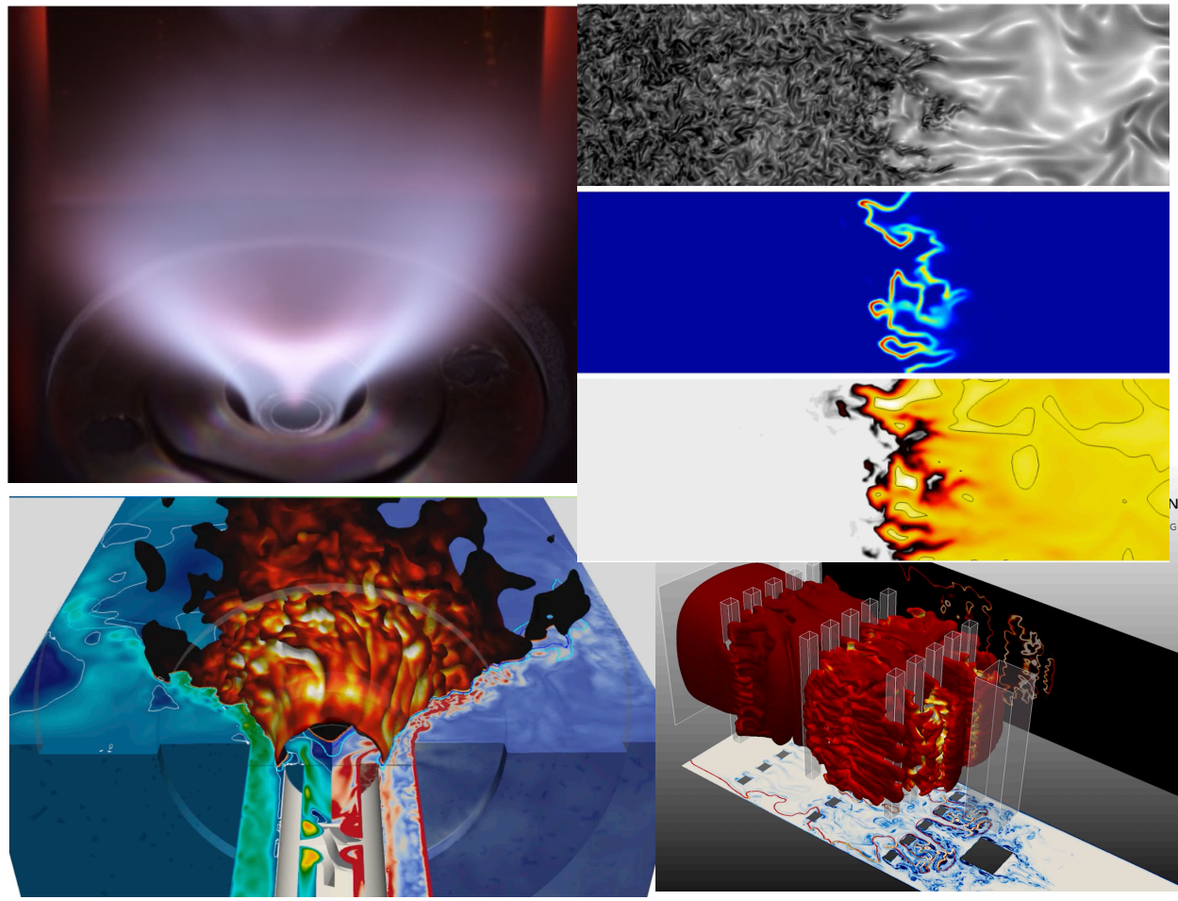
CFD AND HYDROGEN COMBUSTION



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C. Brunet, S. Richard ***Safran Helicopter Engines***

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IMFT
INSTITUT DE MECANIQUE DES FLUIDES DE TOULOUSE

CERFACS

CAN CFD DO WHAT WE EXPECT FOR H2 ?

EVERYONE PLANS TO USE CFD TO EXPLORE ALL POSSIBLE ENGINE GEOMETRIES AND FUEL CHARACTERISTICS BEFORE ENGINES ARE BUILT. SAME EXPECTATION FOR SAFETY SCENARIOS

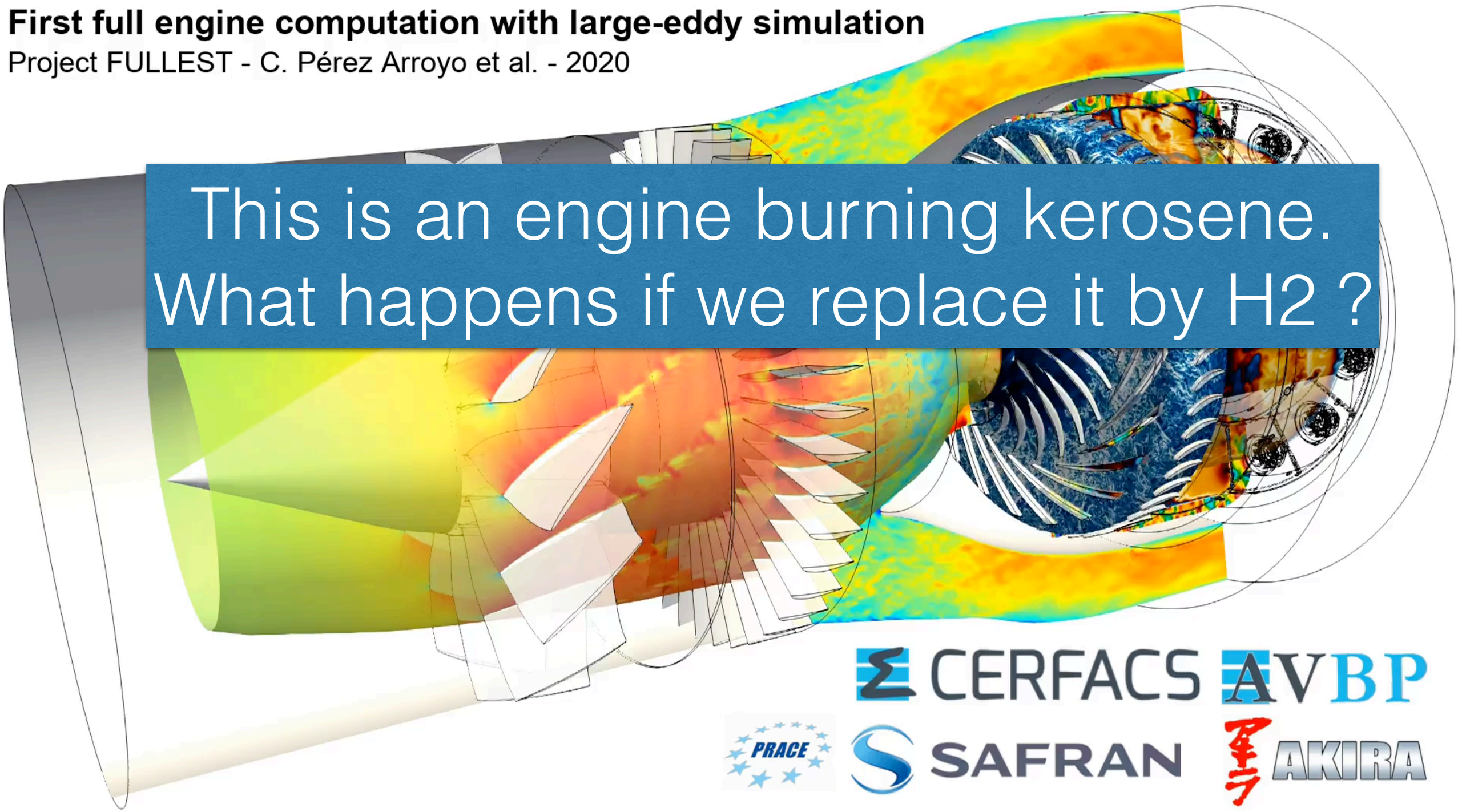
THIS IS DIFFERENT FROM EXISTING KEROSENE-AIR ENGINES WHERE CFD EXPERTS NOW HAVE PLENTY OF EXPERIENCE BASED ON MEASUREMENTS, TRIAL, ERROR AND … TUNING.

IS H2 EASIER ?
ARE OUR CODES READY FOR THIS ?…

CFD OF ENGINES HAS MADE HUGE PROGRESS

First full engine computation with large-eddy simulation

Project FULLEST - C. Pérez Arroyo et al. - 2020



This is an engine burning kerosene.
What happens if we replace it by H2 ?

CERFACS AVBP

PRACE SAFRAN AKIRA

Prix ATOS Joseph Fourier 2021

OUTLINE OF PRESENTATION

★ **Thermodiffusive instabilities and first models in LES (2022 Center for Turbulence Stanford Summer Program + J. Gaucherand, V. Coulon, A. Aniello PhDs at CERFACS and IMFT)**

★ **Walls and hydrogen chemistry (L. De Nardi PhD)**

★ **Flame stabilization processes at the lips of injectors for hydrogen flames (J. Bertsch, M. Chen, A. Aniello PhDs)**

FROM A CFD POINT OF VIEW

★**The good news for CFD experts is that the chemical schemes for H2 air flames are:**

- ➡ **well known**
- ➡ **simple**

★**Unfortunately, with H2, we have other… issues**

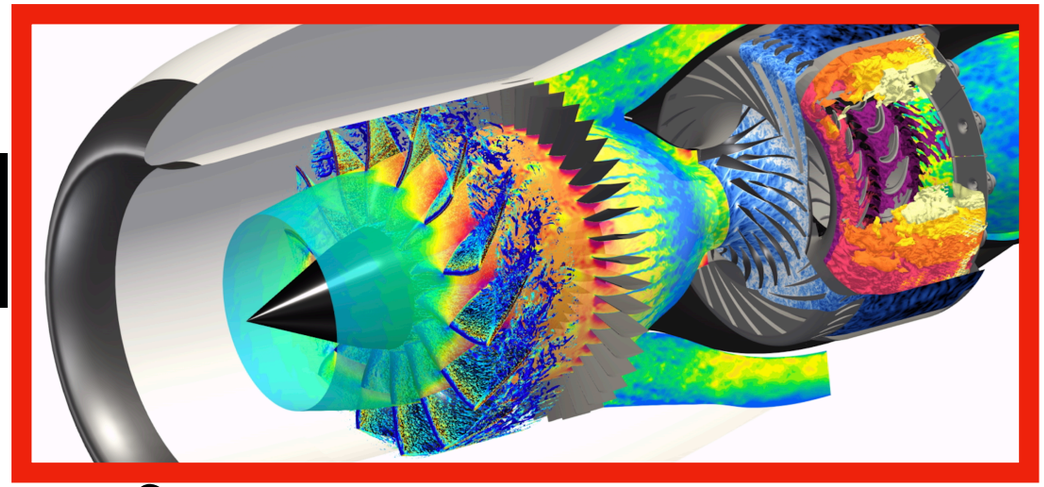
IS H2 SPECIAL FOR CFD ?

COMPUTING H2 SYSTEMS PUSHES US IN TWO DIRECTIONS CFD DOES NOT LIKE:

- ***Small chemical times and thicknesses***
- ***Higher pressure (for engines)***
- ***Larger domains (for explosions)***

The two tough axis for H2 air flames:

Reynolds = SIZE * SPEED / nu
where nu = nu0 Po/P
A Re=ct line in a P-SIZE diagram is a parabola



PRESSURE

REAL COMBUSTION CHAMBERS

Increasing Re

DNS

LES

REAL JET FLAMES AND EXPLOSIONS

1 bar

L

IZE

WE CAN (ALMOST) DO DNS FOR LAB SCALE FLAMES BUT WE NEED LES FOR REAL SYSTEMS

BUT THERE ARE OTHER ISSUES:

- *H2 flames are often a mix of premixed and diffusion flames: not that many models can do 'multimodes'*

- *H2 diffuses very rapidly, creates specific instabilities such as thermodiffusive cells: one paper submitted to Comb. Flame per week -> we love this one*

- *H2 chemistry at walls has problems…*

- *The stabilization of H2 flames at lips is not understood yet*

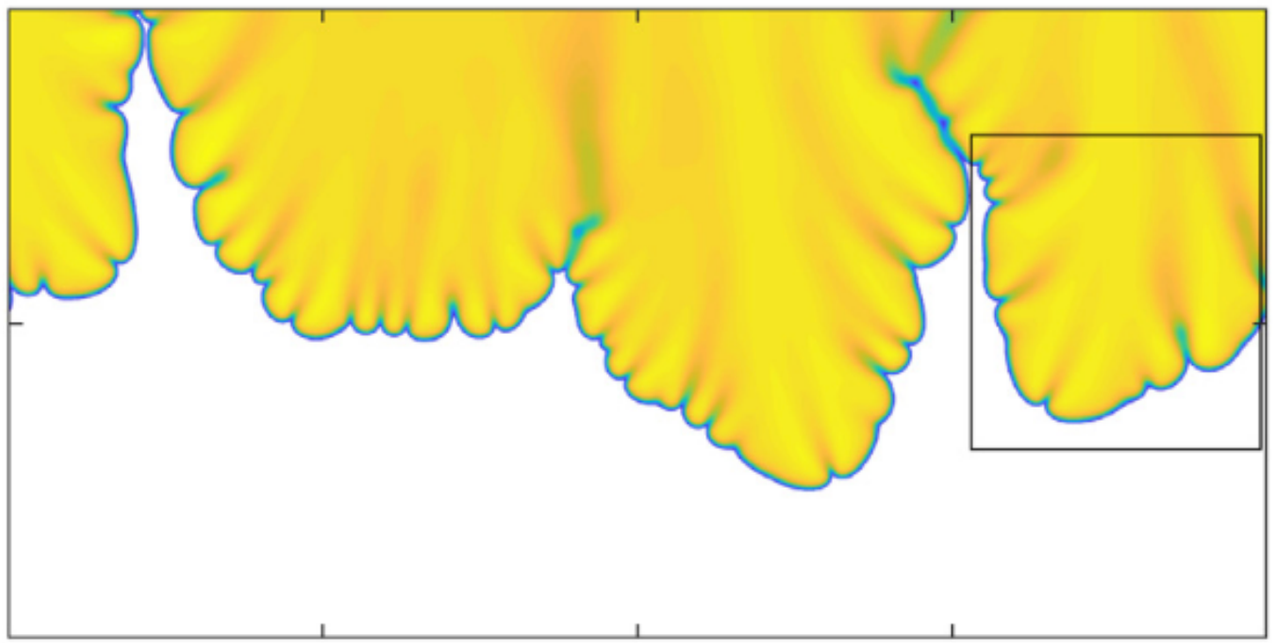
THERMODIFFUSIVE INSTABILITIES

H2 is a small molecule: it diffuses faster than heat.
This is quantified through the Lewis number:

$$L_e^k = \lambda/(\rho C_p D_k) = D_{th}/D_k$$

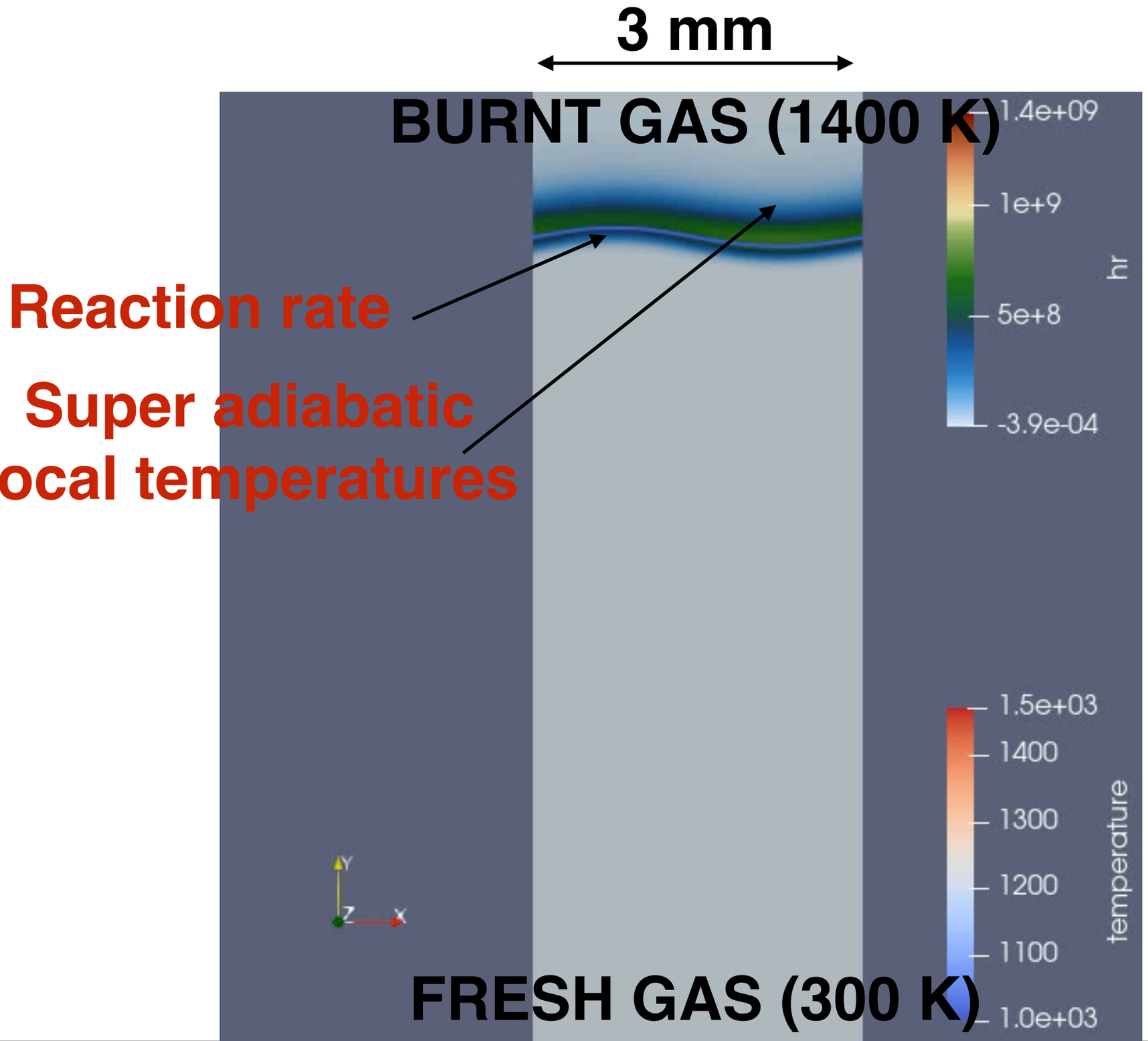
For H2: $L_e^k = 0.3$

Main consequence of this fact: 'thermodiffusive instabilities'



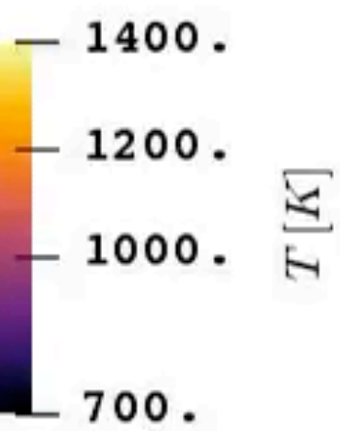
Berger Attili and Pitsch, *Combustion and Flame*, 2021.111936

Flames which should be flat are not ... flat

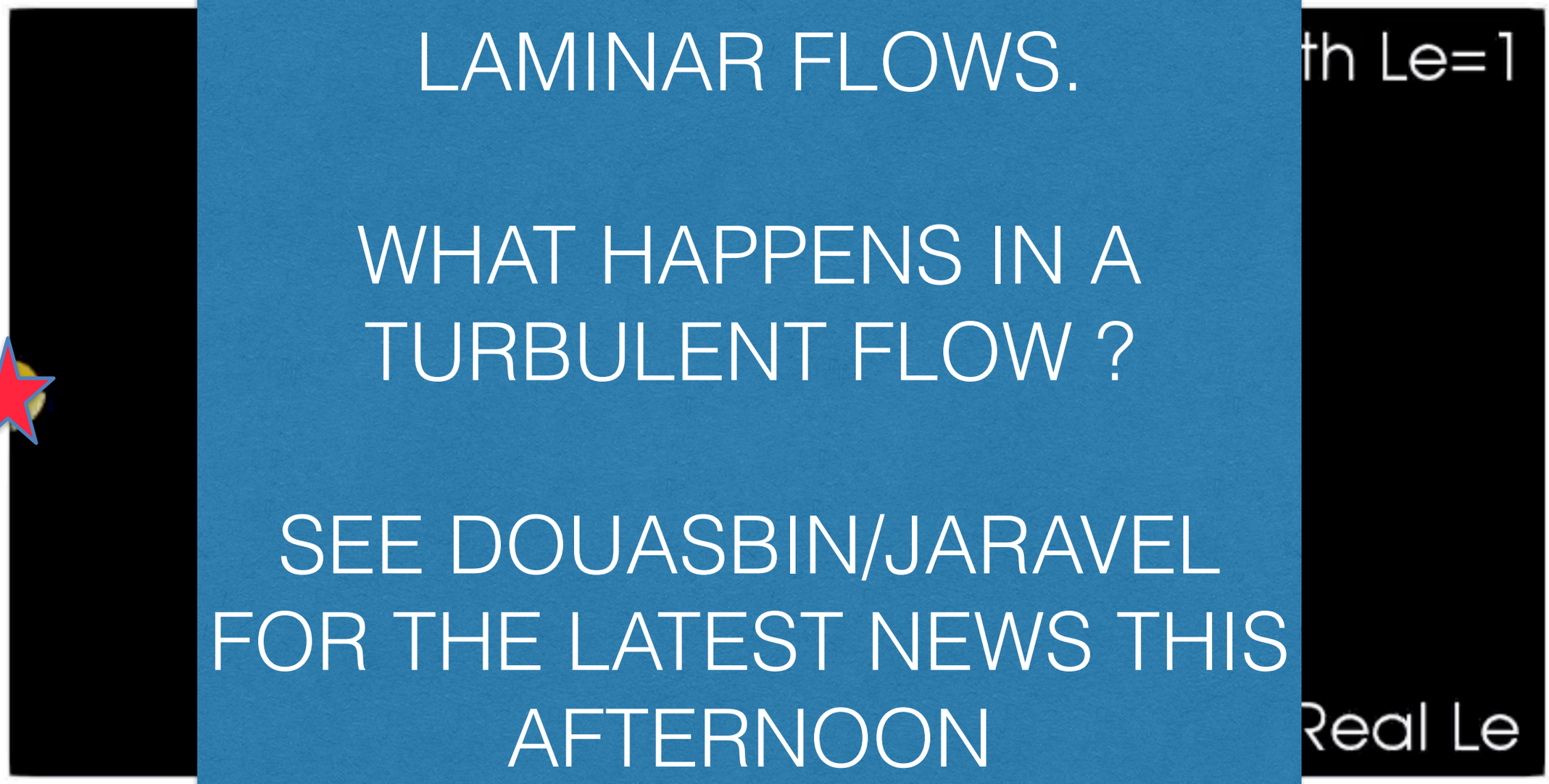


THERMODIFFUSIVE INSTABILITIES

TD stable



TD unstable



THESE CELLS APPEAR IN LAMINAR FLOWS.

WHAT HAPPENS IN A TURBULENT FLOW ?

SEE DOUASBIN/JARAVEL FOR THE LATEST NEWS THIS AFTERNOON

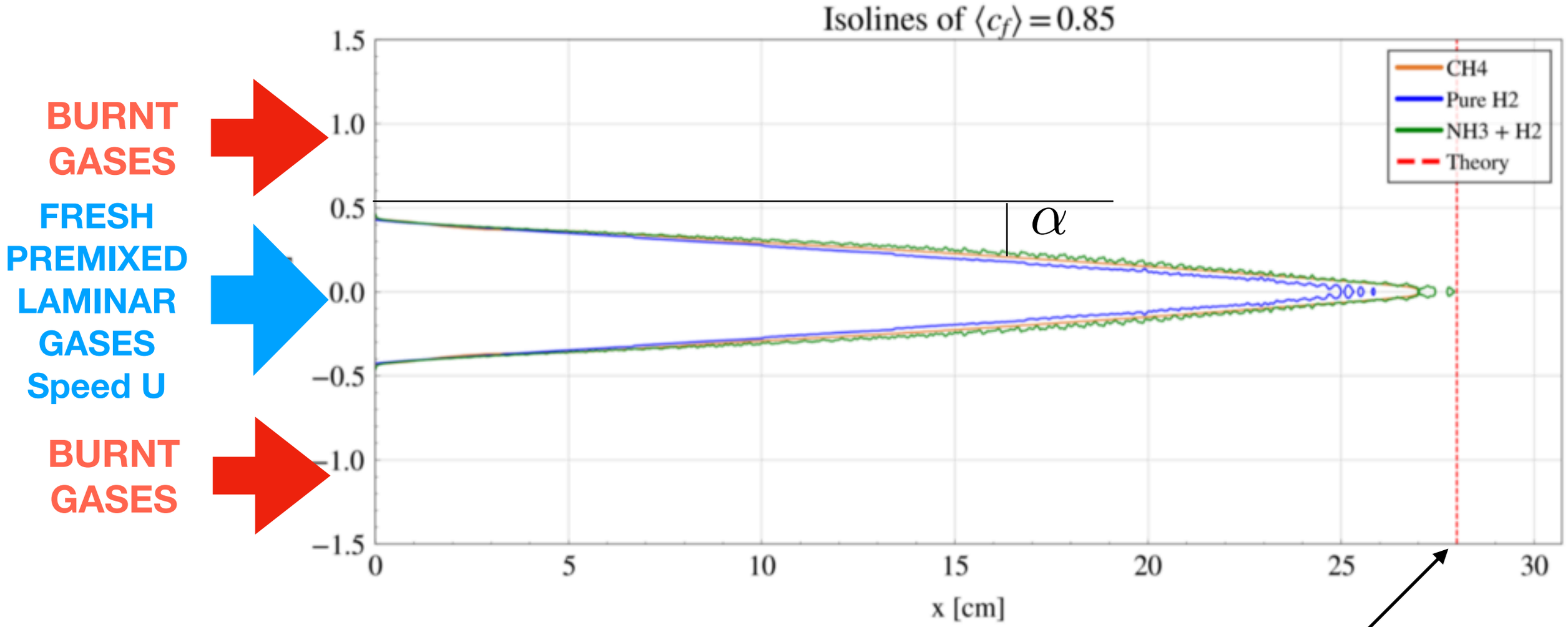
CERFACS

In a turbulent case, TD can interact with flame/turbulence wrinkling and usual models wont work…

How do we know ?: DNS (Attili, Berger, Pitsch or Howarth, Aspden)
Here we show results by CERFACS and NTNU (Gaucherand, Laera, Schulze-Netzer, Poinsot, *Combustion and Flame*, 256, 2023, 112986)

- 3 premixed flames with exactly the **same laminar flame speed (0.38 m/s) and flame thickness**
  - Methane-air flame, $\phi = 1$
  - Hydrogen-air flame, $\phi = 0.45$
  - Ammonia/hydrogen flame, $\phi = 1$, $X_{NH_3} = 0.535$
- Chemistry:
  - CH4: 1-step mechanism with Pfitzner for reaction rate source term (5 species, 1 reaction)
  - NH3-H2: ARC mechanism from CRECK (14 species, 7 QSS, 174 reactions)
  - H2: detailed San Diego mechanism H2 (9 species, 42 reactions)

Laminar flames front: all the same, as expected

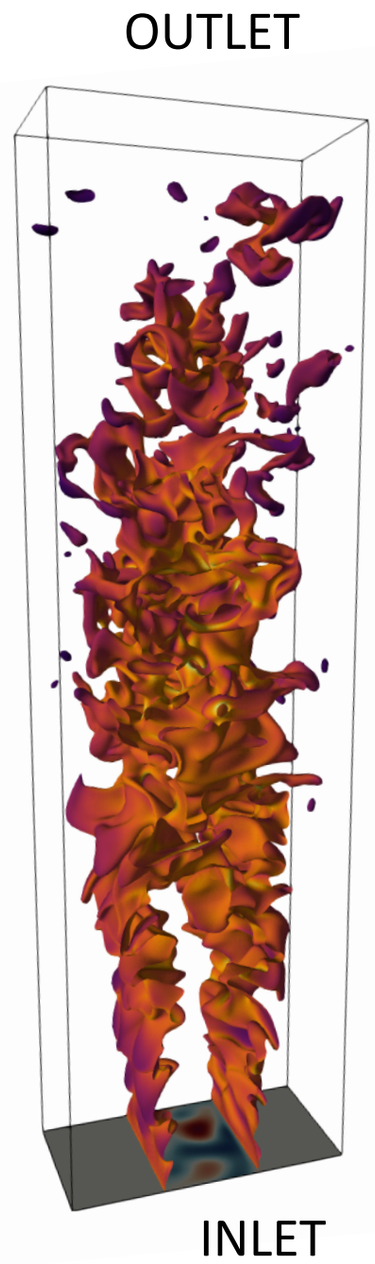


Theoretically, the flame length (given by $sin(\alpha) = s_L/U$) is $L_f = 28\ cm$

IN A LAMINAR FLOW, EVERYTHING IS FINE

Numerical set up of DNS: turbulent cases

	CH4-air	H2-air	NH3/H2-air
Domain size Lx [cm]	**10.24**	**5.12**	**8.96**
Number of points in front flame [-]	**7**	**11**	
Number of points (Nx/Ny/Nz) [-]	**1601/401/201**	**1281/641/321**	**2191/627/314**
Simulation time [ms]	**8**	**4.1**	**7.2**

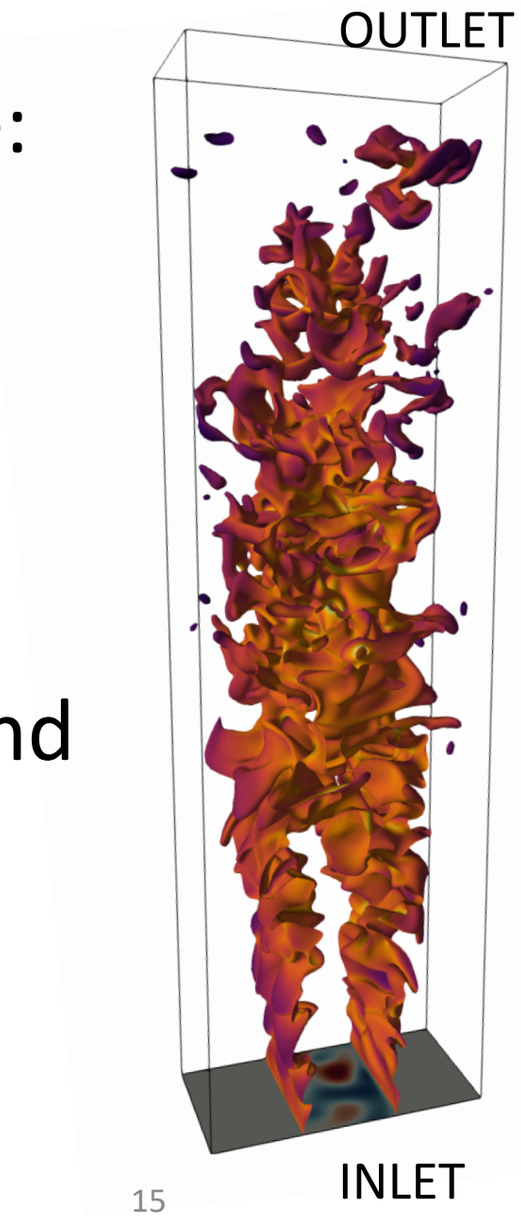


Numerical set up of DNS: turbulent cases

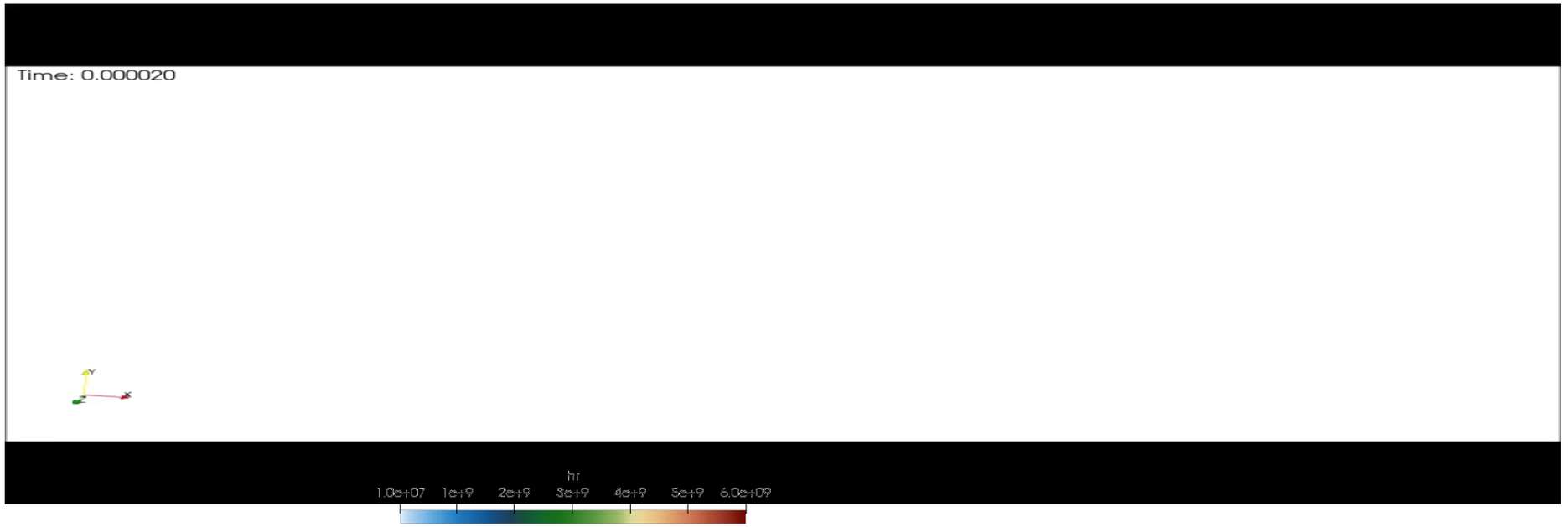
- For most turbulent combustion models, these 3 flames are similar because these models inputs are:
  - *Laminar flame speed s_L and thickness δ_L*
  - *Turbulence RMS speed u' and integral scale L*

- In other words, most existing models would be blind to the differences between these flames

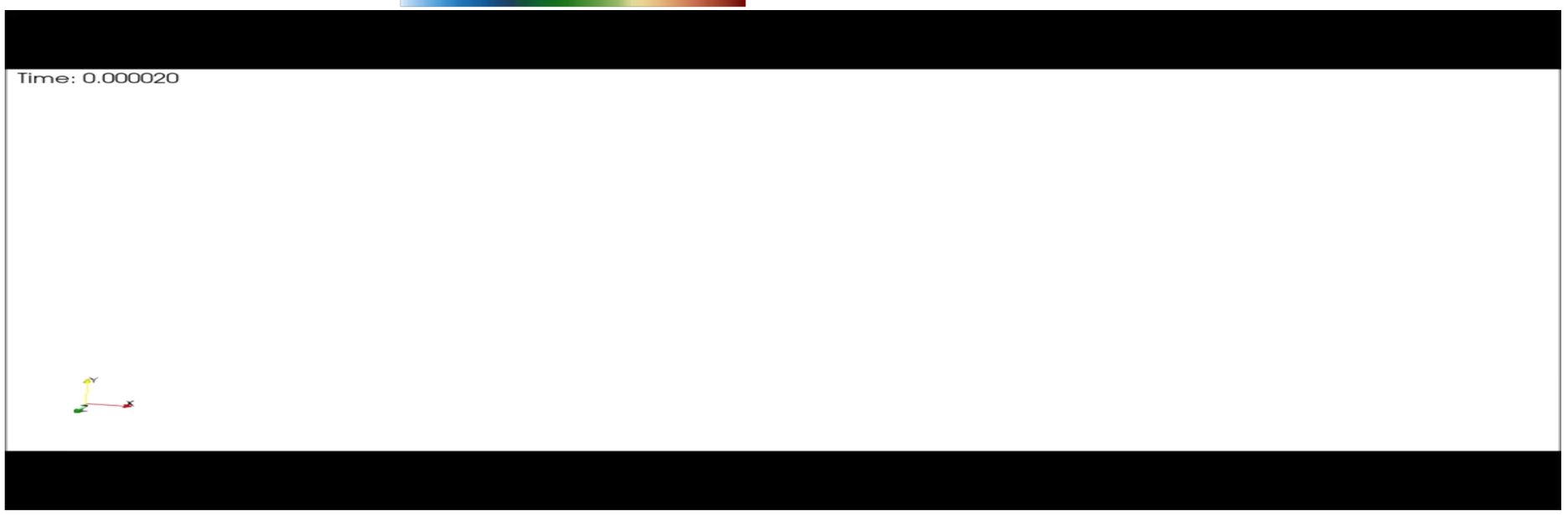
Let us look at the DNS results:



CH4-air flame

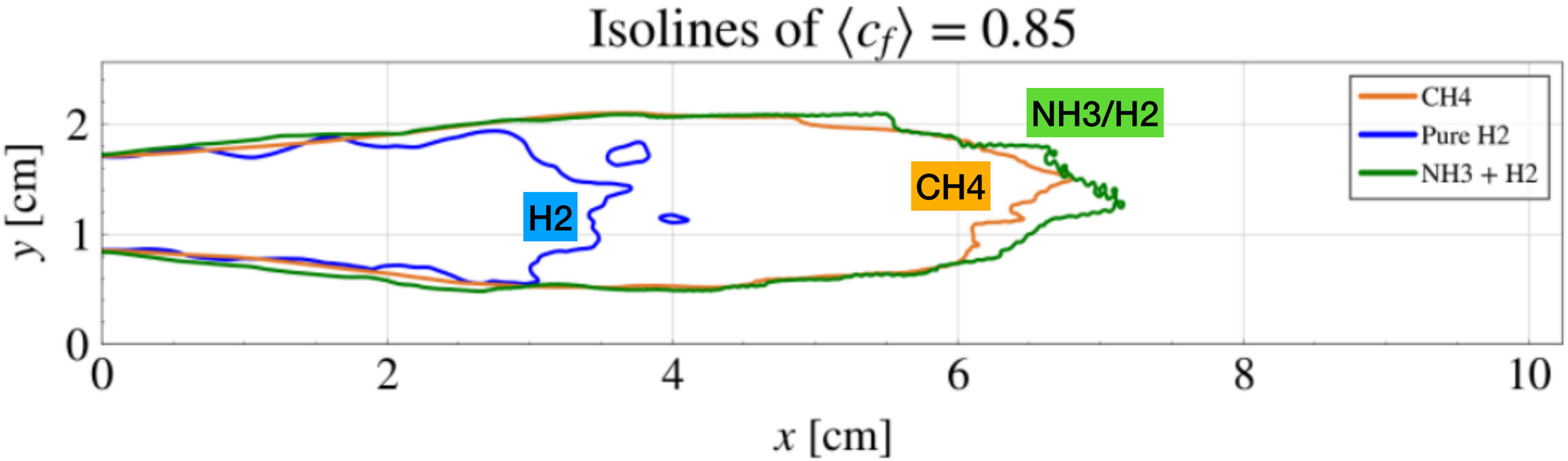


NH3/H2-air flame



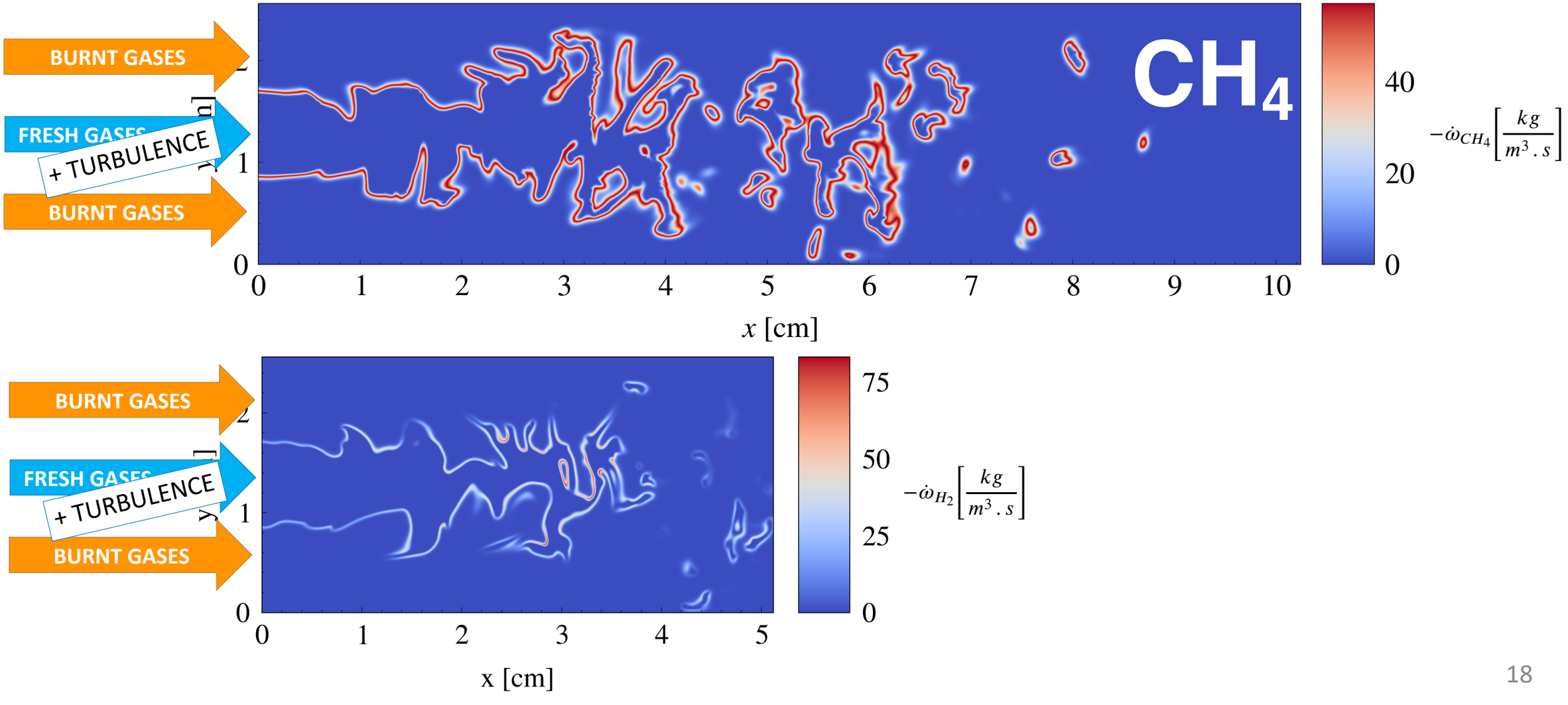
H2-air flame

Turbulent flames: MEAN position

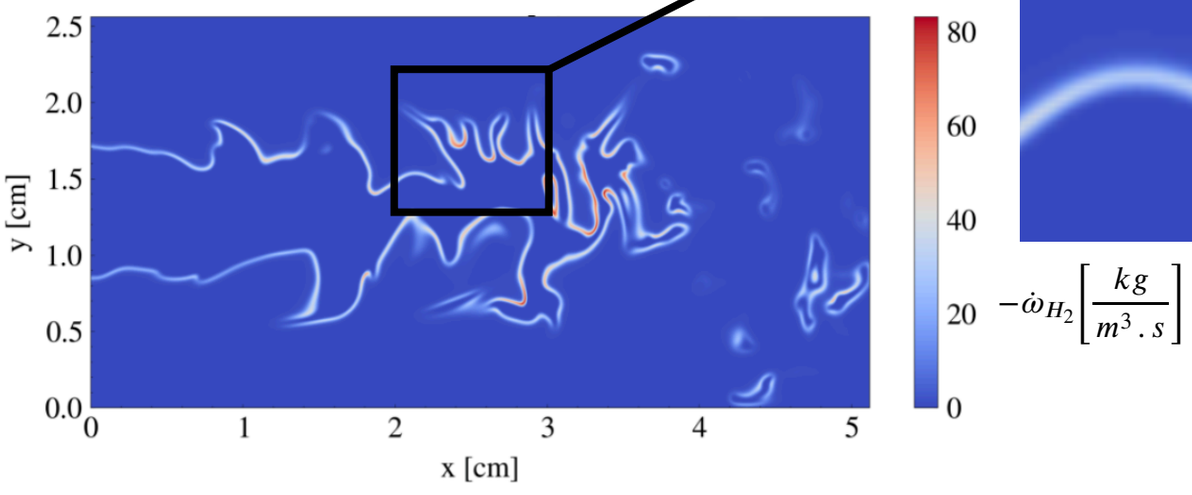


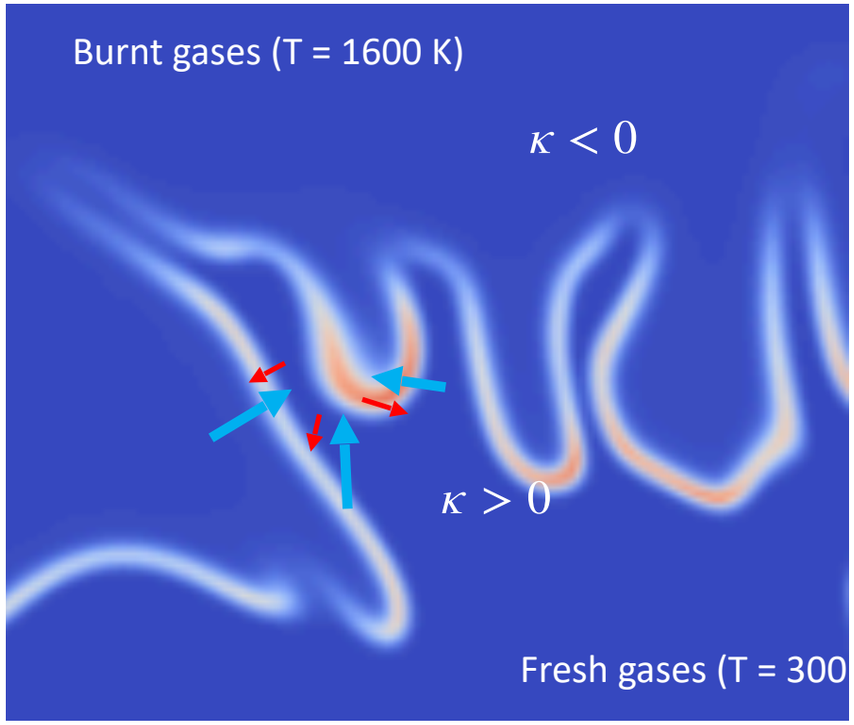
→ Pure H2 / AIR turbulent flame length almost 2 times less compared to CH4 and NH3-H2

→ Flame/turbulence interaction models using ‘only’ u'/s_L and L/δ_L as inputs will be wrong for H2


BURNT GASES
FRESH GASES
+ TURBULENCE
BURNT GASES
CH4
y [cm]
x [cm]
0
1
2
3
4
5
6
7
8
9
10
40
20
0
$-\dot{\omega}_{CH_4}\left[\frac{kg}{m^3 . s}\right]$
BURNT GASES
FRESH GASES
+ TURBULENCE
BURNT GASES
y [cm]
x [cm]
0
1
2
3
4
5
75
50
25
0
$-\dot{\omega}_{H_2}\left[\frac{kg}{m^3 . s}\right]$

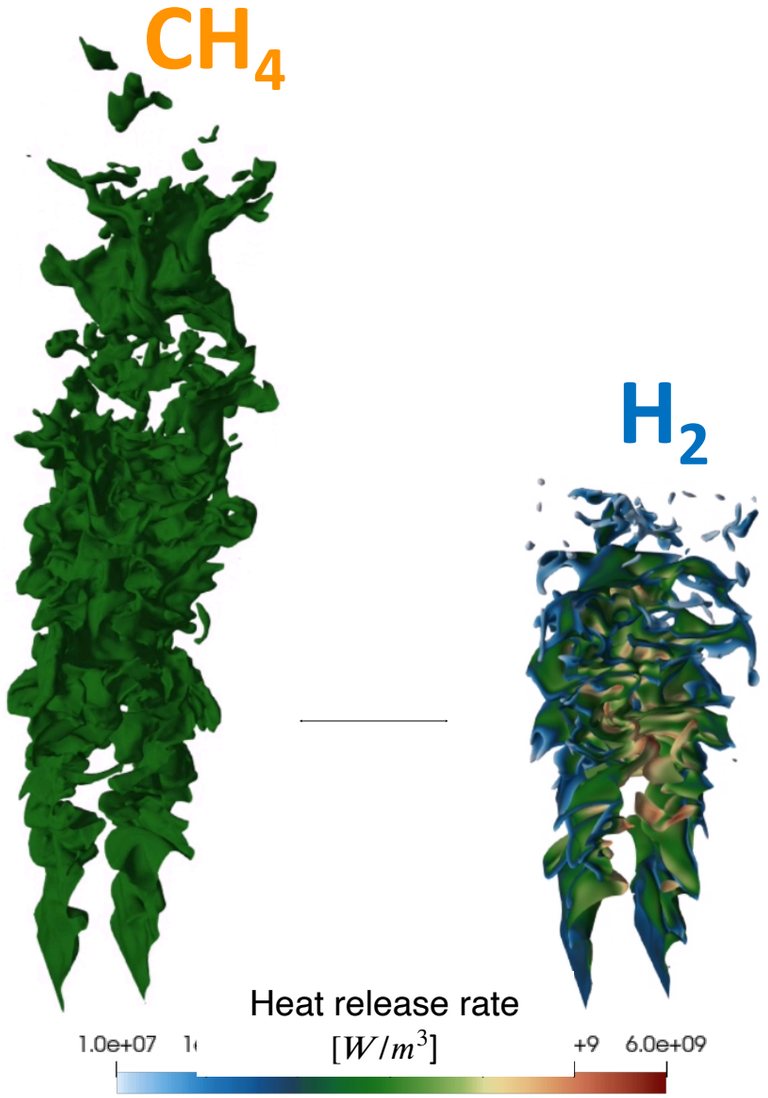
$$Le_{H_2} = \frac{\mathscr{D}_{th}}{\mathscr{D}_{H_2}} \approx 0.3 \qquad (Le_{CH_4} \approx 1)$$





← **H2 mass diffusivity**
→ **Thermal diffusivity**

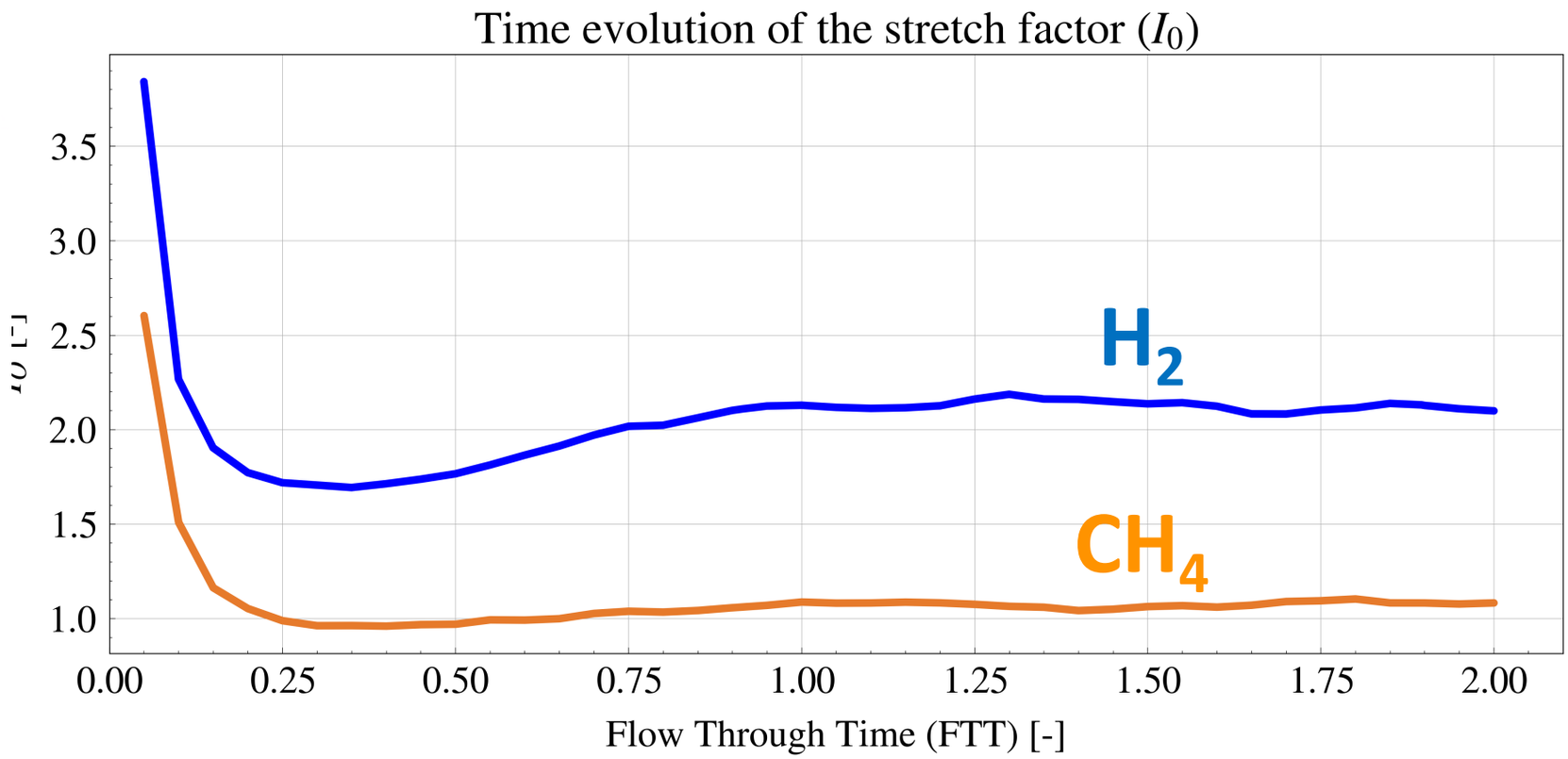
→ What your eyes show you - a strong effect of curvature- is actually misleading: the main effect is NOT that certain curved flame zones burn more than others. The main effect is that ALL flame zones burn much more on average than the laminar flame speed



$$I_0 = \frac{\bar{s}_c}{s_L^0}$$

Consumption speed averaged along the flame

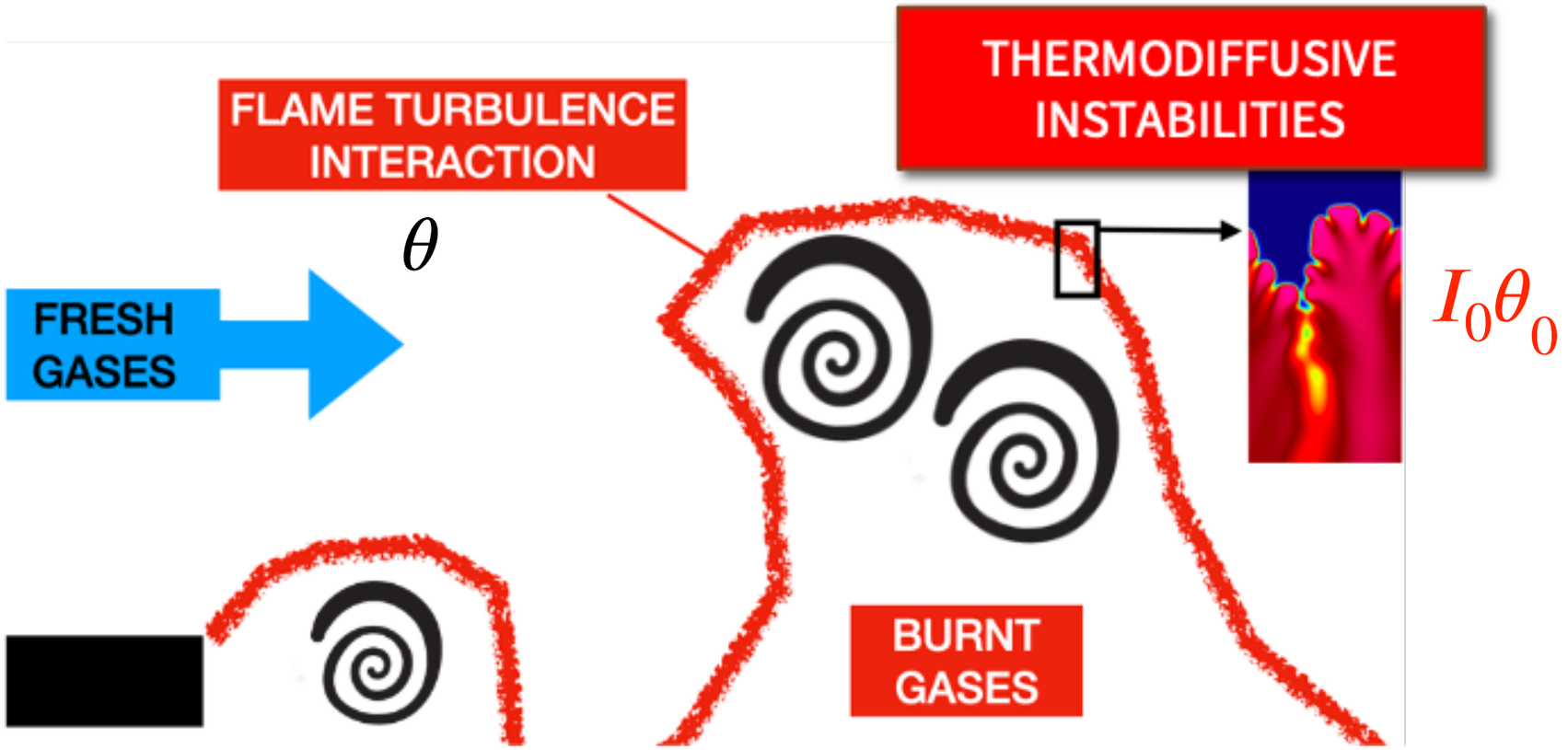
Laminar flame speed



Introducing Thermodiffusive Effects into LES codes

- DNS tells us there is an issue with thermodiffusive effects for lean H2 flames
- HOW DO WE FIX THIS IN LES (we can continue to do DNS but it does not give us a model we can use) ?
- One possible example: the TD TFLES models
  - Implemented in the usual Thickened Flame LES model: *A. Aniello, D. Laera, L. Berger, A. Attili and T. Poinsot. web.stanford.edu/group/ctr/ctrsp22/iv03_Aniello.pdf*
  - Using DNS data produced by Aachen (Dr. Lukas Berger, Dr. Xu Wen, Prof. Heinz Pitsch from Aachen University Dr. Antonio Attili, University of Edinburgh)
  - Assumes scale separation:
    - Small: thermodiffusive effects are supposed to play a role only at very small scales, not seen by the LES.
    - Large: at the LES grid level, standard flame/turbulence models are used.

The TD TFLES model:



The turbulent flame speed s_T becomes:

$s_T = s_L^0 \, \theta \, I_0 \, \theta_0$

With:

s_L^0: laminar flame speed

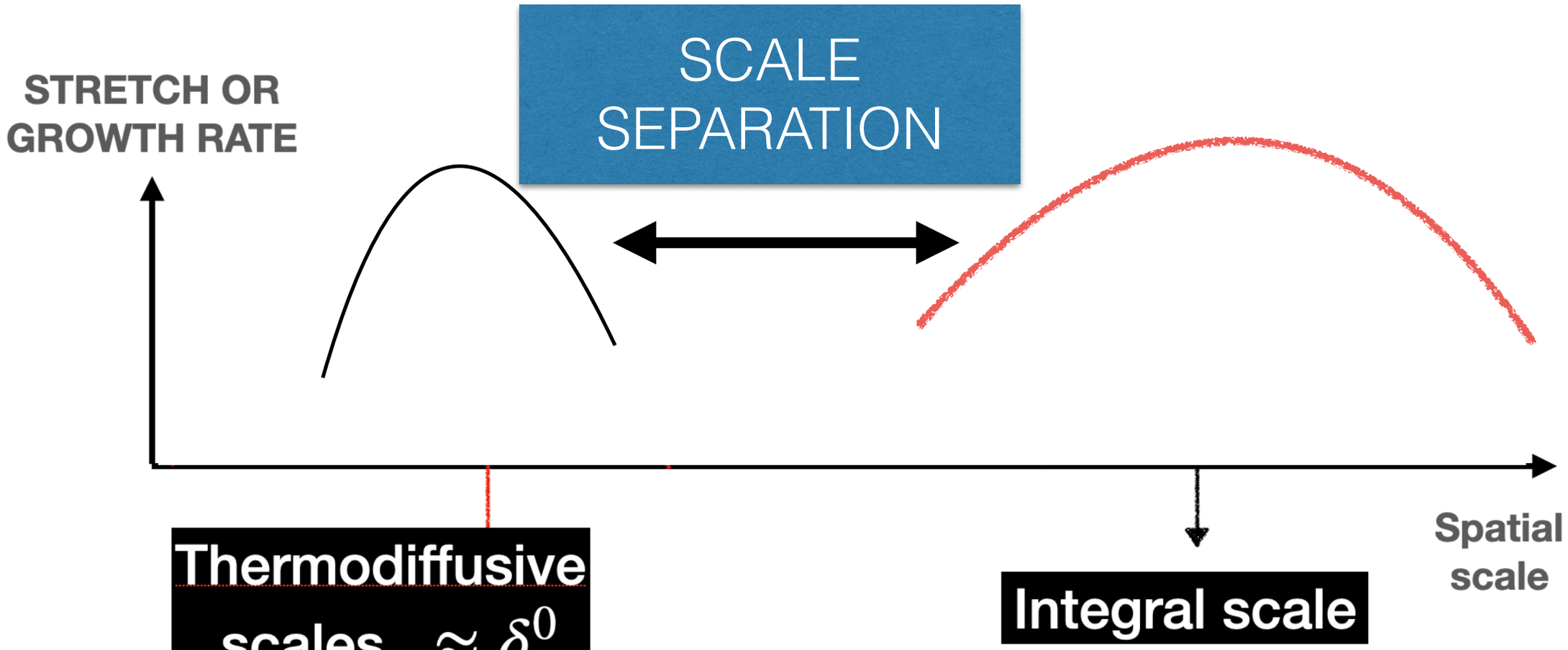
θ: wrinkling due to turbulence

STANDARD TFLES MODEL

I_o: increase of consumption speed due to thermodiffusive instabilities.

θ_O: wrinkling due to instabilities

TD TFLES EXTENSION



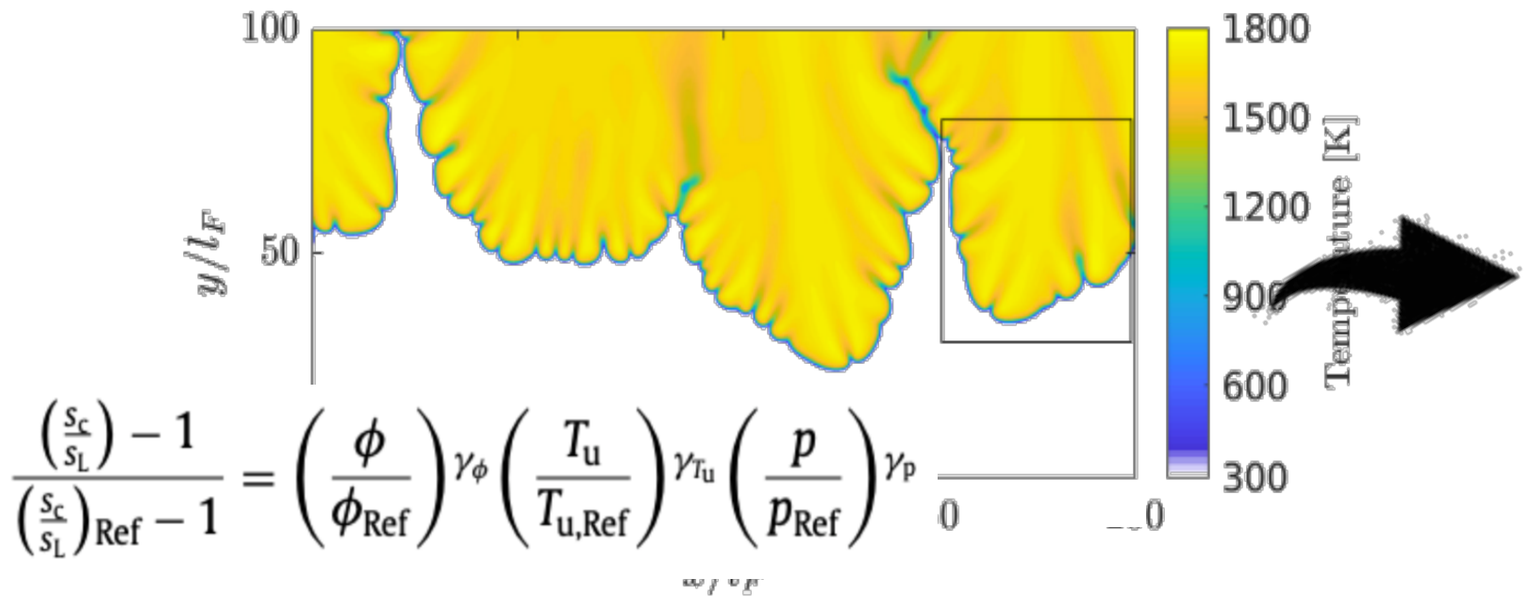
Thermodiffusive effects live only at small scales

Modeled by increasing the local ‘laminar’ flame speed

Flame/turbulence interaction lives at large scales

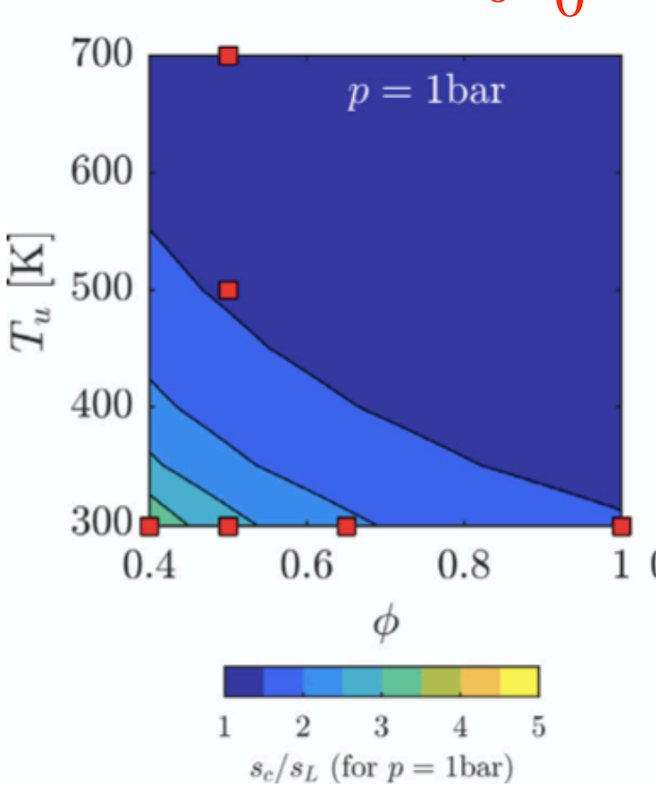
Modeled by using the efficiency function of the TFLES model

How do we obtain $I_0\Theta_0$? From DNS (Aachen group)

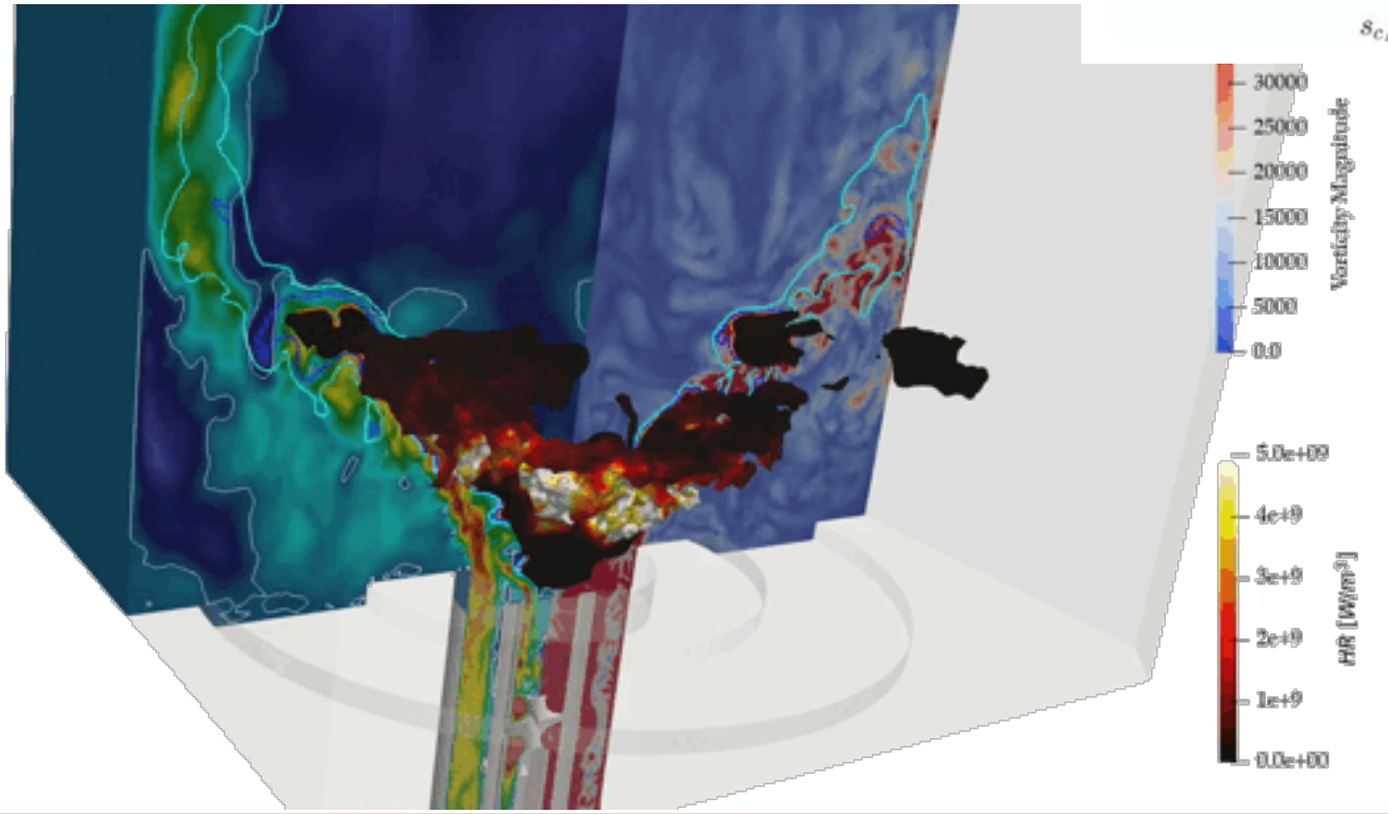


$$\frac{\left(\frac{s_c}{s_L}\right)-1}{\left(\frac{s_c}{s_L}\right)_{\mathrm{Ref}}-1}=\left(\frac{\phi}{\phi_{\mathrm{Ref}}}\right)^{\gamma_\phi}\left(\frac{T_{\mathrm{u}}}{T_{\mathrm{u,Ref}}}\right)^{\gamma_{T_{\mathrm{u}}}}\left(\frac{p}{p_{\mathrm{Ref}}}\right)^{\gamma_{\mathrm{p}}}$$

$I_0\theta_0$



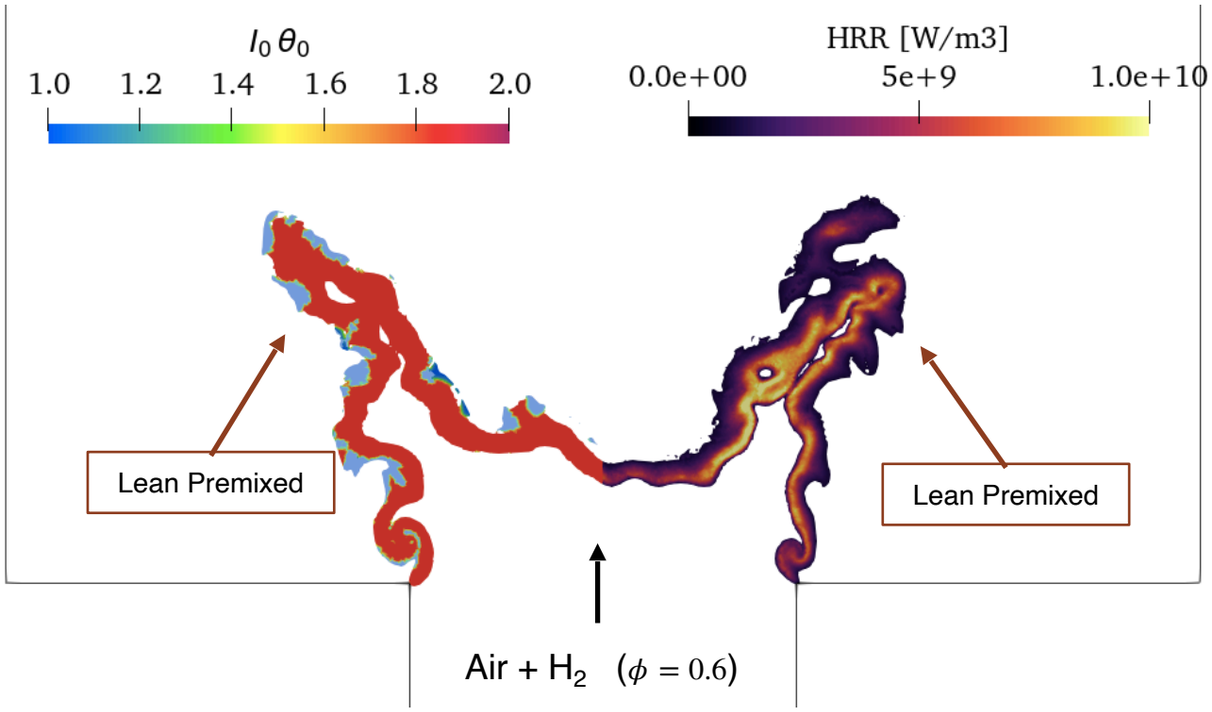
- DNS-based law for $I_o\Theta_o$ from Berger et al. CNF2022.

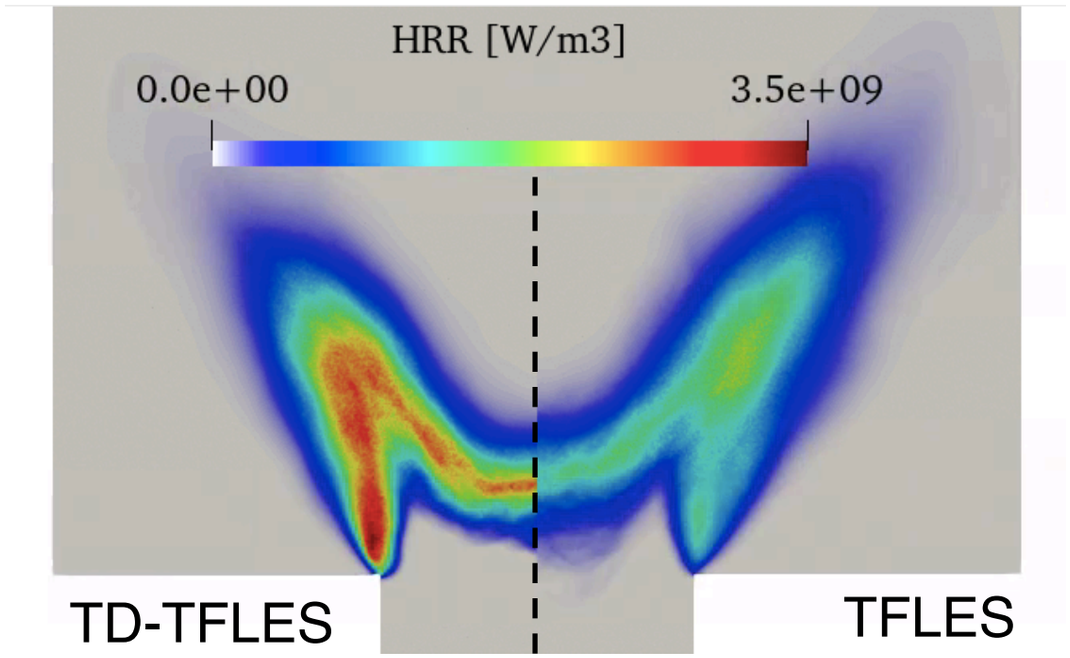


1. Legier, et. Al (2000). In *Proceedings of the summer program* (Vol. 12, pp. 157-168). Center for Turbulence Research Stanford, CA.

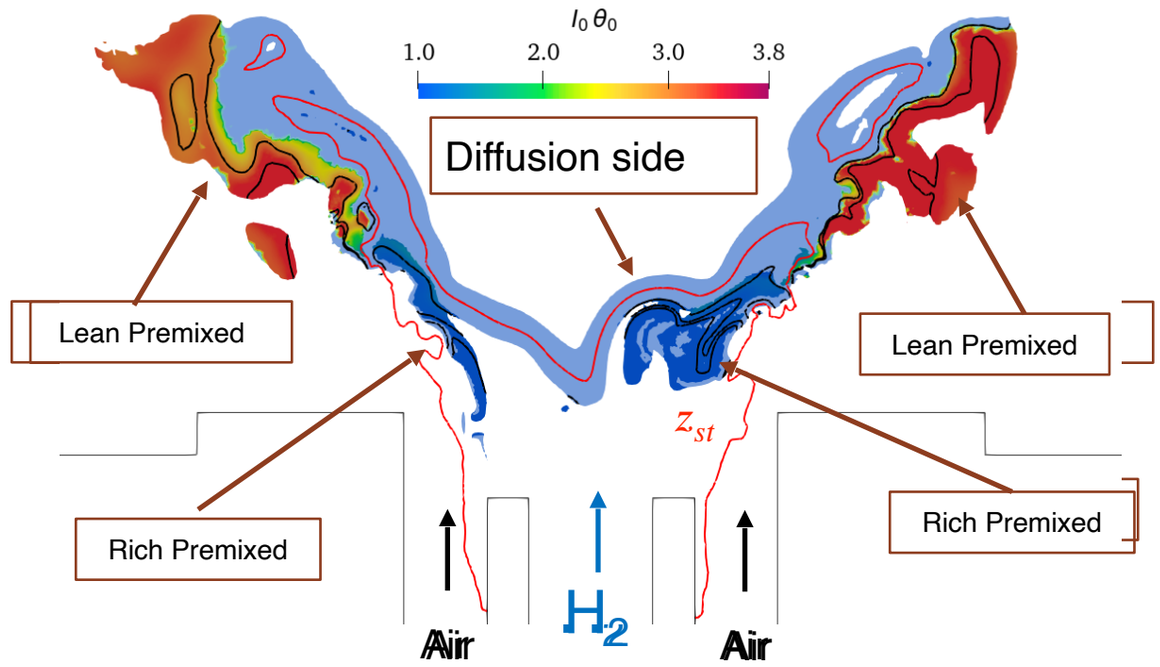
A posteriori test of TD LES for HYLON and TU Berlin flames

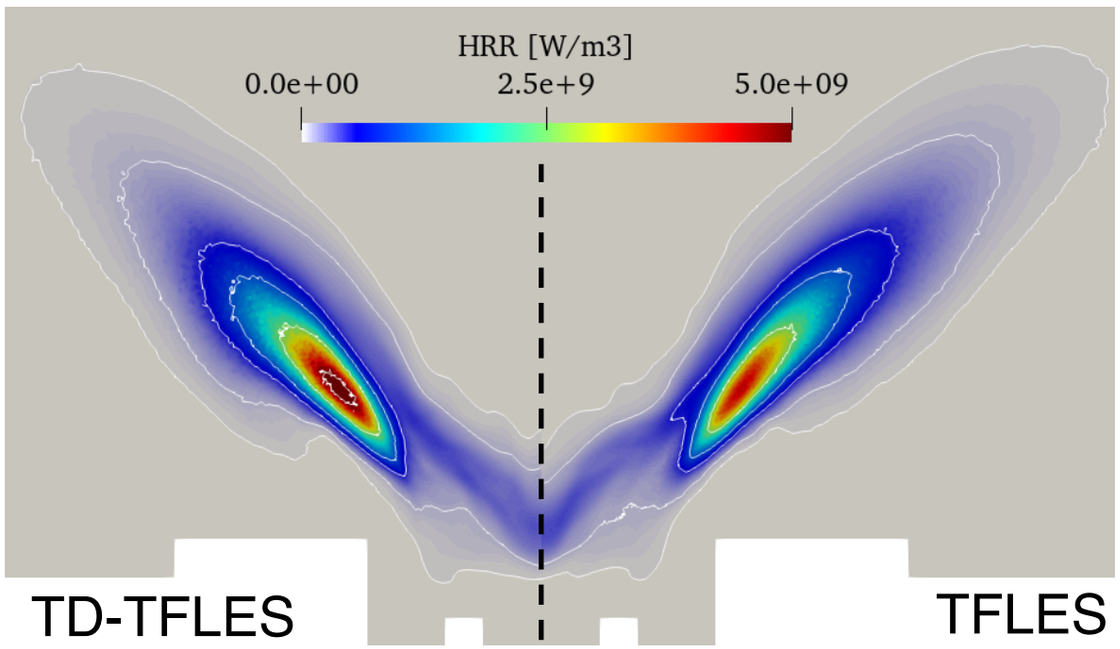
Fully premix lean flame @ TUB





Partially premix flame @ HYLON





Another CFD issue: walls and H2

Why worry about walls?

- The problem of the heat load generated by hydrogen flames is important because hydrogen flames come closer to walls

- For flames stabilized on injector lips: the temperature of the lips is an issue because (1) it controls the stabilization of the flame and (2) the lips should not burn and (3) even if they dont melt, hot walls might encourage flashback

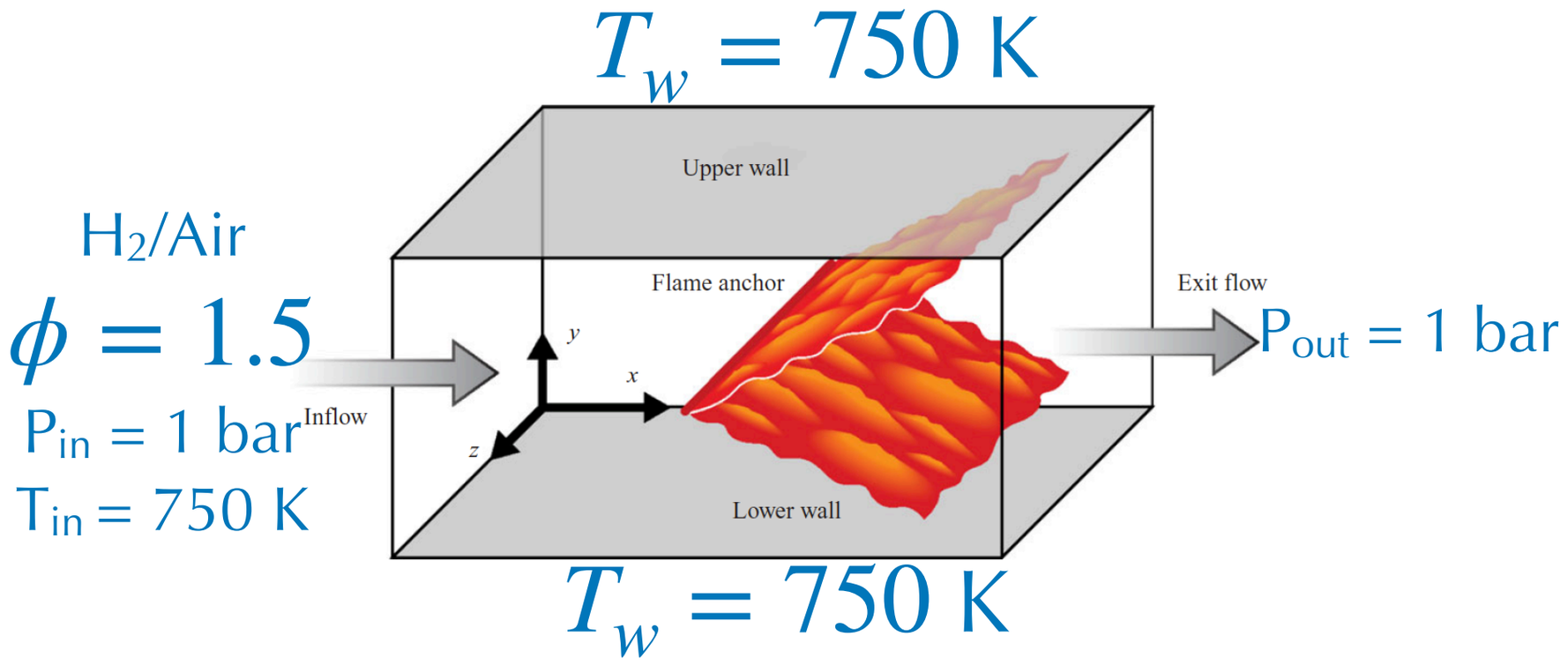
- For flames impacting walls: the walls should not melt - > Safety issue

- In many processes (cement, iron, glass), we need to know the heat transfer to walls and the unpleasant possibility of catalytic reactions on the walls…

Reference: Loic De Nardi, Quentin Douasbin, Olivier Vermorel, Thierry Poinsot. Infinitely Fast Heterogeneous Catalysis Model for Premixed Hydrogen Flame-Wall Interaction. Comb. Flame. 261, 113328, 2024

SO: our CFD codes should predict flame-wall interaction correctly for H2 flames. But they do not...

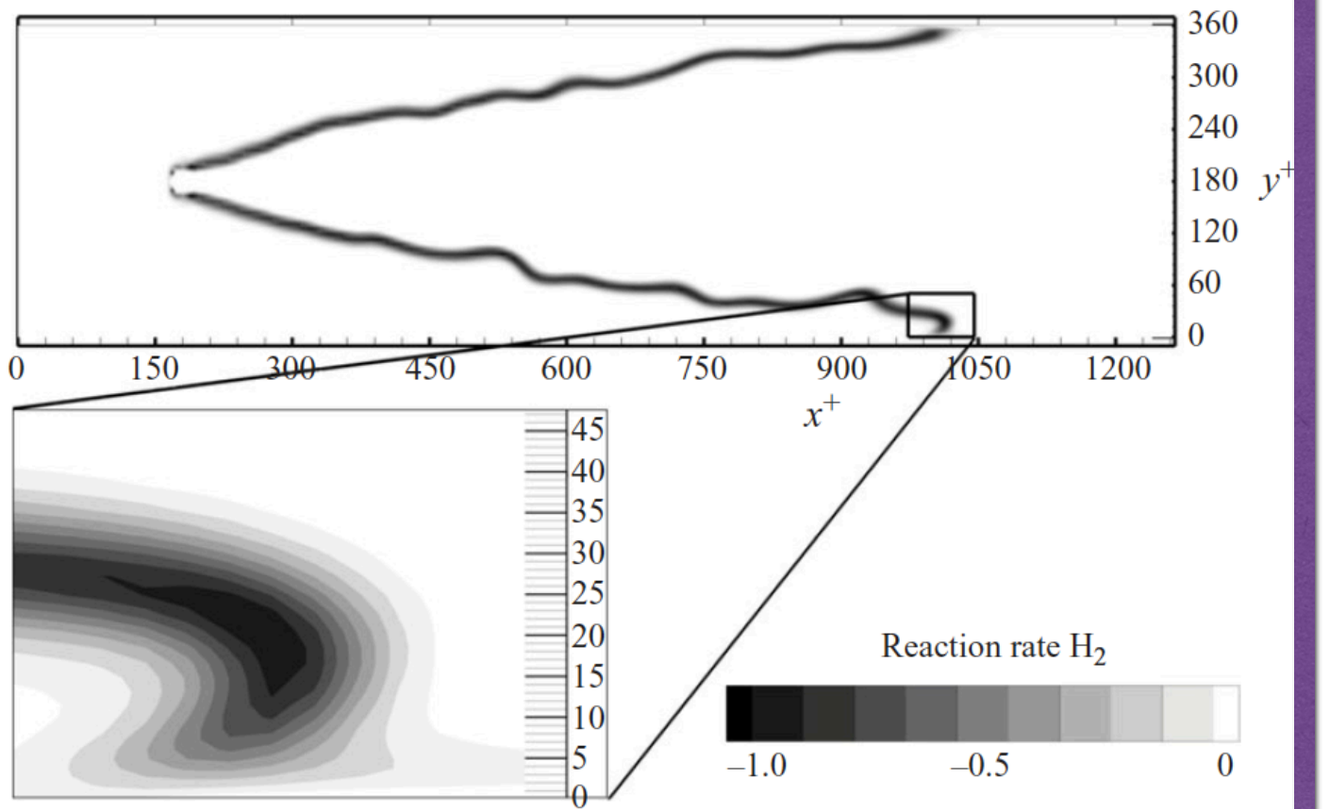
- **A well-known DNS of H_2 FWI [6]**



Laminar FWI - standard wall treatment

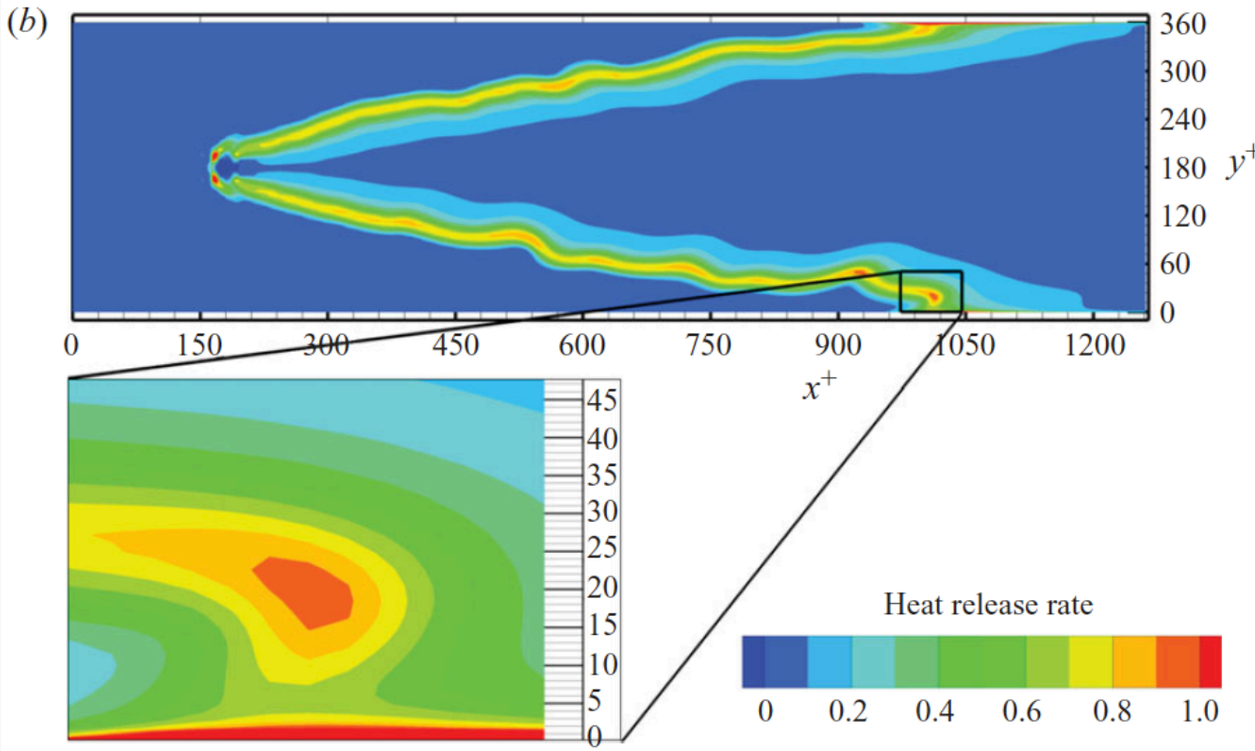
[6] Gruber et al. (JFM, 2010)

$\dot{\omega}_{H_2}$ is correct at the wall



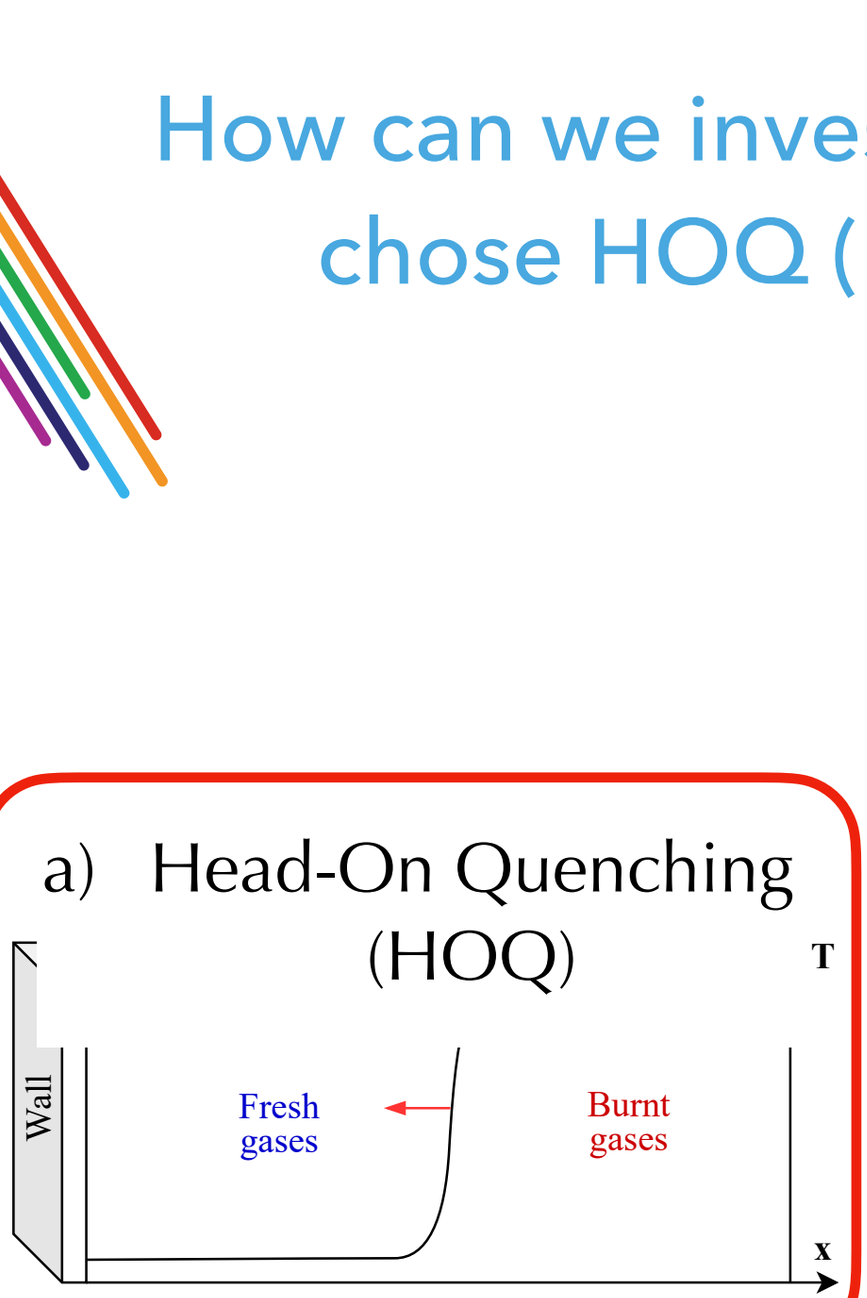
[6] Gruber et al. (JFM, 2010)

But $\dot{\omega}_T$ is not

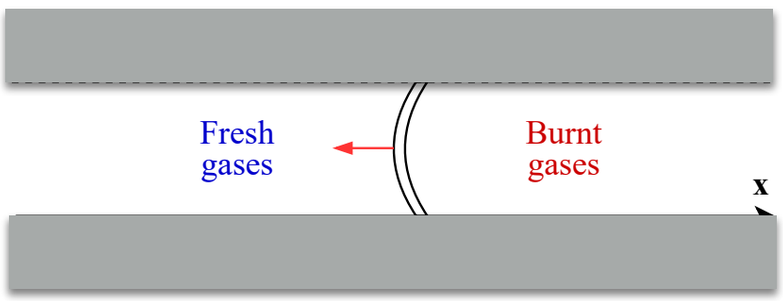


How can we investigate this question simply ?: we chose HOQ (Head On quenching) runs [7]

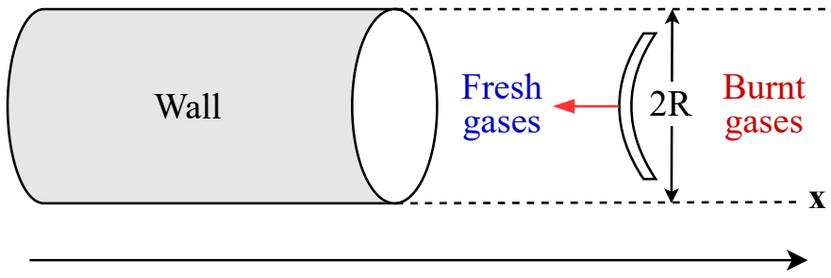
a) Head-On Quenching (HOQ)



b) Side-Wall Quenching (SWQ)

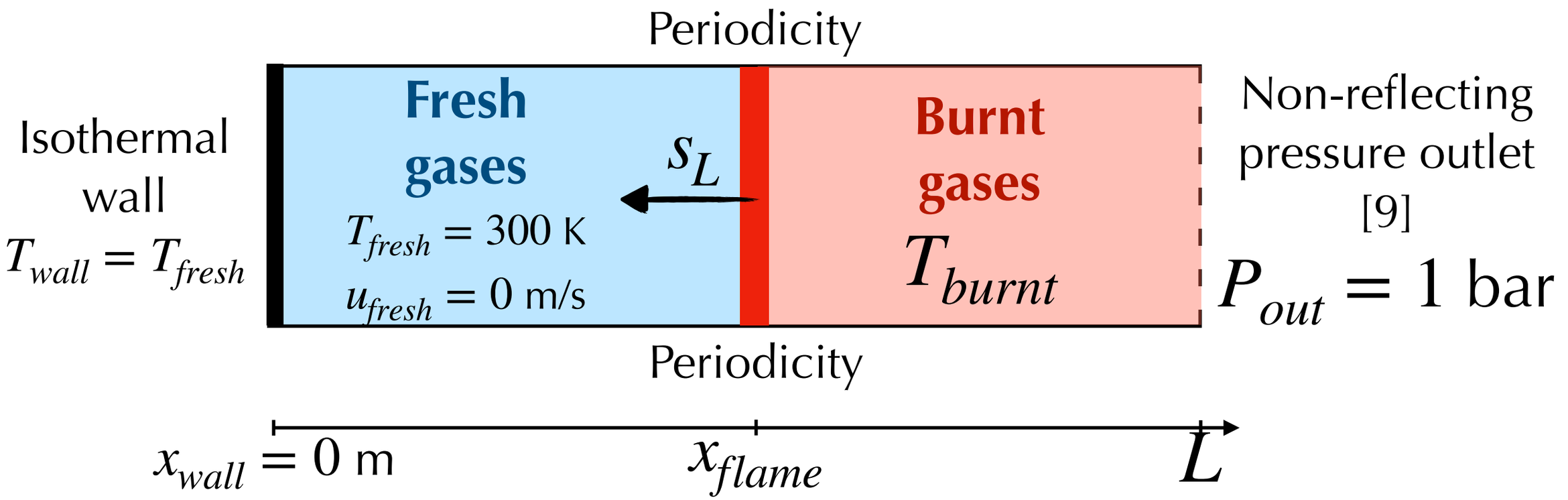


c) Tube quenching



[7] Poinsot and Veynante (TNC, 2012)

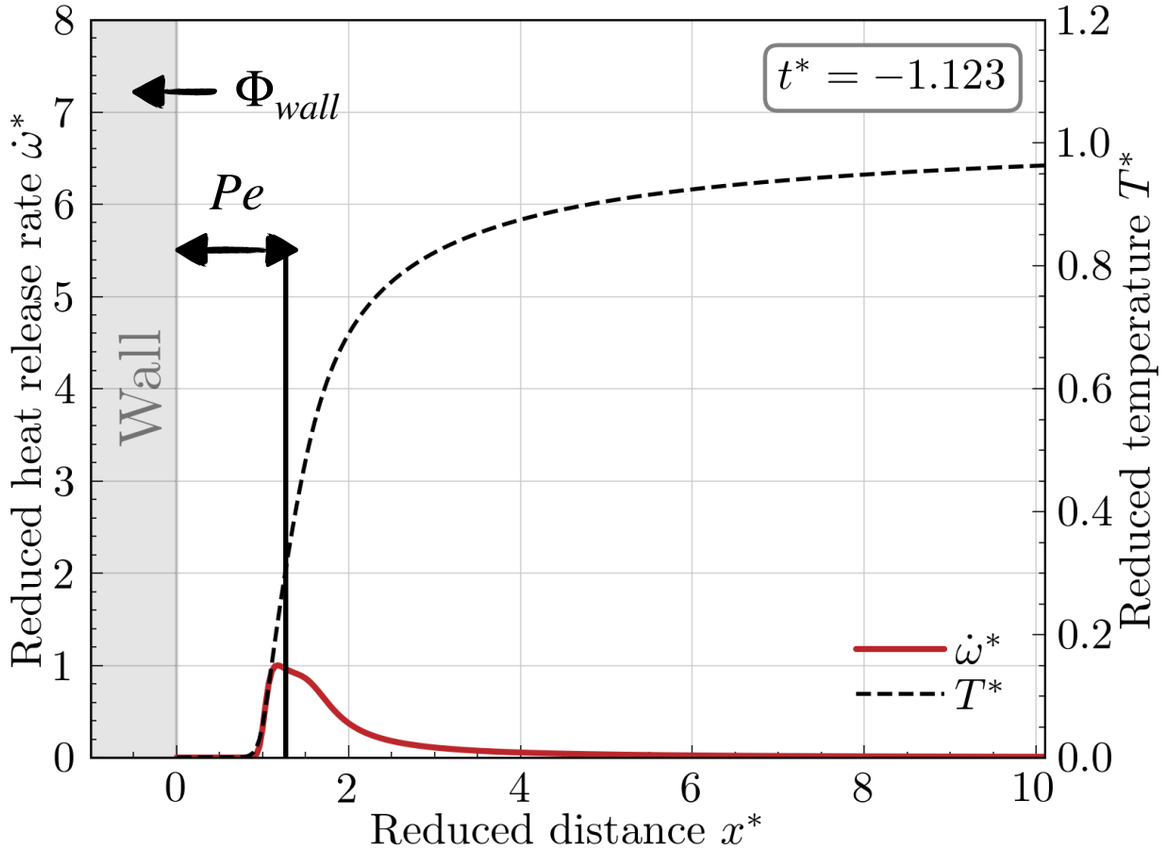
- **1D HOQ simulation with AVBP [8]**



[8] Schönfeld and Rudgyard (AIAA, 1999)

[9] Poinsot and Lele (JCP, 1993)

▸ Definitions



▸ Reduced variables

$$x^* = x/\delta_L$$

$$t^* = (t - t_Q)s_L/\delta_L$$

$$T^* = (T - T_f)/(T_b - T_f)$$

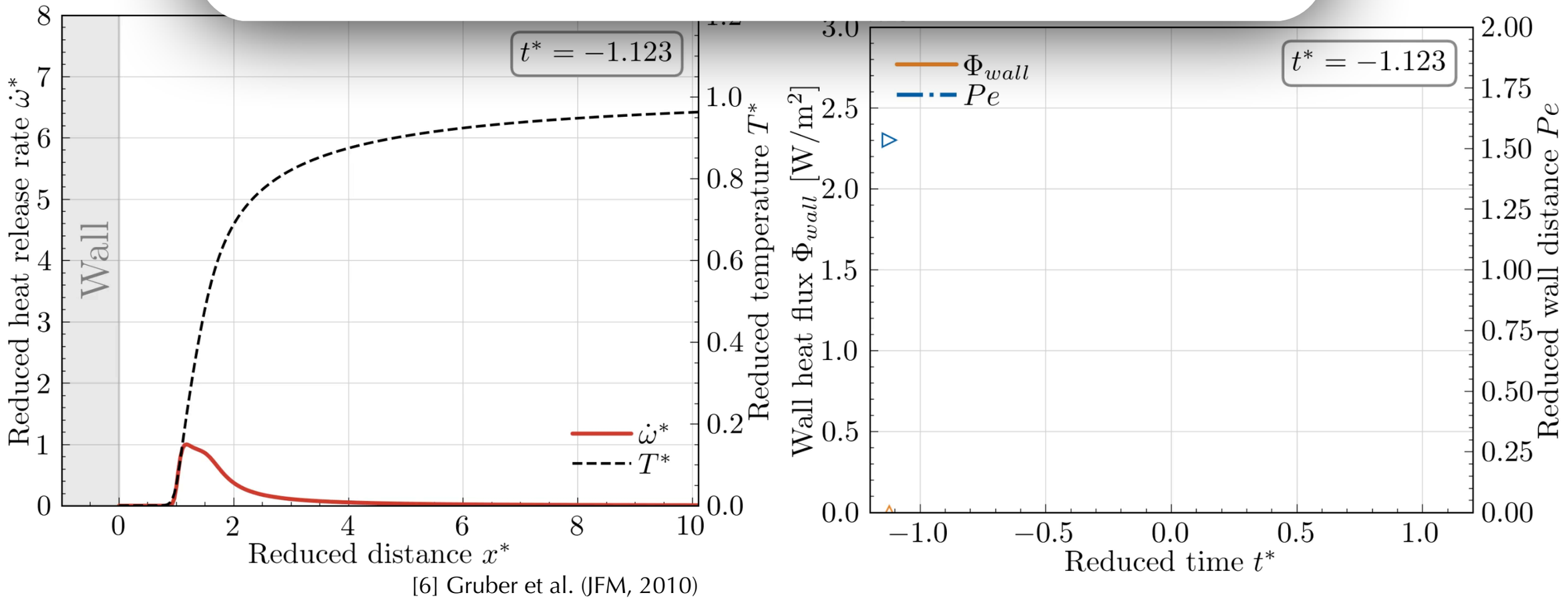
$$\dot{\omega}^* = \dot{\omega}_T/\dot{\omega}_T^0$$

▸ Quantities of interest

$$Pe = x_{flame}/\delta_L$$

$$\Phi_{wall}$$

- Same spiked value of heat release $\dot{\omega}^*$ at the wall at $t^* = 0$ as in [6]
- Also noticed in other studies for H_2 [10-14] and CH_4 [15]



[6] Gruber et al. (JFM, 2010)

[10] Owston et al. (IJHE, 2007)

[11] Mari et al. (CNF, 2016)

[12] Zhao et al. (CNF, 2022)

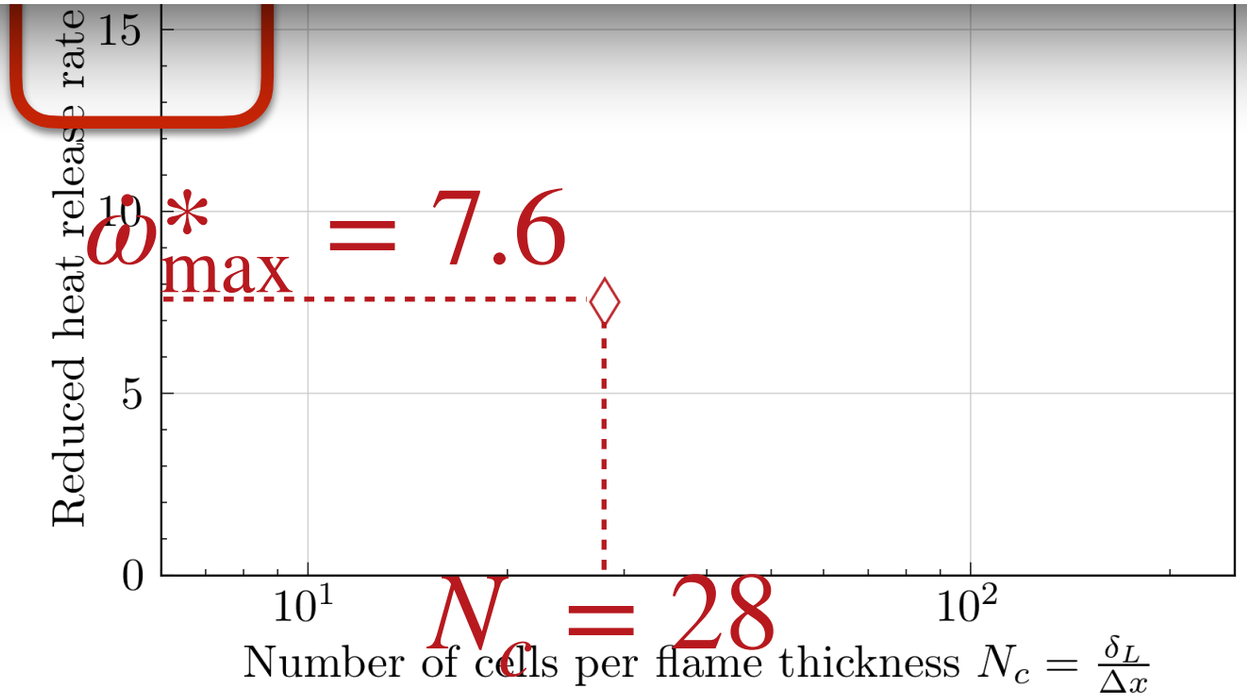
[13] Dabireau et al. (CNF, 2003)

[14] Lai et al. (IJHFF, 2022)

[15] Popp and Baum (CNF, 1997)

- State-of-the-art schemes [16-19] <u>not fitted for FWI</u>
- Tried most chemical schemes and found the same result
- Who is responsible: the H atom

ns!



- 1D HOQ performed for $N_c \in [7;\ 224]$
- $\dot{\omega}^*$ peak at quenching does not converge when the grid is refined

[16] O'connaire et al. (IJHE, 2004)
[17] Li et al. (IJHE, 2004)
[18] Saxena and Williams (CNF, 2006)
[19] Burke et al. (IJHE, 2010)

Who is responsible ?

ID	Reaction	k [cm^3/mol/s/K$^\beta$]	β [-]	E_a [cal/mol]
R1	$H + O_2 \Longleftrightarrow OH + O$	3.52e+16	−0.70	17070
R2	$H_2 + O \Longleftrightarrow OH + H$	5.06e+04	2.67	6291
R3	$H_2 + OH \Longleftrightarrow H_2O + H$	1.17e+09	1.30	3635
R4	$H_2O + O \Longleftrightarrow 2\ OH$	7.60e+00	3.84	12780
R5	$2\ H + M \Longleftrightarrow H_2 + M^*$	1.30e+18	−1.00	0
R6	$H + OH + M \Longleftrightarrow H_2O + M^*$	4.00e+22	−2.00	0
R7	$2\ O + M \Longleftrightarrow O_2 + M^*$	6.17e+22	−0.50	0
R8	$H + OH + M \Longleftrightarrow OH + M^*$	4.71e+18	−1.00	0
R9	$O + OH + M \Longleftrightarrow HO_2 + M^*$	8.00e+15	0.00	0
R10	$H + O_2 + M \Longleftrightarrow HO_2 + M^\dagger$	$k_\infty = 4.65e+12$	0.44	0.0
		$k_0 = 5.75e+19$	−1.40	0.0
R11	$HO_2 + H \Longleftrightarrow 2\ OH$	7.08e+13	0.00	295
R12	$HO_2 + H \Longleftrightarrow H_2 + O_2$	1.66e+13	0.00	823
R13	$HO_2 + H \Longleftrightarrow H_2O + O$	3.10e+13	0.00	1721
R14	$HO_2 + O \Longleftrightarrow OH + O_2$	2.00e+13	0.00	0
		$k_0 = 2.30e+18$	−0.90	−1702
R17	$2\ HO_2 \Longleftrightarrow H_2O_2 + O_2$	3.02e+13	0.00	1386
R18	$H_2O_2 + H \Longleftrightarrow HO_2 + H_2$	2.30e+13	0.00	7950
R19	$H_2O_2 + H \Longleftrightarrow H_2O + OH$	1.00e+13	0.00	3585
R20	$H_2O_2 + OH \Longleftrightarrow H_2O + HO_2$	7.08e+12	0.00	1434
R21	$H_2O_2 + O \Longleftrightarrow HO_2 + OH$	9.63e+06	2.00	3991

The H radical at the wall is the bad guy

IFHC model for H_2 FWI

A simplified approach for FWI

- **There should be zero H radical at the wall surface: they disappear through catalytic reactions with the solid surface**
- **Infinitely Fast Heterogeneous Catalysis (IFHC) [3]**
  - Global surface chemistry: total, irreversible, occurring in 1 timestep:

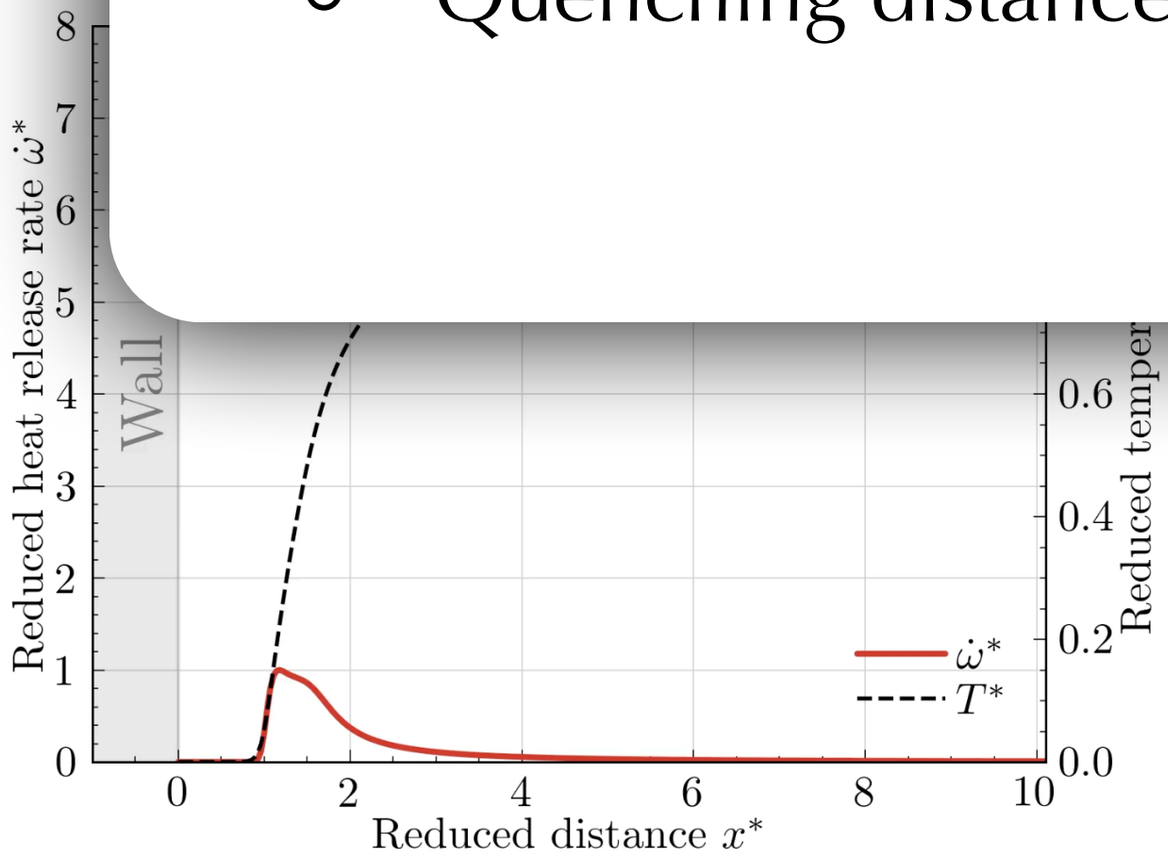
$$2H + O \rightarrow H_2O \quad (1)$$

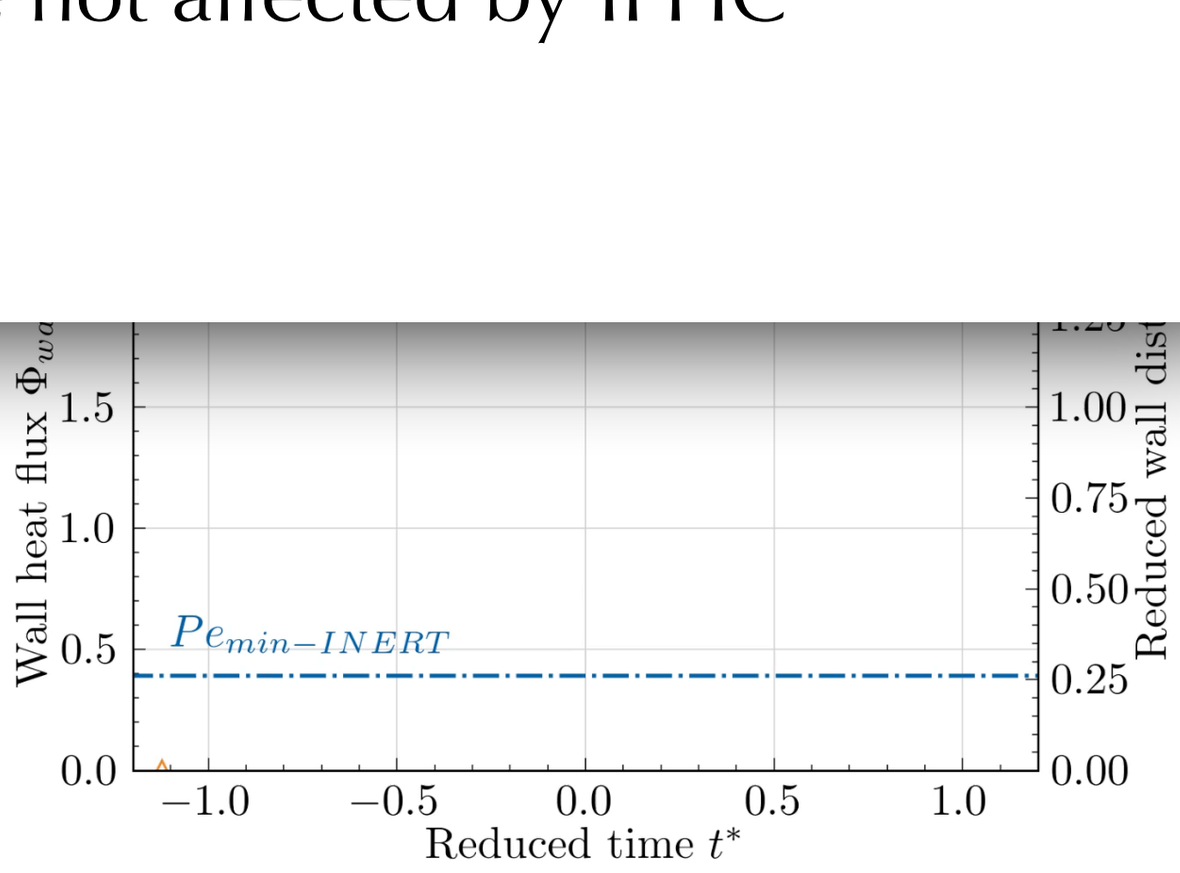
$$H + OH \rightarrow H_2O \quad (2)$$

$$4H + O_2 \rightarrow 2H_2O \quad (3)$$

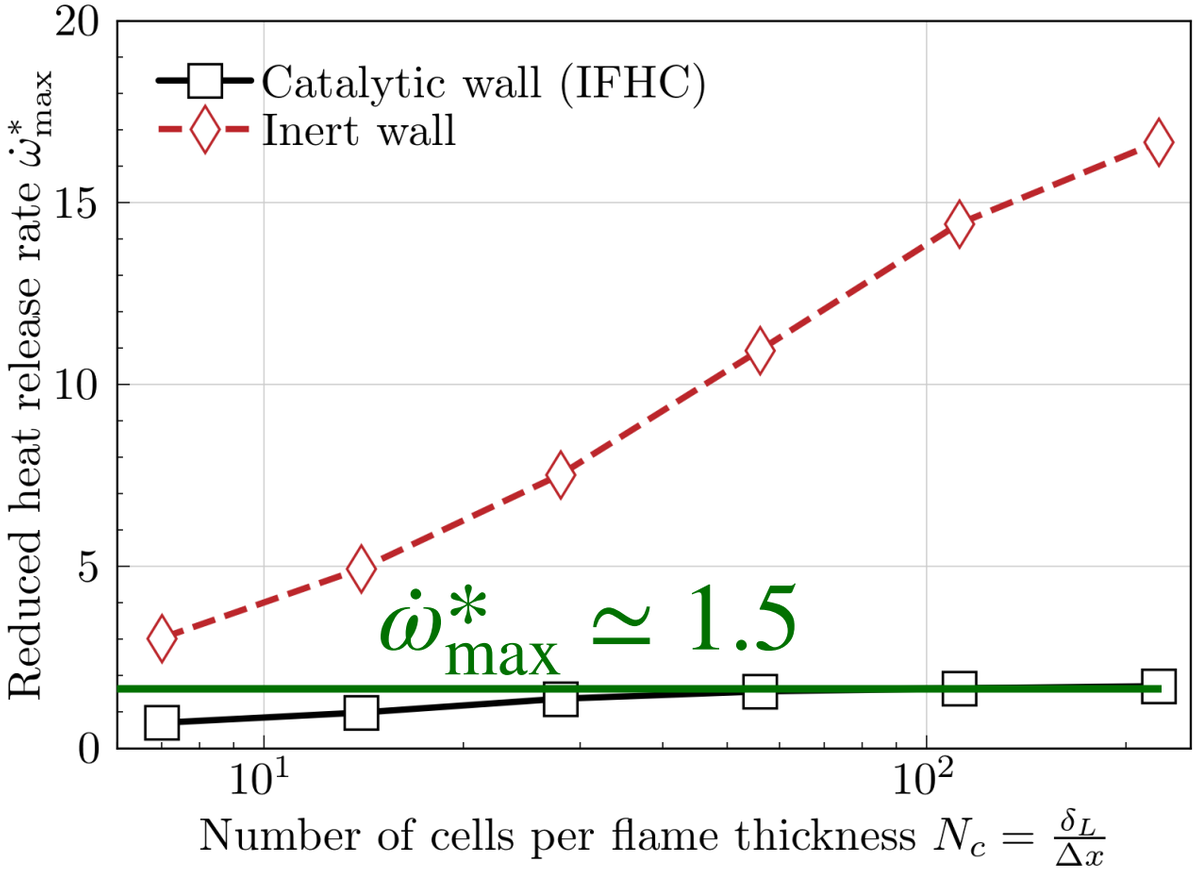
[3] De Nardi et al. (CNF, 2024)

- No crazy heat release rate at the wall with IFHC
- Wall heat flux lowered by ~30% versus inert wall
- Quenching distance not affected by IFHC





- **Results for an isothermal wall with IFHC: well posed, convergent problem**



- Mesh influence with the IFHC model
- 1D HOQ performed for $N_c \in [7;\ 224]$

→ **Grid convergence retrieved**

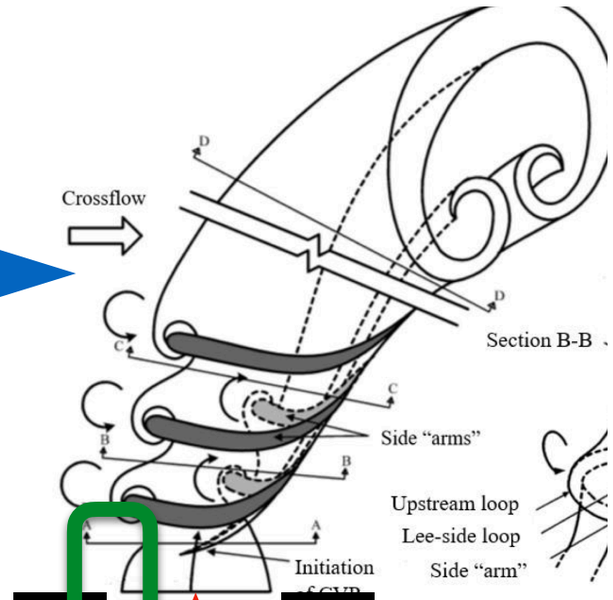
Yet another CFD issue: flame stabilization

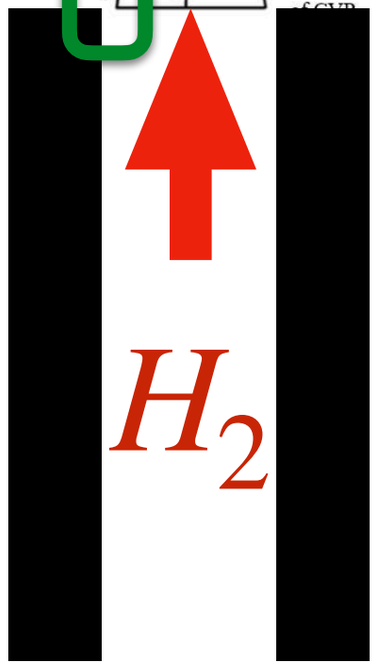
Why worry about stabilization?

- All H2 air concepts rely on ‘some creative method’ to mix H2 and air fast

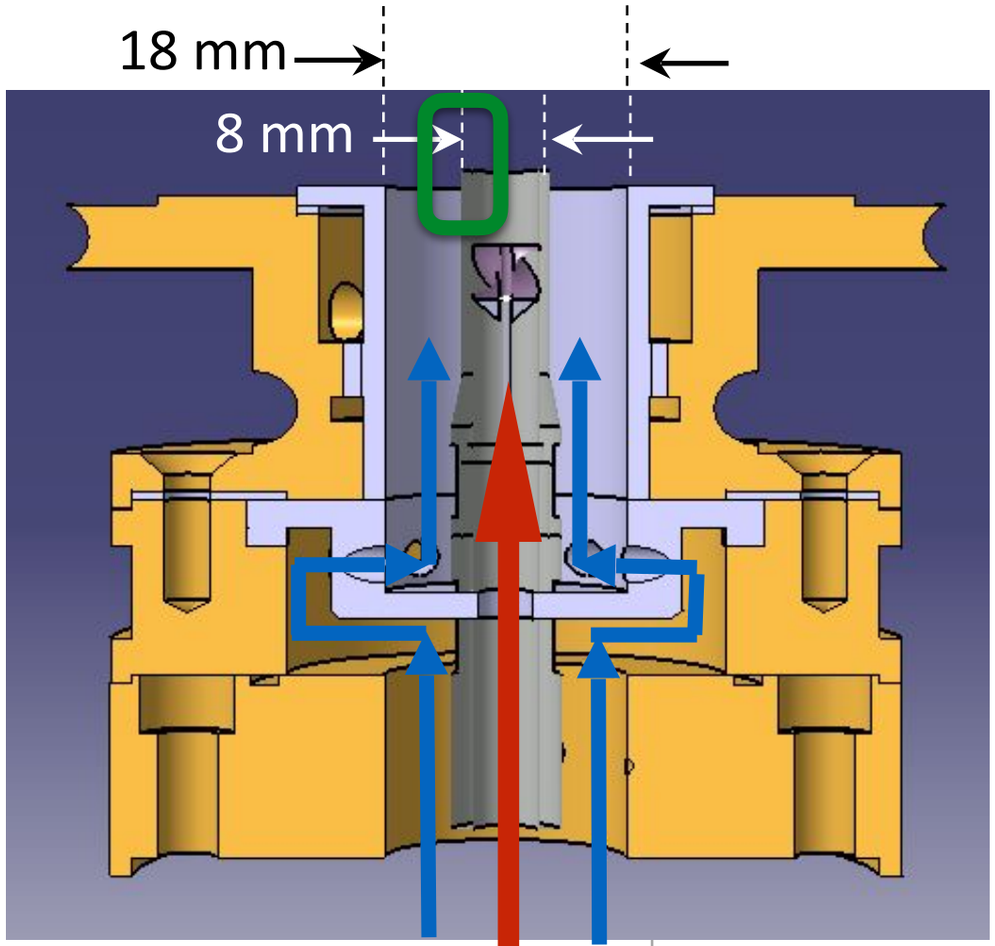
MICROMIX

AIR

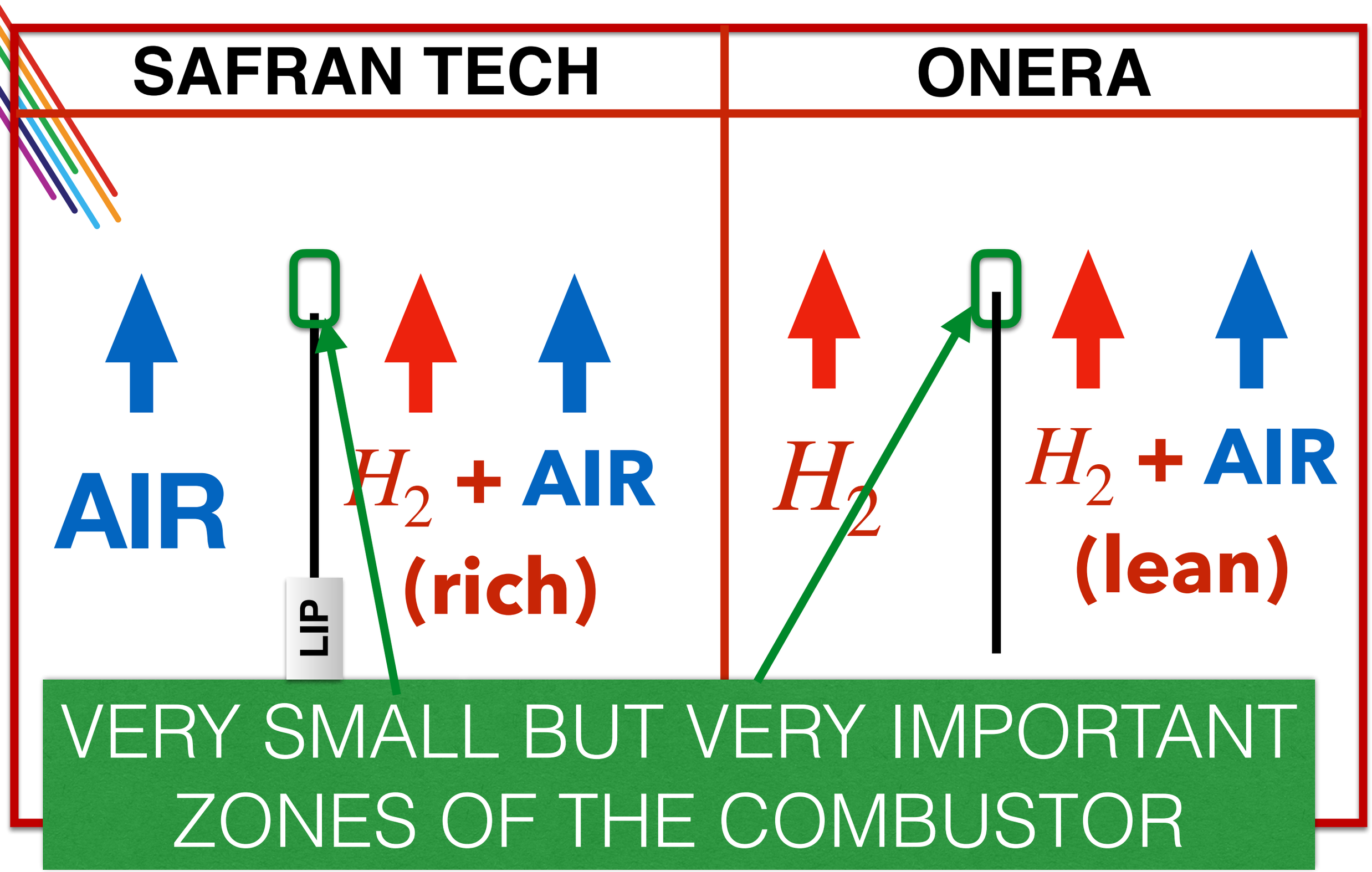




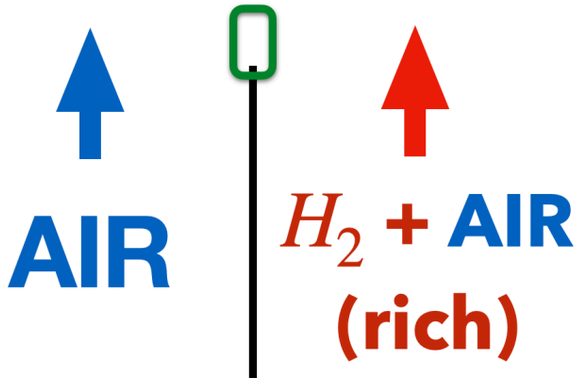
HYLON



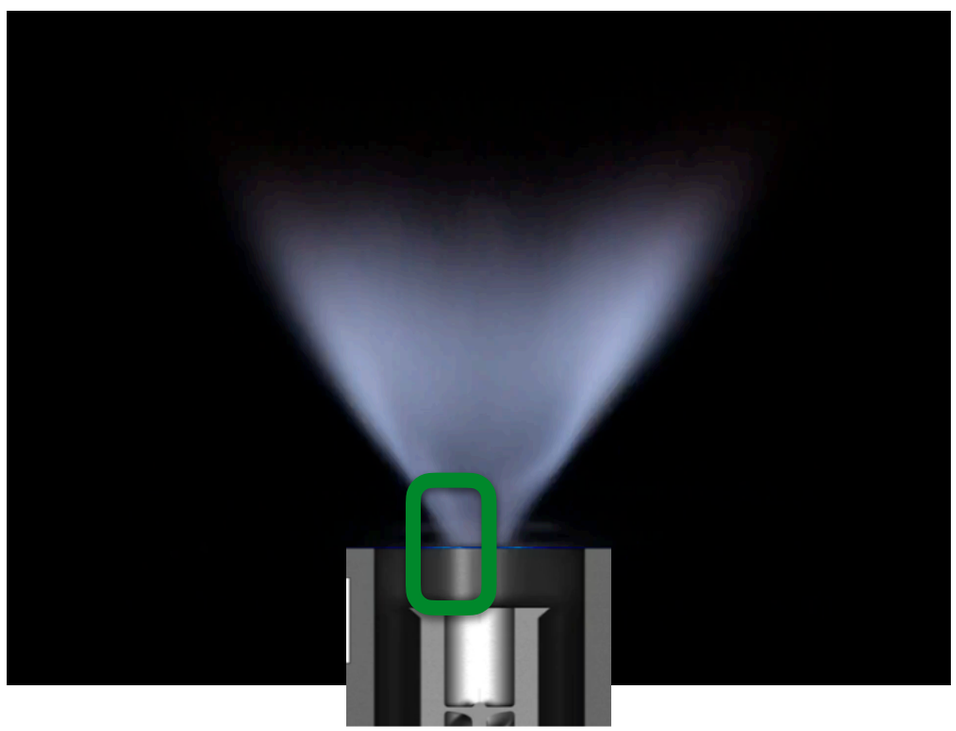
CERFACS

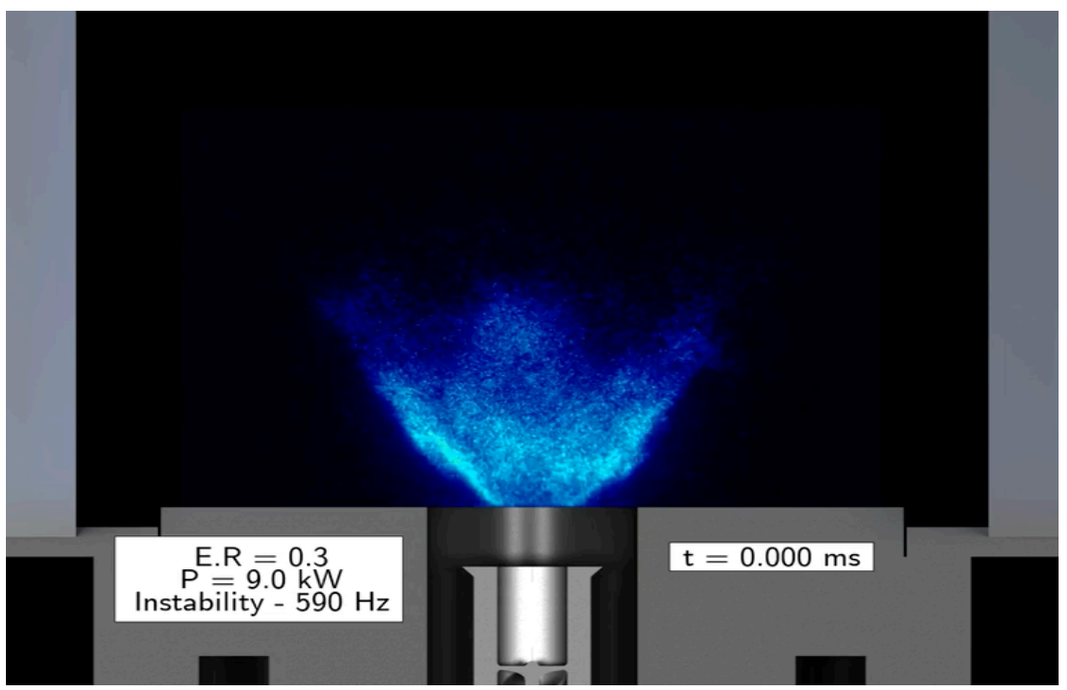

SAFRAN TECH
ONERA
AIR
H_2 + AIR
(rich)
LIP
H_2
H_2 + AIR
(lean)
VERY SMALL BUT VERY IMPORTANT
ZONES OF THE COMBUSTOR

Why should we care ?

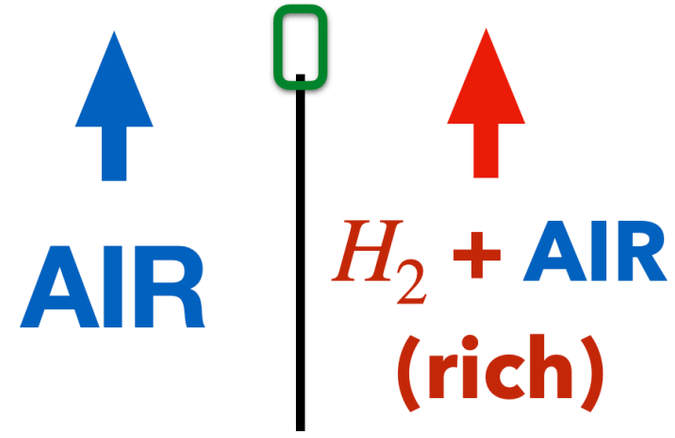


- This zone controls flame anchoring:
  - Flame **too close** to the lips: the lips will burn. If they do not burn, we'll have a diffusion flame and too much NOx. After a while, we may even have flashback
  - Flame **too far** from the lips: the flame might blow off or become unstable -> thermoacoustics



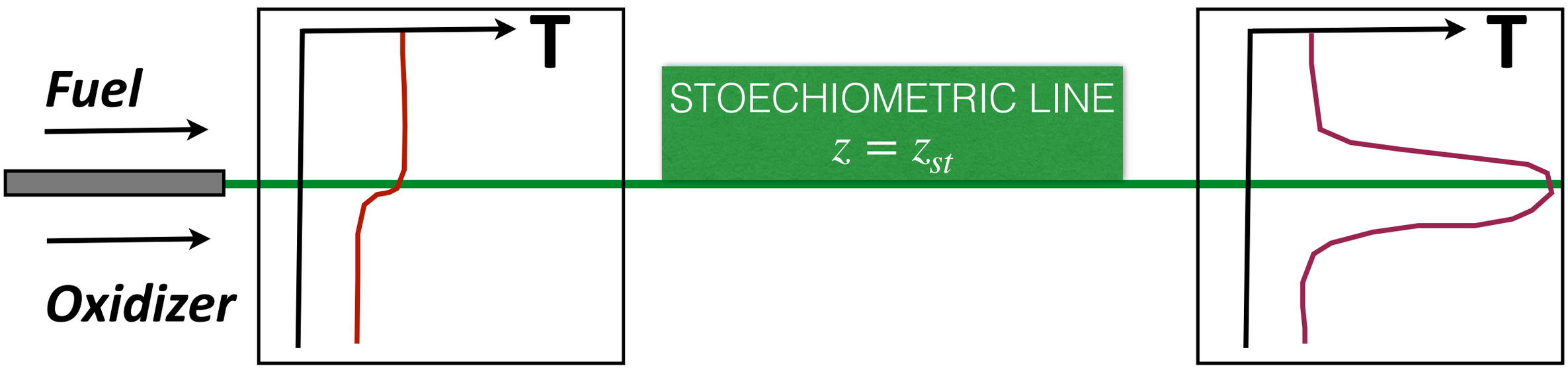


Why is this zone a problem?



- This zone contains flame elements which are beyond our LES models: ‘edge’ flames (among which, the ‘triple’ flames)
- Edge flames are not included in any turbulent combustion model
- Edge flames are very small…

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

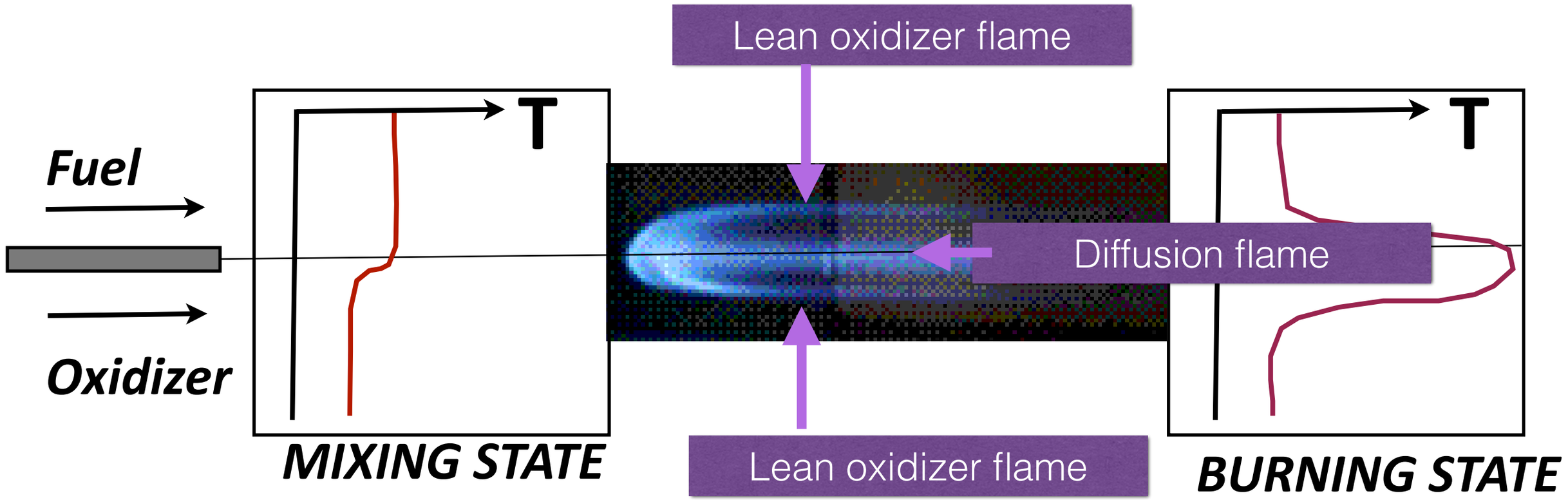


MIXING STATE ***BURNING STATE***

In any system, where you inject pure fuel and pure oxidizer, you start by mixing them with no flame. Later downstream, you burn in a diffusion mode on the stoichiometric line $z = z_{st}$. How ?

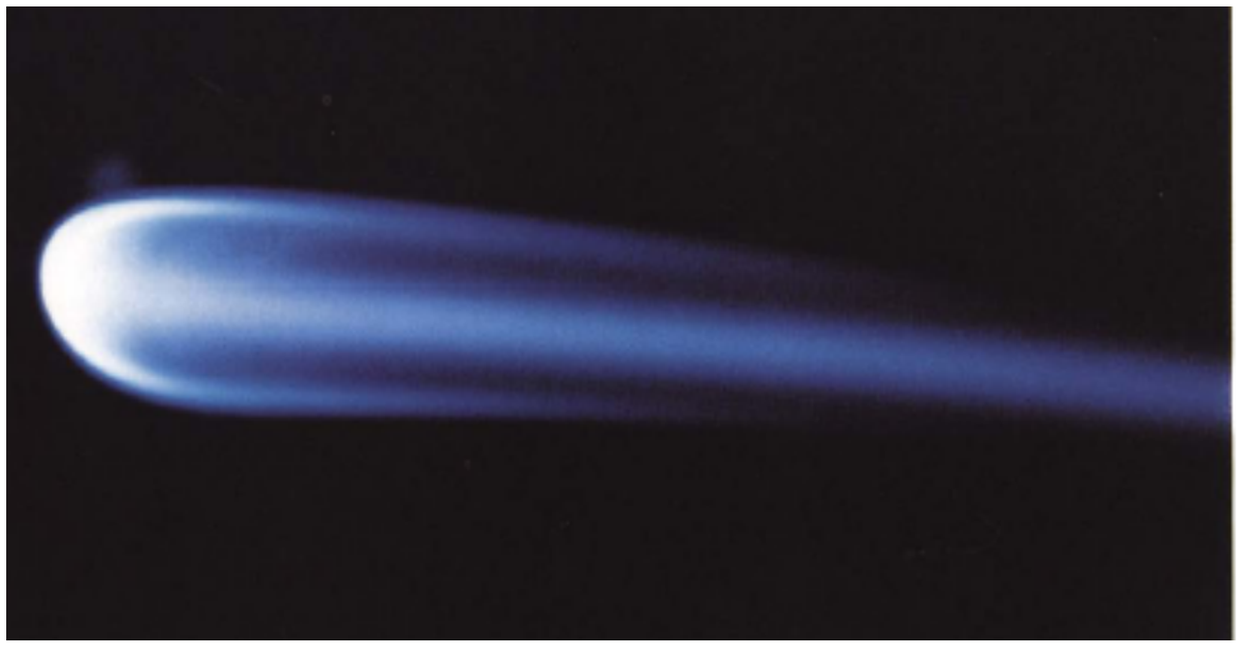
In other words: how does a diffusion flame begin ?

THE CONSENSUS TODAY IS THAT THIS TRANSITION IS PRODUCED BY TRIPLE FLAMES:



P. N. Kioni, B. Rogg, K. N. C. Bray, and A. Liñán, "Flame spread in laminar mixing layers: The triple flame," Combust. Flame 95, 276,1993.

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



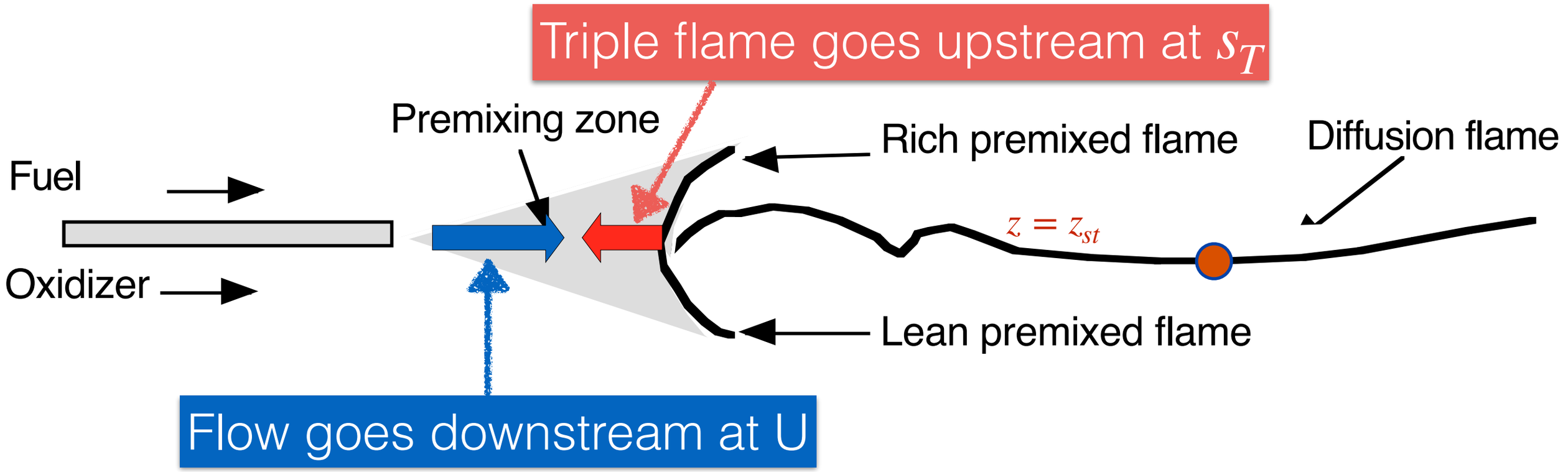
- **A TRIPLE FLAME SPEED SCALES LIKE:**

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

Stoechiometric laminar flame speed

Density ratio

MUNIZ AND MUNGAL: LINK THE STABILIZATION OF DIFFUSION FLAMES TO THE SPEED OF TRIPLE FLAMES



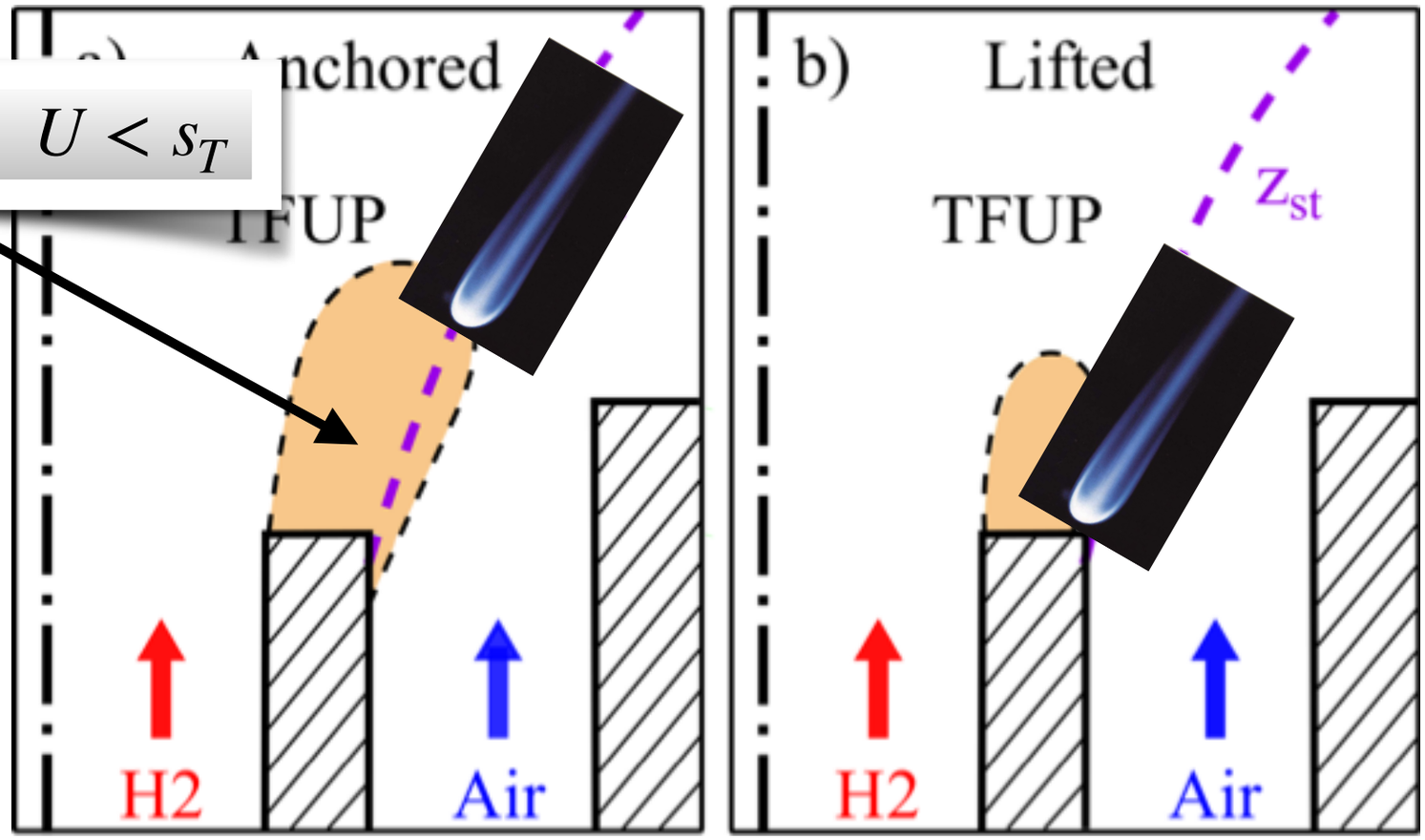
If $U > s_T$ the flame is convected away
If $U < s_T$ the flame goes upstream and attaches to the lips

Remember that the flame MUST travel along the stoichiometric line $z = z_{st}$

L. Muniz and M. G. Mungal. Instantaneous flame-stabilization velocities in lifted-jet diffusion flames. Comb. Flame, 1997, 111, 1-2,16-31

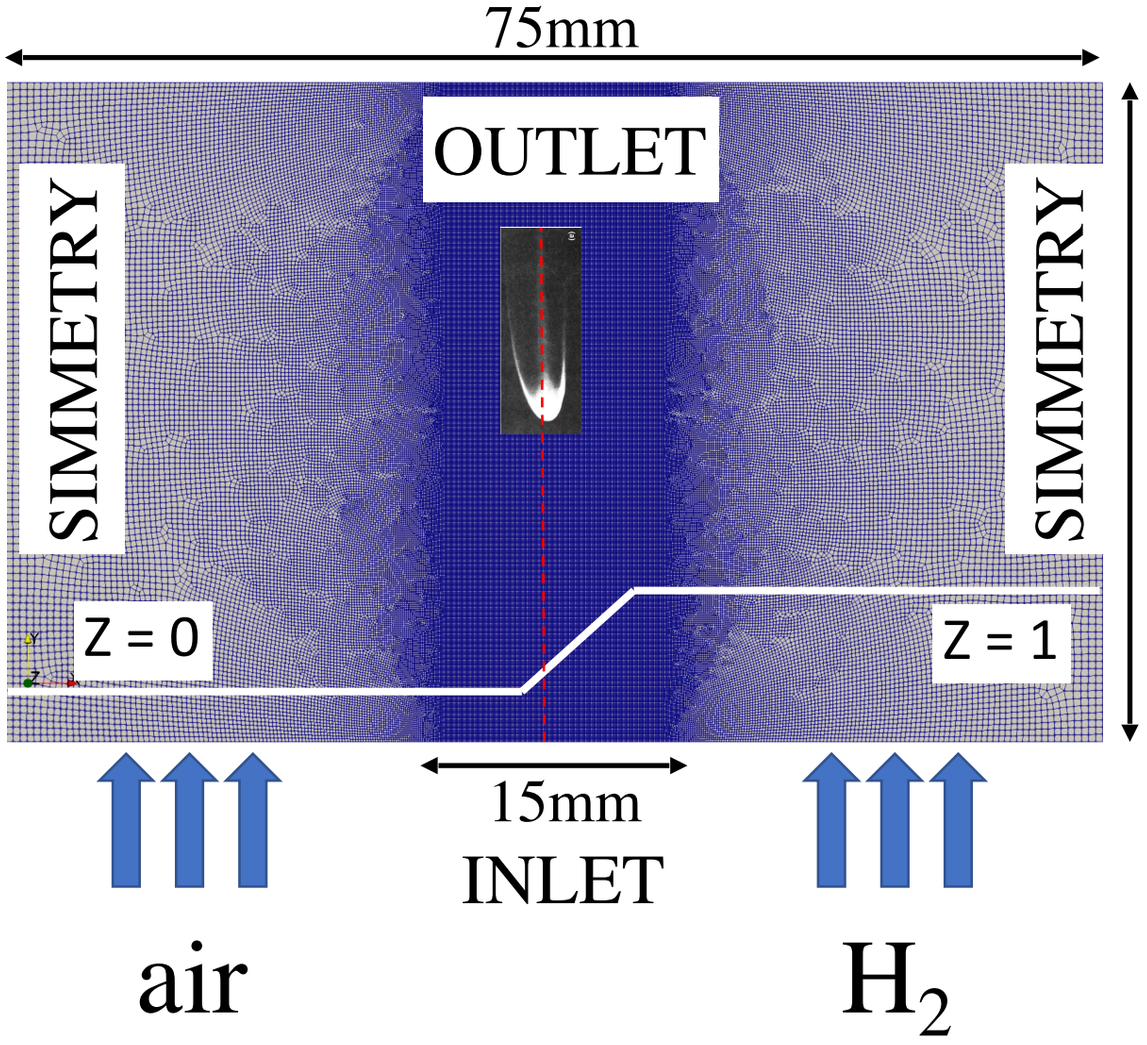
Triple Flame Upstream Propagation (TFUP): for H2 air flames at 1 bar, the triple flame speed $s_T = s_L^0\sqrt{\rho_1/\rho_2}$ is 7 m/s

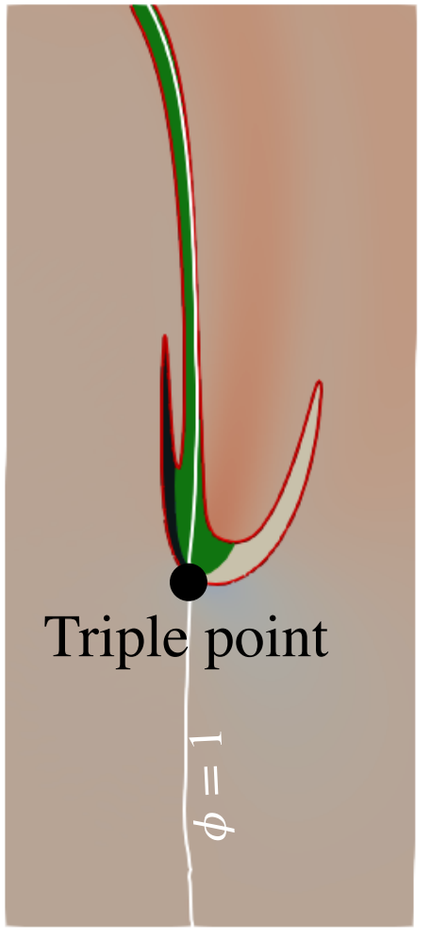
In this TFUP zone, $U < s_T$

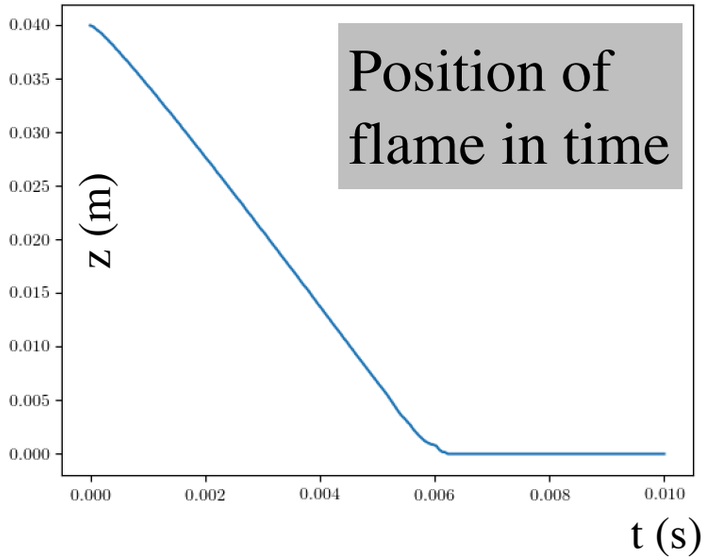


S. Marragou, H. Magnes, A. Aniello, L. Selle, T. Poinsot, T. Schuller. Experimental analysis and theoretical lift-off criterion for H2/air flames stabilized on a dual swirl injector, *Proc. Comb. Inst.*, 2022. 10.1016/j.proci.2022.07.255

DNS of triple H2 air flames (Aniello PhD)

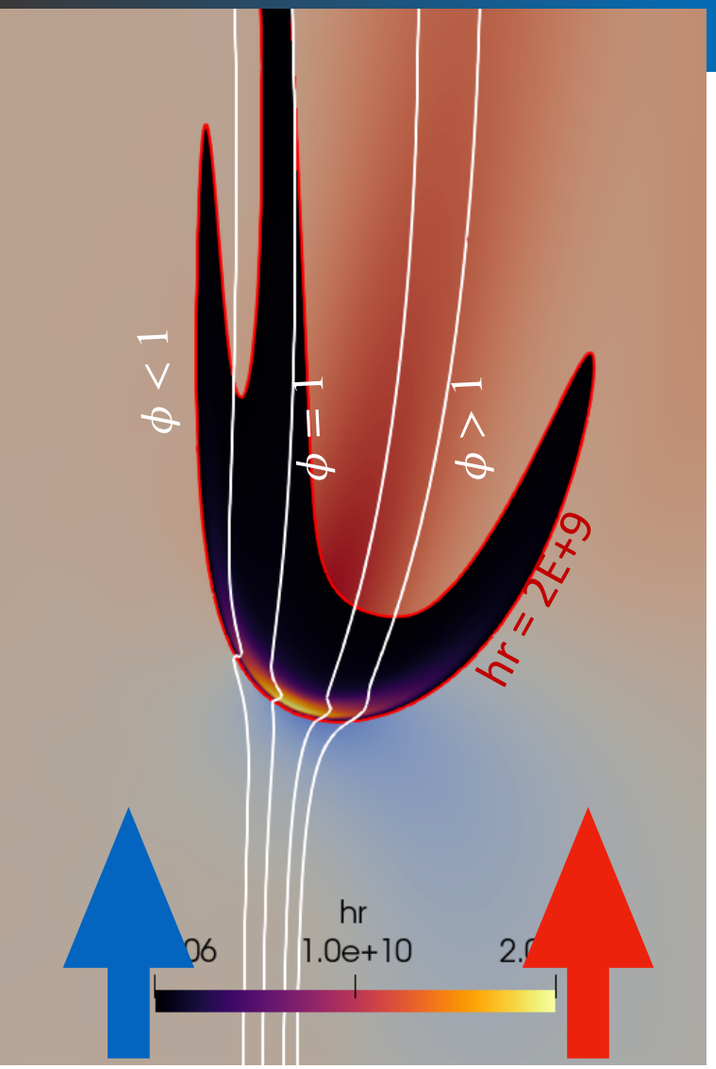






Flame velocity depending on:

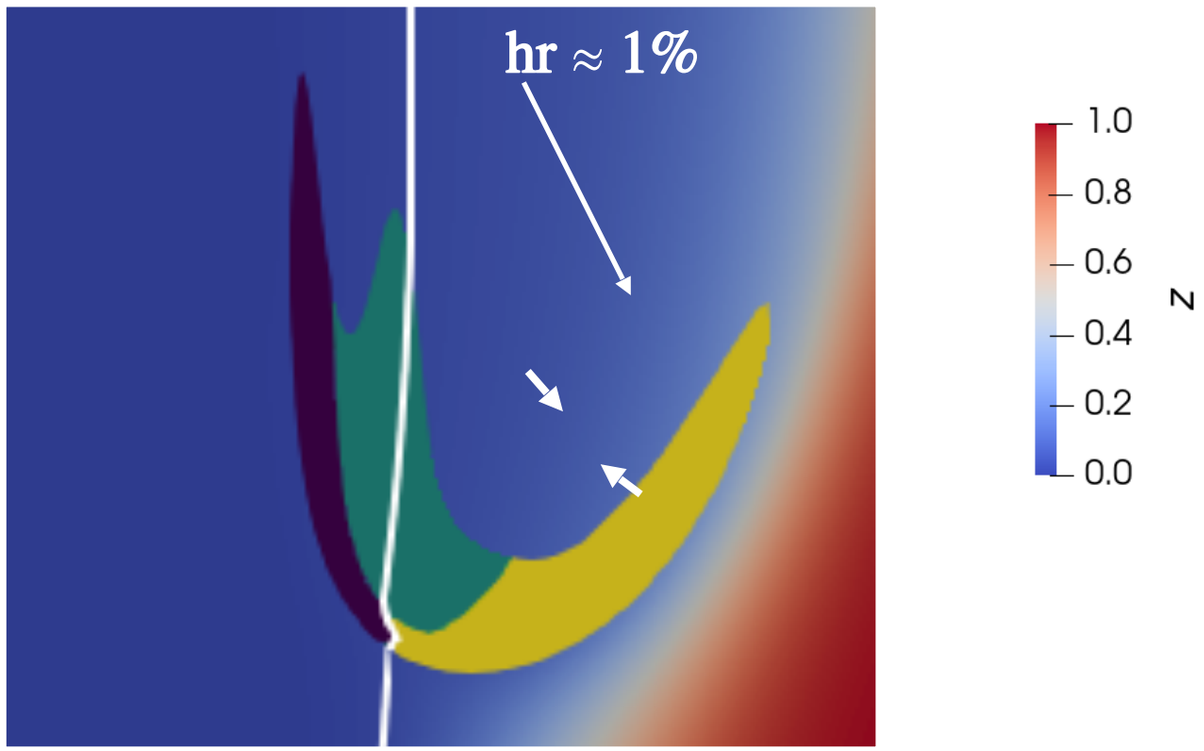
- v_Z
- Fresh gas temperature
- Pressure



- We know that these flames exist and control flame stabilization. They are a bit special for H2
- Experiments confirm that they provide the right scalings for lift off
- Can not capture them with LES models: most LES models do not even know what a triple flame is
- Can capture them with DNS but…

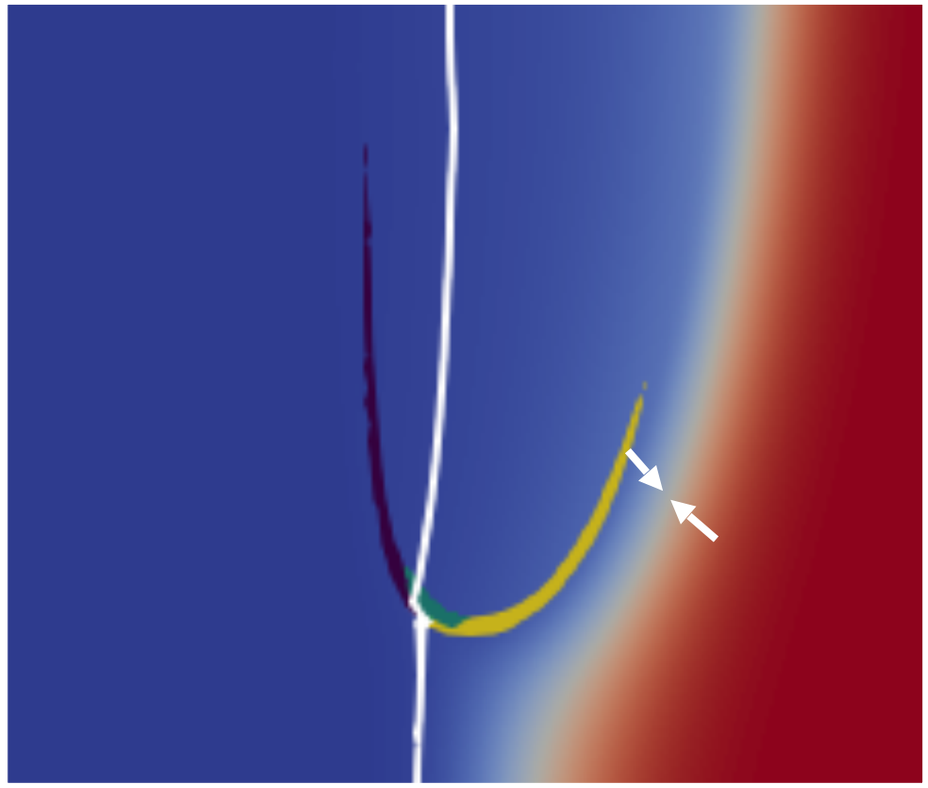
But DNS cant go to high pressures even in 2D…

$\Delta x = 25\ \mu m$



T = 300 K , P = 1 bar

$\Delta x = 8\ \mu m$



T = 300 K , P = 5 bar

Aniello's unpublished results

'Other' edge flames are expected

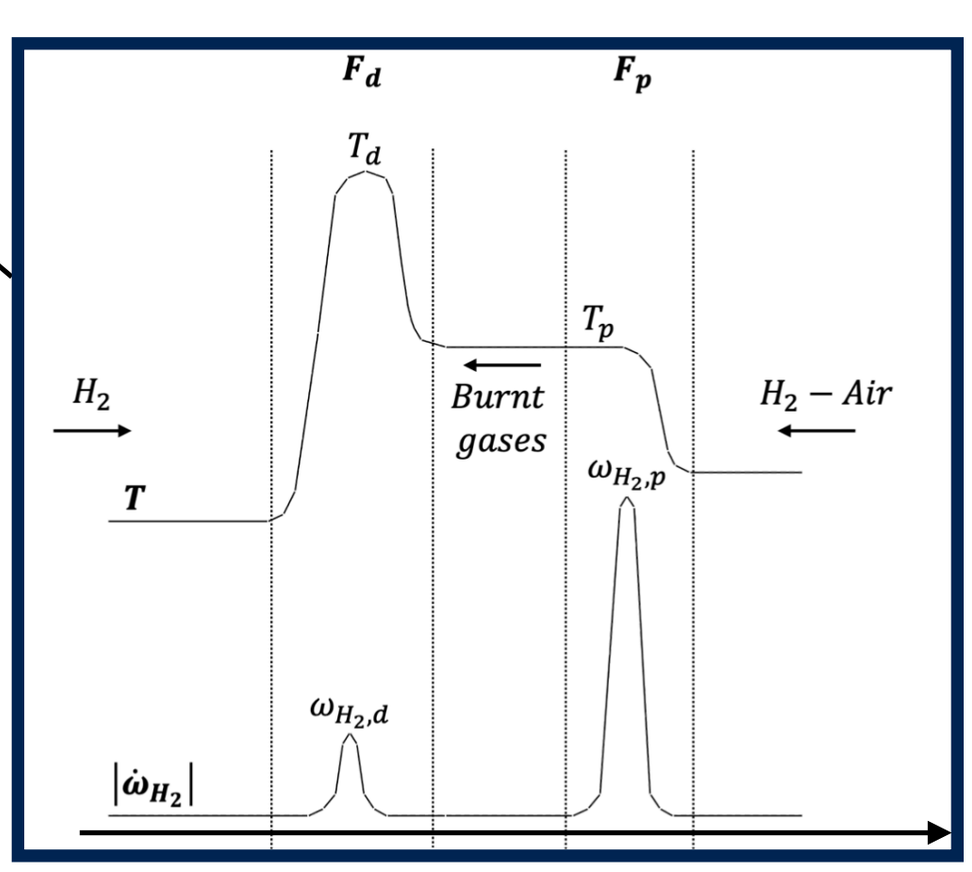
Hot vitiated AIR

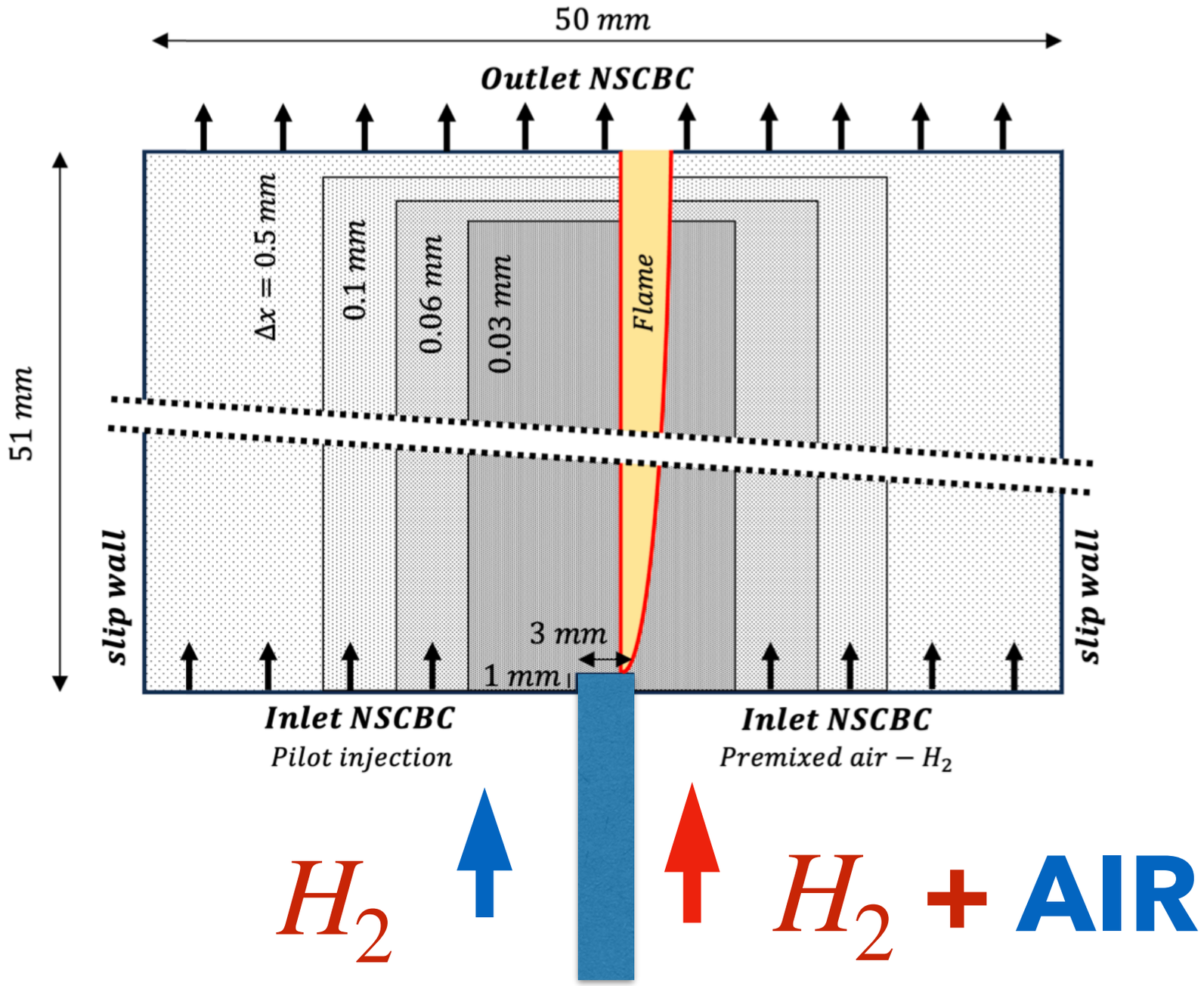
Diffusion H_2/ VITIATED AIR flame

Lean H_2/ AIR flame

H_2

H_2 + AIR (lean)

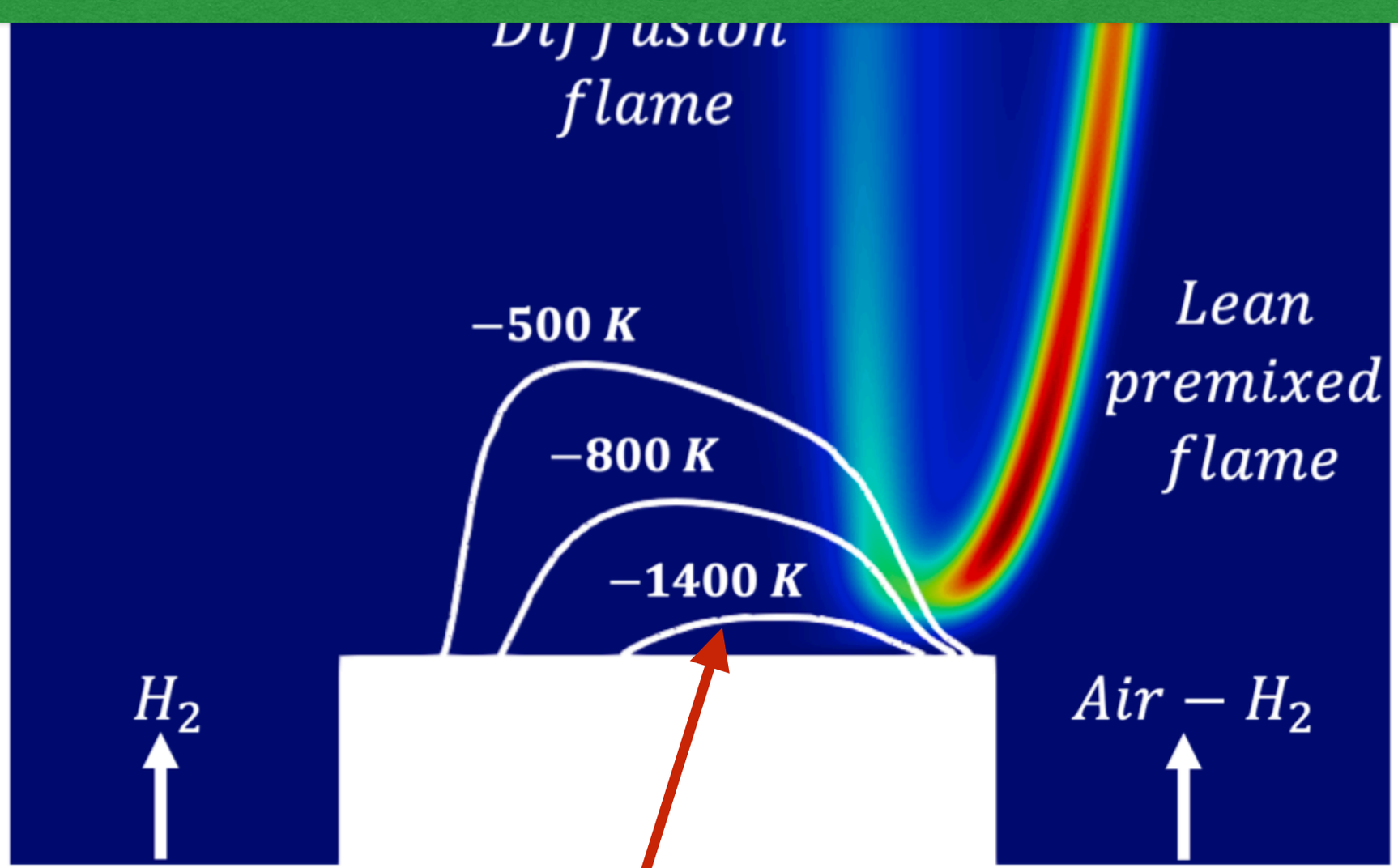




J. Bertsch et al. *40th Symp. Comb.* Stabilization regimes and flame structure at the flame base of a swirled lean premixed hydrogen-air injector with a pure hydrogen pilot injection. Submitted

Source term for H2

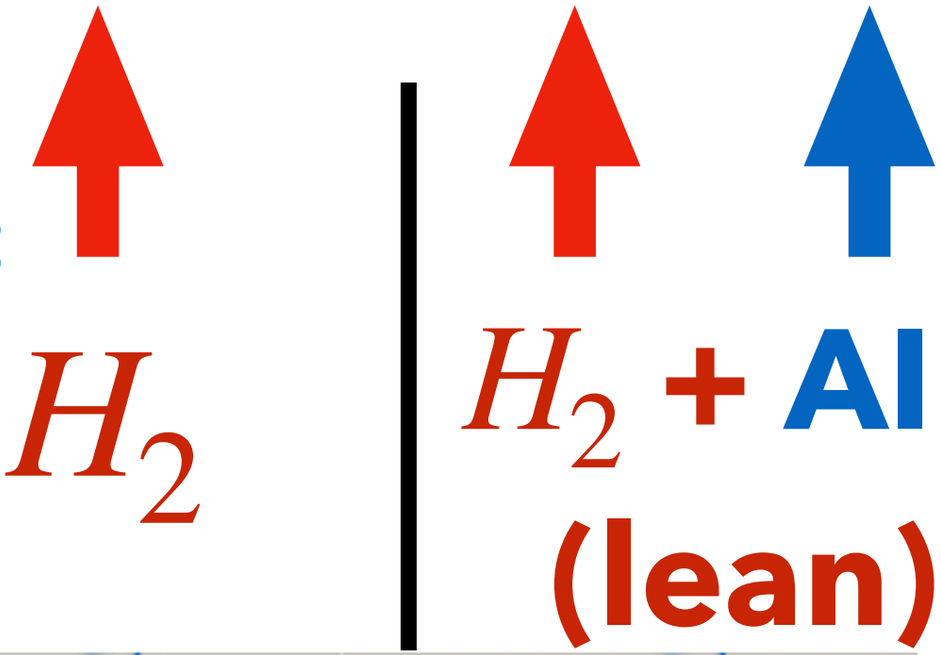
THESE EDGE FLAMES DO NOT PROPAGATE ANY MORE. THEY ARE COOLED BY THE LIP AND LOSE A LOT OF HEAT TO IT -> WE PERFORM CHT COMPUTATIONS

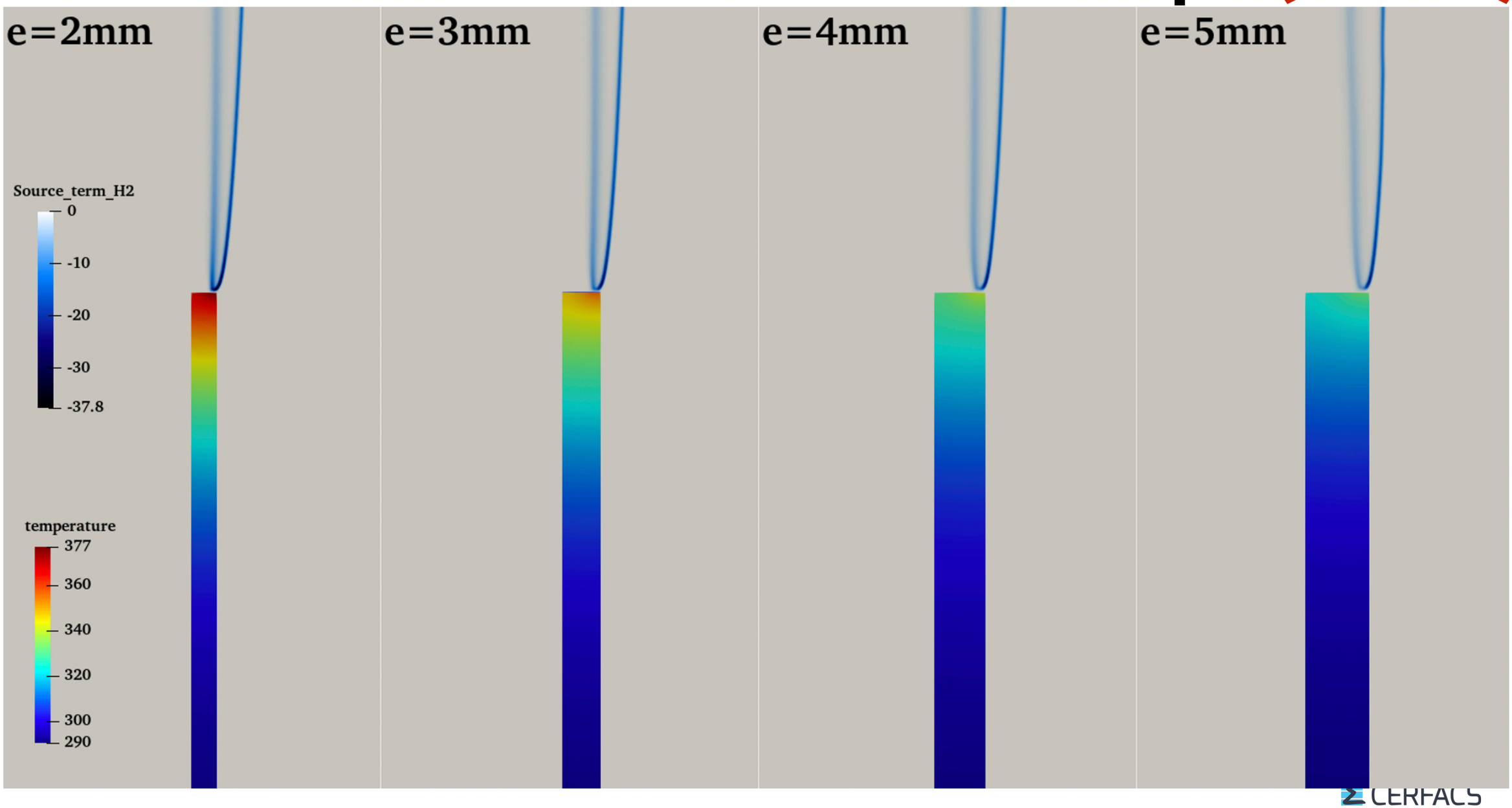


T-Tadia (heat loss)

Bertsch et al, 40th Symp. Comb.

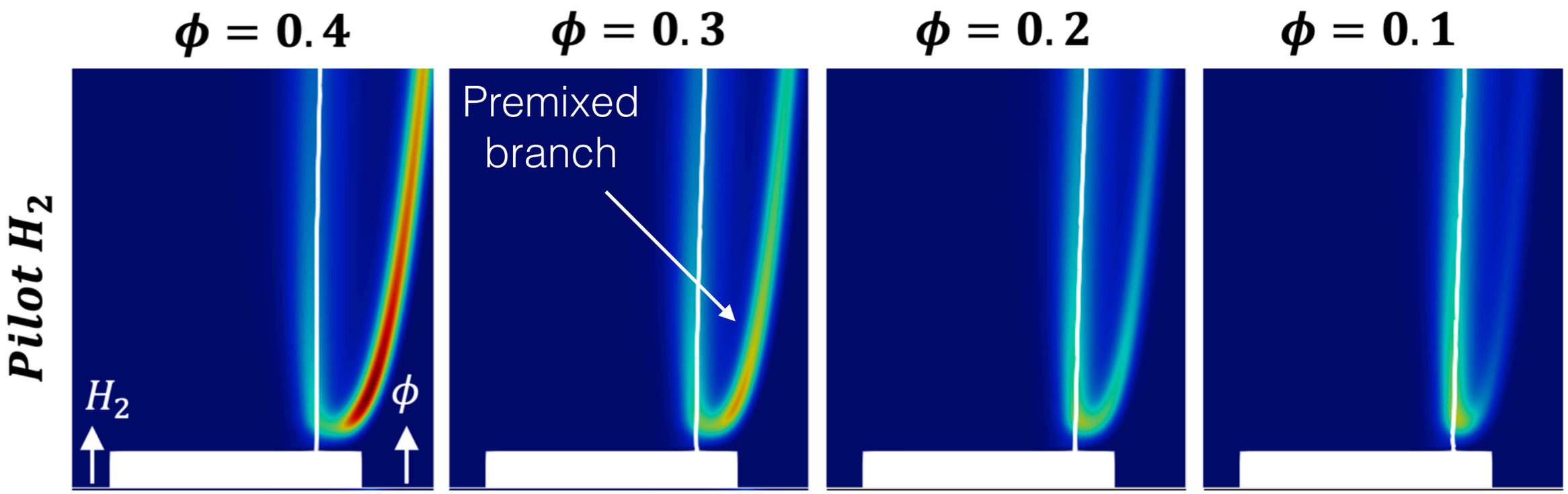
FULL CHT OF 'RIM-STABILIZED EDGE FLAMES:



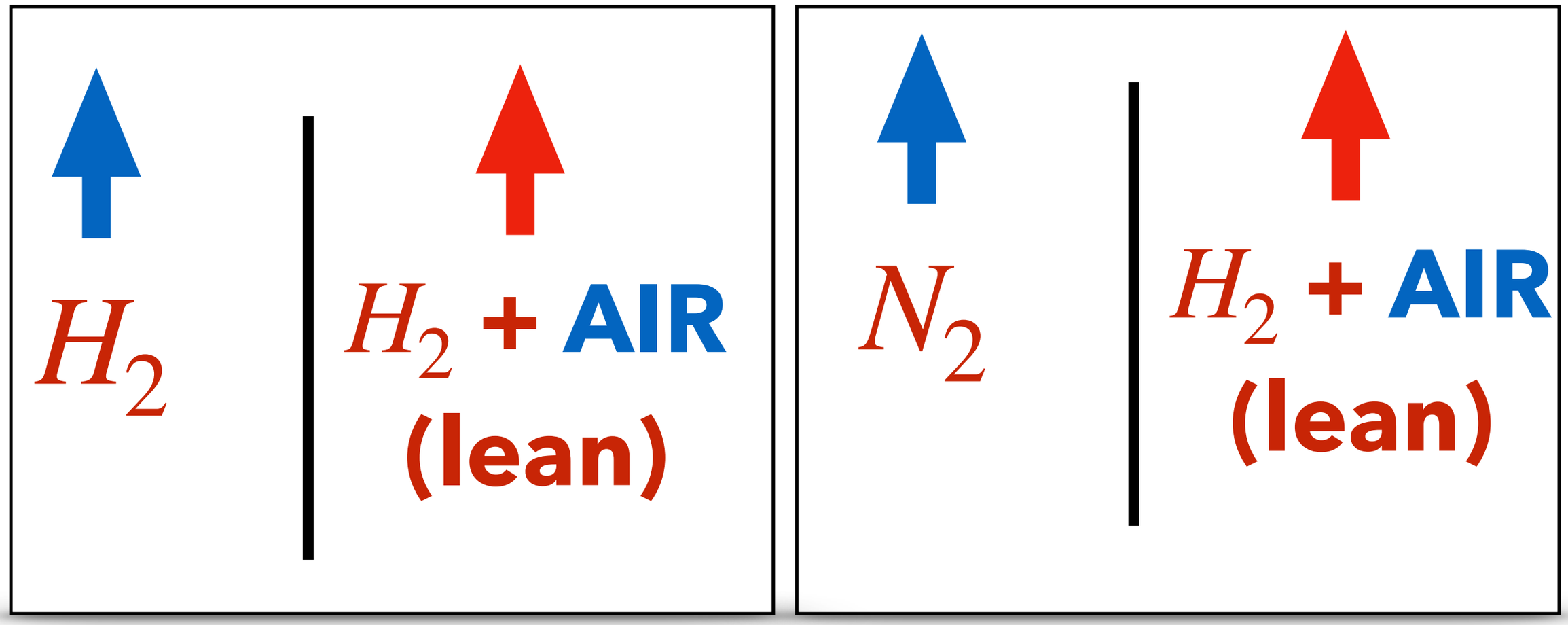


CERFACS

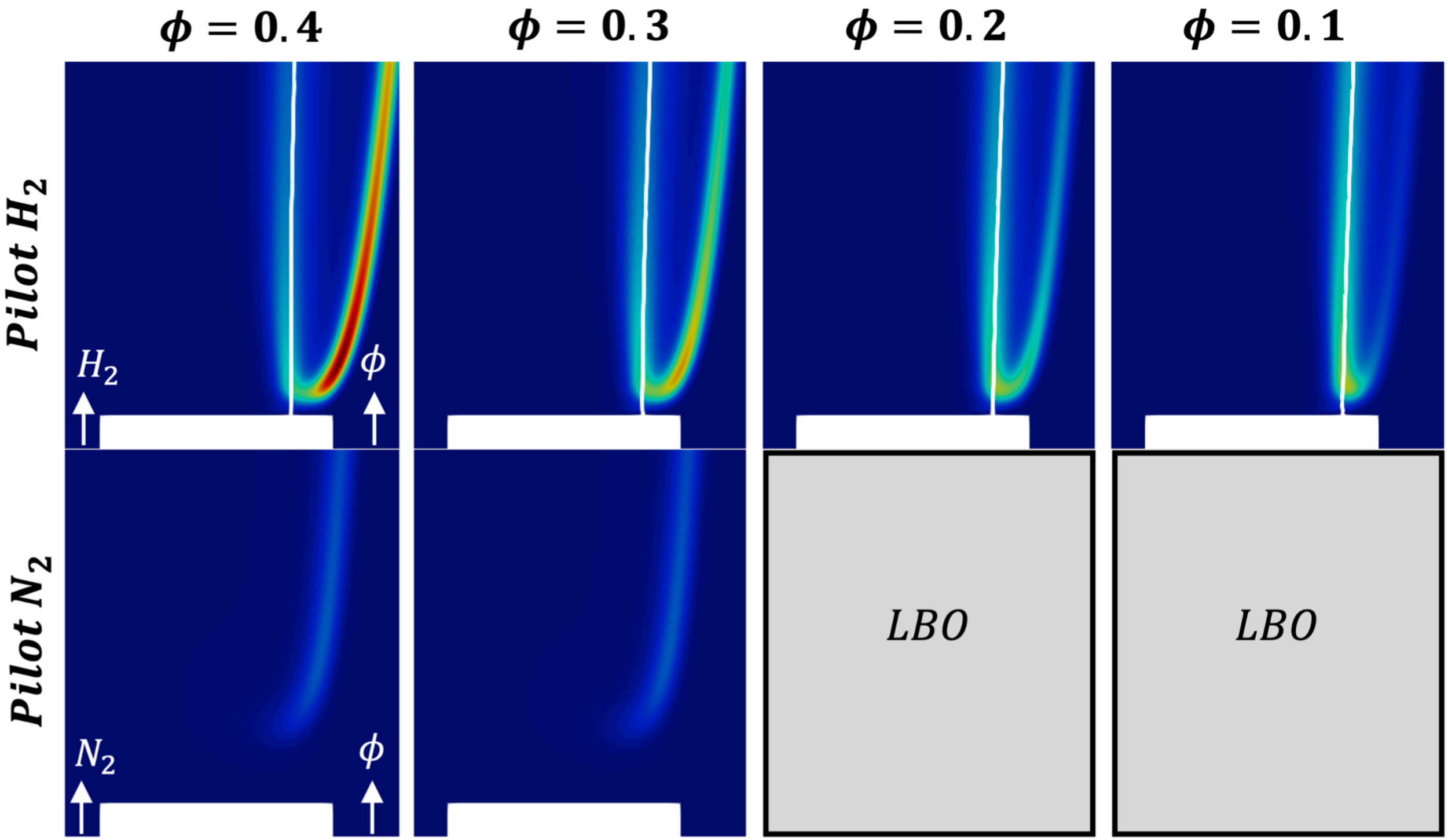
THE STRUCTURE OF THESE RIM STABILIZED EDGE FLAMES DEPENDS ON THE EQUIVALENCE RATIO OF THE PREMIXED BRANCH



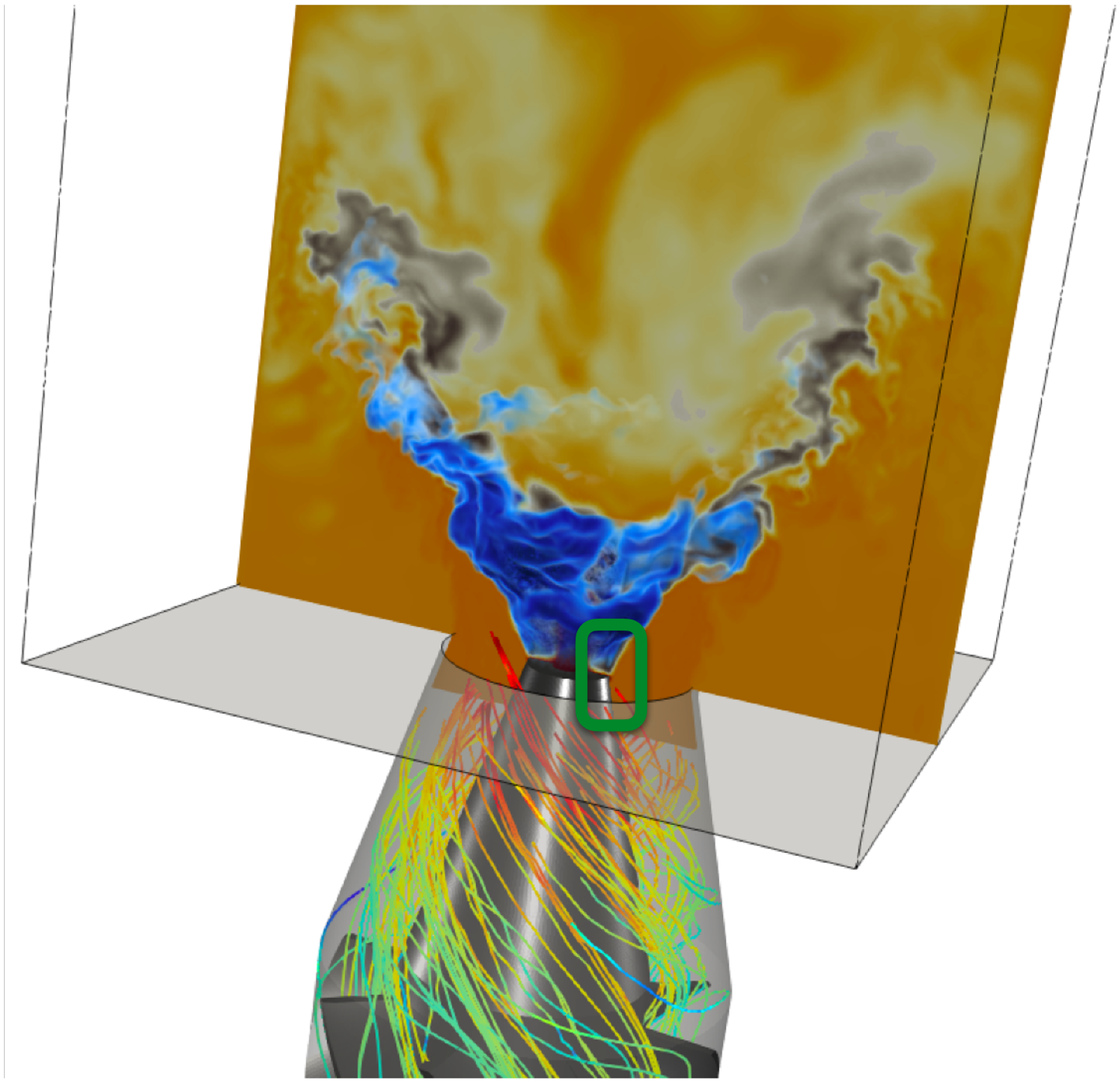
AND THE PURE INJECTION OF H2 HELPS TO STABILIZE THE PREMIXED BRANCH: COMPARING H2 WITH N2 INJECTION IN THE LEFT STREAM

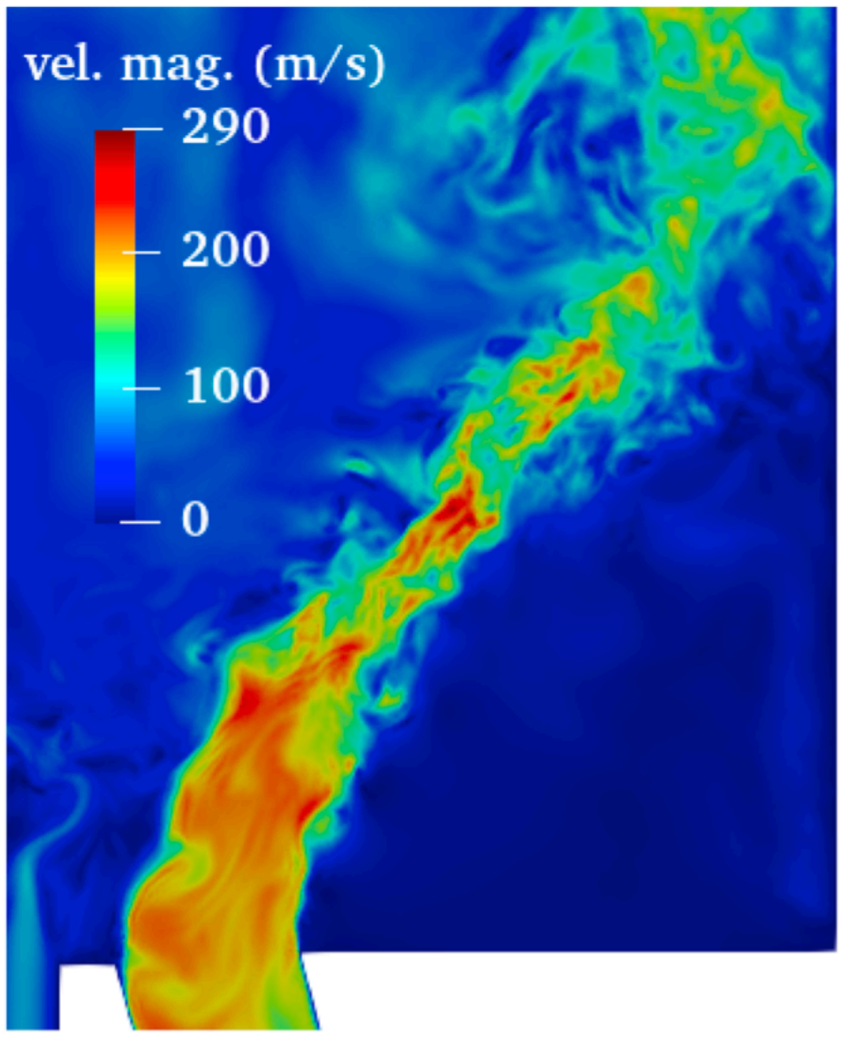


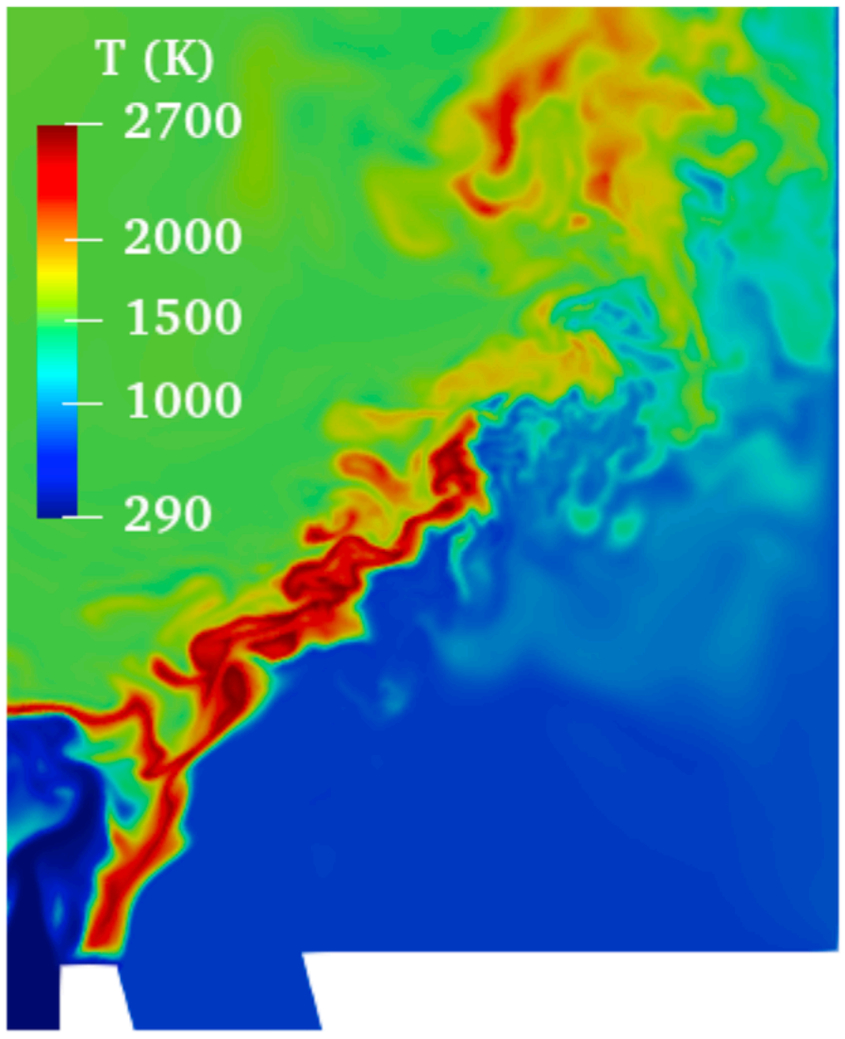
GOING TO N2, THE PREMIXED BRANCH QUENCHES BELOW PHI=0.25, CAUSING LEAN BLOW OFF (LBO)

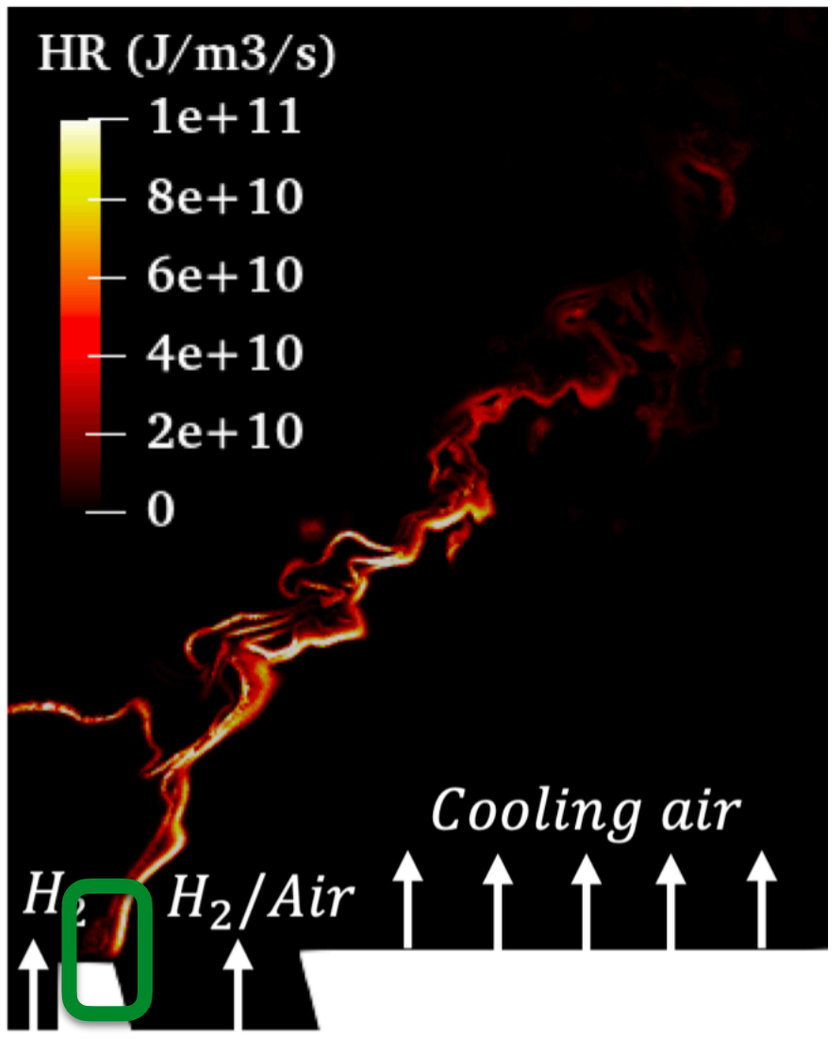


Does LES see these flames ?




vel. mag. (m/s)
290
200
100
0


T (K)
2700
2000
1500
1000
290


HR (J/m3/s)
1e+11
8e+10
6e+10
4e+10
2e+10
0
Cooling air
H_2/Air

CONCLUSIONS

- We must re-design most combustion chambers for H2 flames. Simulations will be essential

- 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…