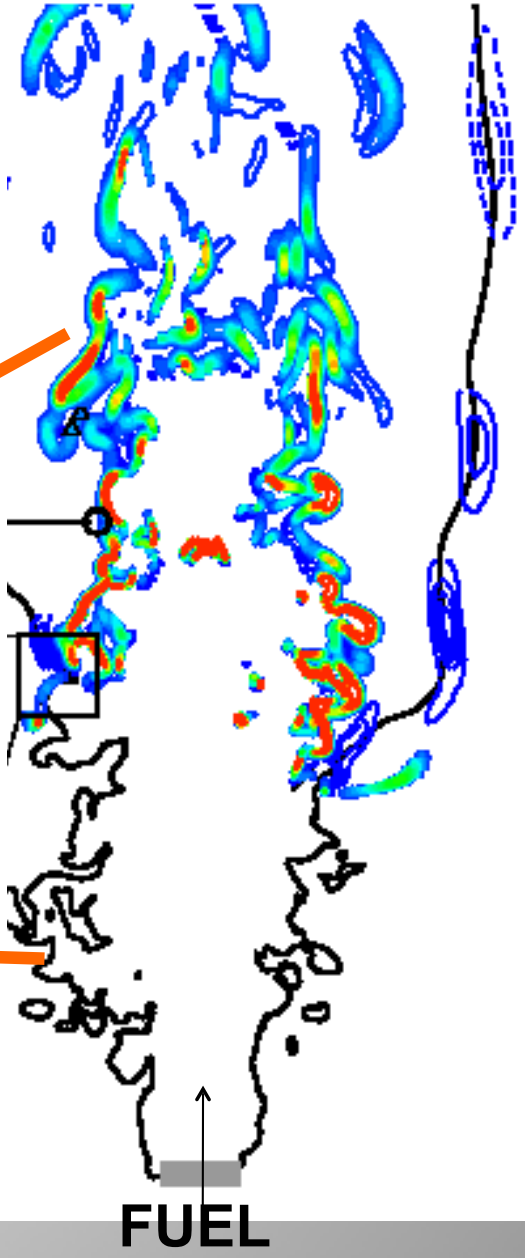
CAUTION: works only if… chemistry is infinitely fast. And if only two streams feed the combustor (otherwise z does not exist)

Typical problem: stabilization of diffusion flames

NEVER USE TABULATED FLAMES VS z IN A FLAME FOR WHICH YOU ARE NOT SURE THAT CHEMISTRY IS FAST.
IN THE REAL WORLD:
- WORKS ONLY FOR SOME H2 FLAMES
- FOR ALL OTHERS, IT IS DANGEROUS

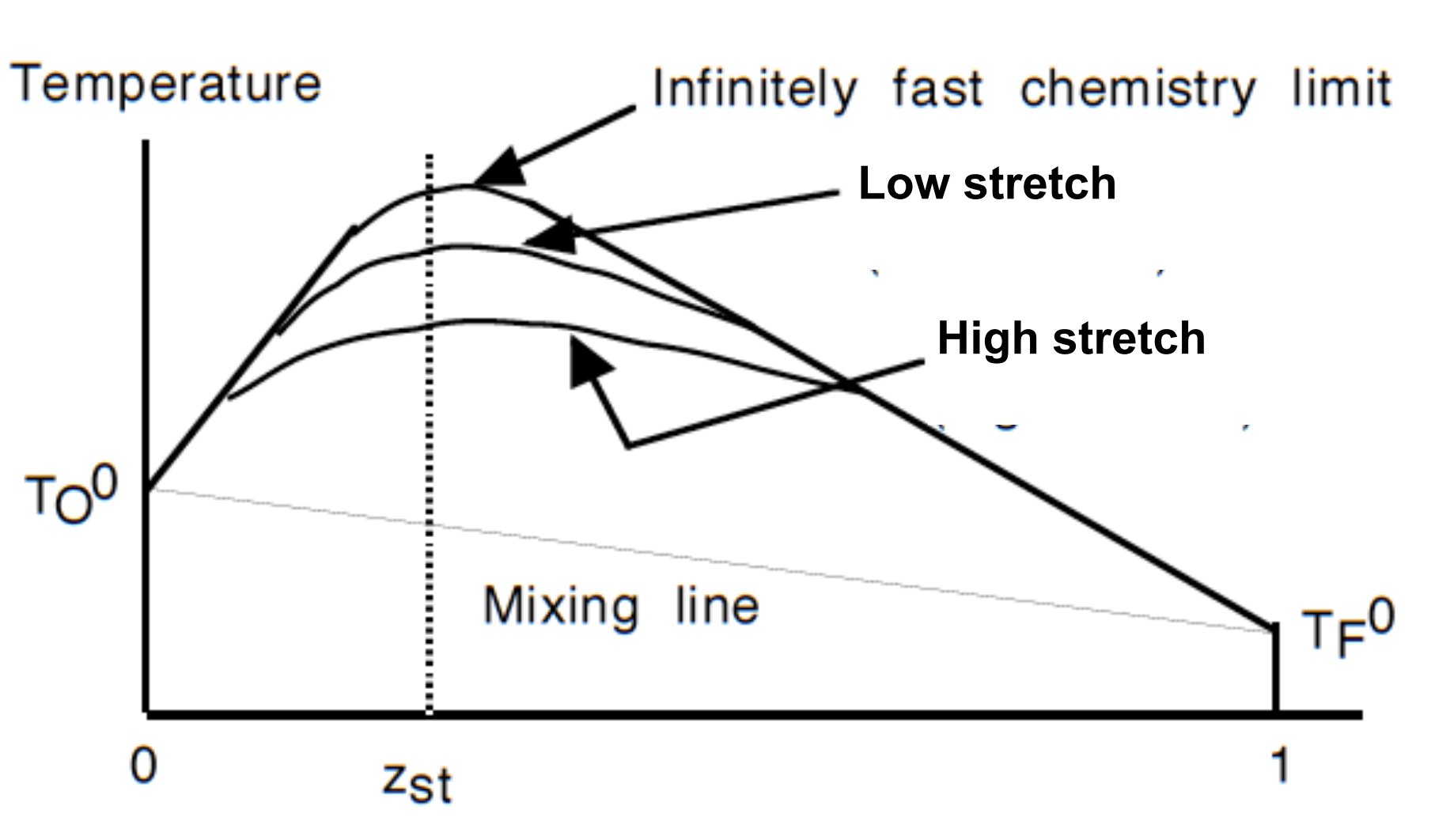


No, here, you cannot !
Chemistry is not 'on' yet

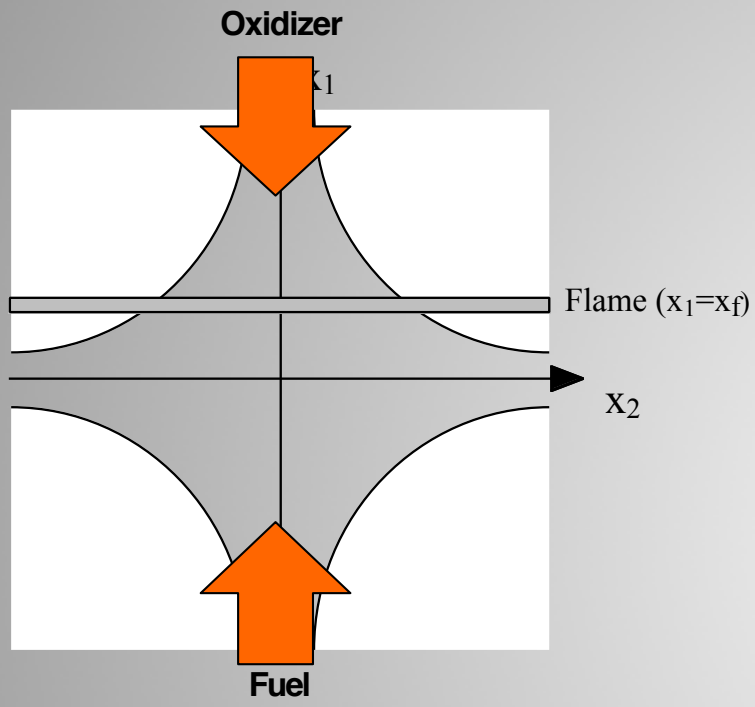


STRETCH: a required extension for most flames:

DNS and experiments show that the flame structure does not depend on z only: an additional parameter must be introduced: this is *flame stretch* (or scalar dissipation)



A required extension for diffusion flames:



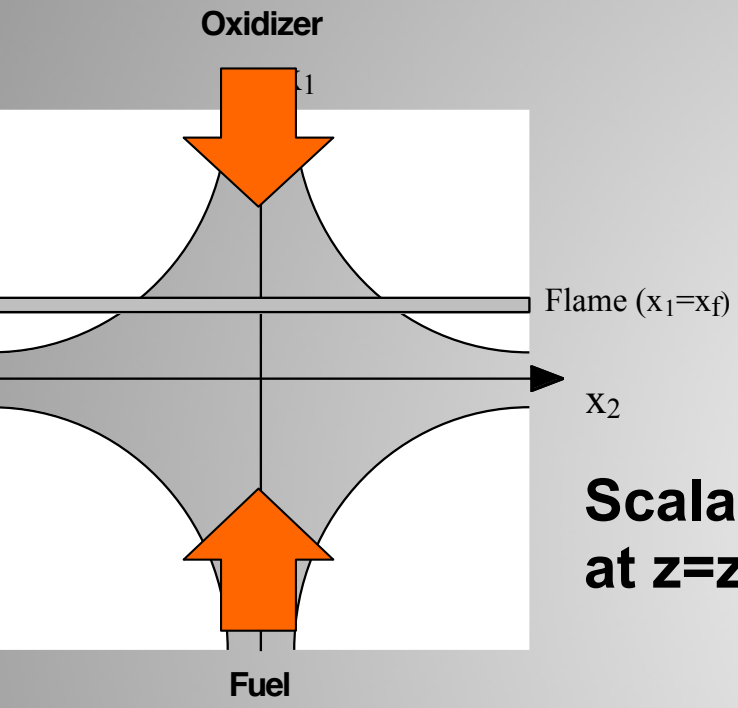
The laminar diffusion flame is a stretched flame and stretch (or equivalently scalar dissipation) controls its structure. Most tabulation methods add scalar dissipation in the table which becomes 2D: χ

$$f(z,\chi)$$

$$\chi = 2\mathcal{D}\left(\frac{\partial z}{\partial x_i}\frac{\partial z}{\partial x_i}\right)$$

While χ **is unambiguously defined for laminar flames, its evaluation in a LES is more difficult.**

Stretch or scalar dissipation ?



Both can be used to characterize the state of a diffusion flame: in a laminar diffusion flame, they are directly linked

Scalar dissipation at z=zstoich

Flame stretch

$$\chi_f = \frac{a}{\pi} \exp\left[-2\left(\mathrm{erf}^{-1}\left(\frac{\phi-1}{\phi+1}\right)\right)^2\right]$$

$$\phi = s\frac{Y_F^0}{Y_O^0}$$

Ch. 3 Sec 3.4.2

Stretch κ or scalar dissipation χ ?

In a turbulent flow, scalar dissipation χ is easier to compute because it does not require to know the flame normal $\overrightarrow{n}$ as needed for stretch. For χ knowing the z field is sufficient

$$\chi = 2\mathcal{D}\left(\frac{\partial z}{\partial x_i}\frac{\partial z}{\partial x_i}\right)$$

$$\kappa = \nabla_t \cdot \vec{\mathbf{u}} + s_d \nabla_t \cdot \vec{\mathbf{n}}$$

The main difficulty in both cases for RANS or LES is to find the sub grid contribution to scalar dissipation or to strain: unsolved problem, dominated by approximations

ANOTHER SIMPLE 'TABULATION': PERFECTLY PREMIXED LEAN FLAMES. 1 species, 1 reaction

Here 'tabulation' can be demonstrated/justified using theory and we did it before in 'Basics':

1- Assume that the flame is so lean that only the fuel limits the reaction rate. Only Y_F needs to be tracked

$$q_1 = A_1 \left(\frac{\rho Y_{CH_4}}{W_{CH_4}} \right)^{n_{1F}} \left(\frac{\rho Y_{O_2}}{W_{O_2}} \right)^{n_{1O}} \exp\left(-\frac{E_{a1}}{RT} \right)$$

↓

Almost constant

2- Assume that the Mach number is small, pressure is constant, Lewis=1. Theory says that in this case, temperature *T* and fuel mass fraction Y_F are linked by:

$$\frac{T - T_1}{T_2 - T_1} + \frac{Y_F}{Y_F^1} = 1$$

Only one independent variable gives everything. Usually take *c* *(also called θ), the progress variable:*

$$\theta = \frac{T - T_1}{T_2 - T_1} = 1 - \frac{Y_F}{Y_F^1}$$

• Most classical theories for turbulent premixed flames are indeed based on methods using θ only.

Tabulation in 3D premixed flames:

Solve at each time step, at each point, the conservation equations for:

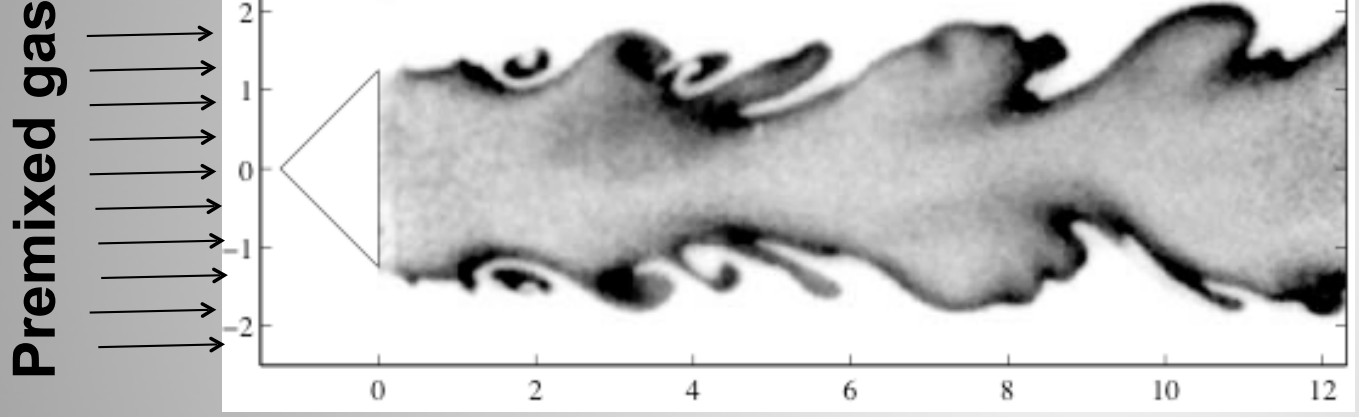
- density, velocities + Progress variable c (also called θ by many authors): with one source term for c

- the expression for the reaction rate is valid for laminar AND turbulent flames. All manyfold assumptions are valid:

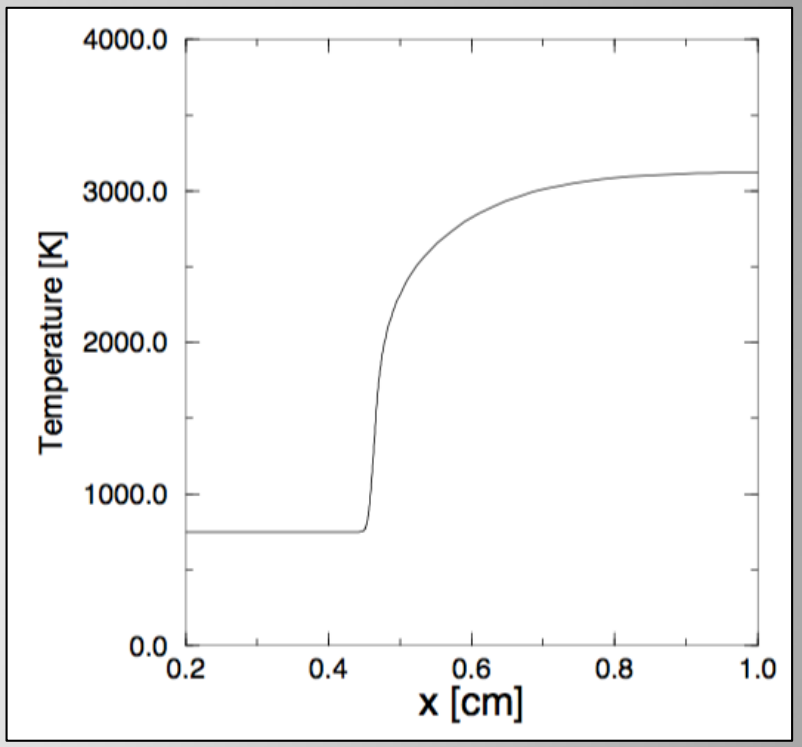
$$\frac{\dot{\omega}_F}{Y_F^1} = B_1 T^{\beta_1} e^{-\beta/\alpha} \rho(1-\Theta) \exp\left(-\frac{\beta(1-\Theta)}{1-\alpha(1-\Theta)}\right)$$

This is the simplest manifold formulation... It can be extended:

Tabulation in premixed flames:



3D turbulent flame

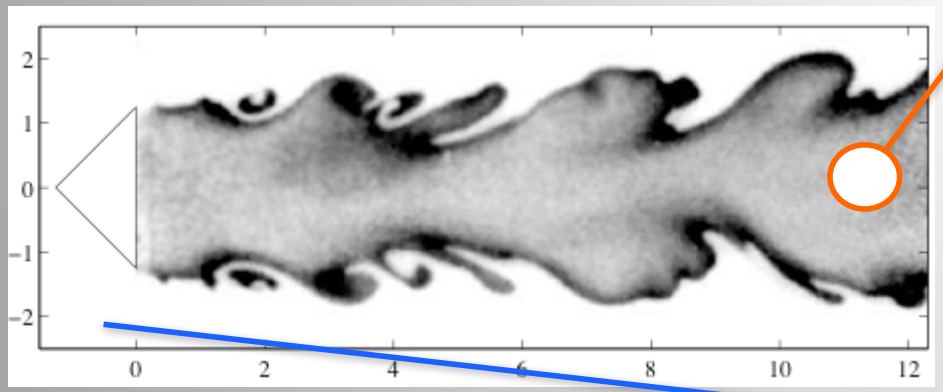


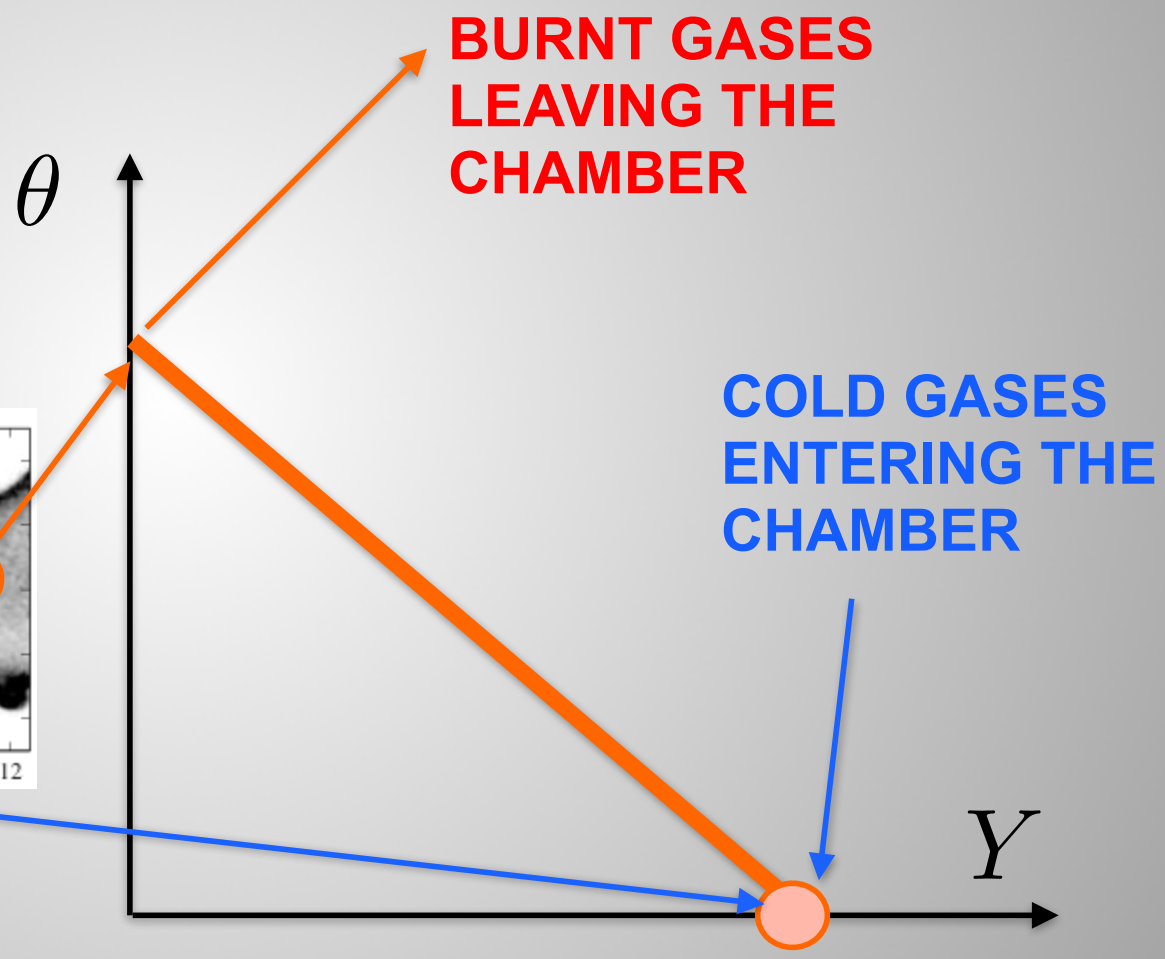
1D laminar flame

We assume that :

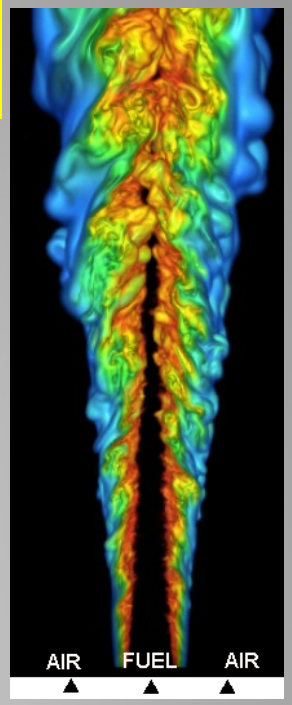
- **Yk and T are functions of c in these two flames**
- **the functions are the same**

The simplest manyfold in adiabatic premixed flames:





Extensions of tabulation methods



We have seen two ‘perfect’ cases where tabulations work:

- Infinitely fast chemistry diffusion flames with z
- Perfectly premixed lean flames with c

This is not sufficient to address all real flames and extensions have been developed to handle more regimes.

The first and most natural extensions are based on the introduction of two variables *at the same time*:

- the progress variable *c*
- the mixture fraction *z*



GENERALIZED TABULATIONS (FPI, FGM): 2 independent variables c and z

Solve at each time step, at each point, the conservation equations for:

- density, velocities,

- progress variable c

- mixture fraction z

All species Yk and temperature are tabulated as fn of z and c but are not solved for in the 3D code.

+ : we have all the other species: complex chemistry is included.

- : it is a 'frozen' complex chemistry. The links between Yk and (z,c) are fixed and obtained on canonical laminar flames.

CAUTION: works only if… flow is adiabatic and is fed by two streams only.

THE SUCCESS OF TABULATIONS

Tabulation methods have had significant success in the last years (see Cornell, EM2C or Eindhoven papers).

They have been applied to many canonical flames (purely premixed adiabatic flames, pure diffusion flames, constant pressure, constant inlet temperature, two-feed system).

FPI: CORIA, EM2C
FGM: EINDHOVEN
ISAT: CORNELL

A nice numerical feature of tabulation:

A tabulation method will provide reaction rates obtained from reading a data base:

$$\dot{\omega} = f(c)$$

This expression will always give a physically reasonable reaction rate

A method based on Arrhenius rates will provide reaction rates from the Arrhenius expression:

$$\dot{\omega} = A Y_f^{n_F} Y_O^{n_O} \exp(-T_a/T)$$

This expression might provide non physical values when small numerical errors develop on mass fractions or temperatures (usually due to dispersion errors)

Bonus: if you have c and z, you ca… read tables to have ALL spe…

Tables can be extended to include a…

NO=f(c,z)
CO=f(c,z)
OH=f(c,z)

Just by pa…ation, all species can be ext… …r 2 quantities (c and z) b…

Cau… …not work very well for species such as NO w… …n the burnt gases where c goes from 0.95 to 0.99… …the tabulation is not precise.

Remember that using a tabulation method based on a complex chemistry scheme is NOT the same as using a complex chemistry scheme

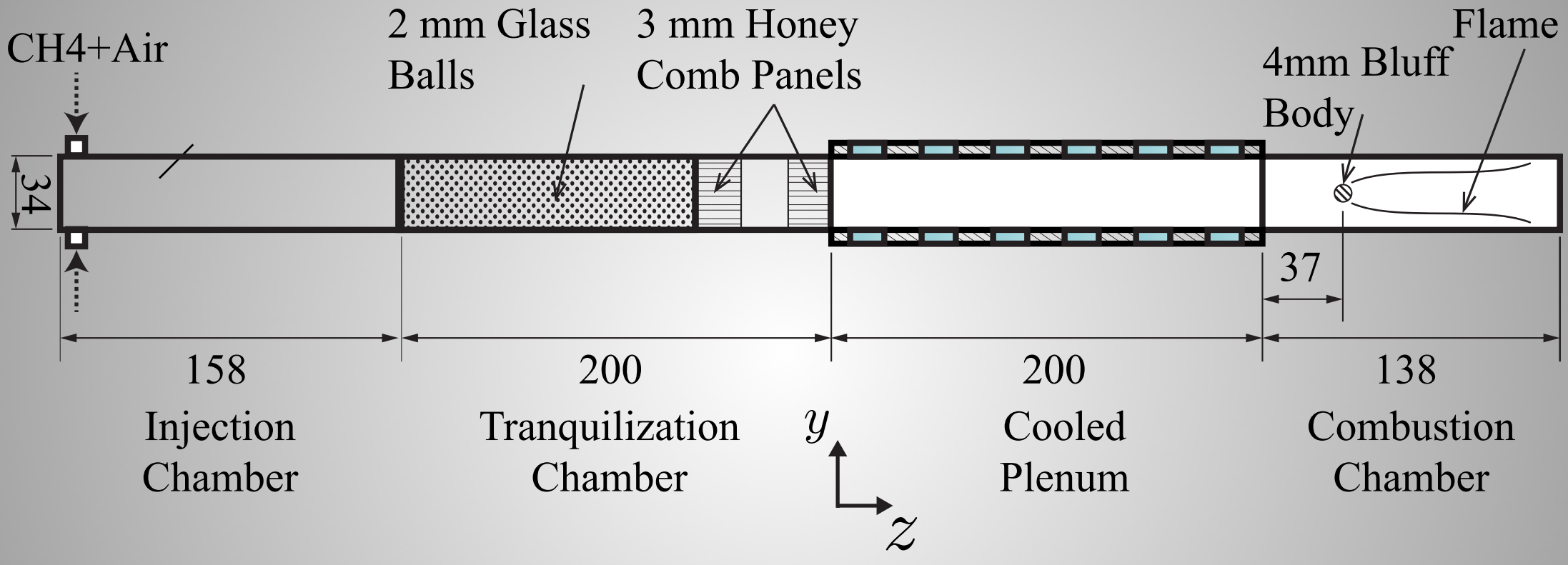
THE LIMITS OF TABULATIONS

In real systems, taking into account:

- Variable pressure (such as in a piston engine)
- Variable dilution (by Exhaust Gas Recirculation for example)
- Cases where more than two streams enter the chamber (so that a mixture fraction z cannot be defined)
- Non adiabatic cases

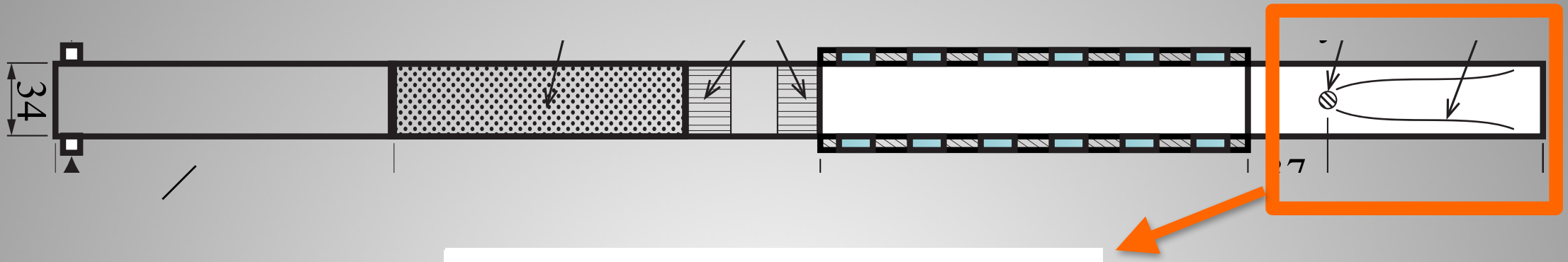
leads to tabulation methods which become difficult and heavy:
- too many control parameters in the table
- finding the relevant flame on which to tabulate data becomes also quite arduous...

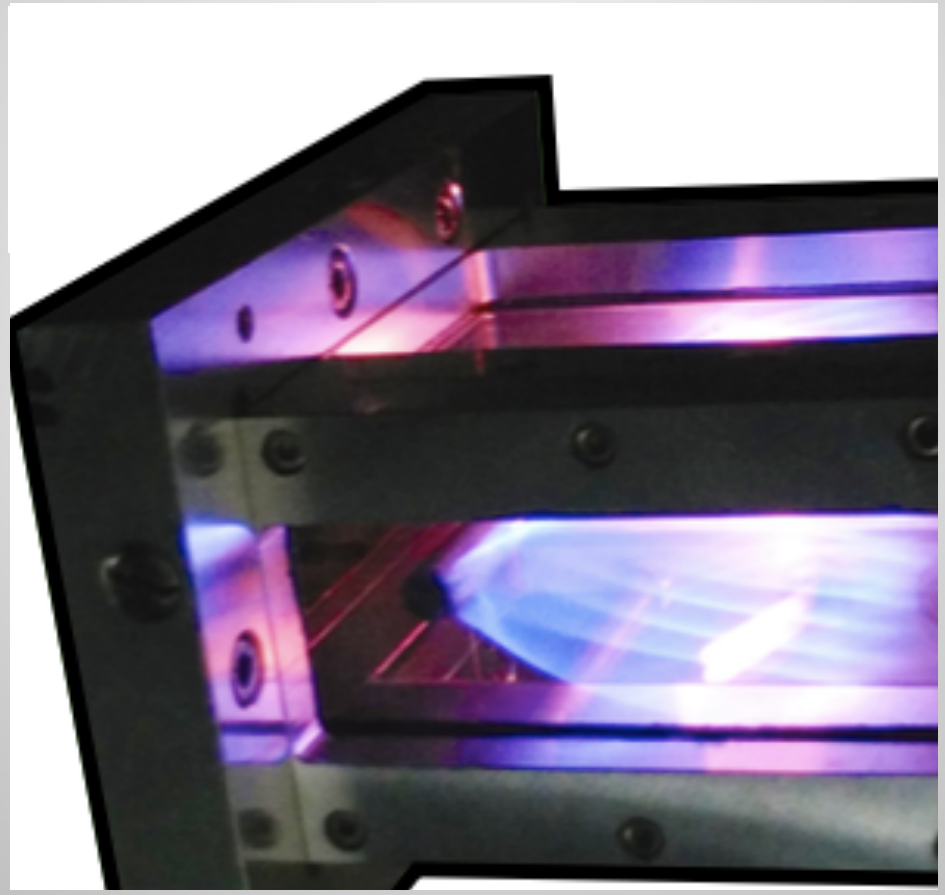
Example of difficulty for tabulation methods: a non adiabatic flame



$$u_b = 1.07\, m.s^{-1}$$
$$T_{in} = 292\, K$$
$$\Phi_{er} = 0.75$$

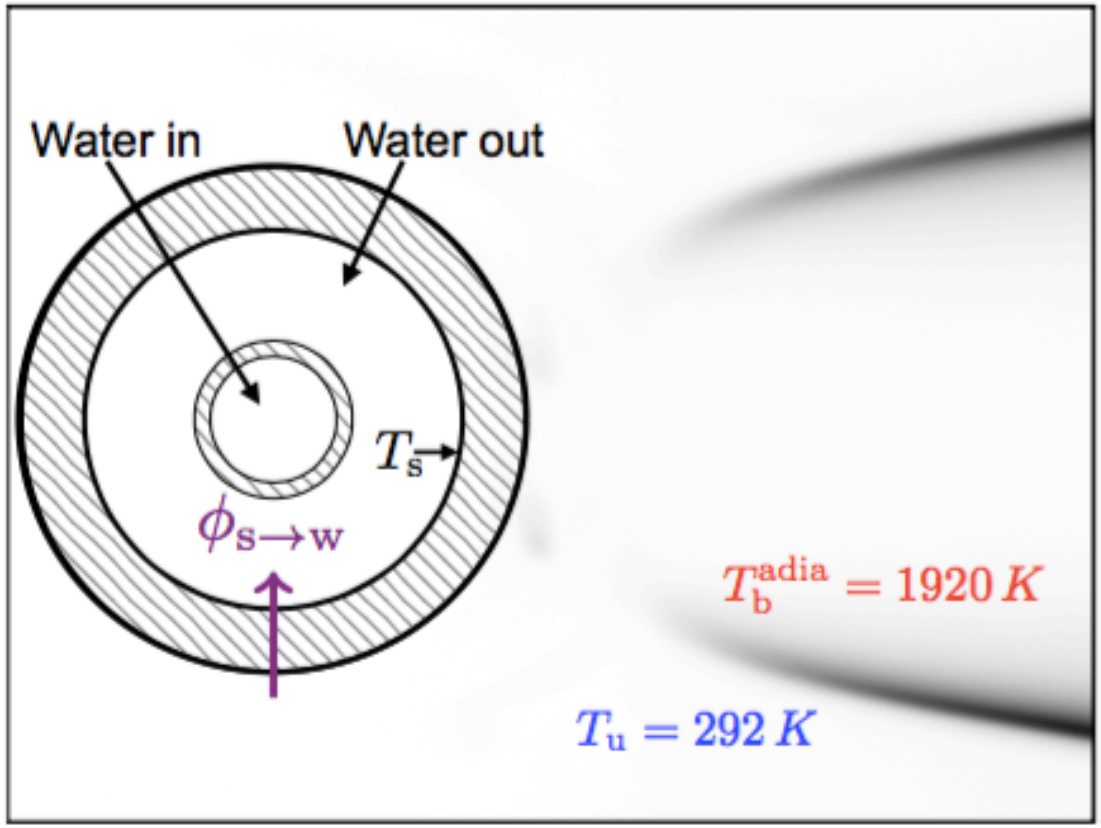
PhD of D. Mejia, M. Brebion, IMF Toulouse

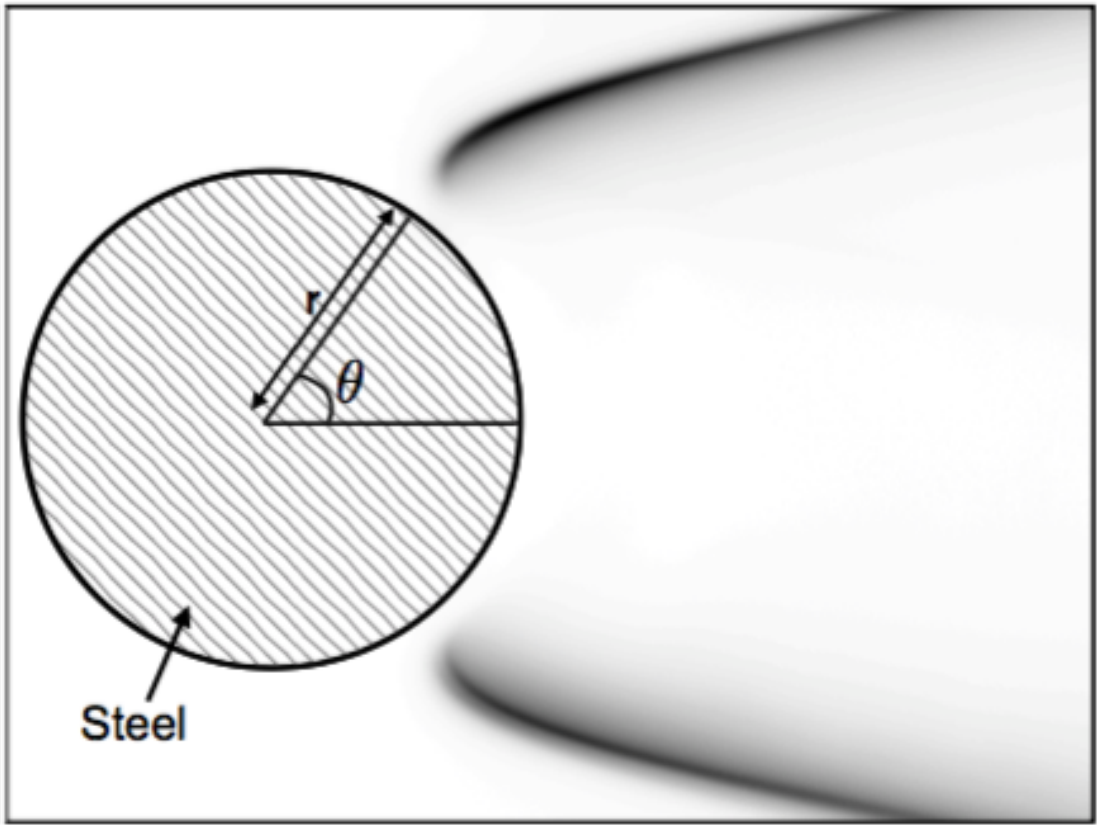

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COOLED FLAME HOLDER

ADIABATIC FLAME HOLDER

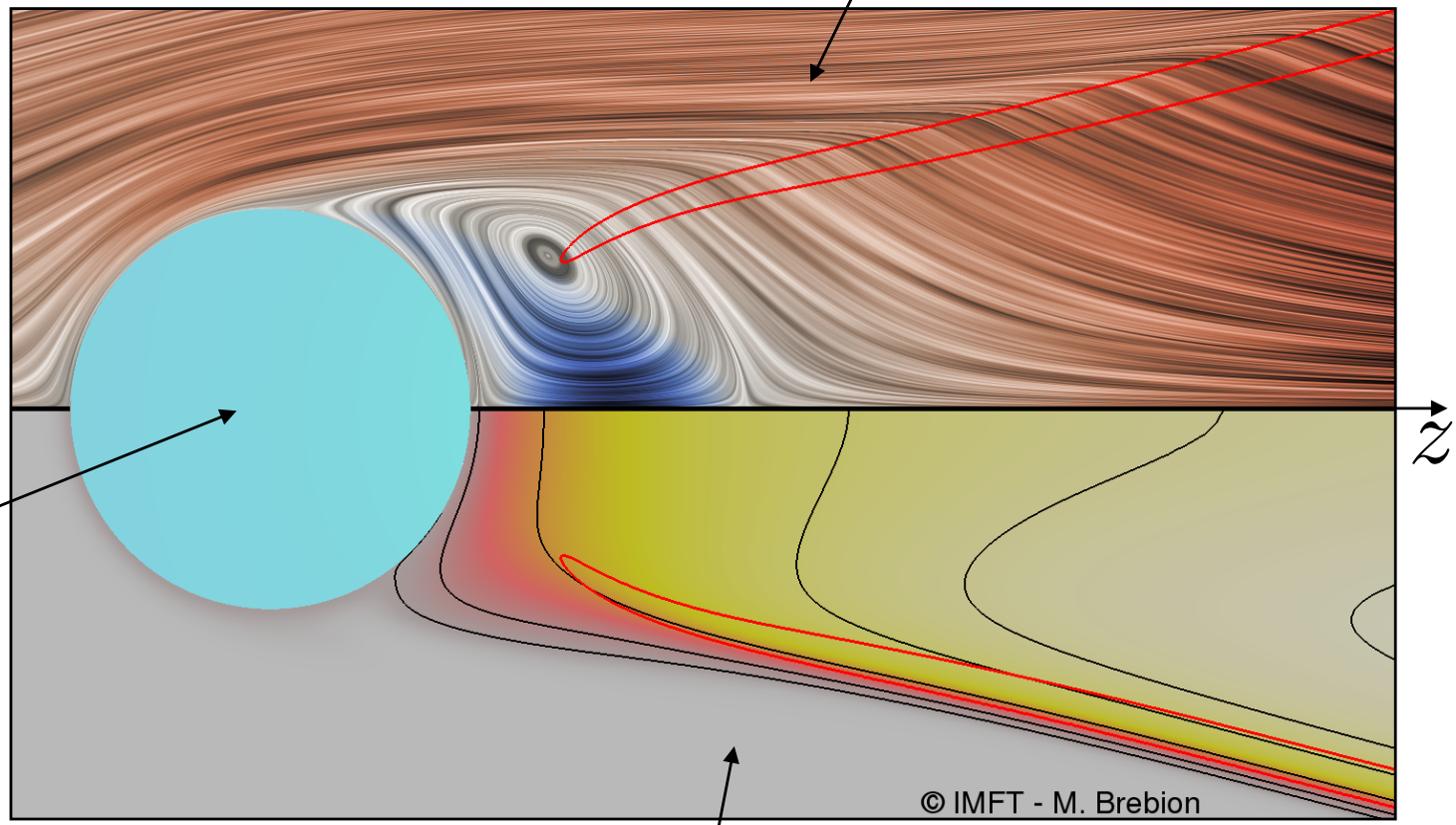




Transition from cooled to uncooled cylinder

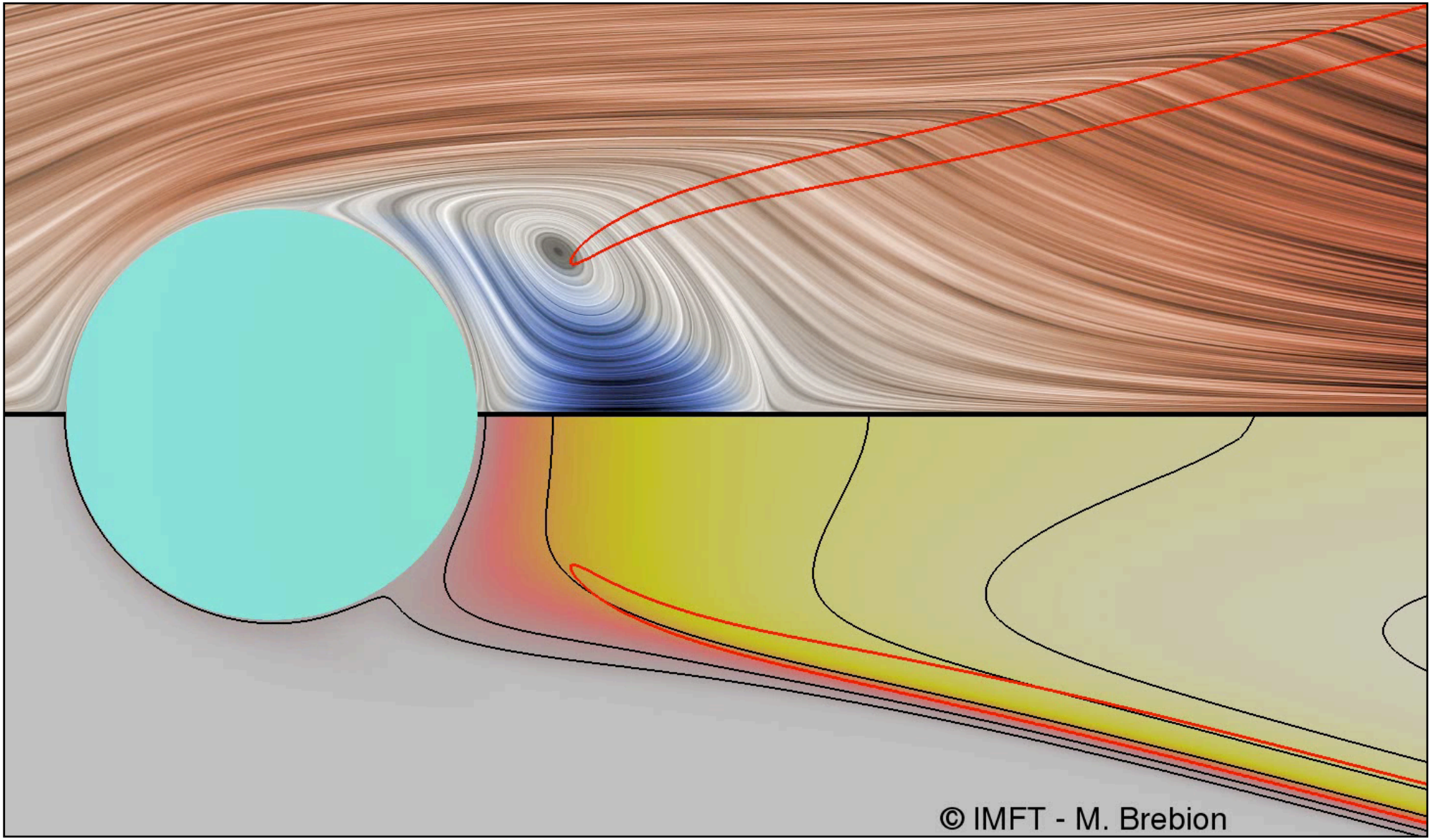
Flow velocity visualisation:
Line integral convolution method colored by u_z

Solid temperature visualisation:
colormap

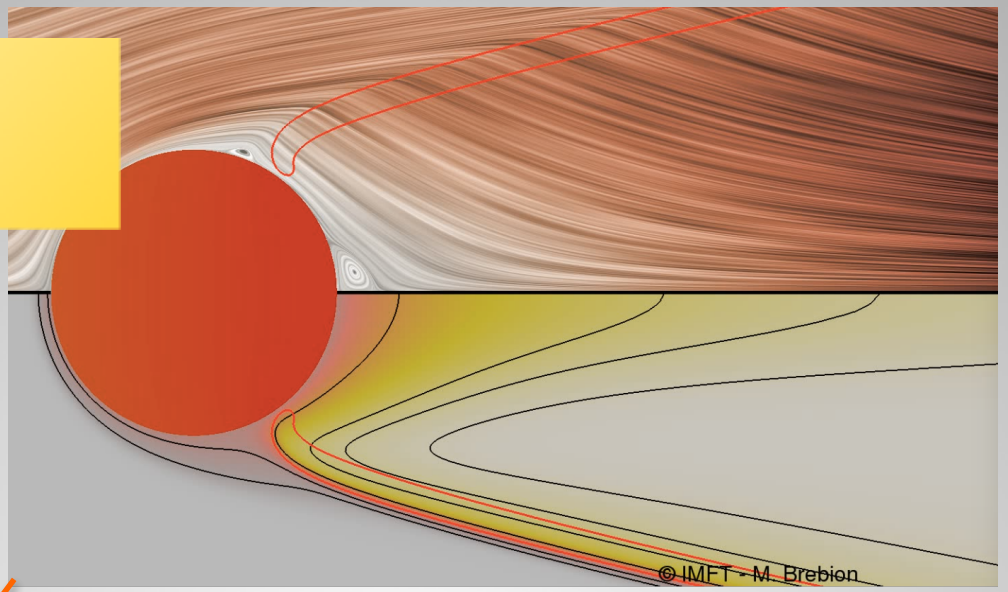


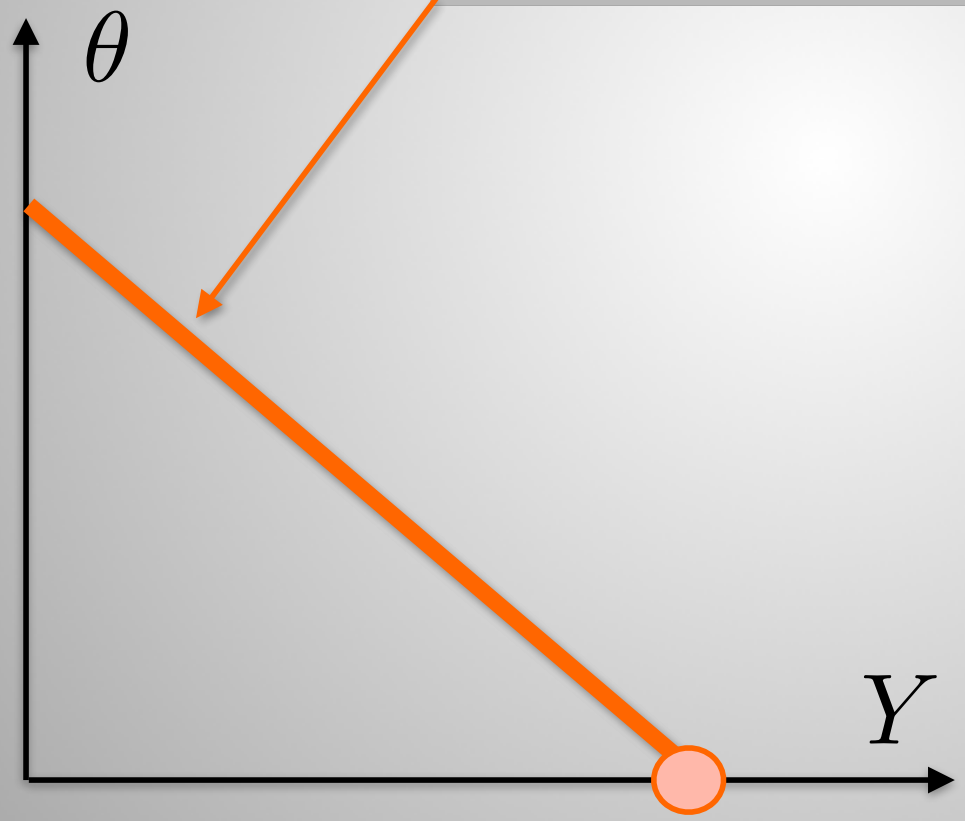
Flow temperature visualisation:
iso-contours + colormap

Transition from cooled to uncooled cylinder



ADIABATIC FLAME HOLDER



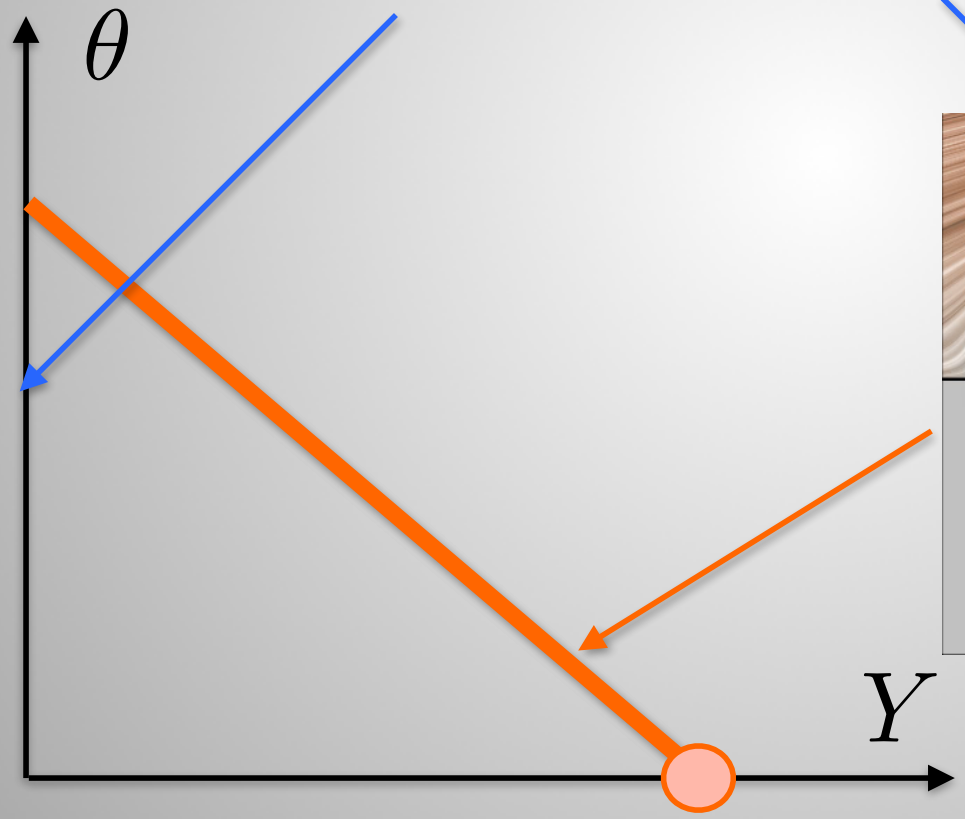


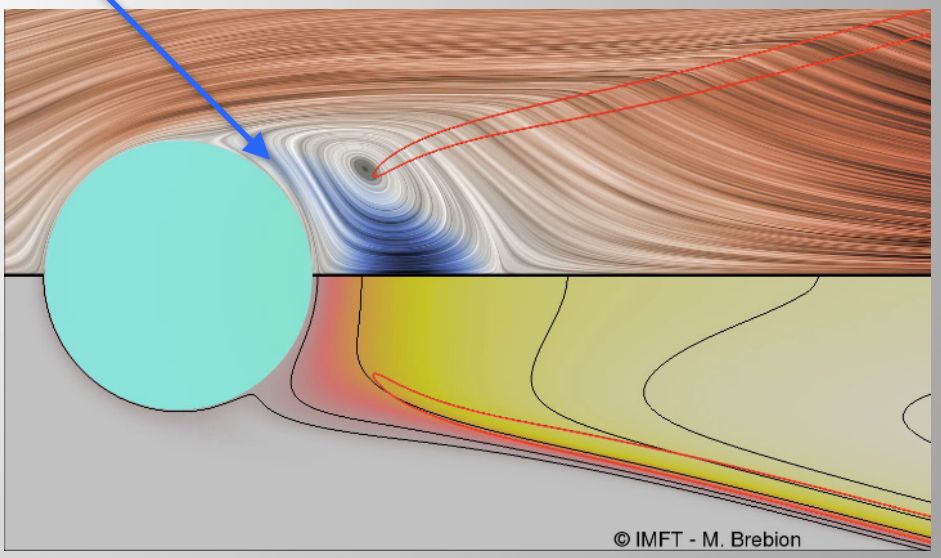
WE ARE ON THE MANYFOLD

COOLED FLAME HOLDER

WE ARE NOT ON THE MANYFOLD ANYMORE

EFFECTS OF HEAT LOSSES: $Y + \Theta < 1$





OUTLINE

1/ BRUTE FORCE METHODS

2/ TABULATION TECHNIQUES

3/ REDUCED SCHEMES

4/ ANALYTICALLY REDUCED SCHEMES

REDUCED SCHEMES: 5 to 10 species, 2 to 10 reactions

Solve at each time, at each point, the conservation equations for:
- Density
- Velocities
- Temperature
- A FEW Chemical species Yk for k= 1 to N (N up to 10)
- A FEW GLOBAL REACTIONS (M from 1 to 4)

All species are solved independently: instead of 2 degrees of freedom (tabulation), we now have N degrees of freedom.

More general but more expensive than tabulation methods.

Can work with non adiabatic flows, multiple streams feeding the combustor.

THE QUEST FOR REDUCED SCHEMES

The search for reduced chemical schemes started long ago:

- Westbrook and Dryer "Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames," *Comb. Science and technology*, 27, 31-43, 1981

- Jones and Linstedt. "Global reaction schemes for hydrocarbon combustion. " *Comb. Flame*, 1988, Vol:73, 233-249.

This is a fitting exercise: if we have a single step reaction, we can fit 5 parameters: preexponential constant A, activation energy T_a, temperature exponent β, species exponents.
How many flame properties can we fit with 5 parameters ?

Answer: not that many if we have only one reaction and we keep the reaction parameters...constant.

But what if we start tuning A, T_a and β ?

If we start tuning A, T_a and β, we can match many flame properties. For ex, if we compute a turbulent premixed flame at a fixed equivalence ratio, we can ask the reduced scheme to match:

- Adiabatic flame temperature
- Laminar flame speed
- CO2 and CO mass fractions in the burnt gases

We use a full chemical scheme as a reference to tune the reduced scheme (this means we need one !) for our 'target flames'. These target flames must be simple enough to be computed with the full scheme.

Main idea: it is very difficult to build a reduced scheme which matches ALL properties of a full scheme over ALL conditions of pressure, composition and temperature.
But it is much easier to match certain properties of a full scheme with a reduced scheme only in a limited range of conditions.

Building reduced schemes for 3D codes

0D or 1D codes (full chemistry)

Full scheme → Compute results on the 'target' flames using full and reduced schemes and adjust reduced scheme constants until they match

Tune reduced scheme → Compute results on the 'target' flames using full and reduced schemes and adjust reduced scheme constants until they match

Complex chemistry stops here. The task of the reduced scheme is to mimic complex chemistry as well as possible on these simple flames which can be computed with simple codes

3D codes (reduced chemistry)

Use the reduced scheme in the 3D code

Why this works ?

Because the whole procedure has a limited ambition. The whole process is performed for a limited range of parameters !

The reduced scheme which is obtained has a limited range of validity: have to re construct a new one every time we change regime (pressure, temperature, equivalence ratio, etc)

DON'T BE A PERFECTIONIST.
RECOGNIZE THAT WE ARE LOOKING FOR A COMPROMISE AND THAT KINETICS APPROXIMATIONS MAY NOT BE THE WORSE ASSUMPTIONS WE USE...

Examples of reduced schemes

For CH4/air or kerosene / air flames

Using 1 or 2 chemical reactions and 5 to 8 species

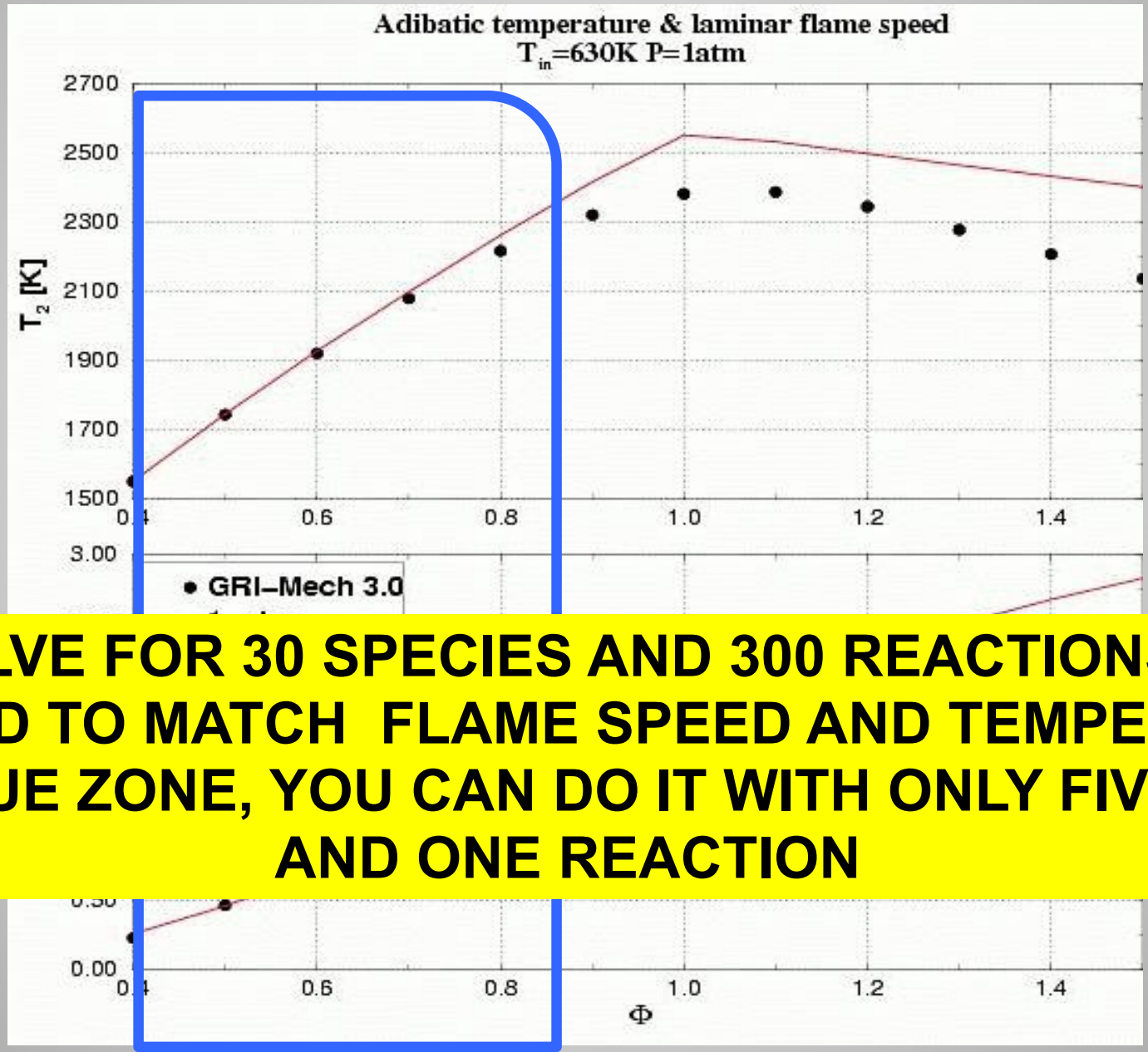
Adjusting ONLY the pre exponential constant A

METHANE / AIR FLAME USING SINGLE-STEP SCHEME: CH4+2(O2+a N2) -> CO2 + 2 H20 + 2a N2

```
ELEMENTS
 H   O    C   N
END
SPECIES
CH4 O2 CO2 H2O N2
END
REACTIONS
CH4+2O2=>CO2+2H2O                          1.100451E+22     0.0   35143.0
FORD / CH4 1.7602 /
FORD / O2 1.2667 /
END
```

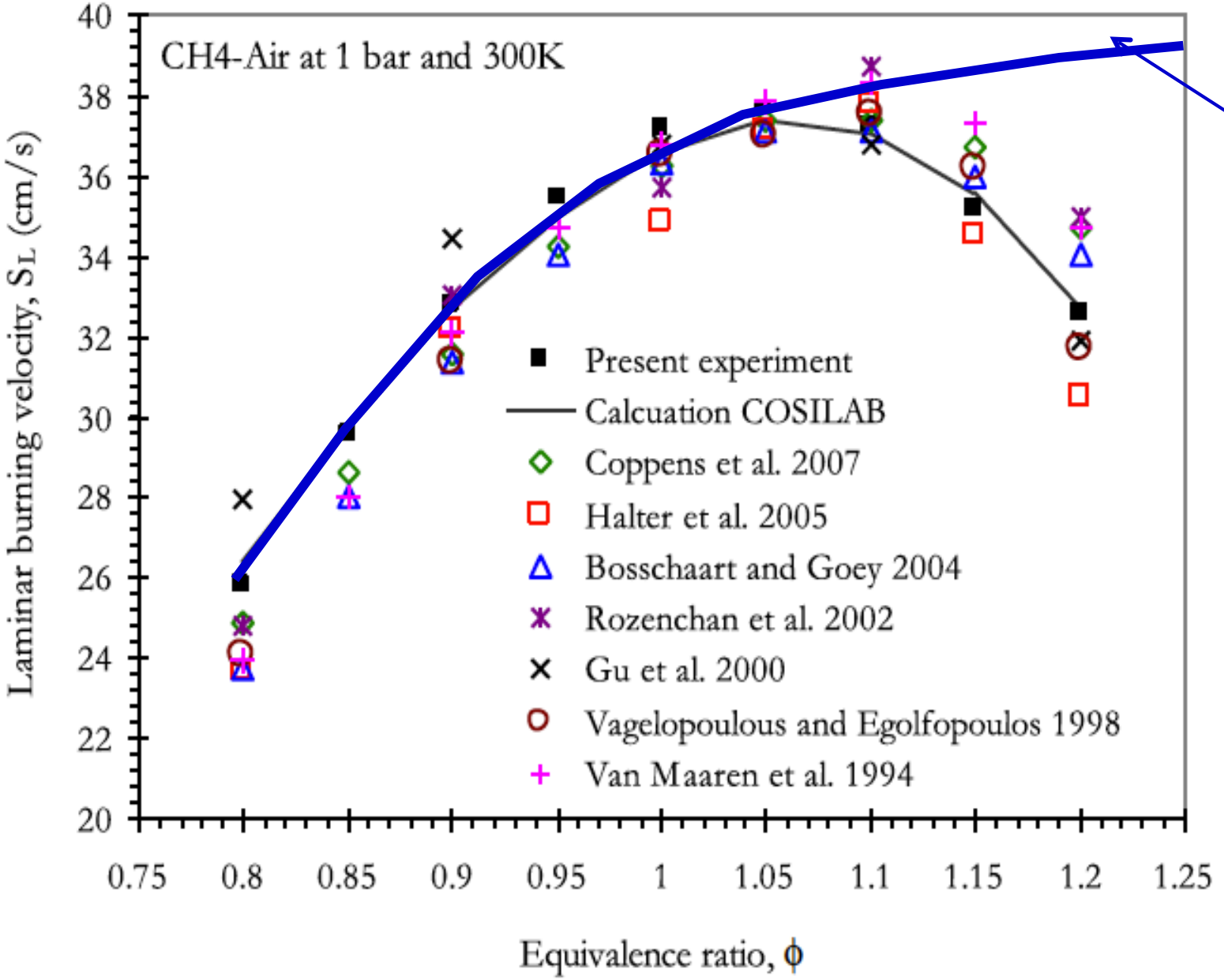
$$q_1 = A_1 \left(\frac{\rho Y_{CH_4}}{W_{CH_4}} \right)^{n_{1F}} \left(\frac{\rho Y_{O_2}}{W_{O_2}} \right)^{n_{1O}} \exp\left(-\frac{E_{a1}}{RT} \right)$$

1-step: T_{in}=630K P=1atm Φ_0=0.5



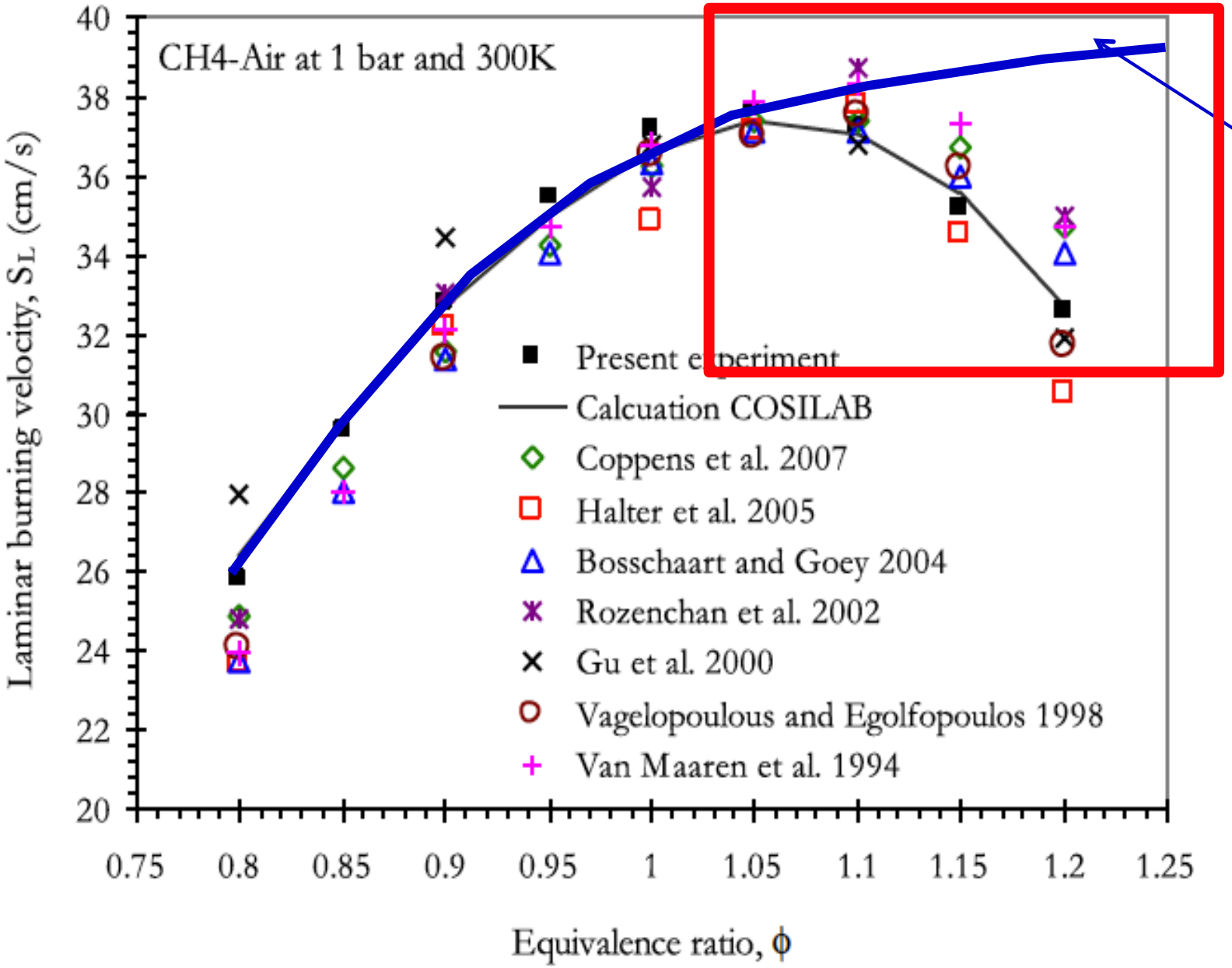
WHY SOLVE FOR 30 SPECIES AND 300 REACTIONS IF YOU ONLY NEED TO MATCH FLAME SPEED AND TEMPERATURE ? IN THIS BLUE ZONE, YOU CAN DO IT WITH ONLY FIVE SPECIES AND ONE REACTION

WE CAN EVEN MAKE IT WORK FOR RICH CASES:



Single step chemistry

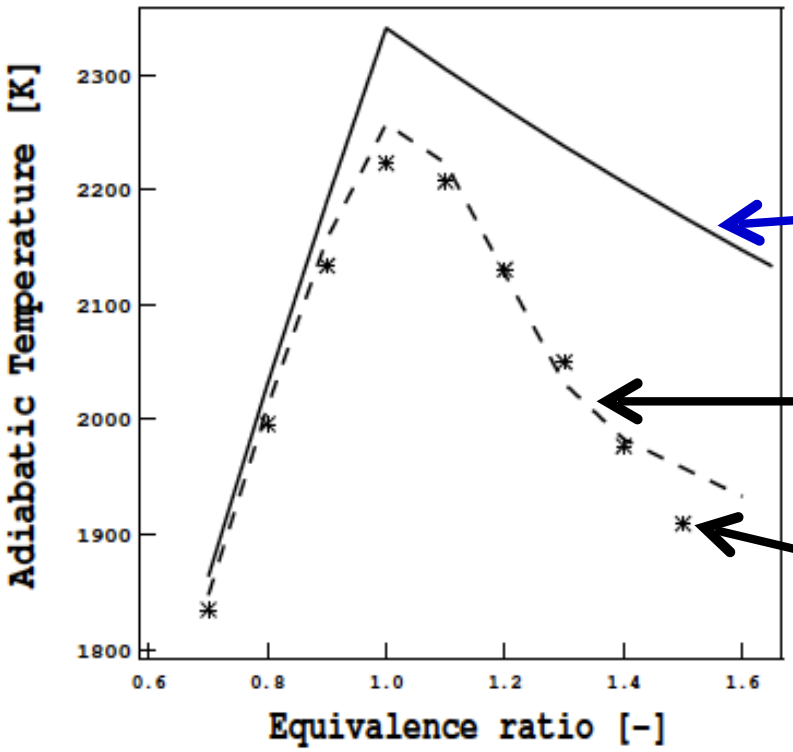
NEVER FORGET THAT THE ERROR MARGIN ON FLAME SPEEDS IS NOT SMALL:



WHY DO WE FAIL HERE ?
BECAUSE WE MISS CO

BUT WE CAN DO BETTER:

- ADD ONE SPECIES (CO) -> CH4,O2,CO2,H2O,N2,CO
- AND ONE REACTION: CO+ 1/O2 <-> CO2

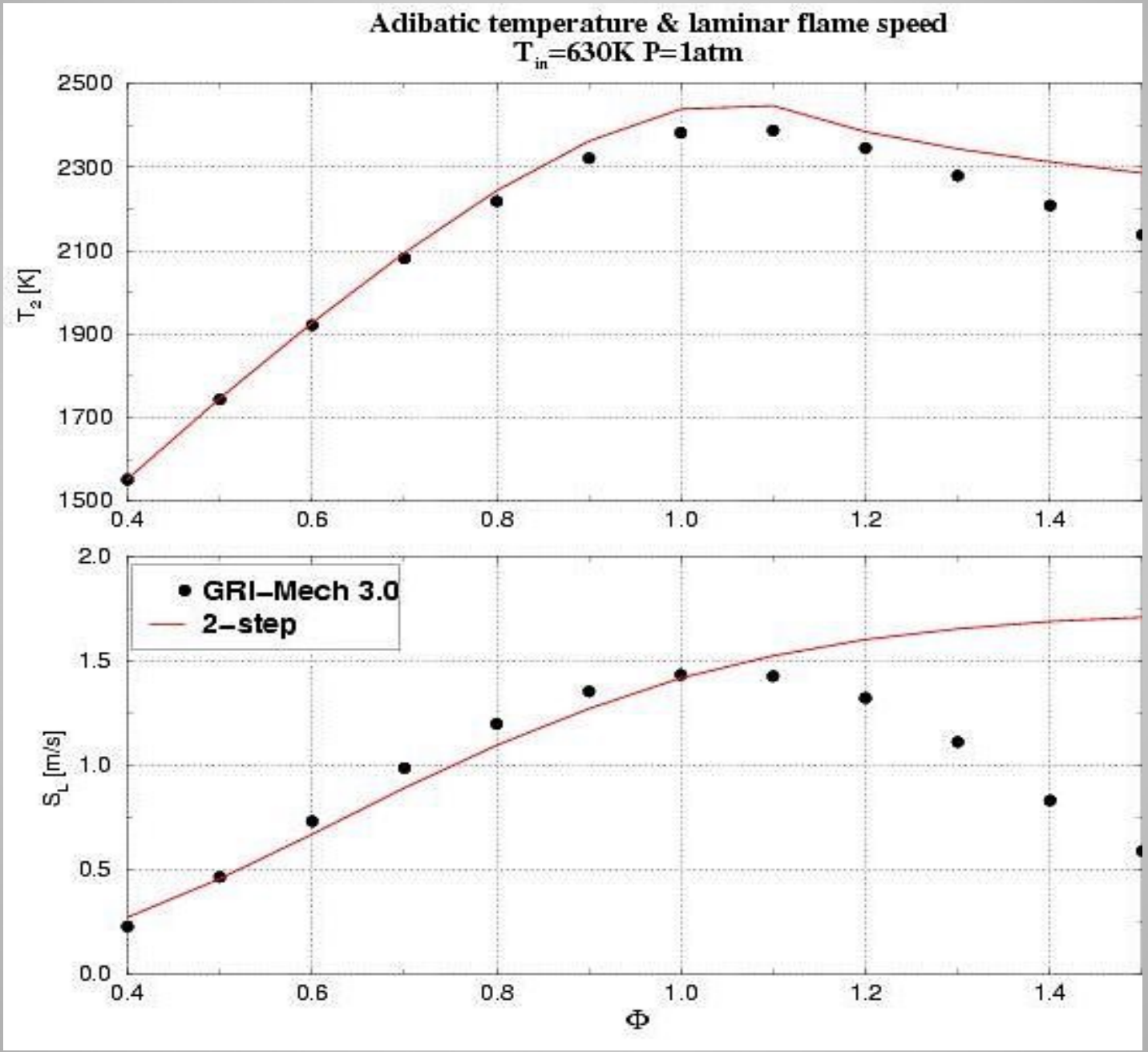


Single step chemistry with 5 species (no CO)

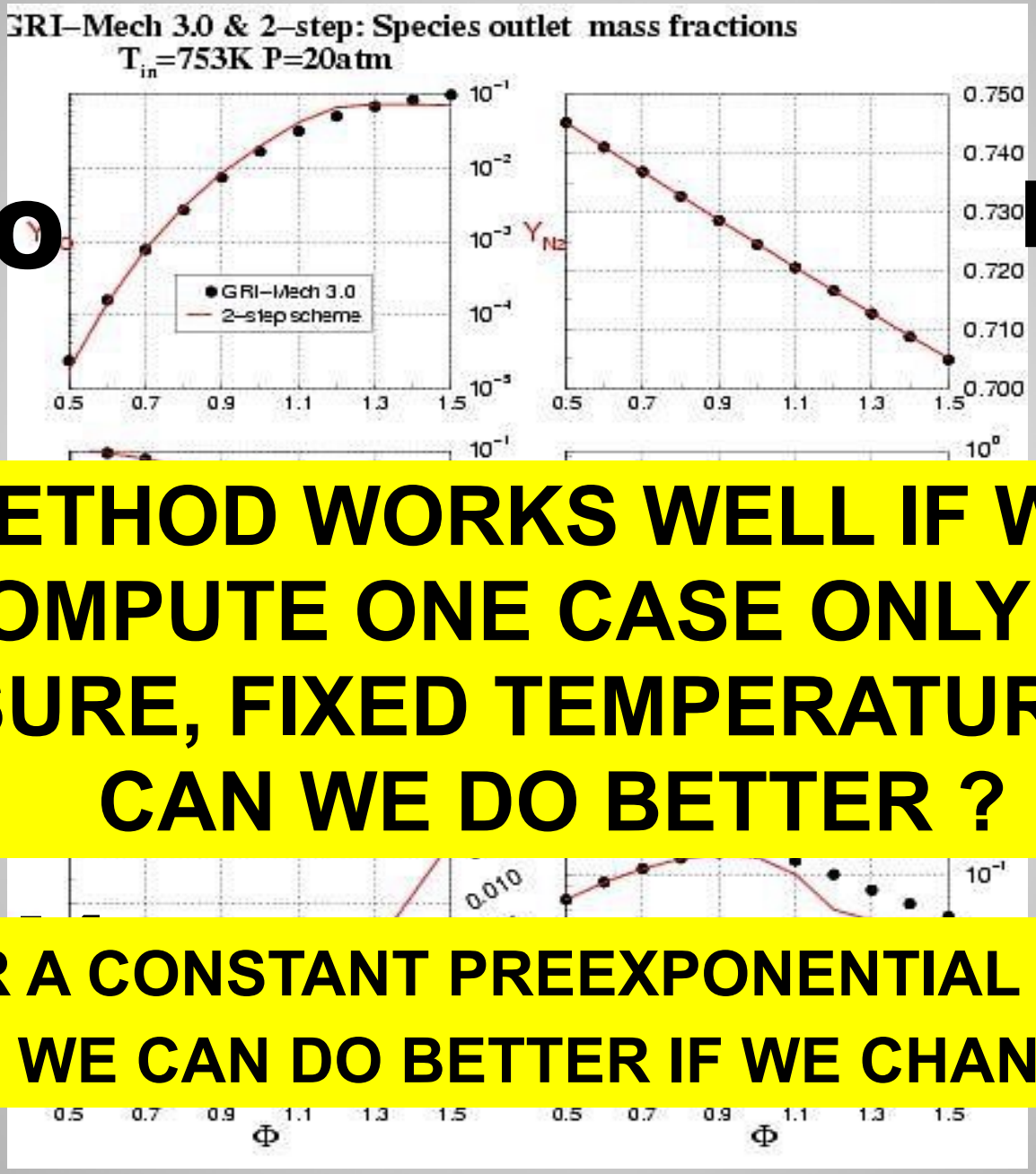
Two step chemistry with 6 species (with CO)

Full chemistry

2-step: T_{in}=630K P=1atm Φ_0=0.5



2-step: T_{in}=630K P=1atm Φ_0=0.5



CO N2

THIS METHOD WORKS WELL IF WE WANT TO COMPUTE ONE CASE ONLY (FIXED PRESSURE, FIXED TEMPERATURE, ETC). CAN WE DO BETTER ?

THIS IS FOR A CONSTANT PREEXPONENTIAL CONSTANT A

BUT WE CAN DO BETTER IF WE CHANGE A !

EXTENSION TO A WIDER RANGE OF EQUIVALENCE RATIOS AND CONDITIONS :

GO FROM

$$q_1 = A(\rho Y_F/W_F)^{\nu_F}(\rho Y_O/W_O)^{\nu_O} e^{-T_a/T}$$

TO:

$$q_1 = A(\phi)(\rho Y_F/W_F)^{\nu_F(\phi)}(\rho Y_O/W_O)^{\nu_O(\phi)} e^{-T_a(\phi)/T}$$

WE CHANGE A AS A FUNCTION OF THE LOCAL EQUIVALENCE RATIO ϕ

EXTENSION TO A WIDER RANGE OF EQUIVALENCE RATIOS AND CONDITIONS :

Tune each constant as a function of equivalence ratio:

- **Fernández-Galisteo, Sánchez, Liñán, and Williams. One-step reduced kinetics for lean hydrogen–air deflagration, *Comb. Flame* 2009, 156. MODIFY ALL CONSTANTS OF THE SCHEME**

- **Franzelli et al *Comb. Flame* 157, 1364. MODIFY ONLY PREEXPONENTIAL CONSTANTS**

$$q_1 = A(\phi)(\rho Y_F/W_F)^{\nu_F}(\rho Y_O/W_O)^{\nu_O} e^{-T_a/T}$$

A becomes A(ϕ) where ϕ is the local equivalence ratio

Example for methane: the BFER scheme for CH4 and for kerosene

The 2S_CH4_BFER mechanism is composed of six species (CH_4, O_2, CO_2, CO, H_2O et N_2) and takes into account two reactions:

$$CH_4 + 1.5\ O_2 \quad => \quad CO + 2\ H_2O \tag{13}$$

$$CO + 0.5\ O_2 \quad <=> \quad CO_2 \tag{14}$$

- first reaction: it controls the flame speed and the ignition delay;
- second reaction: it is needed to predict burnt gas temperature for rich mixtures.

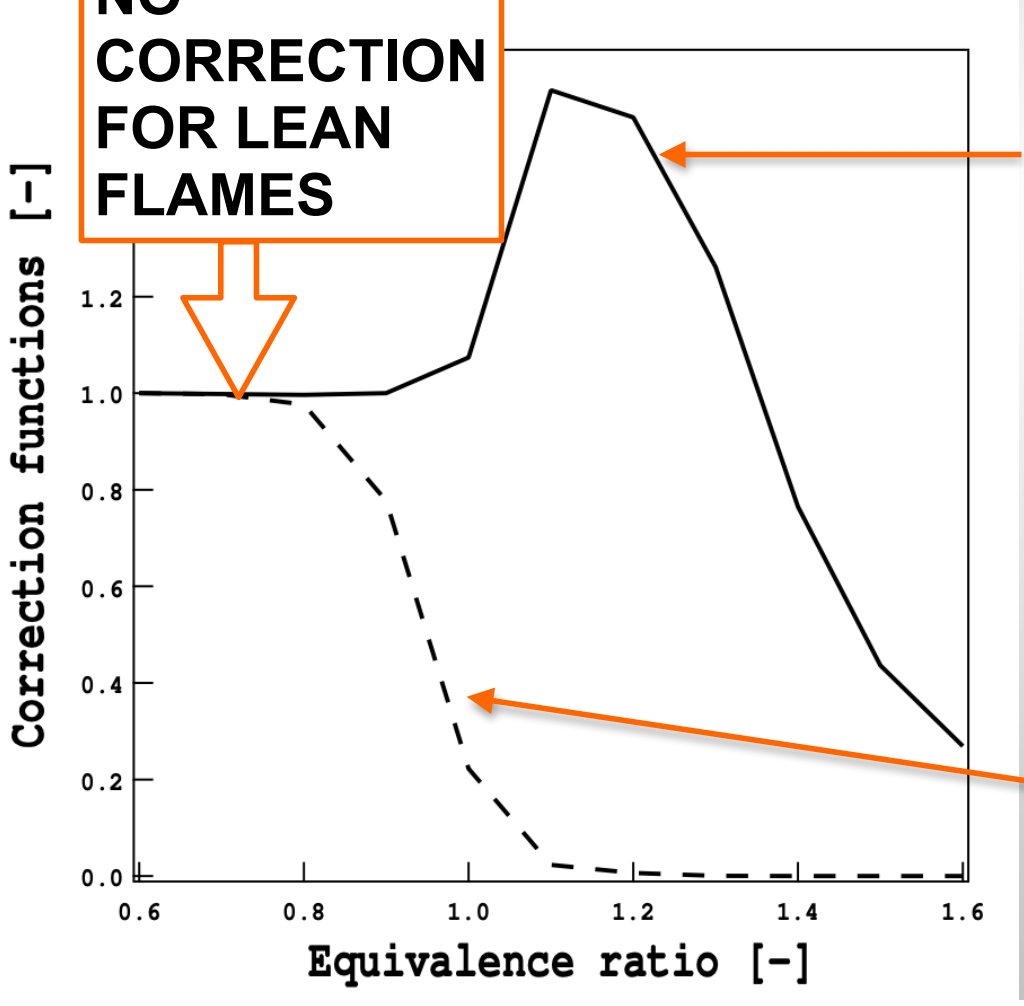
Validated for a wide range of pressure $1\ atm < P < 10\ atm$, initial temperature $300\ K < T_f < 800\ K$ and equivalence ratio $0.7 < \phi < 1.6$.

The general methodology described in B.Franzelli, E.Riber, M. Sanjosé and T. Poinsot, *A two-step chemical scheme for kerosene-air premixed flames*, Combust. Flame, 157 (2010) 1364-1373 has been used to build this scheme.

THE CORRECTION FUNCTIONS FOR A TWO-STEP SCHEME FOR CH4 AIR-FLAMES:

$$k_{f,1} = A_1 f_1(\phi) \exp^{(-E_{a,1}/RT)} [CH_4]^{n_{CH_4}} [O_2]^{n_{O_2,1}},$$
$$k_{f,2} = A_2 f_2(\phi) T^{0.7} \exp^{(-E_{a,2}/RT)} [CO]^{n_{CO}} [O_2]^{n_{O_2,2}}$$

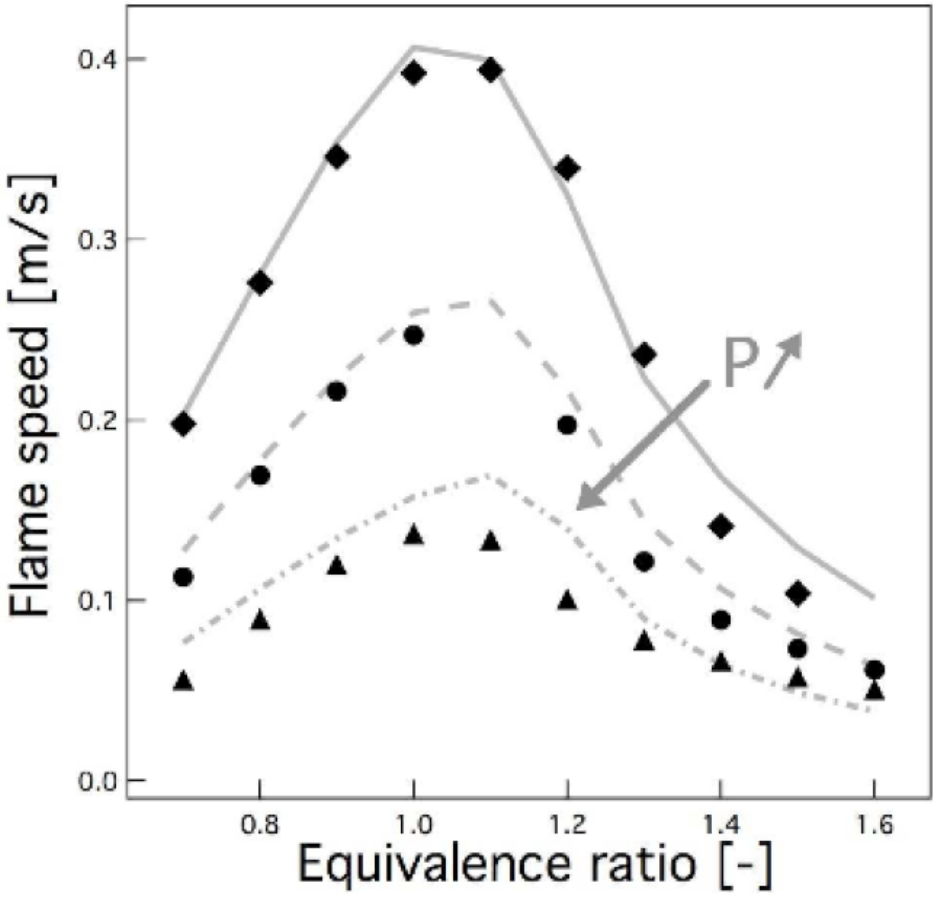
NO CORRECTION FOR LEAN FLAMES



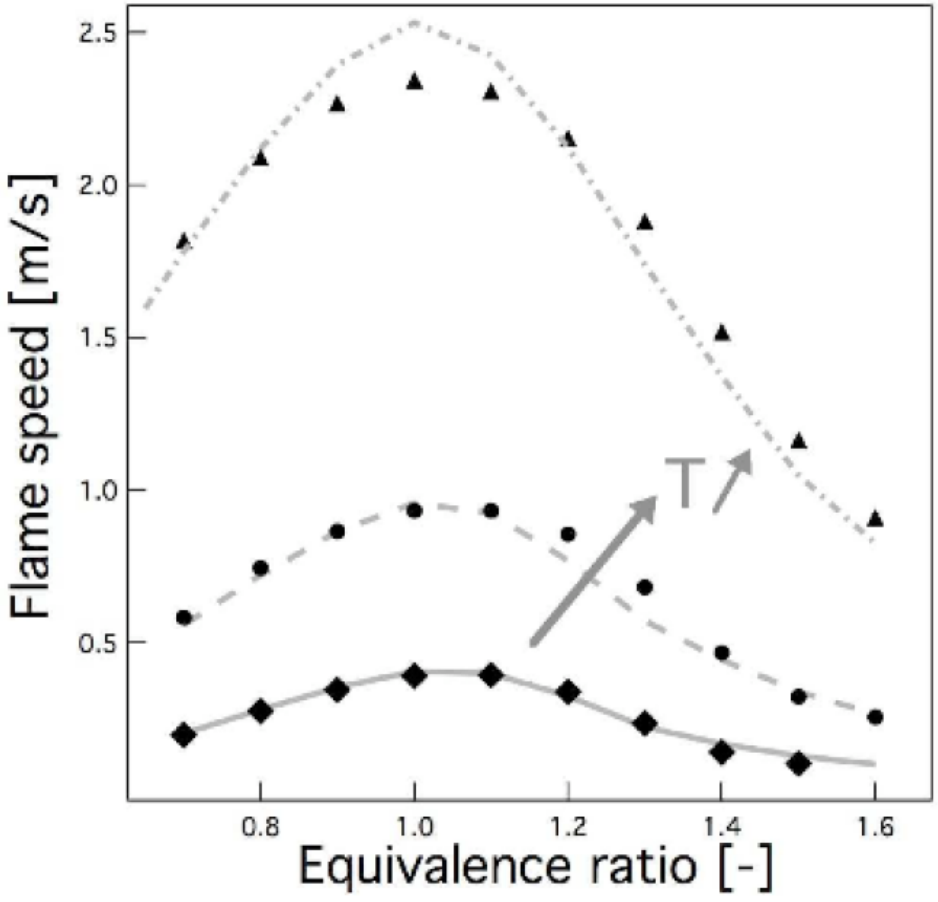
$f_1(\phi)$

$f_2(\phi)$

A two-step scheme for CH4/air flames (Franzelli et al CF 157, 1364):



a.



b.

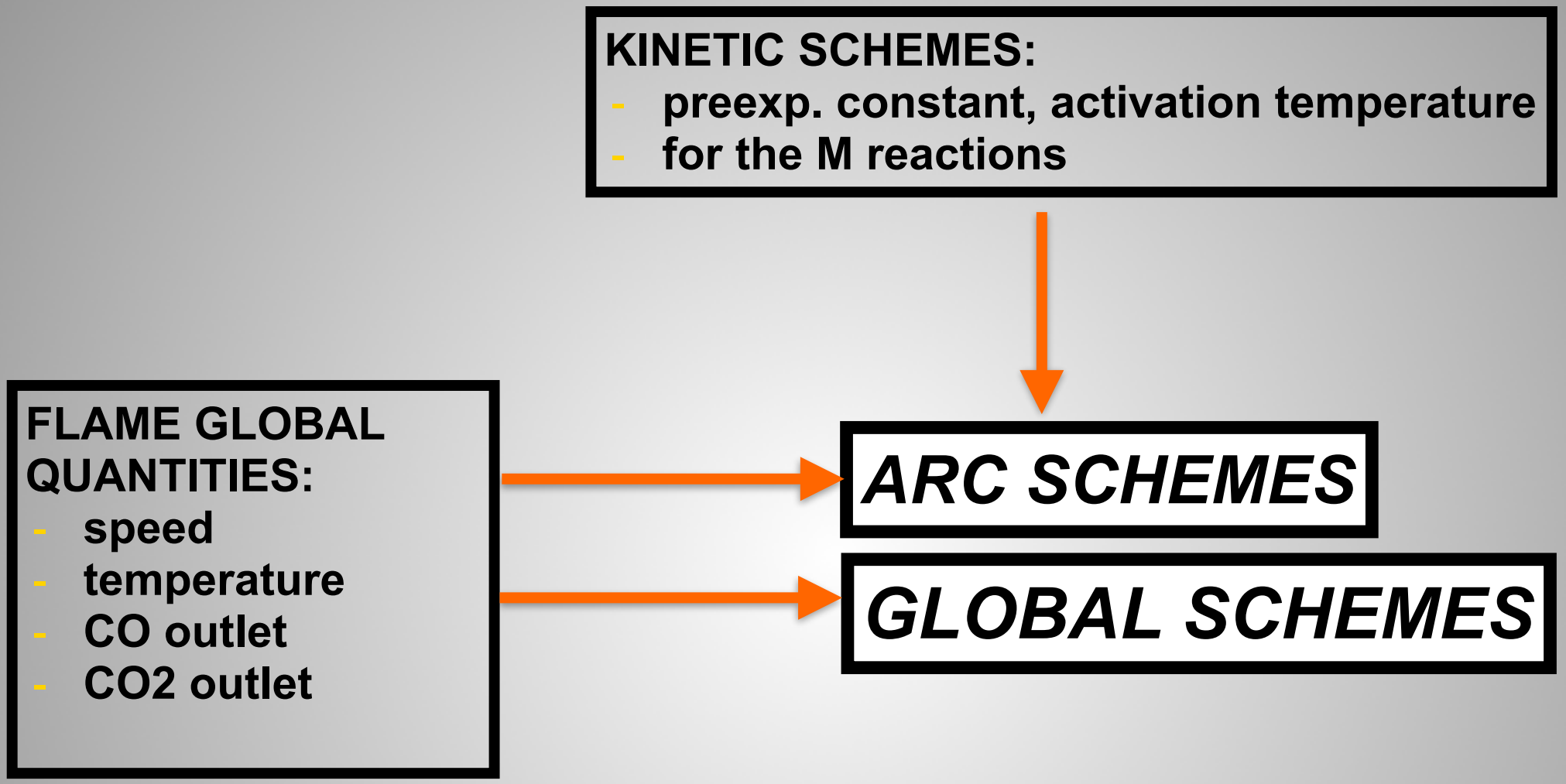
Works for lean and rich flames, over a wide range of pressures and temperatures
Exists also for kerosene/air flames

A NEW TREND FOR REDUCED SCHEMES: ANALYTICAL SCHEMES

Fitting schemes with 1 to 4 reactions is purely a mathematical exercice: we did not use any of the chemical information available in a full scheme.

We can do better : use schemes which have been « reduced analytically » (10 to 20 reactions), starting from full schemes:

- **Advantage: physically based schemes, much more general**
- **Drawback: more expensive**


KINETIC SCHEMES:
- preexp. constant, activation temperature
- for the M reactions
FLAME GLOBAL QUANTITIES:
- speed
- temperature
- CO outlet
- CO2 outlet
ARC SCHEMES
GLOBAL SCHEMES

ANALYTICALLY REDUCED SCHEMES

- The main idea is to use ‘analytically’ reduced schemes with more species and reactions:
  - instead of 2 steps, go to 20.
  - Instead of 6 species, go to 25.

- Important point for LES: such schemes are coded in 200 Fortran lines… No table needed, no space required, no human intervention before each run

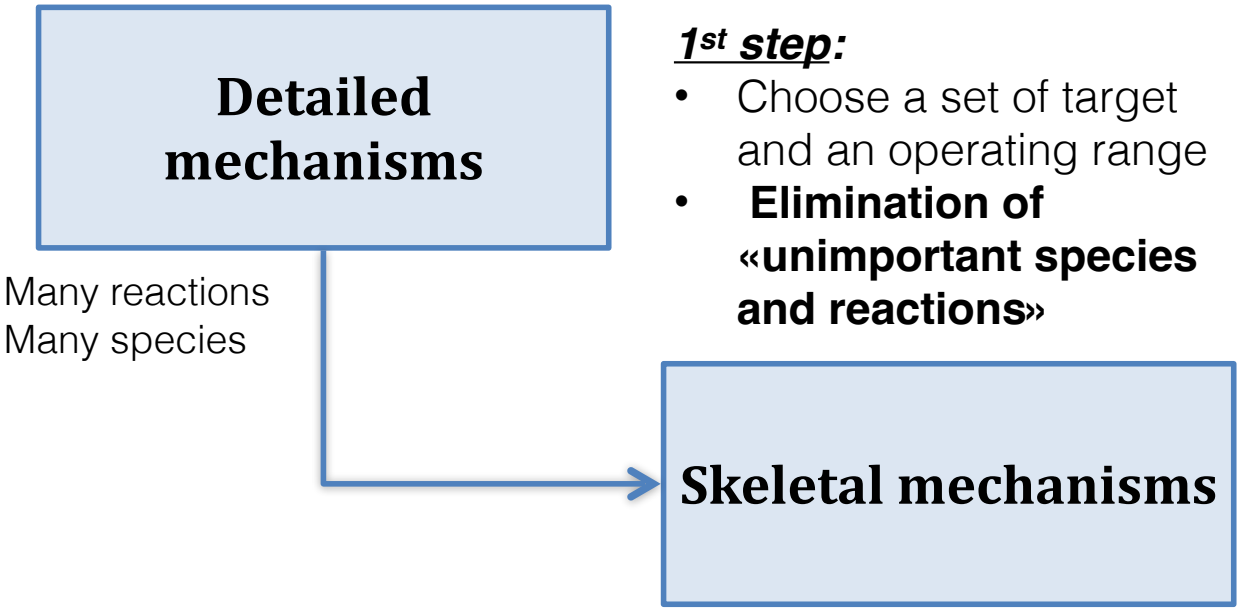
ARC is not new

Already proposed by T. Lu, for example:

R. Sankaran, E.R. Hawkes, J.H. Chen, T.F. Lu, C.K. Law, "Structure of a spatially developing turbulent lean methane–air Bunsen flame," Proc. Comb. Inst. 31 (2007) 1291.

T.F. Lu and C.K. Law, "A criterion based on computational singular perturbation for the identification of quasi steady state species: A reduced mechanism for methane oxidation with NO chemistry," Combustion and Flame, Vol.154 No.4 pp.761–774, 2008.

- **Derivation of ARC schemes**



1st step:

- Choose a set of target and an operating range
- **Elimination of «unimportant species and reactions»**

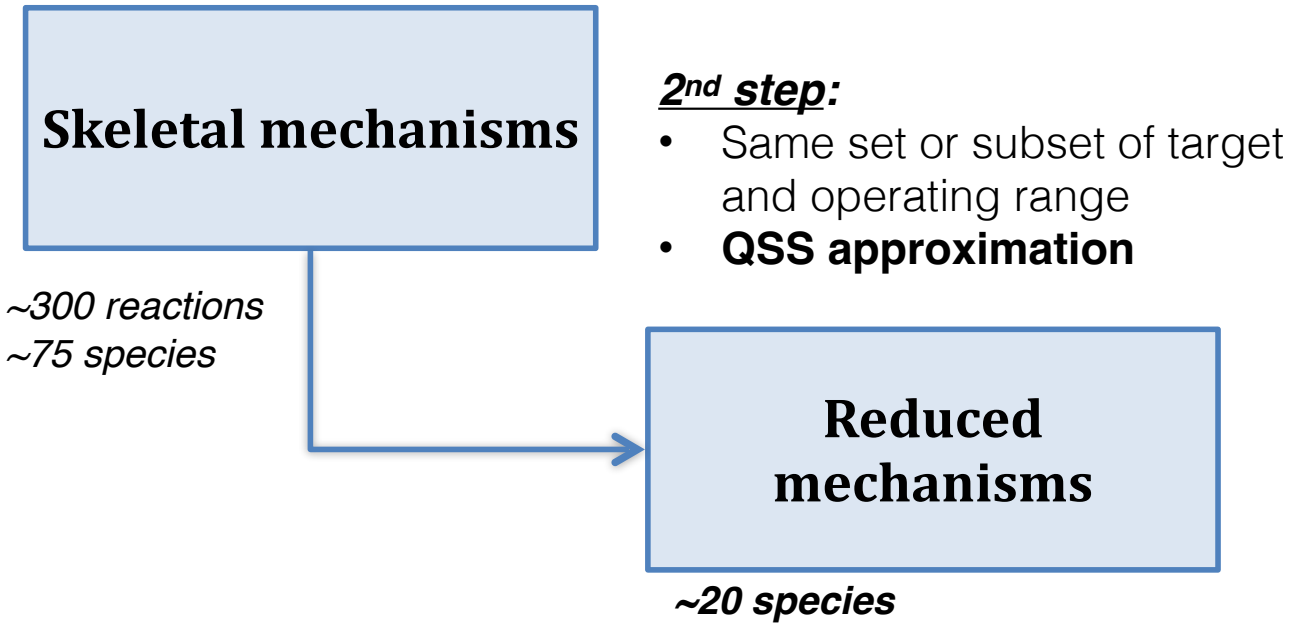
~300 reactions
~75 species

Techniques:

- **Directed Relation Graph method (DRG)**
- **Lumping**
- Path Flux Analysis
- Principal Composant Analysis
- Sensitivity Analysis
- ...

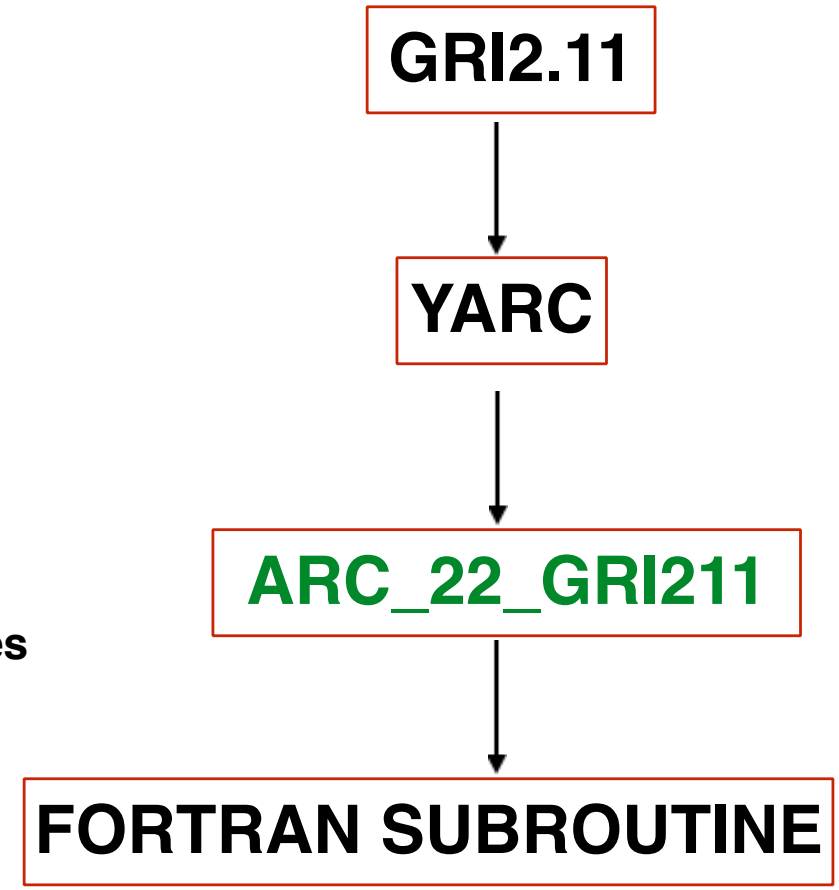
Techniques:

- Jacobian investigations (**Level Of Importance (LOI),** Computational Singular Perturbation, ...)
- Sensitivity Analysis



ARC: the example of CH4

- **YARC reduction tool [1]:**
  - **1st step: Skeletal reduction**
    - **Directed relation graph method [2]**
    - **Reduces the number of species**
  - **2nd step: Quasi Steady State approximation**
    - **Level of Importance criterion [3]**
    - ➔ **Reduces the number of transported species**
    - ➔ **Reduces the numerical stiffness**



[1] Pepiot, PhD thesis, 2008
[2] Pepiot, C&F, 2008
[3] Lovas, PCI, 2000

Advantages of ARC

Information of initial full mechanism is preserved

- **No assumption on flame structure: the species are all independent**
- **CO and NO directly obtained: no additional model needed**
- **Once a scheme is implemented in a 3D solver, it can handle a very wide range of flames and regimes without change.**

Advantages of ARC

- **Heat losses, dilution effects, quenching, ignition can be captured directly**
- **Two phase flow combustion is also easy to add**
- **Numerically, the stiffness of chemistry can be mastered: reactions which are too fast are handled via QSS assumptions so that the 3D code does not have to deal with them.**

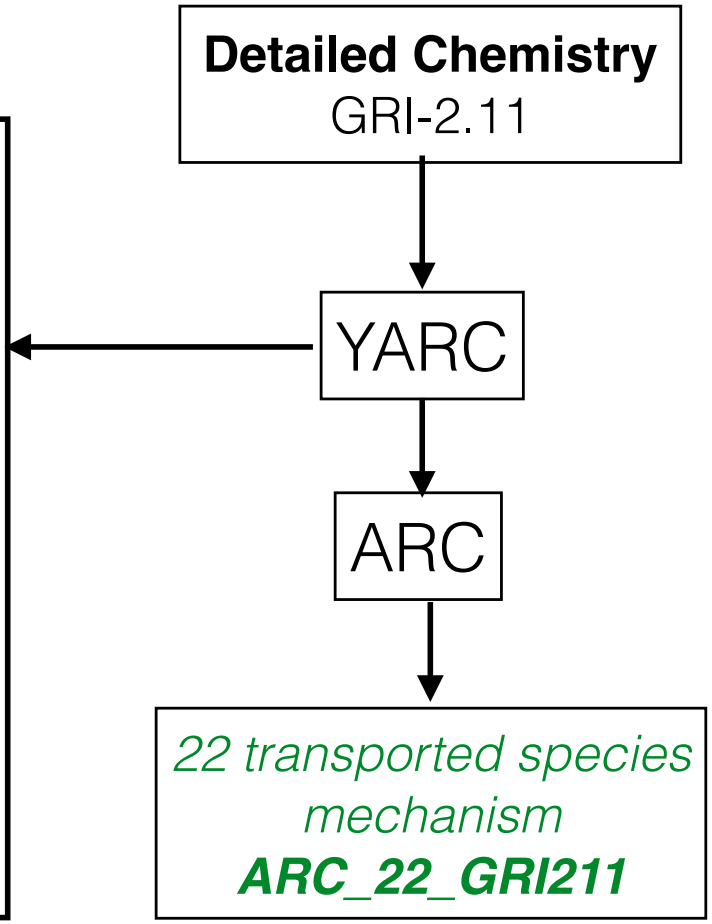
EXAMPLE OF ARC DERIVATION FOR METHANE/AIR CHEMISTRY (INCLUDING NOx AND CO)

[1] Pepiot, PhD Thesis, 2008

- **YARC** reduction tool [1]
- Goal: build a scheme able to reproduce **NO and CO formation** (**methane-air** mixture)

- Target problem
  - **Premixed flame:** ϕ=0.6 → 1.4
  -->Target conditions: *1 bar, 300K*
- Target quantities :
  - Global quantities: flame speed
  - Local quantities: Heat release, **CO** and **NO** concentrations

Objective: **Relevant chemical routes** preserved in the reduced mechanism



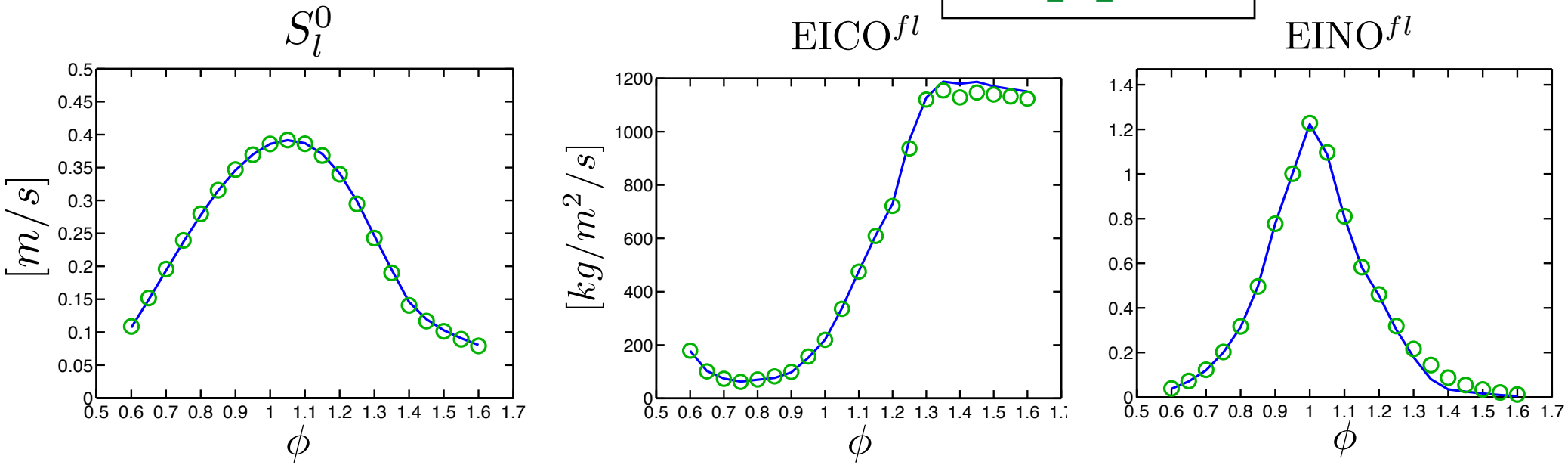
CERFACS

SPECIES in ARC_22_GRI211

- **TRANSPORTED (22): CH4, O2, N2, CO, CO2,H2O, H2, H, O, OH, HO2, CH3, CH2O, H2O2, CH3OH, C2H2, C2H6, C2H4, NO, NO2, HCN, N2O.**
- **QSS (15): CH2, CH2(S), HCO, CH2OH, C, CH, C2H3, C2H5, CH3O, HCCO, NH2, NCO, HNCO, HNCO, HOCN.**

300 K, 1 bar (Scheme derivation conditions)

— GRI2.11
O ARC_22_GRI211

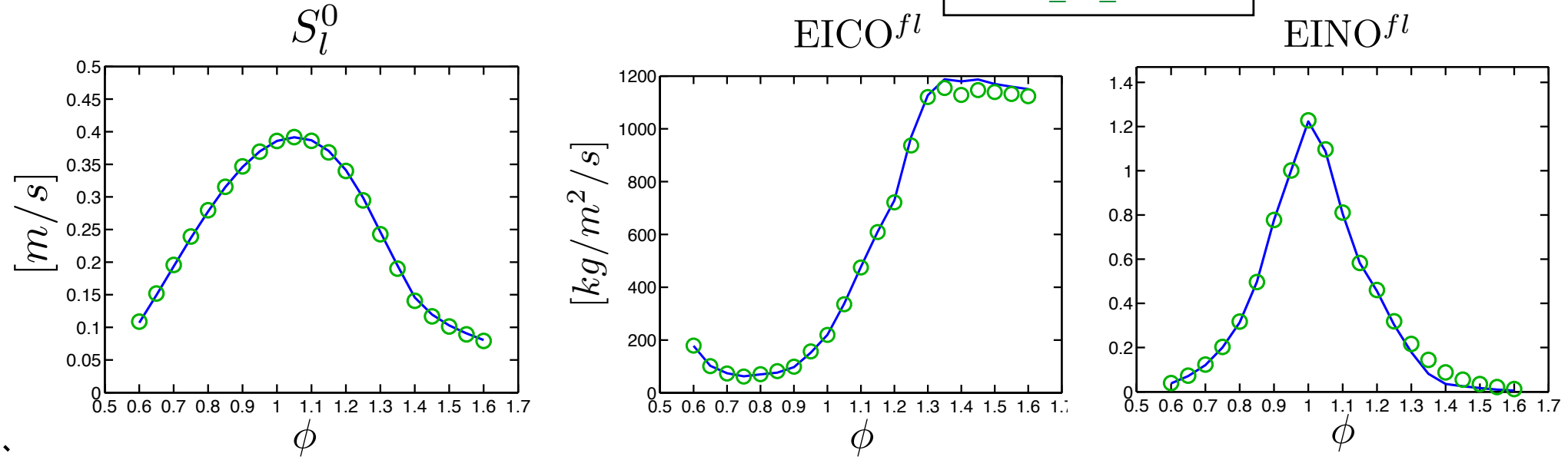


CERFACS

ARC EVALUATION - CHANGING OPERATING POINT:

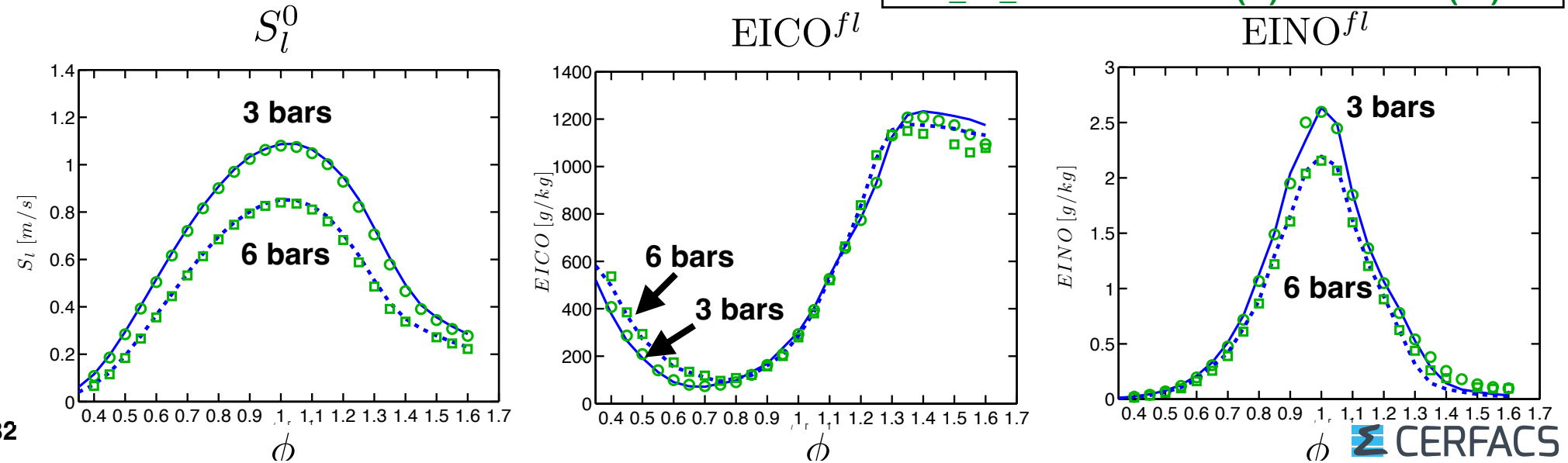
300 K, 1 bar (Scheme derivation conditions)

— GRI2.11
O ARC_22_GRI211



680 K, 3-6 bars (Gas turbine conditions)

GRI2.11: 3 bars (—) and 6 bars (- - -)
ARC_22_GRI211: 3 bars (O) and 6 bars (□)



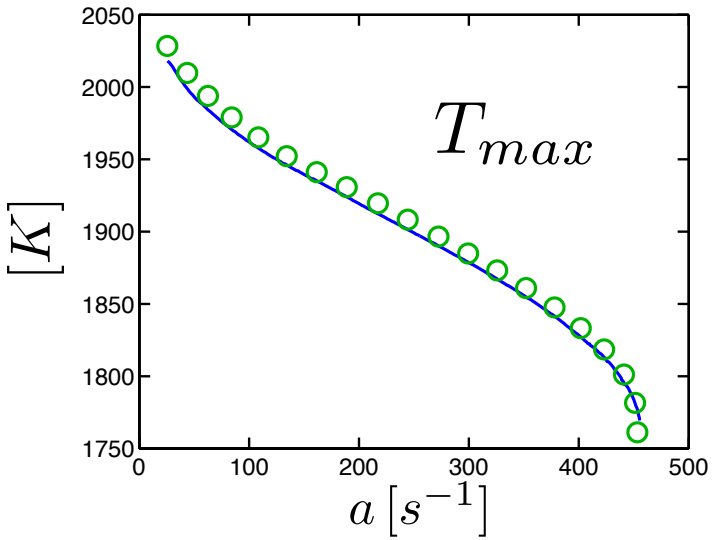
CERFACS

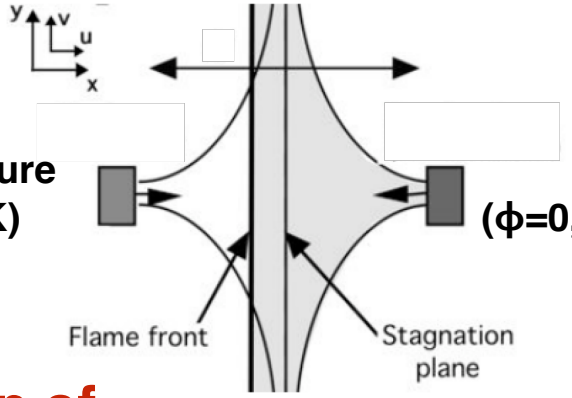
ARC EVALUATION - CHANGING FLAME TYPE:

Sandia Flame D [1]
Non-premixed combustion regime

→

Validation on strained counterflow flames



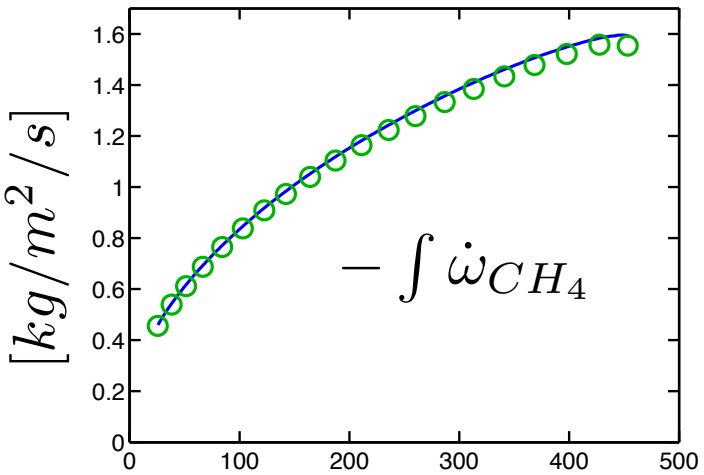


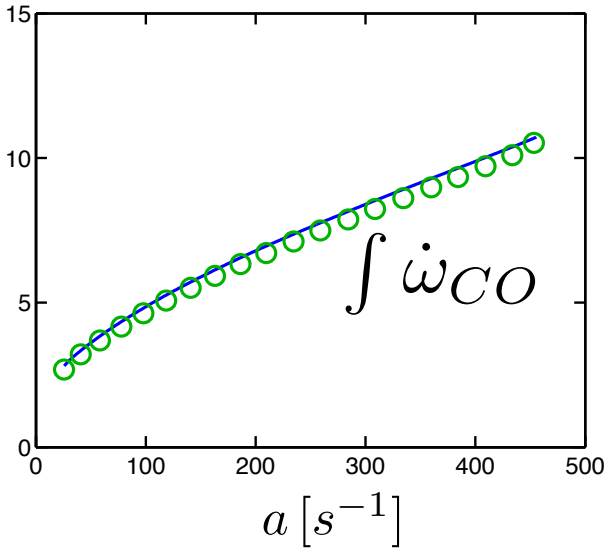
Rich air-fuel mixture
(ϕ=3.2, T=300 K)

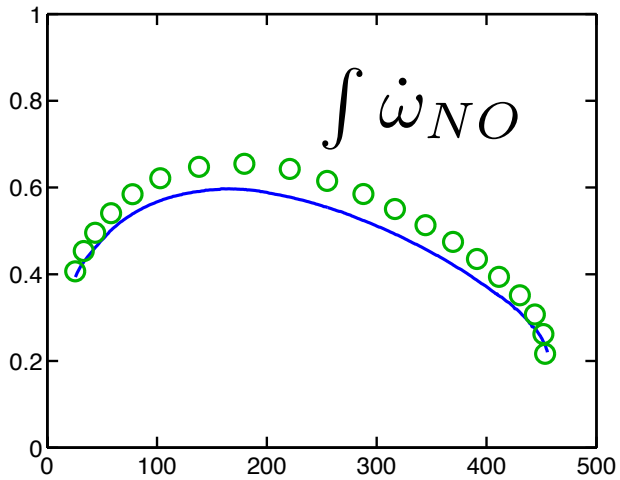
Air
(ϕ=0, T=300 K)

➡ **Response to strain of diffusion flames accurately reproduced by ARC**

— GRI2.11
O ARC_GRI_211







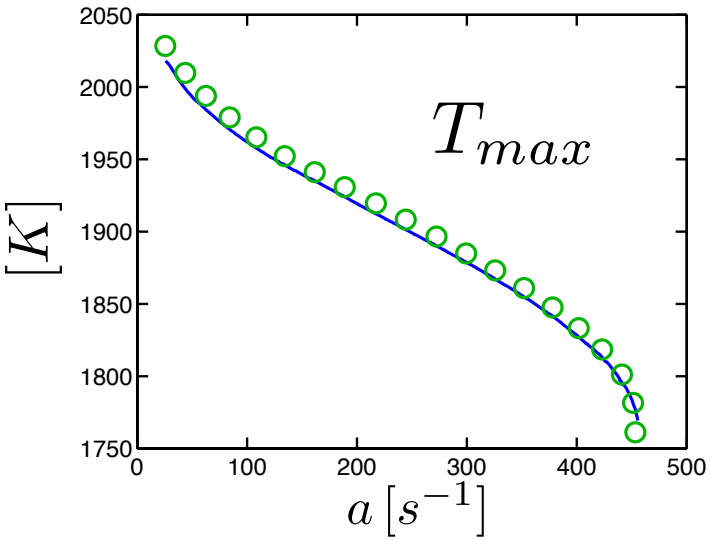
CERFACS

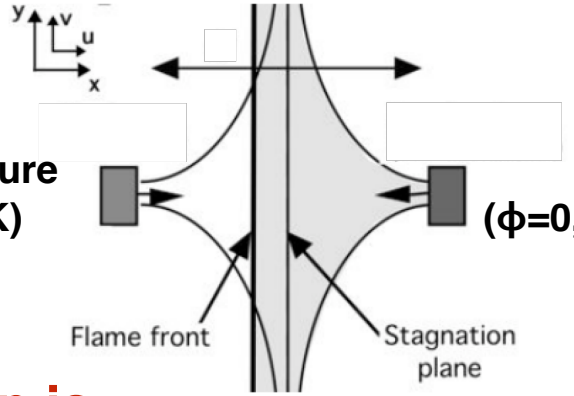
ARC EVALUATION - LAMINAR NON-PREMIXED FLAMES

Sandia Flame D [1]
Non-premixed combustion regime

→

Validation on strained counterflow flames



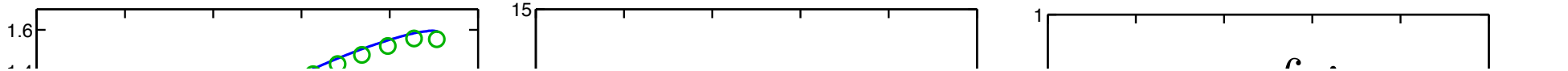


Rich air-fuel mixture
(ϕ=3.2, T=300 K)

Air
(ϕ=0, T=300 K)

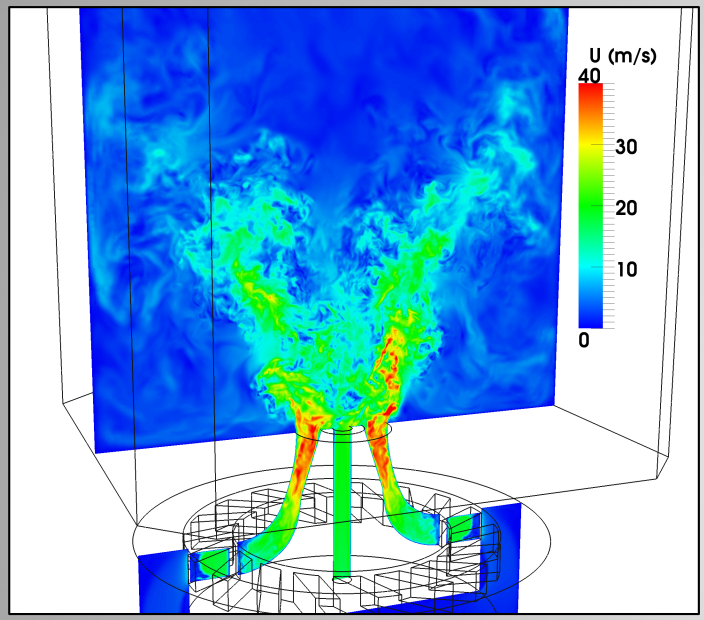
➡ **Response to strain is accurately reproduced by the ARC**

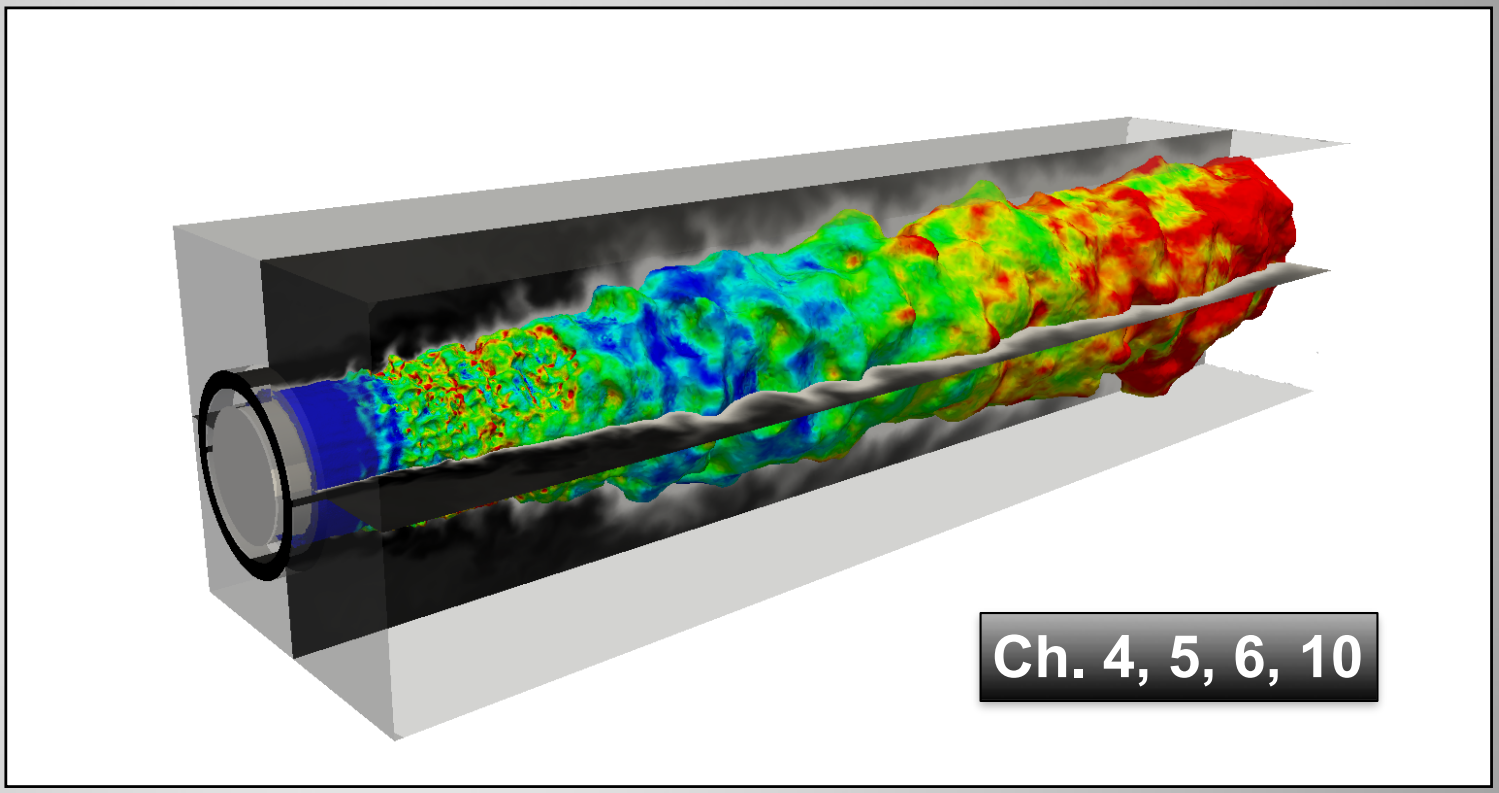
— GRI2.11
O ARC_GRI_211

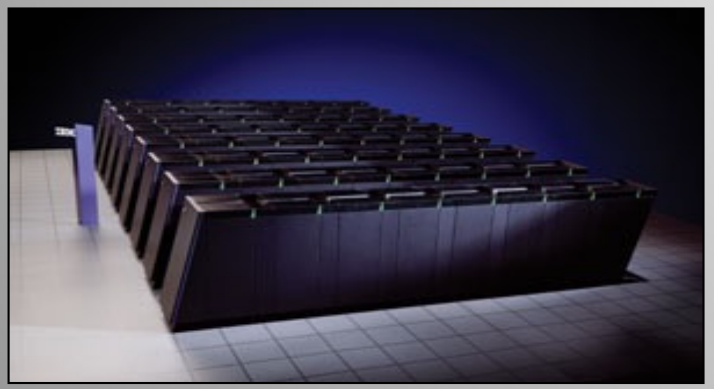


Since the ARC scheme is built on a full scheme, it retains most of its qualities. Once built for a premixed flame at a given (P,T) set, it works for other conditions and for other flames

High Performance Computing







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Combustion instabilities



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CNRS, Université de Toulouse, France



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INSTABILITIES ARE EVERYWHERE IN MECHANICS: MANY SYSTEMS CAN BE IN ‘UNSTABLE‘ EQUILIBRIUM





IN REACTING FLOWS, THIS IS WORSE: THE AVAILABLE POWER IS HUGE

Reacting flows are dominated by mechanisms which exhibit instabilities:

- hydrodynamics --> Kelvin Helmholtz in shear layers.
(C. M. Ho and P. Huerre *JFM* 1984, 16.)

- instabilities at interfaces between liquid fuel and air

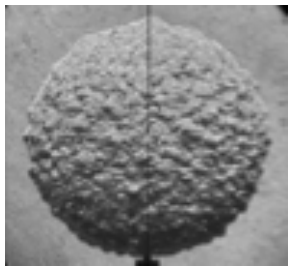
- kinetics: the existence of chemical reactions leads to additional instabilities of flame fronts --> thermodiffusive instabilities in lean H2 flames, formation of cells

- structures: the vibration of the combustor walls can couple with the flames

Ch. 9, 10

Classification of instabilities in combustion (Barrere, Wiliams, Putnam) introduced in the 60s based on the size of the components involved in the instability:

- Intrinsic: modes which are due only to local, short distance interactions between kinetics and flow. Ex: formation of cells (small size, high frequencies)



- Chamber: modes due to the whole flame where vortices, created by the instabilities of the shear layer, couple with the flame front (mid size, mid frequencies)

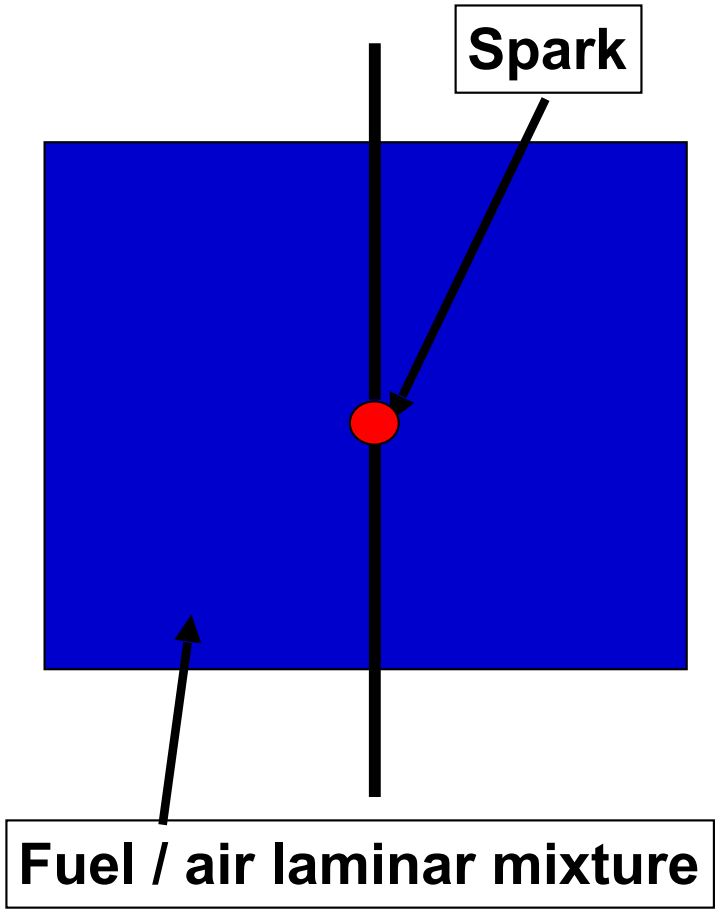


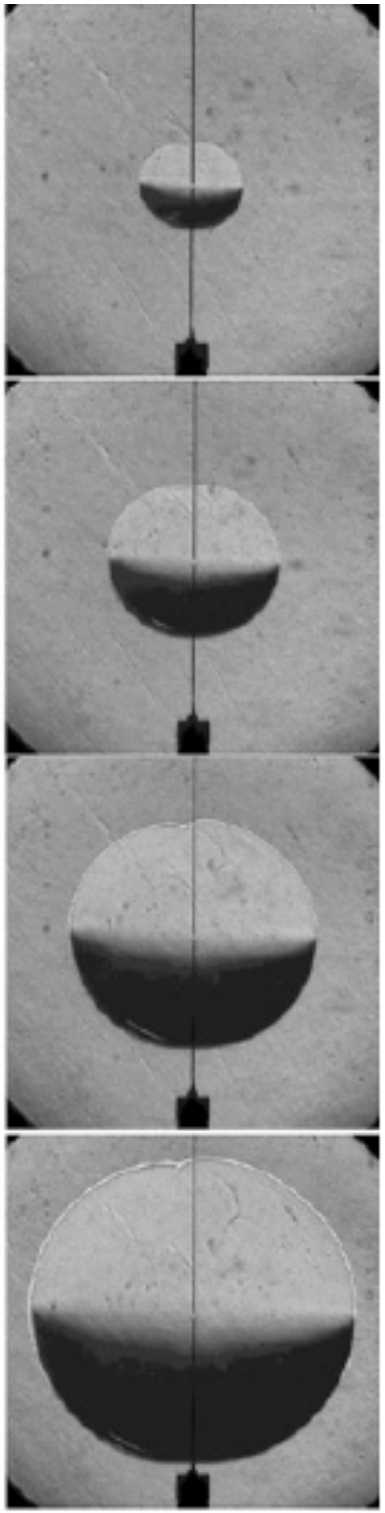
- System: modes where the whole combustor is involved: long wavelengths, low frequency



INTRINSIC INSTABILITY

Growth of a spherical laminar flame ignited by a spark.

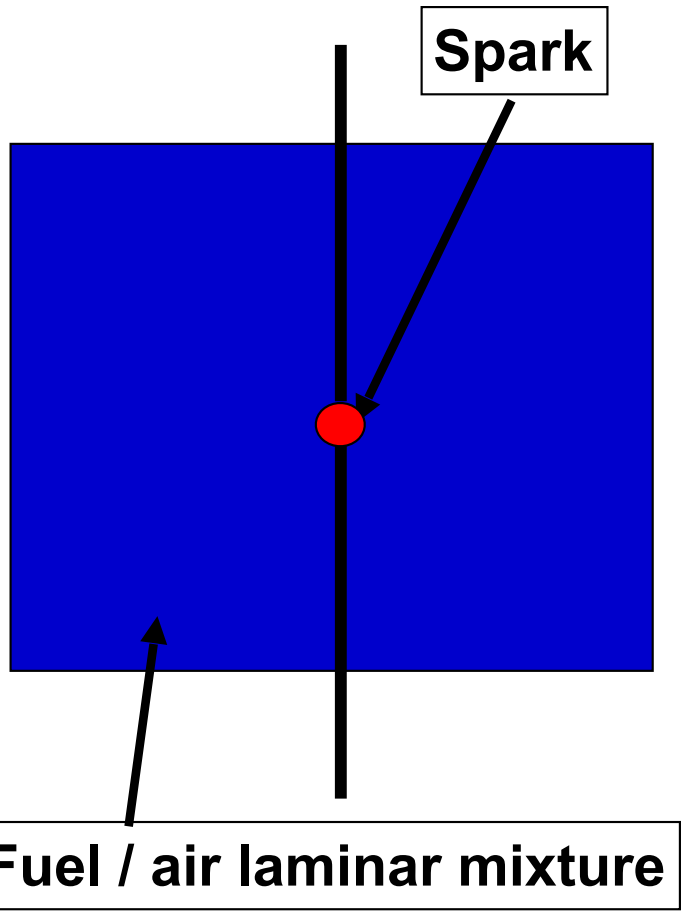


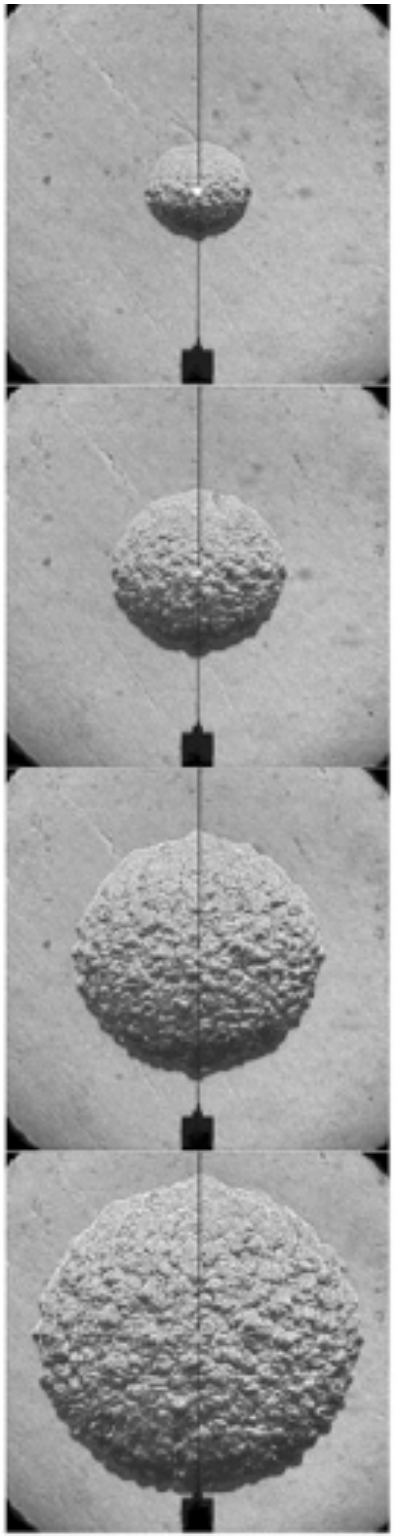


PROPANE / AIR: Perfectly smooth laminar spherical front

Time

Law et al 30th Symp. (Int.) on Comb.

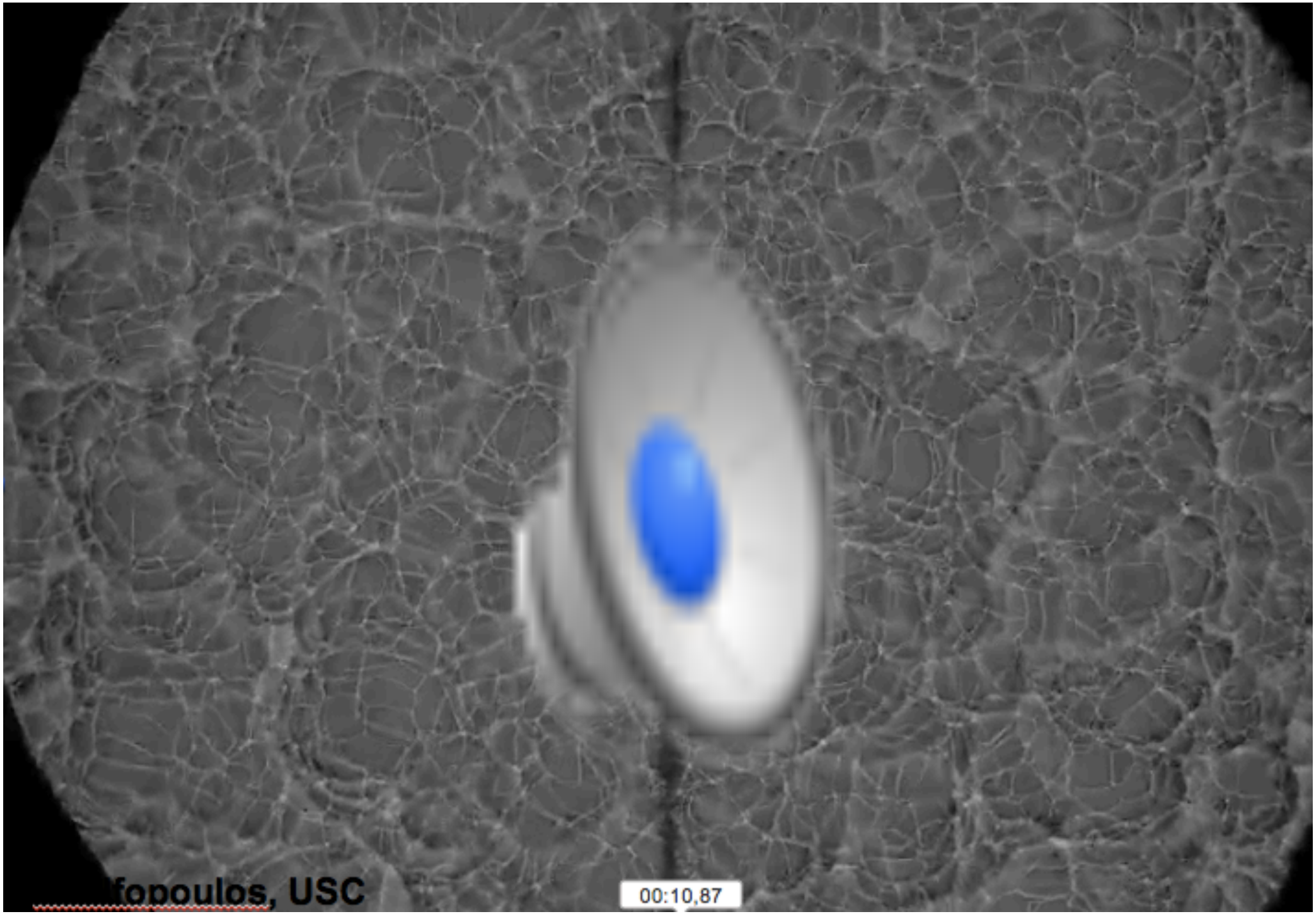




HYDROGEN / AIR: Formation of cells on the flame front

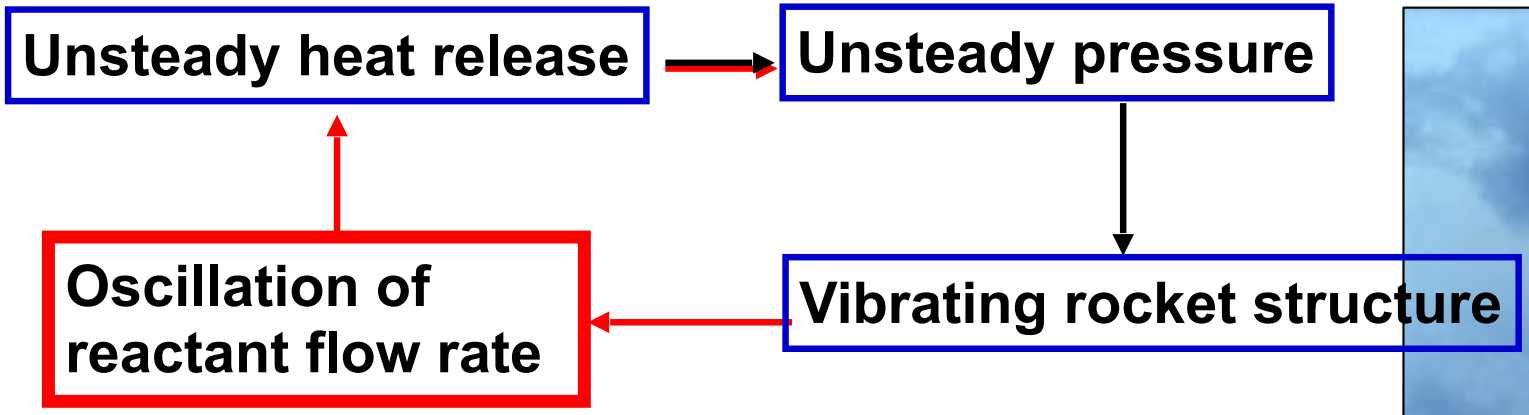
Time

Law et al 30th Symp. (Int.) on Comb.



Pr Egolfopoulos, USC

EXAMPLE OF SYSTEM INSTABILITY: THE POGO EFFECT

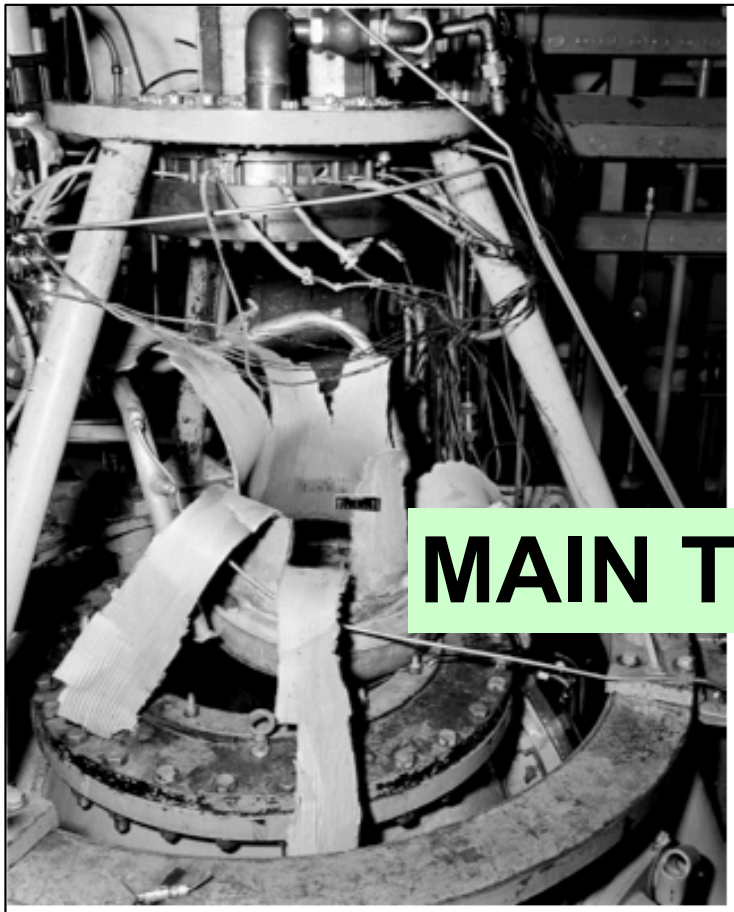


Saturn V fist stage
Soviet Union's N1-L3 rocket

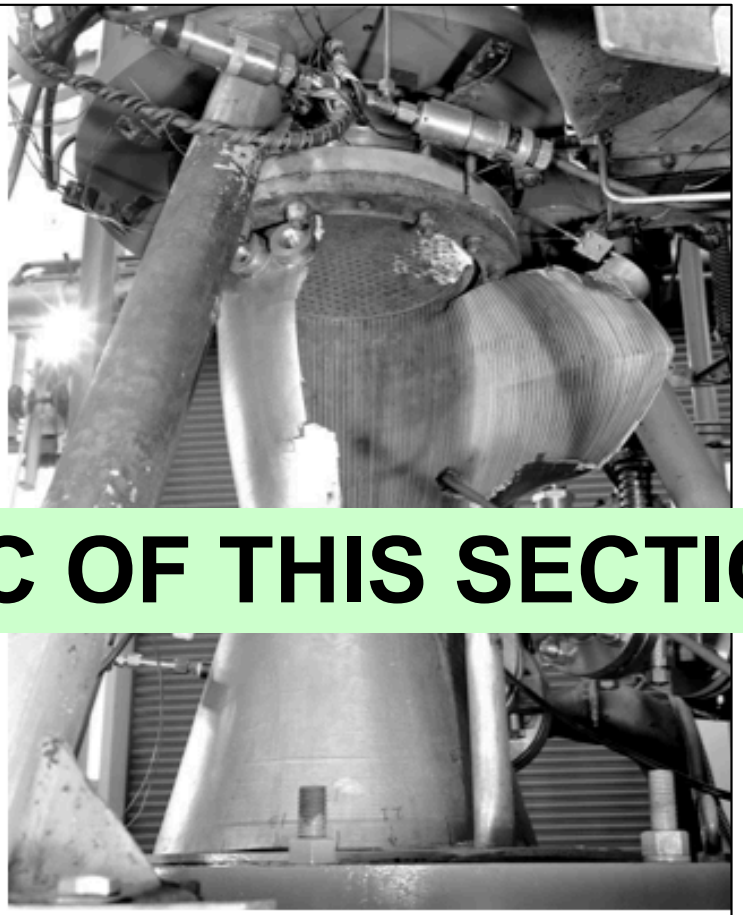


A specific class of chamber instabilities: « thermoacoustics »

In combustion chambers, acoustics and combustion can couple, leading to dramatic consequences....



Liquid rocket engine (NASA 1957)



Liquid rocket engine (NASA 1963)

MAIN TOPIC OF THIS SECTION

Mechanisms:

The interaction betweeen flame and noise is totally different for free and for confined flames.

FREE

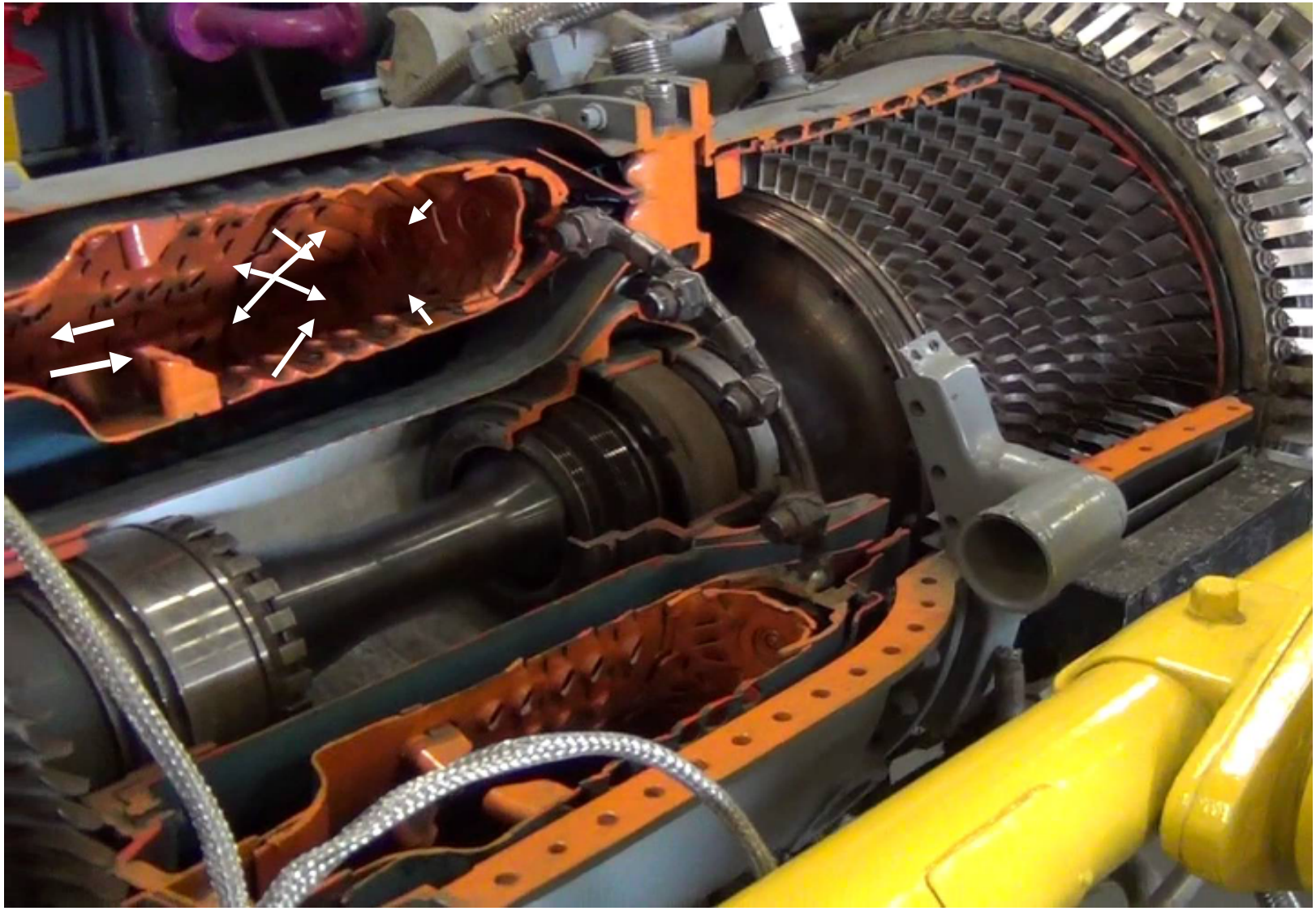
FLAME:



- **Sound propagates away from the flame and never reflects on anything: this is only a ‘far-field’ aeroacoustic problem**

CONFINED

FLAME:

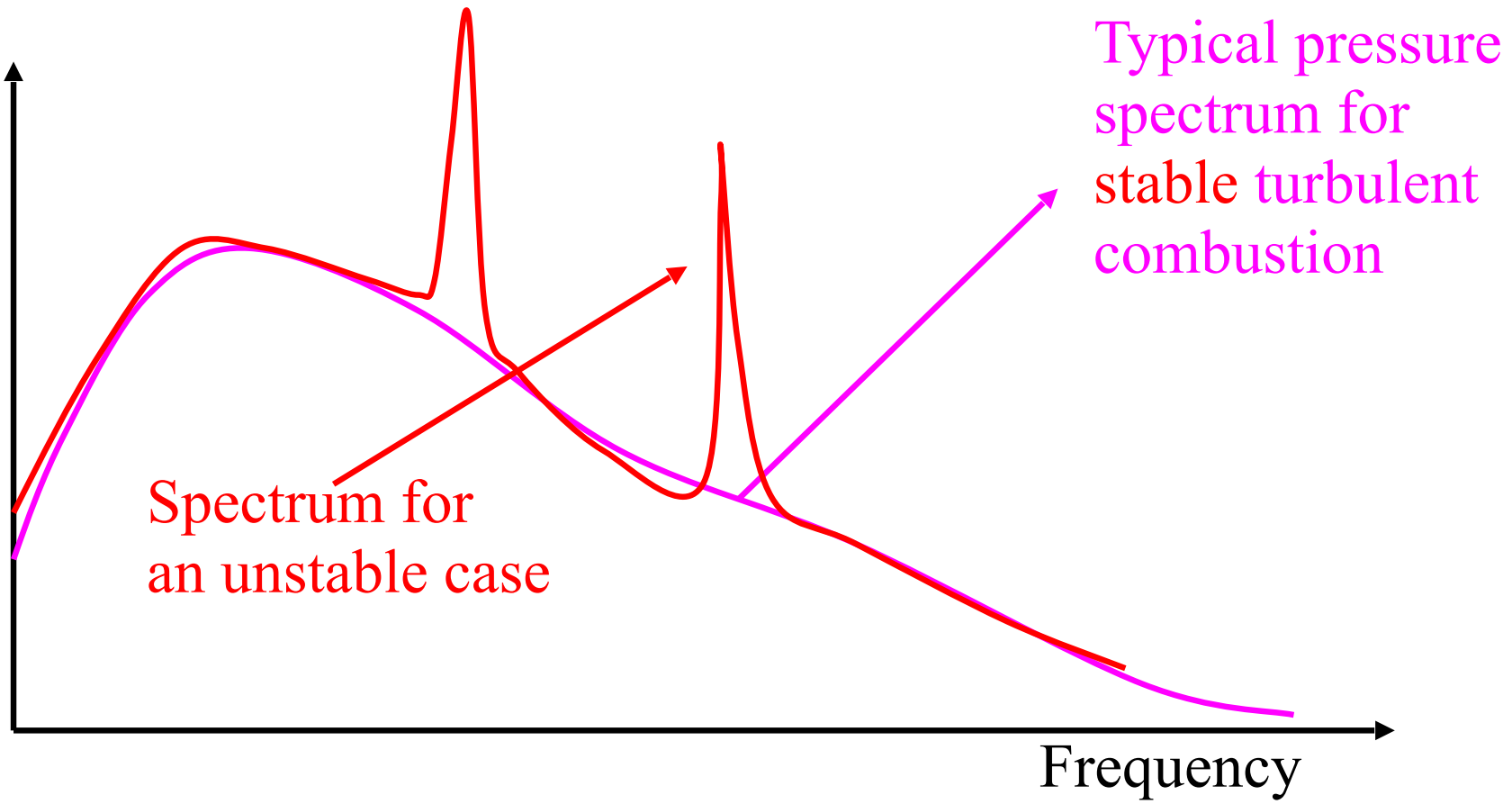


- **Sound propagates away from the flame, reflects on walls, and may come back to the chamber**

Are these acoustic waves a problem ?

- generally no. The flow remains stable. Acoustic waves induce noise and that is all ==> combustion noise

- but in certain cases, yes ! The flow becomes unstable ==> the engine explodes or cannot be operated at all !



Simple scalings:

The velocity induced by acoustic wave u_a is linked to the pressure oscillation level p_a by:

$$u_a = \frac{1}{\rho c} p_a$$

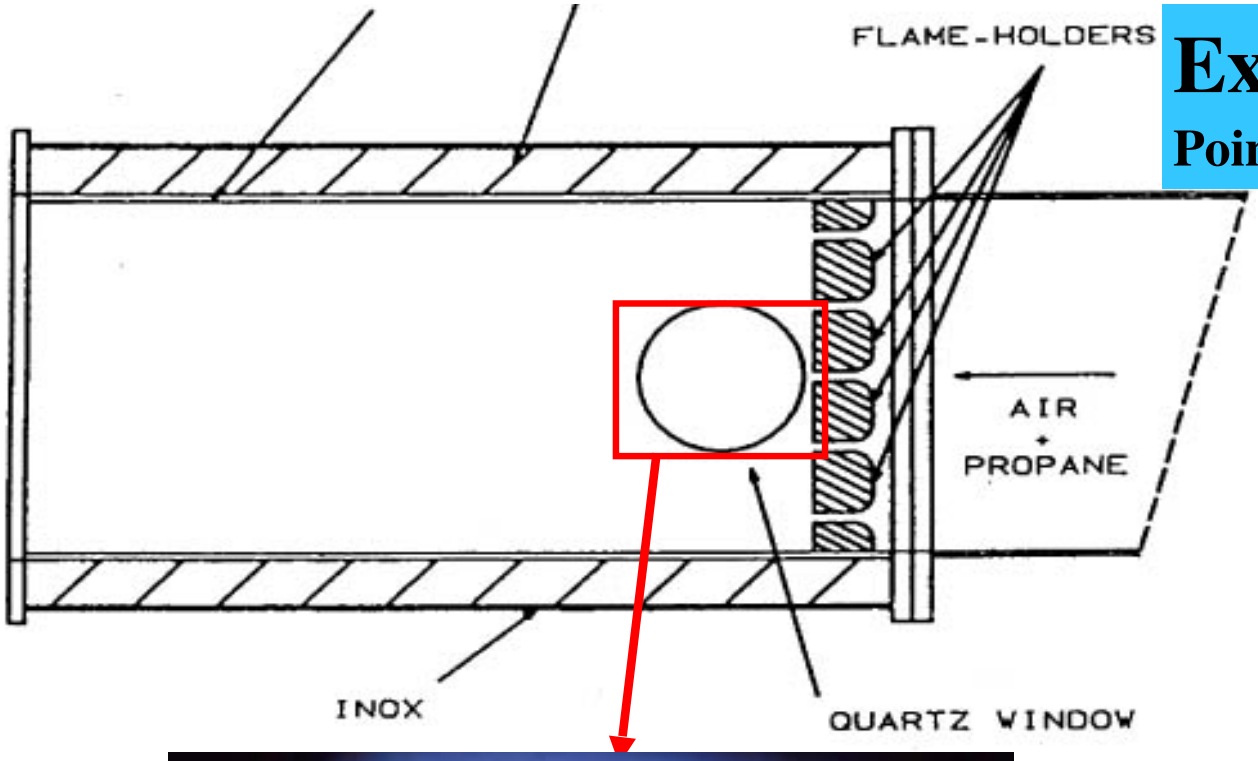
When combustion instabilities begin, typical levels of pressure oscillations are 1000 to 20000 Pa for burners operating at one atmosphere (200 dB… with dB = 20 log {p'/2 10-5})):
since ρc is of the order of 400 uSI, u_a varies between 2 and 20 m/s.

These velocities are larger than 'turbulent' velocities. Their wavelength is also larger (typically the size of the burner). The effect of acoustic waves can be huge: for example, large enough to cause total flashback or quenching in the burner.

Turbulent combustion OR acoustic combustion ?

Example 1 (experiment)

Poinsot et al *J. Fluid Mech.* 1987



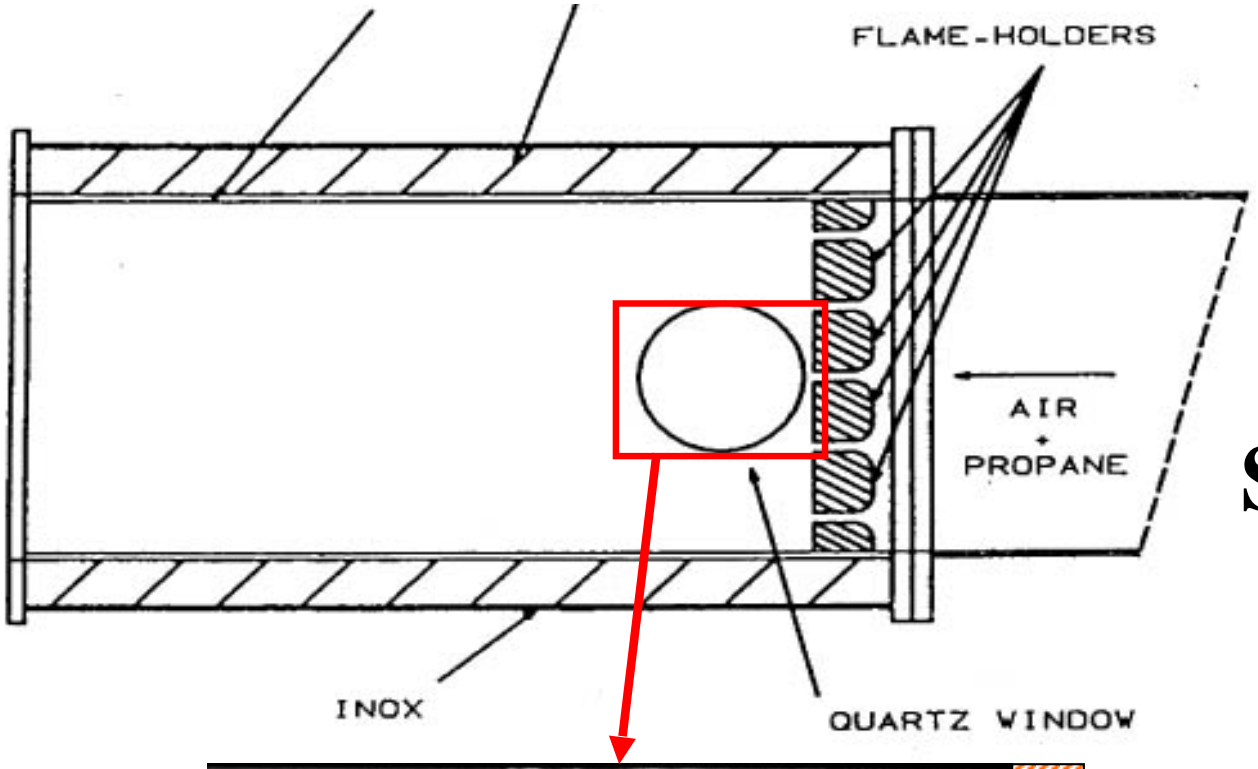


Direct view

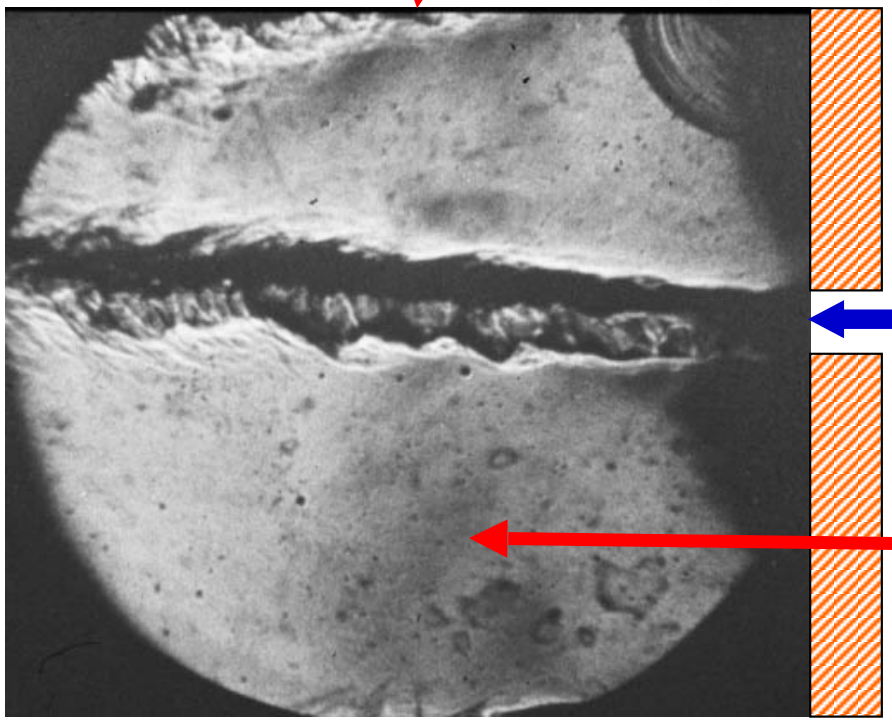
STABLE REGIME

Fresh premixed gas

Hot recirculating gases



STABLE REGIME



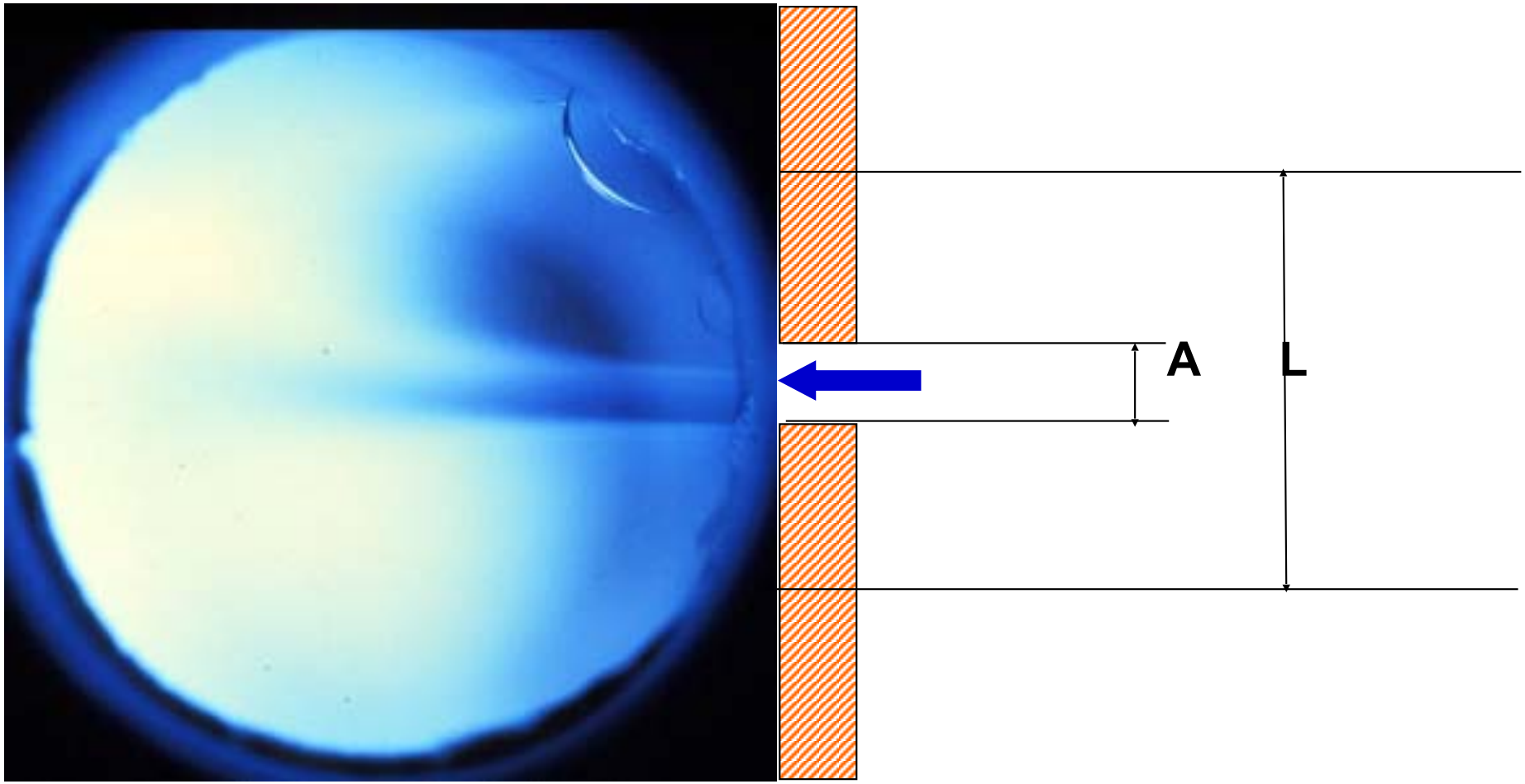
Fresh premixed gas

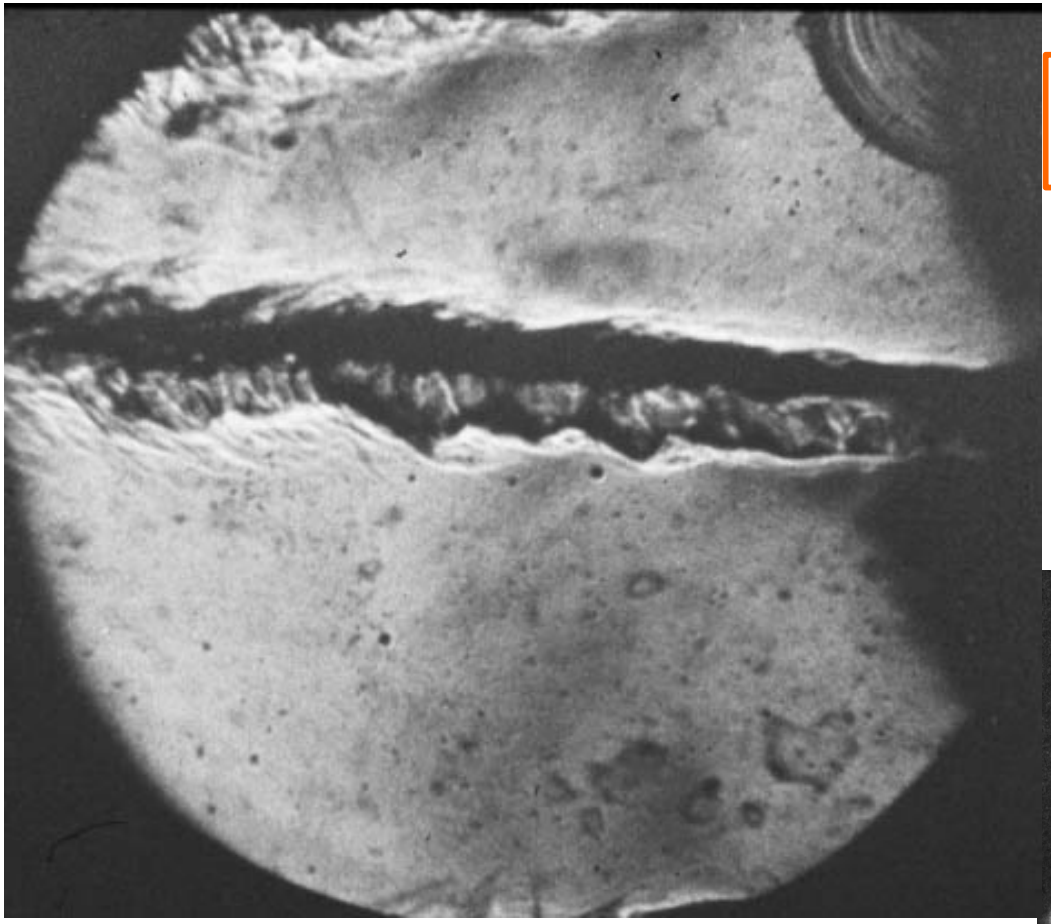
Hot recirculating gases

Schlieren visualization

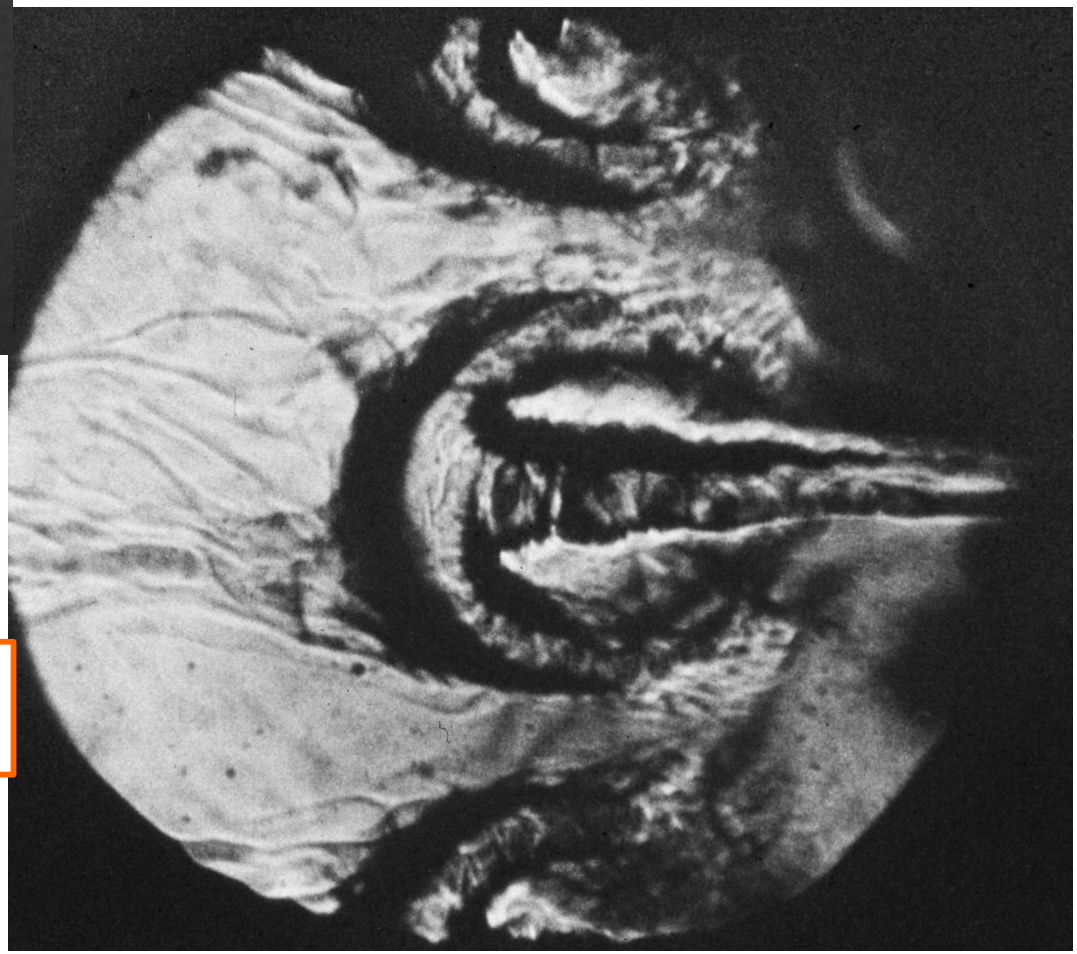
If equivalence ratio is changed by 3 percent:

- **unstable regime at 530 Hz**
- **very high noise levels**
- **walls become red...**
- **limited lifetime of chamber (15 minutes)**

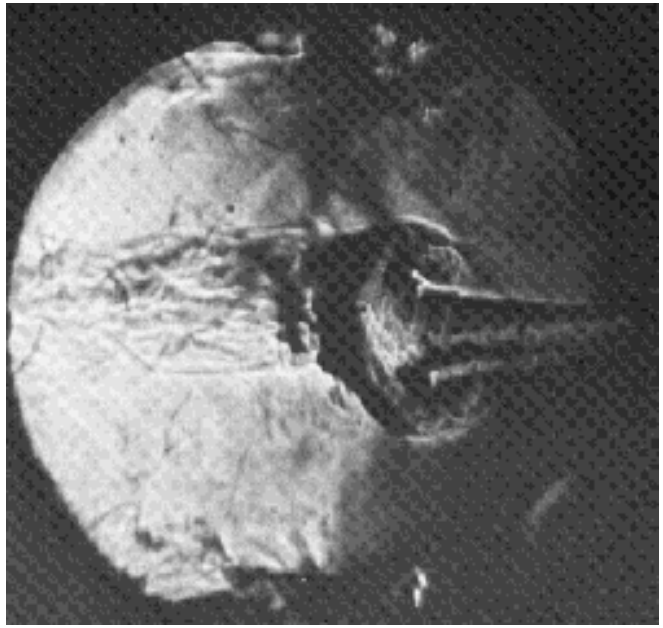
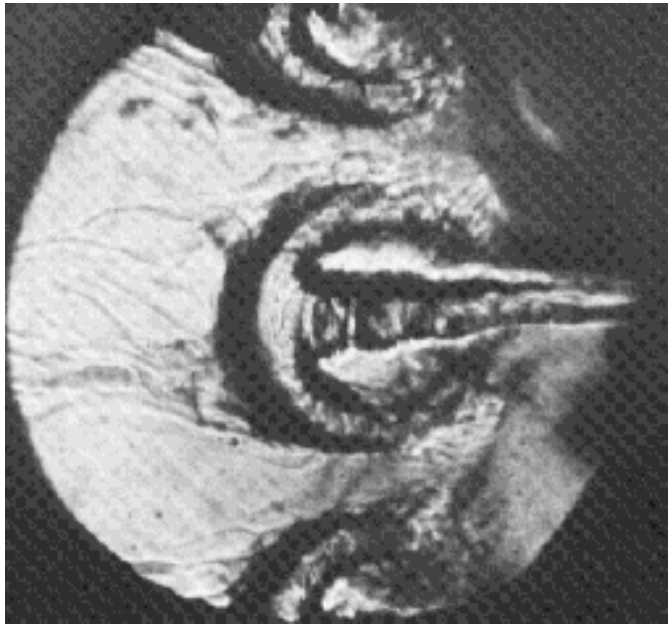


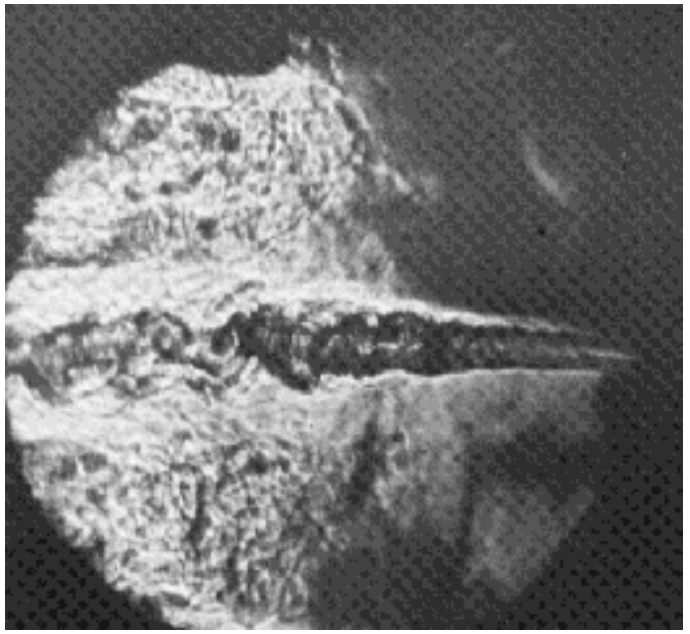


STABLE



UNSTABLE

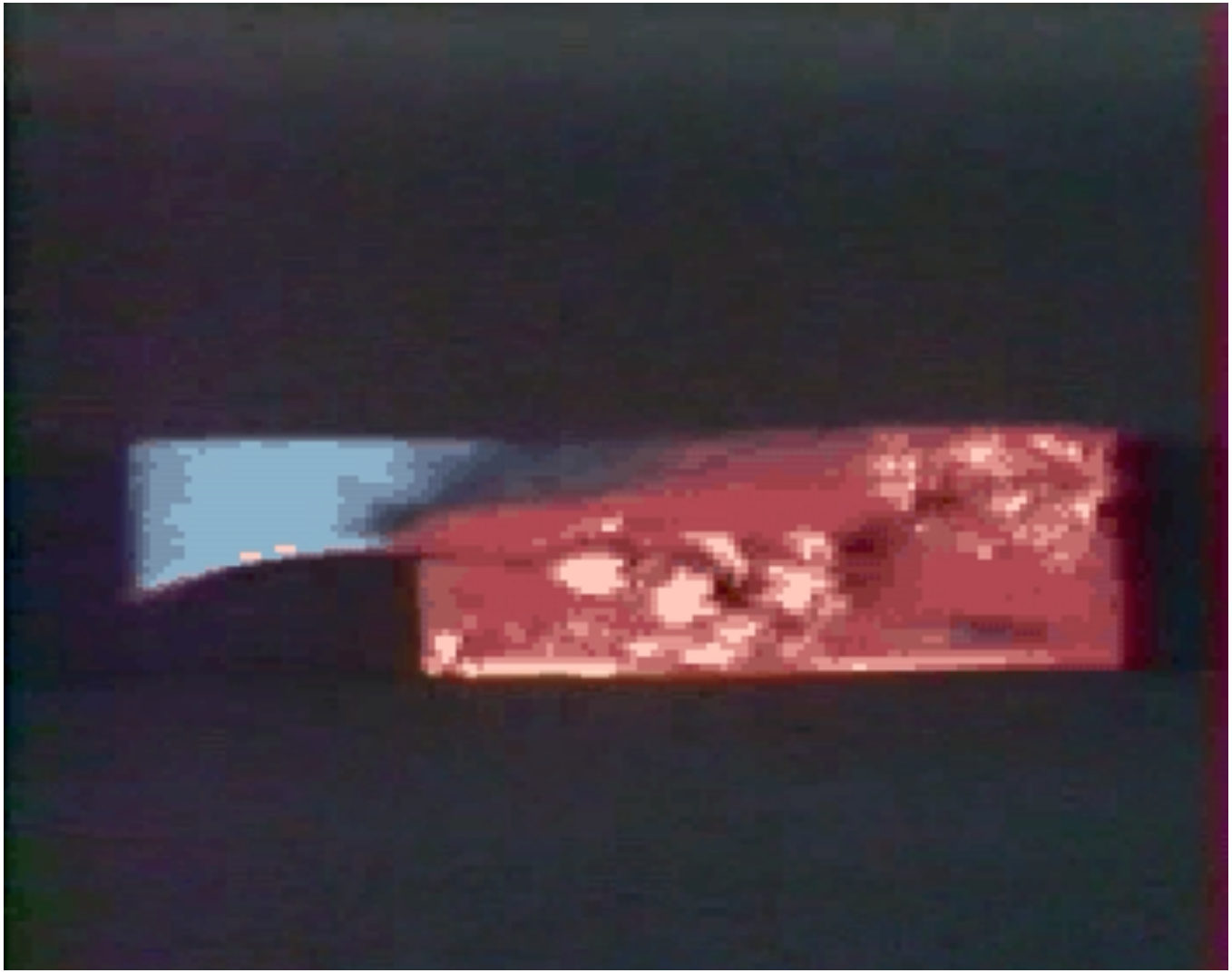


Four snapshots of the 530 Hz cycle (self excited mode)
The 530 Hz is an acoustic mode of the combustor

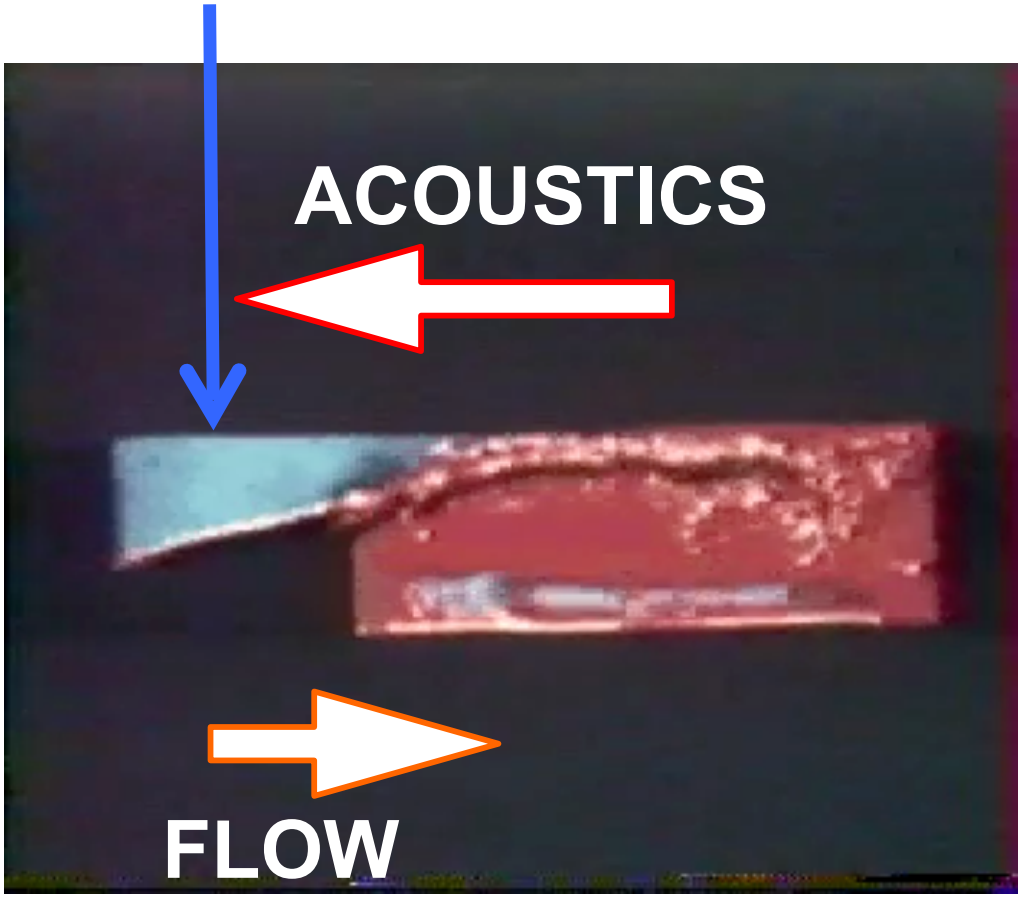
Example 2 (experiment)

The Berkeley step…

The previous example had a strong blockage
For smaller blockage, flashback threatens:



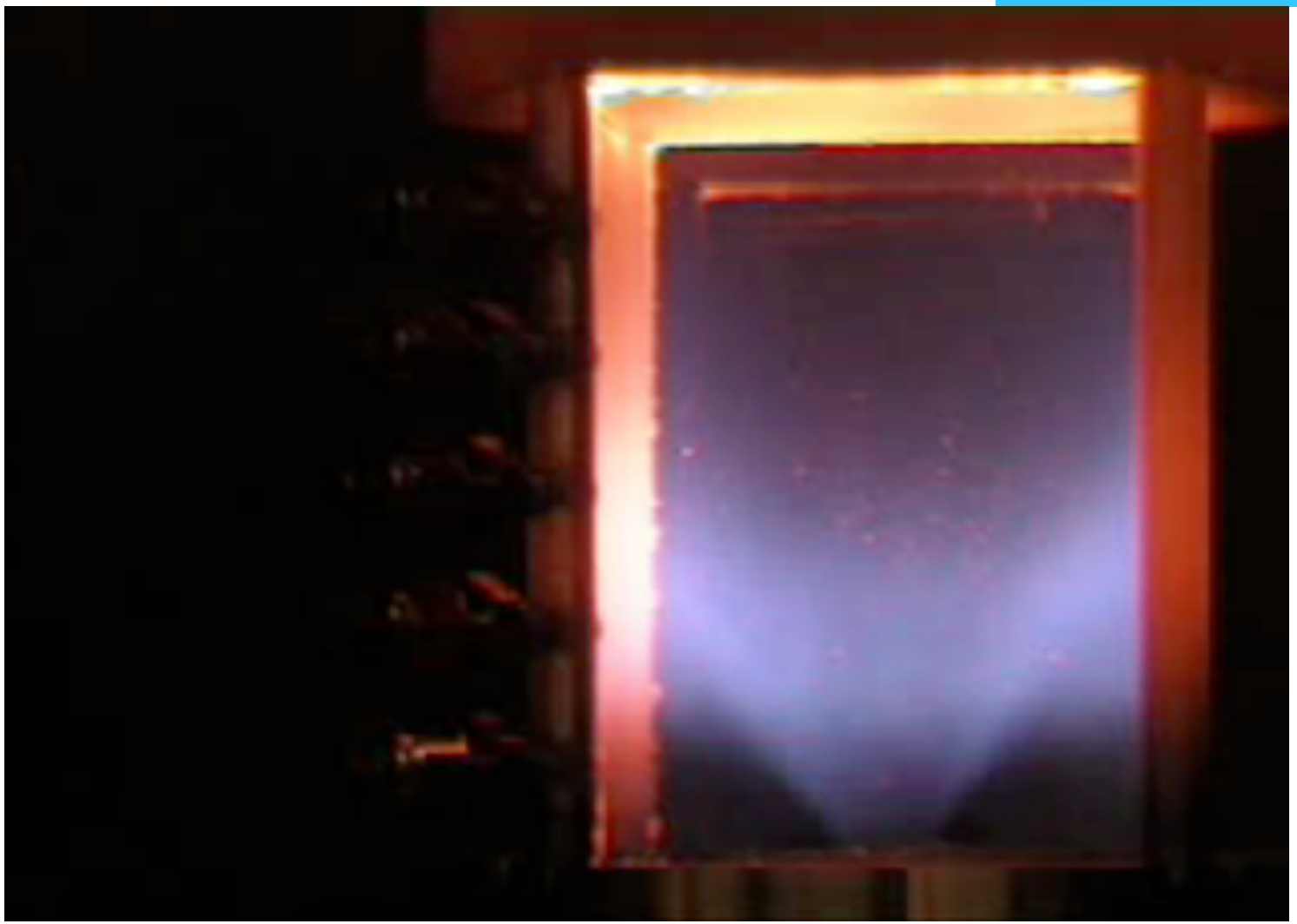
The acoustic velocity here is larger than the mean inlet velocity: the flow is going upstream !



So: yes,indeed, we need to care about acoustics !

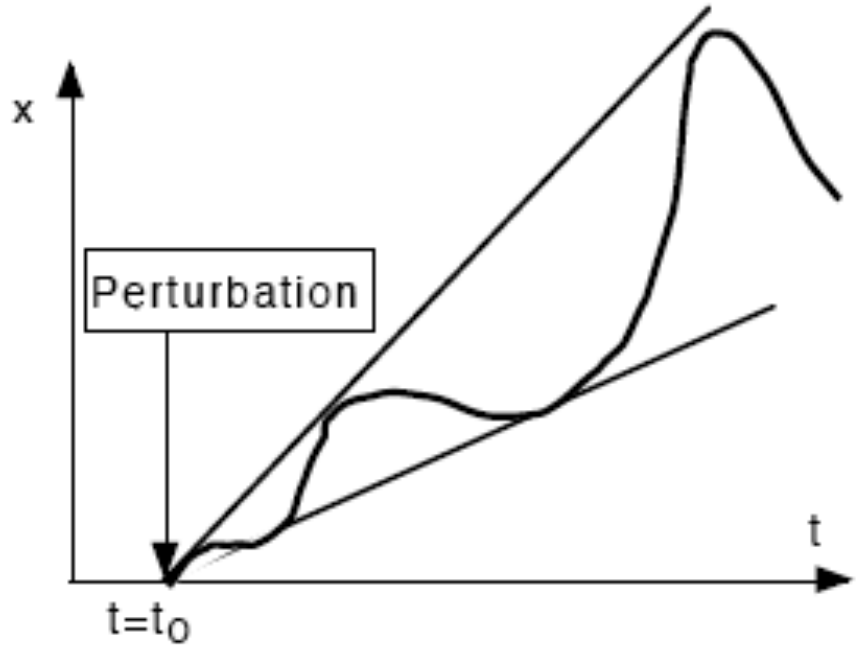
Example 3 (experiment)

What you see if you are in the room:

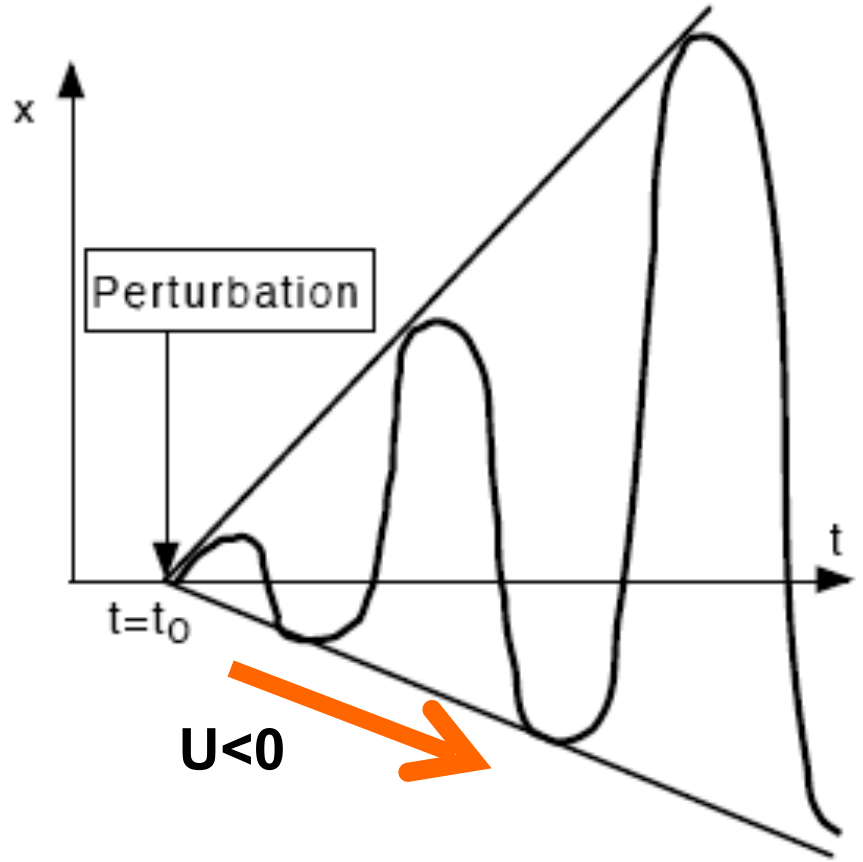


A DLR chamber with multiple modes. Note the natural bifurcations: the flow regime is unchanged but the chamber mode changes

The two main classes of instabilities in flows (Monkewitz, Huerre):



CONVECTIVE (*AMPLIFIER*)

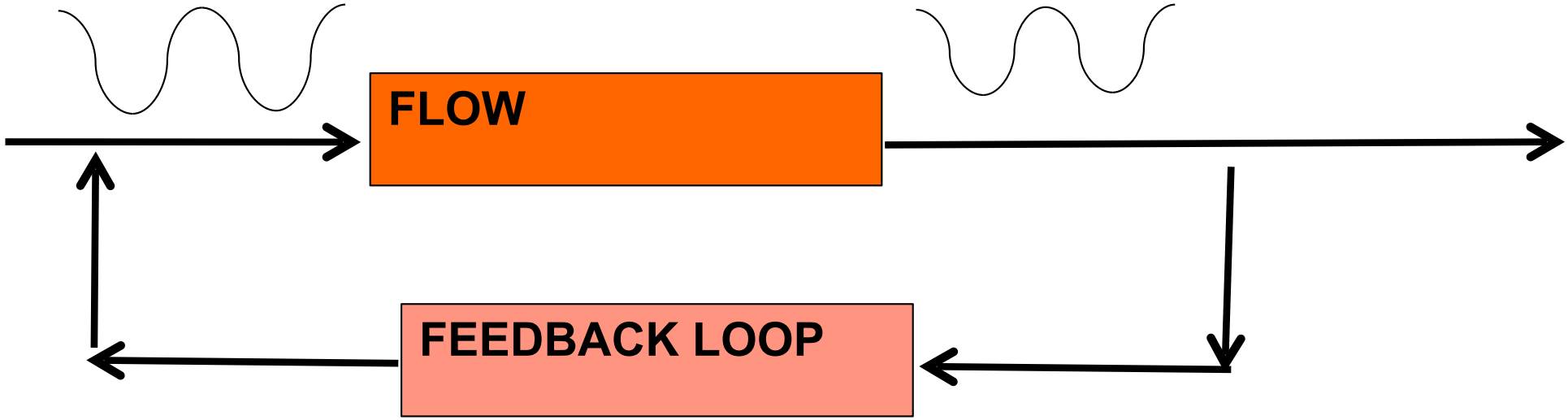


ABSOLUTE (*RESONATORS*)

Absolute instabilities usually are linked to 'information' propagating upstream

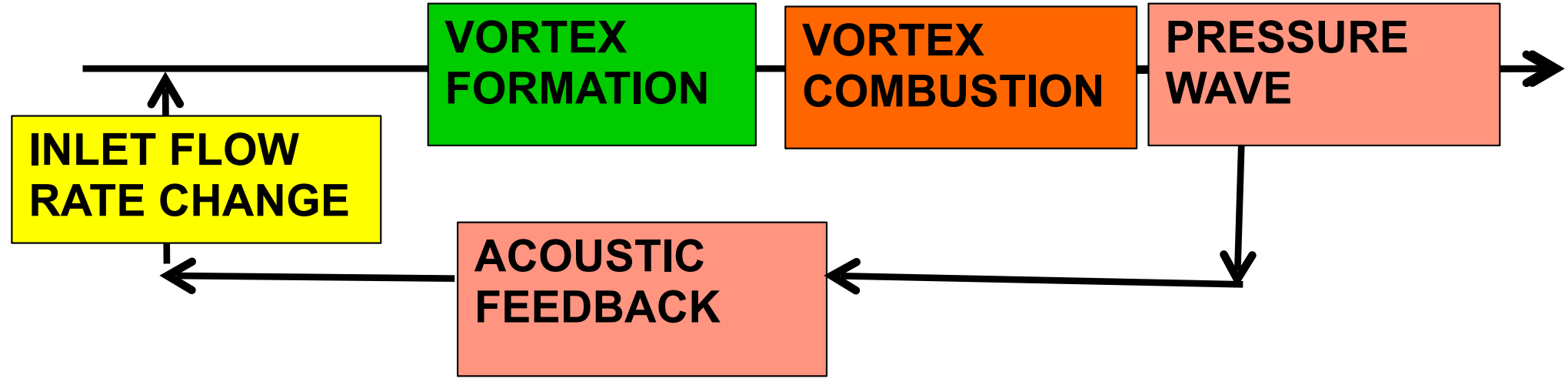


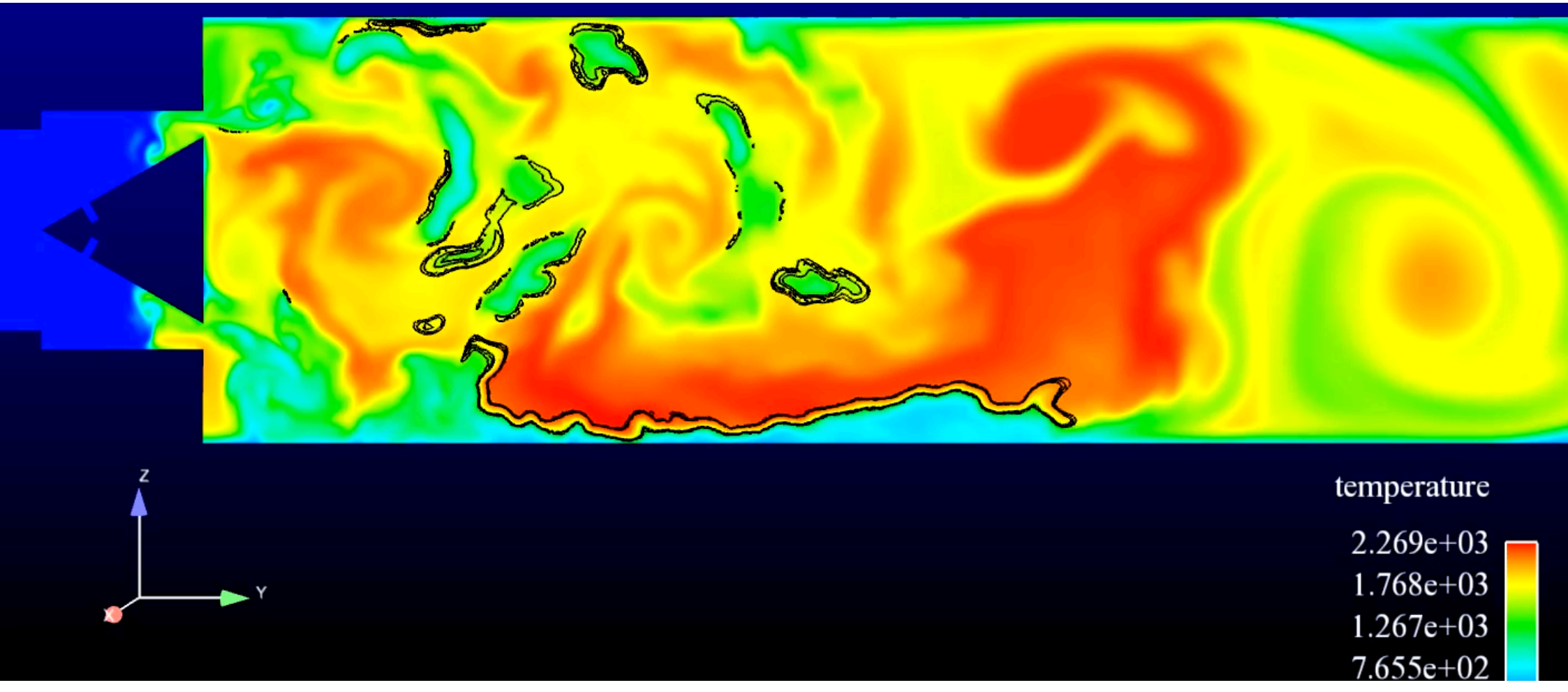
Convective instability (amplifier)



Absolute instability (resonator)

Ch. 8 Sec. 8.5.2

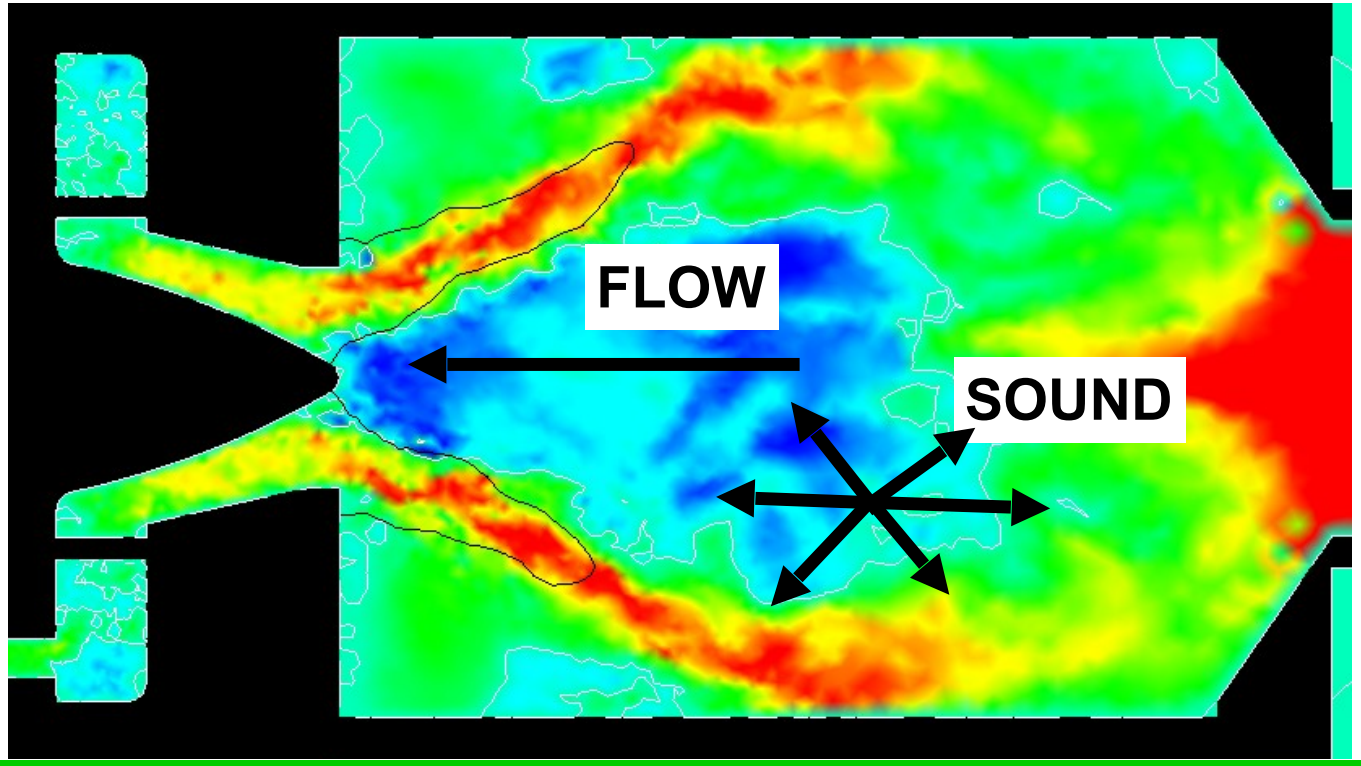

VORTEX FORMATION
VORTEX COMBUSTION
PRESSURE WAVE
INLET FLOW RATE CHANGE
ACOUSTIC FEEDBACK


Z
Y
temperature
2.269e+03
1.768e+03
1.267e+03
7.655e+02

In combustion chambers, we find:

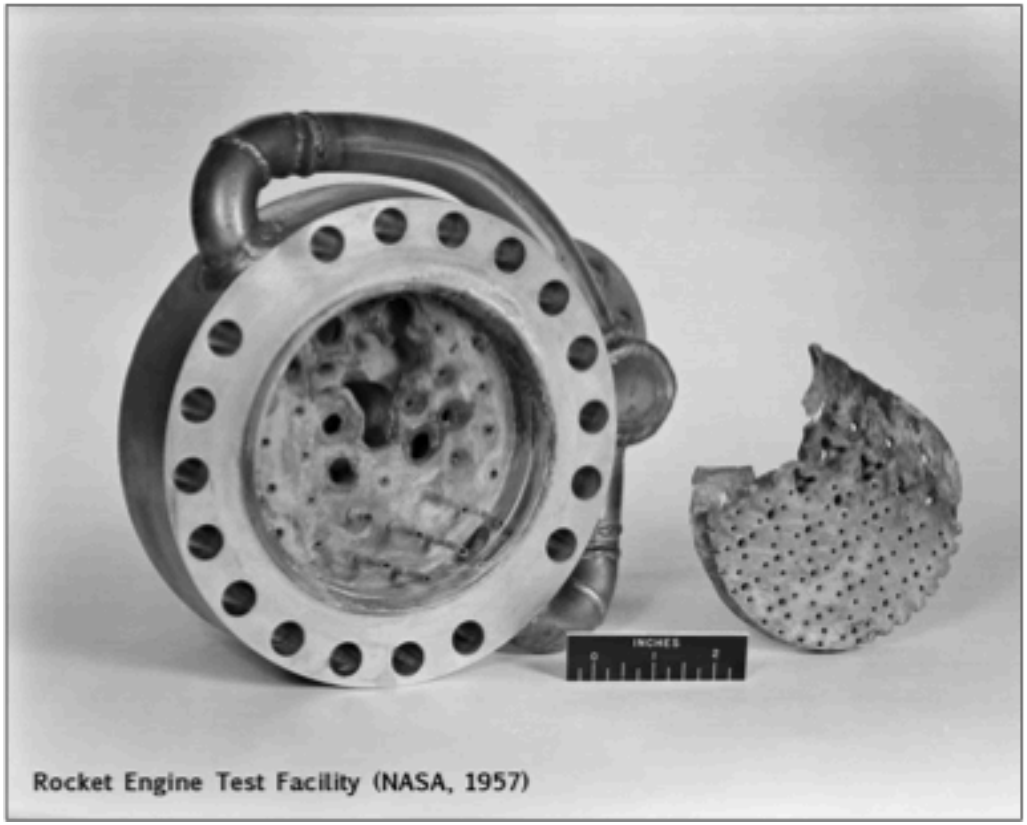
- **Acoustics because the flames are confined**
- **Recirculation zones**

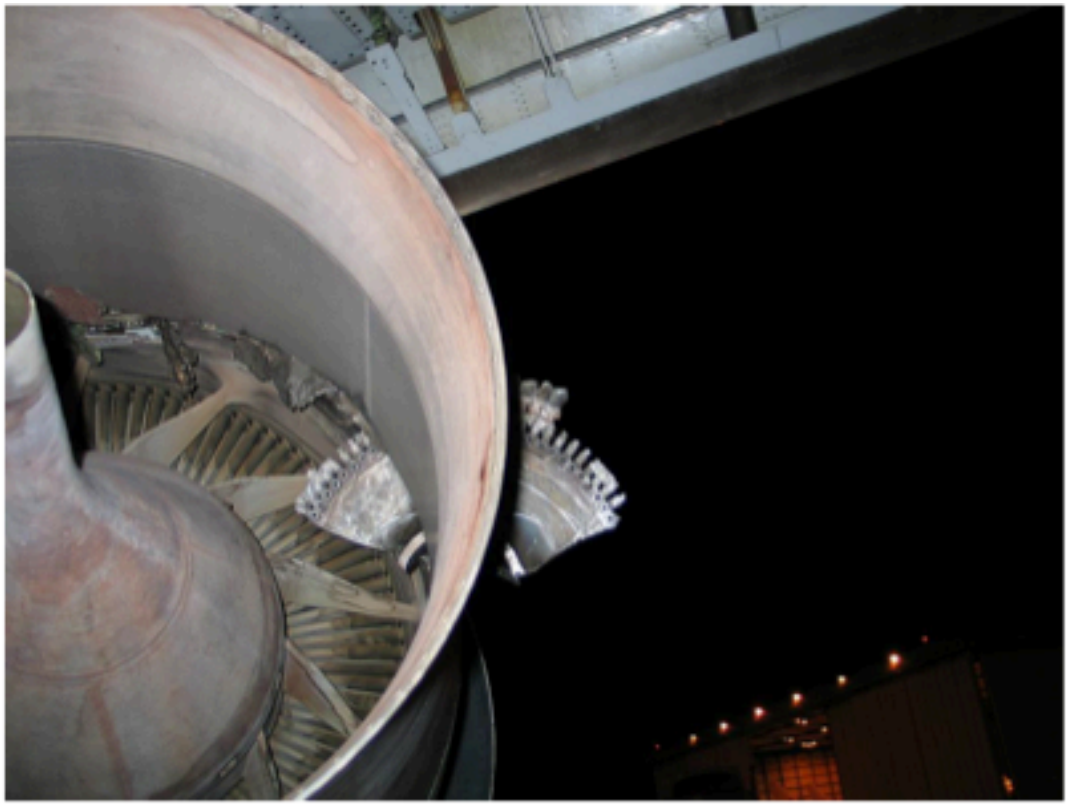
==> information can propagate upstream by convection or by acoustic waves



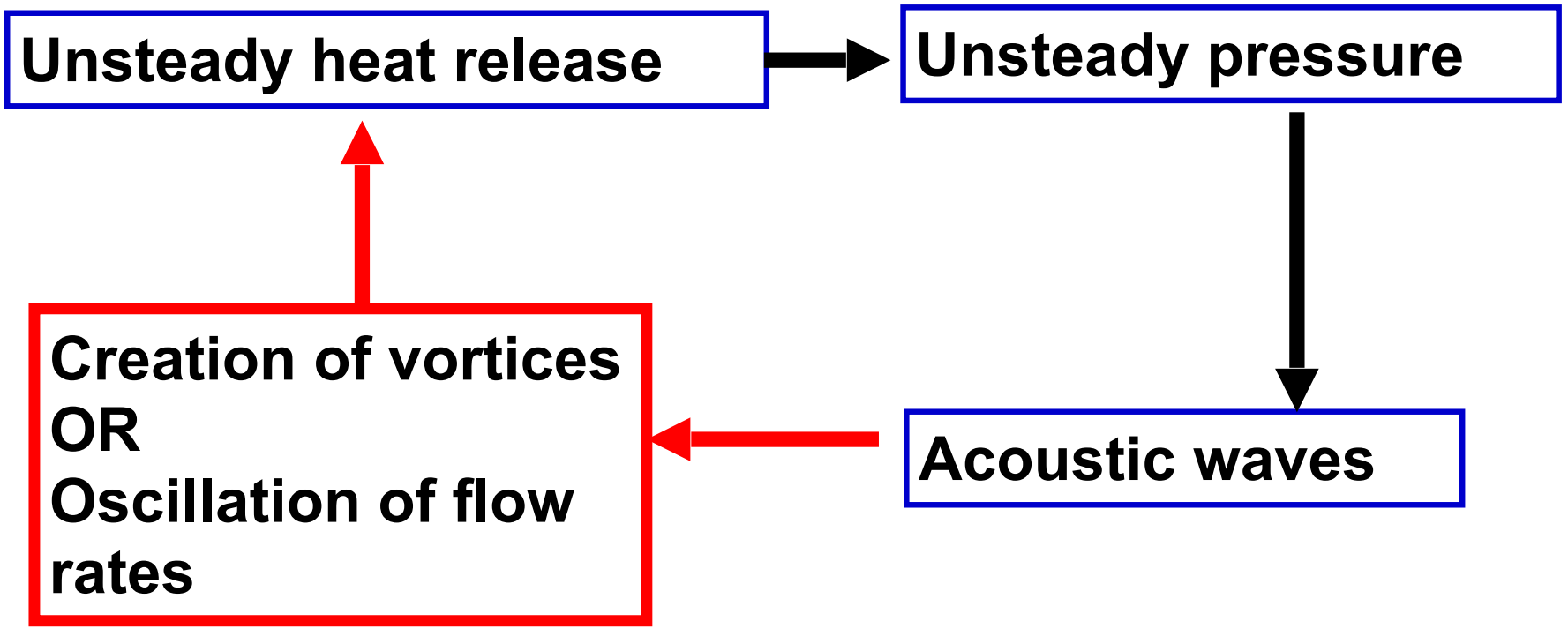
ABSOLUTE INSTABILITIES ARE EXPECTED !

Concentrate on confined flames in combustion chambers surrounded by walls:
‘Thermoacoustics’ (coupled instabilities between acoustics and combustion) become possible -> these absolute instabilities are the most dangerous





Not a new problem: Thermoacoustics are known since Lord Rayleigh *Nature* 1878.



Why acoustics and flame can couple:

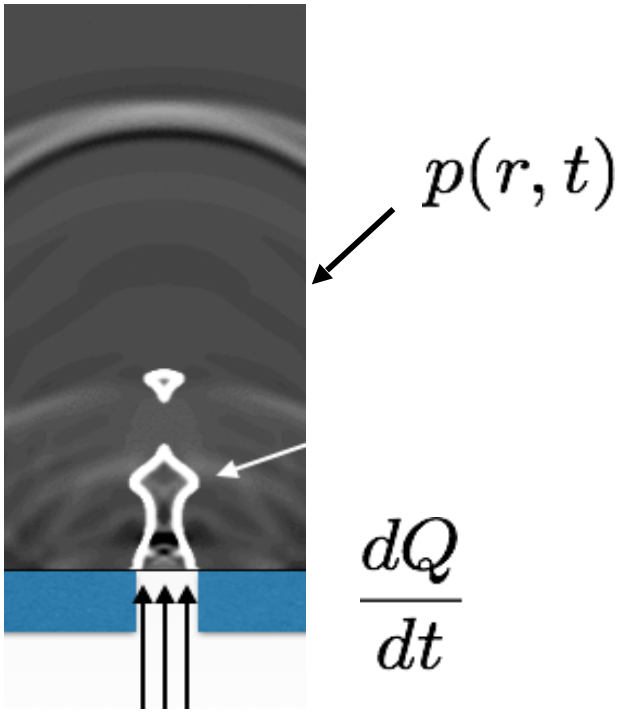
1/ Flames make noise...

➡ Unsteady flames create acoustic waves: unsteady heat release acts like an acoustic monopole

$$p(r,t) = \frac{\rho_\infty}{4\pi r}\left(\frac{\rho_u}{\rho_b} - 1\right)\left[\frac{dQ}{dt}\right]_{t-\tau}$$

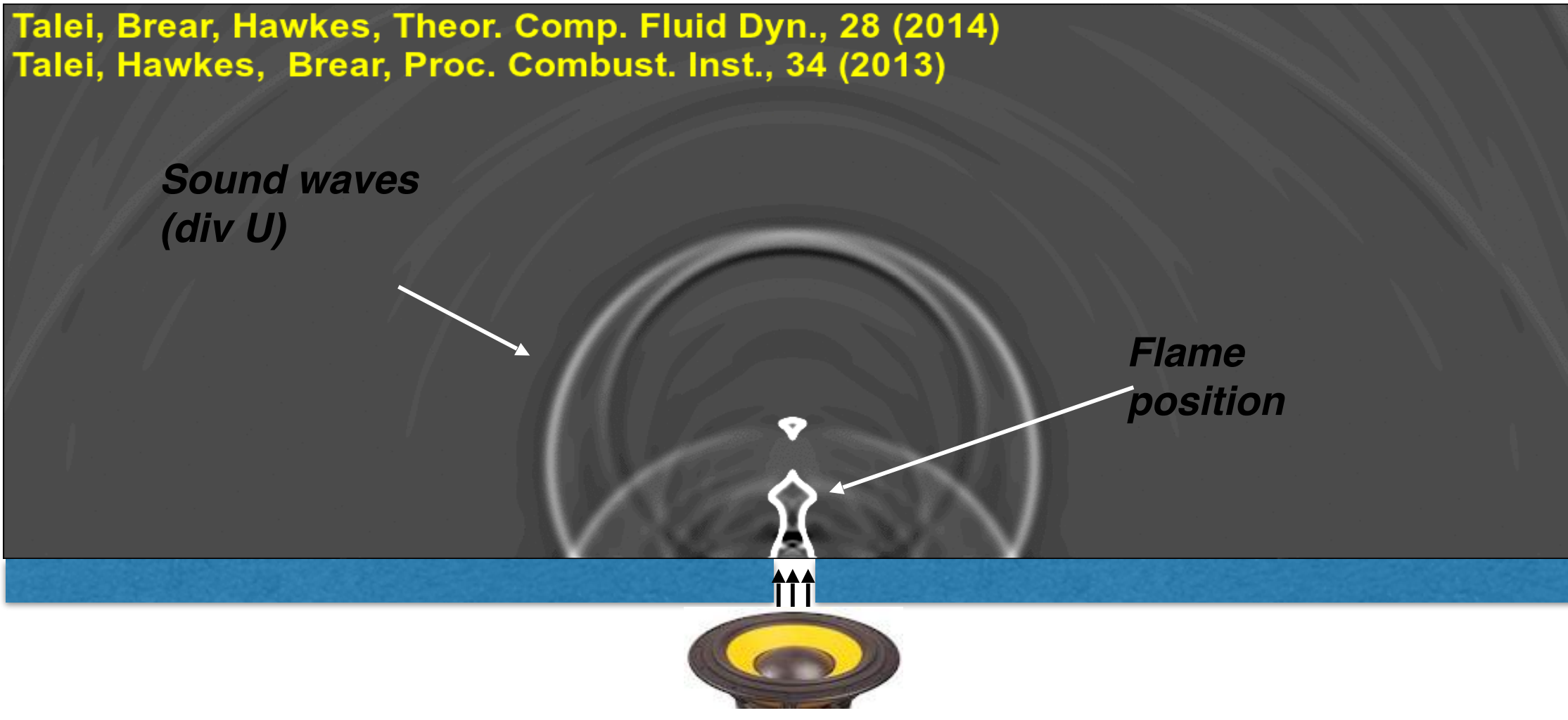
Far field unsteady pressure

Unsteady heat release



Price et al, 12th Symp. (Int.) Comb. 1969
Schuller et al, Comb. Flame 128, 2002

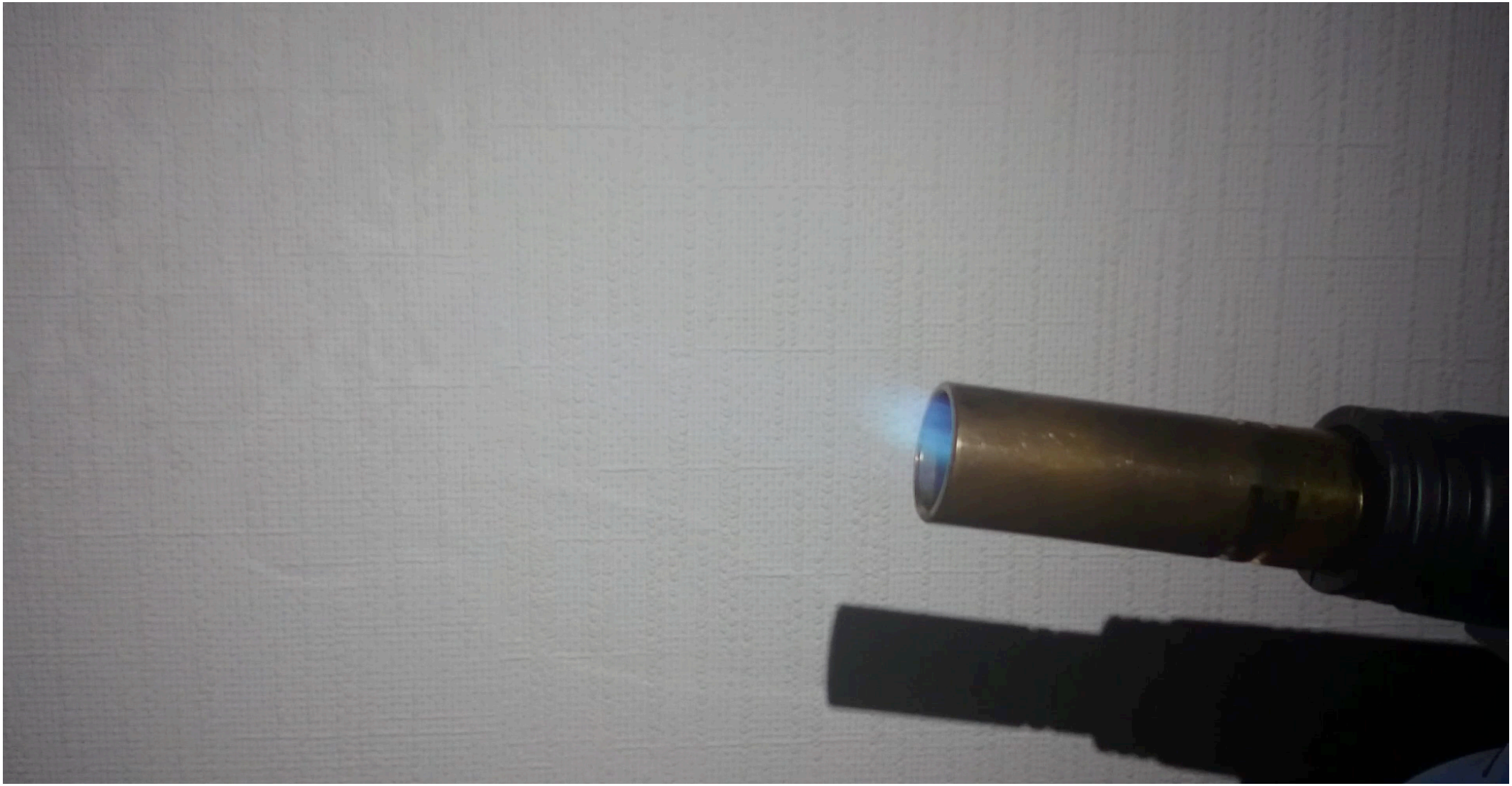
Visualization of sound waves created by a premixed pulsated laminar V flame:



JET NOISE WITH NO FLAME



JET NOISE WITH FLAME:





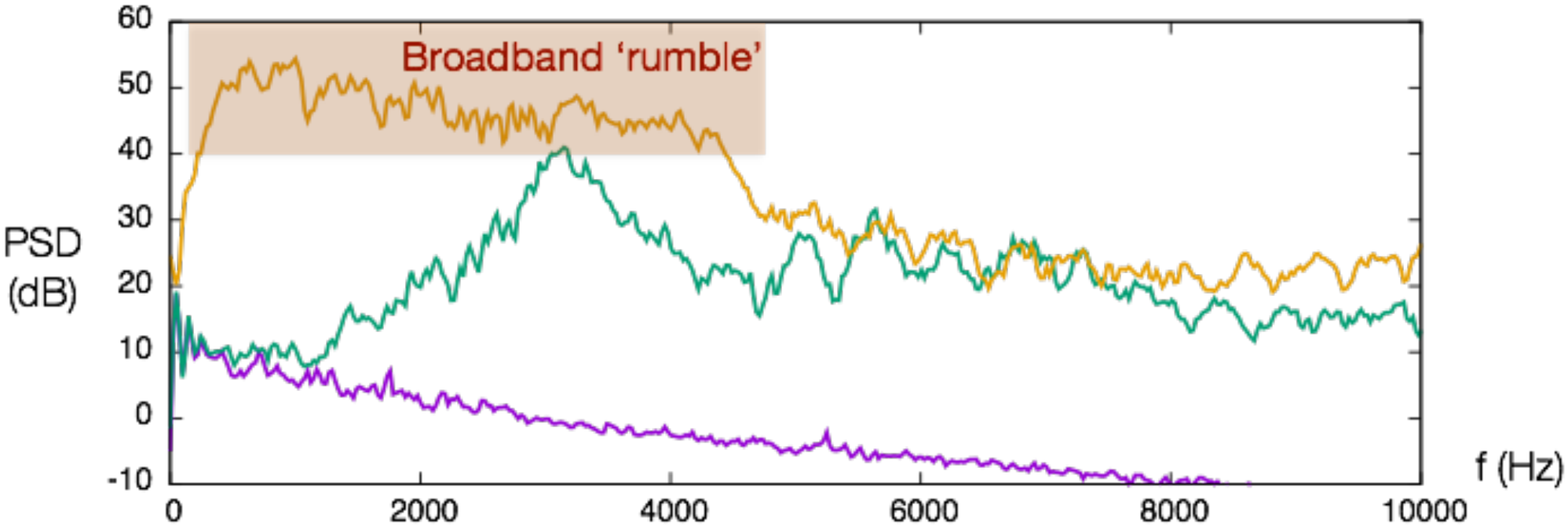
Laminar flame



Full throttle

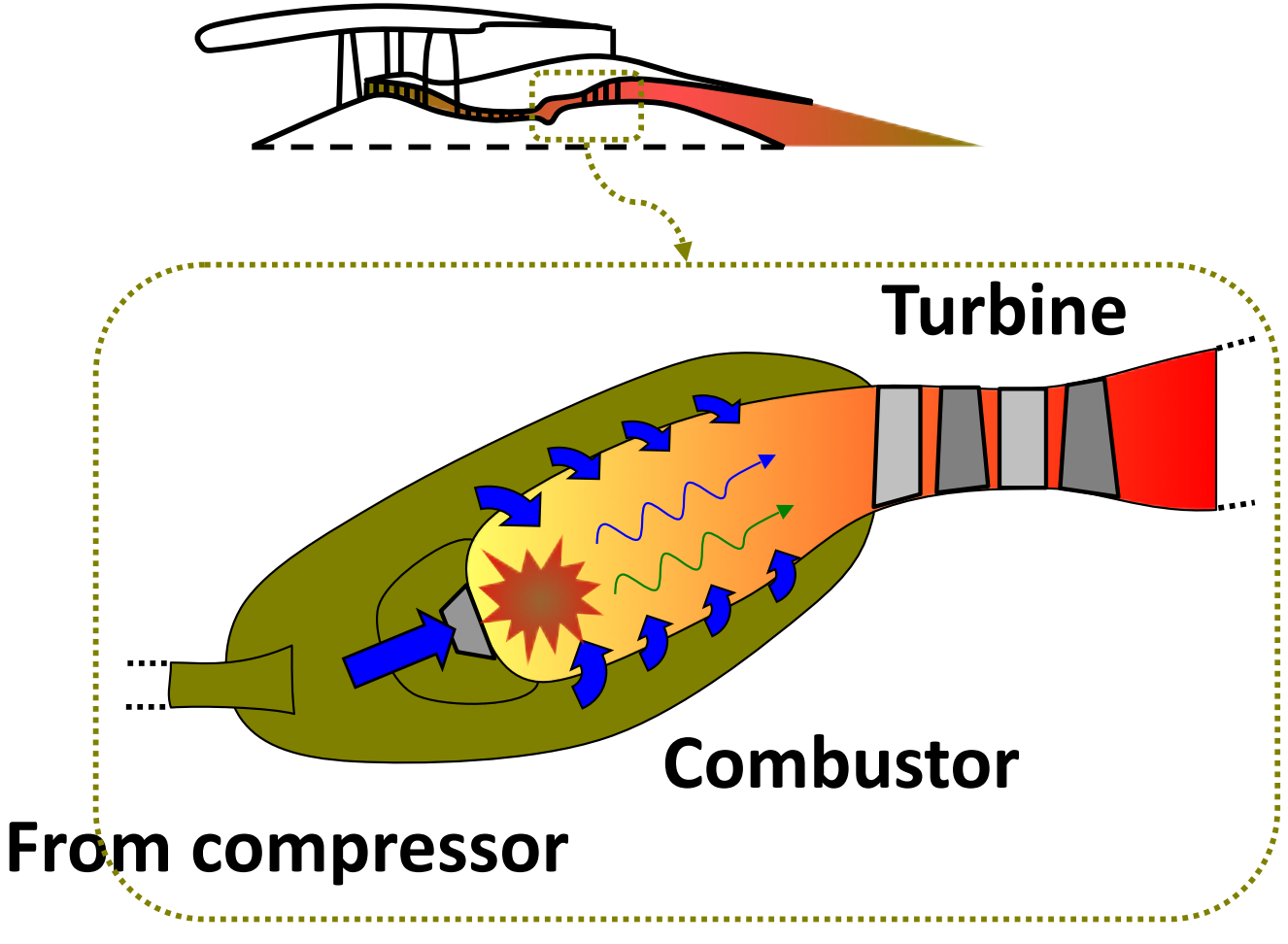


Full throttle - no combustion



2/ In a confined domain (as in most combustors), noise travels and comes back

The acoustic waves produced by combustion can reflect on walls, inlets, outlets… and come back to the flame zone.



3/ Flames are sensitive to noise

Flames feel the acoustic field and react to it

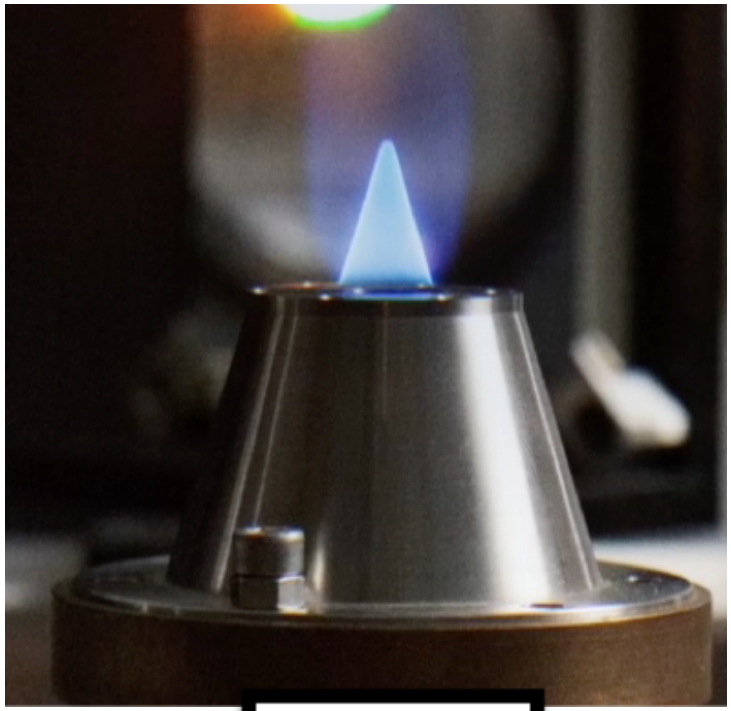
The Dancing Flame

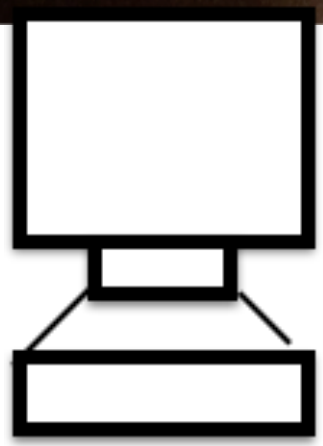
Daniel Durox

Laboratoire EM2C
Ecole Centrale Paris
CNRS (UPR 288)

With the help of :
EM2C technical staff : Y. Le Teno

Soundtrack :
Jeremy Weisman





Loudpe

Pyrophone ou orgue à gaz // 1876

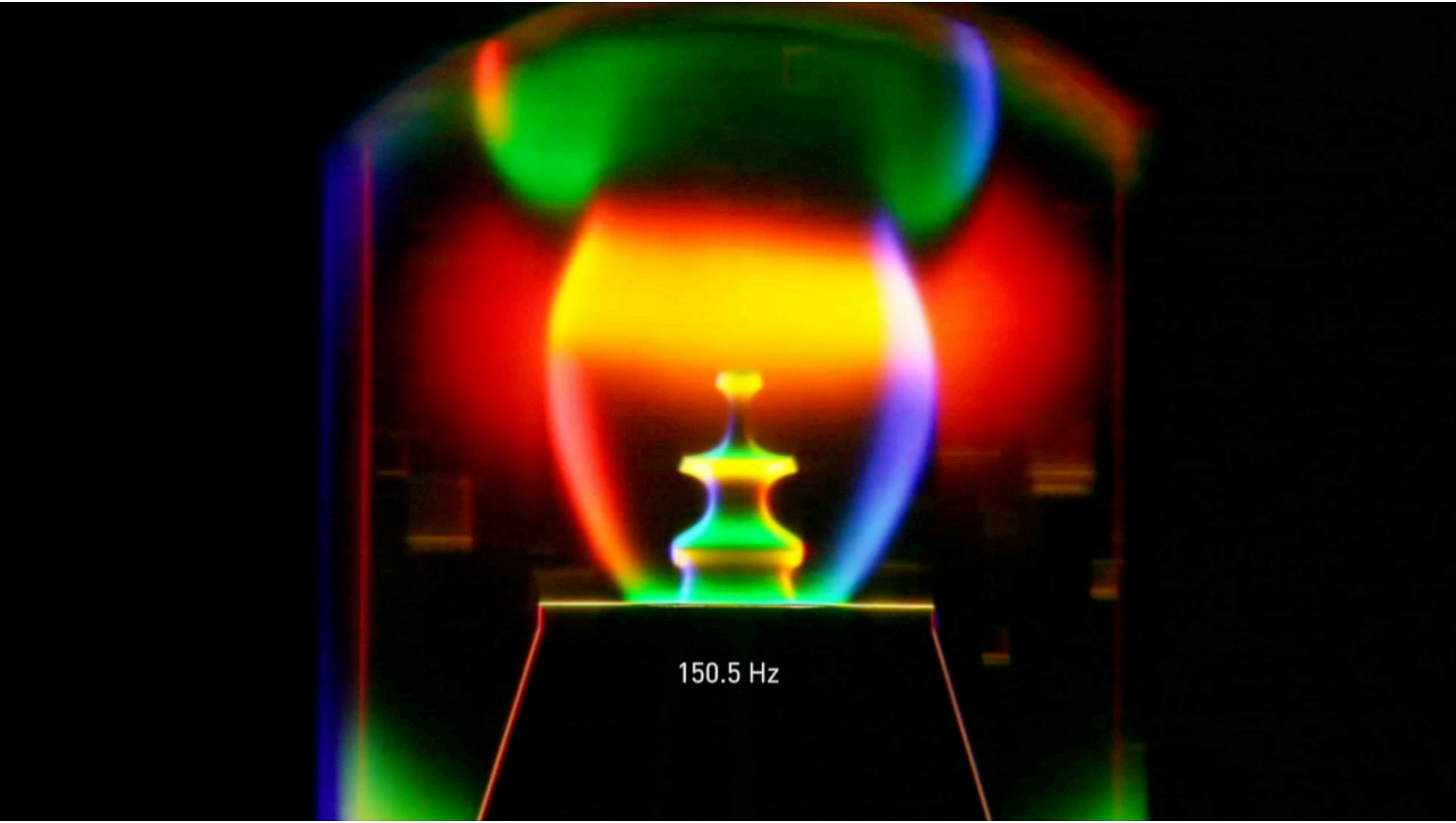
SCMHA 1019

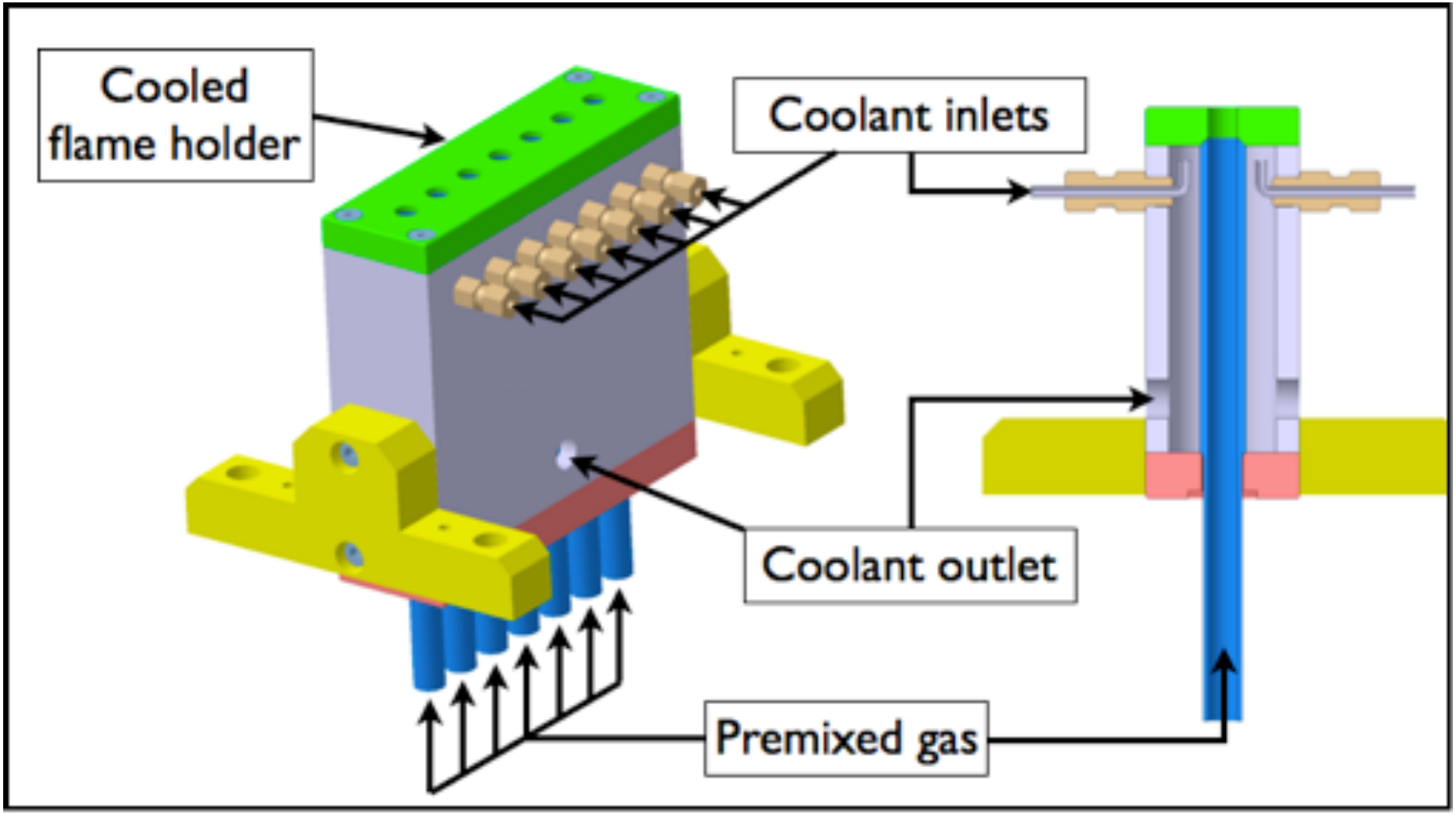
Frédéric Kastner (1852-1882)
Les touches du clavier commandent l'ouverture et le débit de chaque bec. L'action de la flamme sur l'air produit des sons. Cet instrument rarissime fut présenté à l'Académie des Sciences à Paris. César Franck, Charles Gounod et Wendelin Weissheimer composèrent pour ces « flammes chantantes ».

Pyrophon (Flammenorgel) // 1876

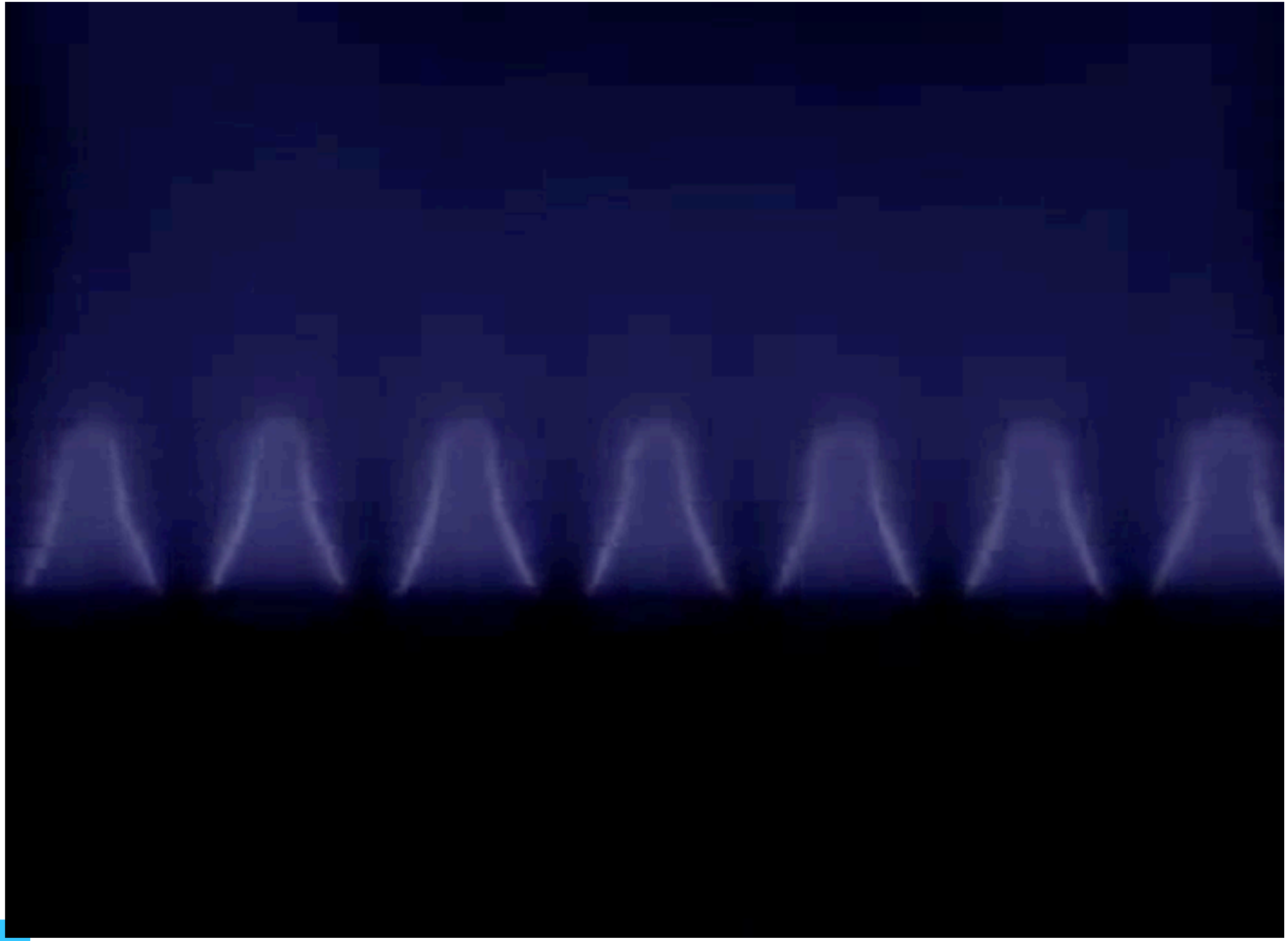
Frédéric Kastner (1852-1882)
Öffnung und Durchsatz der Brenner wurden mit



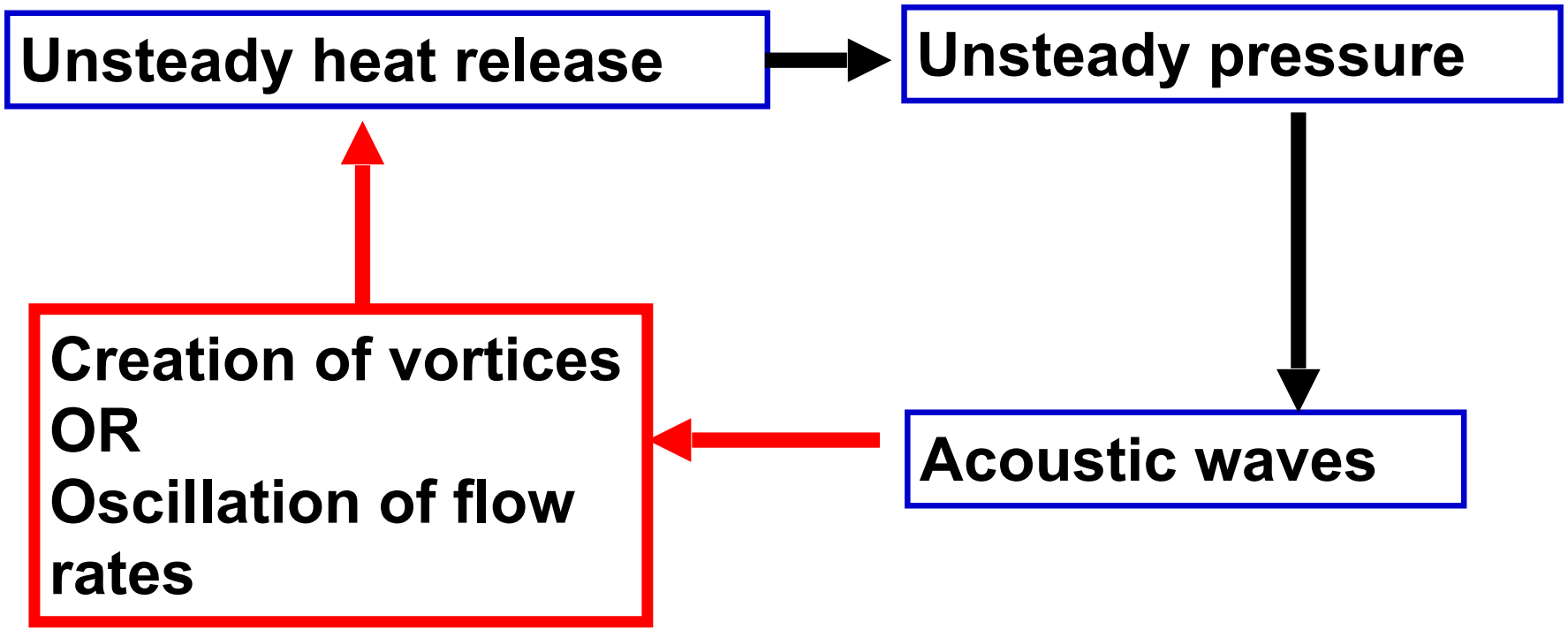

150.5 Hz


Cooled
flame holder
Coolant inlets
Coolant outlet
Premixed gas





As a result, coupling may occur: chamber instability



École Centrale Paris
leader, entrepreneur, innovateur

Flame Organ

Daniel Durox

Laboratoire EM2C
Ecole Centrale Paris
CNRS (UPR 288)

With the help of :
ECP students : L. Martin, M. Pelletier, A. Rachih
EM2C technical staff : E. Jean-Bart, Y. Le Teno

10 kW burner

Dr Durox
EM2C



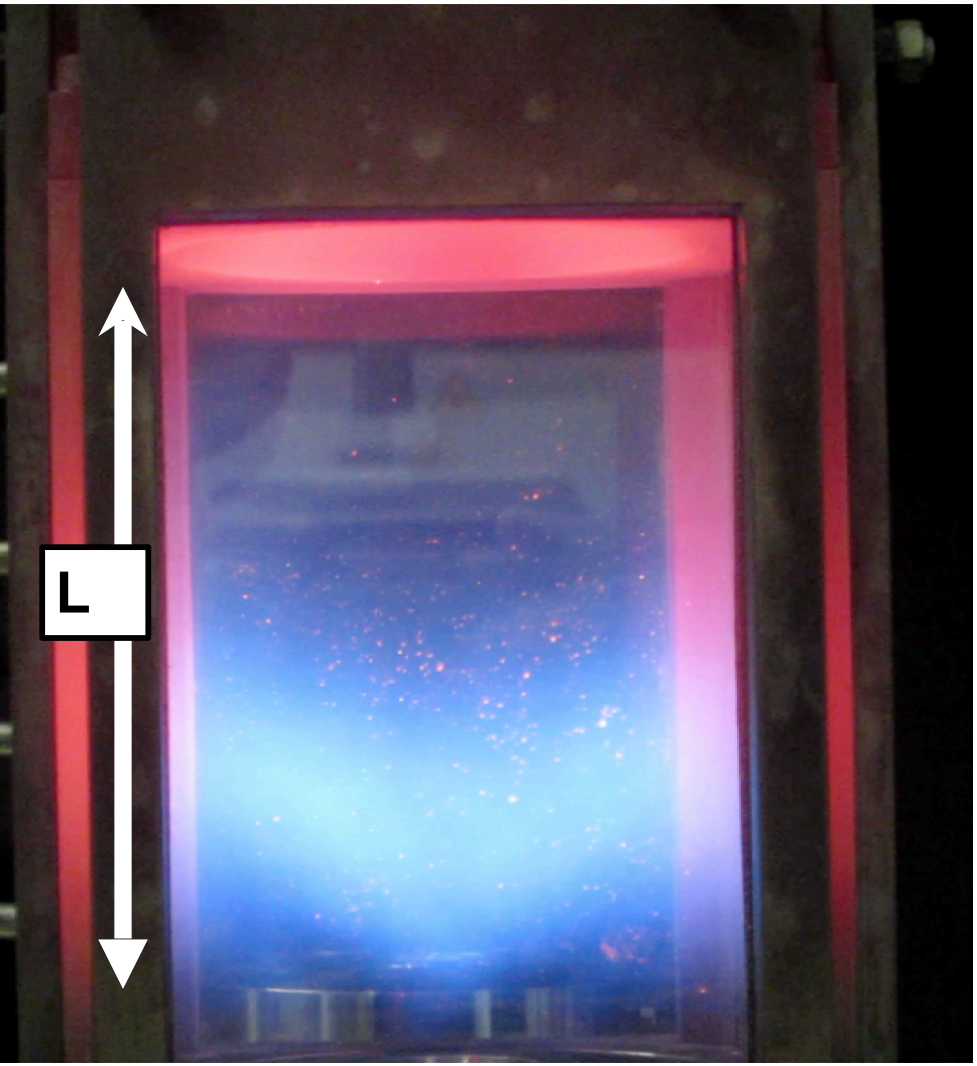






100 kW annular burner
EM2C

Frequency of unstable acoustic modes



Sound

Time to go from inlet to outlet ands come back for sound

$$\tau = 2L/c$$

Sound speed

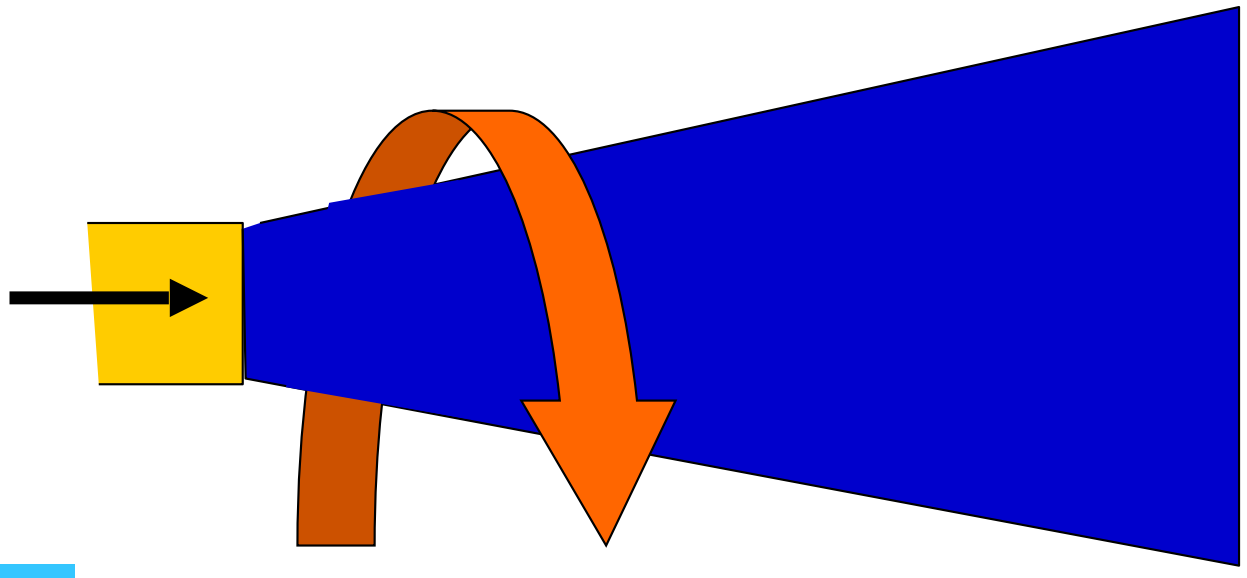
$$f = 1/\tau = \frac{c}{2L}$$

C= 700 m/s, L= 0.5 m:

$$f = \frac{c}{2L} = 700Hz$$

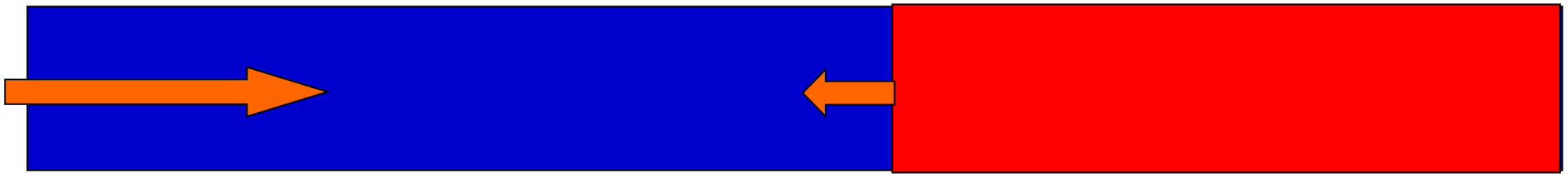
Before describing acoustic instabilities, we must discuss a specific feature of combustion chambers: SWIRL.

Swirl is a rotation of the flow along its axis



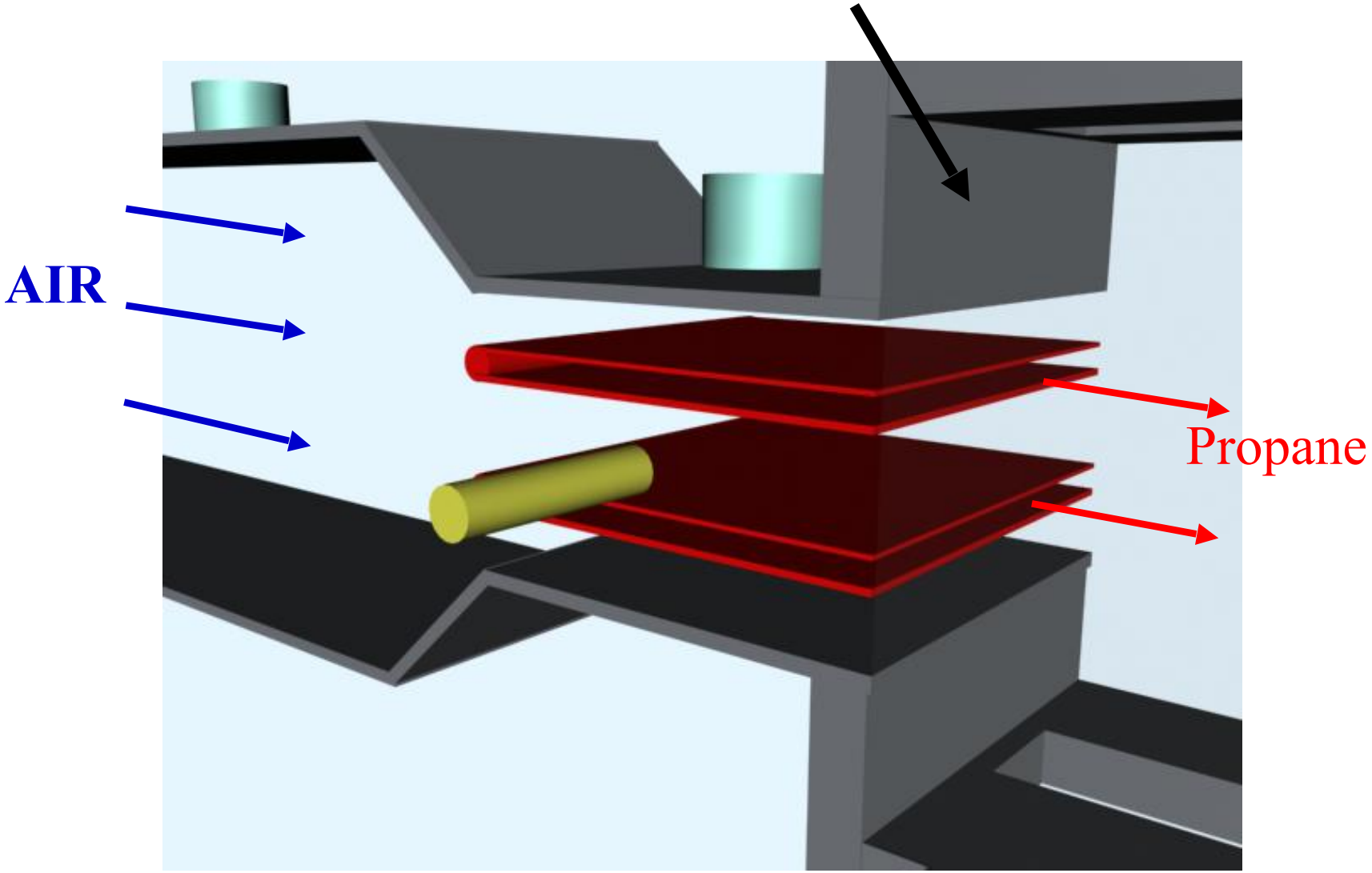
Swirl: why ?

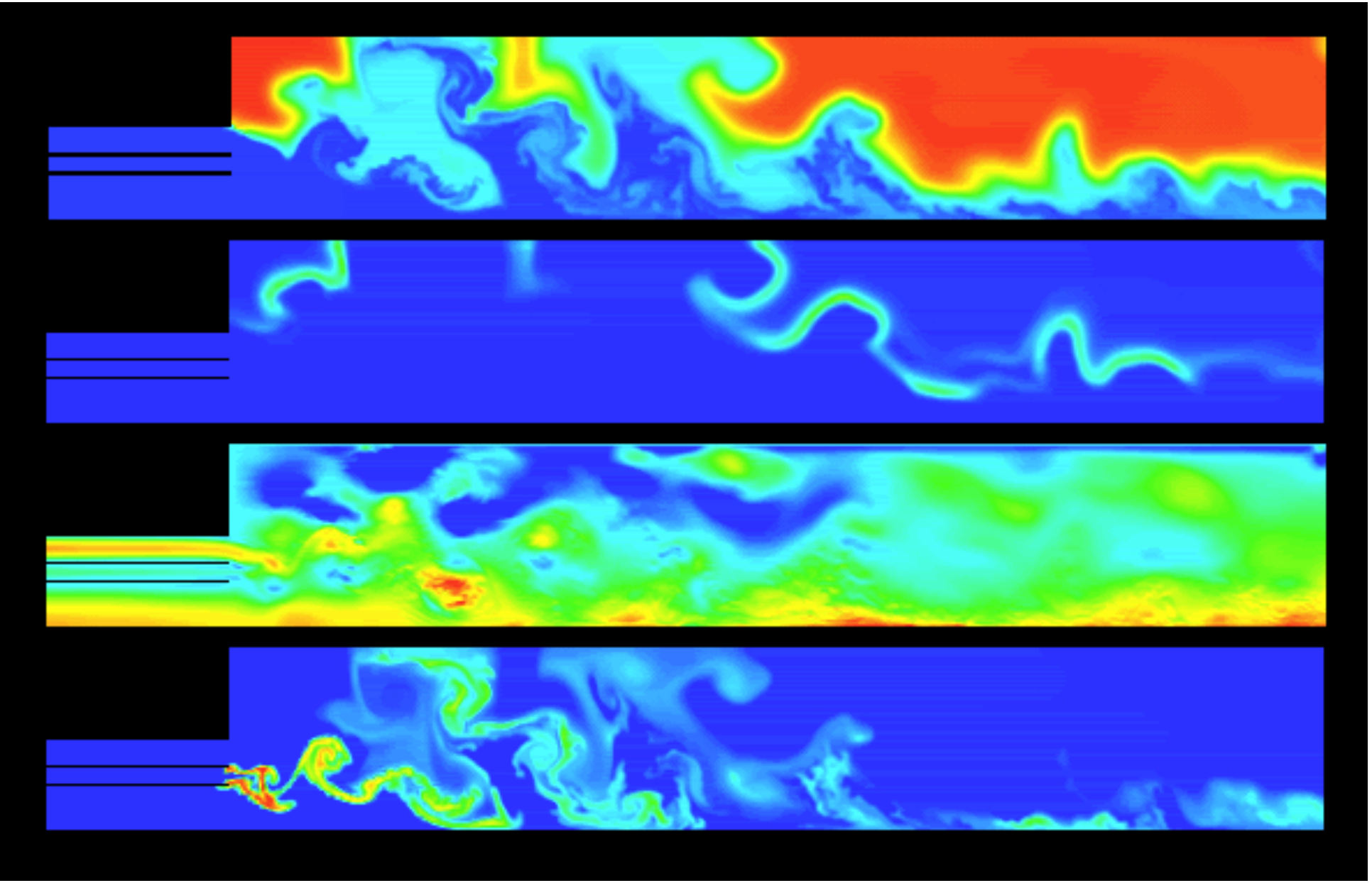
Flame stabilization !: flames do not propagate at high speeds. Typically CxHy+Air flames move at sL=50 cm/s. CxHy/O2 flames at a few m/s.



As soon as the flow speed is larger than a few m/s, flames can be stabilized only by a recirculation zone containing burnt bases to ignite the incoming gases.

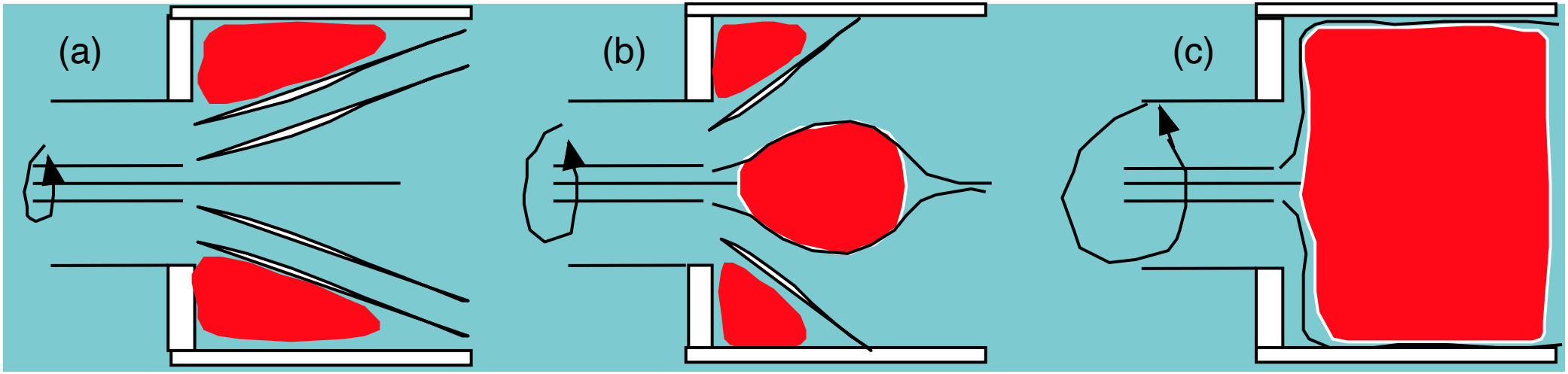
How do you create a recirculation zone ?
Solution 1: dump geometry. Backward facing step




Temp
Reaction
Velocity
Mixing
Yf Yo

Another solution to create recirculation is SWIRL:

- Swirl creates a low velocity region in the jet axis.
- Strong swirl allows to create recirculation zones
- These zones do not touch walls.



Low swirl

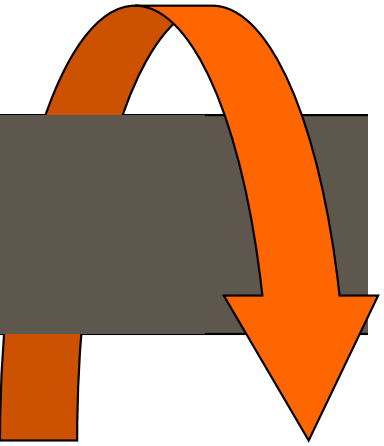
Medium swirl

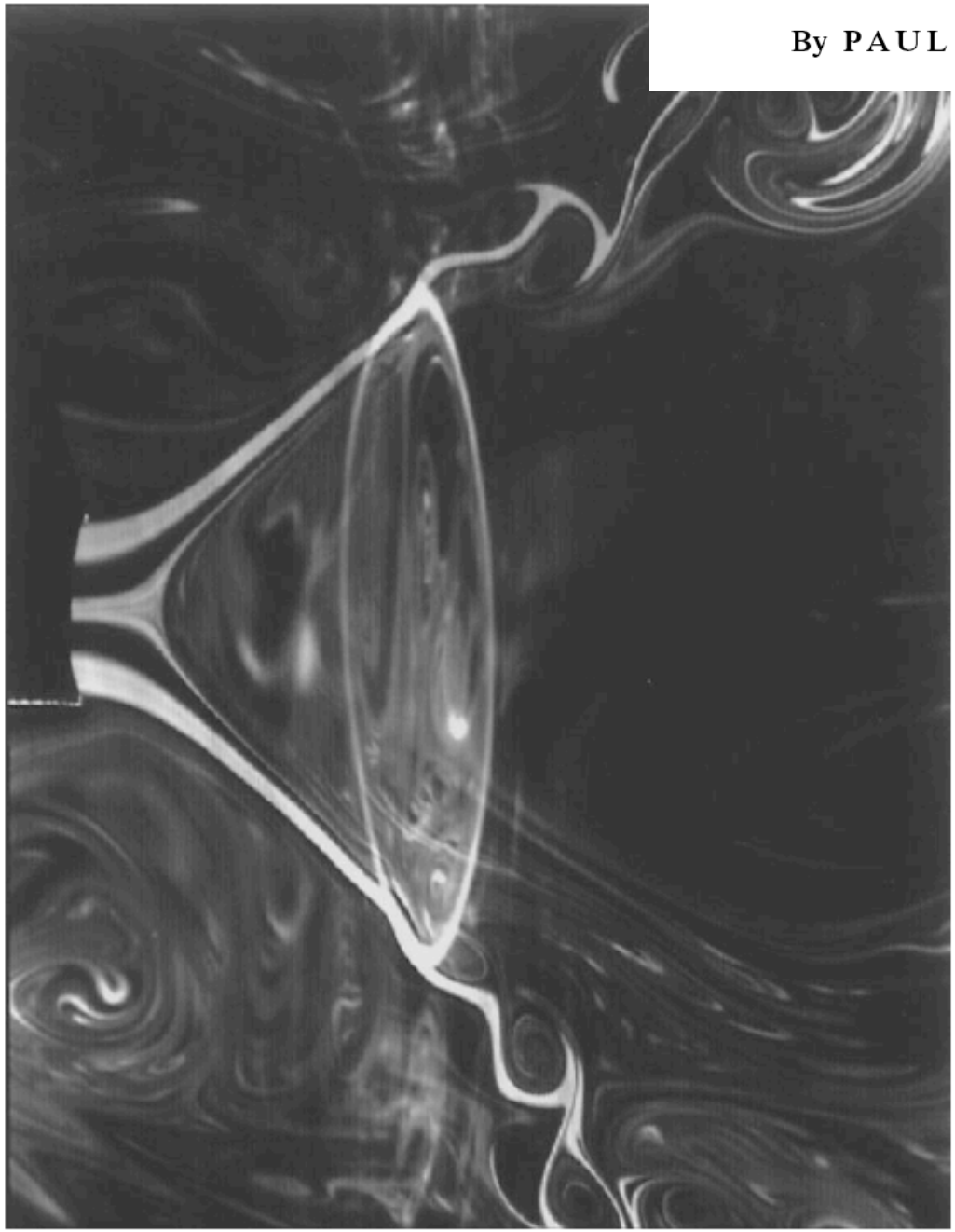
High swirl

J. Fluid Mech. (1998), *vol.* 376, *pp.* 183–219. Printed in the United Kingdom
© 1998 Cambridge University Press

Experimental study of vortex breakdown in swirling jets

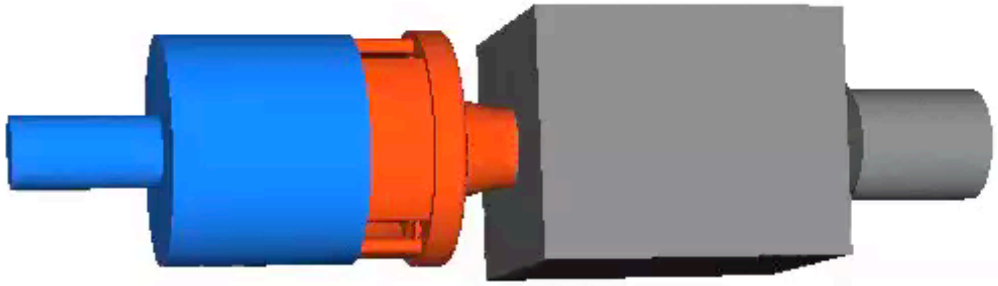
By PAUL BILLANT[1,2], JEAN-MARC CHOMAZ[1] AND PATRICK HUERRE[1]





How is swirl introduced ?

PRECCINSTA EU project

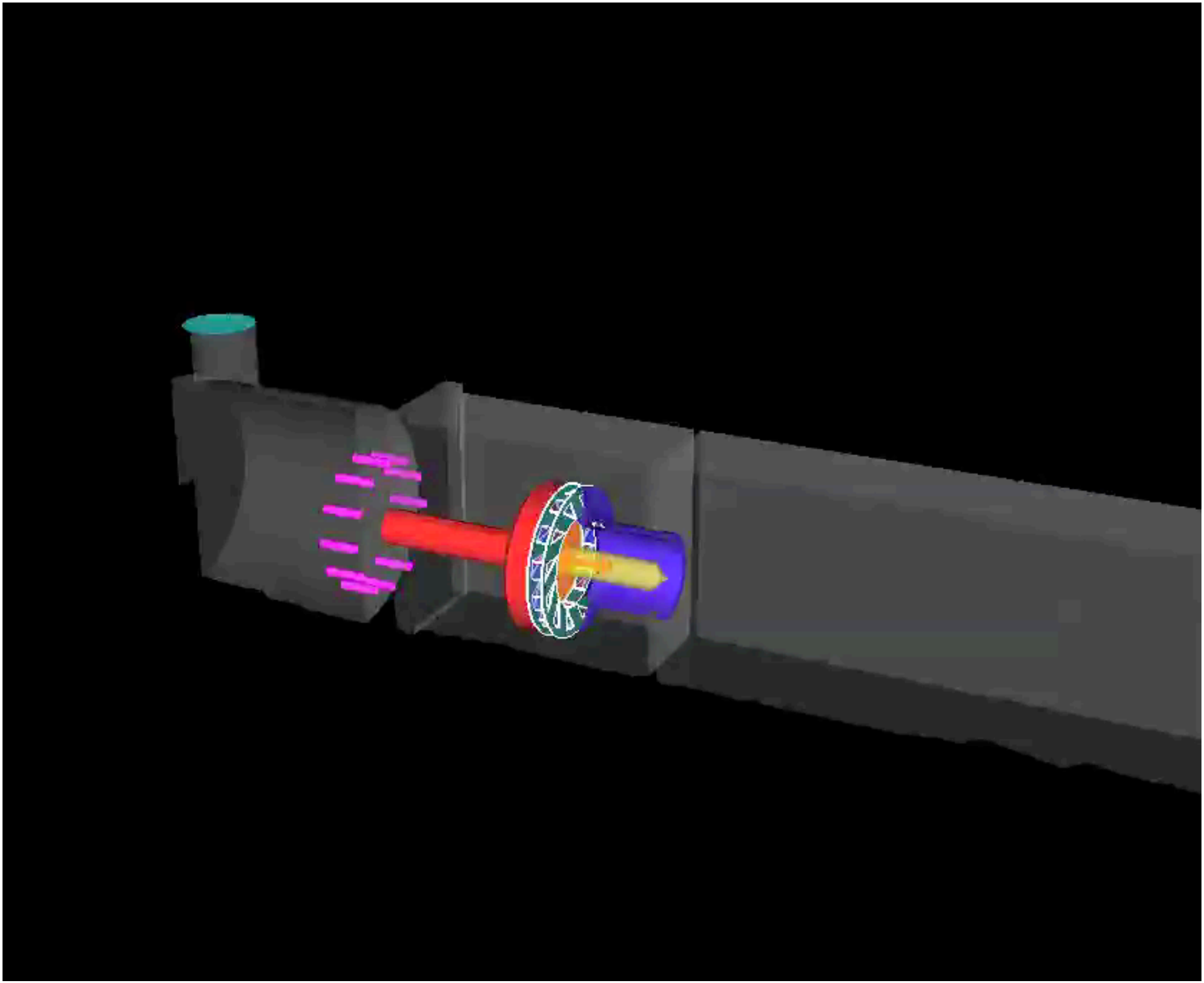


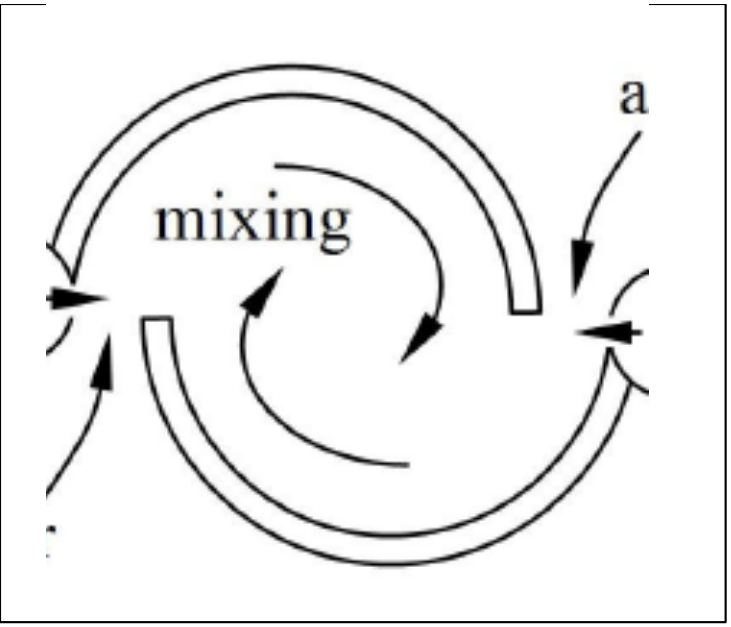
Mesh	device fully meshed
	3 million cells
	3D unstructured

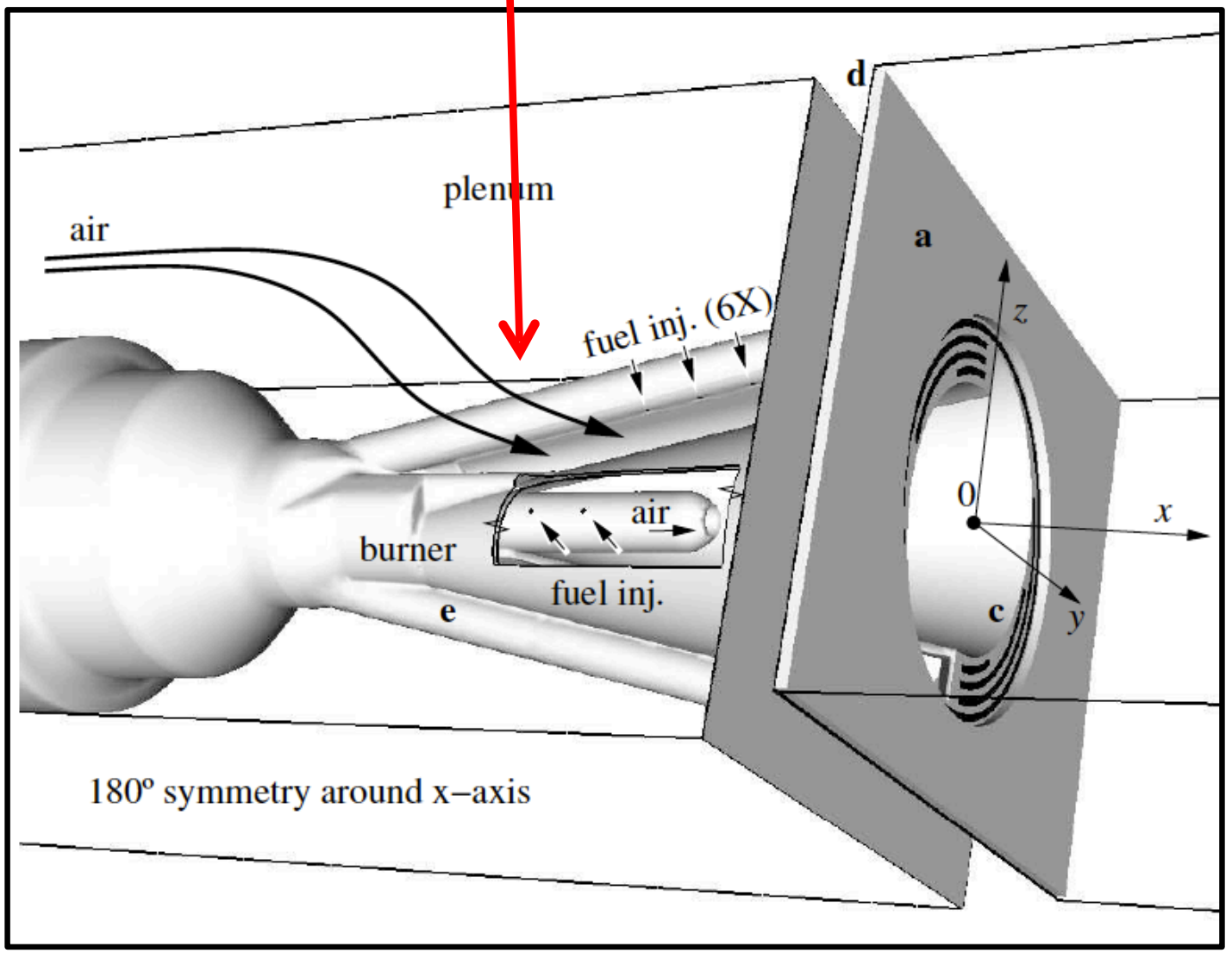
Measurement performed by DLR

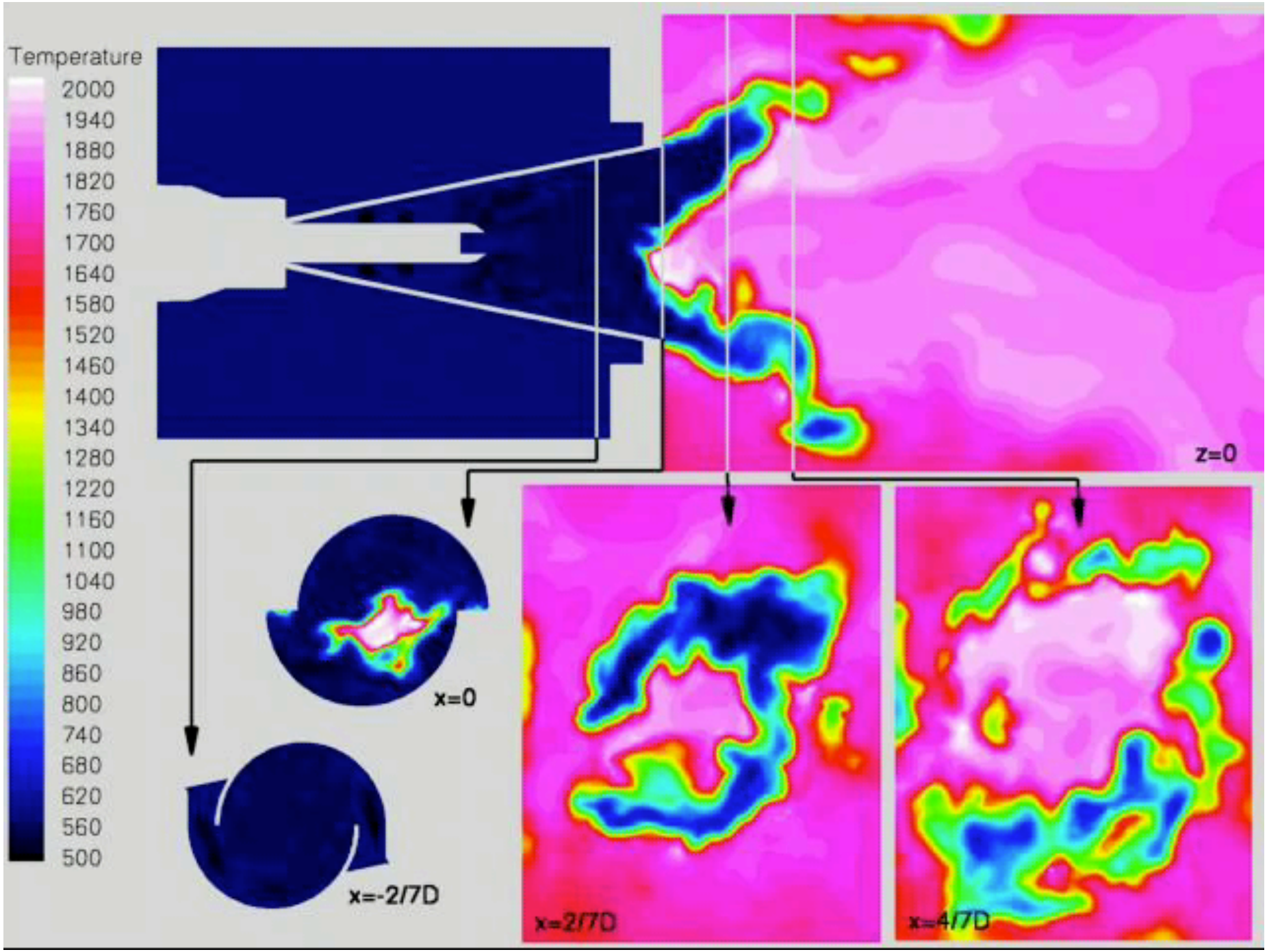
CERFACS

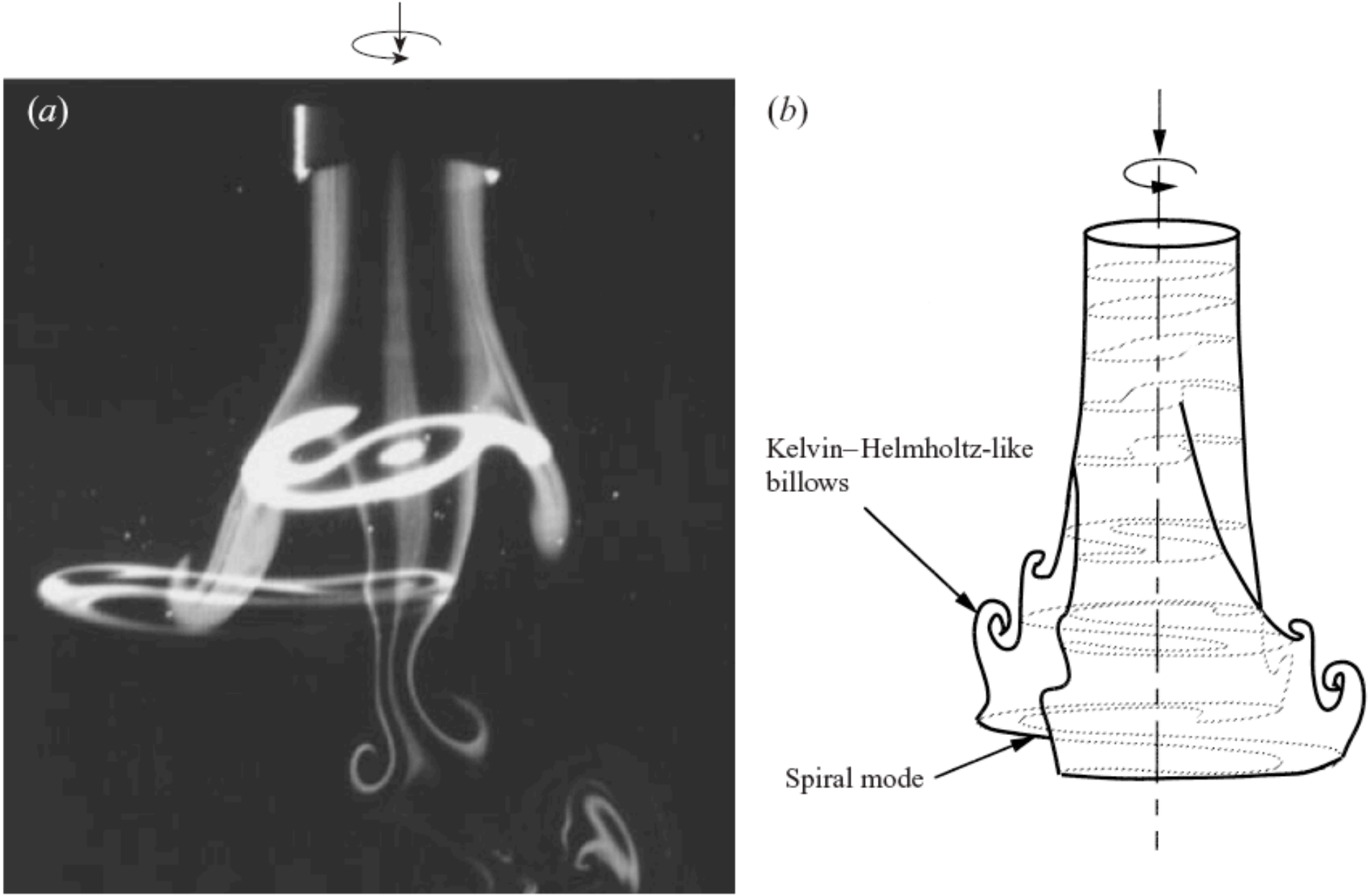
Turbomeca
groupe snecma




a
mixing

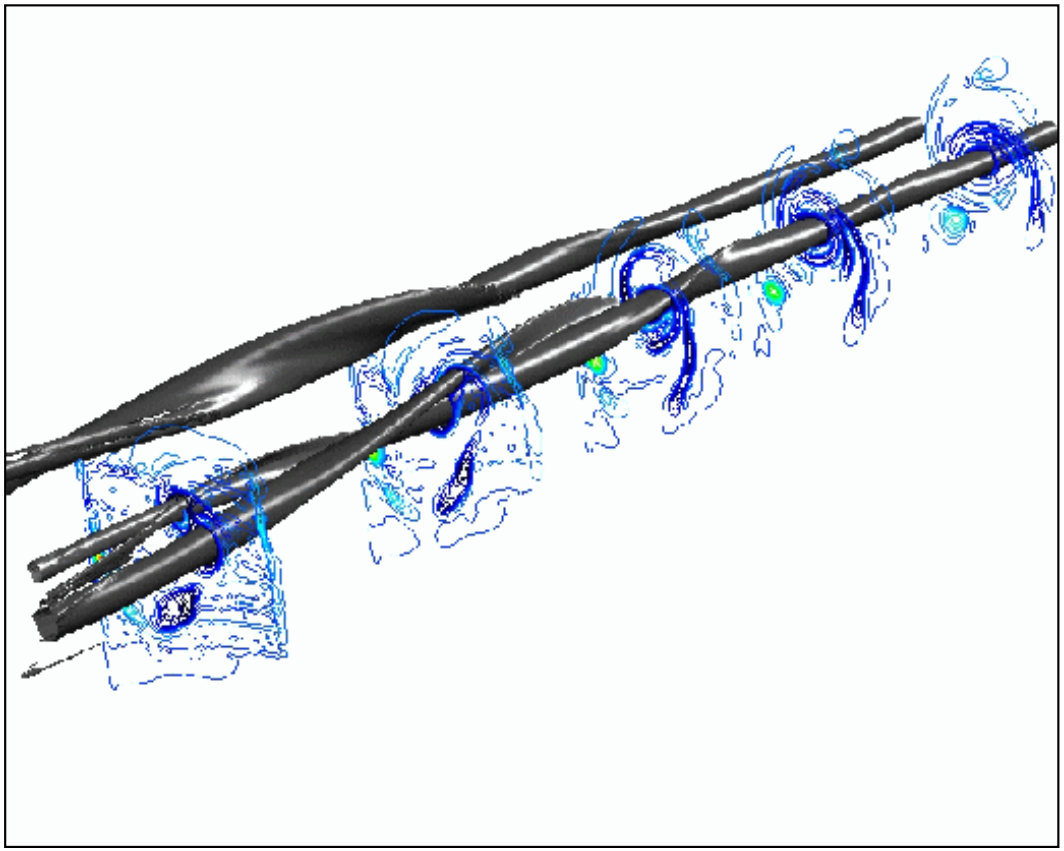

plenum
air
fuel inj. (6X)
d
a
z
0
x
y
c
air
burner
fuel inj.
e
180° symmetry around x–axis


Temperature
2000
1940
1880
1820
1760
1700
1640
1580
1520
1460
1400
1340
1280
1220
1160
1100
1040
980
920
860
800
740
680
620
560
500
z=0
x=0
x=-2/7D
x=2/7D
x=4/7D


(a)
(b)
Kelvin–Helmholtz-like billows
Spiral mode

Have you seen swirled jets before ? Yes, in the sky !





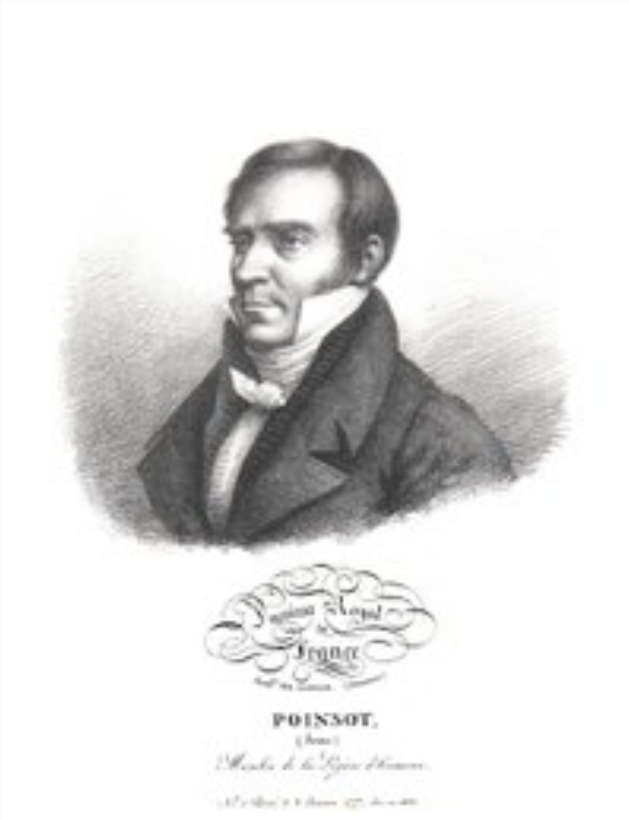
Something that turns can lead to ‘precession’:





For a swirled flow: the rotation axis itself turns. Not necessarily in the same direction as the mean flow

Louis Poinsot



Naissance : 3 janvier 1777
Clermont-en-Beauvaisis
(France)

Décès : 5 décembre 1859
Paris (France)

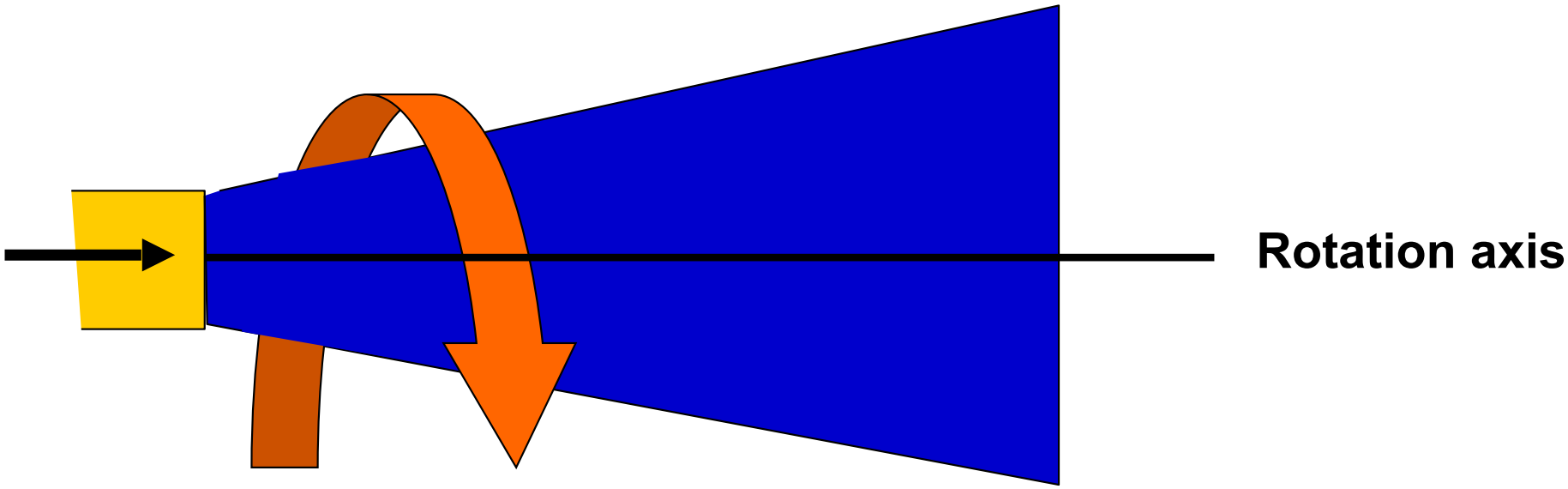
So SWIRL is good for combustion chambers !

But a swirled flow exhibits instabilities:

- the same as in jets: Kelvin Helmholtz

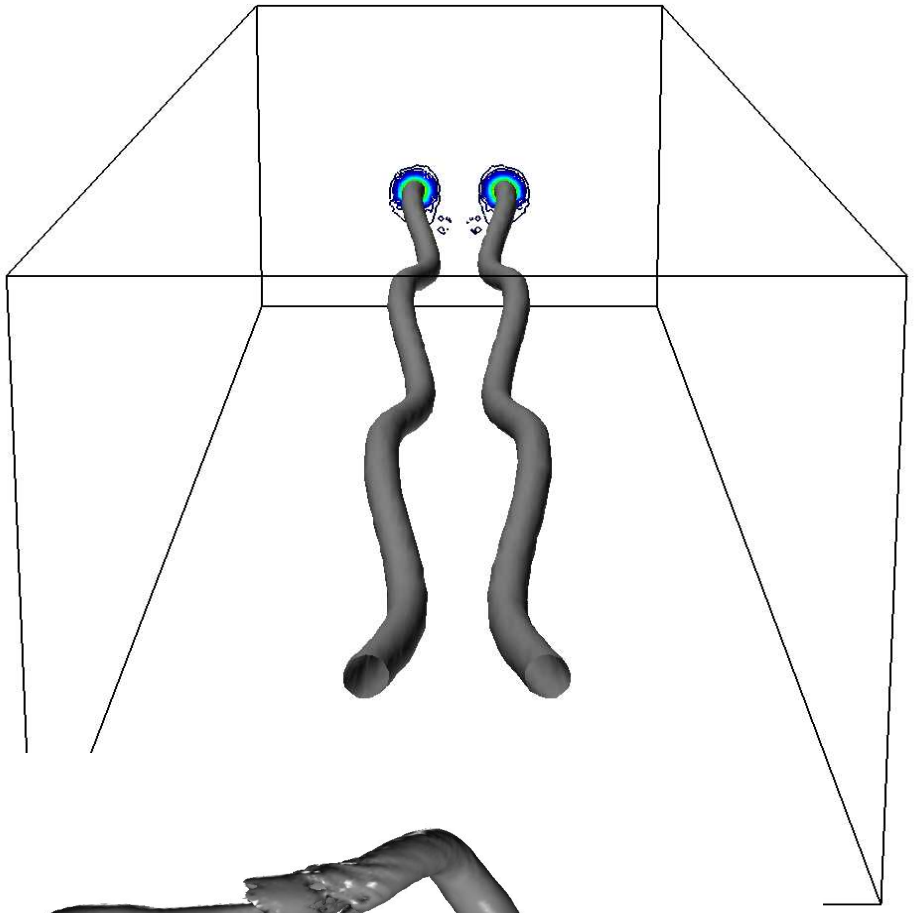
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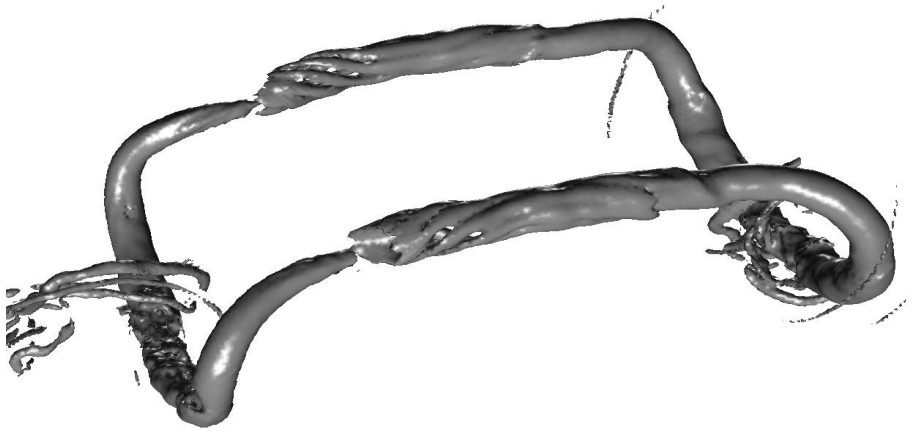
- new modes due to rotation (and since we have introduced negative velocities, absolute modes !)

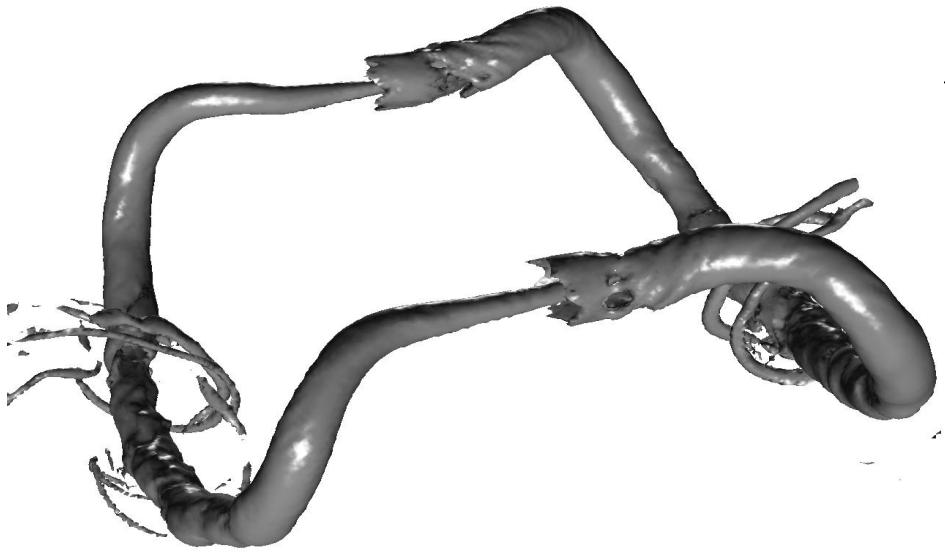


One example of swirled flow instabilities: the Crow mode.

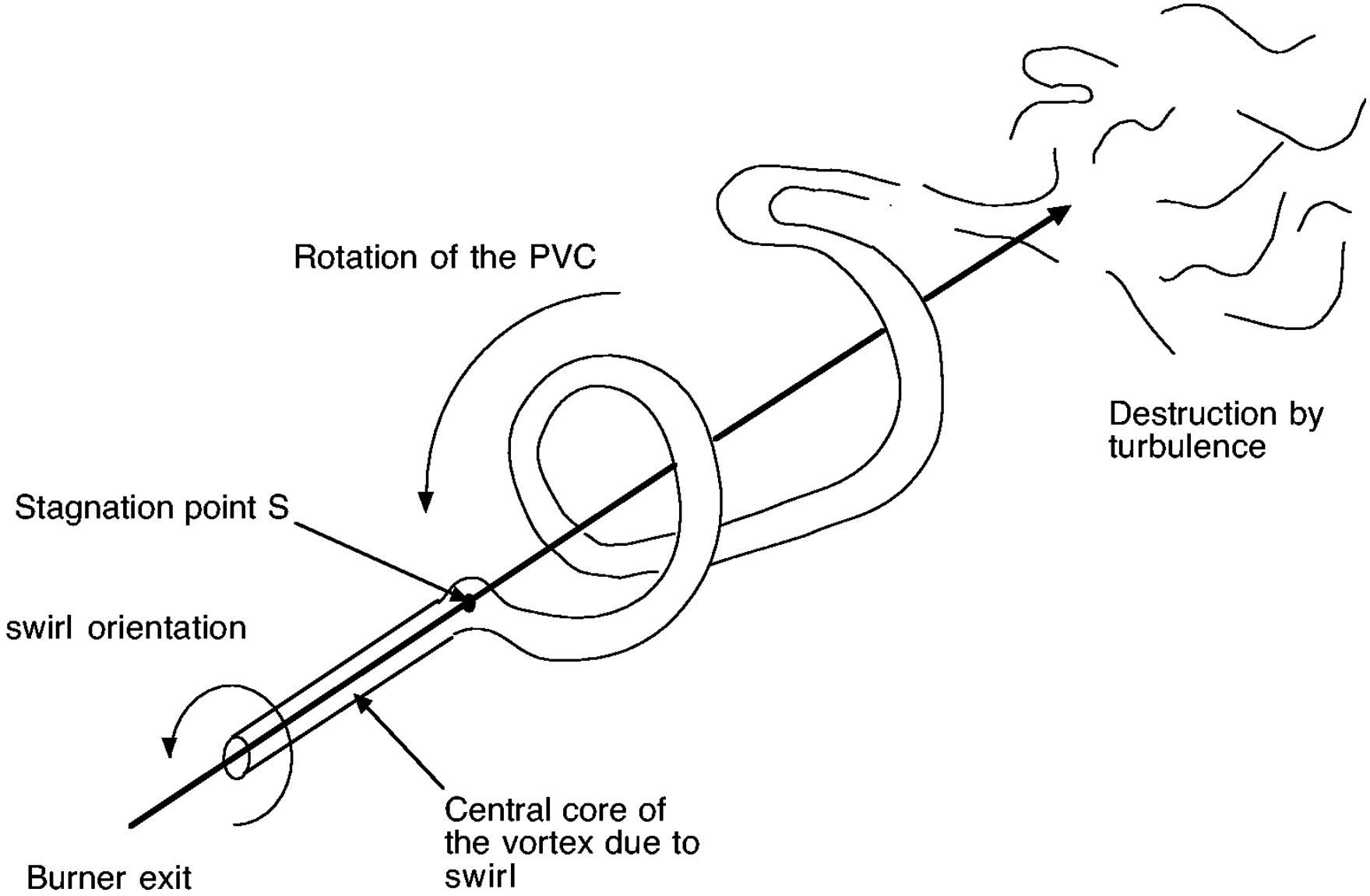




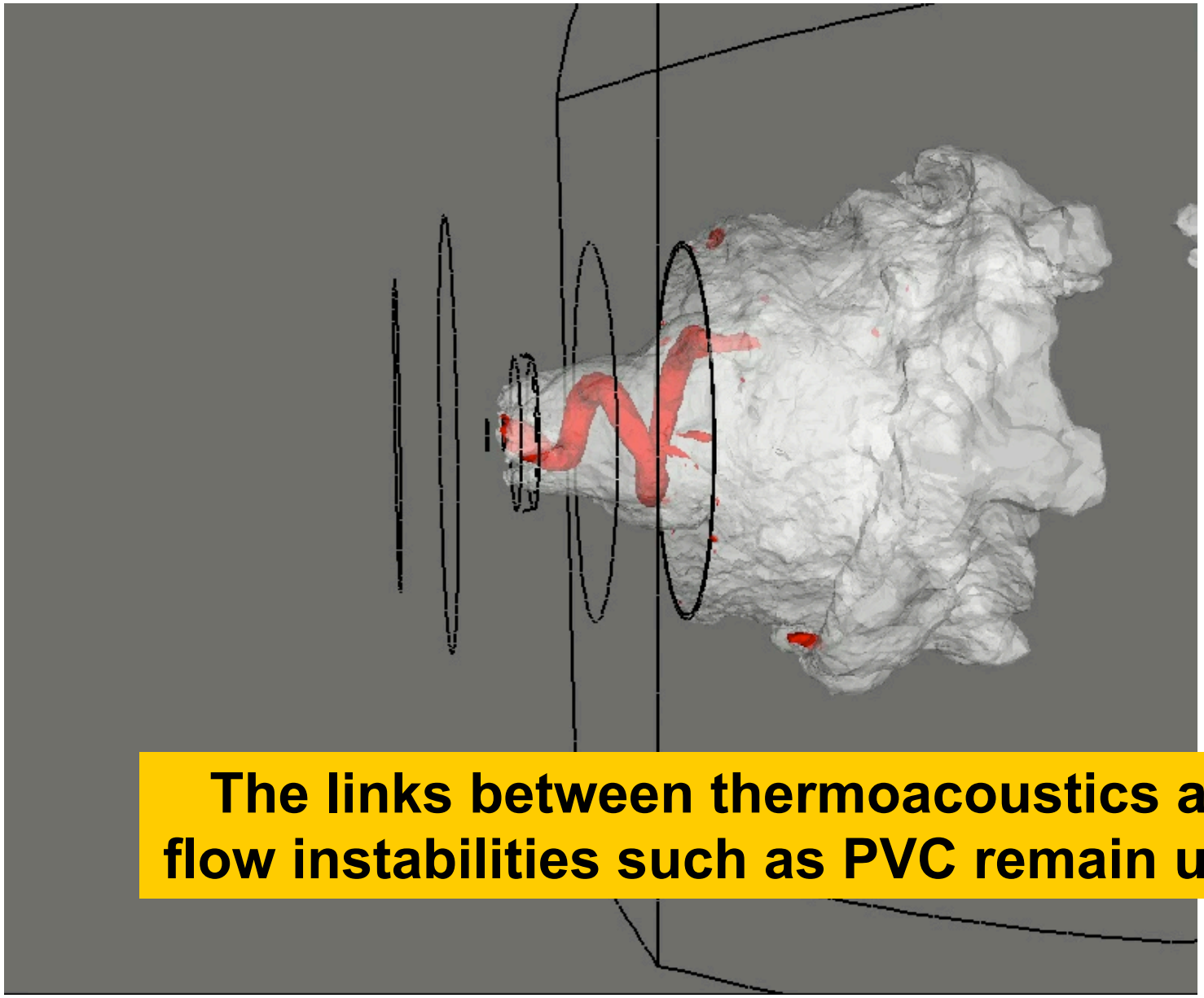




Swirled flows have another specific instability: precessing vortex cores



PVC visualized in LES of a swirled reacting flow:



White surface: flame surface

Red surface: low pressure surface

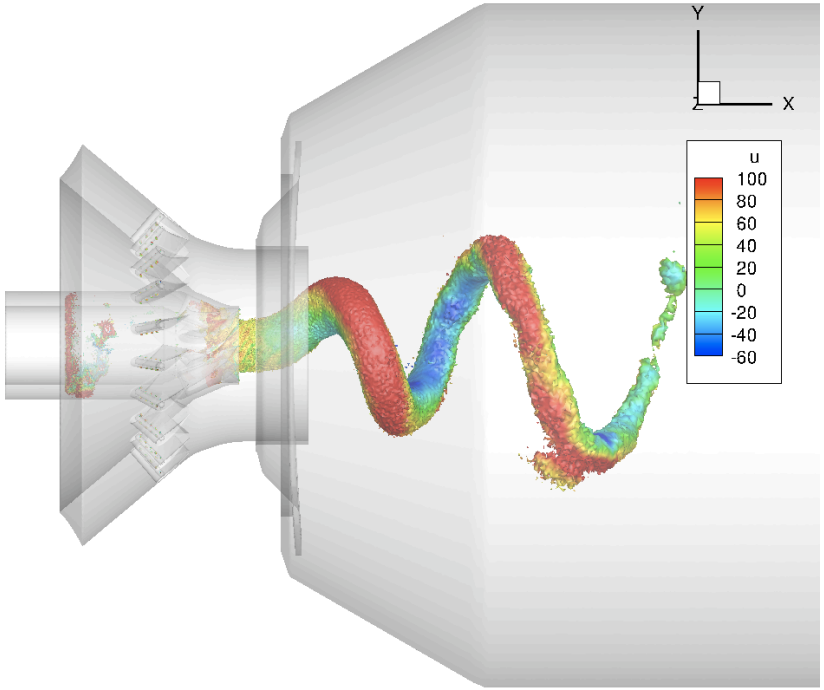
The links between thermoacoustics and swirling flow instabilities such as PVC remain unclear today.

THE TOOLS TO STUDY THERMOACOUSTICS :

Why acoustics and combustion interact

Effects of combustion instabilities in gas turbines

Examples of studies of combustion Instabilities in gas turbine configurations



Ch. 8

Interaction acoustics / combustion

Not a classical topic: USUALLY, pressure waves are not important in subsonic flames. They are a by-product of combustion and produce noise (combustion noise can be important !) but there is no need to account for them in computing the flames themselves.

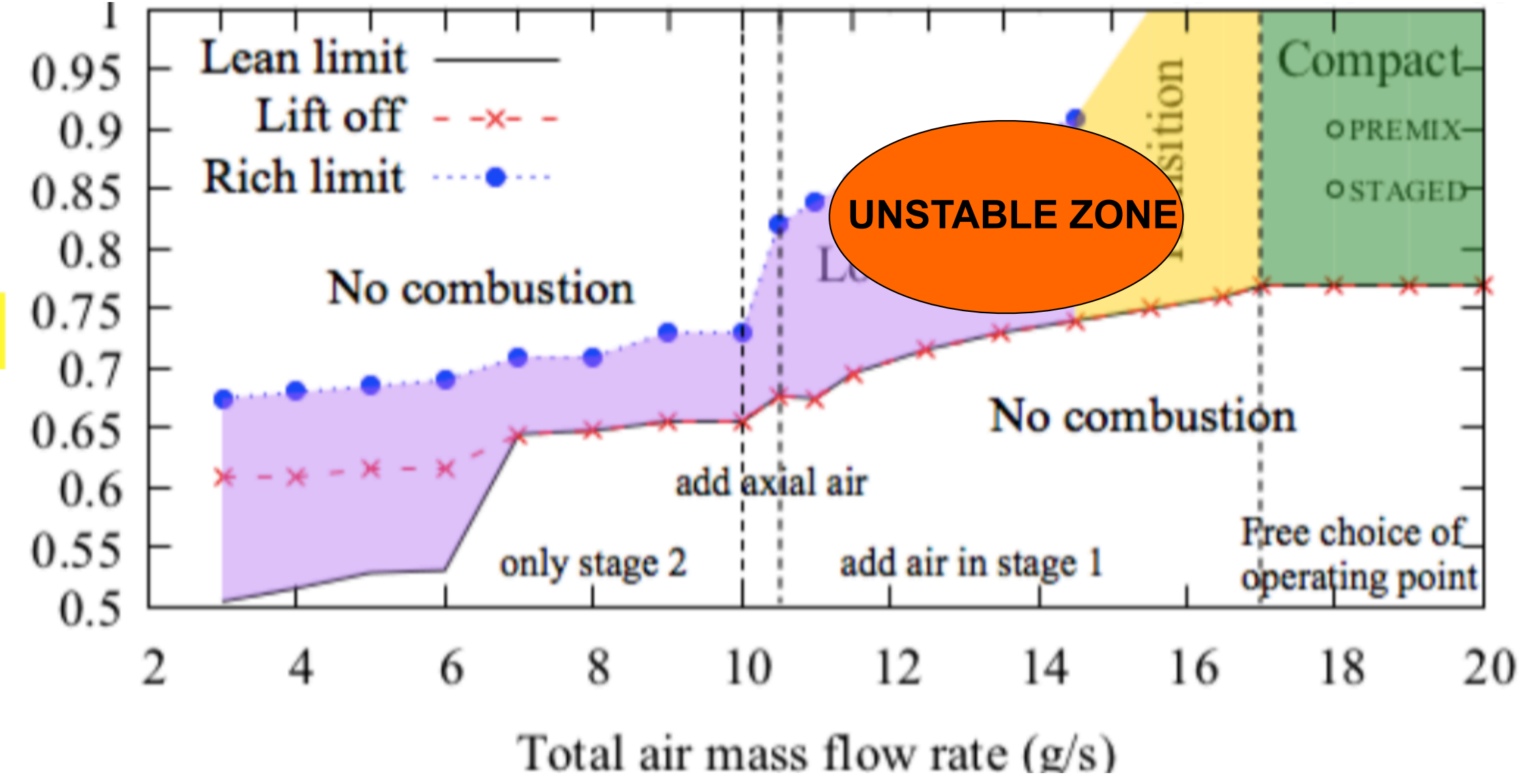
In thermoacoustics, when acoustics DO modify flames, we need to develop a theory able to compute reacting flows and acoustics.

<u>Textbooks:</u>
Crighton, Dowling, Ffowcs Williams,Heckl and Leppington « *Modern methods in analytical acoustics* » 1992, Springer -> acoustics

Poinsot and Veynante *« Theoretical and numerical combustion* »
-> combustion theory and simulations

Williams *« Combustion theory »* 1985. -> theory

STABILITY MAPS: IN GENERAL A FUNCTION OF AIR AND FUEL FLOW RATES, OR OF AIR FLOW RATE AND EQUIVALENCE RATI



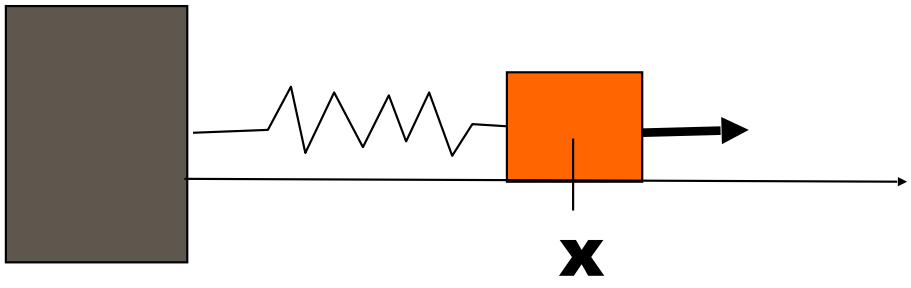
CLASSICAL METHODS TO STUDY RESONATORS:

Two approaches:

- <u>Approach 1:</u> take the conservation equations, linearize them, look for eigenmodes. Objective: find frequency and growth rate as well as mode structure (p'(x))
- <u>Approach 2:</u> define a proper energy of the system: assume it changes harmonically, find the frequency and growth rate. Objective (less ambitious): find instability criteria

Before looking at flames: let us do a small exercice on the pendulum…

The linear oscillator with no forcing:



$$m\ddot{x} + kx = 0$$

Spring force: F = -kx

Mass m

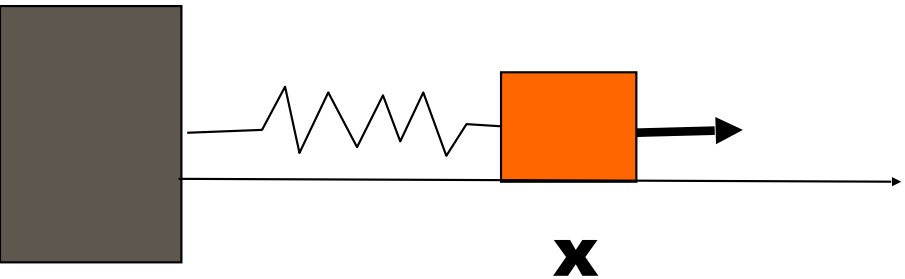
v=dx/dt

Approach 1: just solve it !

$$x = \hat{x}e^{i\omega t}$$

With: $\omega = (k/m)^{1/2}$

The linear oscillator with no forcing: energy definition



x

v=dx/dt

$$m\ddot{x} + kx = 0$$

Multiply by the velocity v=dx/dt and integrate:

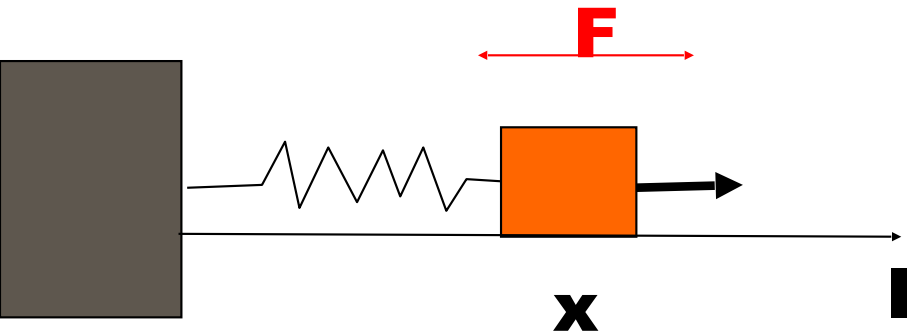
$$\frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = E$$

E is the total energy of the system

Here E is constant.

The linear oscillator with forcing:

$$m\ddot{x} + kx = F$$



$$\omega = (k/m)^{1/2}$$

If we do not know F, cant say much

==> Approach 1 is limited

v=dx/dt

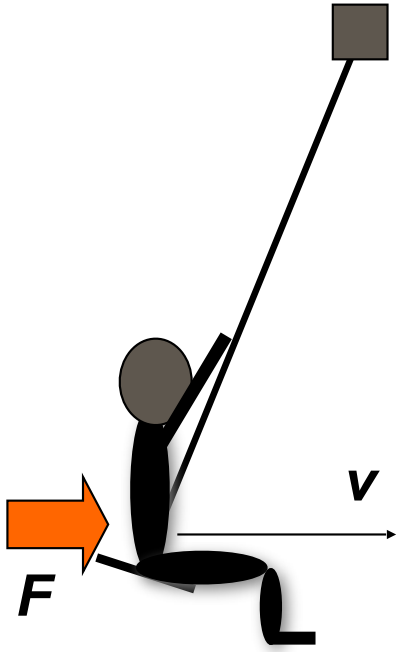
BUT Approach 2 can be used:

Multiply by v and integrate:

$$\frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = E + \int_0^t F v dt$$

This is the total energy of the system

$$\frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = E + \int_0^t F v dt$$



The total energy of the system will grow if:

$$\int_0^t F v dt > 0$$

This is an 'instability' criterion: if the force F and the velocity v are such that the integral of their product is positive (ie if F and v are 'in phase'), instability will grow because the total system energy grows.

If you have a swing at home, you knew this already ?

STABILITY OF A COMBUSTION SYSTEM:

- Idea is similar to the pendulum

- Derivation is a bit more complicated: we need to define an energy for acoustics. Two steps:
  - Define acoustic energy in a non reacting flow
  - Then extend it to reacting flows.

Acoustics in a non reacting flow:

Acoustic waves exist in all fluids…. Start from :

$$\frac{\partial \rho}{\partial t} + \nabla(\rho u) = 0$$

$$\frac{\partial u}{\partial t} + u\nabla u + \frac{1}{\rho_o}\nabla p = 0$$

Consider a mean state in which there is no flow:

u=0 and $p=p_o$

Assume perturbations around this state and write

u= u' and $p=p_o+p'$

Assume isentropic flow (no combustion):

$p= k\,\rho^{\gamma}$ ==> $p' = c_o^2\,\rho'$

Linearize equations to obtain:

$$\frac{1}{c_0^2}\frac{\partial p'}{\partial t} + \rho_o \nabla(u') = 0$$

$$\frac{\partial u'}{\partial t} + \frac{1}{\rho_o}\nabla(p') = 0$$

A useful tool : the acoustic energy

Combine equations:

$$\frac{1}{c_o^2}\frac{\partial p'}{\partial t} + \rho_0 \nabla u' = 0 \quad \Rightarrow \quad p'/\rho_0$$

$$+$$

$$\frac{\partial u'}{\partial t} + \frac{1}{\rho_0}\nabla p' = 0 \quad \Rightarrow \quad u'\rho_0$$

Summing:

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho_o u'^2 + \frac{1}{2}p'^2/(\rho_o c_o^2)\right] + \nabla(p'u') = 0$$

$$\frac{\partial}{\partial t}E + \nabla F = 0$$

E: local acoustic energy
F: acoustic flux = p' u'

What happens with combustion ? We cannot suppose that the flow is isentropic anymore.

Add the temperature equation:

Ch. 8 Sec. 8.3

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} = -\frac{\partial p}{\partial x}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x}\right) = \dot{\omega}_T + \frac{\partial p}{\partial t}$$

+ the state equation: $p = \rho r T$

Linearize around mean state (take Mach=0 for simplification)

$$\rho = \rho_0 + \rho' \qquad p = p_0 + p'$$

$$u = u' \qquad T = T_o + T'$$

Keep only first order terms:

$$\frac{\partial \rho'}{\partial t} + \rho \frac{\partial u'}{\partial x} = 0$$

Continuity

$$\rho_0 \frac{\partial u'}{\partial t} = -\frac{\partial p'}{\partial x}$$

Momentum

The energy and state equations become:

$$\rho_0 C_p \frac{\partial T'}{\partial t} = \dot{\omega}'_T + \frac{\partial p'}{\partial t}$$

$$\frac{1}{p_0}\frac{\partial p'}{\partial t} = \frac{1}{\rho_0}\frac{\partial \rho'}{\partial t} + \frac{1}{T_0}\frac{\partial T'}{\partial t}$$

Which can be combined to obtain:

$$\frac{1}{\rho_0}\frac{\partial \rho'}{\partial t} = \frac{1}{p_0}\frac{\partial p'}{\partial t} - \frac{1}{T_0}\frac{\partial T'}{\partial t} = \frac{1}{c^2}\frac{\partial p'}{\partial t} - \frac{\dot{\omega}'_T}{C_p T_0}$$

where $c^2 = \gamma \frac{p_0}{\rho_0}$ c is the sound speed

Multiply by

$$\frac{1}{c^2}\frac{\partial p'}{\partial t} + \rho\frac{\partial u'}{\partial x} = \frac{\dot{\omega}'_T}{C_p T_0} \quad \rightarrow \quad \frac{p'}{\rho_0}$$

$$\rho_0\frac{\partial u'}{\partial t} = -\frac{\partial p'}{\partial x} \quad \rightarrow \quad \rho_0 u'$$

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho_0 u'^2 + \frac{1}{2}\frac{p'^2}{\rho_0 c^2}\right] + \frac{\partial u' p'}{\partial x} = \frac{p'\dot{\omega}'_T}{\rho_0 C_p T_0}$$

The acoustic energy equation in a reacting flow:

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho_0 u'^2 + \frac{1}{2}\frac{p'^2}{\rho_0 c^2}\right] + \frac{\partial}{\partial x}(u'p') = \frac{\gamma - 1}{\gamma P_0} p' \dot{\omega}'_T$$

Acoustic energy

Acoustic flux

Source term (Rayleigh)

This local equation can be integrated spatially to give:

$$\frac{\partial}{\partial t}\mathcal{E} + \nabla \mathcal{F} = \iiint \omega' p' dV$$

Heat release perturbations

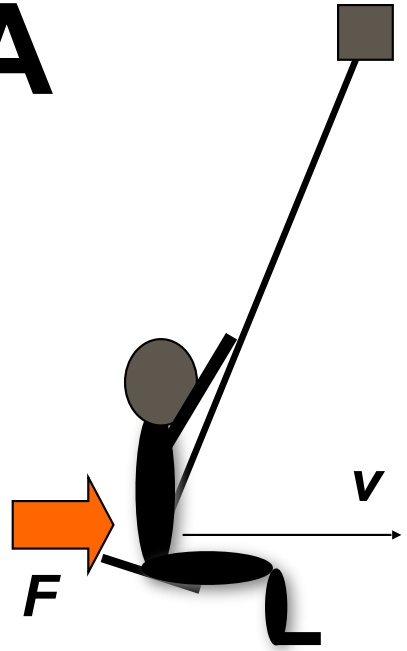
Pressure perturbations

If ω' and *p'* are in phase in enough places in the combustor, it feeds the acoustic energy (local extension of the Rayleigh criterion) ==> combustion instabilities start…

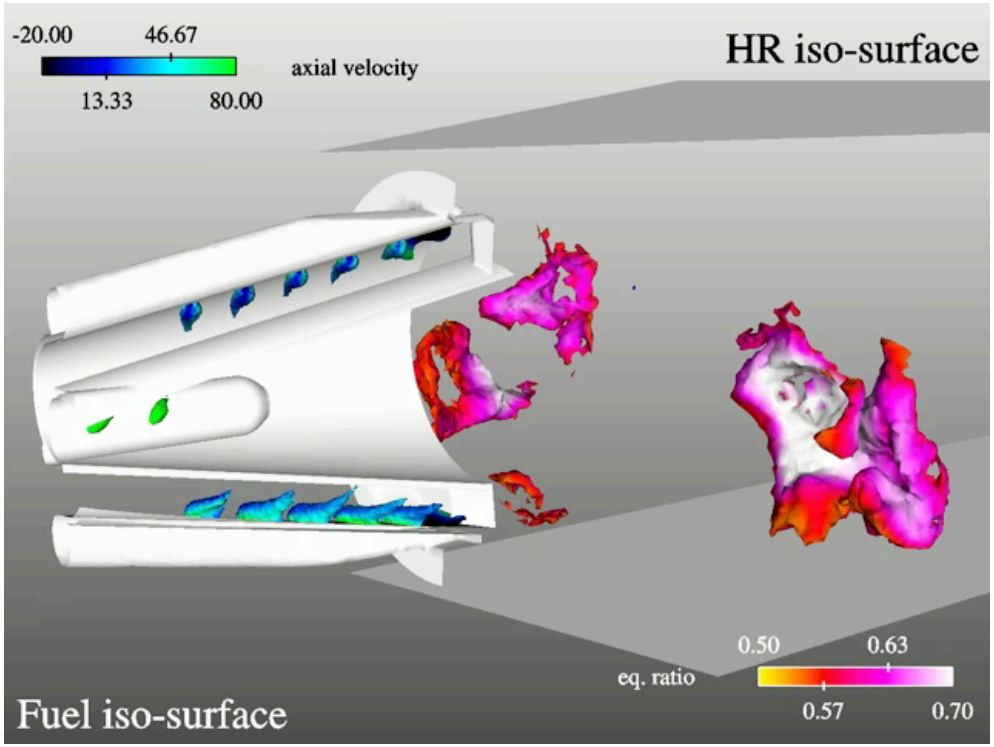
$$\iiint \omega' p' dV > 0 \qquad \text{(Rayleigh)}$$

STABILITY CRITERIA

$$\int_0^t F v dt > 0$$



$$\iiint \omega' p' dV > 0$$



$$\iiint \omega' p' dV > 0$$

Heat release Pressure

« If heat be given to the air at the moment of greatest condensation, or be taken from it at the moment of greatest rarefaction, the vibration is encouraged.
On the other hand,if heat be given at the moment of greatest rarefaction, or abstracted at the moment of greatest condensation, the vibration is discouraged »

Lord Rayleigh
Nature, 1878, July 18
(Phenomenon of singing flames already identified before 1800 but Rayleigh was the first to formulate a stability criterion)

What determines the existence of combustion instabilities in a burner is:

- **not the fuel type**
- **not the size**
- **not the shape**
- **not the equivalence ratio**
- **not….**

BUT ONLY THE FACT THAT:

- the Rayleigh criterion is satisfied (it is necessary but not sufficient)

The Rayleigh criterion is a phase criterion between:
- **unsteady heat release q'**
- **unsteady pressure p'**

The Rayleigh criterion may be negative at an equivalence ratio of 0.6 and become positive at 0.61
-> we change q'

Or it may be negative for a given exhaust diameter and become positive for a very slightly different other one
-> we change p'

The classical story of Mr x, combustion engineer:

- **I have this great burner which I have used in different combustion chambers for years with no problem**
- **I have sold it two months ago to be used in a new but very similar chamber**
- **Now this chamber is 'howling' (buzzing, hooting, screaming: other names for 'too much noise') and can melt or explode after 10 minutes.**
- **WHAT HAPPENED ?**

BURNER + COMBUSTION CHAMBER

= CHANGING RAYLEIGH CRITERION

= **POTENTIAL BIG TROUBLE**

The Rijke tube at home: kitchen experiments !

Take a gas bottle fitted to a ‘burner’







Combustion chambers:

Introduce the burner in simple cylinders: these ‘combustion chambers’ will contain the flame



Small size tube



Long tube

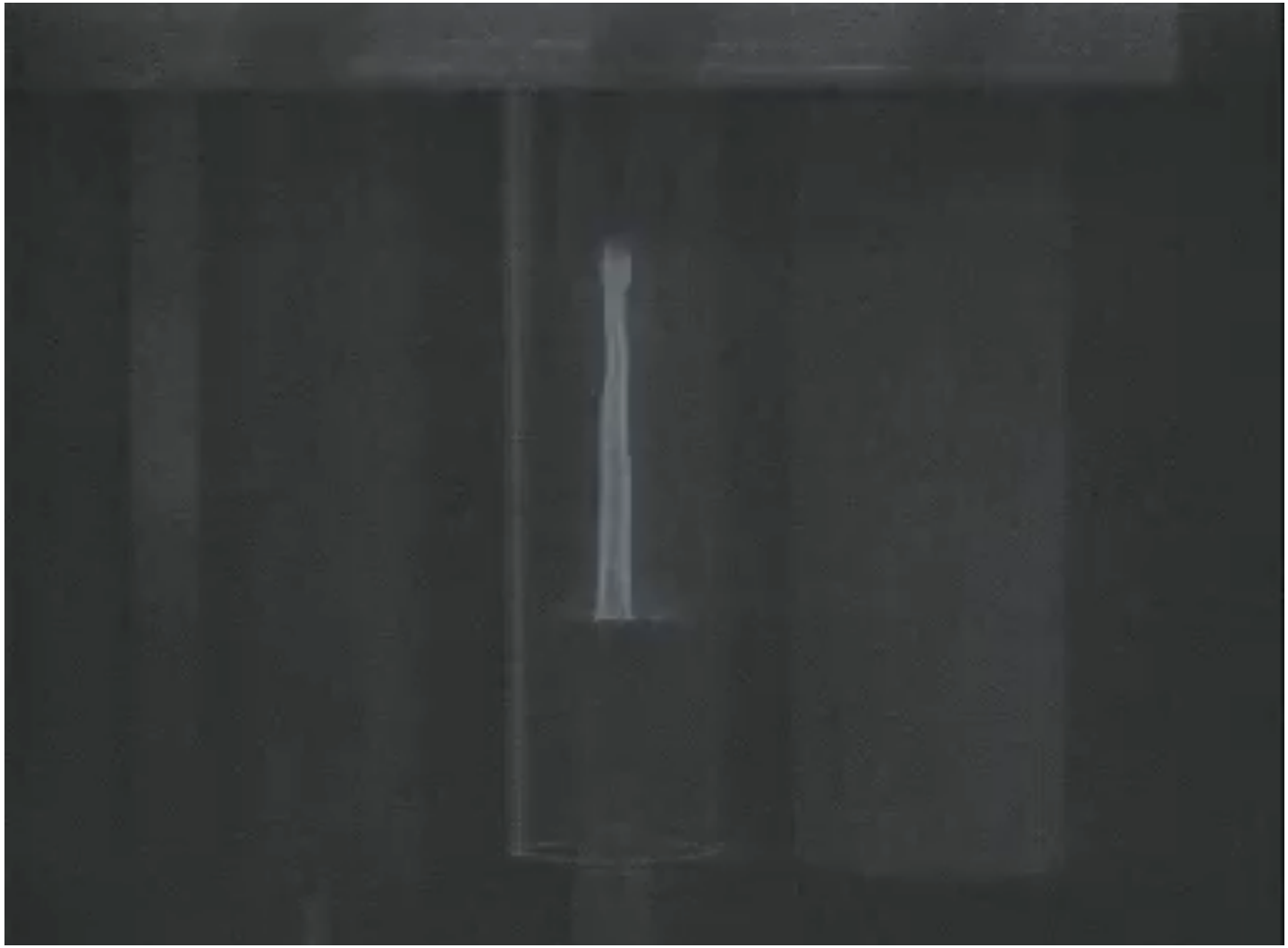


Medium size tube:



What is happening inside ?

A view on the same type of experiment with transparent ducts (Dr Durox, EM2C Paris)



Linear vs non linear. Exp. growth vs limit cycles

The previous equations are linear.

They can tell us whether:

- The system is unstable: $\mathrm{Im}(\omega) < 0$

- The system is neutral: $\mathrm{Im}(\omega) = 0$

- The system is stable: $\mathrm{Im}(\omega) > 0$.

$$x = \hat{x} e^{i\omega t}$$

If the system is unstable (the instability criterion is fulfilled), the instability will grow. Where it will stop cannot be predicted with this linear approach. After the instability starts, different outcomes can be obtained at longer times:

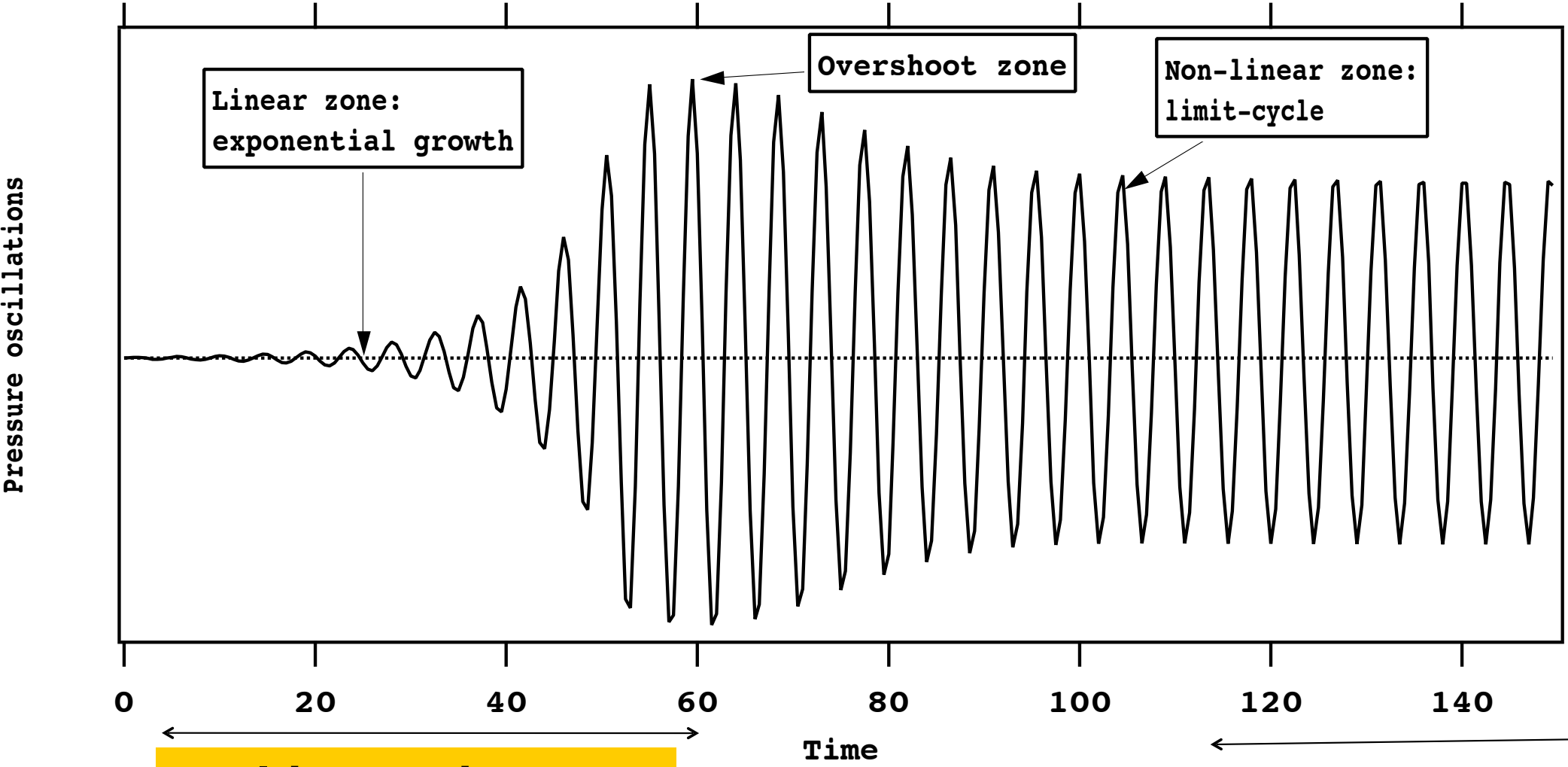
- The system can reach a limit cycle

- The combustor can explode

- The operator may stop combustion because of vibrations

- The system may quench

LIMIT CYCLES



Linear phase
Exponential growth of the amplitude

Non linear phase
Limit cycle

Acoustic solvers

?

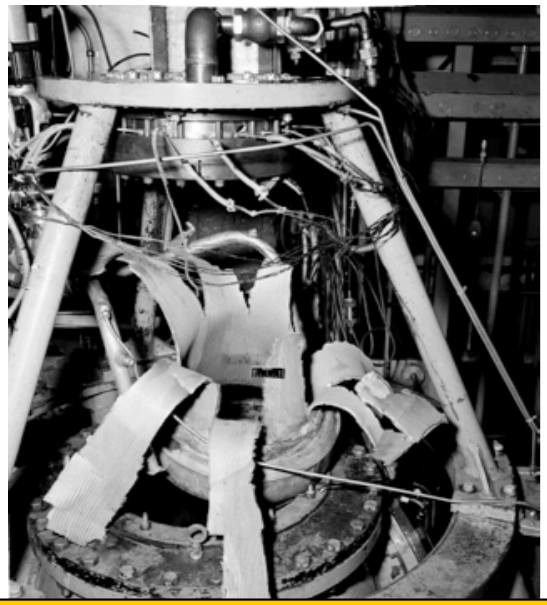
LES and expts

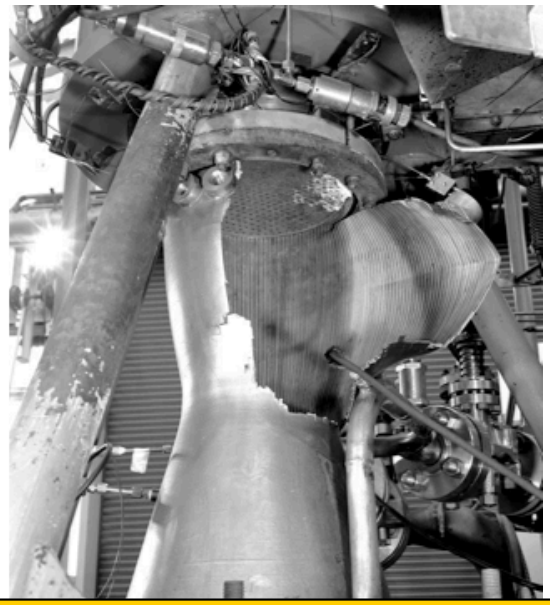
DESTRUCTION

Limit cycles are only ONE form of final results in thermoacoustics:

If the loss term is not sufficient, the amplitude of oscillations might grow until something really unpleasant occurs:

1- the combustor can explode





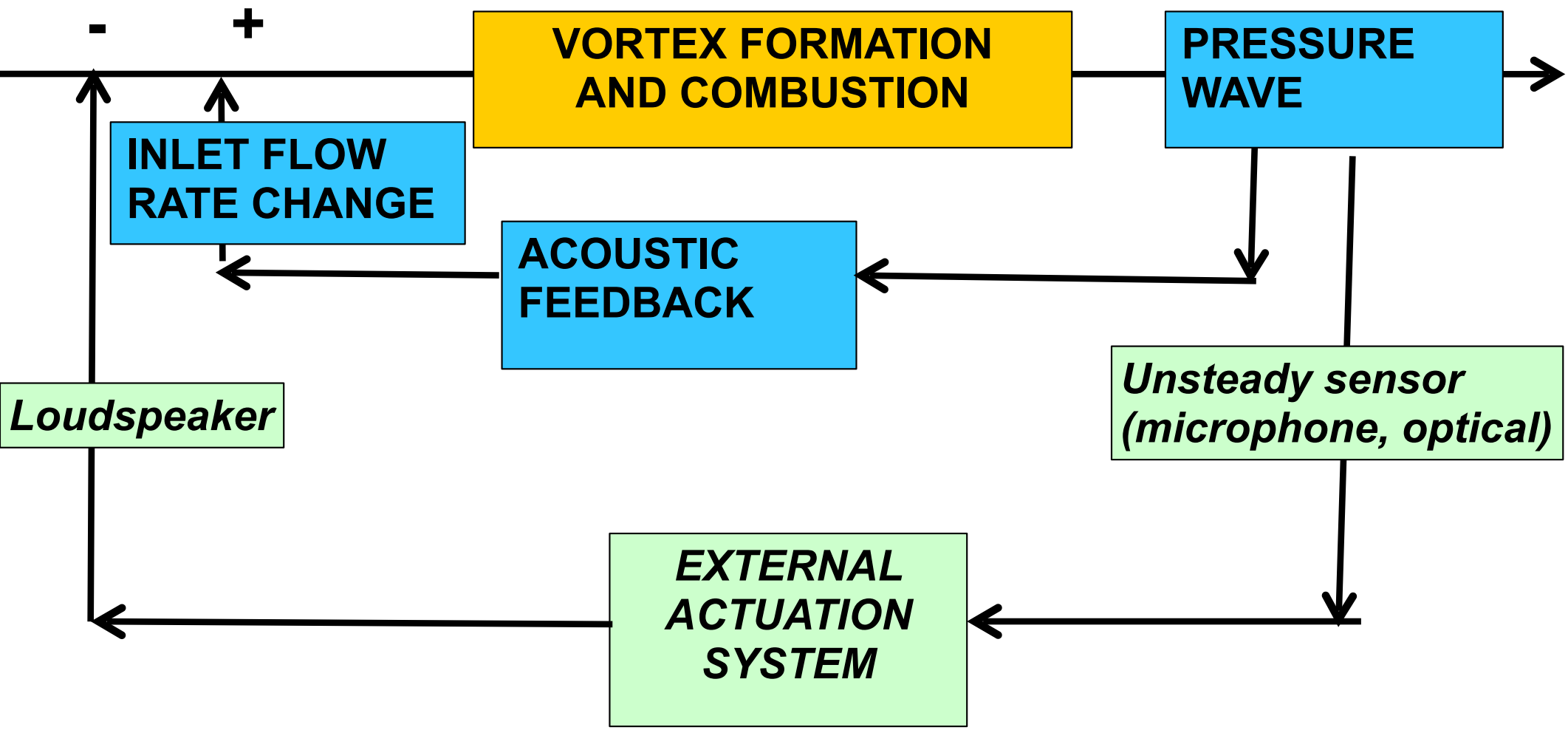
In industrial gas turbines, the system switches off when pressure oscillation or structure vibration levels are too high

2- the flame can also quench, unable to resist to the oscillations it has created. This can happen without making any noise.

3- the flame can also move to another place (flashback), where it is not supposed to be

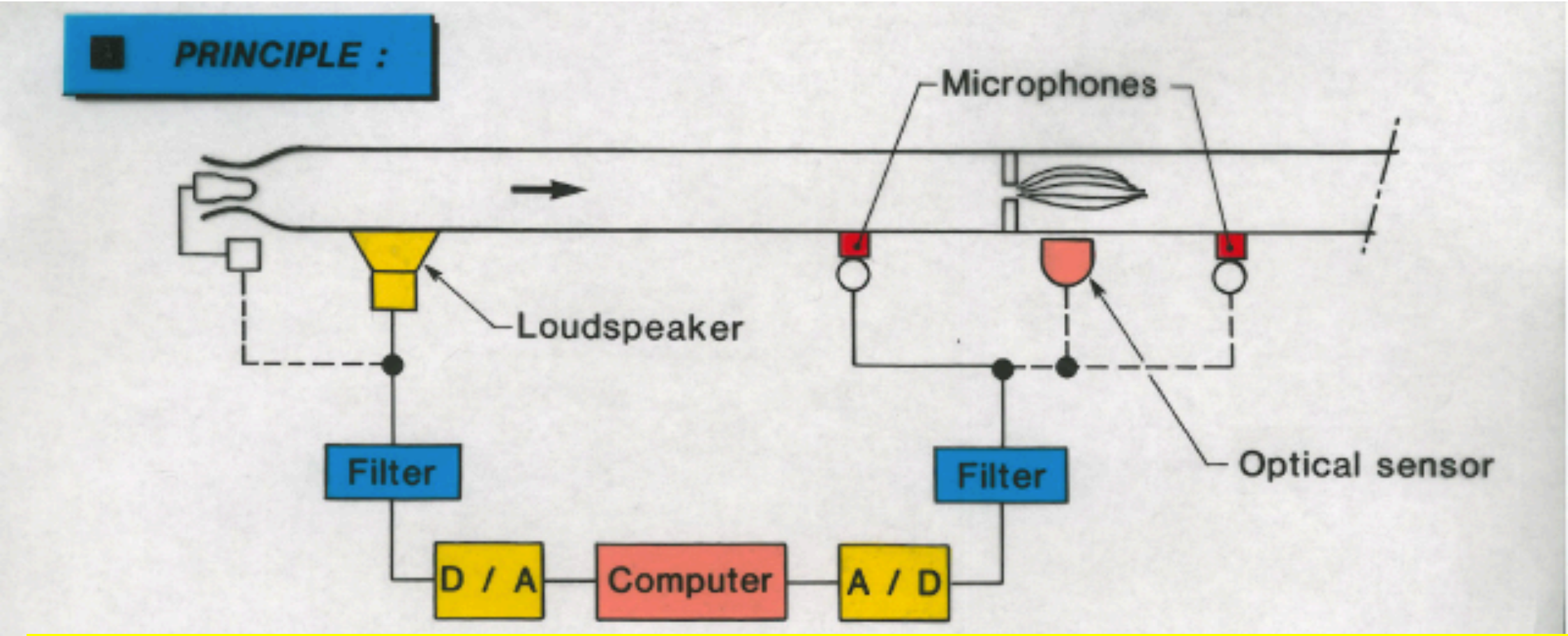
How do we know ? Thanks to active control (see review paper on active control of combustion: McManus, Poinsot and Candel, PECS, 1993, 19), a method which was studied intensively in the 90s.

ACTIVE CONTROL OF COMBUSTION INSTABILITIES:



What is active control of combustion instabilities ?

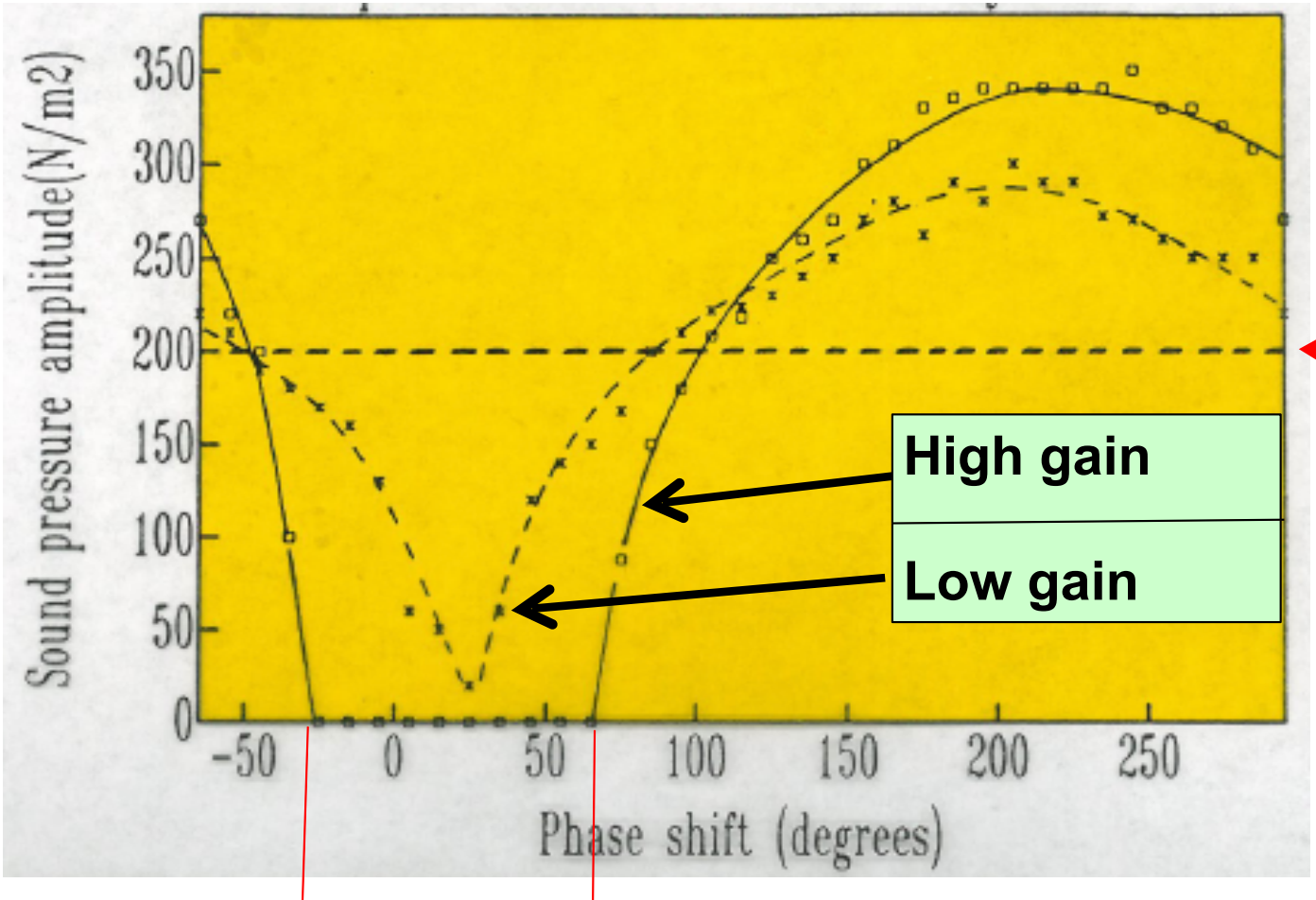
Example for a laminar Bunsen flame



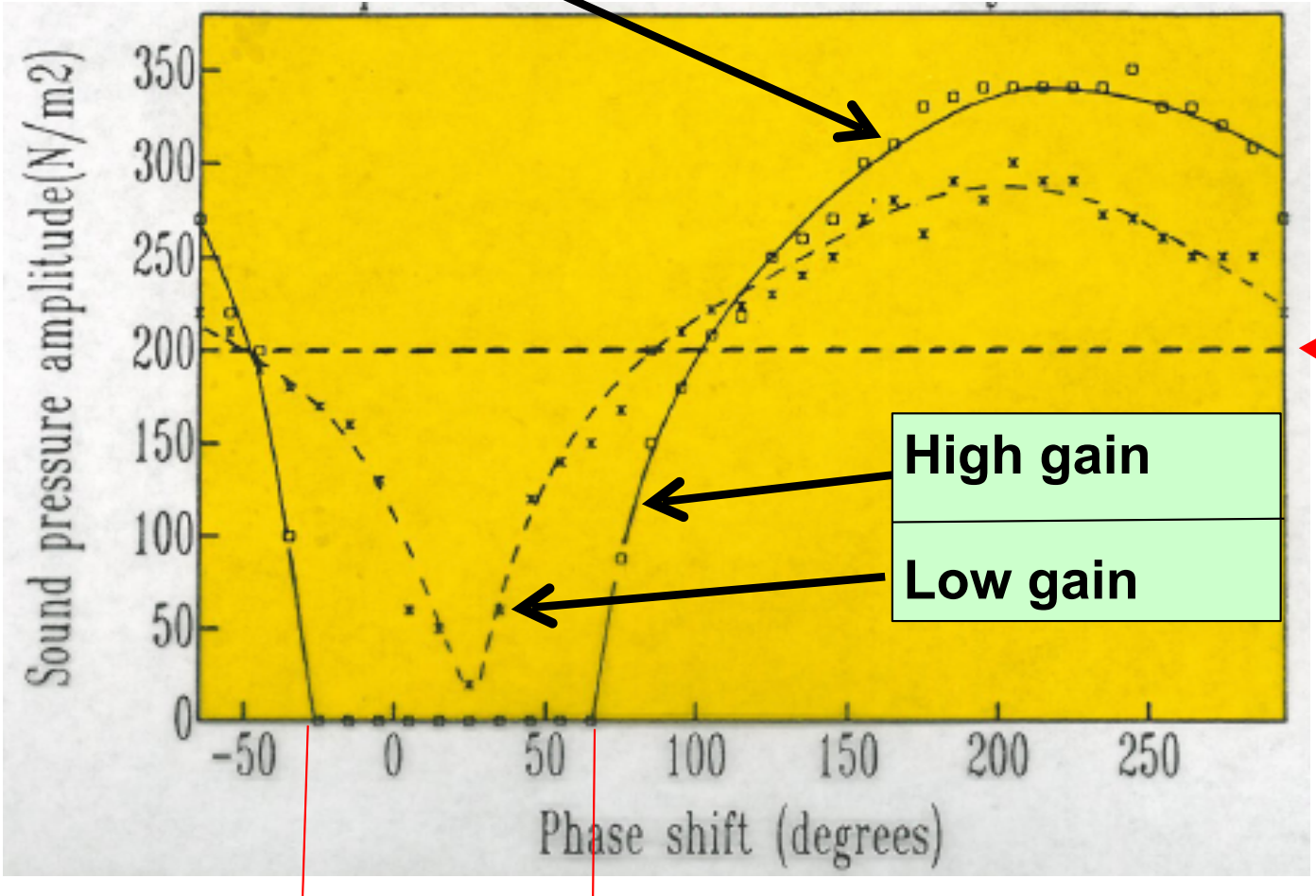
Sending back to the flame, its own acoustic production

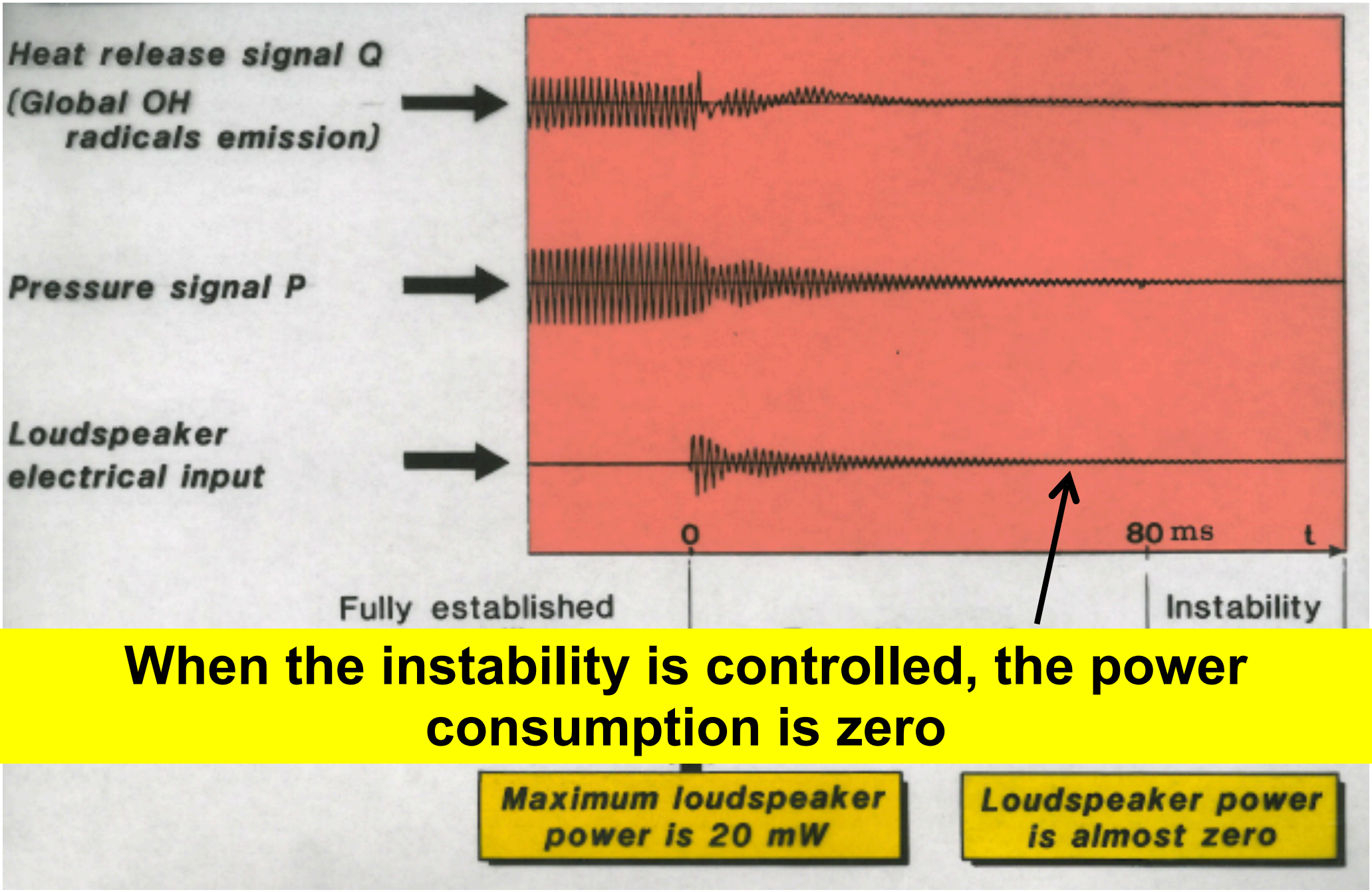
Similar to antinoise in the field of acoustics

When the gain is small, the instability is reduced
When the gain is larger, the instability is killed



When the phase is in the right range, the instability is reduced BUT if the phase is not in the right range, the instability is amplified ! -> efficient method but delicate





When the instability is controlled, the power consumption is zero

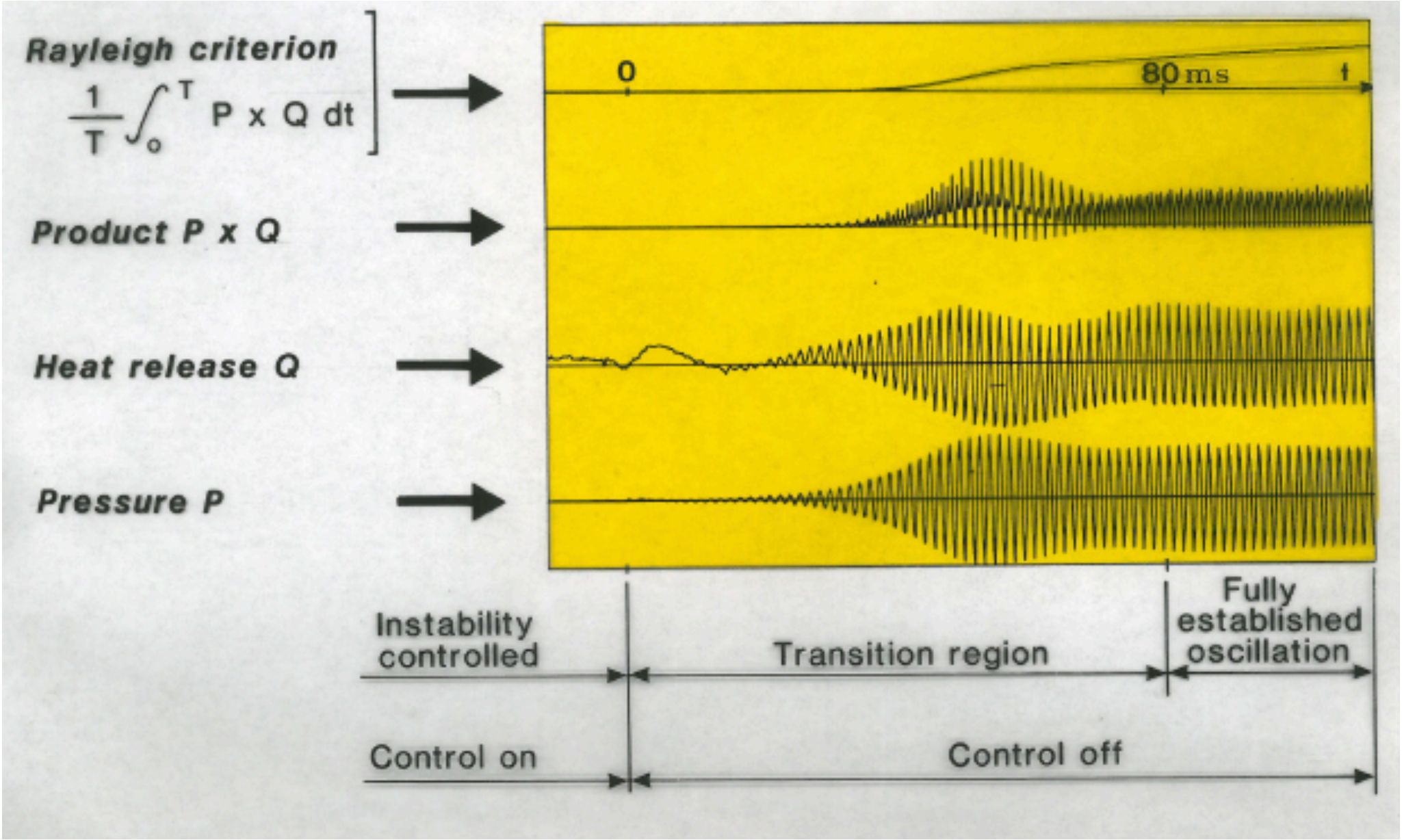
Active control research for thermoacoustics was strong in the 90s: patents taken in labs (EM2C) and companies (GE). Demonstrations on real engines worked:

- **Industrial gas turbines: active control was used in Siemens gas turbines** (Seume, J., Vortmeyer, N., Krause, W., Hermann, J., Hantschk, C., Zangl, P., Gleis, S., and Vortmeyer, D. Application of active combustion instability control to a heavy duty gas turbine. ASME Journal of Engineering for Gas Turbines and Power 120 (1998), 721–726.)

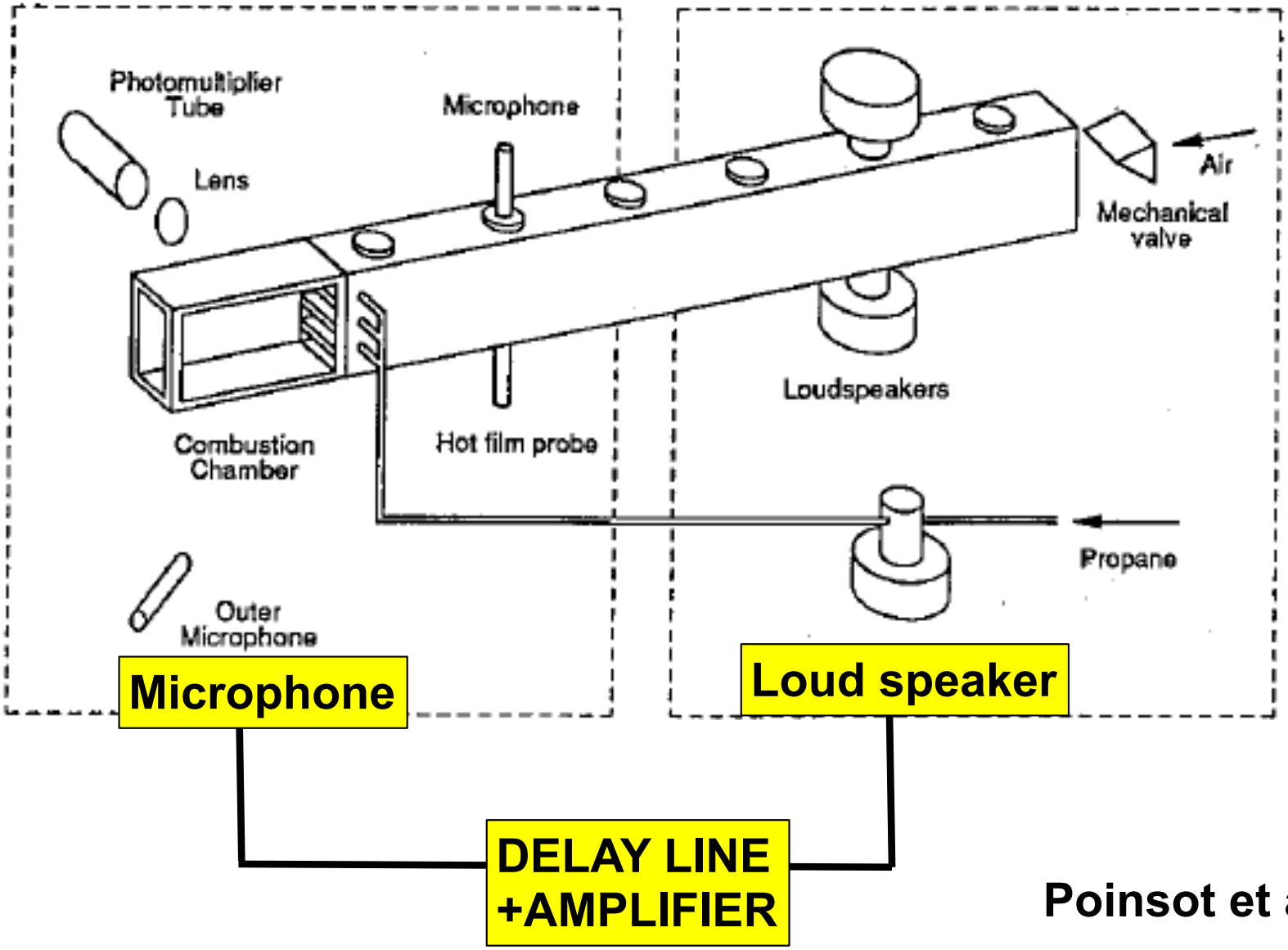
- **For aeroengines, tests worked at GE or SNECMA but certification issues killed the idea**

But for scientific investigations, active control remains a great tool because it allows to let the instability start 'on request'

Initiating an instability on demand with active control:

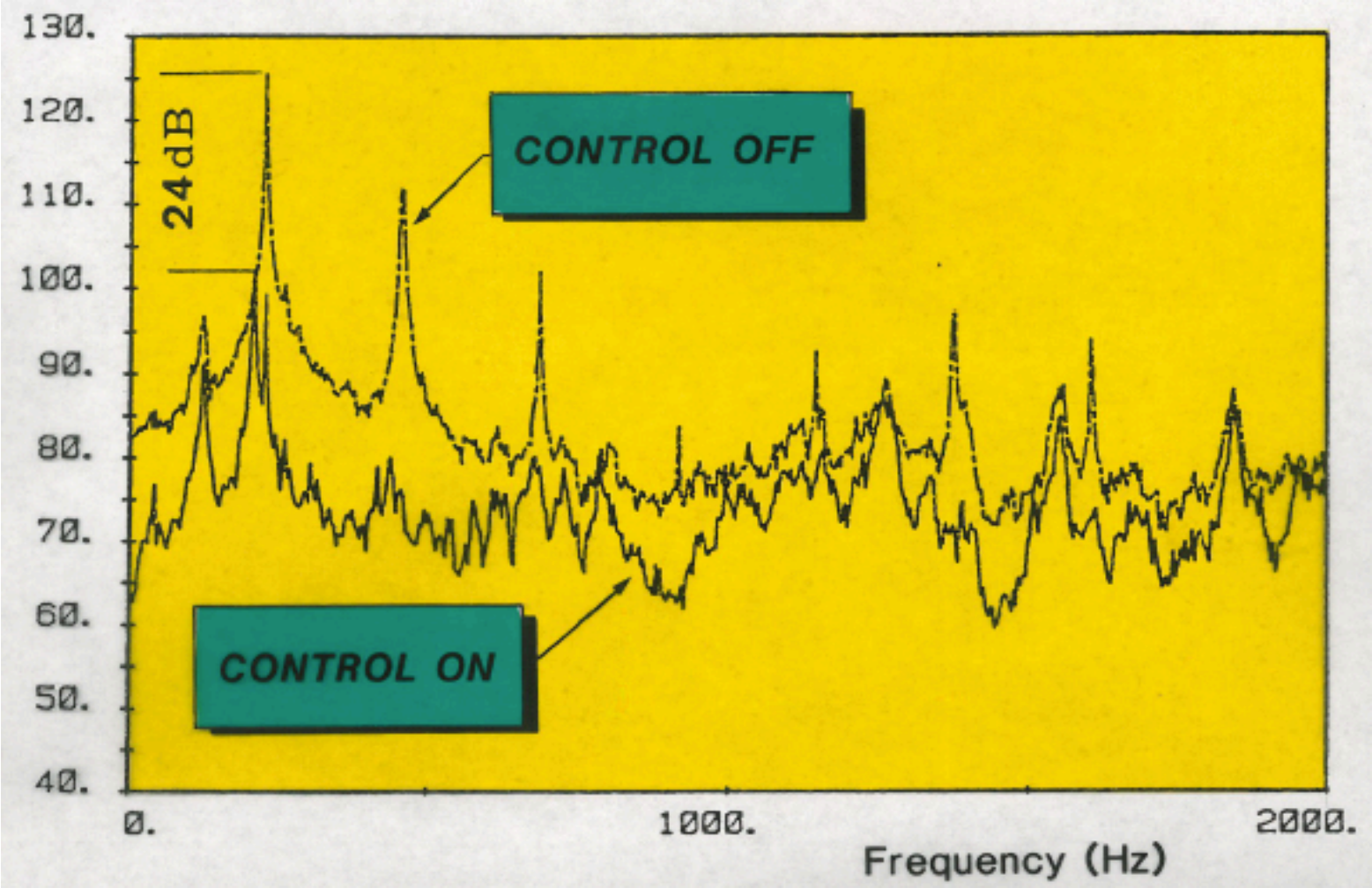


Other example: a turbulent burner. This combustor is unstable but it can be stabilized using active control:



Poinsot et al J. Phys. 1992

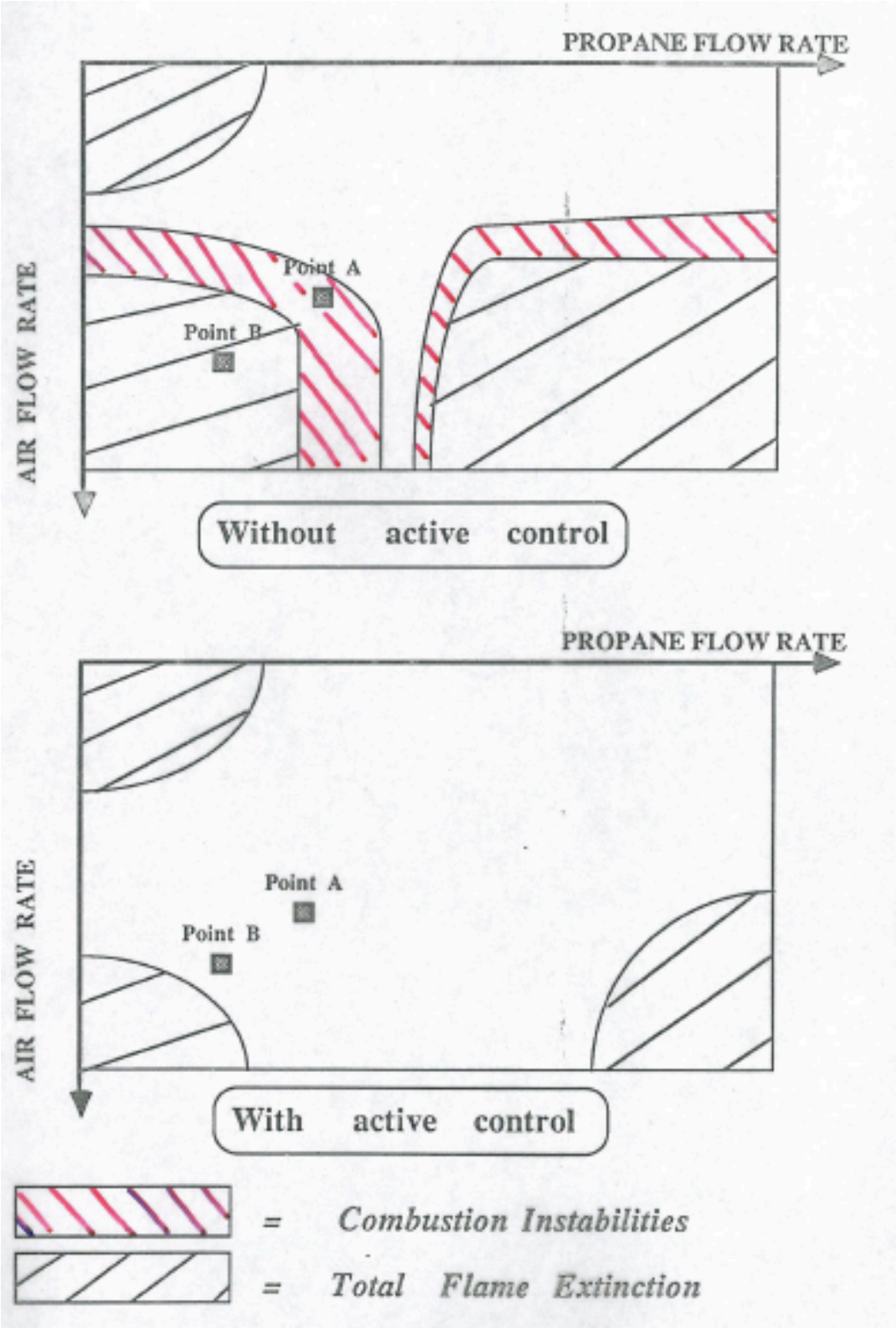
Point A: with and without control



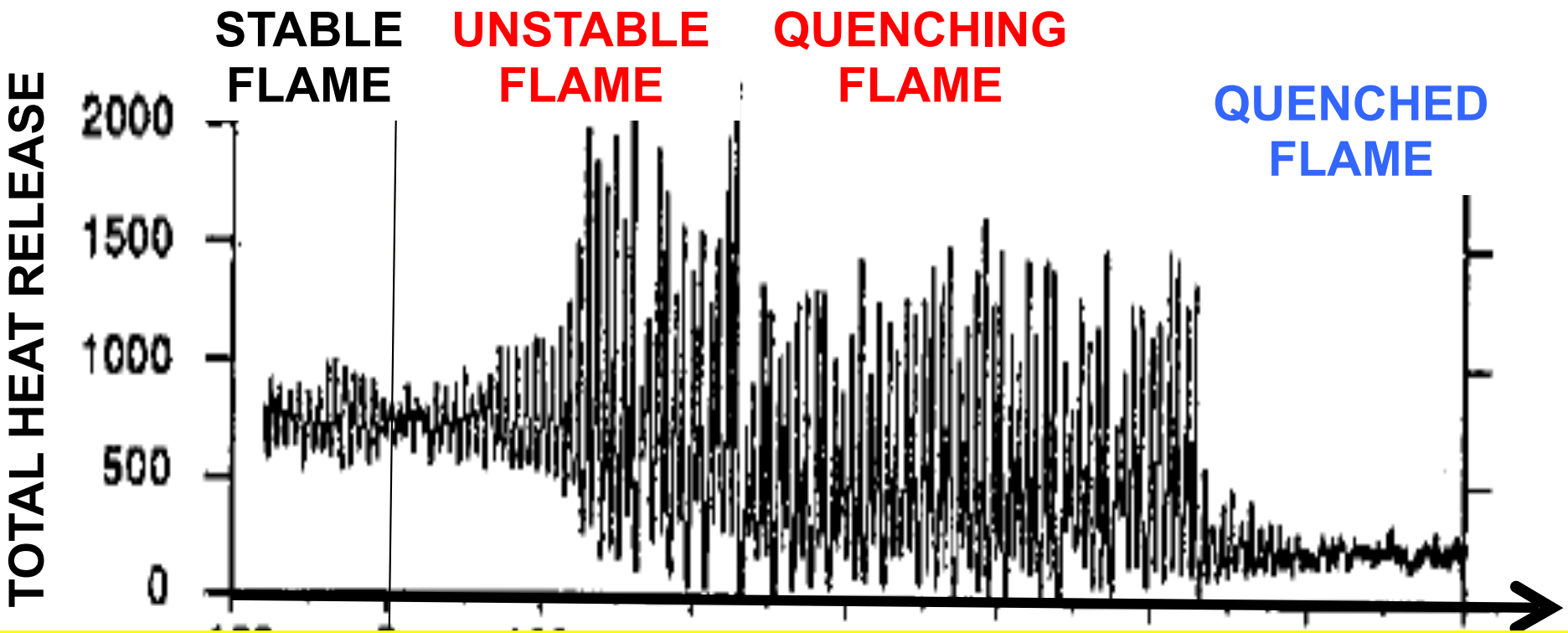
Active control allows not only to control unstable modes but also to extend the domain of operation of the burner (in a fuel/ air flow rate diagram):

- with control, point A is unstable (limit cycle) without control and becomes stable with control

- with control, point B does not burn without active control. With control it burns and is stable

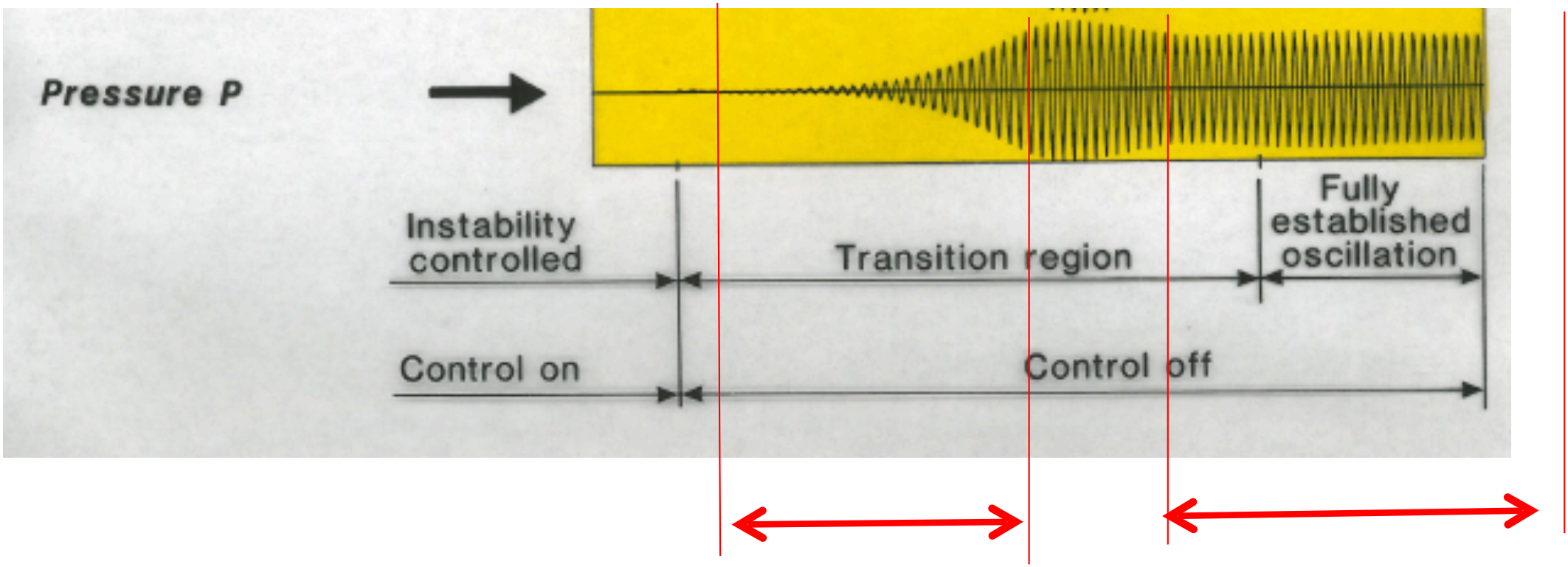


For point B: the flame starts oscillating and ... quenches !



THIS IS AN EXAMPLE WHERE 'FLAME QUENCHING' IS DUE TO FLAME INSTABILITIES

Another capacity of active control: measure the growth rate in the linear phase



Linear phase (exponential growth)
This is what models usually predict

Limit cycle (zero growth)
This is what experimentalists see

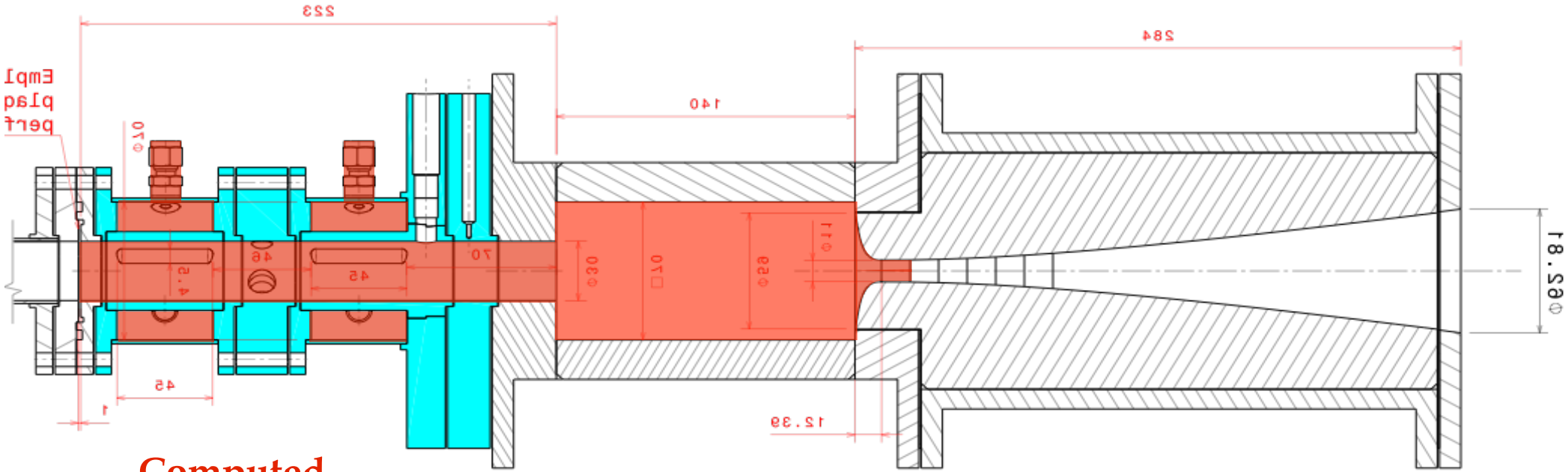
Instabilities and flashback

Another possible event for a flame submitted to acoustic instabilities is to flashback

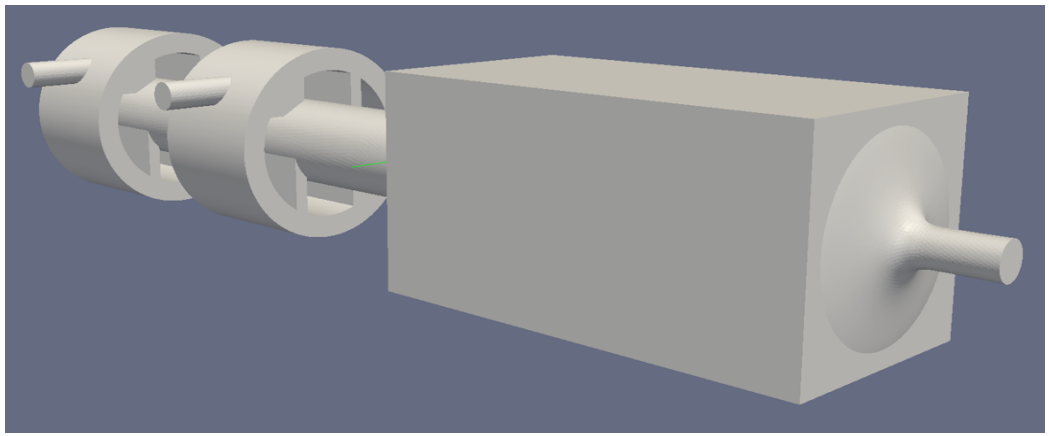
Why ? Because acoustic velocities can be large enough to push the flame upstream from the chamber

Example: an EM2C turbulent flame. Stabilization behind a dump plane.

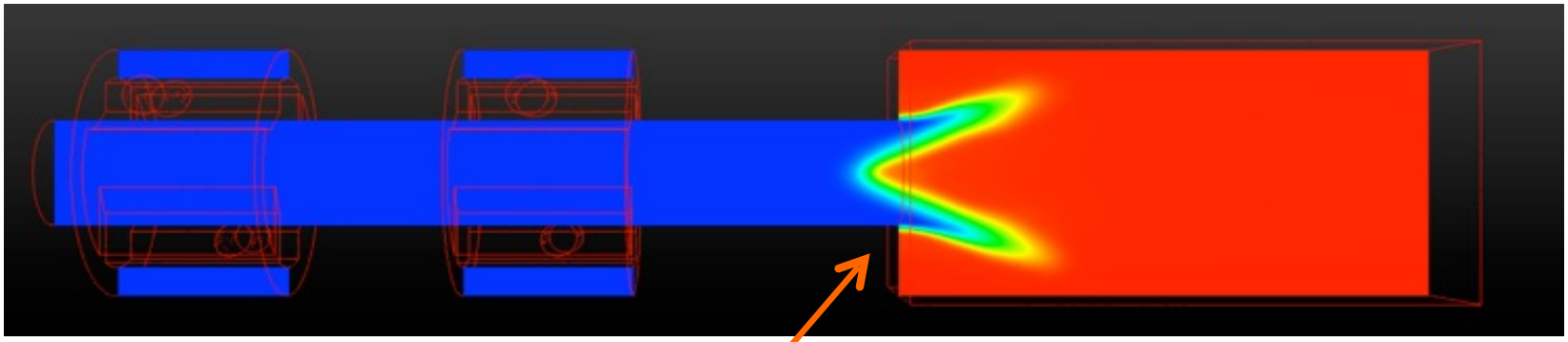
II - The CESAM-HP setup at Ecole Centrale Paris



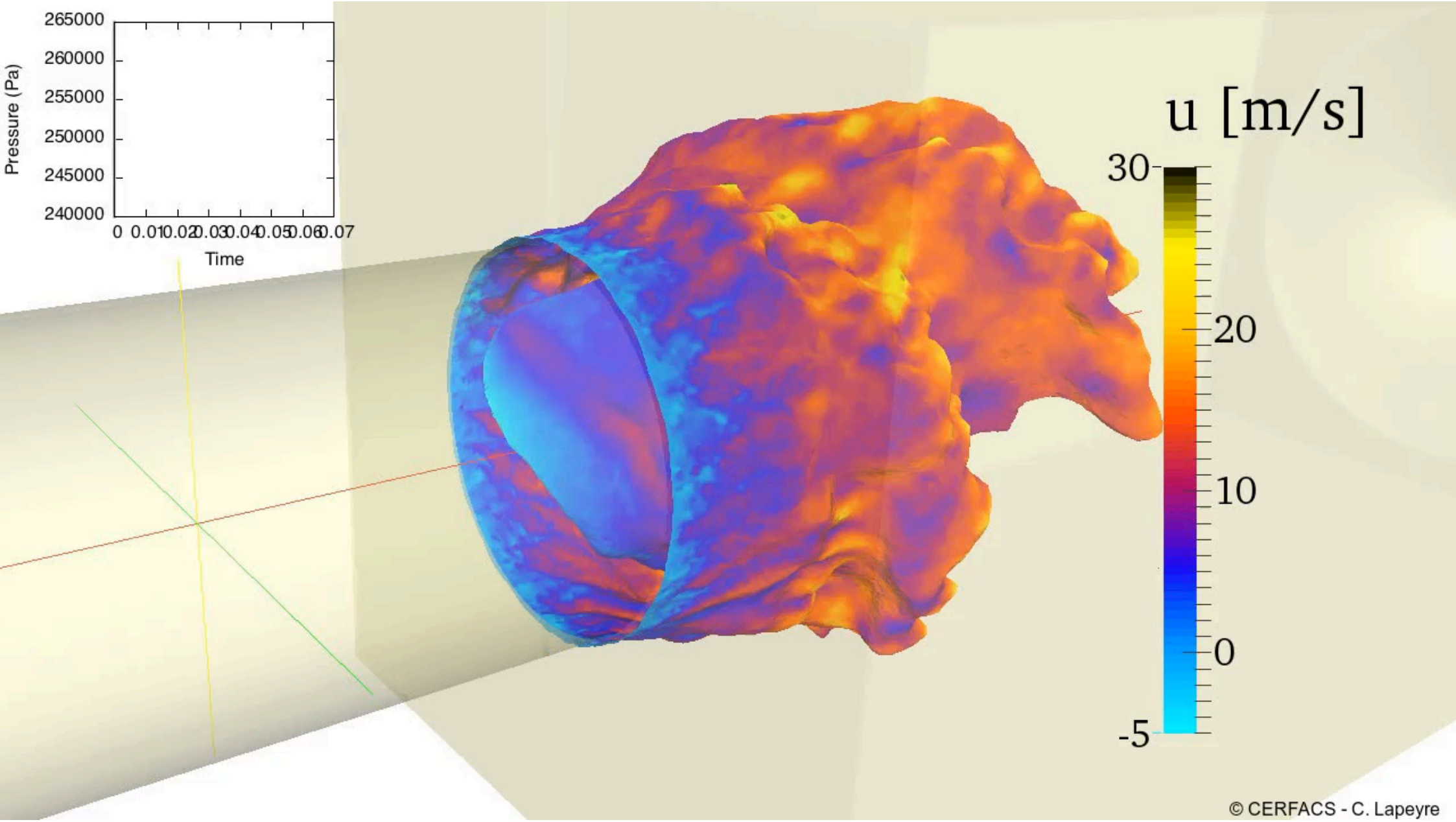
Computed Domain



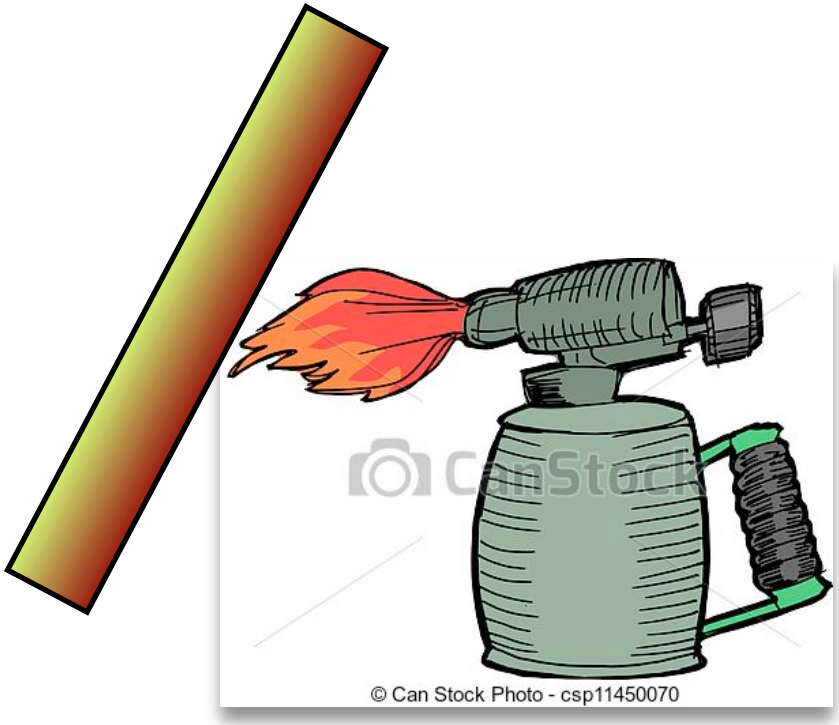
Mean temperature field

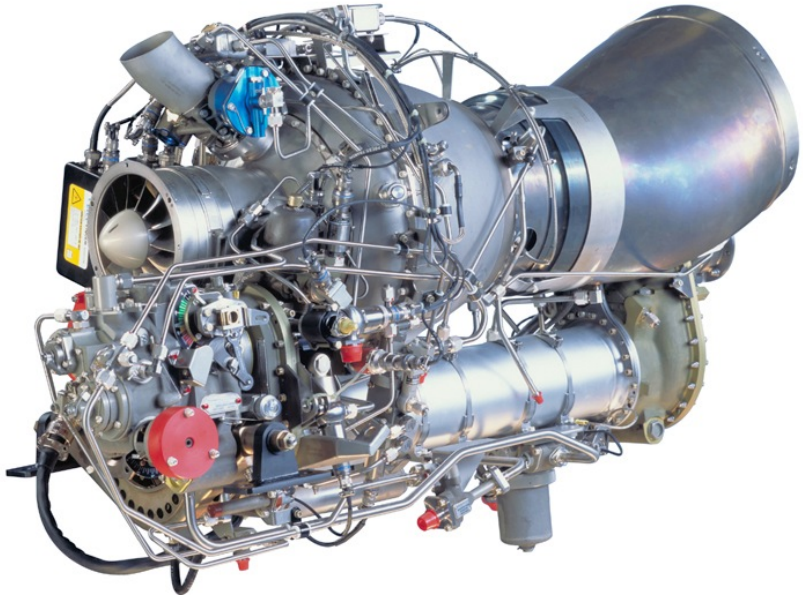


This is where the flame SHOULD be


265000
260000
255000
250000
245000
240000
Pressure (Pa)
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07
Time
u [m/s]
30
20
10
0
-5
© CERFACS - C. Lapeyre

Flame / wall interactions





T. Poinsot, *IMF Toulouse, CNRS and INPT, CERFACS*
L. Gicquel, G. Staffelbach, O. Vermorel, P. Wolf, M. Boileau, O. Colin, D. Veynante, L. Selle, C. Sensiau, L. Benoit, E. Gullaud, C. Berat, V. Moureau

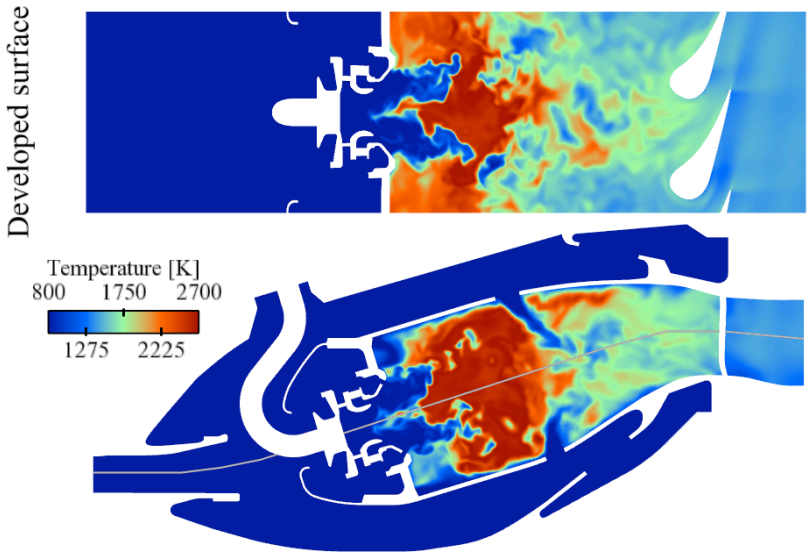
Copyright Dr T. Poinsot 2023

FLAMES AND WALLS: WHY DO WE CARE ?

FLAMES ⇄ **WALLS** → ***POLLUTANTS***

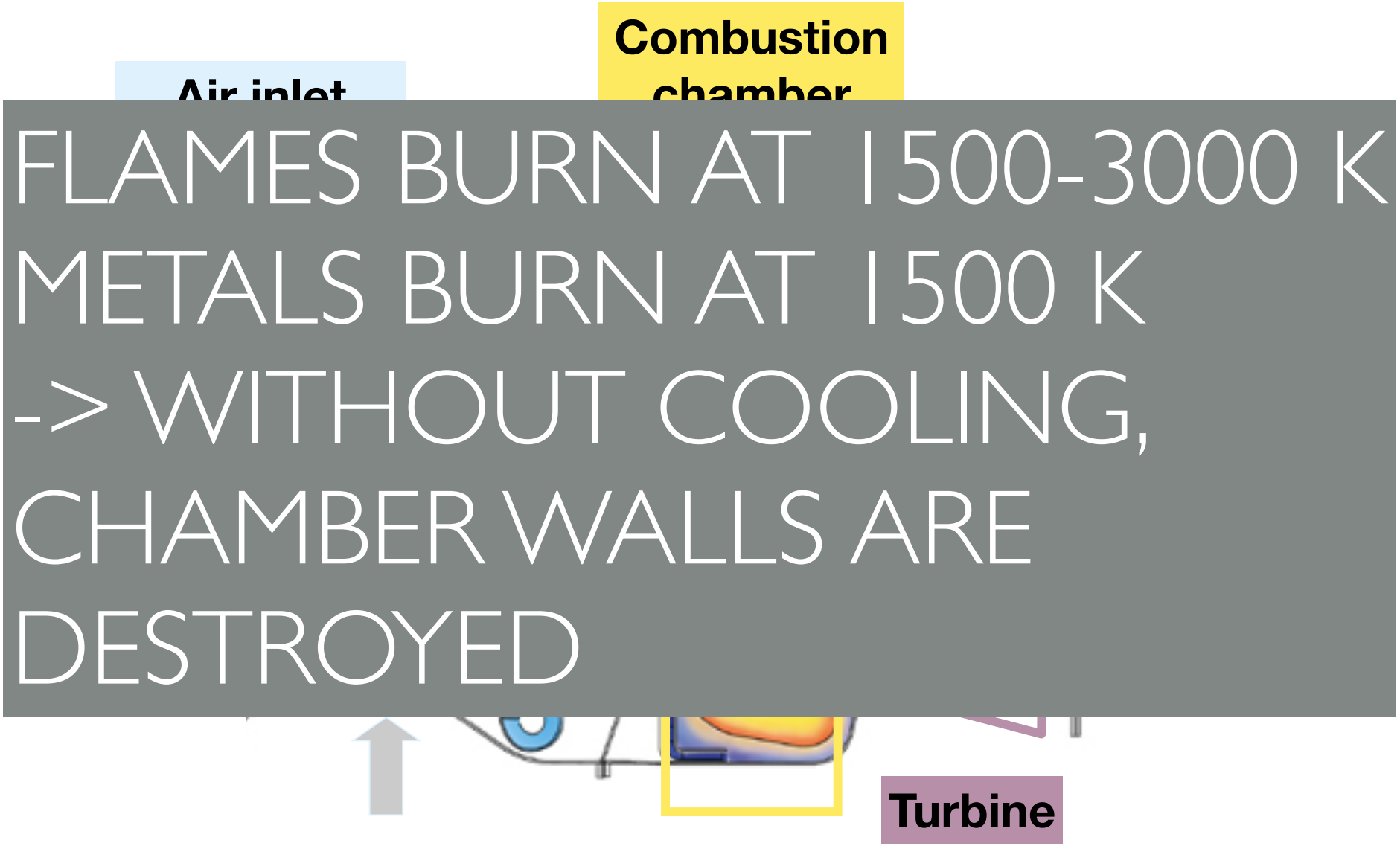
WALLS → ***ACOUSTICS*** → ***INSTABILITIES*** → **FLAMES**

Ch. 7



DEM21 - AVBP

Context: many walls in most combustors:



FLAMES BURN AT 1500-3000 K
METALS BURN AT 1500 K
-> WITHOUT COOLING, CHAMBER WALLS ARE DESTROYED

Combustion chambers in a gas turbine:

1- Must burn all the injected fuel with high efficiency (99 %)

2- Must limit pollutant emission

3- Must **NOT** burn walls.

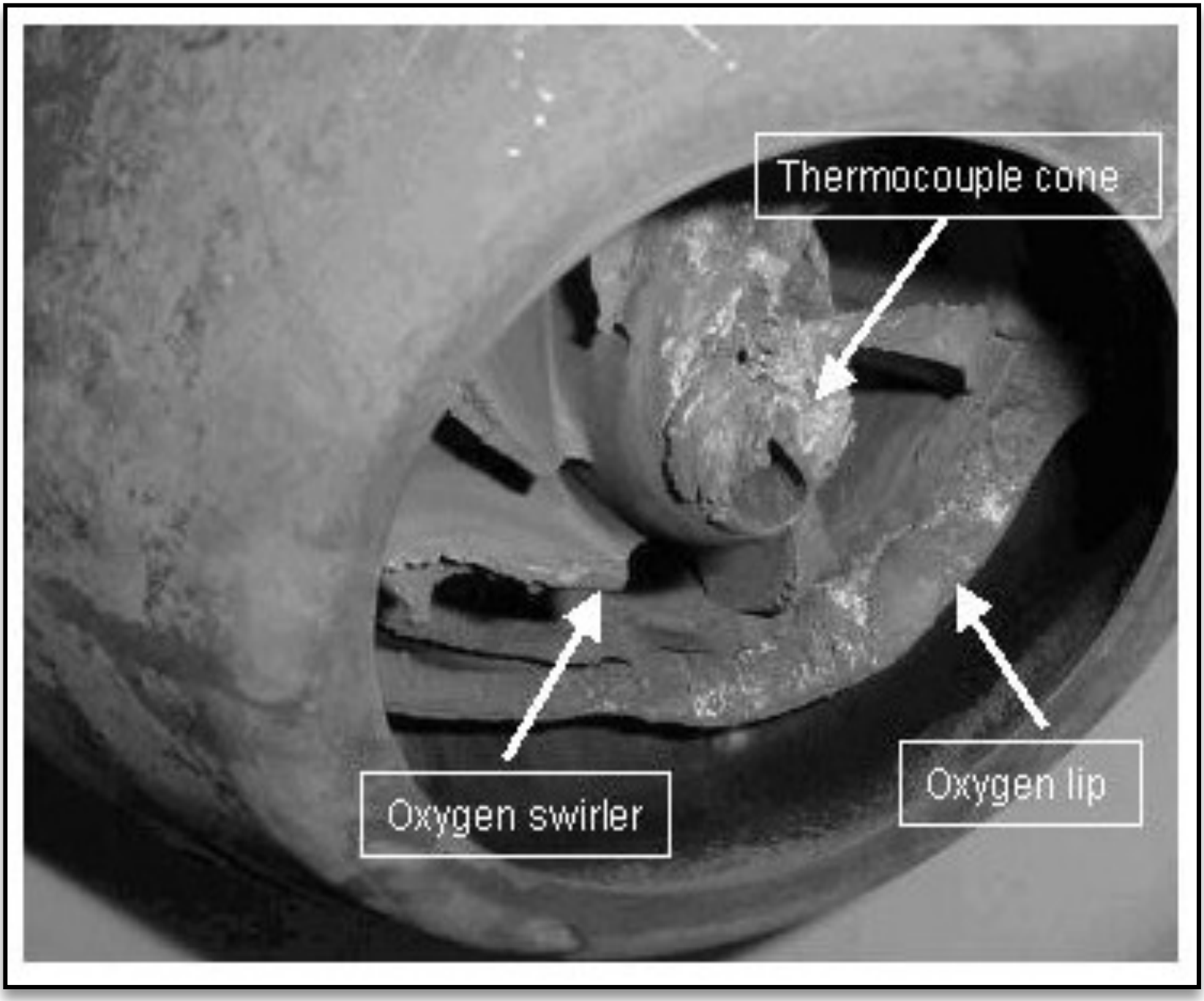


1 is easy

2 is difficult

3 is mandatory

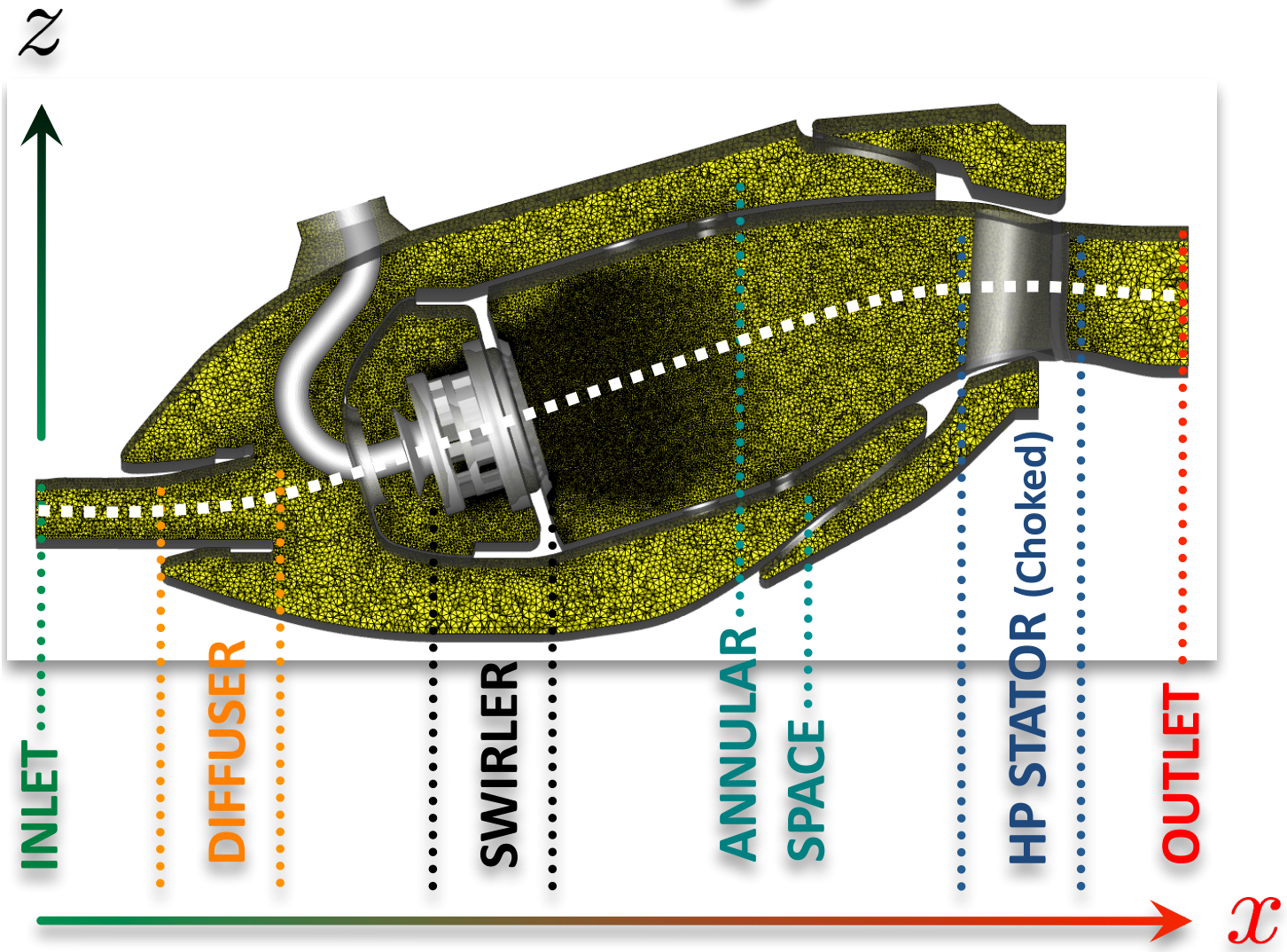
CATASTROPHIC FLAME-WALL INTERACTION

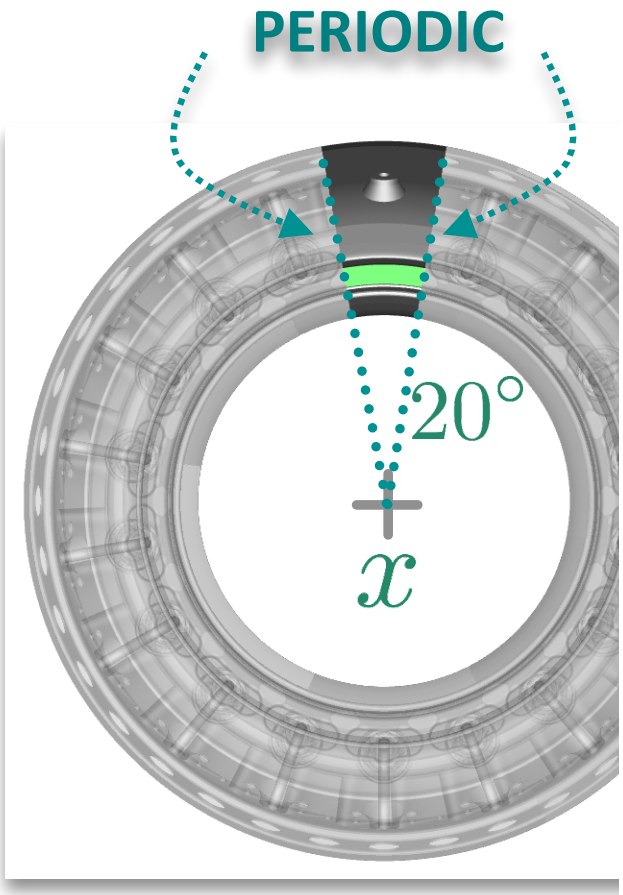




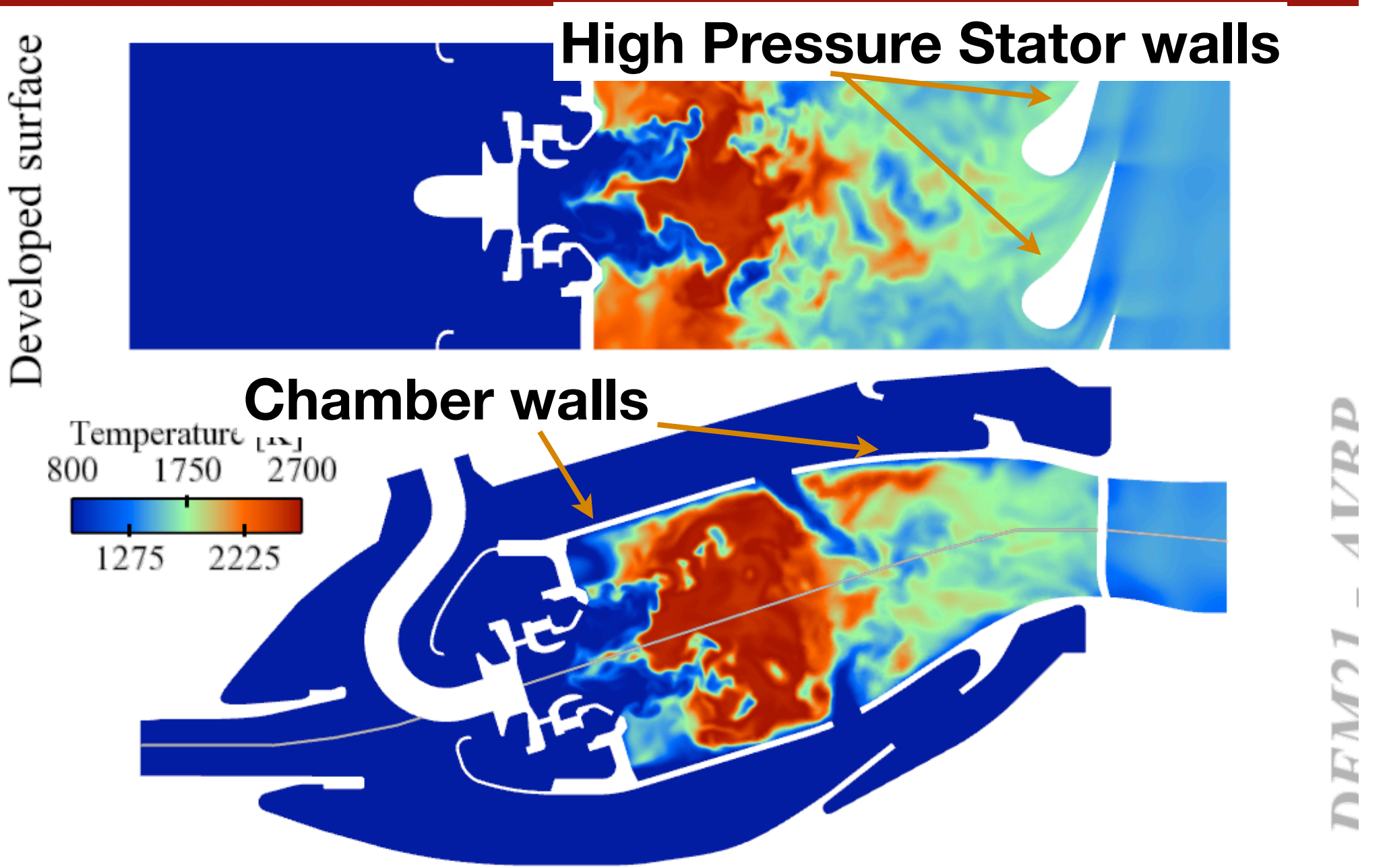
Walls ?

Aero-engine combustor sector





Which walls ?


High Pressure Stator walls
Chamber walls
Developed surface
Temperature [K]
800
1750
2700
1275
2225

Which walls ?

- Combustion chamber walls see high gas temperatures: must be cooled and protected by multiperforated films
- High Pressure stator walls: cooled by internal air circulation (and sometimes films)
- Turbine vanes: cooled in aircraft engines but not in helicopters
- Rocket engines: the walls of the nozzle

The design of cooling systems controls the lifetime

Which type of flame / wall interaction ?

- In this talk: walls do NOT (should not...) burn: no chemistry takes place at the wall surface

- The problem is to make sure that this does not happen. The wall must remain cold -> the flux must remain limited

WHAT IF THE WALL REALLY CANNOT REMAIN COLD?

Then chemical reactions will take place at the wall: the wall ... burns

Sometimes, this is done on purpose: for example, in carbon/carbon nozzles for rocket engines



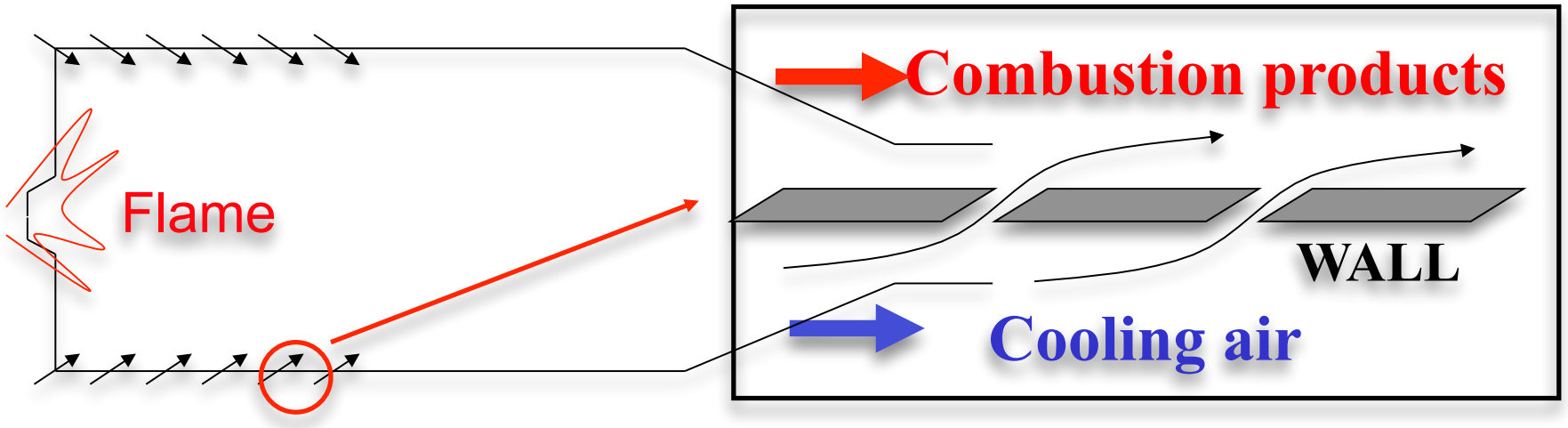
See Popp, P., M. Smooke, et Baum M. (1996) “Heterogeneous/ homogeneous reactions and transport coupling during flame-wall interaction”, Proc. of the Combustion Institute 26: 2693-2700.

Protecting walls by air: multiperforation (effusion cooling)

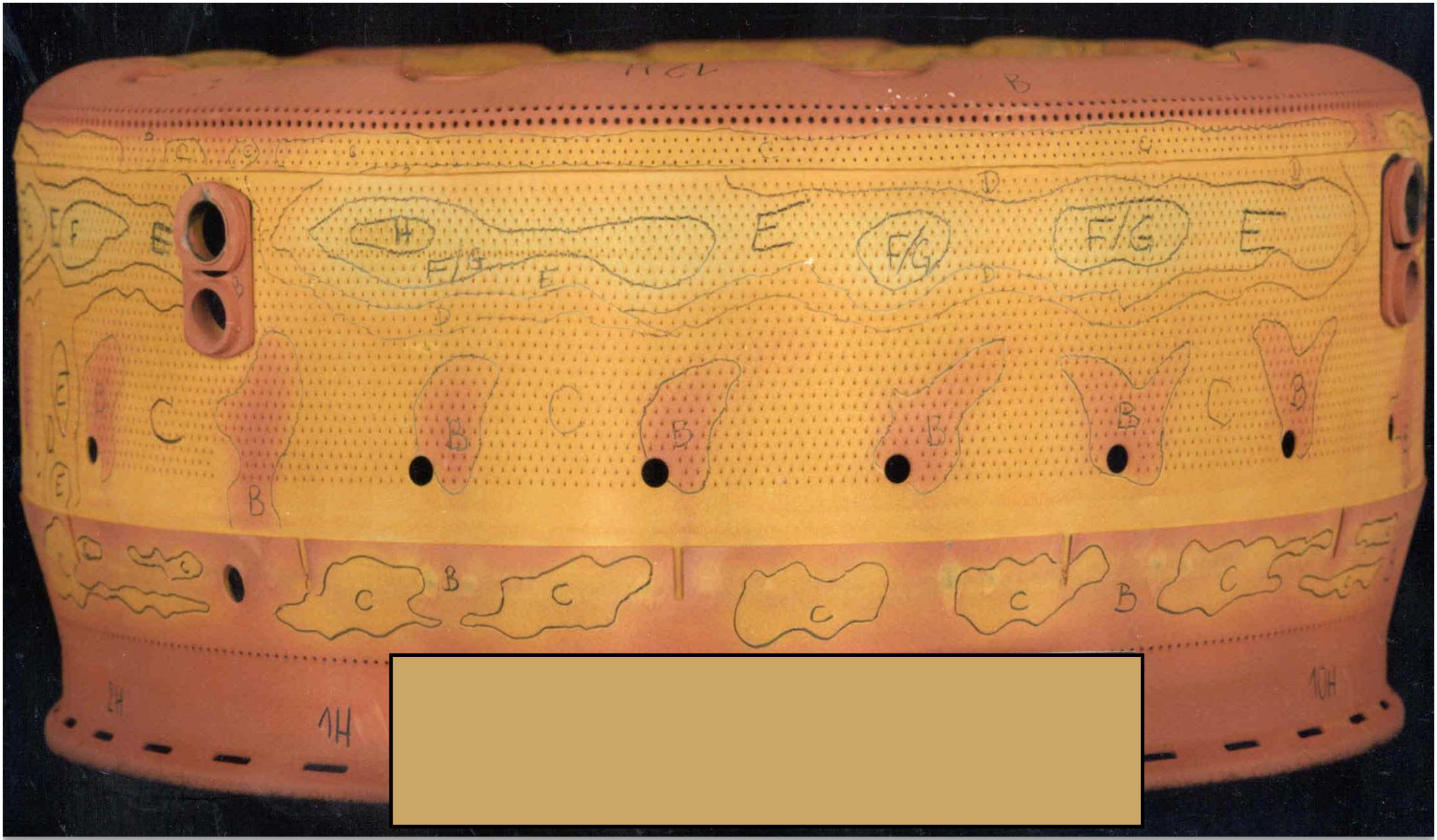
Effusion cooling:

Cooling air injected in the chamber through small holes (typically 0.5 mm)

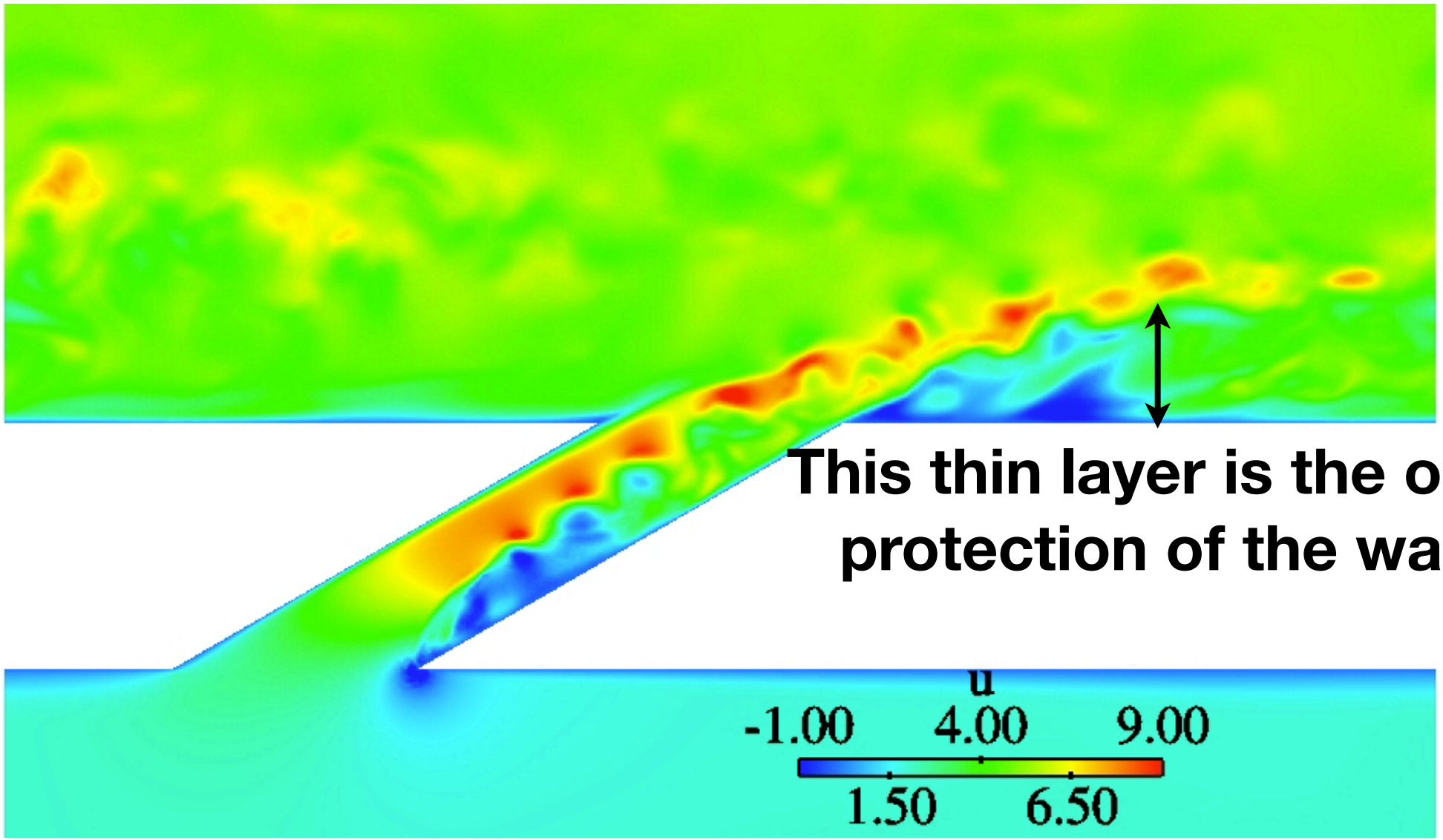
=> Protecting film at the wall



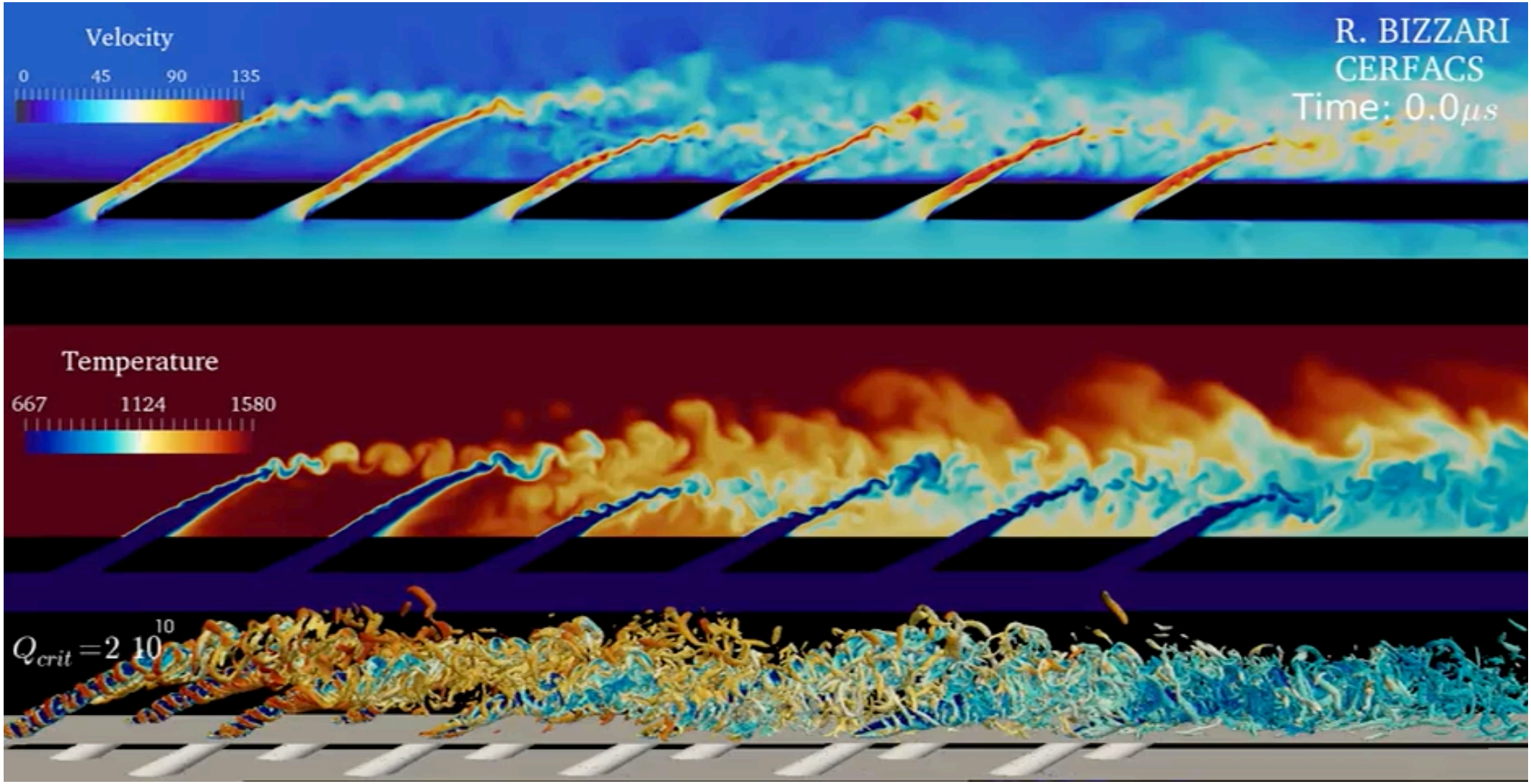
Multiperforated chamber

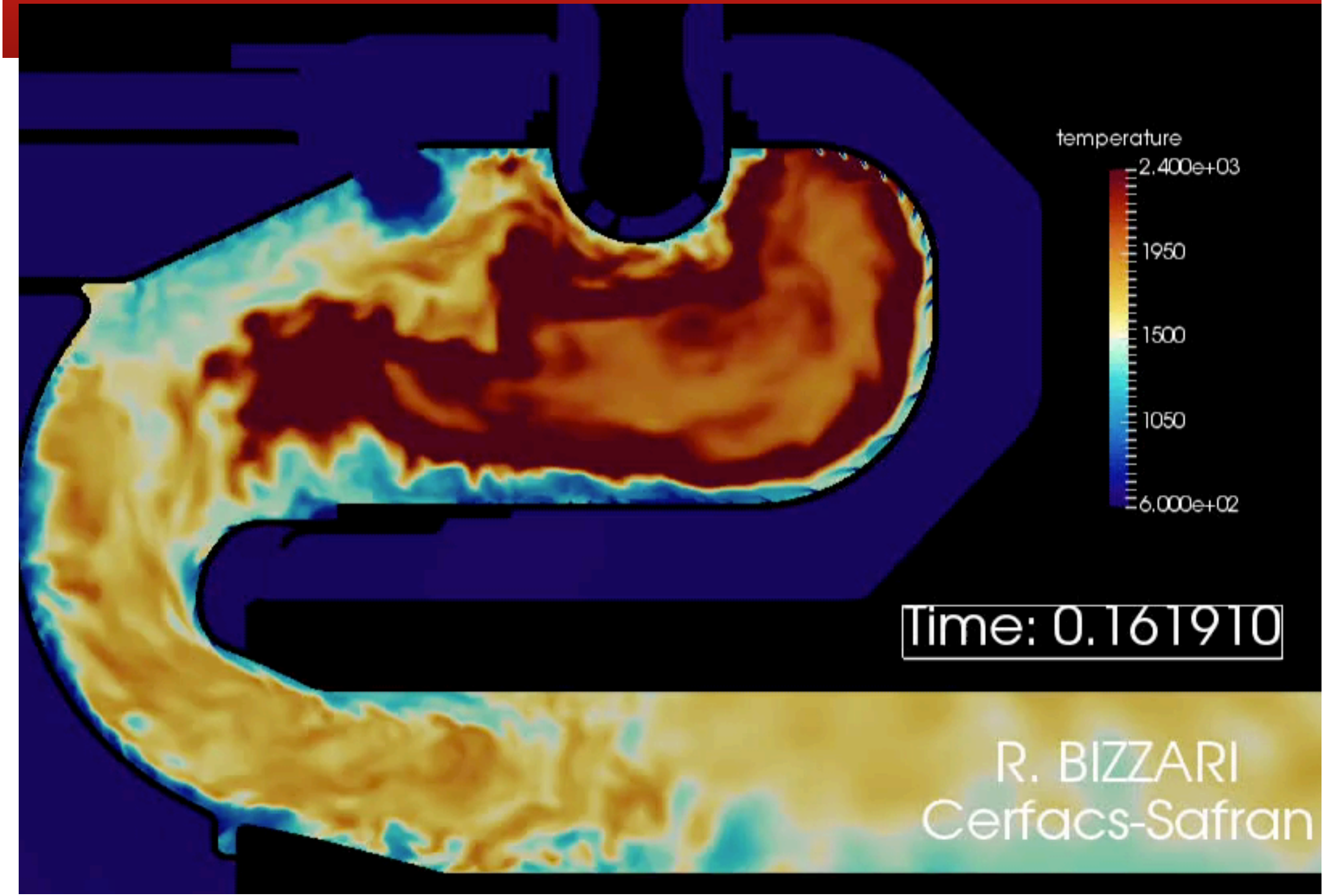


Flow in ONE hole:

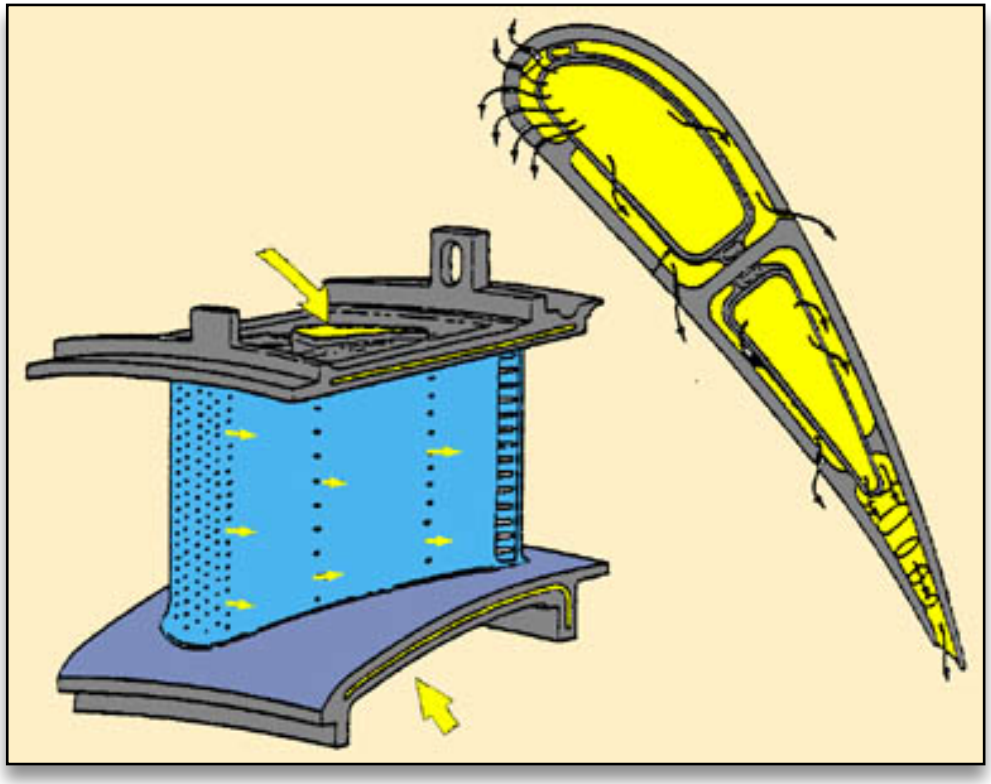


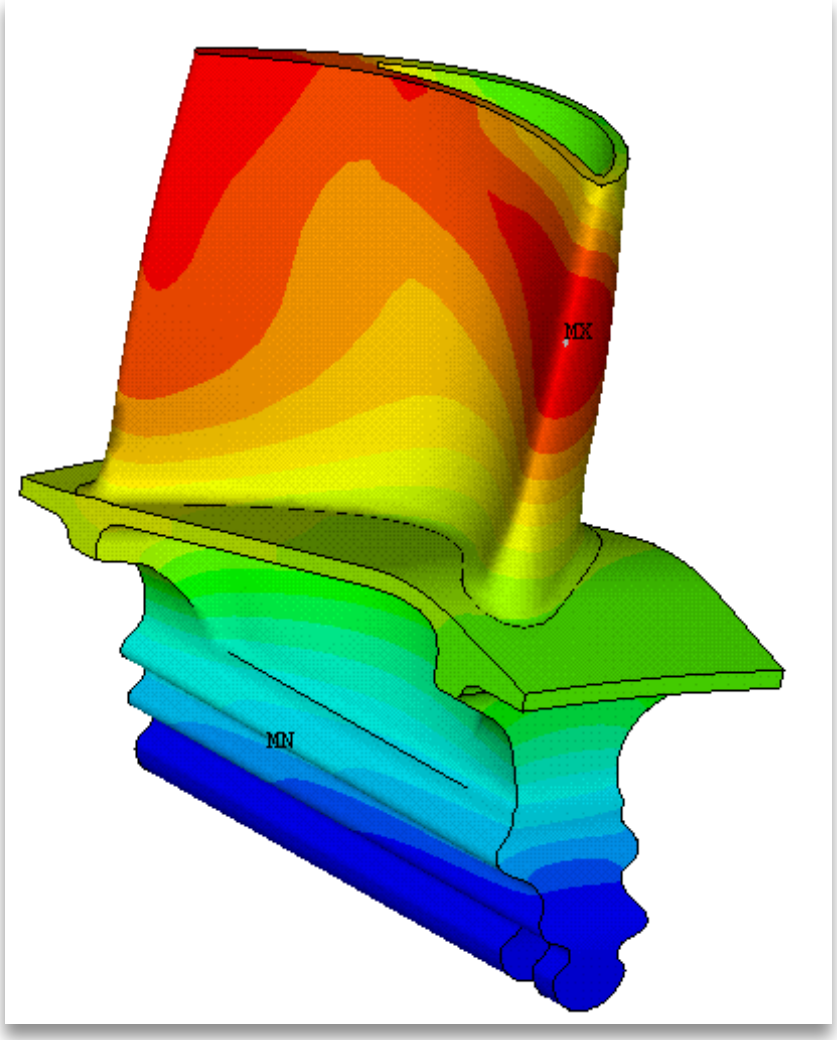
This thin layer is the only protection of the wall


Velocity
0
45
90
135
R. BIZZARI
CERFACS
Time: 0.0μs
Temperature
667
1124
1580
$Q_{crit} = 2\ 10^{10}$

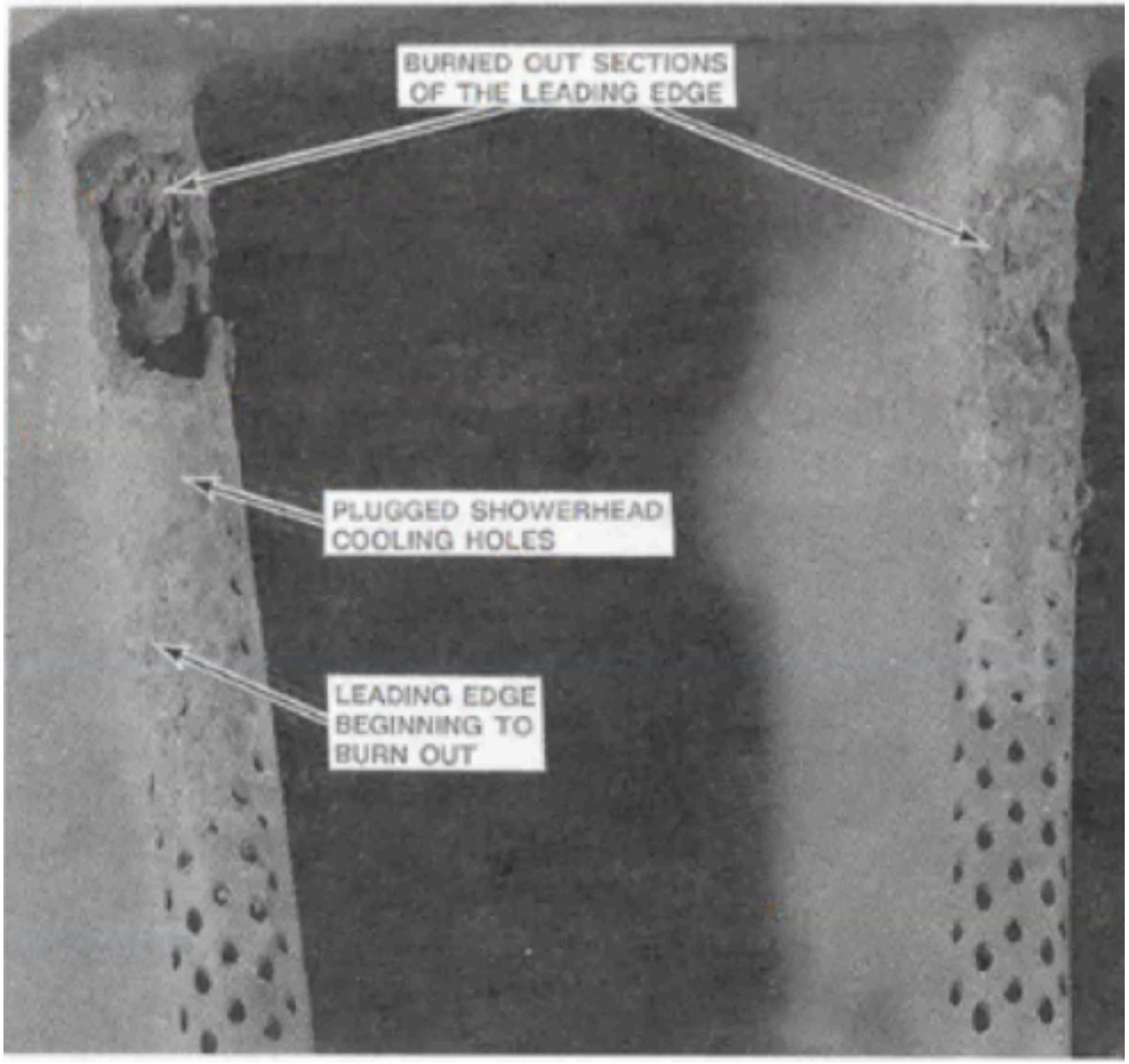

temperature
2.400e+03
1950
1500
1050
6.000e+02
Time: 0.161910
R. BIZZARI
Cerfacs-Safran

High Pressure stator: can be multiperforated too !





Dont block these holes !



When flames meet walls:

Three types of events on a dry (no fuel film), inert, wall (without multiperforation):

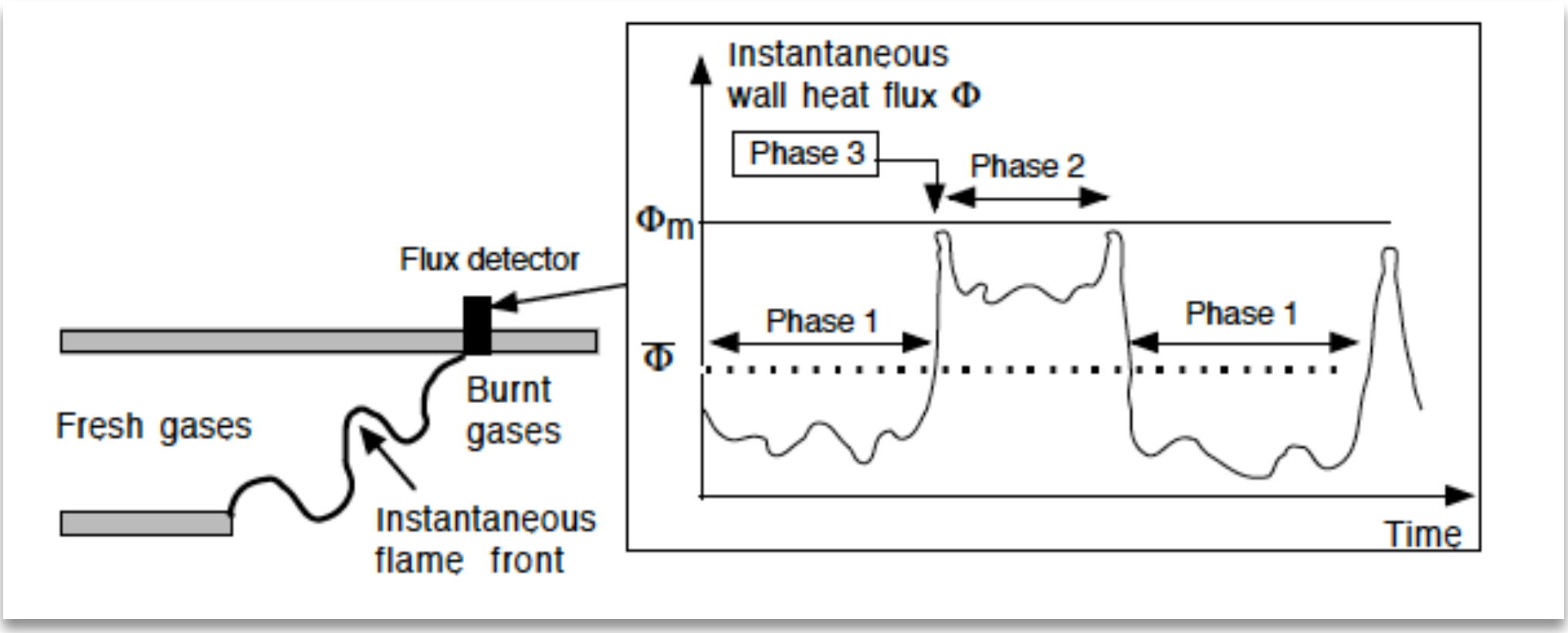
1. Wall is touched by non-reacting gases: no problem

2. Wall is touched by burnt gases: high fluxes for long times

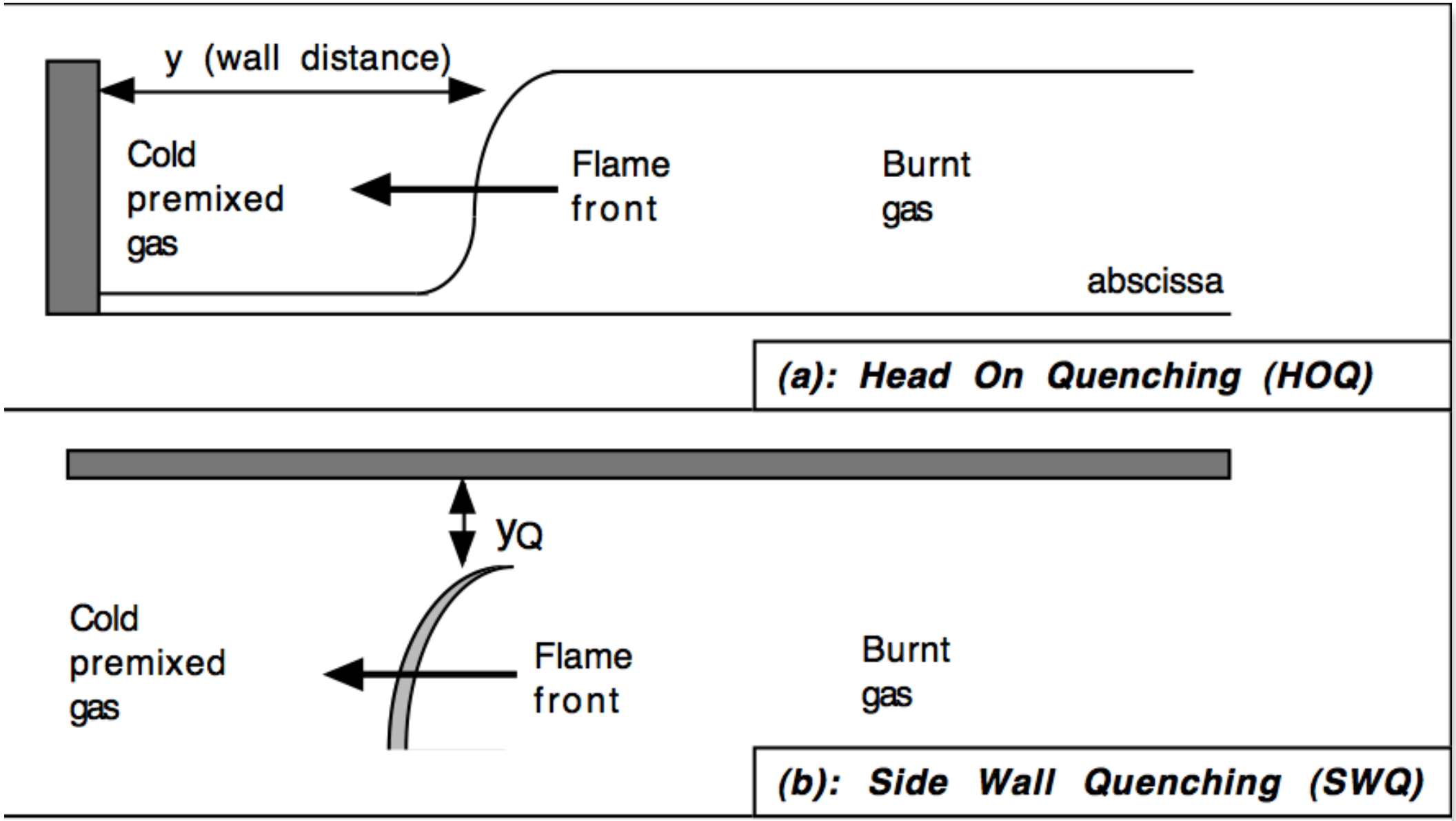
3. Wall is touched by a flame front: very high heat fluxes for very short times

Flame-wall interactions:

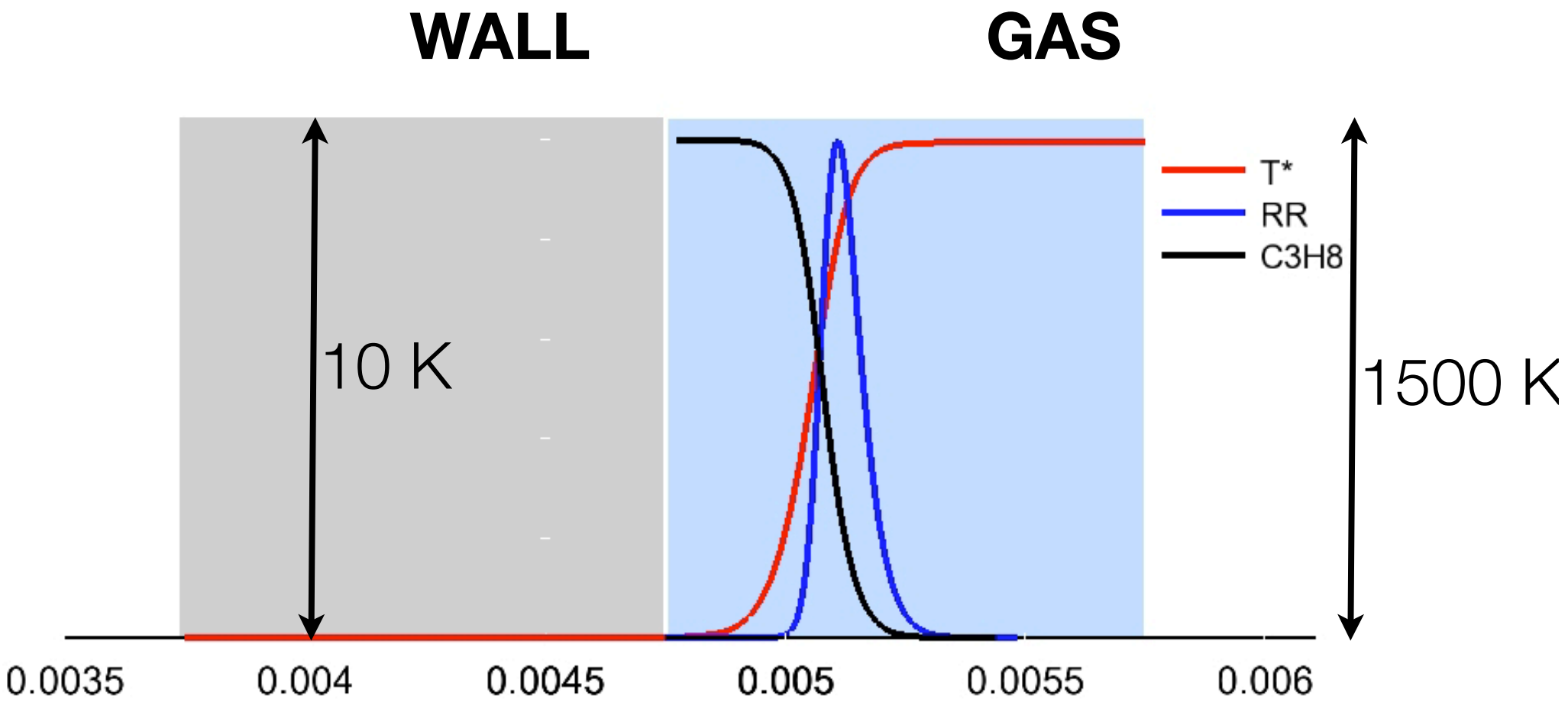
Ch. 7 Sec 7.2



Phase 3 events: an active flame touches a wall

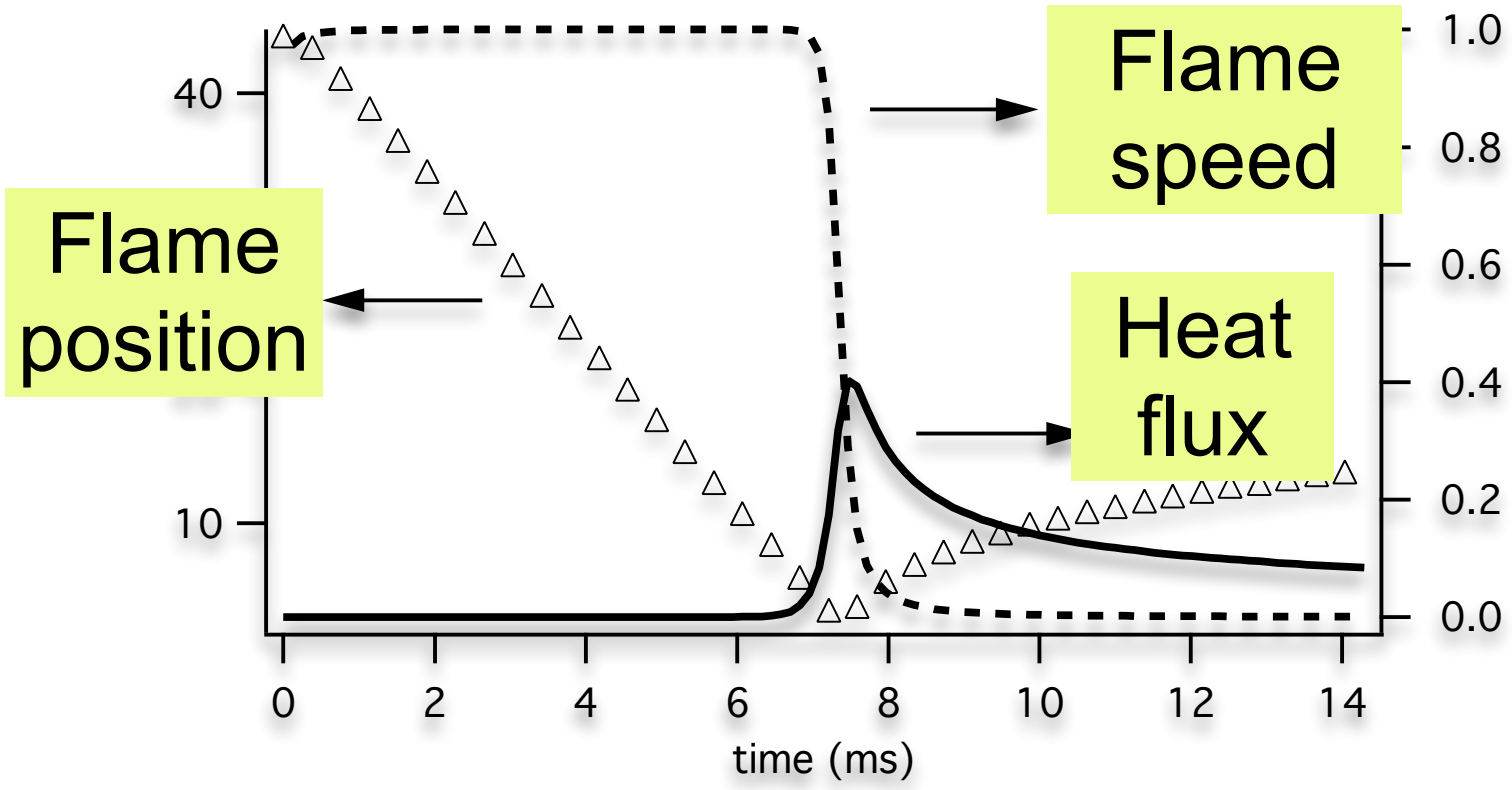


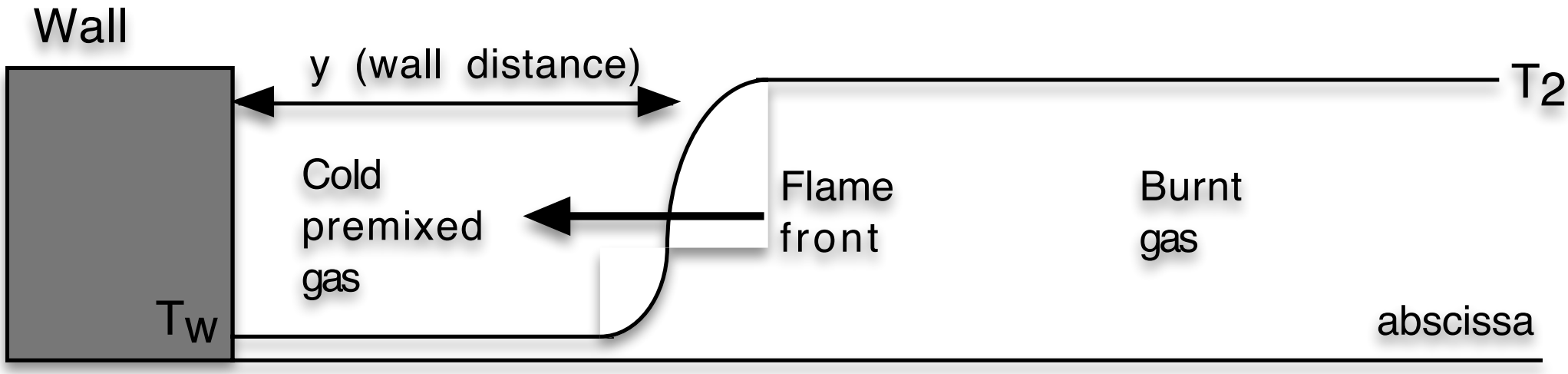
Head on quenching simulation:



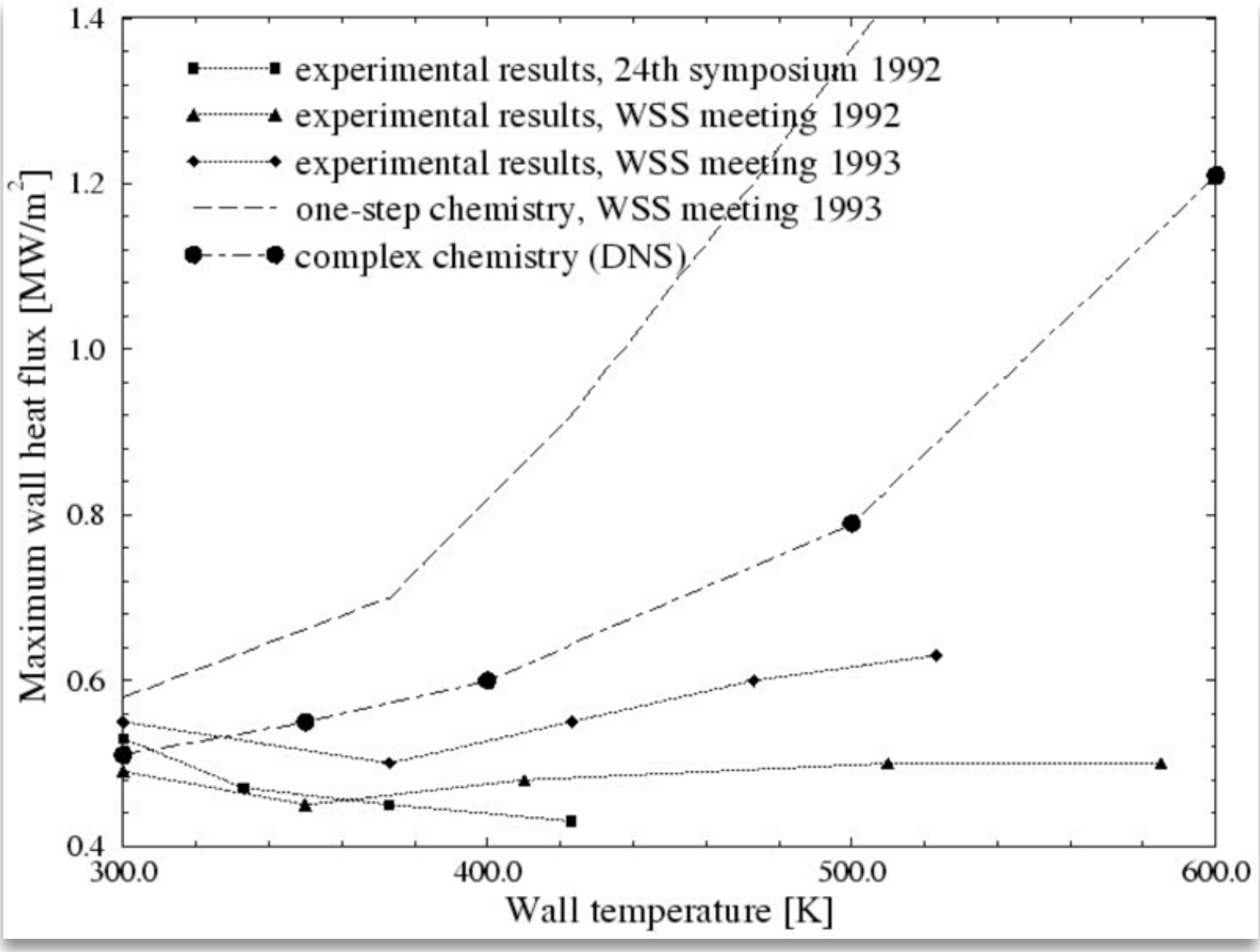
PROPANE / AIR FLAME AT 1 BAR

Classical head on quenching (HOQ)





Maximum heat flux through the wall



Popp, P. and M. Baum (1997) "An analysis of wall heat fluxes, reaction mechanisms and unburnt hydrocarbons during the head-on quenching of a laminar methane flame", *Comb. Flame* 108(3) : 327 - 348.

Simple scaling for maximum wall heat fluxes during flame-wall interaction:

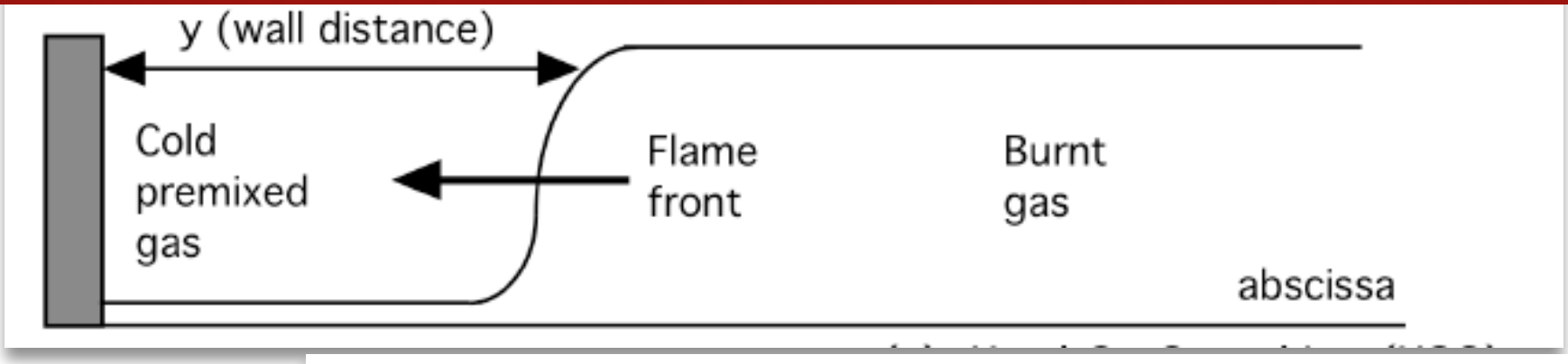
Initial reference	Overall reaction	Approach	Chemical model	Flux Φ MW/m^2	Reduced flux F
Wichman & Bruneaux	$F + O \rightarrow P$	Theory	Simple		0.33
Poinsot et al 1993	$F + O \rightarrow P$	DNS	Simple		0.34
Popp & Baum 1997	CH_4/air - 1 bar	DNS	Complex	0.5	0.4
Vermorel 1999	H_2/O_2 - 1 bar	DNS	Complex	4.85	0.13
Hasse et al 2000	C_8H_{18}/air 10 bar	DNS	Complex	10	0.41

The maximum flux through the wall scales like the flame power:

F= Maximum wall heat flux / Flame Power

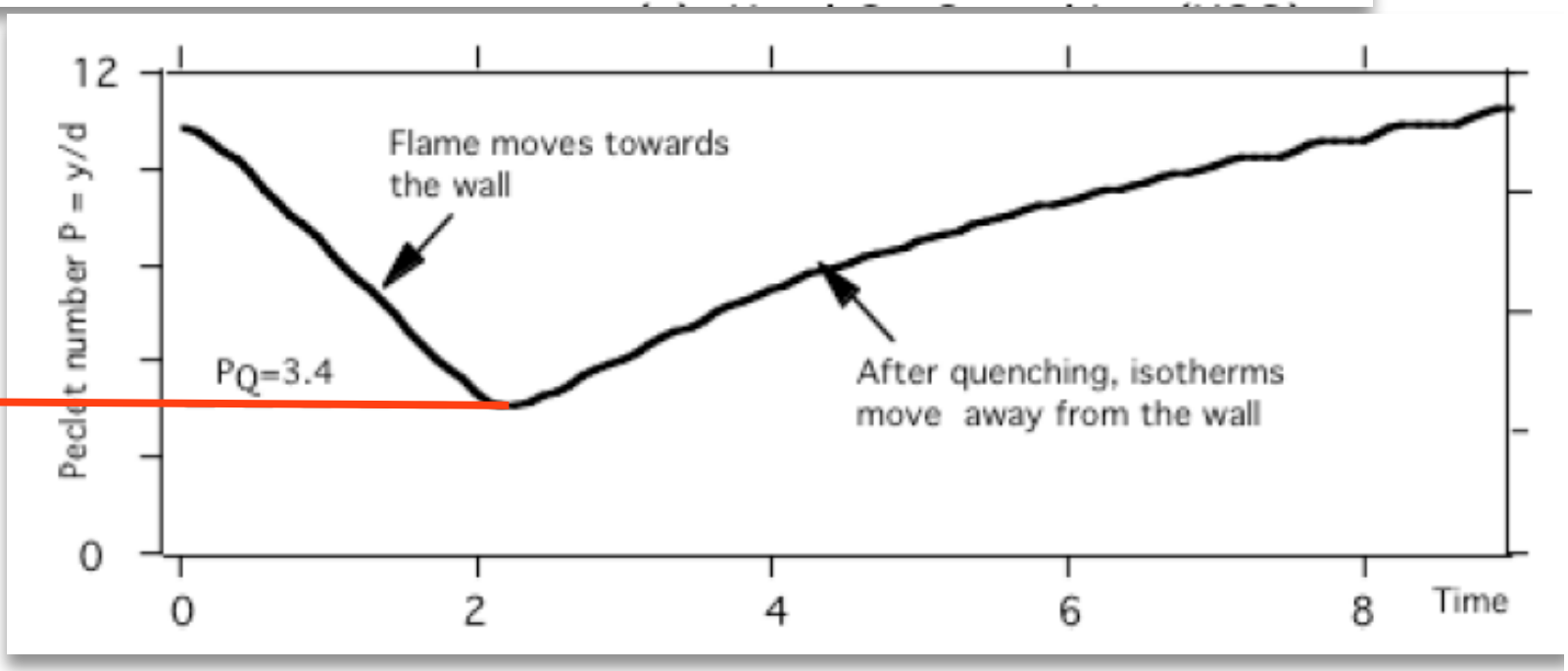
When a flame touches a wall, it delivers 1/3 of its power to the wall (and it dies...)

Simple scaling for minimum distance between flame and wall



$$P = y/\delta$$

$$P_Q = 3.4$$



During Head On quenching, the flame stops at approx 3 flame thicknesses away from the wall

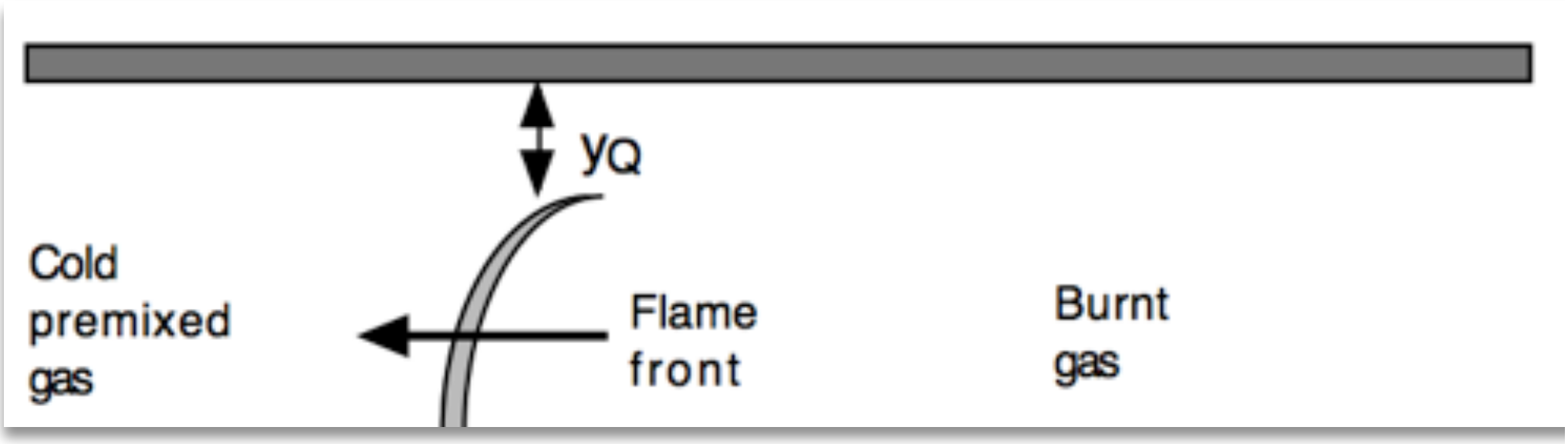
CONSEQUENCES:

- During HOQ, the flame never really touches the wall (if the wall is cold)

- There is unburnt fuel left near the wall: this will lead to pollution (CHx). In a piston engine for example, this fuel will leave the walls during the exhaust phase. This phenomenon is amplified by fuel trapped in crevices

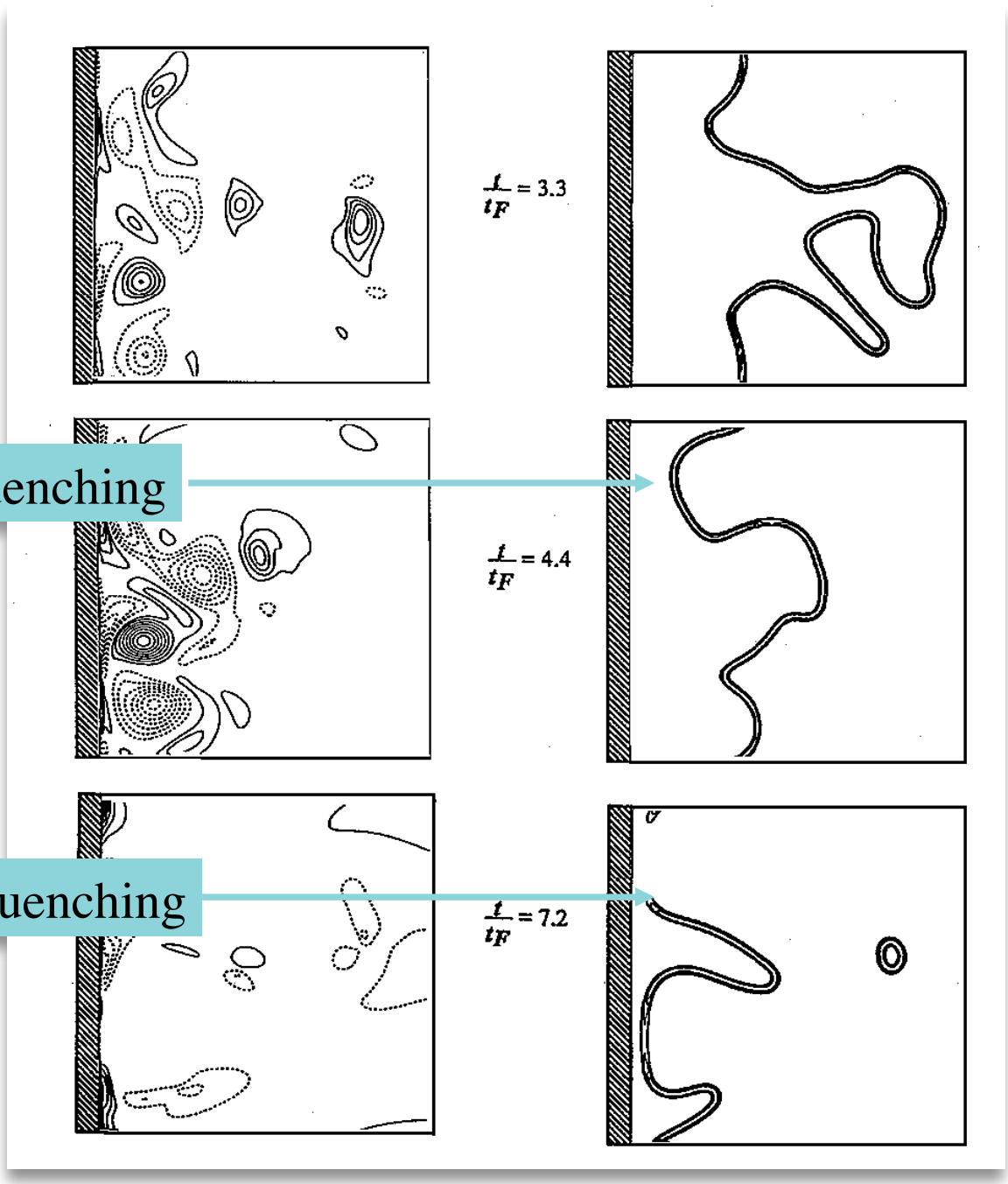
SIDE-WALL INTERACTION

Less studied



Leads to smaller fluxes (F=0.15) and larger minimum flame wall distances (Pe=7)

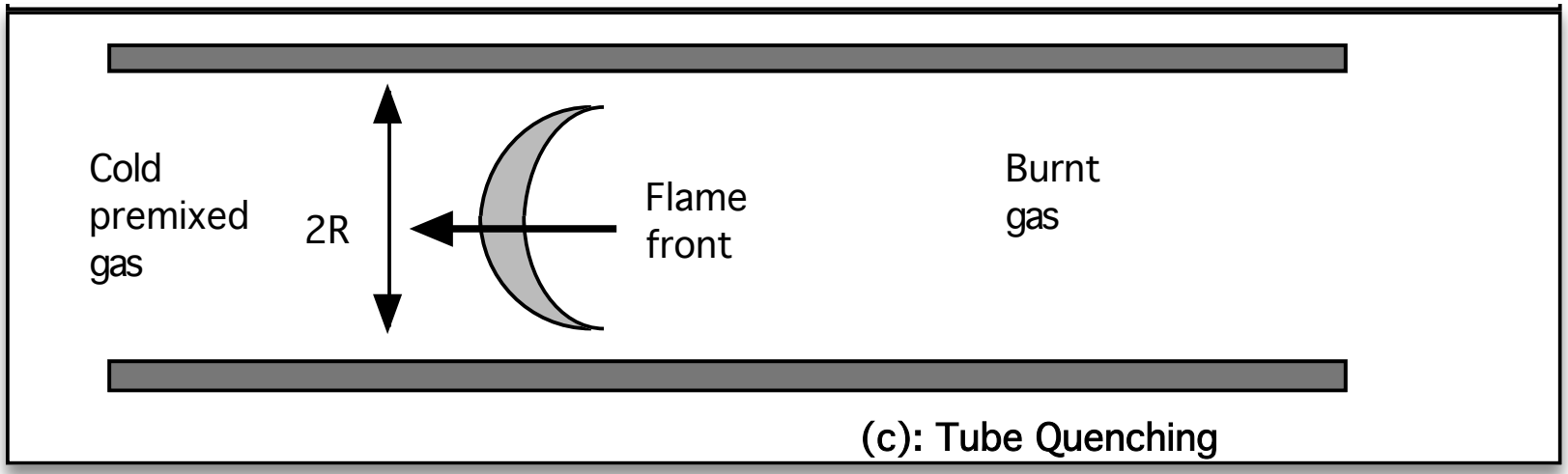
TURBULENT FLOW: both HOQ and SWQ



Head on quenching

Side wall quenching

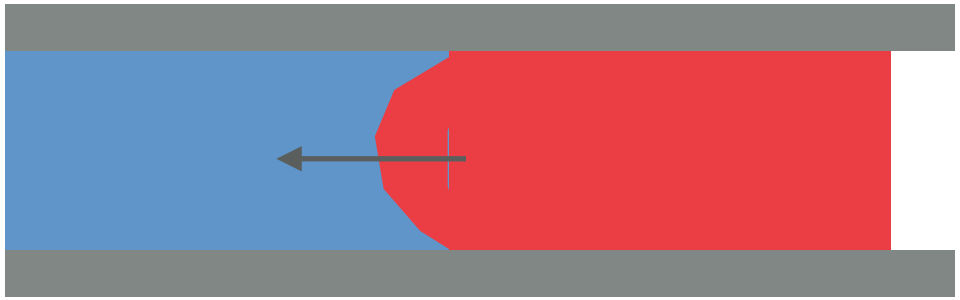
ANOTHER INTERESTING FLAME/WALL INTERACTION CASE: Tube Quenching



In a duct, with a wall on each side, the flame speed is modified and goes to zero if the two sides are too close. Critical distance: $P_Q = 2R/\delta = 50$

This was discovered in the early days of laminar flame studies because experimentalists were obtaining different flame speed values in tubes: they were using different tube diameters

Flames in tubes $\delta = D/s_L^0$



$$\frac{2R}{\delta} > 200$$

Flame moves at the laminar flame speed



$$50 < \frac{2R}{\delta} < 200$$

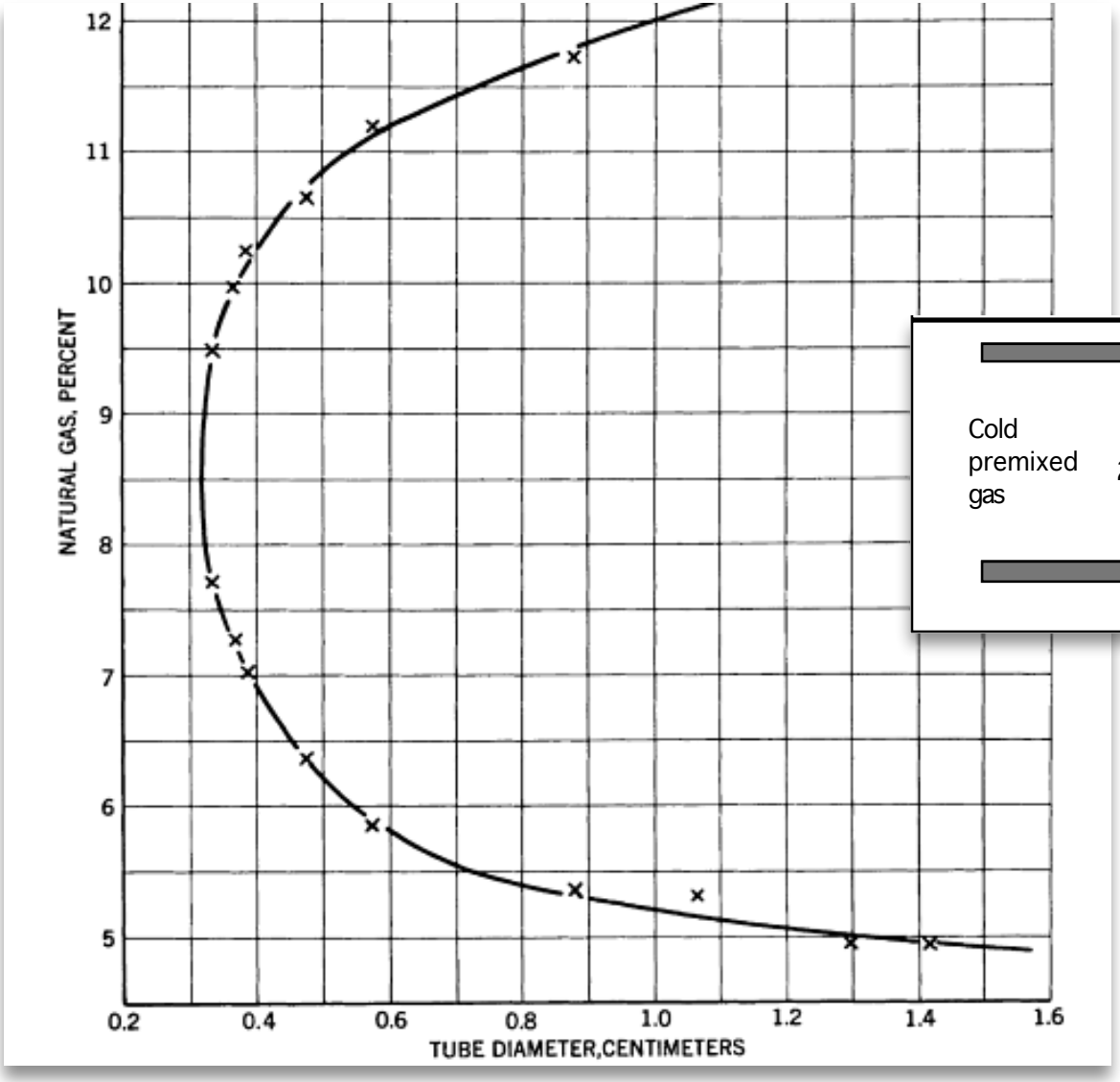
Flame moves at a speed < laminar flame speed



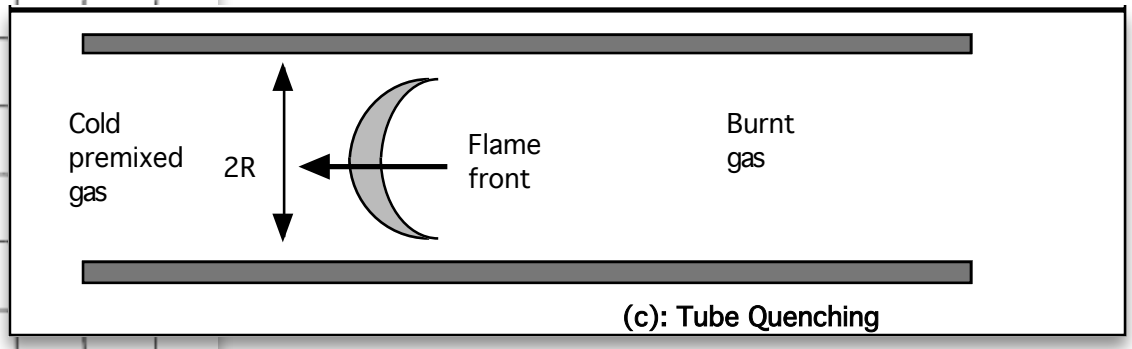
$$\frac{2R}{\delta} < 50$$

Flame is quenched. No propagation at all

MEASUREMENTS OF QUENCHING DIAMETER IN TUBES



$$2R < 50\delta$$



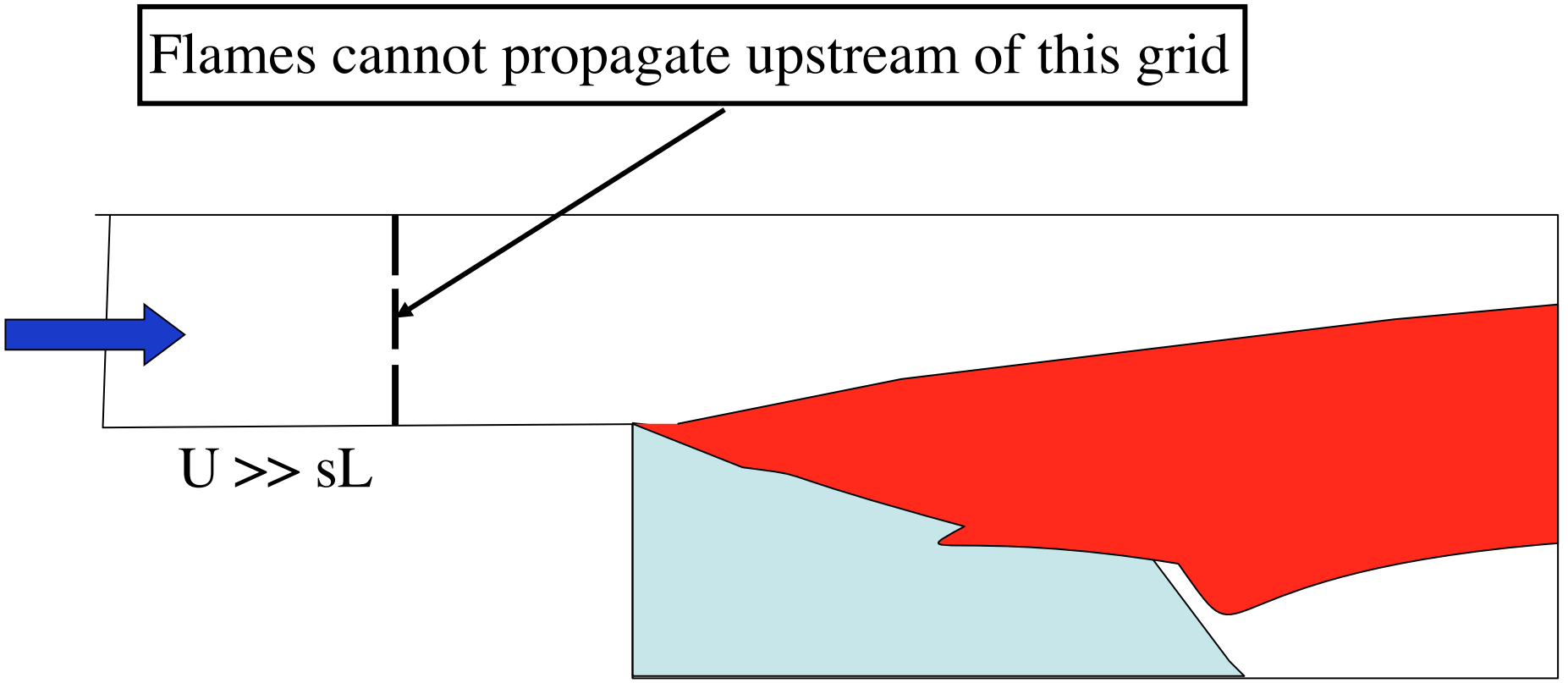
Lewis and von Elbe, 1987

TWO APPLICATIONS OF TUBE QUENCHING

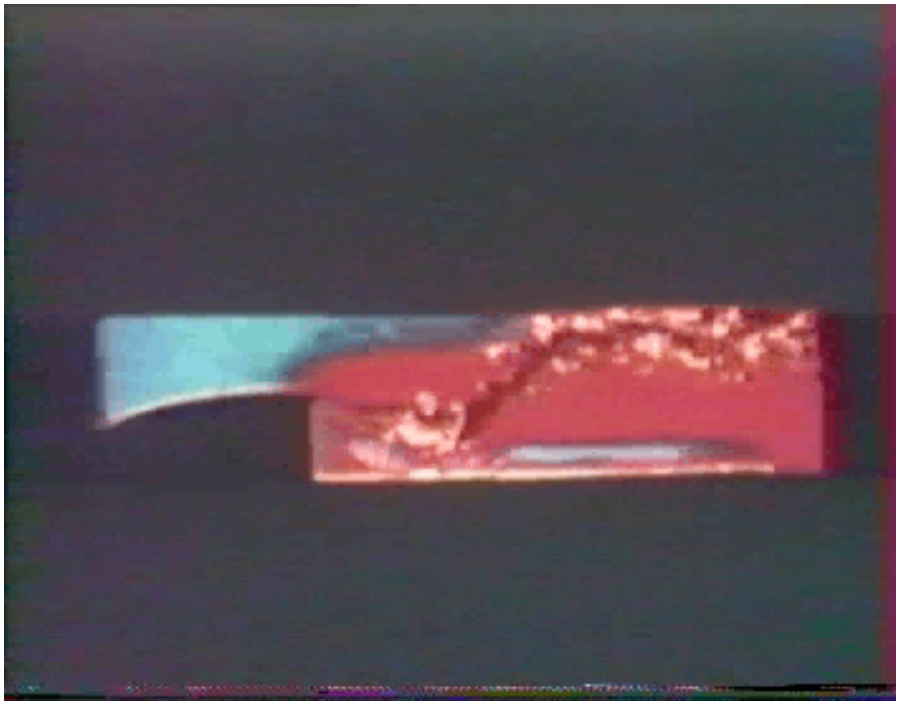
- 1 Flashback protection

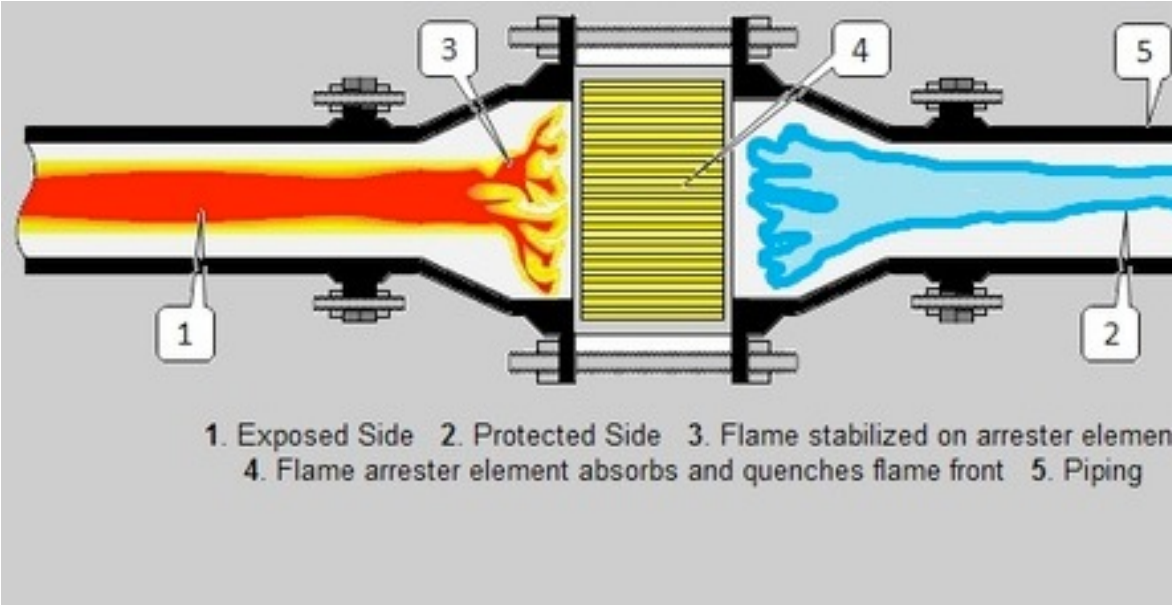
- 2 Mine lamps

Application 1: flashback protection by a perforated plate - flame arrestors



Useful for a case like this

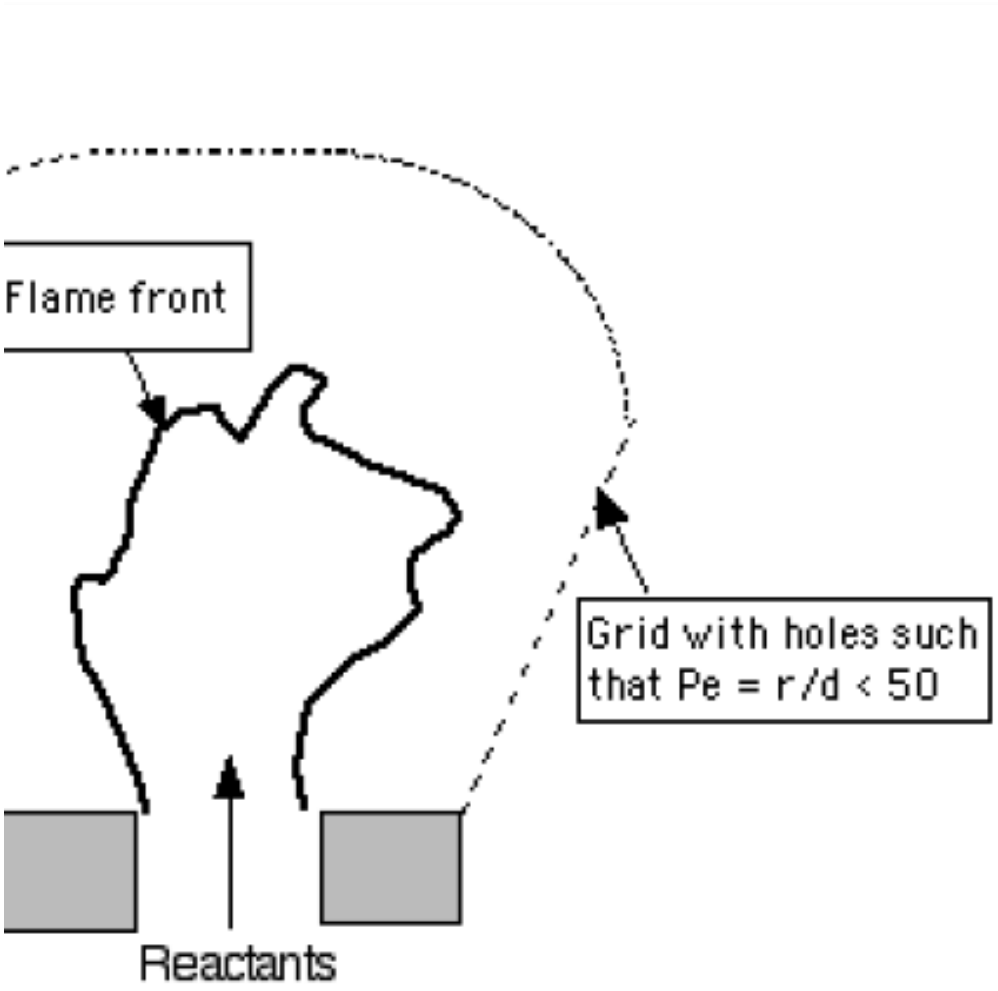


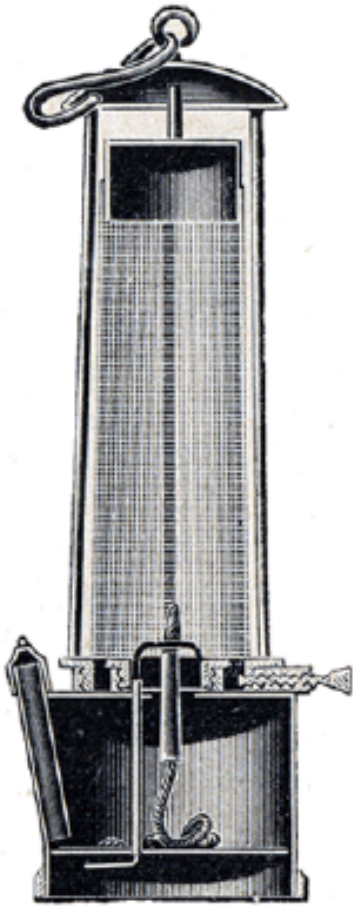


Careful: this usually works only once !

After a flashback, the flame arrestor may be burnt and not be able to work a second time

Application 2: mine lamp

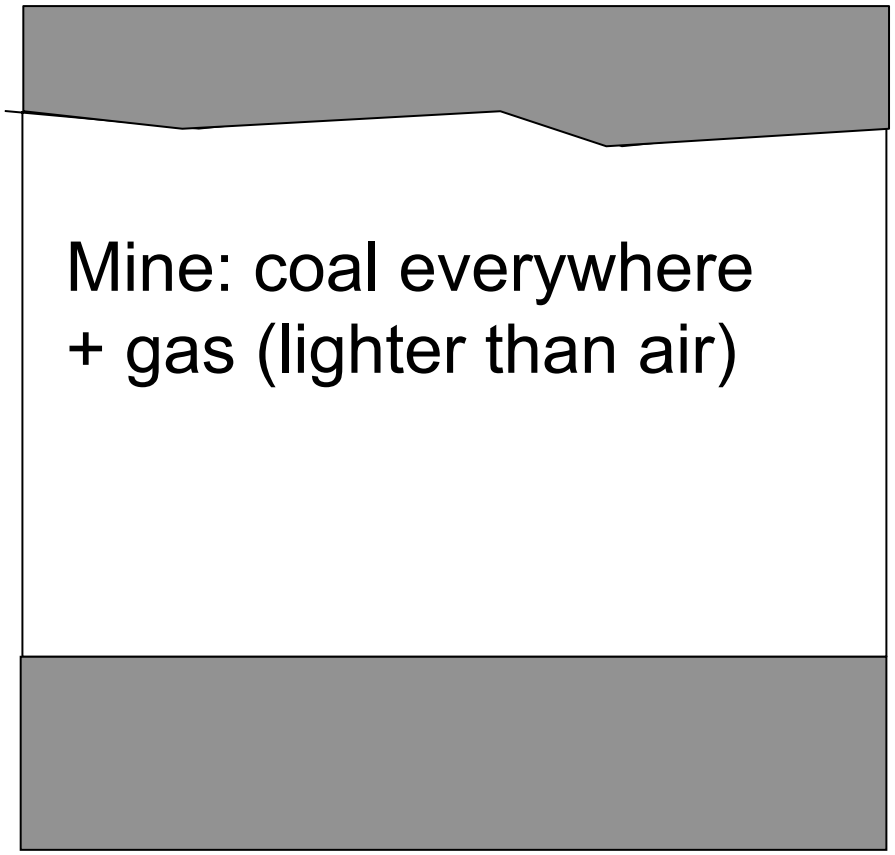






Stephenson
Davy 1817

A (nice ?) example of combustion science: premixed, diffusion flames, triple flames and mine's lamps: explosions in mines



When you have gas (usually CH4) in a mine, you cant work anymore.

The boss says it is your fault and he stops paying you... Need to get this gas out !

You cant pump the gas but... you can burn it !

Good and bad methods to burn the gas trapped in the mine:

- **Explosion**: any accidental spark can ignite the gas and lead to an explosion.





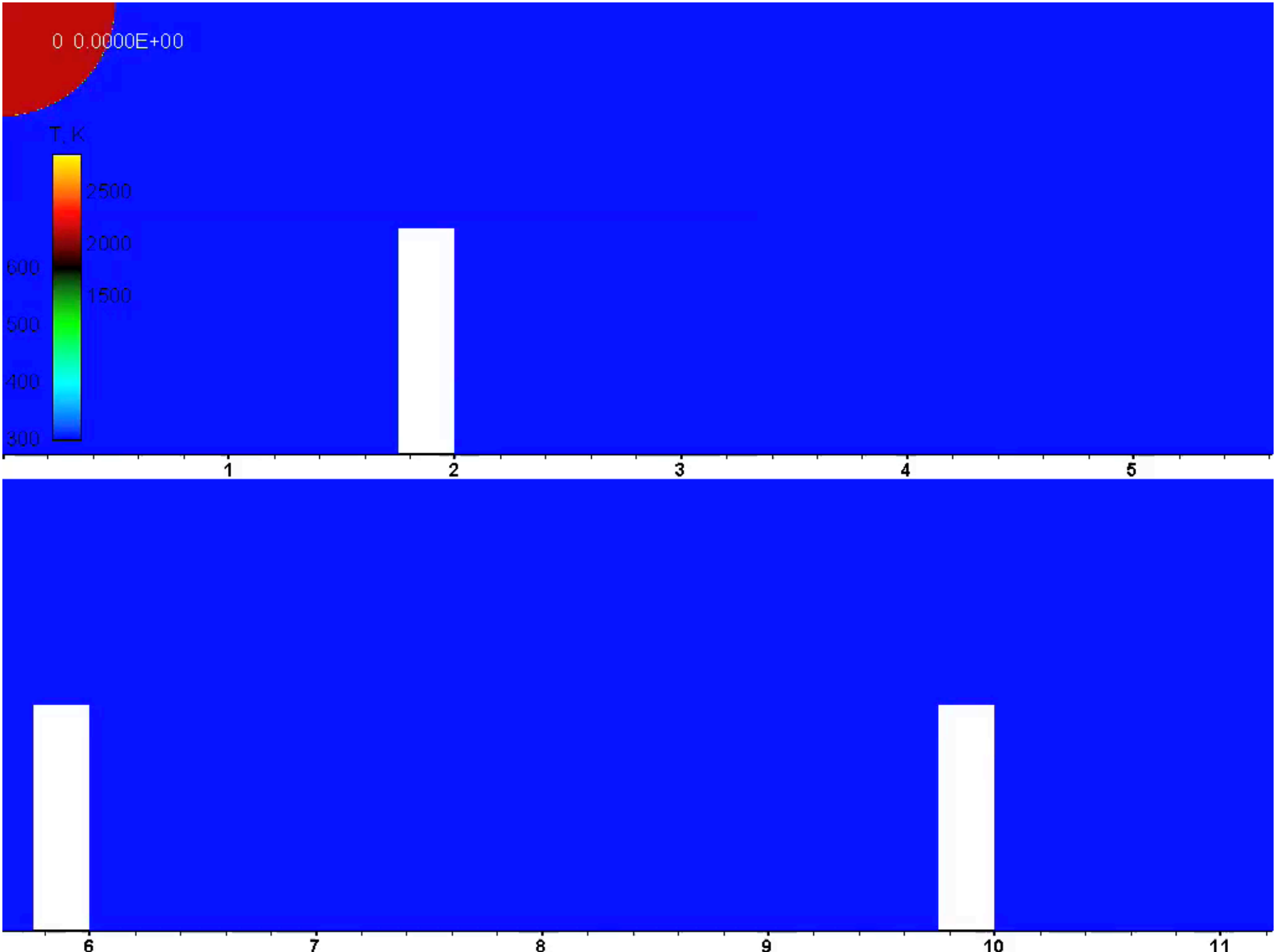
BAD WAY:EXPLOSIONS IN MINES

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 Yuzhou, dans la province de Henan[31,32]	Chine	au moins 20
26 janvier 2011	Mine La Precios		
29 octobre 2011	Mine Xialiuchong à Hengyang[34]	Chine	29
10 novembre 2011	Mine Shizong province du Hunan[35]	Chine	34





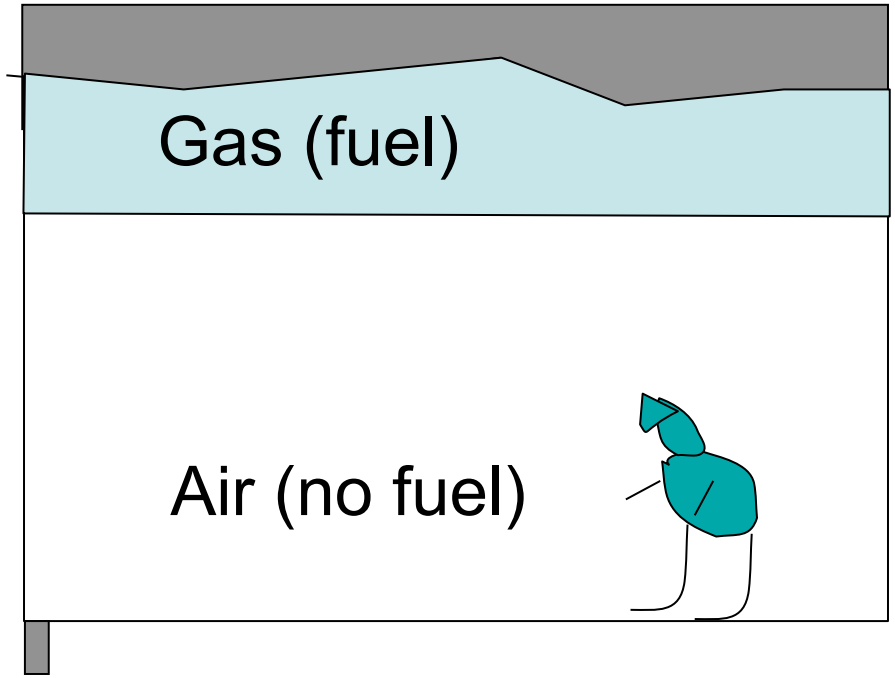
Worse accident: China, 1942, 1565 deaths


0 0.0000E+00
T, K
2500
2000
1500
600
500
400
300
1
2
3
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8
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11

Good and bad methods to burn the gas trapped in the mine:

- BAD: Explosion - any accidental spark can ignite the gas and lead to an explosion

- GOOD: Controlled combustion - burn the methane «slowly»



If you wait long enough, gas and air will be segregated by gravity

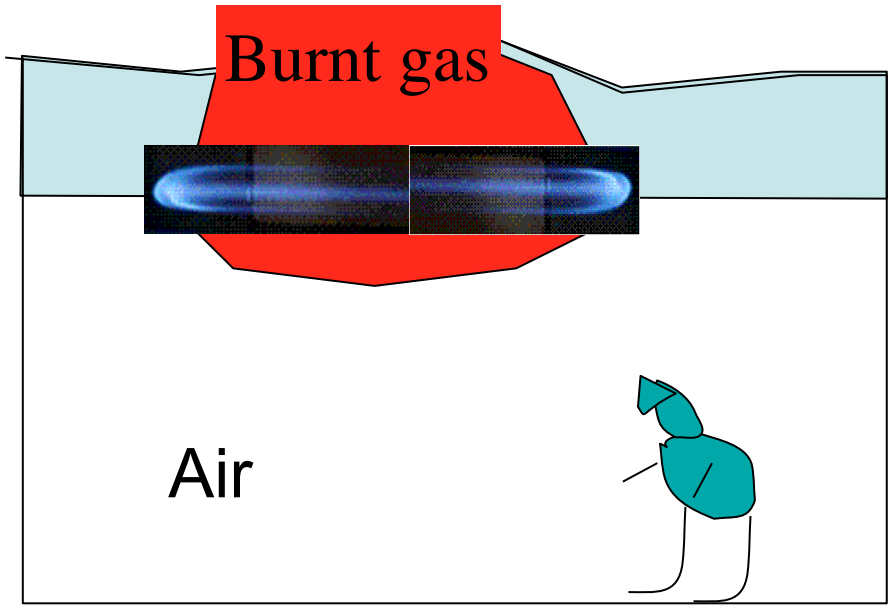
In this segregated situation, a diffusion flame can burn the fuel slowly and safely

But how can you ignite it ?

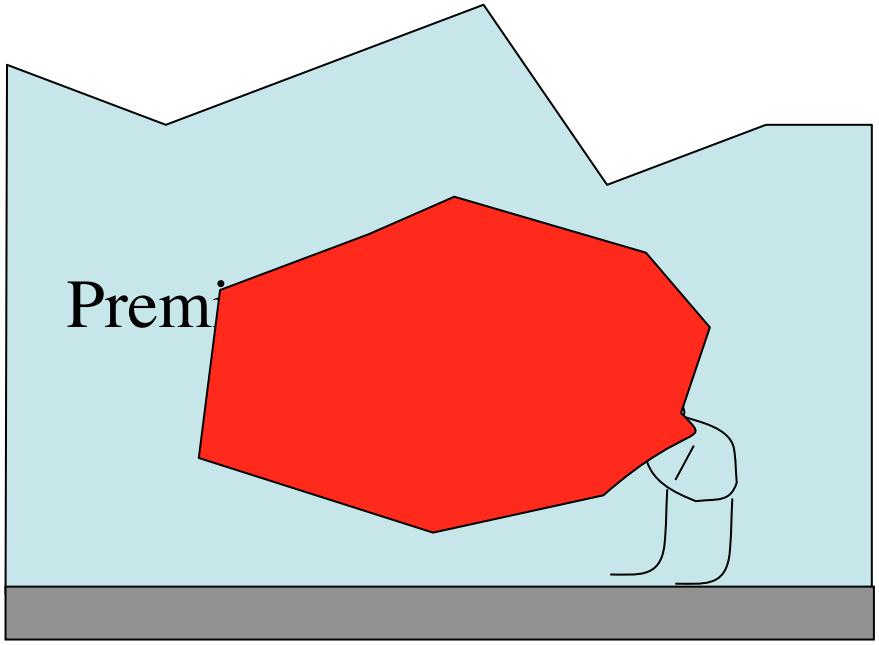
Solution:
- take the youngest worker
- give him a Davy lamp
- send him (crawling) in the mine
- at the place where there is fuel, remove the grid from the Davy lamp
- stand up and raise hand !

TWO SOLUTIONS

1/ Fuel and air were really segregated. The lamp ignites a triple flame which propagates and leaves a diffusion flame. All the fuel is burnt. Noone dies. **The mine can start operating again.**



2/ Fuel and air were not segregated and are still premixed ! In this premixed zone, the lamp ignites a fast premixed flame which goes to detonation. All the fuel is burnt. The young guy dies. **The mine can start operating again.**



In all cases, it works...

BUT THAT IS NOT THE END OF THE STORY:

1/ In many cases, there is a **fire left in the mine** after the explosion. These coal fires sometimes cannot be extinguished once they have been ignited.
In the world, there are numerous coal mines which have been burning for a long time.
Example: the coal mine near the city of Centralia, Pennsylvania, has been burning since 1962. Population went from 1000 in 1962 to 7 in 2013…

2/ Just after a fire, the temptation was big for the owners of **quenching the fire with water** to stop the fire as fast as possible. Even if certain workers were still trapped in the mine…
Example: in Prussia, 22000 deaths from 1886 to 1906.

RADBOD, WESTPHALIA, 1908



At 4.20: explosion in mine maybe due to the opening of one of the lamps

400 people were in the mine. Only a few escape, all attempts to rescue those trapped in the mine are vain because of the heat and of the destruction

At 19.00: to stop the fire, and be able to exploit the mine again later: the mine is…. flooded with river's water. No other survivors.



FLAME WALL INTERACTION AND TURBULENT COMBUSTION MODELS

A topic which is often ignored by theoreticians but not by those who run codes

Most models for turbulent combustion are not built for flames near walls:

➡they assume adiabatic flows

➡they use models based on isotropic turbulence

Both assumptions fail near a wall

Ex: the EBU model

For premixed turbulent combustion, the mean reaction rate is written:

$$\overline{\dot{\omega}}_{\Theta} = C_{EBU}\,\overline{\rho}\,\frac{\varepsilon}{k}\widetilde{\Theta}\left(1-\widetilde{\Theta}\right)$$

At a wall, k goes to zero, and the reaction rate goes to infinity: the flame propagates much faster at the wall than anywhere else. Obviously wrong.

Fixing the EBU model:

Most code developers end up writing things like:

« In the first cell near the wall, the reaction rate is zero (the EBU model is forgotten) »

Clearly a good fix but a bad model: results will depend on the mesh size at the wall.

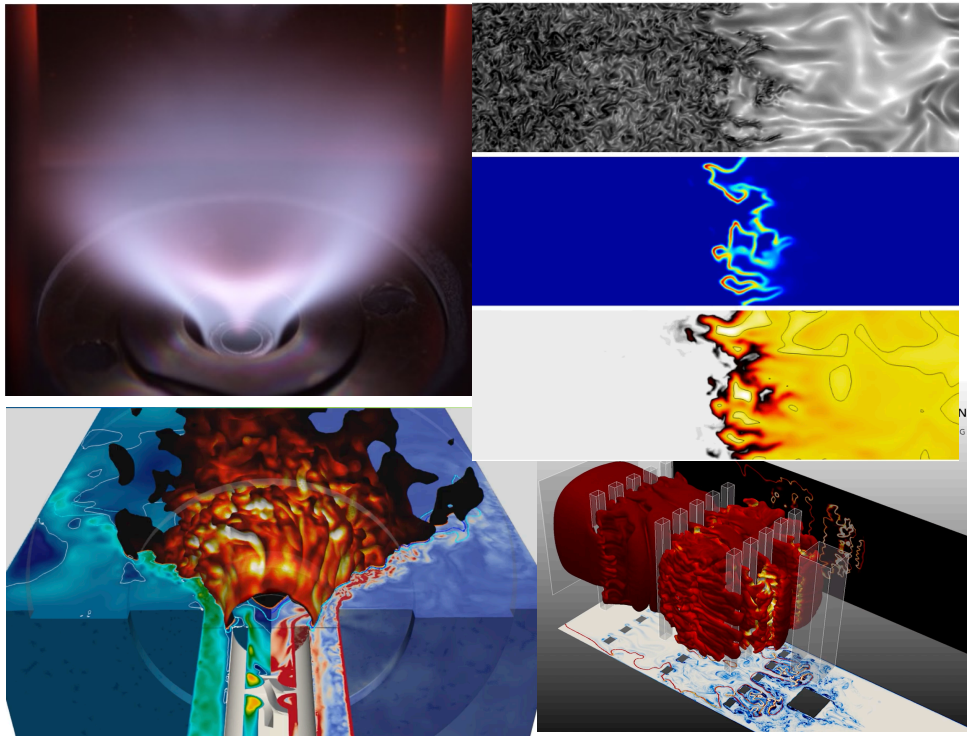
What should be done

Write law of the wall models for combustion as done for aerodynamics

Use models which do NOT assume adiabaticity -> this eliminates many of them

Ch. 7

HYDROGEN COMBUSTION



Thierry Poinsot

- CNRS, Institut de Mécanique des Fluides de Toulouse (IMFT)
- CERFACS, Toulouse
- Stanford University
- French Academy of Sciences
- Editor in chief, Combustion and Flame (with Pr Egolfopoulos, USC)

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C. Brunet, S. Richard ***Safran Helicopter Engines***

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IMFT
INSTITUT DE MECANIQUE DES FLUIDES DE TOULOUSE

CERFACS

We MUST minimize fossil fuel combustion… but how ?

First, burn less and burn better

We MUST go to renewable energies

Problem: renewable energies are intermittent

ENERGY STORAGE IS A MAJOR ISSUE

HOW CAN WE STORE ENERGY ?

★ **SURPRISE: WITH COMBUSTION AGAIN !**

★ **STRATEGIES CALLED POWER TO X TO POWER:**

- Use renewable energy to produce gas (H2 for ex)
- Use H2 later to produce power when needed

POWER TO GAS ? One example:





Electrolysis





STORED IN TANKS

WHAT IS POWER TO GAS ? One example:





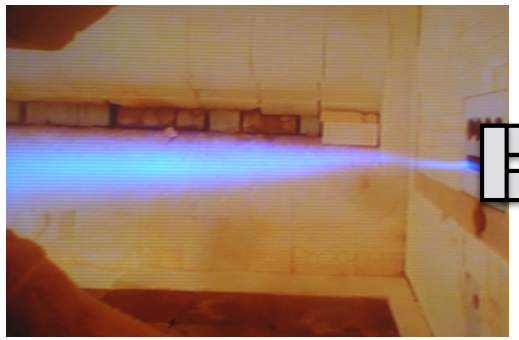
Electrolysis

H_2

O_2

Renewable fuel

Fossil fuel



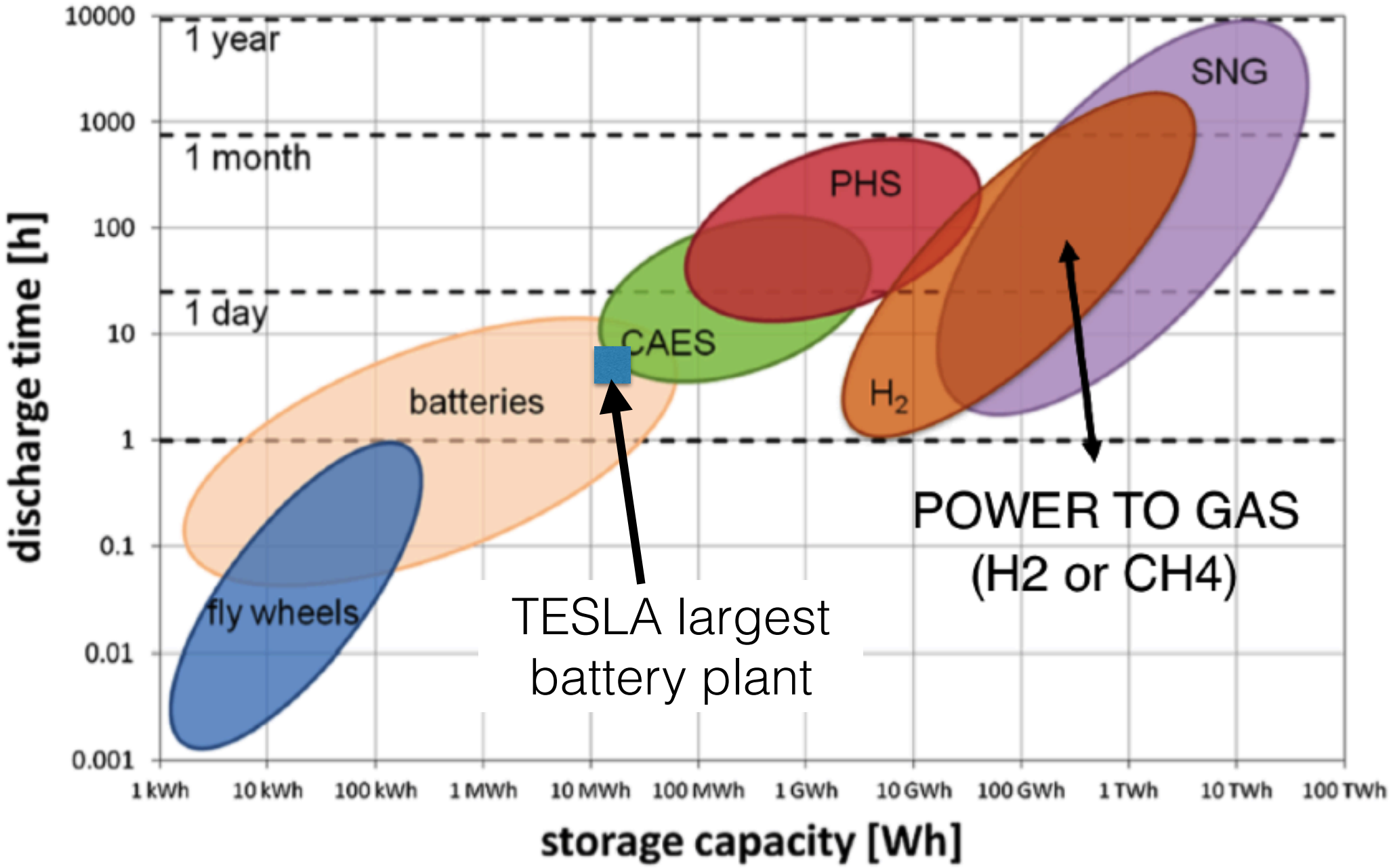
Air

Combustor

HEAT

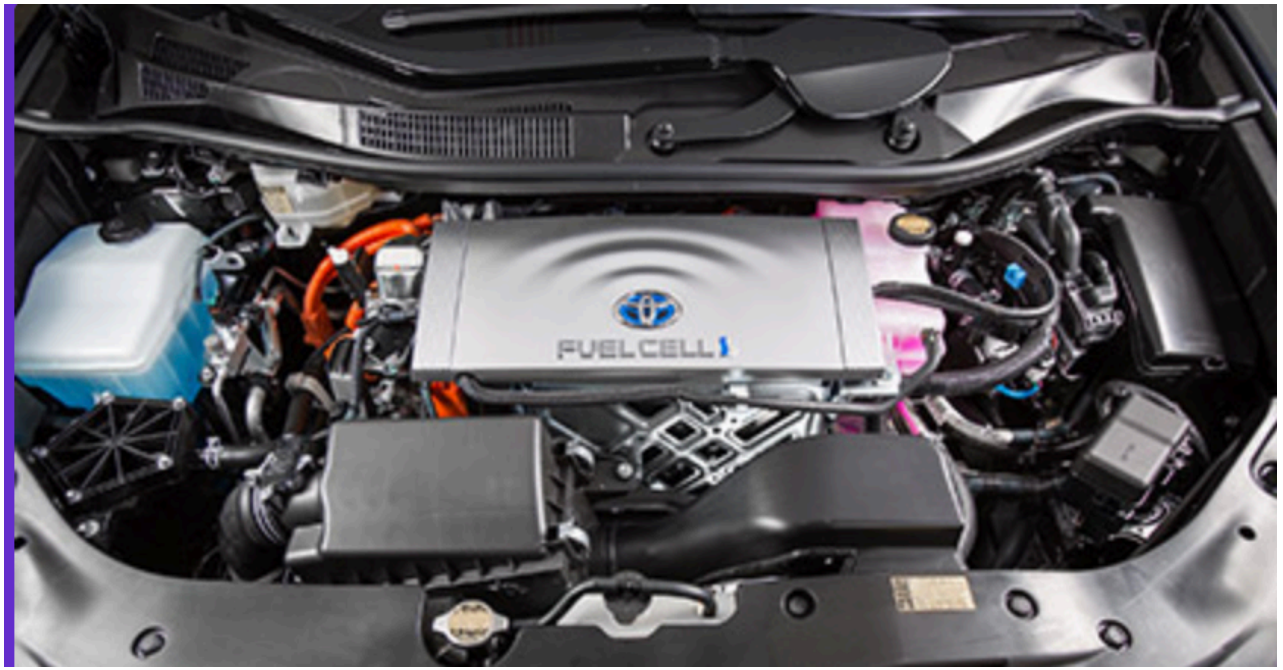
POWER

FUELS CAN STORE A LOT OF ENERGY:



ONCE WE HAVE H2 SAFELY STORED….

★ CAN USE IT IN A FUEL CELL



★CAN CONVERT IT TO CH4 OR NH3 (EASIER FOR STORAGE)

ONCE WE HAVE H2….

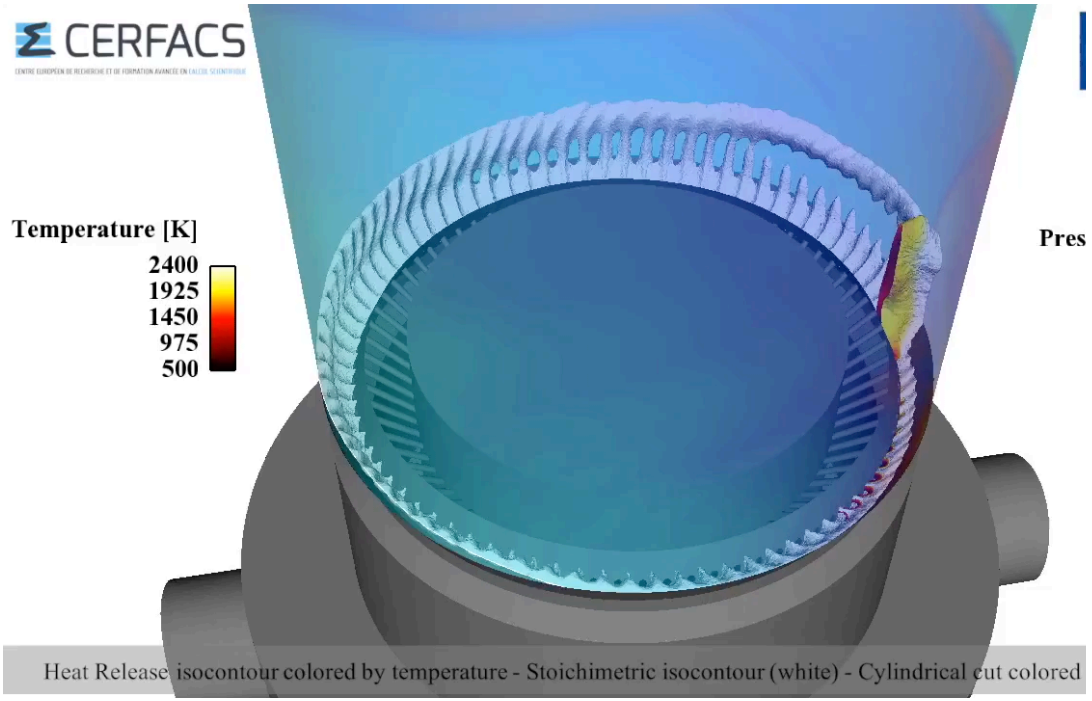
WE CAN ALSO BURN DIRECTLY :

- ★IN A FURNACE
- ★IN HEATING SYSTEMS
- ★IN A PISTON ENGINE (TEN TIMES CHEAPER THAN A FUEL CELL) FOR CARS OR BUSES
- ★TO MAKE YOUR COFFEE OR YOUR BBQ

ONCE WE HAVE H2….

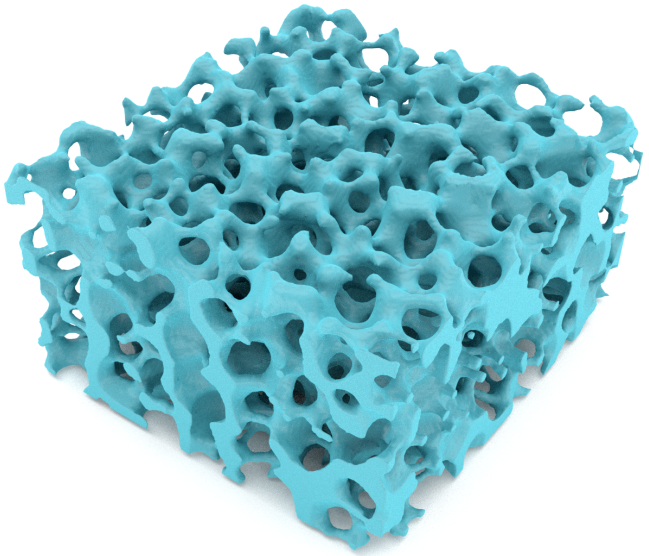
IN ENGINES USING NEW IDEAS:

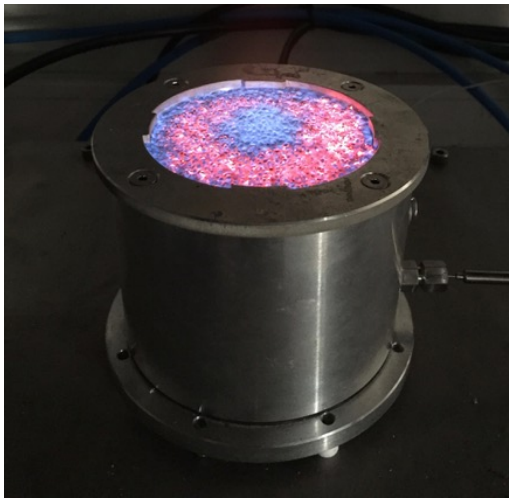
➡ROTATING DETONATION ENGINES



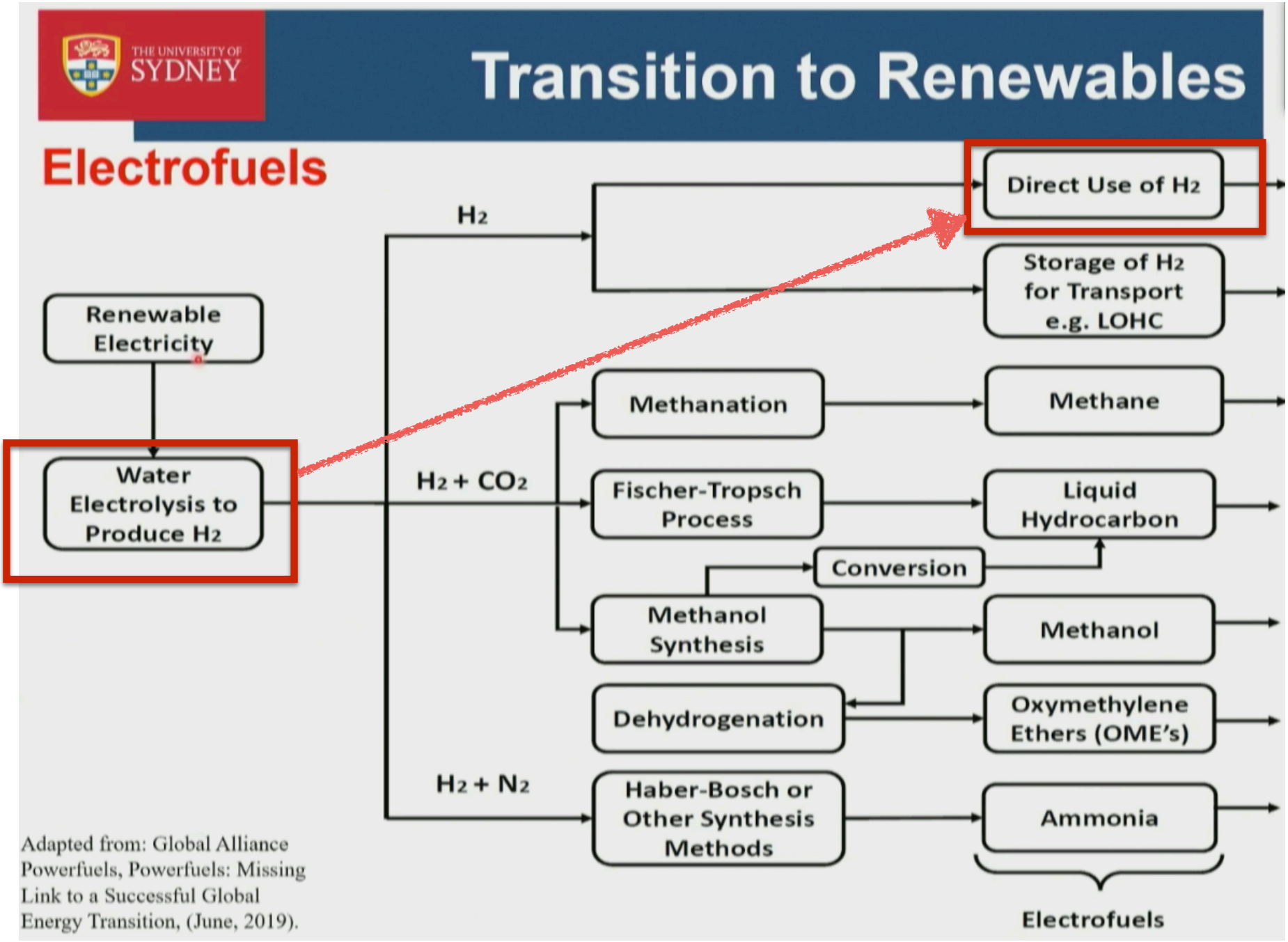
Heat Release isocontour colored by temperature - Stoichimetric isocontour (white) - Cylindrical cut colored

➡POROUS BURNERS





H2 IS ONLY THE ENTRY GAS:….



CERFACS
CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

HYDROGEN…
A short history





Copyright Dr T. Poinsot 2023

H2 STARTED WITH BALLOONS

Started in Paris in 1783: Just needed a light gas able to fill a balloon efficiently

They did not even know it was H2. just saw that it was a light gas

Since they produced it by water: HYDRO(water)… GENerated



BALLOONS STARTED IT:

Balloons in 1783:

- ***4 june 1783: first flight by Montgolfier in Annonay (but not with H2)***
- ***27 aug 1783: Charles and Robert (with H2 obtained with 500 kg of iron and 250 liters of H2SO4)***
- ***1st dec 1783: first human flight by Charles and Robert in Versailles***

HOW DID THEY DO H2 FIRST?

‘Aux tonneaux’ (in a barrel):
- mix iron and sulfur acid in a ‘tonneau’
- recover H2 by a tube on top and store it in the balloon

Iron + H2SO4 -> H2 +…



Fig. 5. Gonflement du premier ballon à l’Hydrogène selon le procédé dit

FIRST PROBLEM: PRODUCE H2

« White » H2 may exist but we don't have much today so that H2 is produced usually by multiple ways from other sources:

Electrolysis:

H_2O + electricity —> H_2 + O_2

H. Davy 1800, Faraday 1833, Arrhenius 1884

Davy and Arrhenius are among the most famous combustion guys

FIRST PROBLEM: PRODUCE H2

$C + H_2O \rightarrow CO + H_2$ Gillard 1850

$CO + Ca(OH)_2 \rightarrow CaCO_3 + H_2$ Griesheim 1900

$CO + H_2O \rightarrow H_2 + CO_2$ Oppau

-> 500 dead, 2000 wounded in Sept 1921, first 'big' accident

$Si + Ca(OH)_2 - 2\,Na(OH) \rightarrow Na_2SiO_3 + CaO + H_2$

$Si + 2\,NaOH + H_2O \rightarrow Na_2SiO_3 + 2\,H_2$

PRODUCE H2

But methane reforming remains the main method to produce H2 today… (more than 98 %):

CH4 + not too much O2 -> CO2 + H2

without carbon capture, it is absolutely not green…

PROBLEM: SAFETY

As soon as we started using H2, we had ‘problems’:

- ***4 june1783: first flight by Montgolfier in Annonay (but not with H2)***
- ***27 aug 1783: Charles and Robert (with H2 obtained with 500 kg of iron and 250 liters of H2SO4)***
- ***1st dec 1783: first human flight by Charles and Robert in Versailles***

SECOND PROBLEM: SAFETY

As soon as we started using H2, we h… oblems':

- ***4 june1783: first flight by … Annonay (but not with H2)***
- ***27 aug 1783: Ch… ert (with H2 obtained wi… on and 250 liters of H2SO4)***
- ***26… rch too close to the H2 … ystem ignites the whole set up***
- ***1… 1783: first human flight by Charles and Robert in Versailles***

H2 AND SAFETY IS A BIG ISSUE
AND IT IS A COMBUSTION ISSUE

AFTER BALLONS: ROCKETS AND AIRCRAFT

USSR

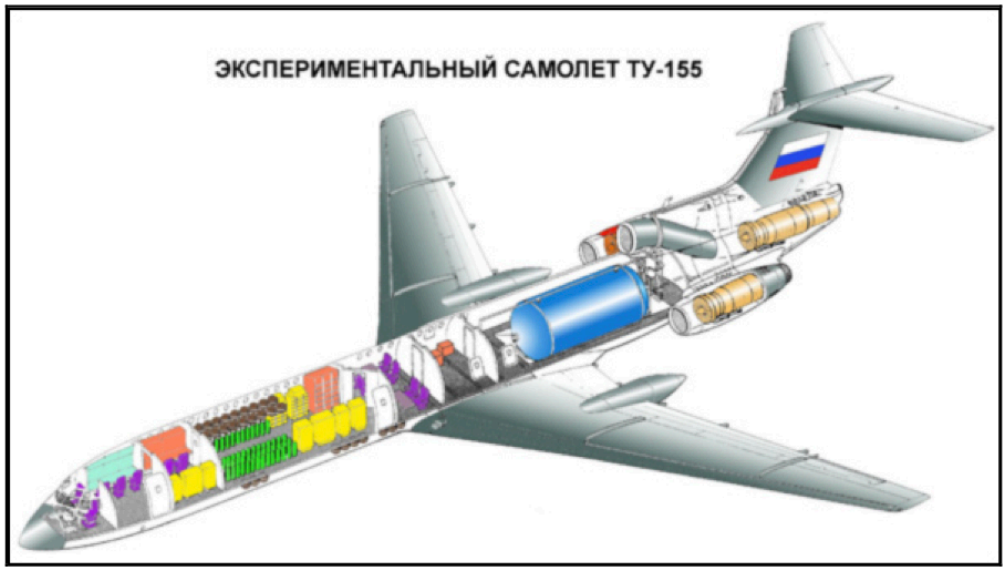
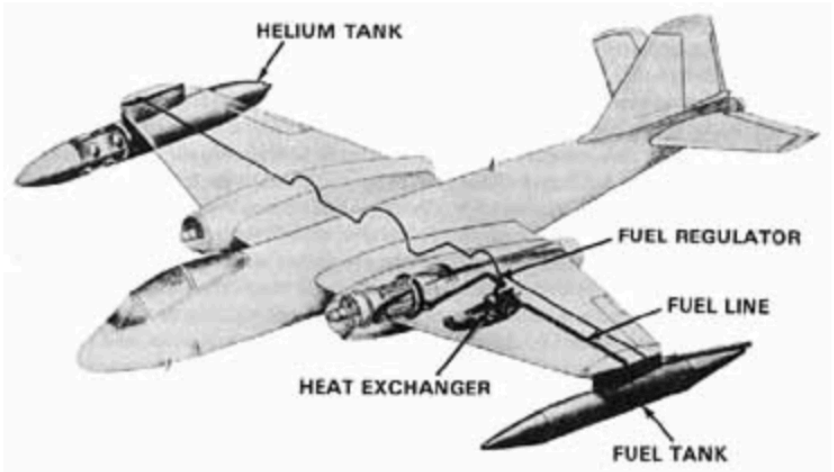


Fig.1 Tupolev-155 airplane layout.

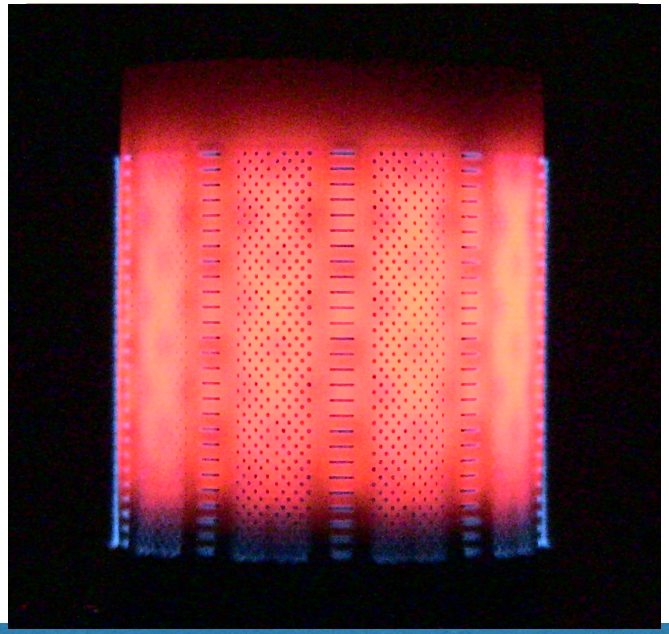
USA



. Liquid-hydrogen fuel system for one engine of a B-57 airplane installed by the NACA Lewis laboratory.

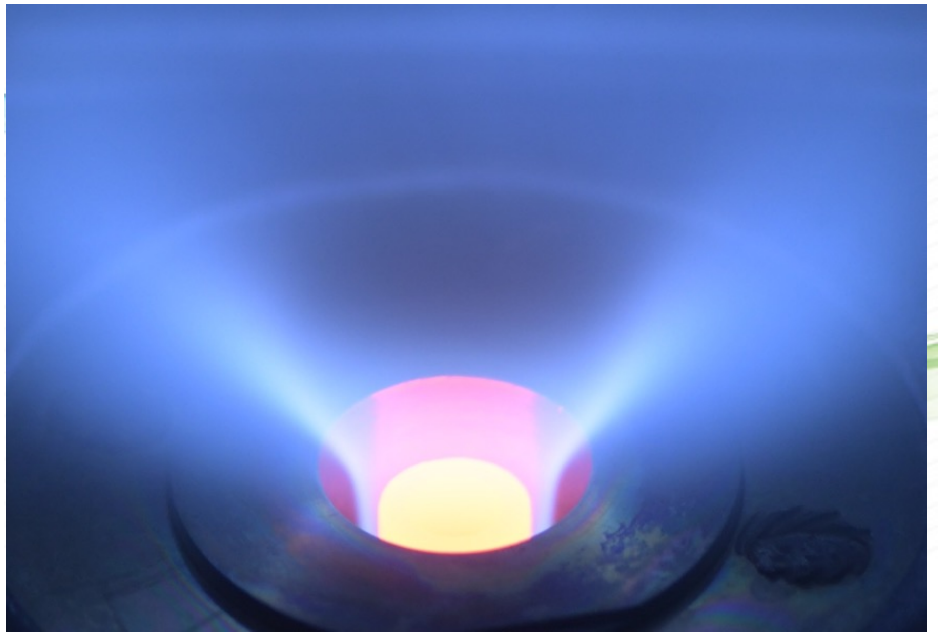
Tomorrow: applications in all fields:

Domestic boilers



p=1 atm
T= 20°C, ambiant air
Laminar flames stabilized on perforated plates

Gas turbines



p= 20-40 atm
T=700-900 K
Swirling flames
Some turbines already handle 50-100% H_2 in the fuel blend (Siemens)

+ heavy industry: quartz, iron, glass

FOR THE COMBUSTION COMMUNITY:

Yes, there will be more hydrogen…

Which leads to the next questions:

Can we use H2 everywhere ?

Can we use it for transportation ?

Can we use it to fly ?

Flying commercial planes with H2 is probably the most difficult thing we can do with H2:
this is an interesting case study…



How do we store H2 on a plane ?

- Cryogenic tanks or
- High pressure gas tanks



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Cryogenic ?

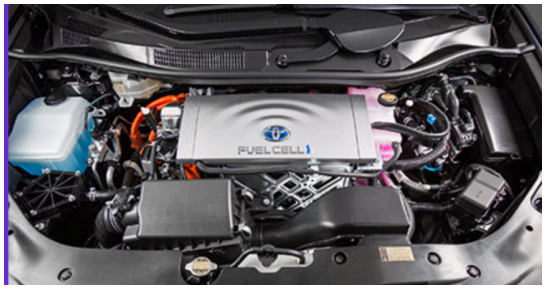
Cryogenic tanks (20 K, 1 bar):
Heat of reaction per unit mass of H2 = 2.2 of kerosene
But even in cryogenic form, H2 is not very dense:

- **Density of liquid H2 = 70 kg/m3**
- **Density of kerosene = 800 kg/m3**

=> Replacing 200 tons of kerosene (220 m3) by H2 will lead to 'only' 80 tons of H2 but to a tank of volume 1100 m3 … at 20 K.



HIGH PRESSURE TANKS?



$$P = \rho RT/W \qquad \rho = (P/RT)W$$

$$W = 0.002\text{kg/mole}$$

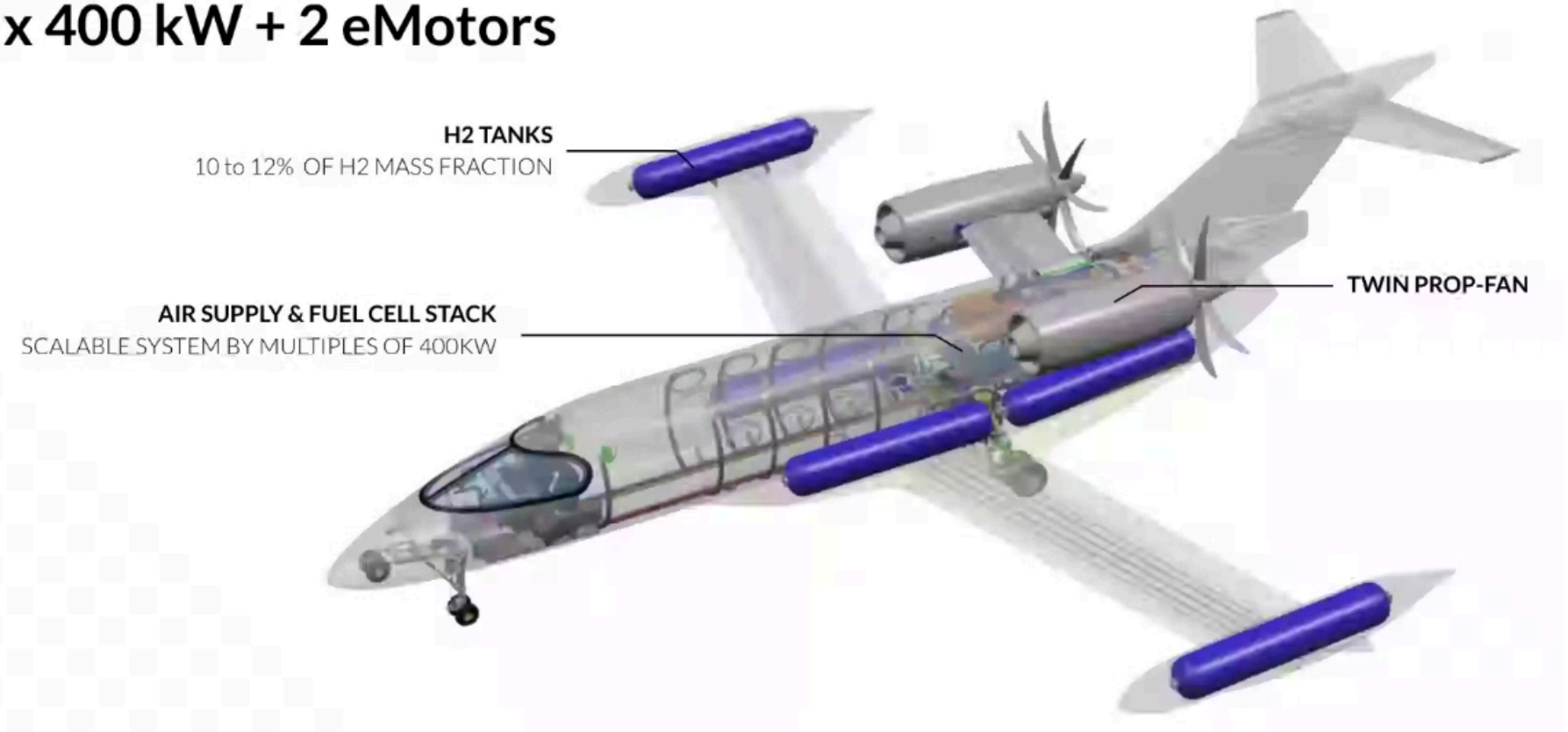
High pressure (700 bars) tanks are heavy: they can't fly easily. In a H2 car (Toyota), tank weight is 130 kgs for a few kgs of H2).

Most companies plan to store H2 as cryogenic..

HIGH PRESSURE TANKS?

Scaling the prototype to a

6 x 400 kW + 2 eMotors



For small planes, maybe high pressure tanks: 700 bar
BEYONDAERO company: fuel cells and gaseous H2


Building the first electric light jet hydrogen-powered
High-level requirements
F-WBYA
Max. range 880 NM
Max. speed 360 KTAS
Max. power generated 2.4 MW
Emissions 0.0 CO_2 eq IN FLIGHT
Max. passengers 8 PAX
MTOW 9.6 t

BACK TO SCIENCE: H2 IS VERY DIFFERENT FROM OTHER FUELS

★ Hydrogen leaks…

★ Hydrogen ignites much more easily

★ Hydrogen burns much faster than all other fuels

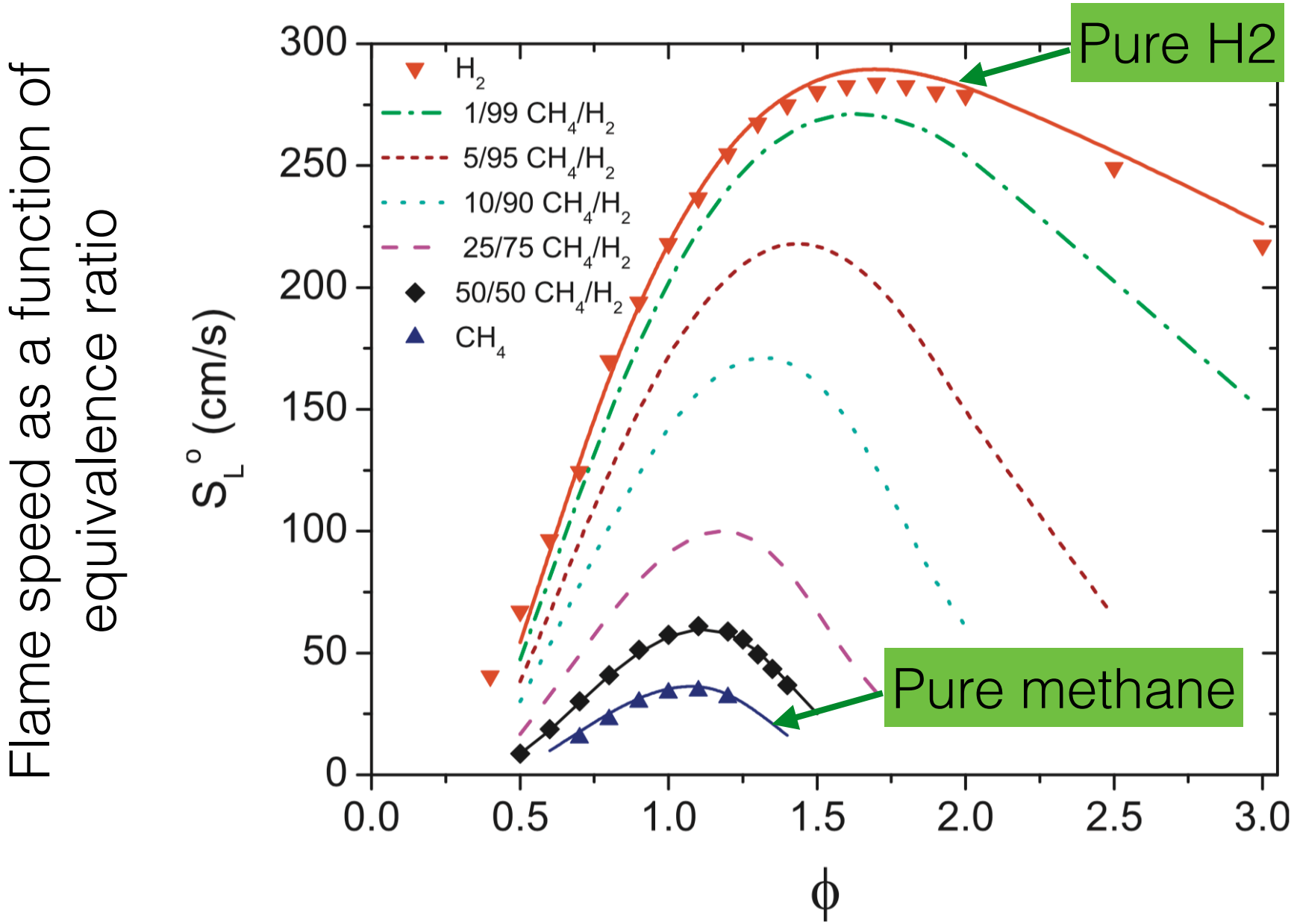
★Hydrogen explodes…

FLAMMABILITY LIMITS:

	LEAN FLAMMABILITY LIMIT	RICH FLAMMABILITY LIMIT
CH4 methane	5 %	15 %
C3H8 propane	2,1 %	9,5 %
H		

The MIE (minimum ignition energy) is also ten times less for H2 than for other fuels

H2 BURNS MUCH FASTER THAN ALL FUELS: example in air



IN PRACTICE:

Yes, there will be hydrogen but we have two key problems:

- ➡Redesign combustion systems adapted to H2 because it is a different fuel
- ➡Ensure that these systems and all those around them (tanks, lines, controllers, etc) are safe

H2 ENGINES WILL HAVE TO BE DIFFERENT:

★H2 burns very fast so that it can not be directly mixed with other fossil fuels in existing systems beyond a certain value (< 10 to 20 % in volume)

★Tests show that injecting pure H2 in existing gas turbines may be difficult: instabilities, noise, flashback, NOx, violent ignition

★To use H2, we have to change the combustion chambers

REDESIGNING COMBUSTORS TO BURN PURE H2:

The example of H2 in gas turbines (just two technologies discussed here - there are many other ideas around):

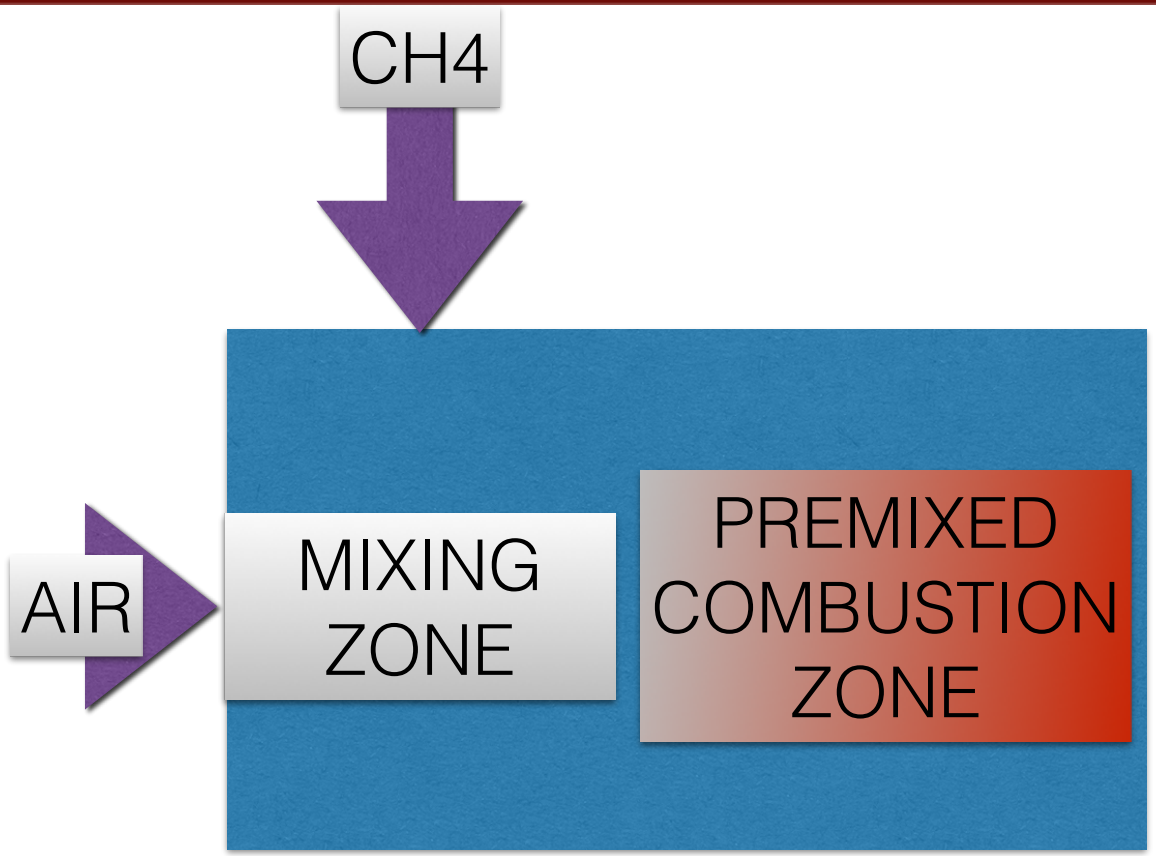
➡The MICROMIX injector of Cranfield

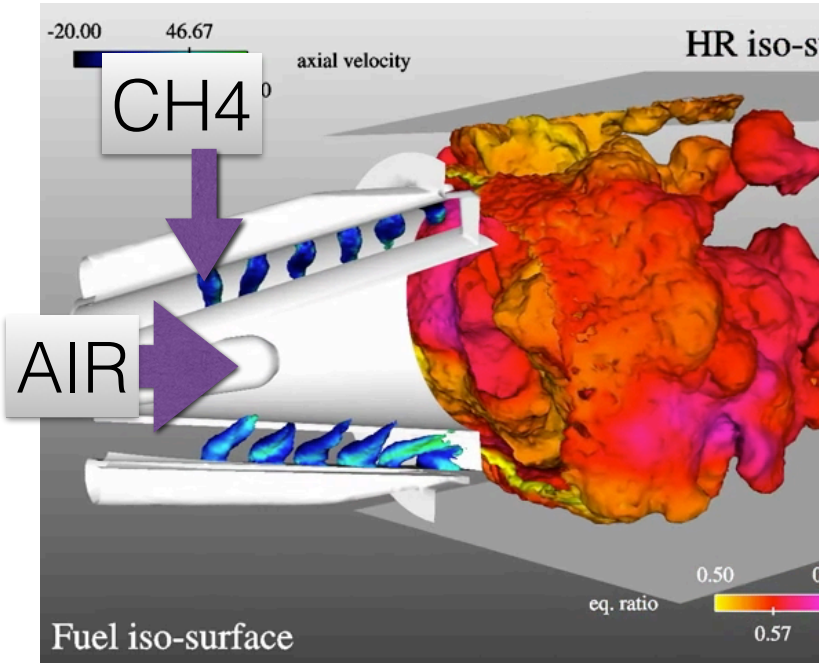
➡The HYLON injector of IMFT

First problem ?: « Mixing vs burning »

This is where this SPOC is useful to understand WHY we have a problem here

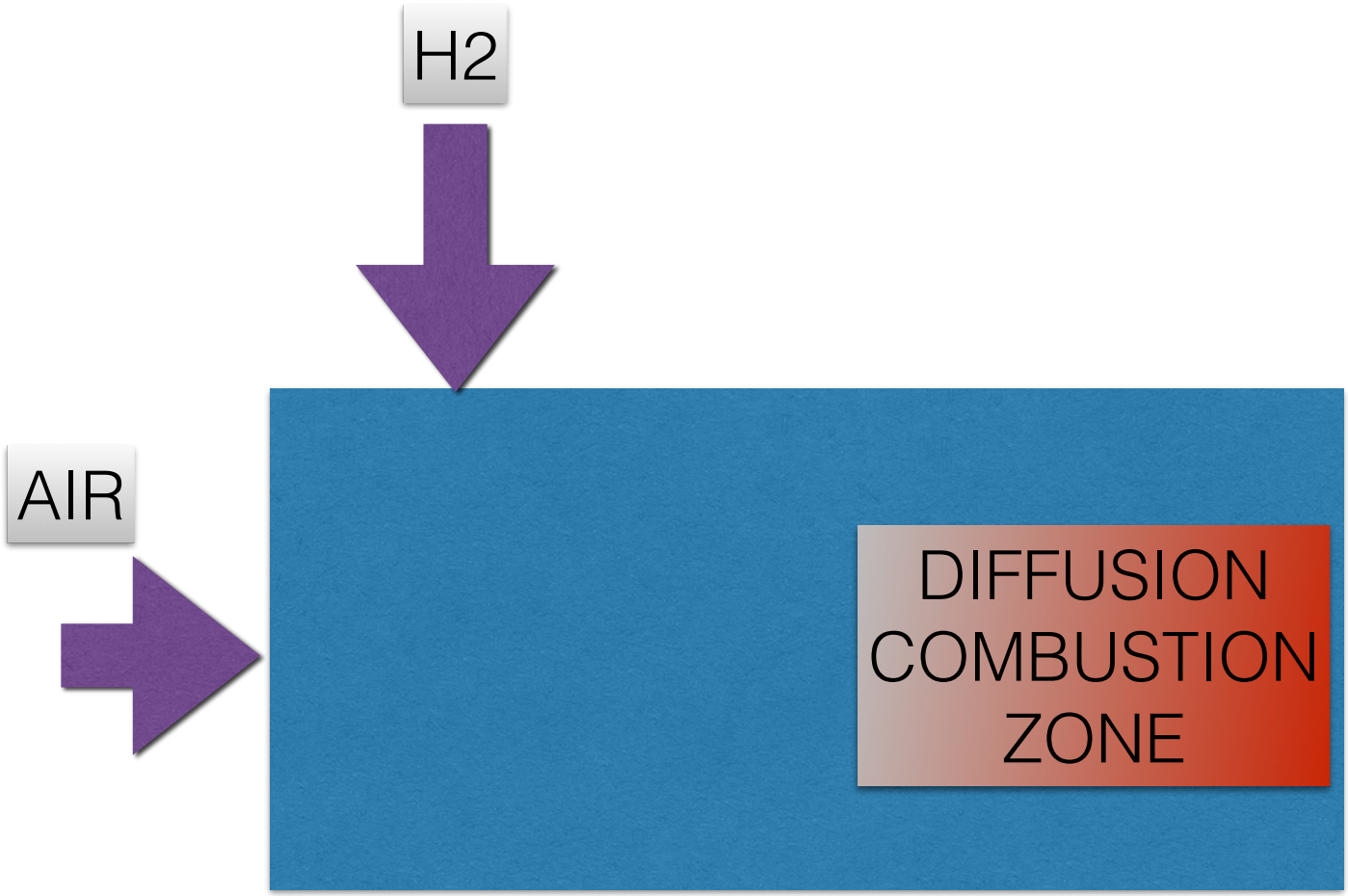
METHANE (or other usual fuels) COMBUSTION





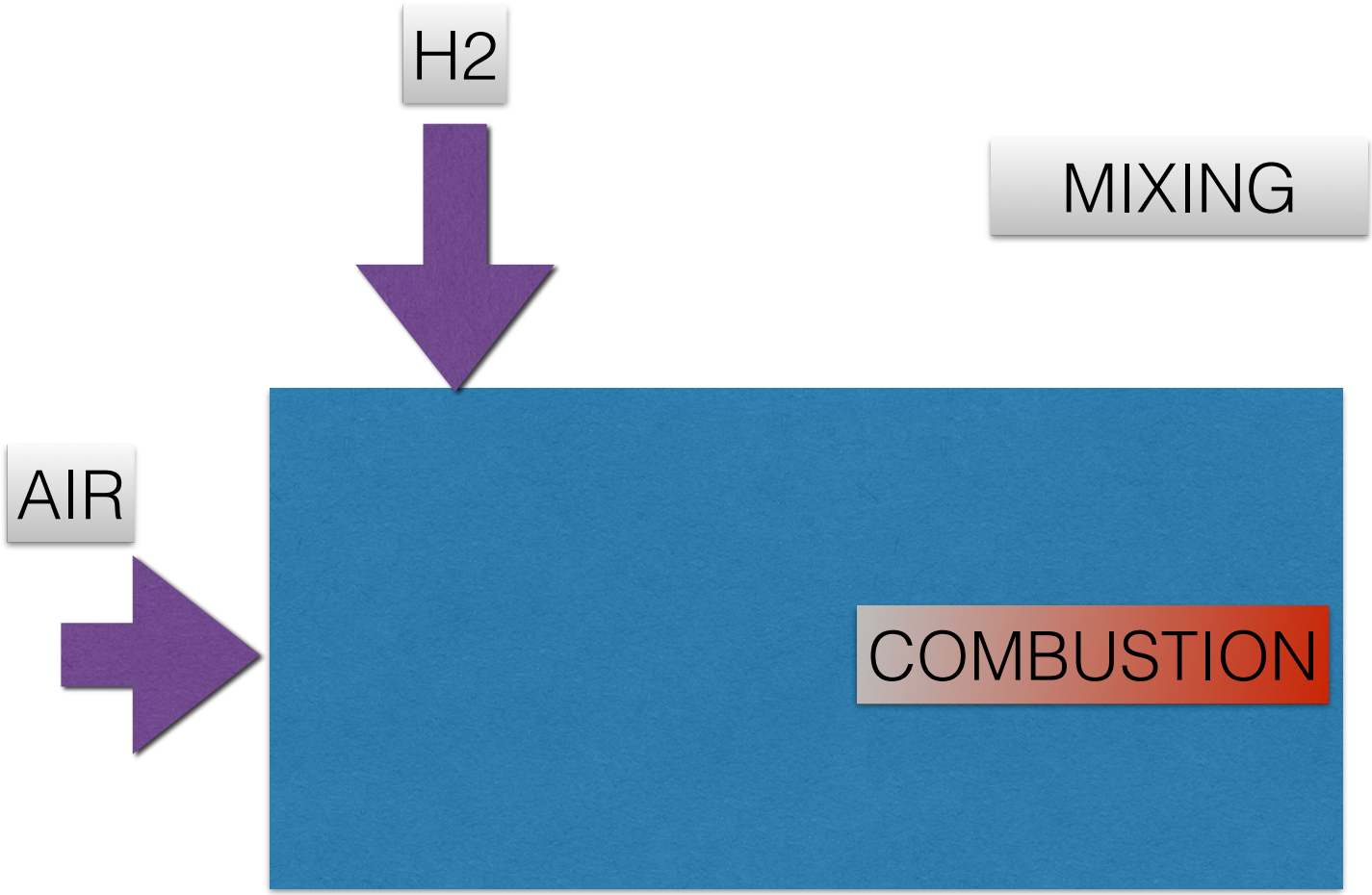
We do not want a diffusion flame to appear. Fortunately, those fuels burn slowly enough to allow mixing to take place before combustion begins.

HYDROGEN COMBUSTION



★**H2 burns so fast that it comes back to the injectors, creates a diffusion flame: too hot, too much NOx, too much heat load on walls**

HYDROGEN COMBUSTION

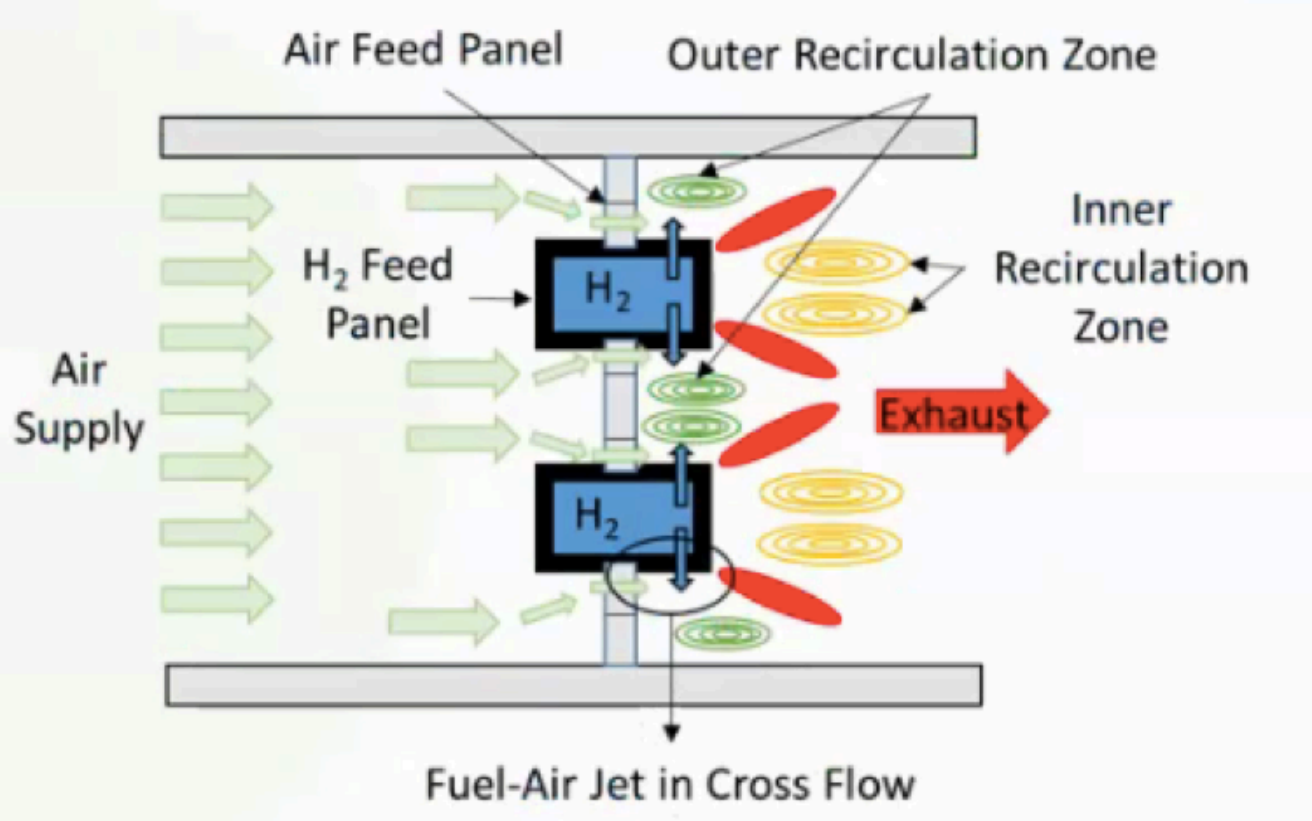


★**The injectors must provide a mixing which is faster than combustion: fundamental fluid mechanics problem. How can we mix fast enough ?**

ONE PATH: MICROMIX

★Use very high flow speeds: diminish flow time scales

★Very small jets of H2



MICROMIX

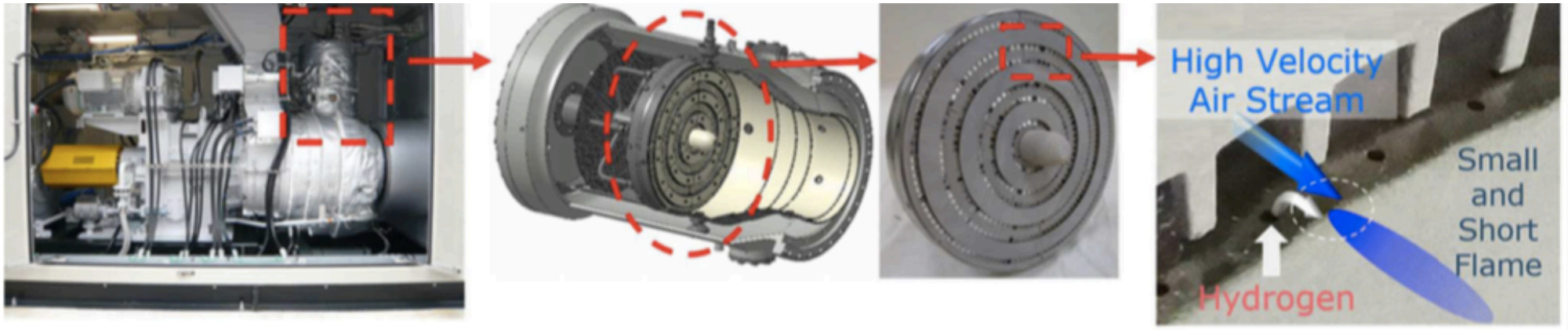
July 21, 2020

New Energy and Industrial Technology Development Organization

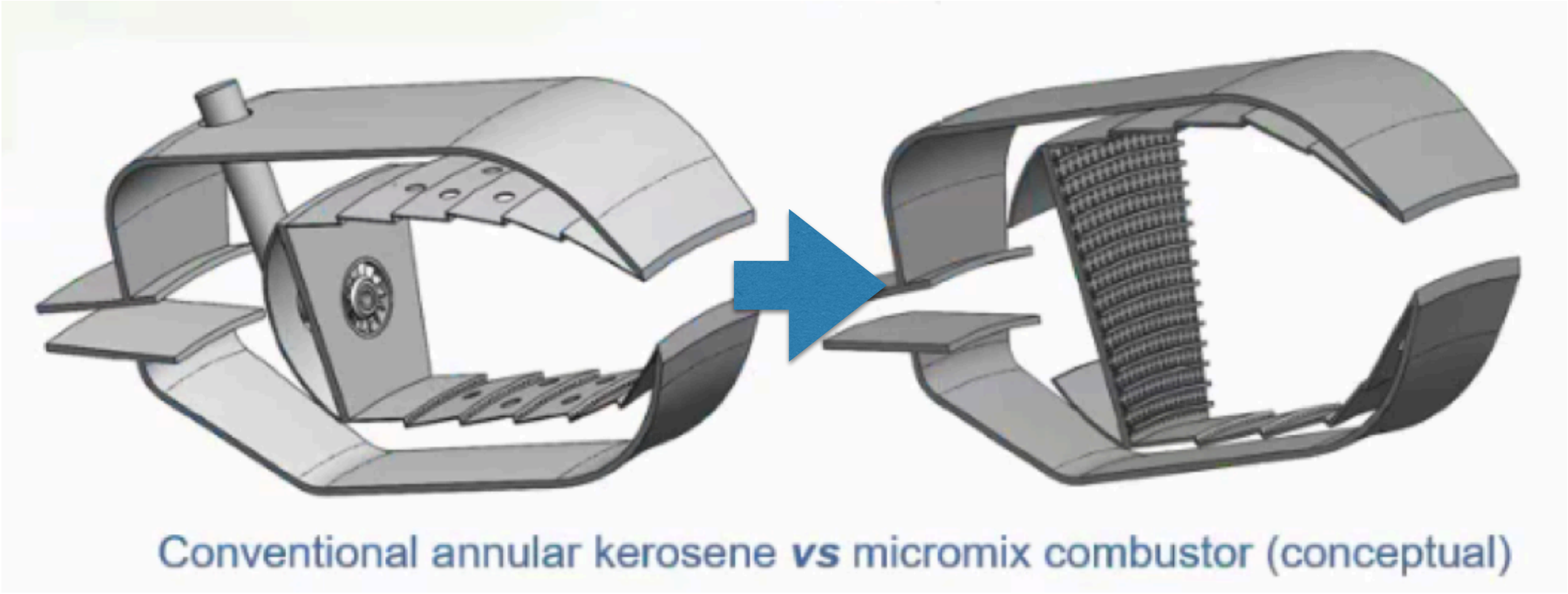
Kawasaki Heavy Industries, Ltd.

Obayashi Corporation

World's First Successful Technology Verification of 100% Hydrogen-fueled Gas Turbine Operation with Dry Low NOx Combustion Technology Improving Power Generation Performances to Realize a Hydrogen Society



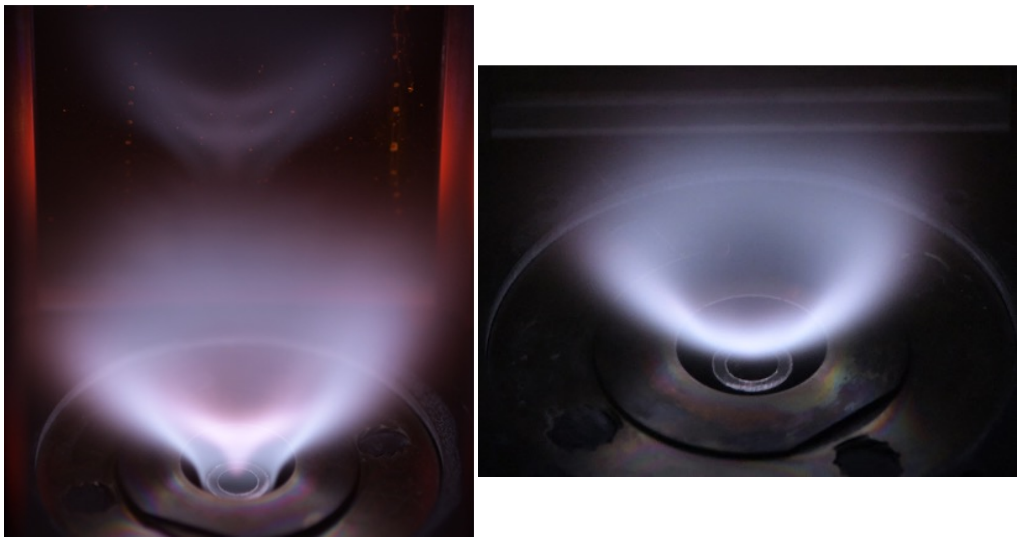
Then we need MANY injectors

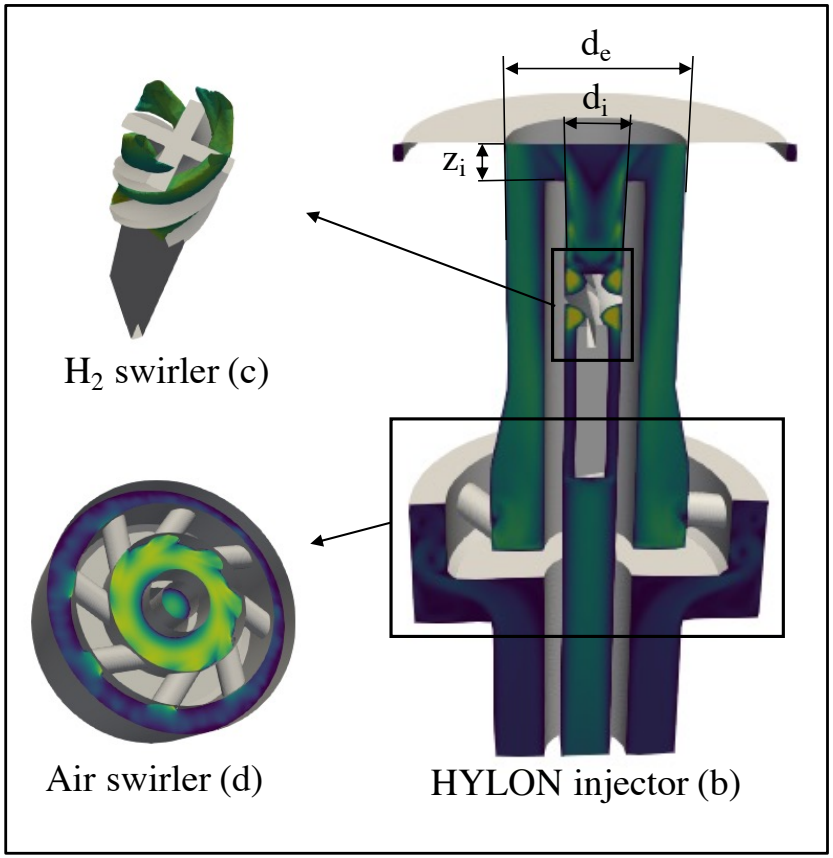


Conventional annular kerosene ***vs*** micromix combustor (conceptual)

ANOTHER PATH: HYLON

Developed in two ERC advanced grants SCIROCCO (2019-2024) and SELECT-H (2023-28) at IMFT and CERFACS
Patented with Safran Helicopter Engines





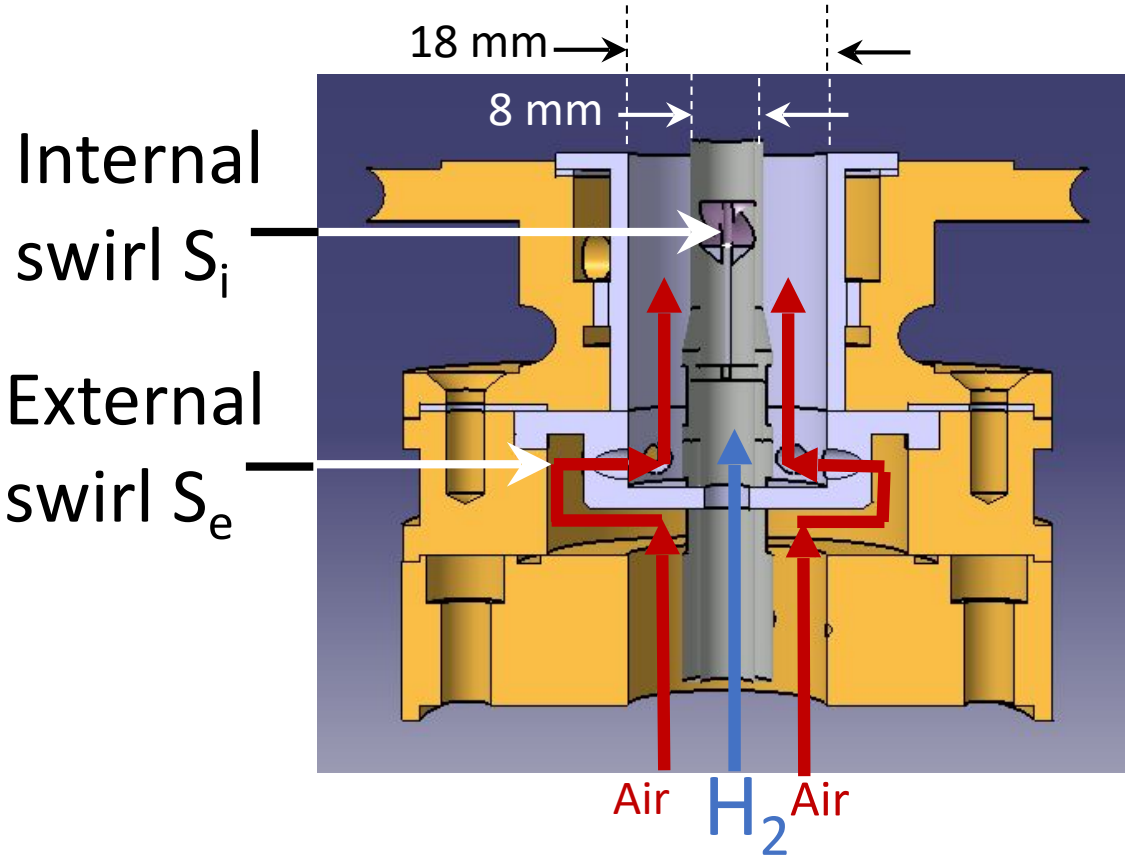
European Research Council
Established by the European Commission

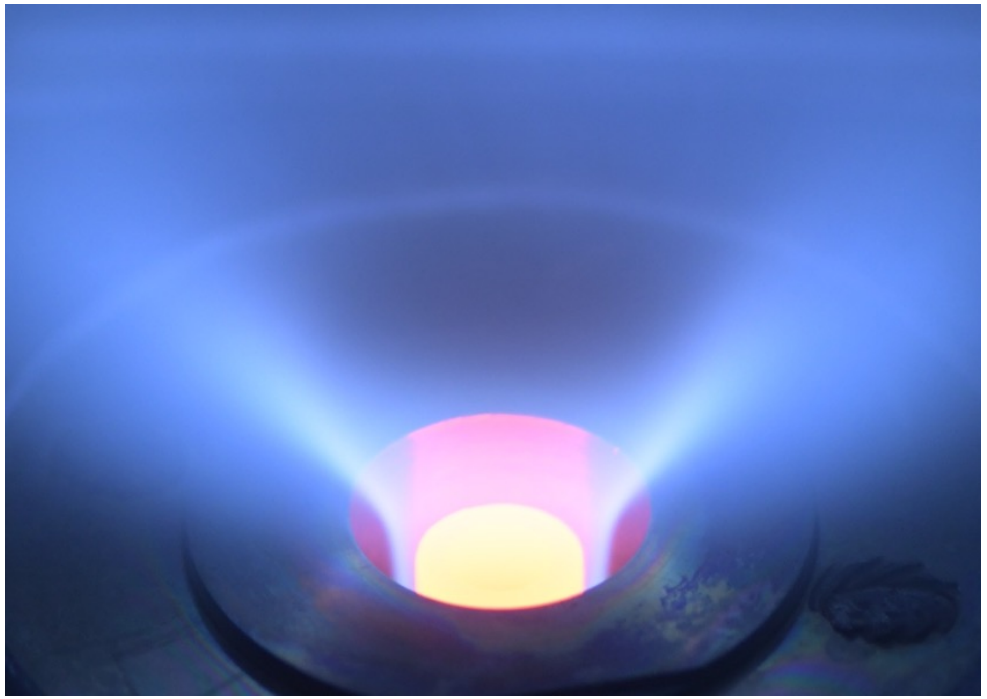
INSTITUT DE MECANIQUE DES FLUIDES DE TOULOUSE

CERFACS

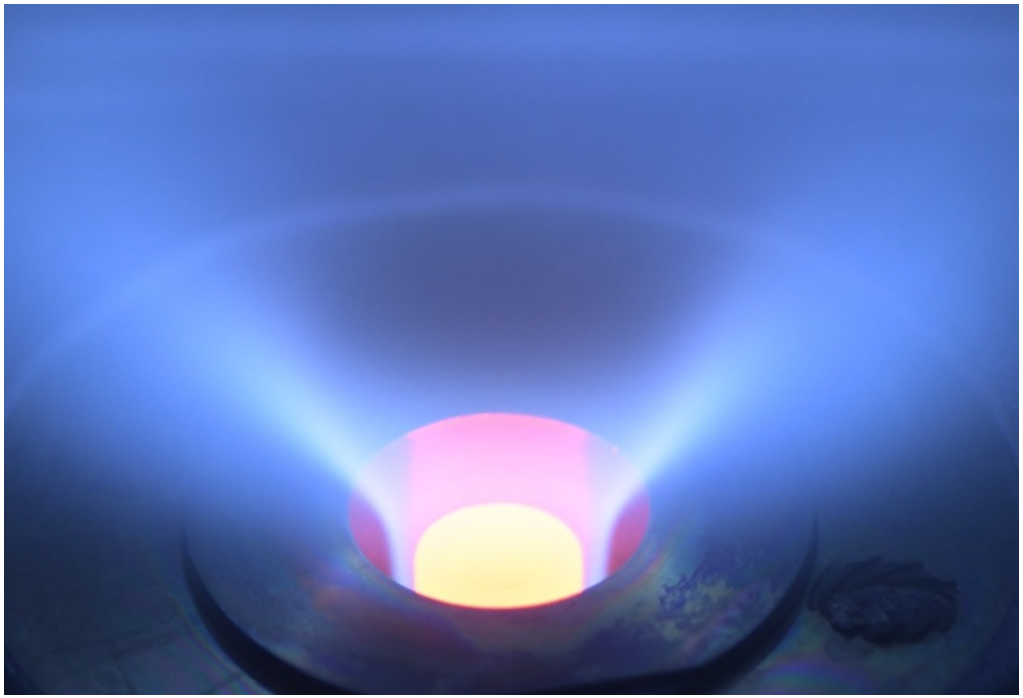
THE HYLON INJECTOR

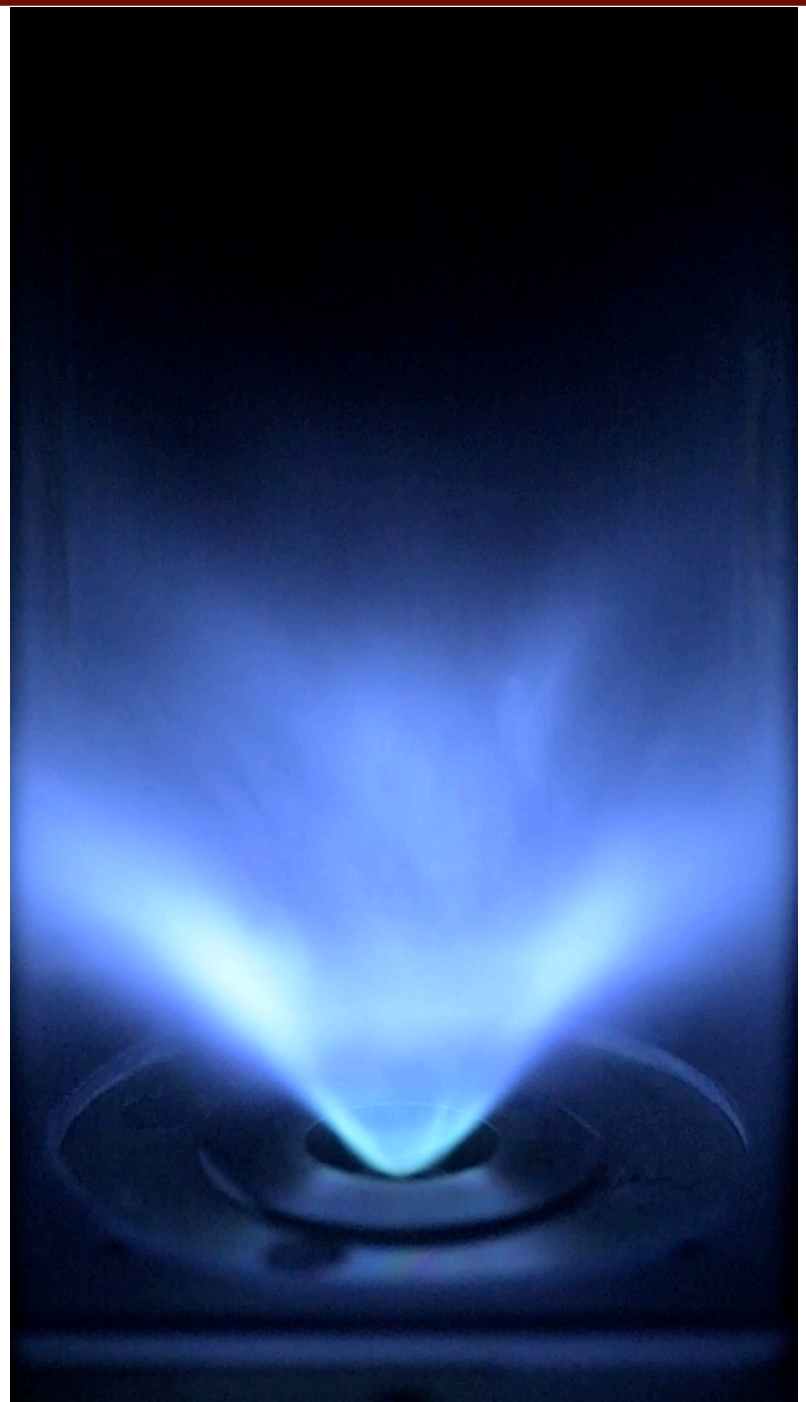
Dual swirl non-premixed injector: a solution for H2 chambers



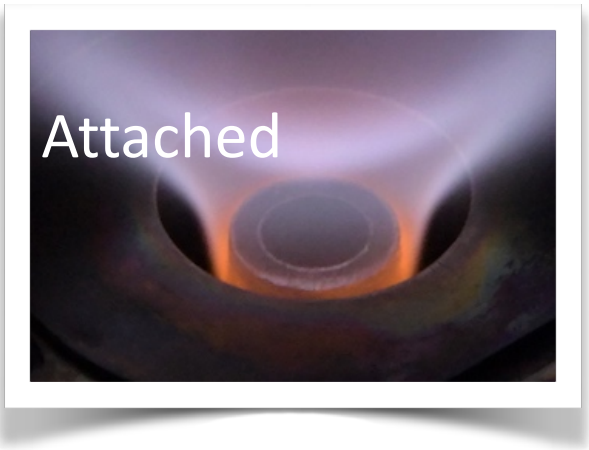


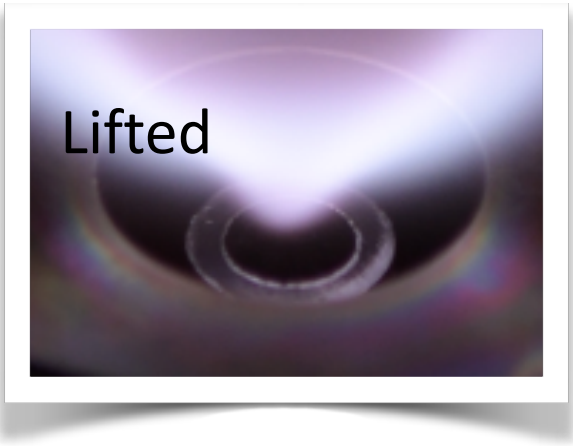
THE HYLON INJECTOR

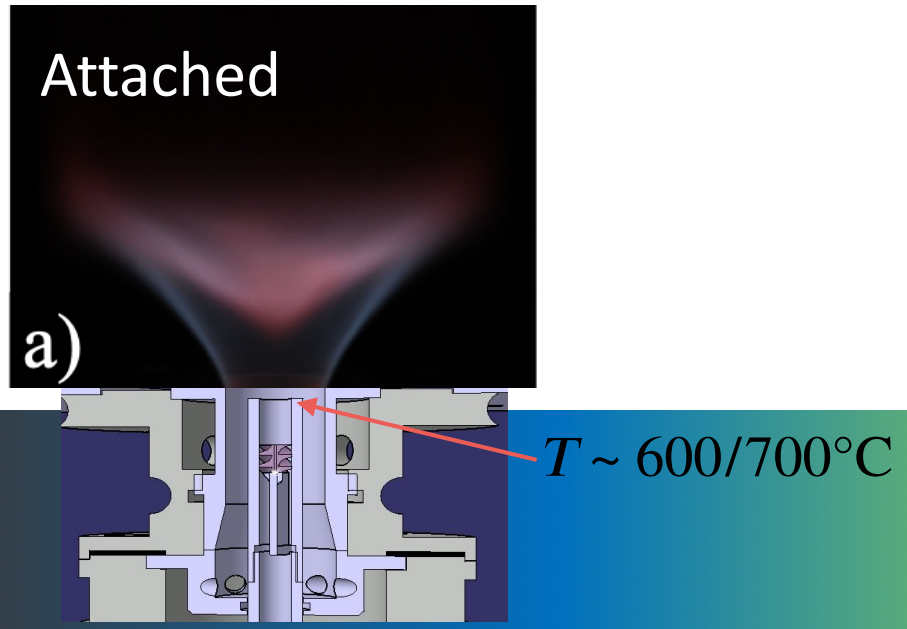


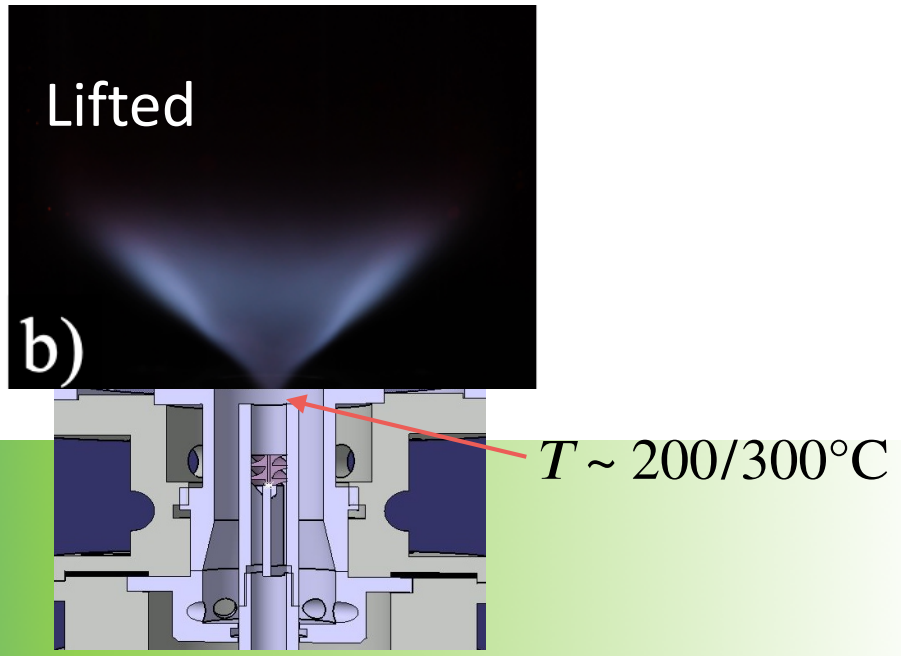


Attached (diffusion) and lifted (premixed) flames
-> different heat loads on lips
-> different flame efficiencies

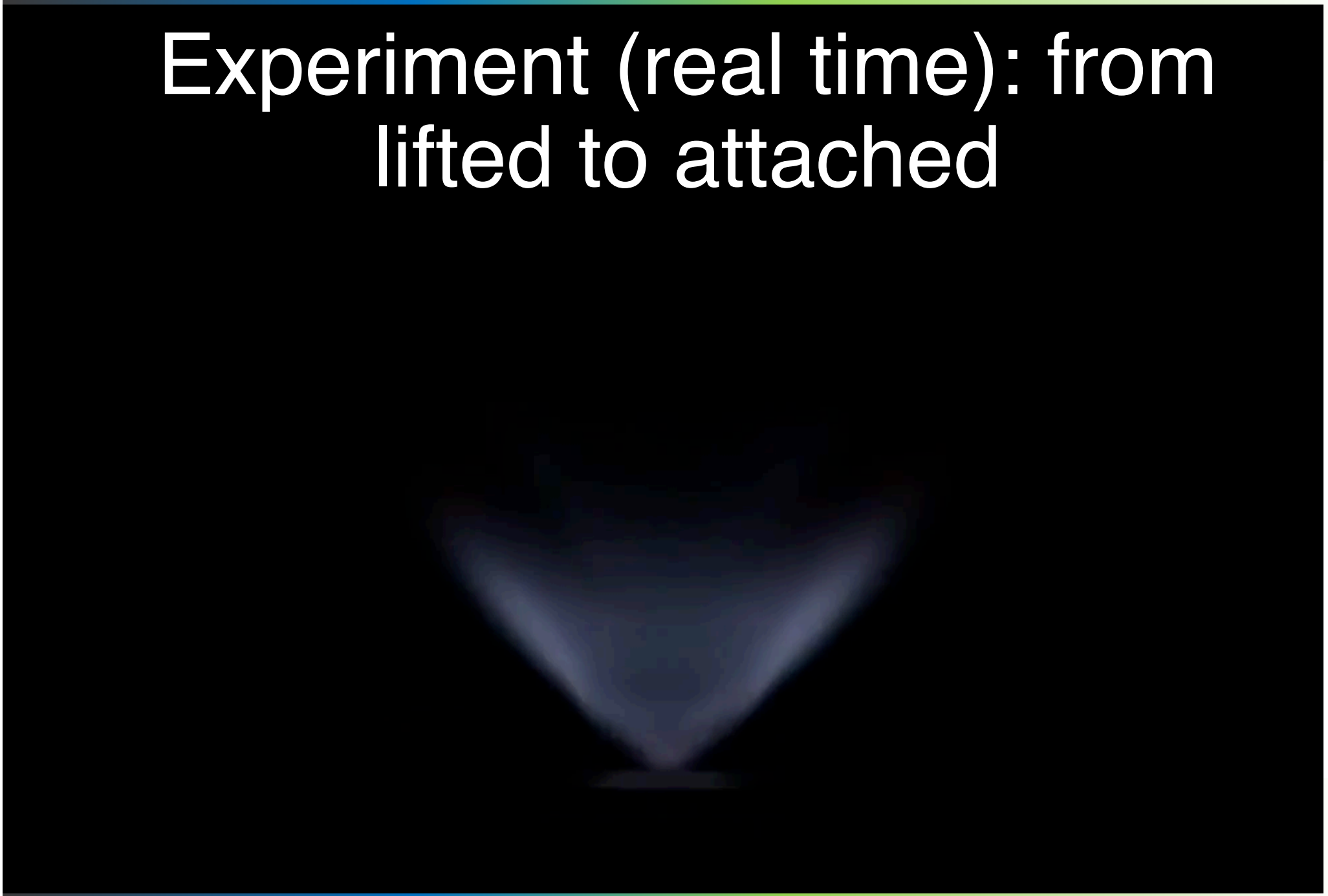




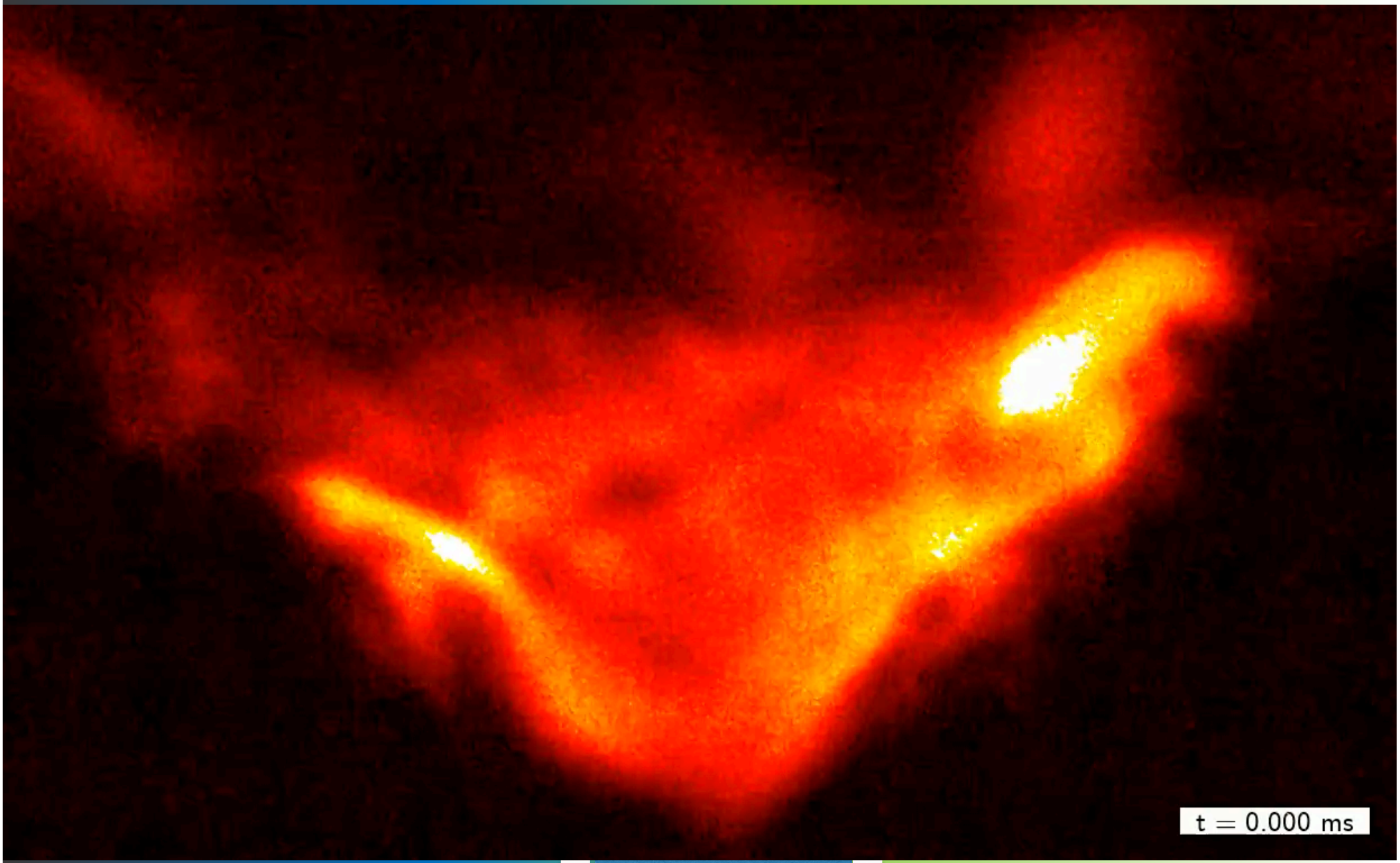




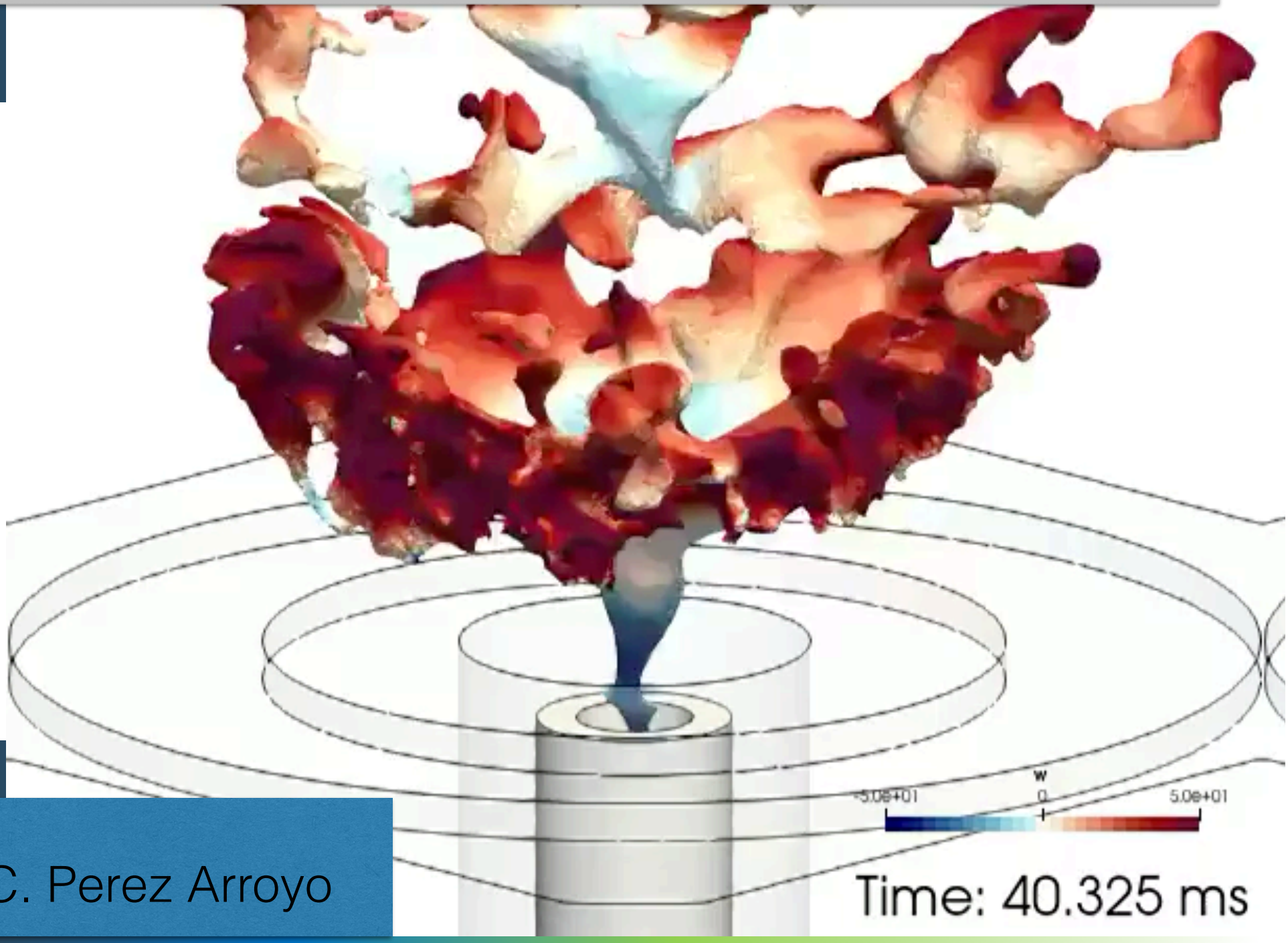
Experiment (real time): from lifted to attached



Experiment (16 kHz camera)



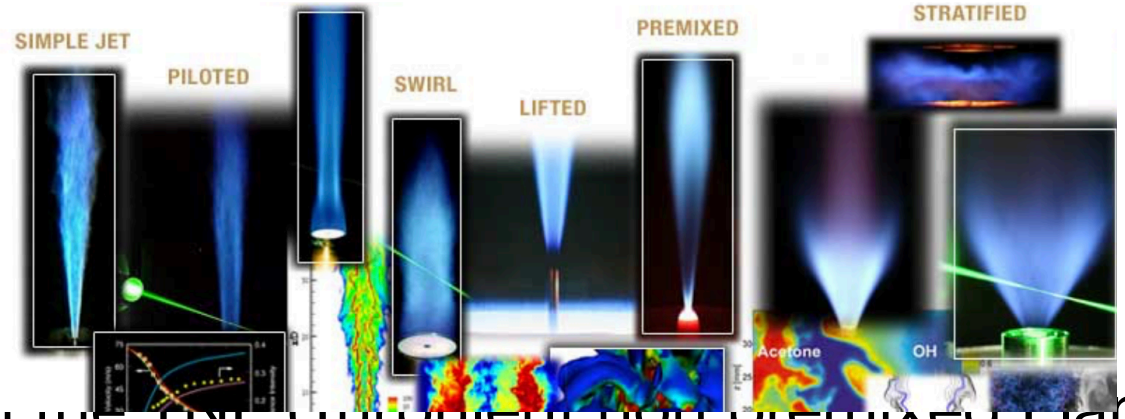
LES transition



C. Perez Arroyo

Comparison workshop for H2 flames

- Ongoing work to organize comparison workshop on H2 flame supported by Clean Aviation (European Union project)



- Results are in the TNF (Turbulent non premixed Flames) workshop. Presented at the TNF workshop in Milano 2024 and Kyoto 2026

- You can participate to HYLON Phase 1 or 2: simply go to tnfworkshop.org/hylon2/ to download the experimental data and send us a mail

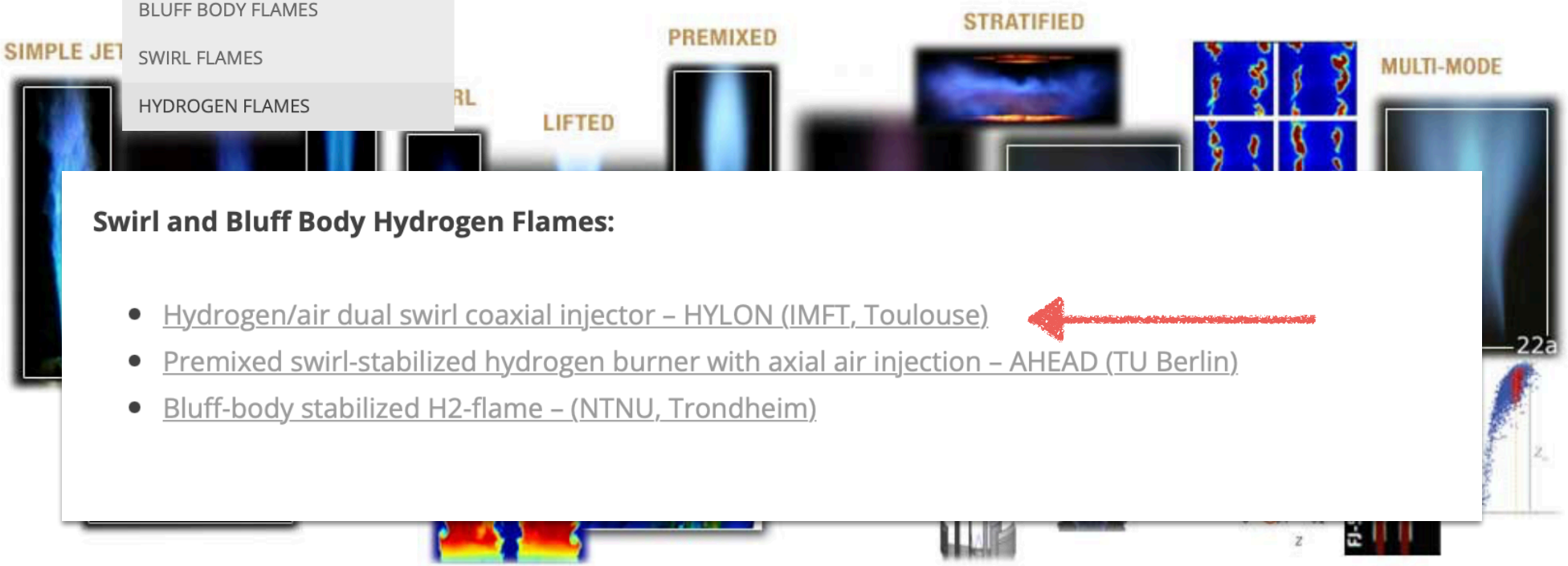
https://tnfworkshop.org/hydrogen-flames/

TNF Workshop

International Workshop on Measurement and Computation of Turbulent Flames

HOME | DATA ARCHIVES | WORKSHOP PROCEEDINGS | CONTACT

- COMPUTATIONAL
- SIMPLE FLAMES
- PILOTED JET FLAMES
- BLUFF BODY FLAMES
- SWIRL FLAMES
- HYDROGEN FLAMES



Swirl and Bluff Body Hydrogen Flames:

- Hydrogen/air dual swirl coaxial injector – HYLON (IMFT, Toulouse)
- Premixed swirl-stabilized hydrogen burner with axial air injection – AHEAD (TU Berlin)
- Bluff-body stabilized H2-flame – (NTNU, Trondheim)

HYDROGEN AND SAFETY

- Need to discuss safety issues: these issues exist for all H2 systems (trains, cars, furnaces, heaters…)
  - Filling H2 tanks, transporting and storing large quantities of H2
  - Leaks of H2: detection and protection
  - *What happens if there is a leak ?*
  - *IS IT SAFE ? We have been using other gases before ! What is different for H2 ?*

CATS or TIGERS ?

CATS IN HOMES



THIS IS SAFE

Kerosene, CH4, C3H8, gasoline

TIGERS IN ZOOS



THIS IS SAFE, TOO

H2

Four legs, one tail, a few teeths… well they look similar, dont they ?

WANT TO HAVE TIGERS AT HOME ? SERIOUSLY ?



IS THIS SAFE ?

Tiger already biting. Norway 2019

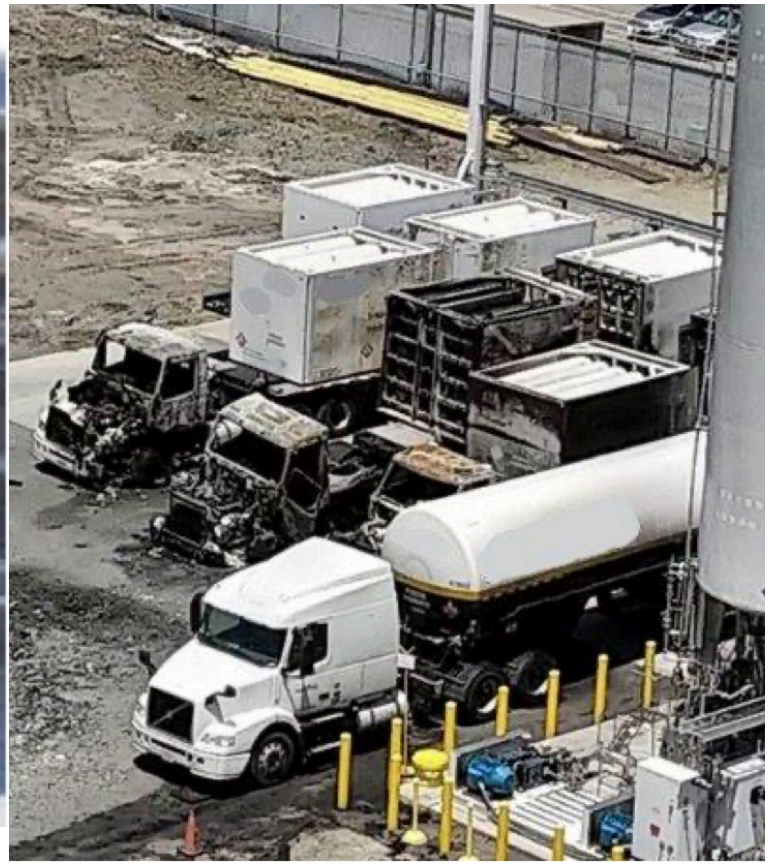
Bernard DEBOYSER / 20 Juin 2019 3:27 / 97

Hydrogène, Voiture hydrogène

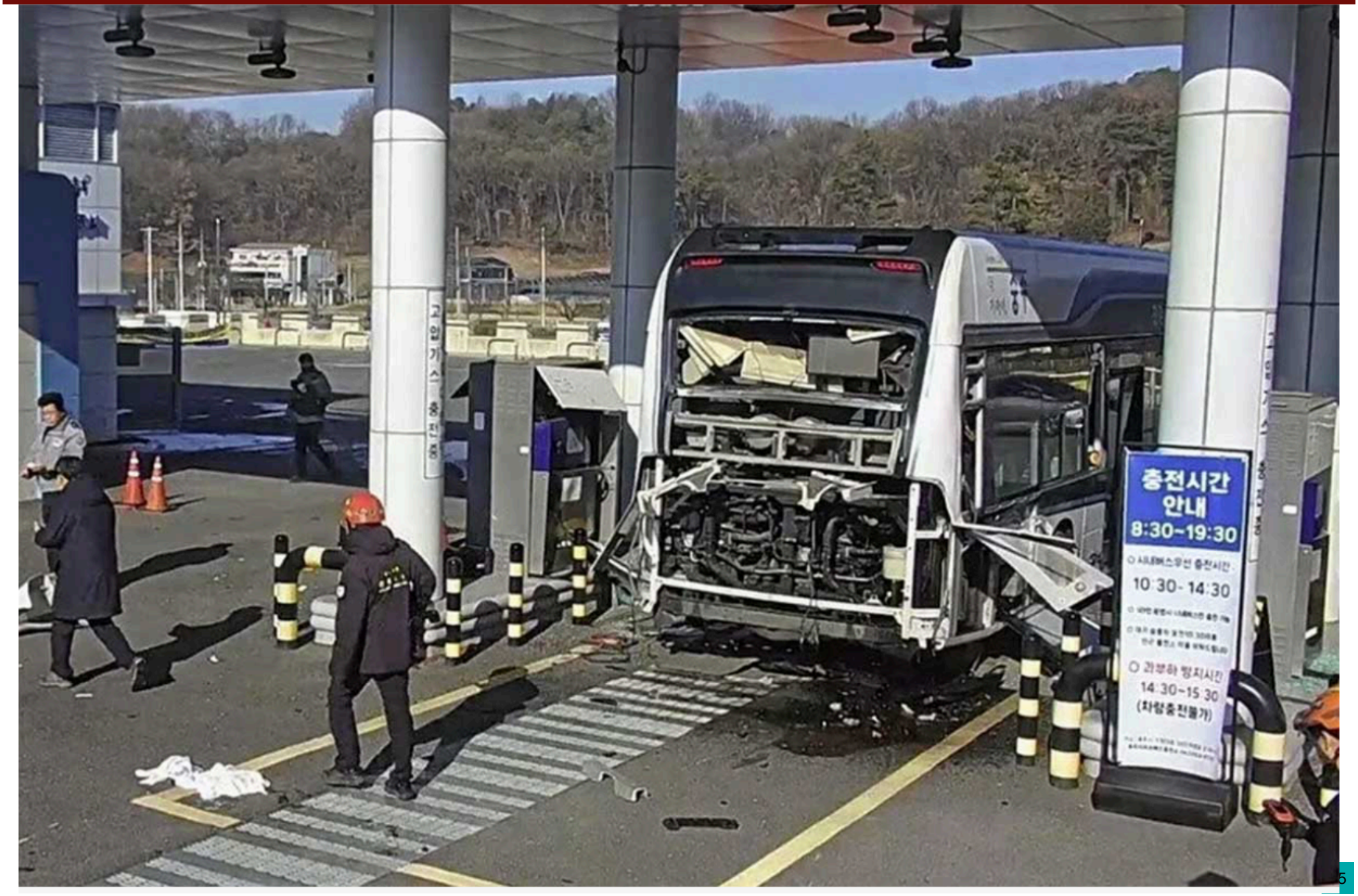


Santa Clara 2019: H2 trailers





South Korea 2024: bus



France 2025: buses again



Another comment on safety

- NOTHING IS ‘SAFE’: IT DEPENDS ON THE MONEY WE ARE READY TO USE TO MAKE IT SAFE. MILLIONS ON TONS OF H2 ARE ALREADY BURNT EVERY YEAR
- WE ALL USE NATURAL GAS EVERY DAY AT HOME: 200 YEARS AGO, MANY WERE WORRIED ABOUT NATURAL GAS SAFETY AND STILL… IT WORKS NOW
- TODAY, SHOW DANGEROUS SITUATIONS LINKED TO H2. THIS DOES NOT MEAN THAT WE CANNOT MASTER THEM. BUT WE MUST UNDERSTAND ALL MECHANISMS TO CONTROL THEM
- THE REAL QUESTION IS: « WHO WILL BE ABLE TO USE H2 SAFELY, AT REASONABLE COST ? »

SIMULATION AND HYDROGEN SAFETY

- USING H2 LEADS TO NEW QUESTIONS ON SAFETY
- CFD IS ESSENTIAL: WE CANT HAVE EXPERIMENTS FOR ALL POSSIBLE REAL ACCIDENTS SCENARIOS

HYDROGEN: Scenarios

H2 LEAK

EXPLOSIONS: DOES NOT IGNITE RIGHT AWAY: ACCUMULATES THEN IGNITES…

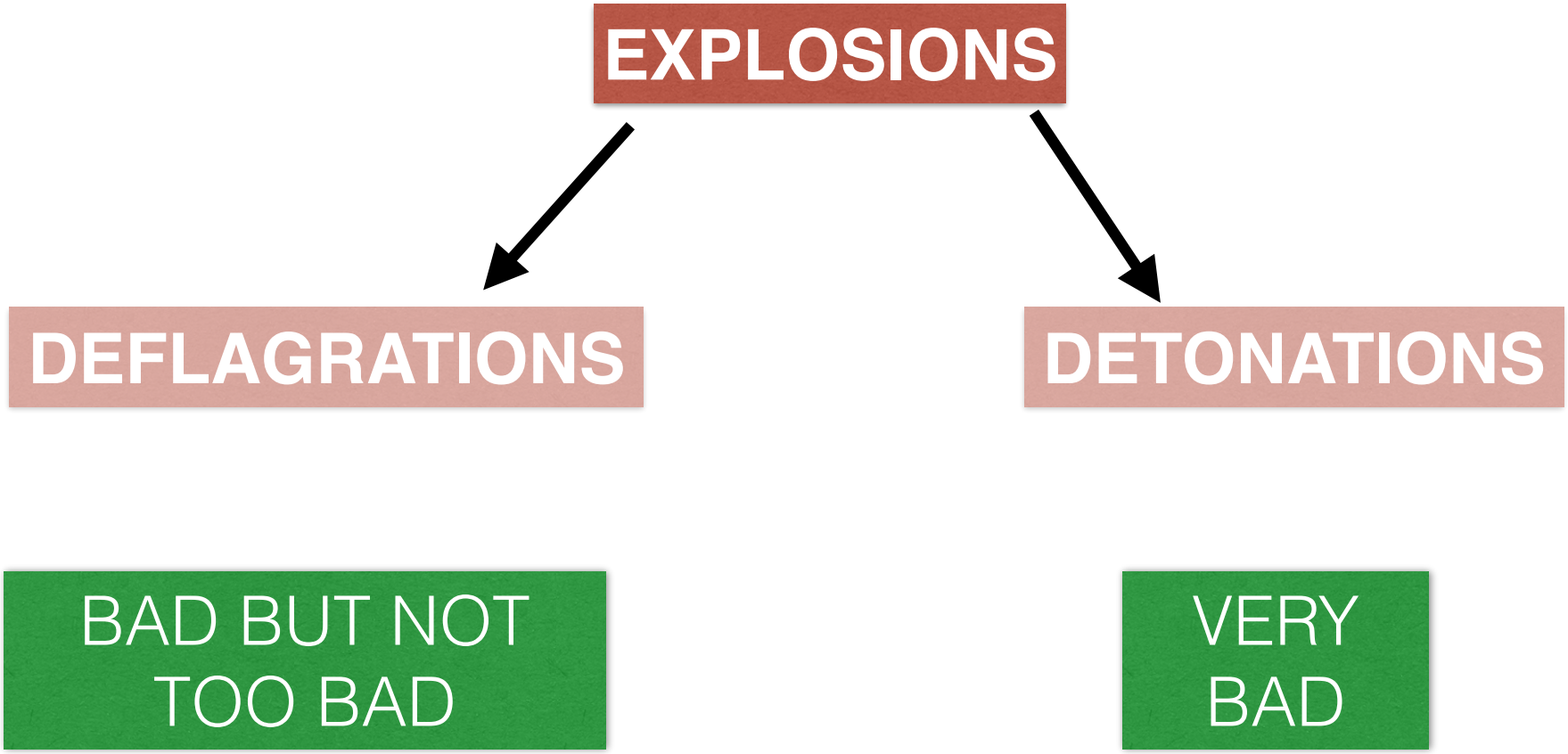


FIRES/FLAMES: IGNITES RIGHT AWAY





EXPLOSIONS COME INTO TWO FAMILIES:



HYDROGEN LEAKS AND EXPLODES:

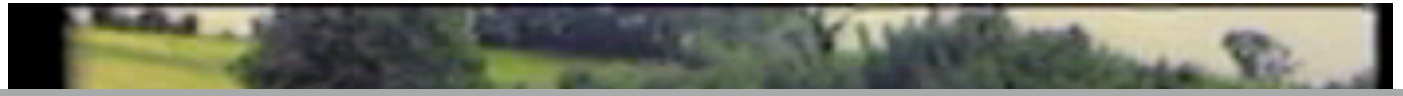
★ANY LEAK OF H2 INTO A CONFINED SPACE CAN LEAD TO EXPLOSIONS.





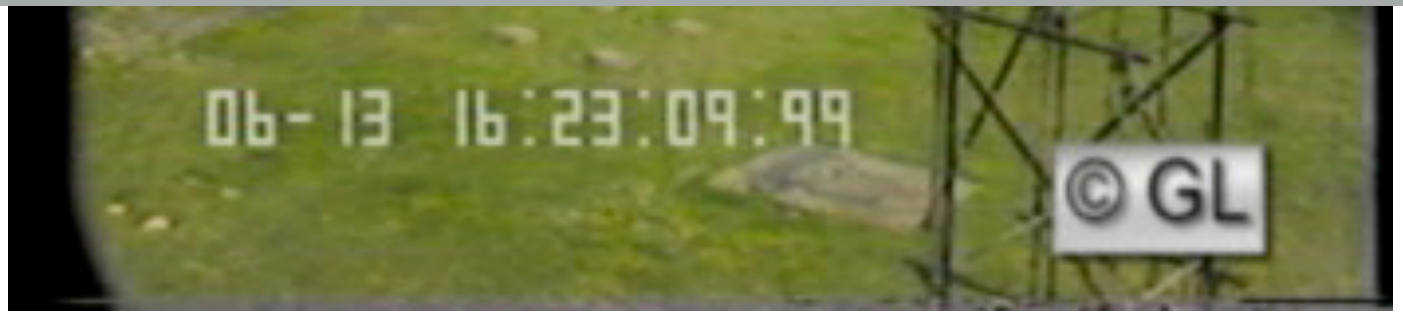
HYDROGEN LEAKS AND EXPLODES:

DEFLAGRATION:



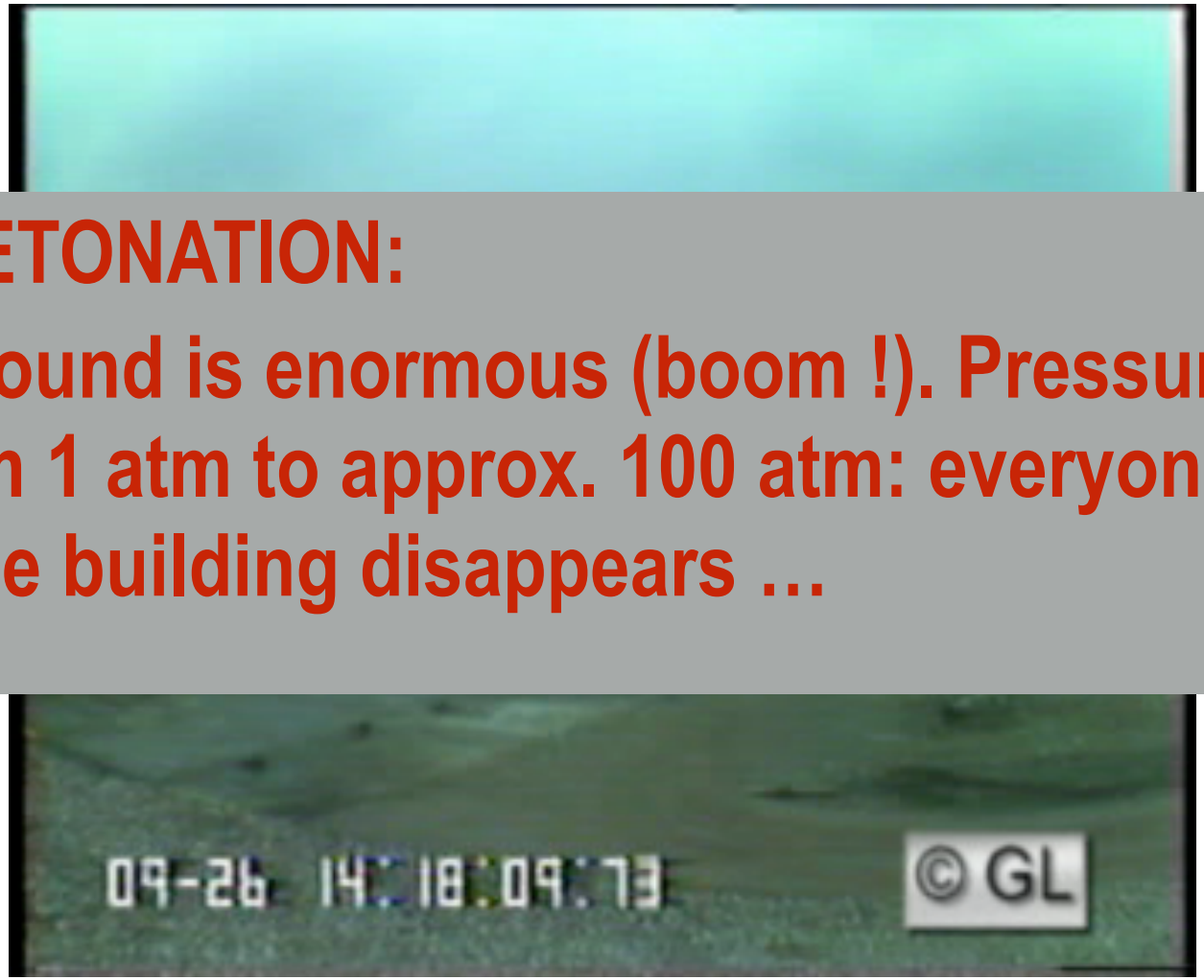
IN A DEFLAGRATION:

- No noise, no ‘boom’
- Pressure goes up from 1 atm to approx. 1.05 atm: no problem for the building to survive
- People die where the flame passes but global damage remains controlled



HYDROGEN LEAKS AND EXPLOSIONS

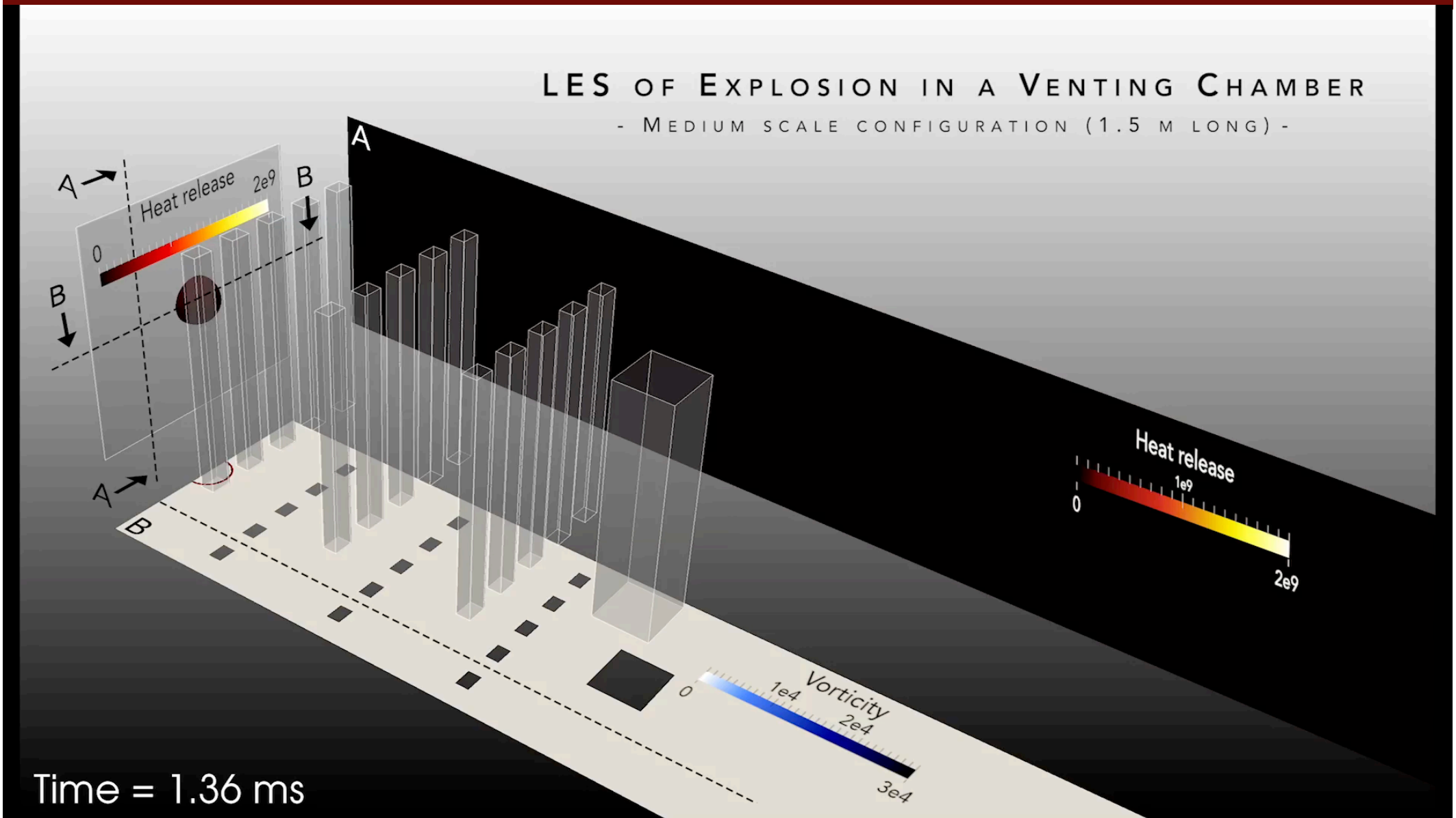
★DETONATION

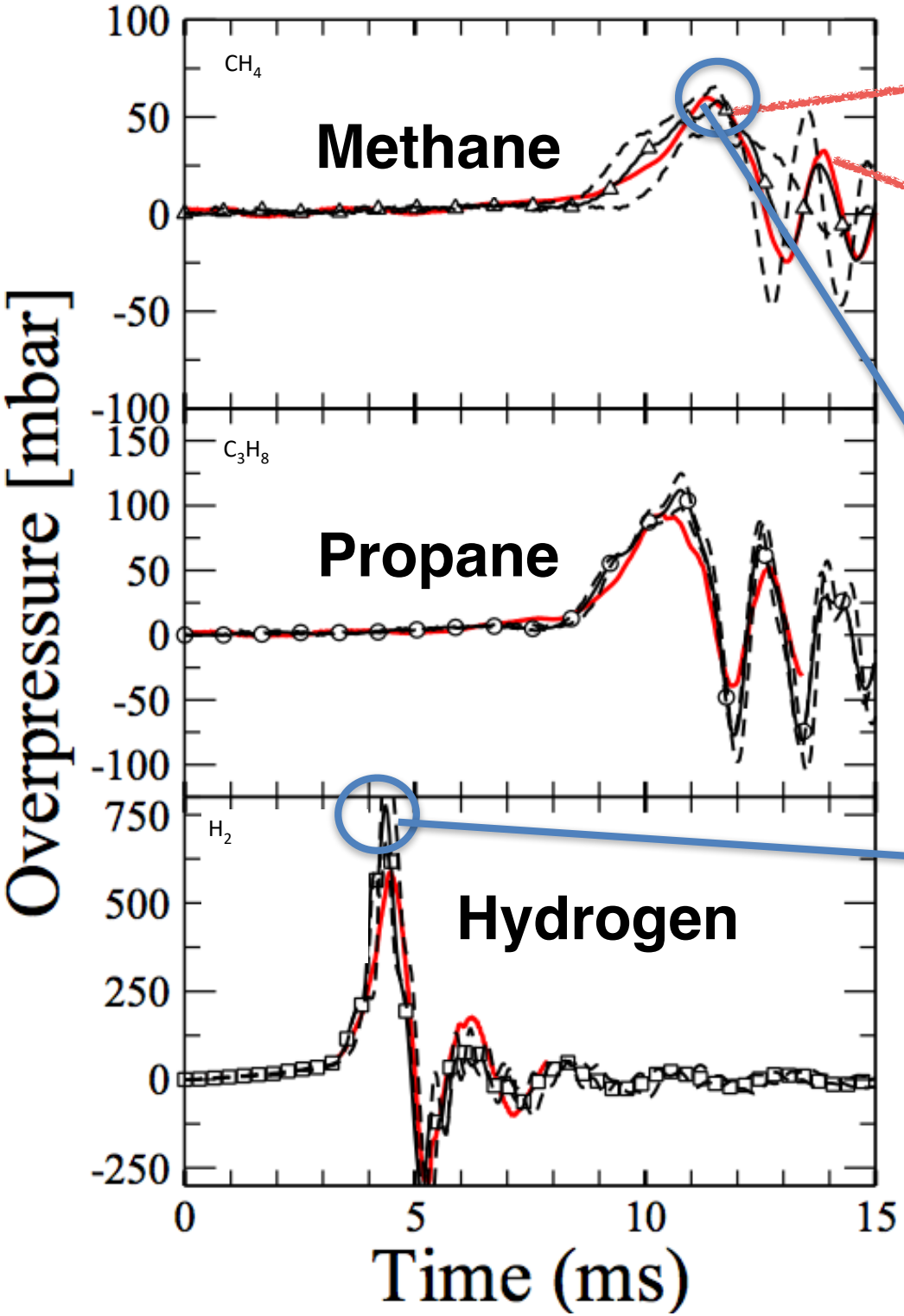


IN A DETONATION:

- The sound is enormous (boom !). Pressure goes up from 1 atm to approx. 100 atm: everyone dies AND the building disappears …

LES OF DEFLAGRATION IN THE SYDNEY (Masri) SETUP ON INCITE MACHINES (USA): 2 BILLION POINTS





Exp (Sydney)

LES (CERFACS)

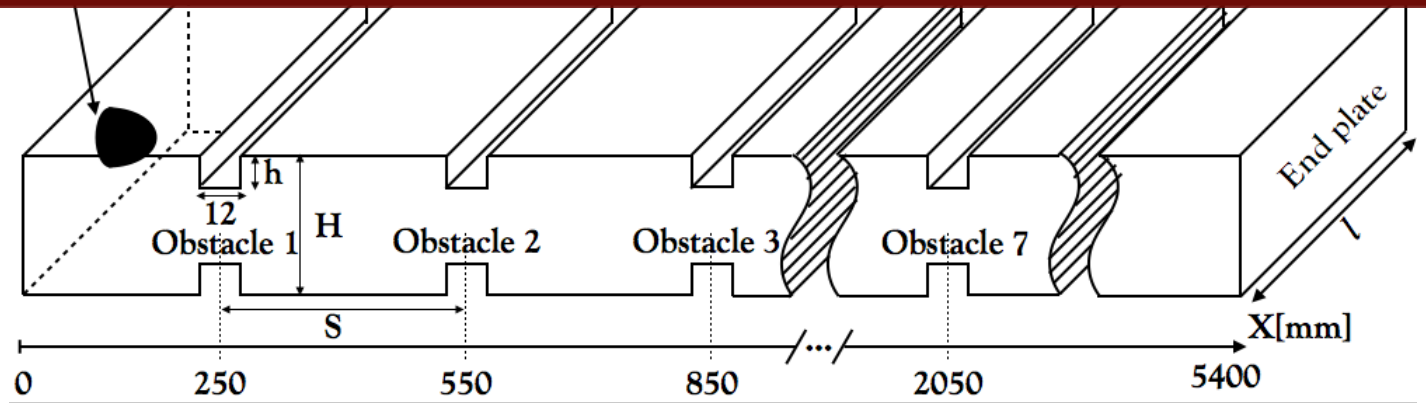
Simulation captures effects of fuel very well. H2 leads to powerful explosions:

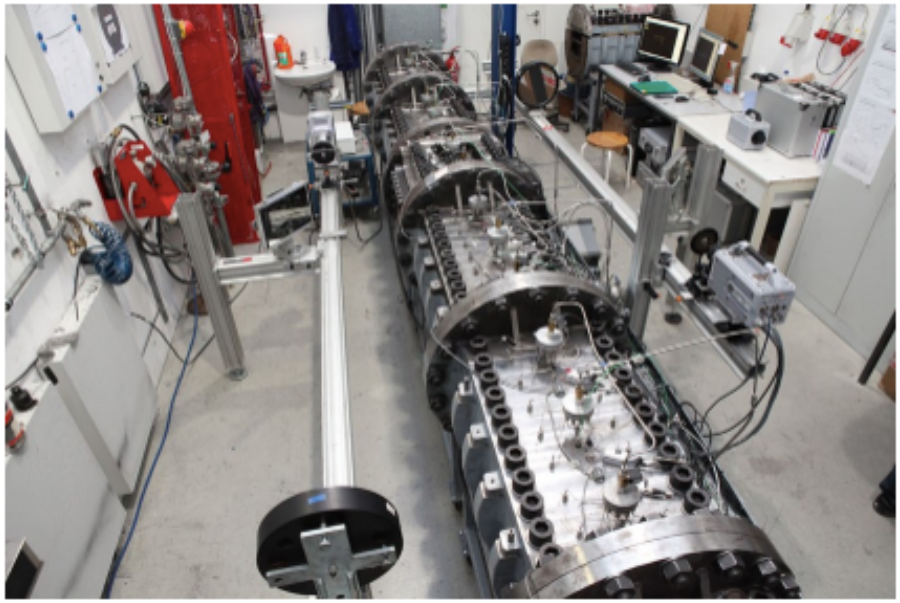
CH4: 60 mbar

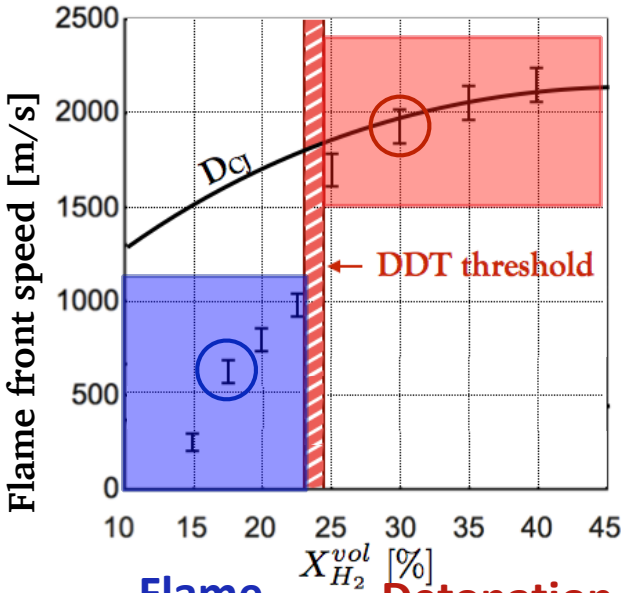
H2: 750 mbar

LES OF EXPLOSIONS IN GRAVENT SETUP AT TU MUNICH

- H_2/air mixture
- Blockage ratio 0.3







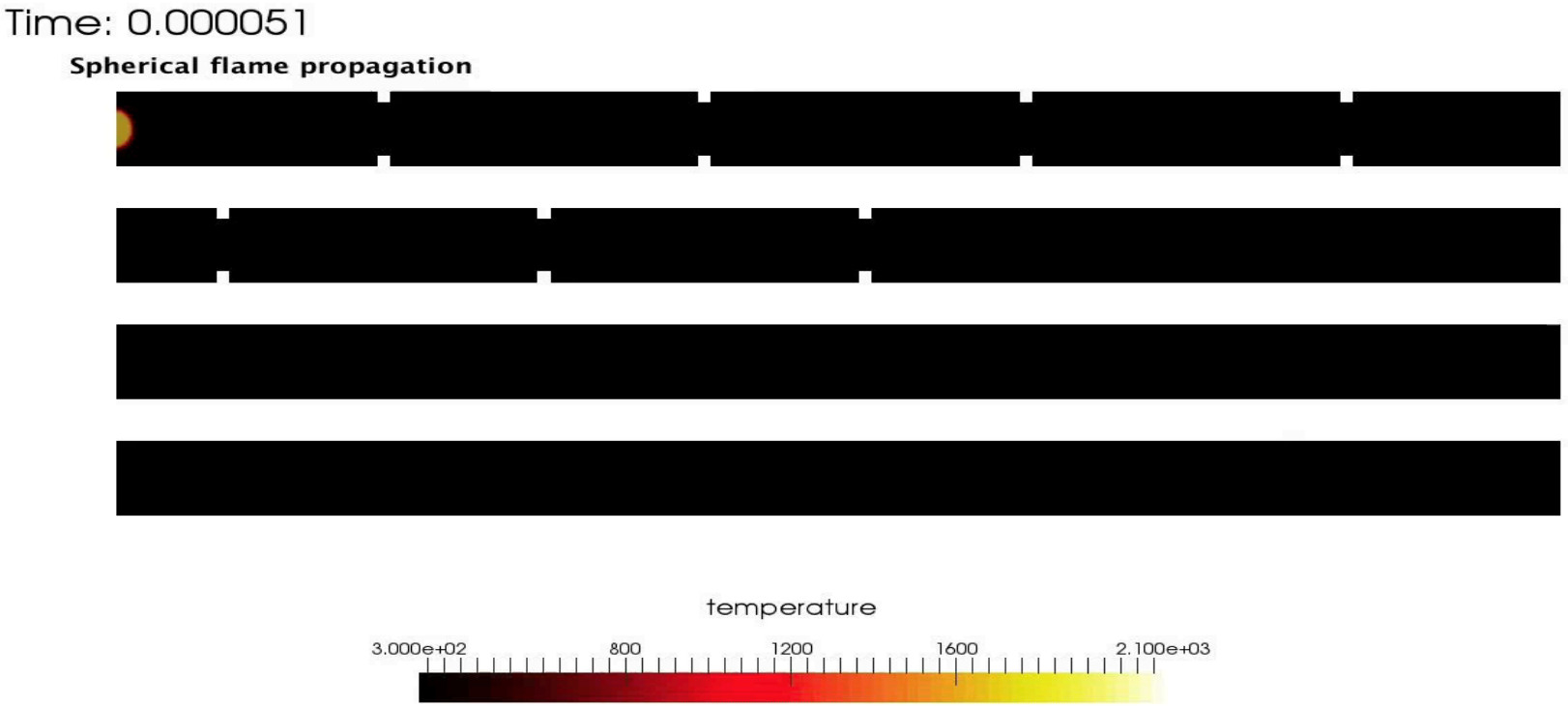
Theoretical detonation velocity D_{CJ}

Flame acceleration

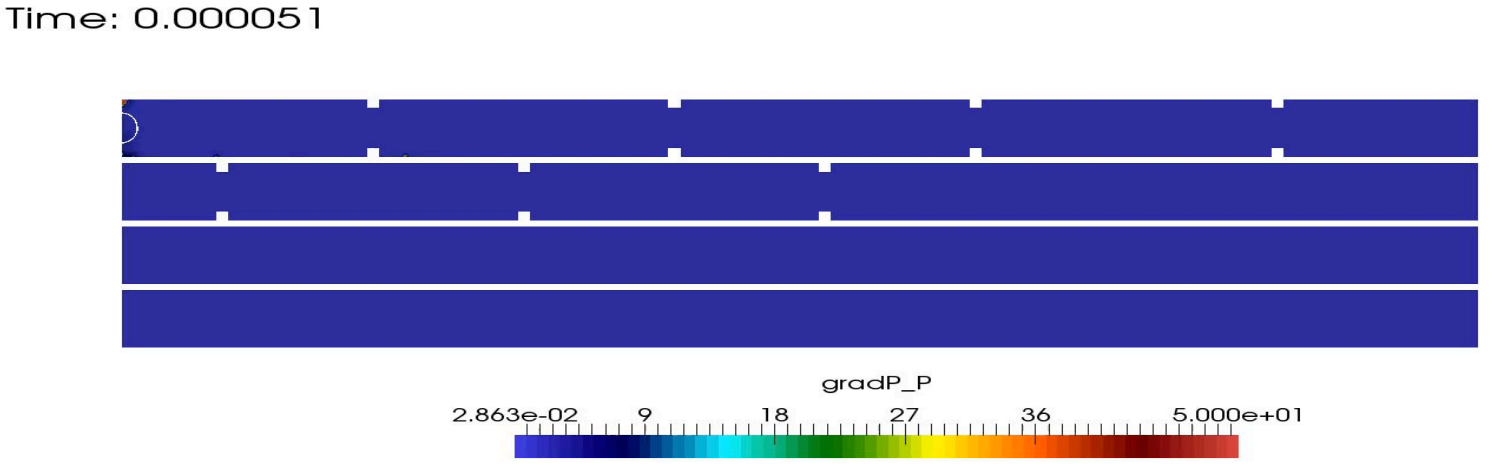
Detonation

Deflagration case (phi=0.52)

Temperature

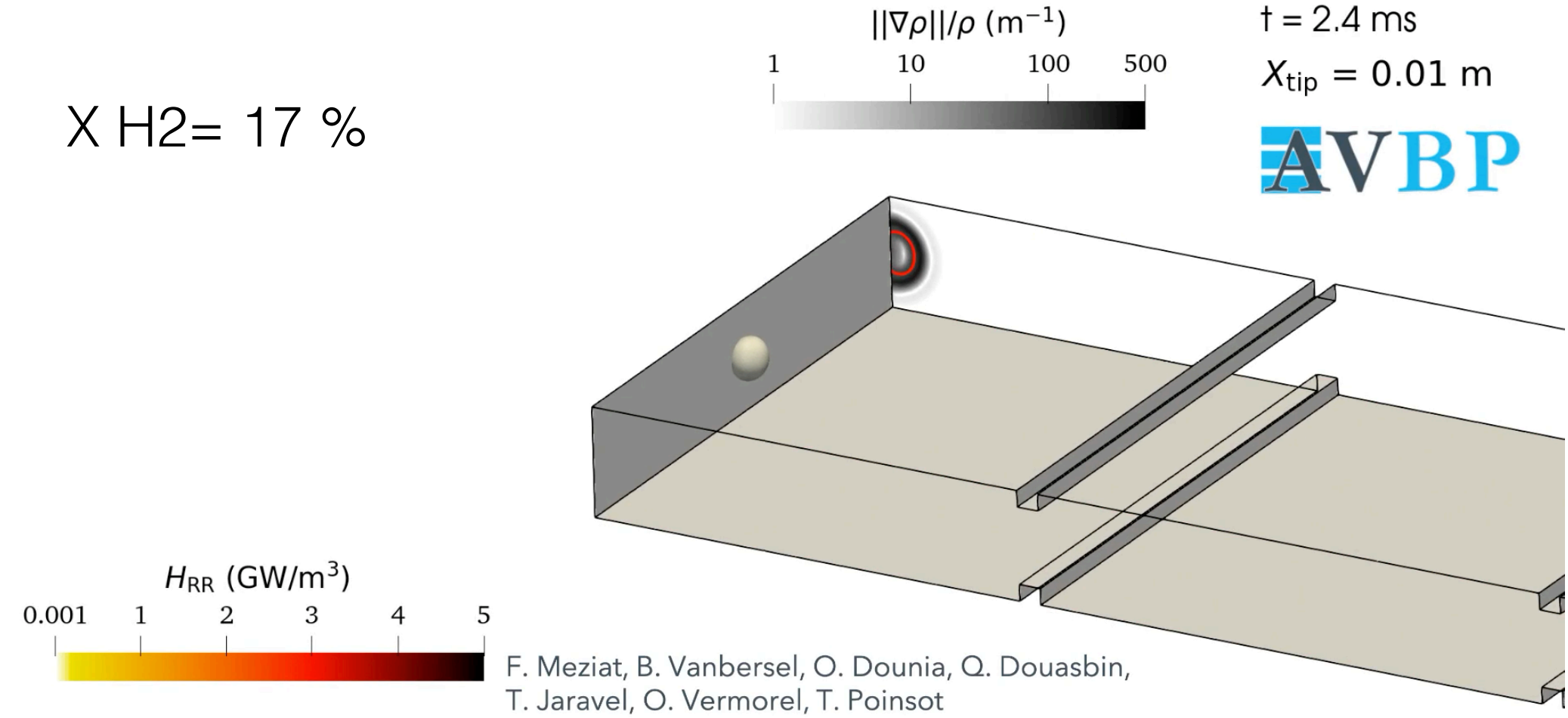


Grad(P) / P



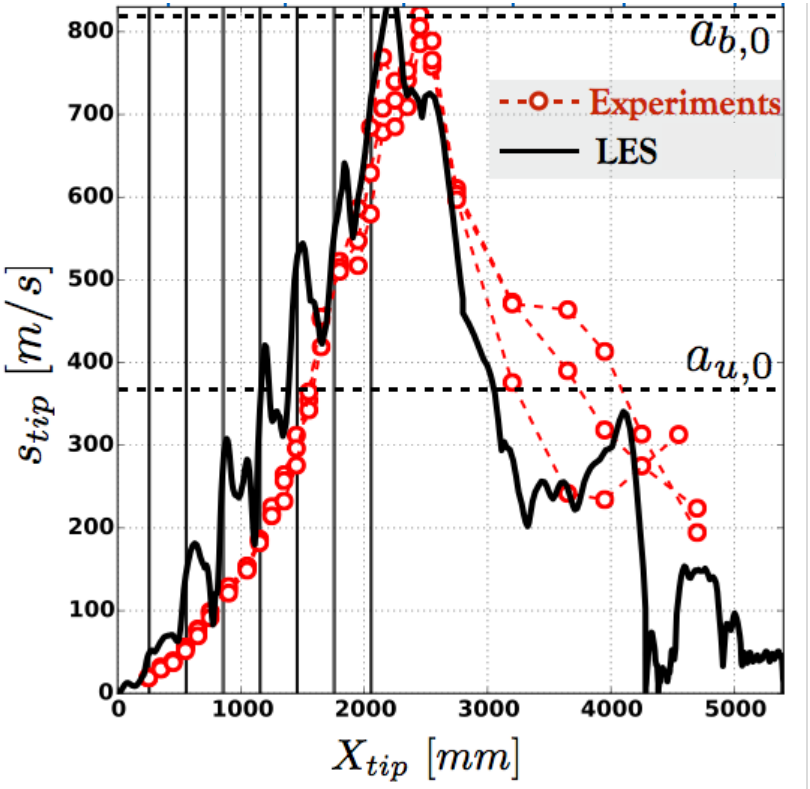
A DEFLAGRATION FIRST:

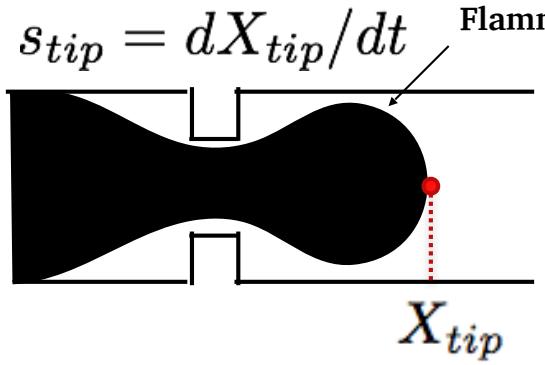
X H2= 17 %

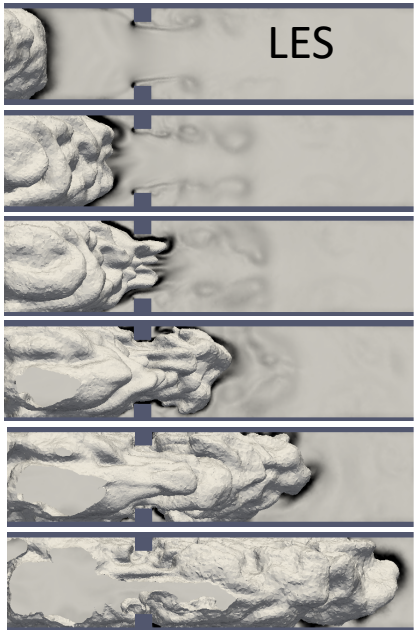


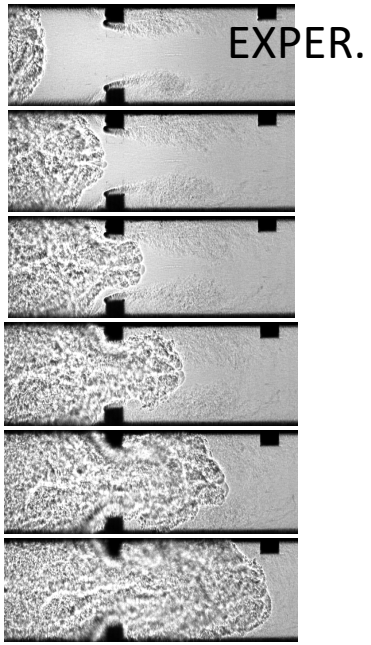
F. Meziat, B. Vanbersel, O. Dounia, Q. Douasbin, T. Jaravel, O. Vermorel, T. Poinsot

Deflagration case (phi=0.52)

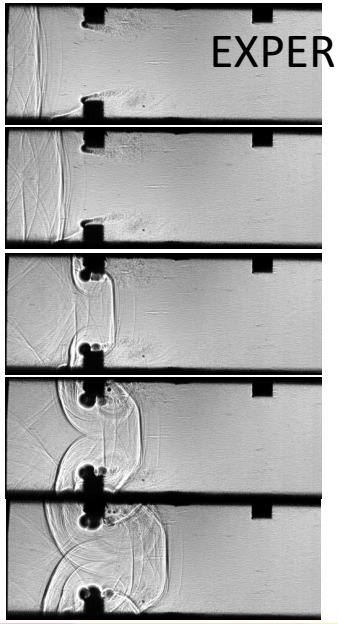




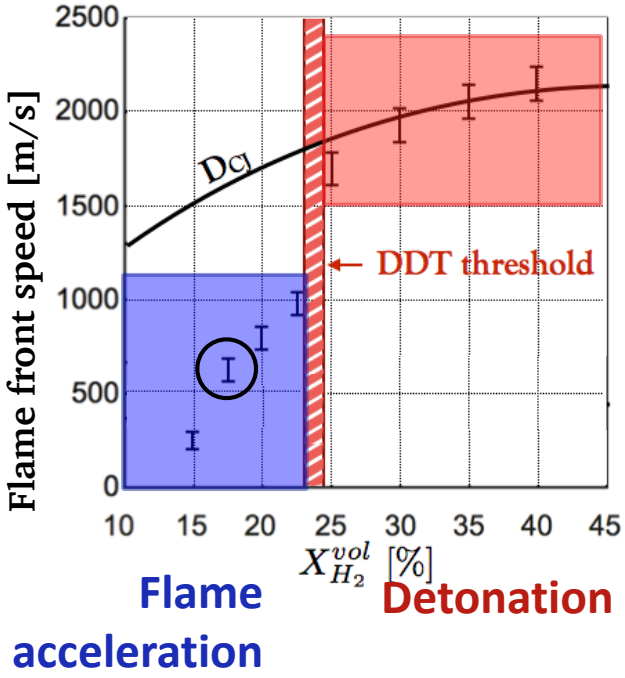




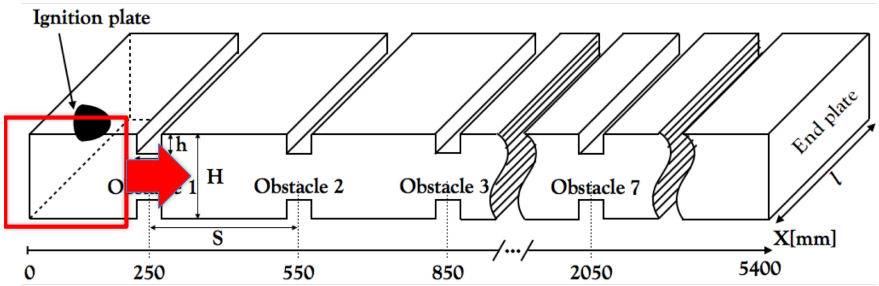




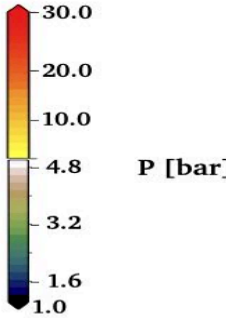
Detonation case (phi=1.0): put more H2 in the duct



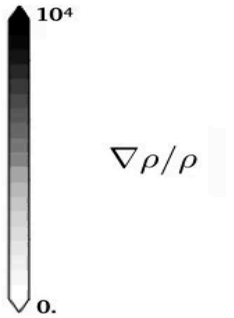
Detonation case (phi=1.0)

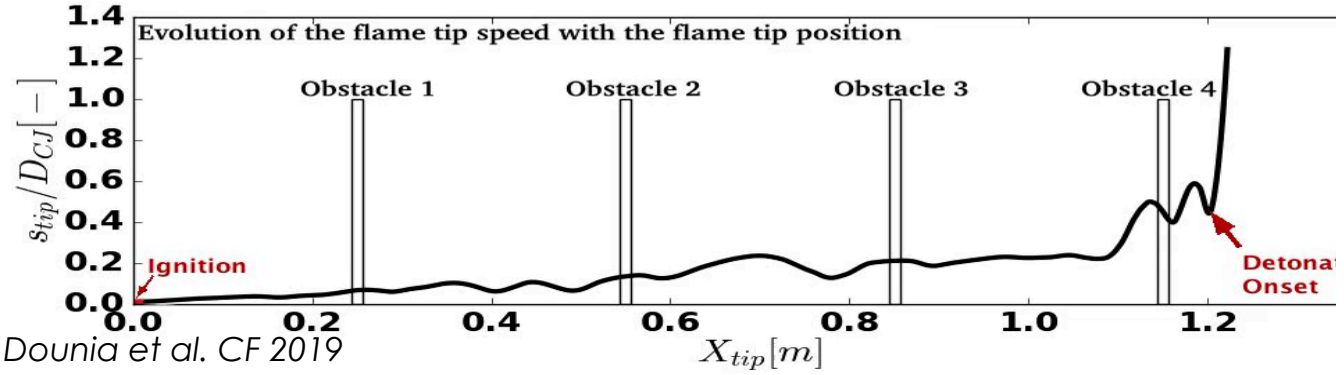












CERFACS

O. Dounia et al. CF 2019

O. Dounia, Q. Douasbin, O. Vermorel

HYDROGEN: Scenarios

H2 LEAK

EXPLOSIONS: DOES NOT IGNITE RIGHT AWAY: ACCUMULATES THEN IGNITES…



FIRES/FLAMES: IGNITES RIGHT AWAY





Typical SAFETY issue for an aircraft

- **A FIRE DUE TO H2 LEAK MAY BE ACCEPTABLE IN AN AIRCRAFT IF IT STARTS AND ENDS AS A *DEFLAGRATION***

- **IT IS DEFINITELY NOT ACCEPTABLE IF IT BECOMES A *DETONATION***

Explosions are not the only problem: if pressure goes up in a H2 tank, we may have to vent it out through a tube:

THEN TWO THINGS MAY HAPPEN -
the example of an in-flight venting:

NO IGNITION



IGNITION

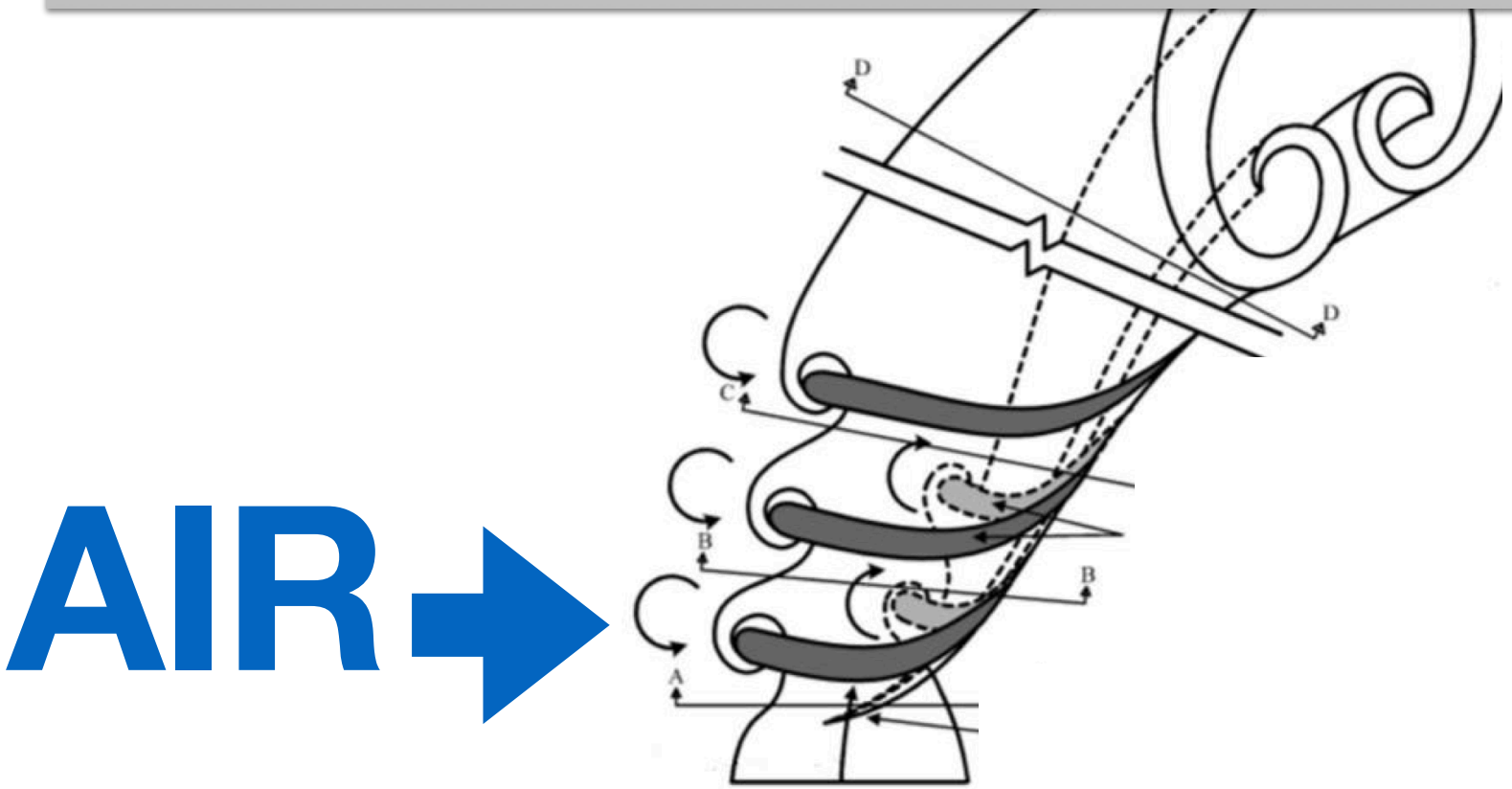


AN ANCHORED FLAME ON AN AIRCRAFT:



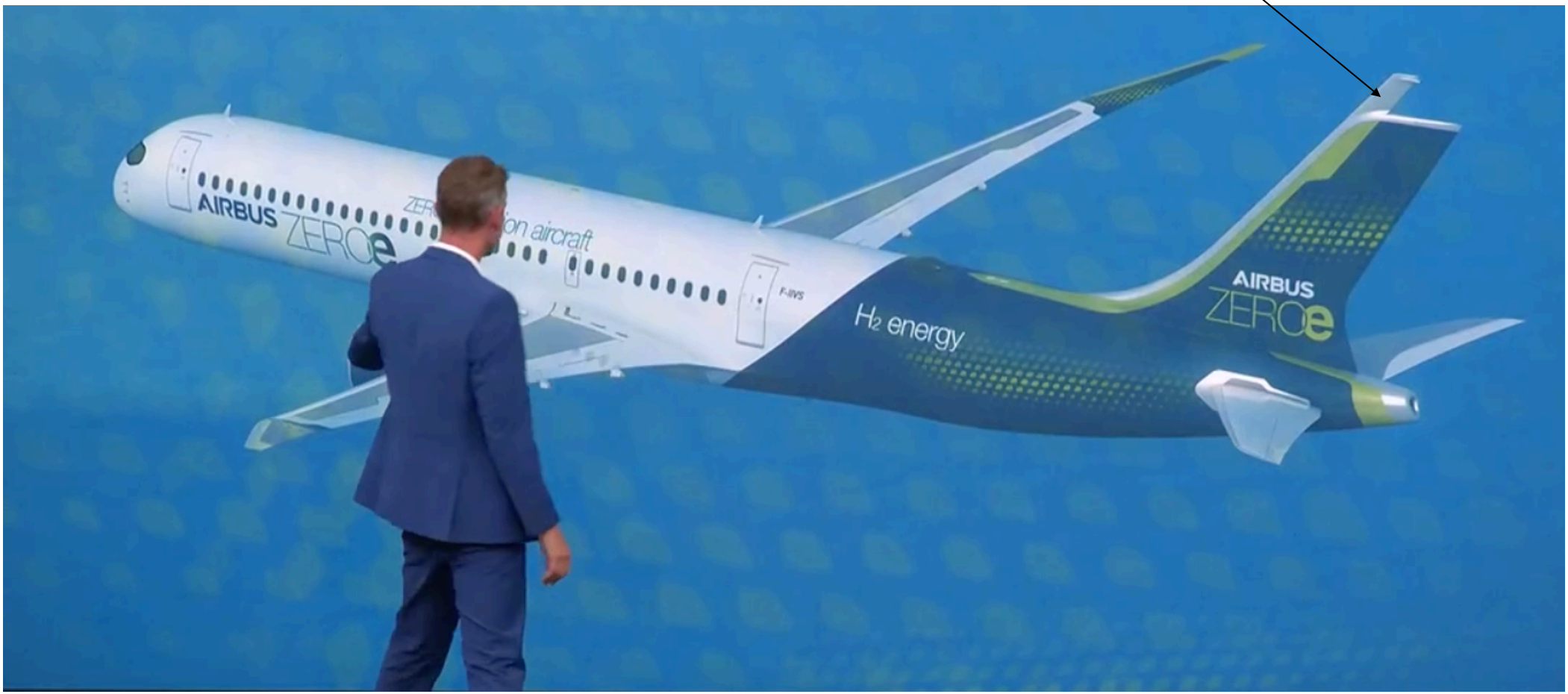


A FUNDAMENTAL PROBLEM OF FLUID MECHANICS:





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



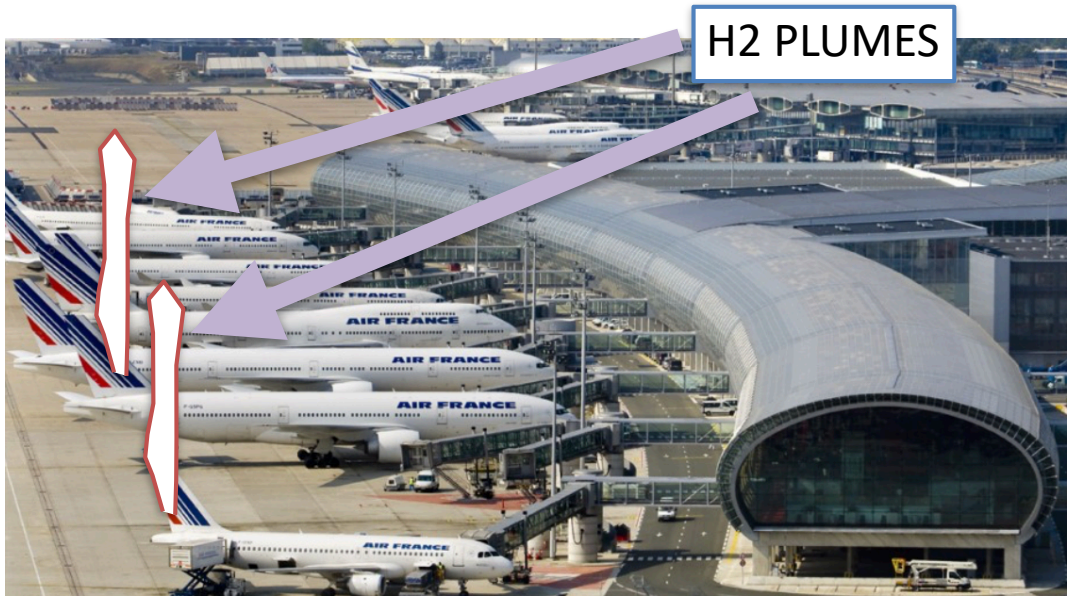
This is for a H2 jet produced at a place WE chose…
If we have a mechanical failure and the leak takes places anywhere in the engine for ex, similar problem… but more complicated to predict and control

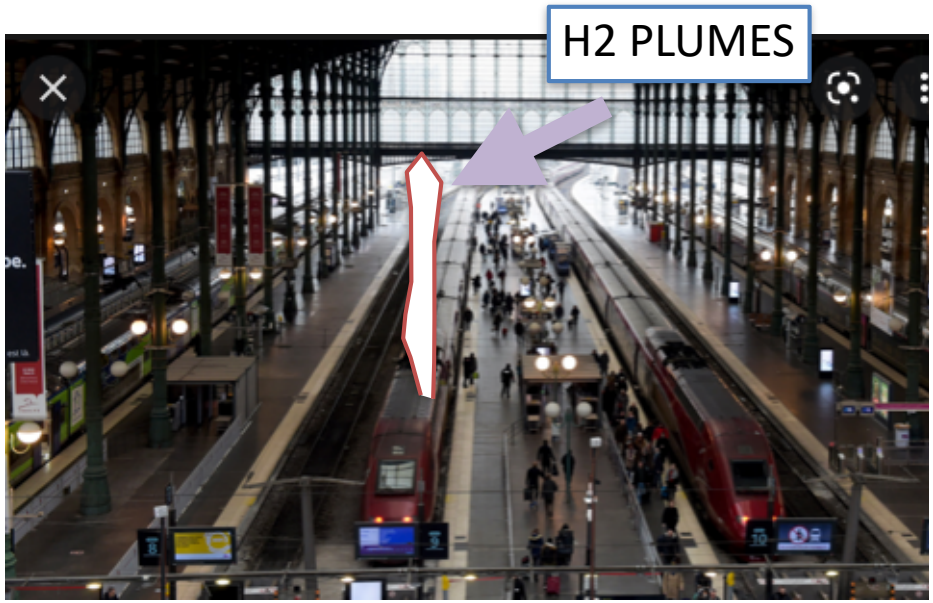

DGEN 380 - Cross Section
PRICE INDUCTION


CORADIA LINT

Even if leaks are always produced through events we control, what about the overall effect of airliners releasing H2 in an airport or trains in a station (or in a tunnel)?

- **Mixing with air will depend on weather and ventilation.**
- **Ignition sources will become an issue**
- **Mitigation (sprinklers) will be possible in certain cases**



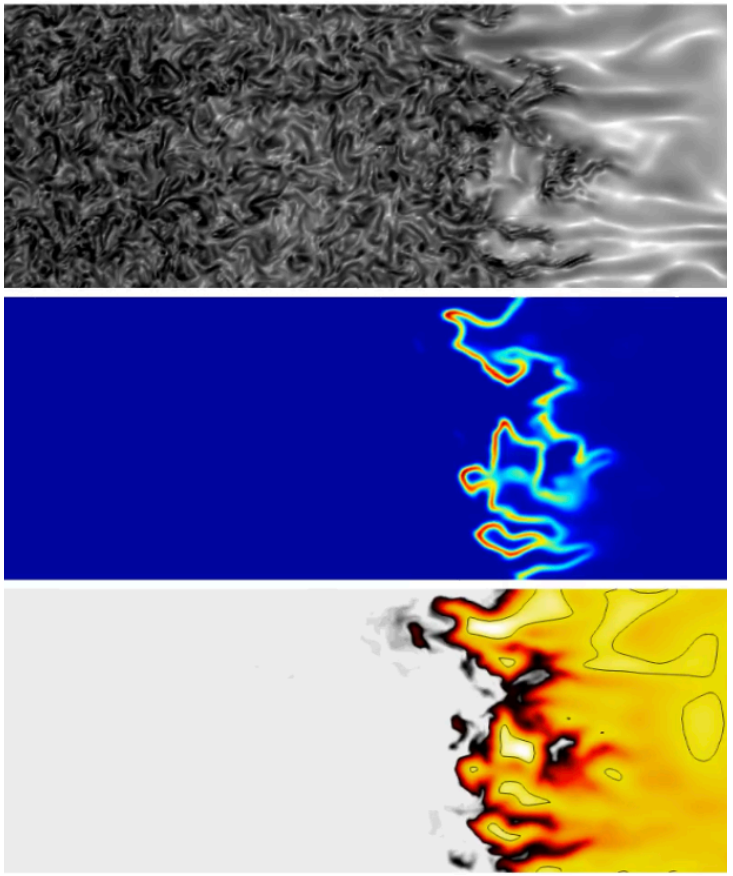


Accidental H2 jets will be MUCH faster because H2 tanks will be at very high pressures



CONCLUSIONS

- H2 will have a great societal potential as an energy vector. It will increase significantly so that using it for transportation and even for aircraft will be possible
- But it will require re-designing most combustion chambers
- Ensuring safety will raise multiple fundamental challenges
- For the first time ever, simulations will be central for engine designs and safety scenarios: this will not be so easy as H2 combustion gathers all exotic concepts in combustion theory: multi-regime flames, thermodiffusive instabilities, detonations, edge flames, ultra fast flames + (of course) turbulence…
- High pressure will make everything more difficult





清华大学燃烧能源中心

Center for Combustion Energy