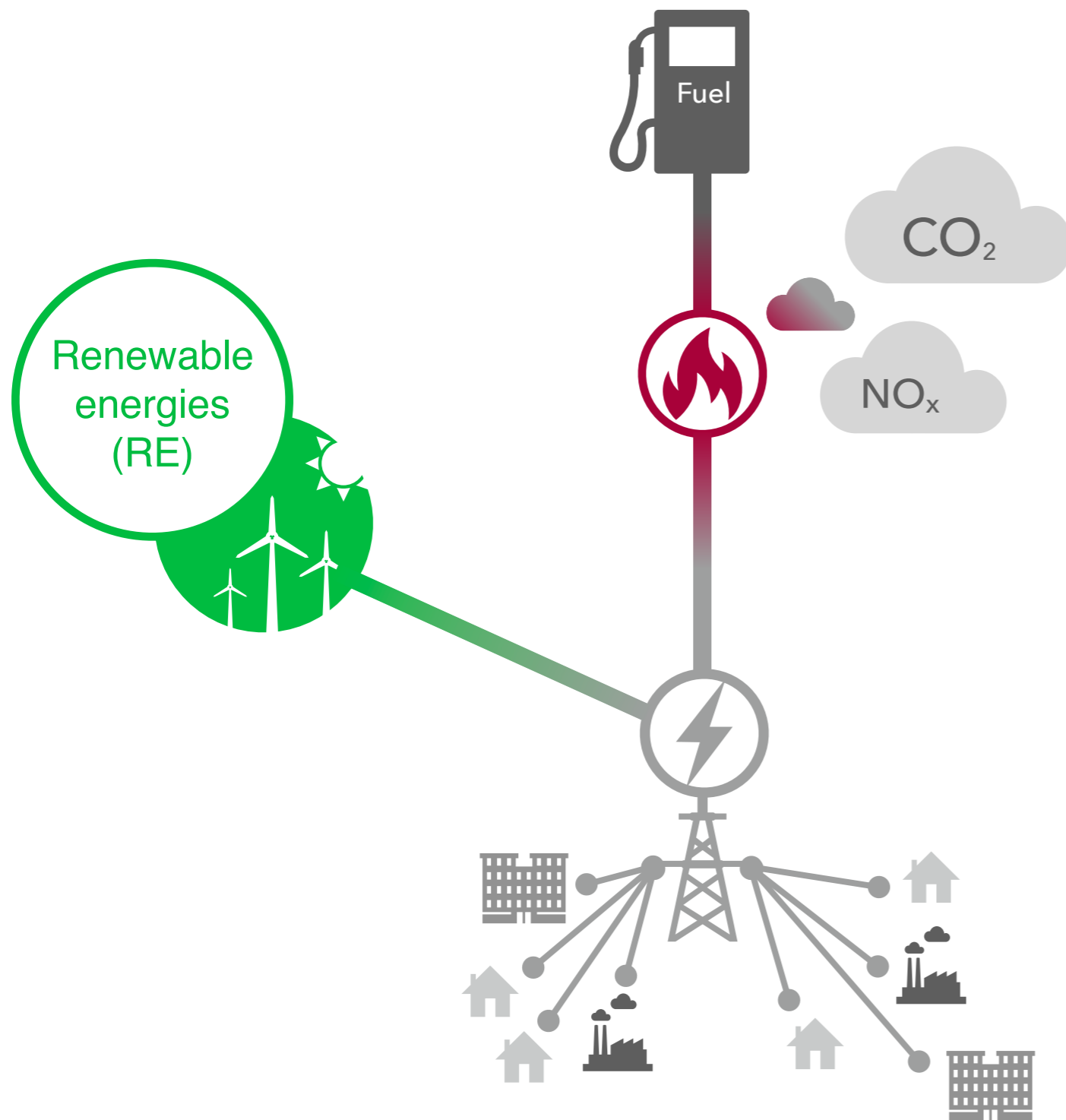


Flashback prevention in a micro Gas Turbine fueled by hydrogen without any combustor redesign

Alessio Pappa
Laurent Bricteux
Ward De Paepe

ERCOFTAC Autumn Festival 2023

12th October 2023

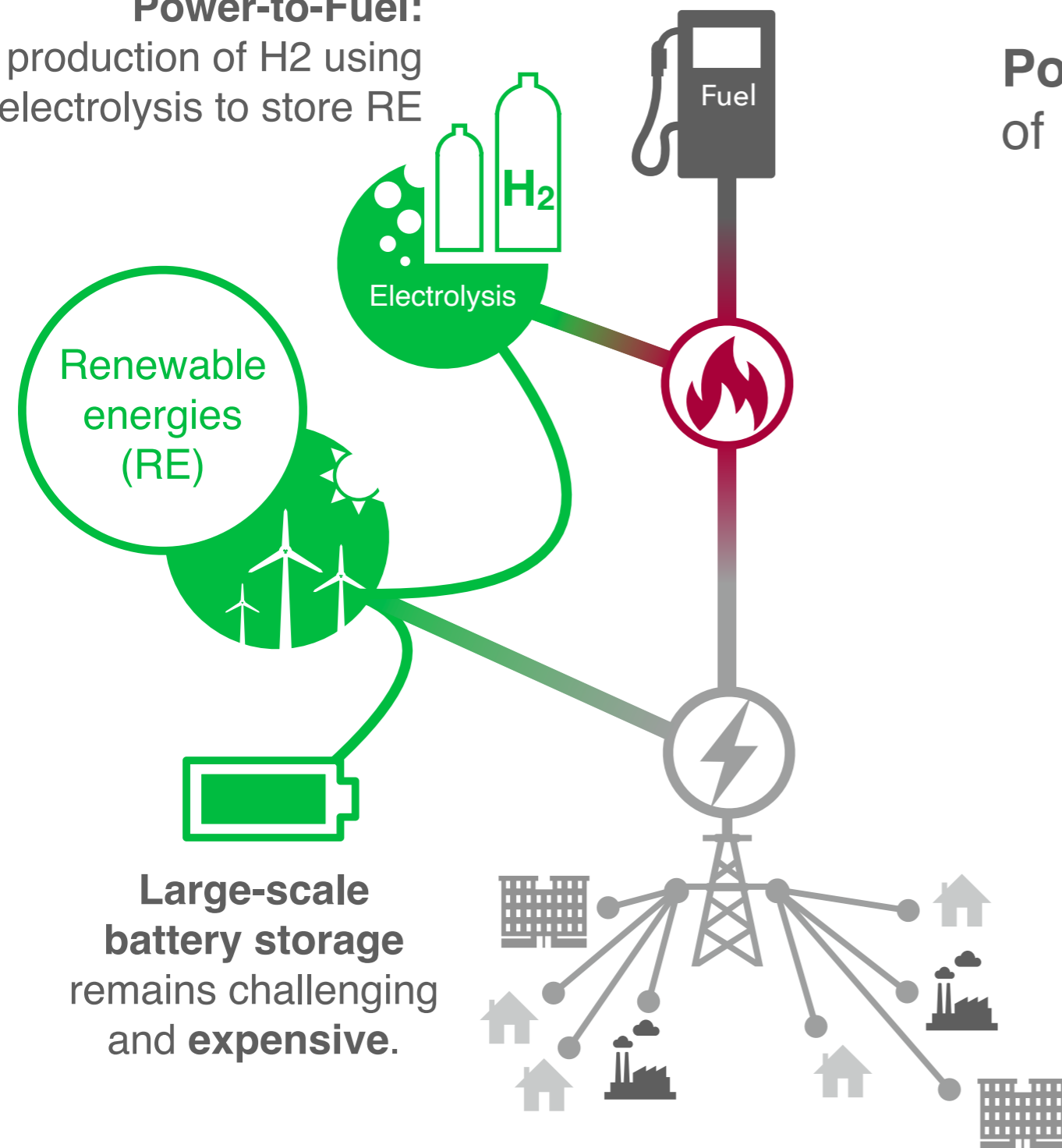


Combustion processes
inherent to
pollutant emissions.

Increased RE contribution
in electricity production
to **reduce CO₂** levels.

Fuel flexibility in micro Gas Turbines towards decarbonification

Power-to-Fuel:
production of H₂ using
electrolysis to store RE



Power-to-fuel to overcome fluctuations of RE (despite their lack of reliability). Unpredictable nature of RE sources.

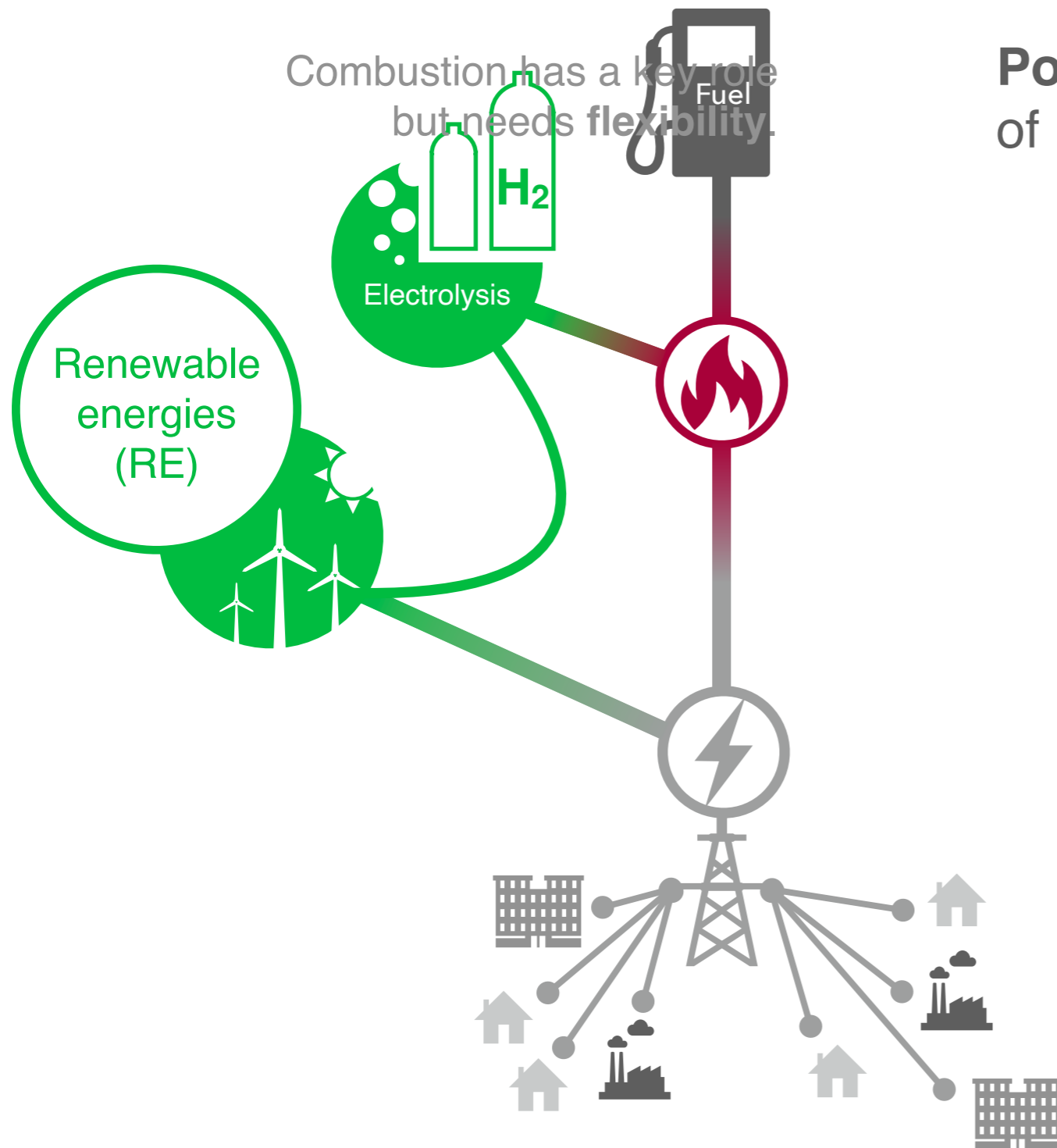
➔ **Fluctuations**

Strong trend towards
storing the excess of
renewable electricity

Fuel flexibility in micro Gas Turbines towards decarbonification

Combustion has a key role but needs flexibility.

Power-to-fuel to facilitate the incursion of RE (intermittent behavior).

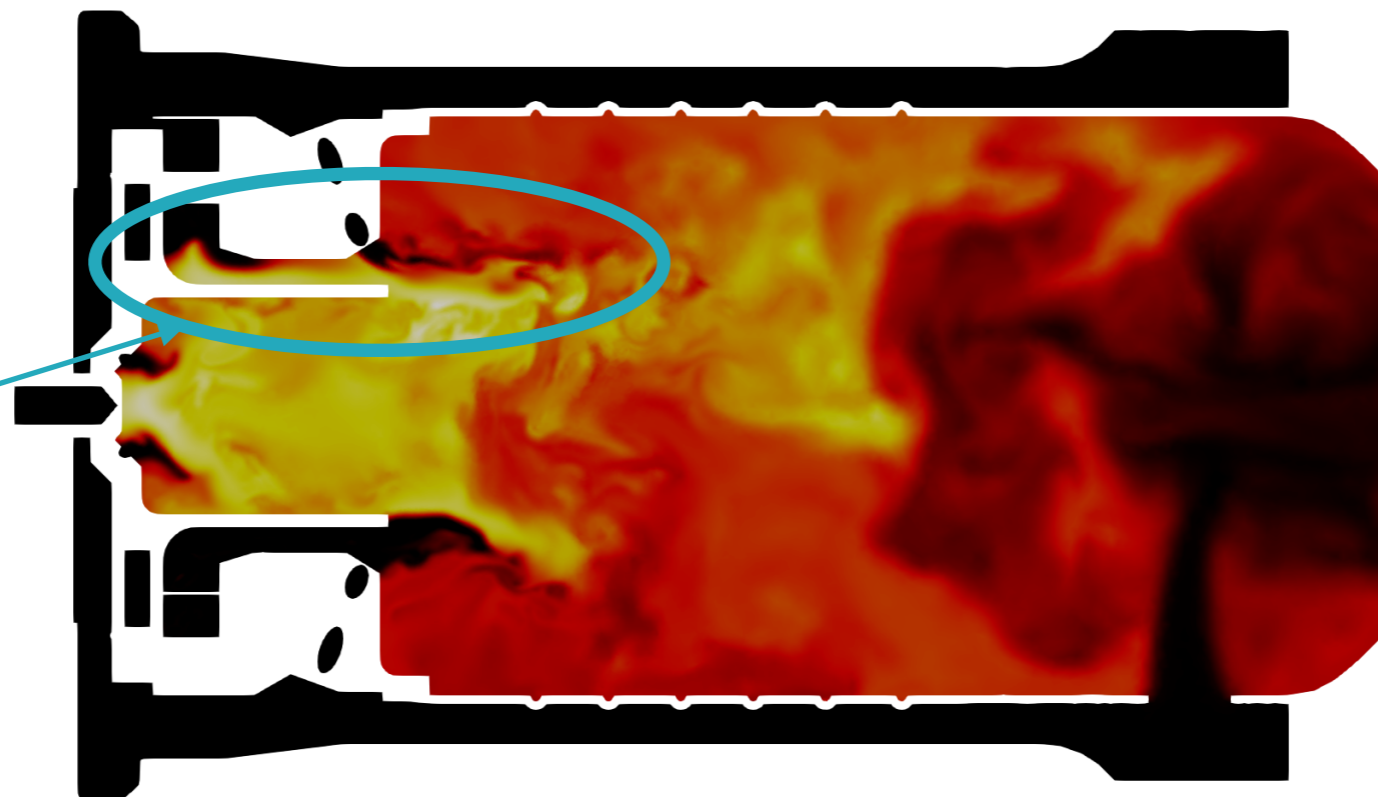


Fuel flexibility in micro Gas Turbines towards decarbonification

Power-to-fuel to facilitate the incursion of RE (intermittent behavior).

Premixed burners not adapted to burn hydrogen blends.

Hydrogen combustion leads to flame instabilities (risk of **flashback**).



Flame front going back in the fuel/air premixing room

Fuel flexibility in micro Gas Turbines towards decarbonification

Power-to-fuel to facilitate the incursion of RE (despite their lack of reliability).

Hydrogen combustion leads to flame instabilities (risk of **flashback**).

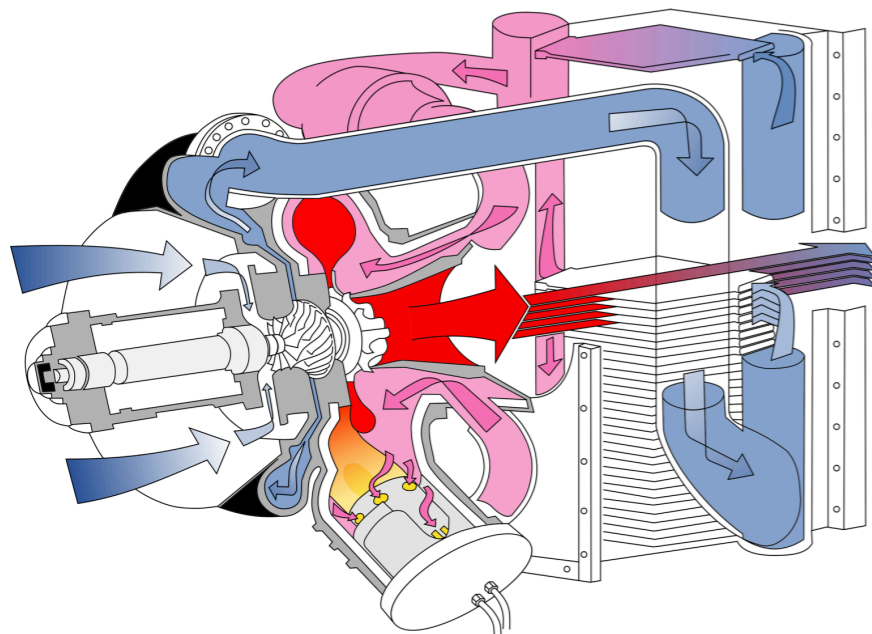
Using diluted conditions from **existing** advanced cycles.

For more flexibility, stabilization achieved **without any redesign** of the combustor.



Humidification & EGR to slow down the reaction rate, temperature & flame speed.

mGTs have a large field of application for small-scale CHP production

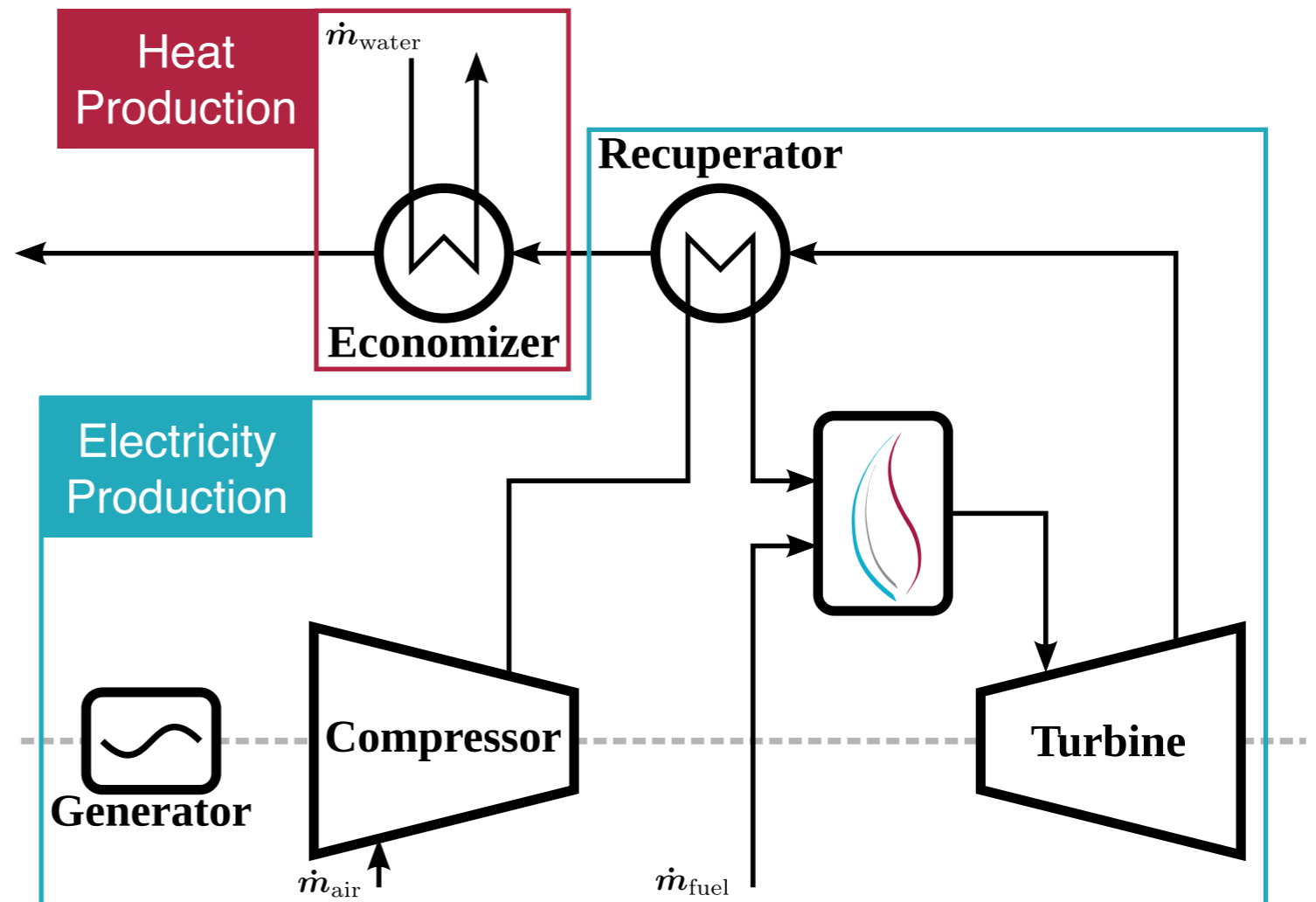


Sketch of Turbec T100

Global efficiency: ~80%
Electrical efficiency: ~30%

Micro Gas Turbines for small-scale
Combined Heat and Power (CHP)
production.

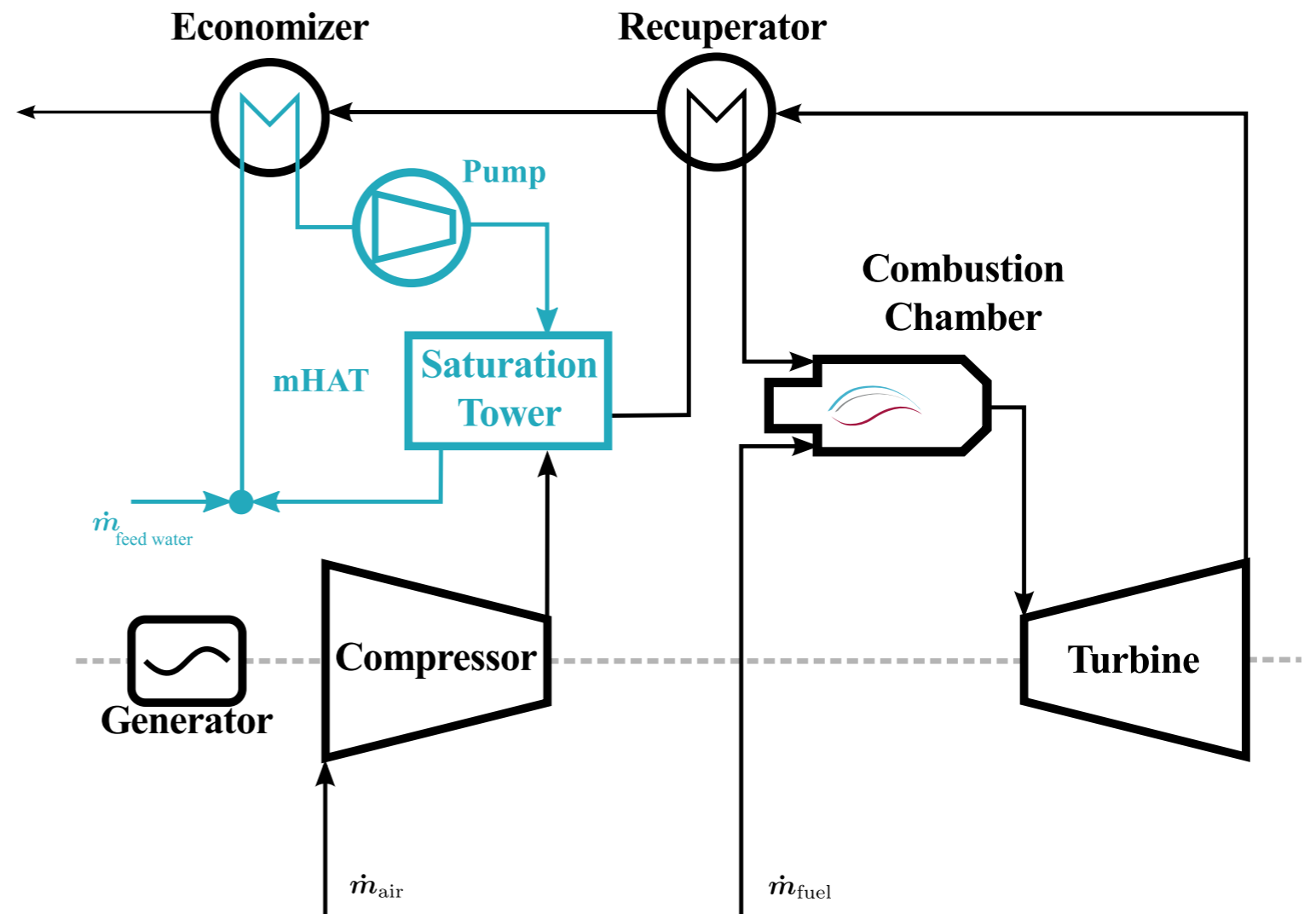
Net heat and electrical production
ranging from 1kW up to a few 100kW



Taking benefit of existing advanced cycle modifications to avoid flashback

Allows advanced cycle modifications:

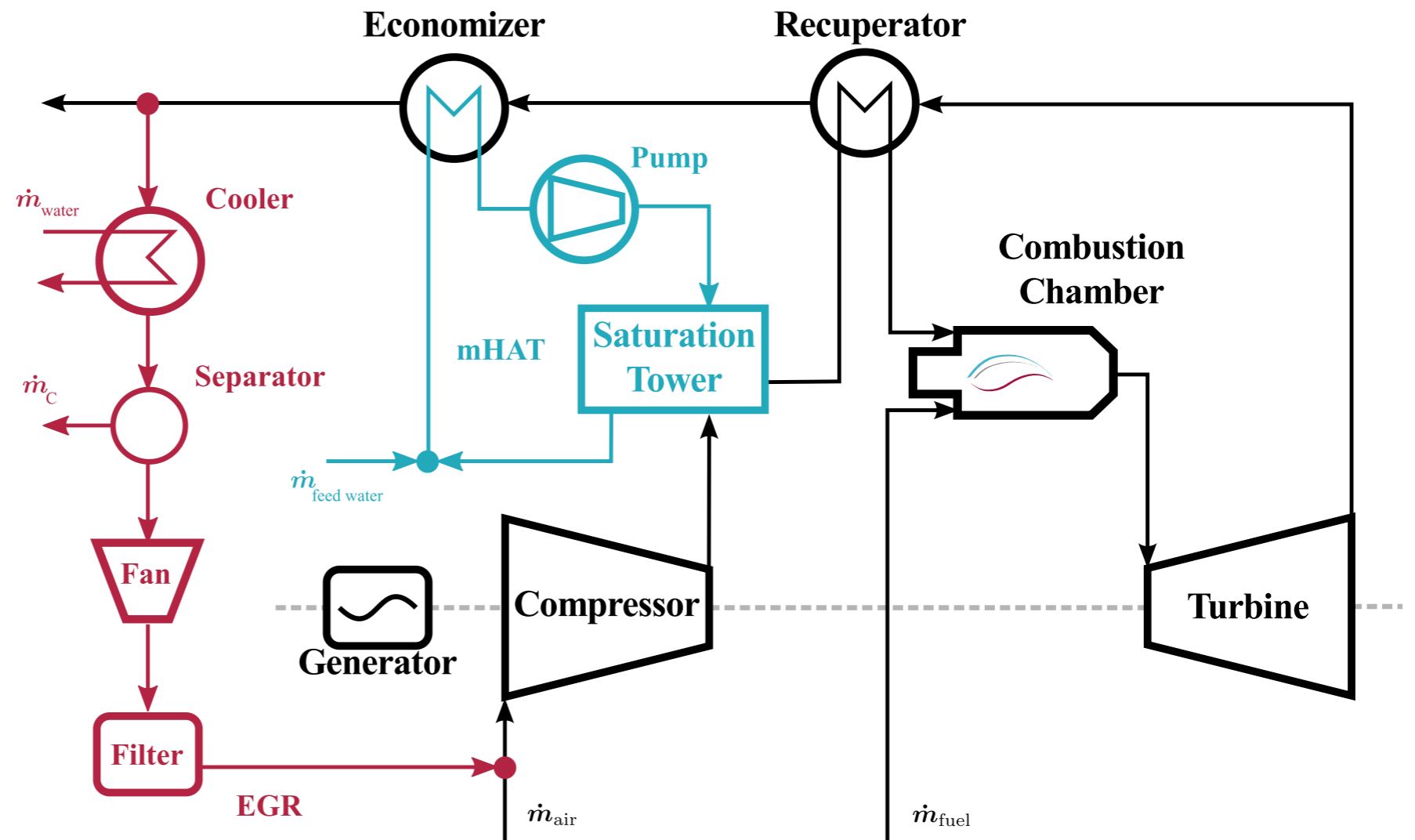
- ➔ **Humidification:** decoupling heat & electricity for increased electrical efficiency (when there is no heat demand).



Taking benefit of existing advanced cycle modifications to avoid flashback

Allows advanced cycle modifications:

- ➔ **Humidification:** decoupling heat & electricity for increased electrical efficiency (when there is no heat demand).
- ➔ **Exhaust Gas Recirculation (EGR)** for CO₂ reduction & performing Carbon Capture & Storage.



These diluted conditions have proven effective in reducing reaction rate, temperature, and flame speed.

Target

Flashback prevention for various H₂ blends without any redesign of a mGT combustor.

Considering humidification & EGR as solution.

1) 0D Chemical Reactor Network /1D Flame model.

- Low-cost chem & thermo flow properties assessment.
- Predetermination of the operating conditions to avoid flashback.

2) Large Eddy Simulations on the Turbec T100 geometry.

- Flashback phenomenology.
- Verification of the low-cost predetermination.
- Stability analysis.

Target

**Flashback prevention for various H₂ blends
without any redesign of a mGT combustor.**

Considering humidification & EGR as solution.

Outline

**Burner layout &
operating conditions**

Large-Eddy Simulations

Conclusions

Target

Flashback prevention for various H₂ blends without any redesign of a mGT combustor.

Considering humidification & EGR as solution.

Outline

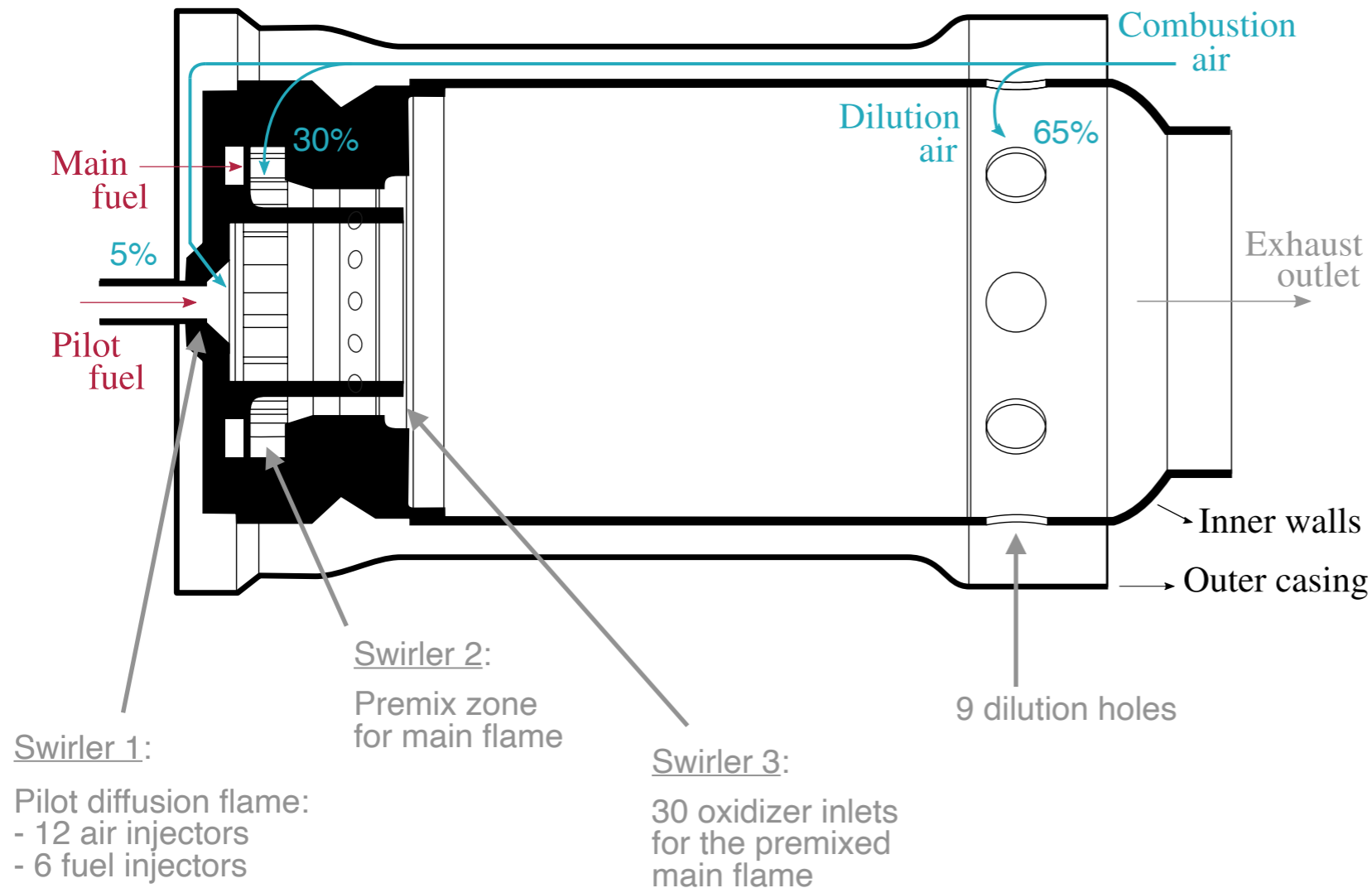
Burner layout & operating conditions

- mGT burner description
- 0D/1D hybrid model
- Optimized operating conditions

Large-Eddy Simulations

Conclusions

The combustor layout of the Turbec T100 mGT is a reverse (or counter-current) flow can burner.



Nominal conditions:

$$P_{th} = 333 \text{ kW}_{th}$$

$$\dot{m}_{air} = 800 \text{ g/s}$$

$$p = 4 \text{ bar}$$

$$T_{air,in} = 865 \text{ K}$$

$$T_{f,in} = 300 \text{ K}$$

For REF case (100% CH₄):

$$\phi_{global} \sim 0.14$$

$$\phi_{local,main} \sim 0.41$$

**Mainly premixed burner:
not adapted to H₂ combustion**

0D CRN to emulate the burner behavior using Perfectly Stirred Reactors.

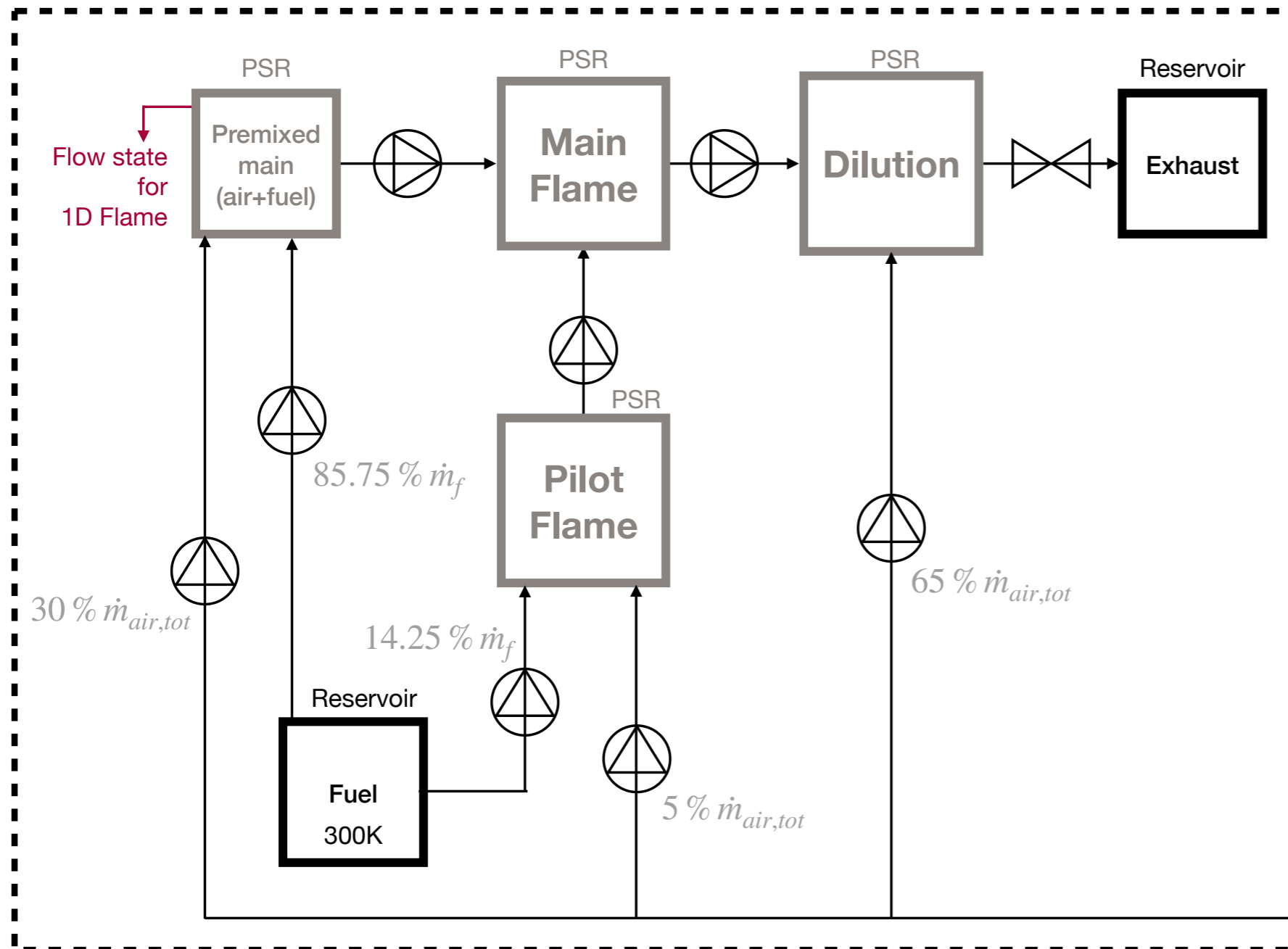
1D Flame to compute the flame speed.

Detailed Chemical Reactor Network model: humidification & EGR emulation

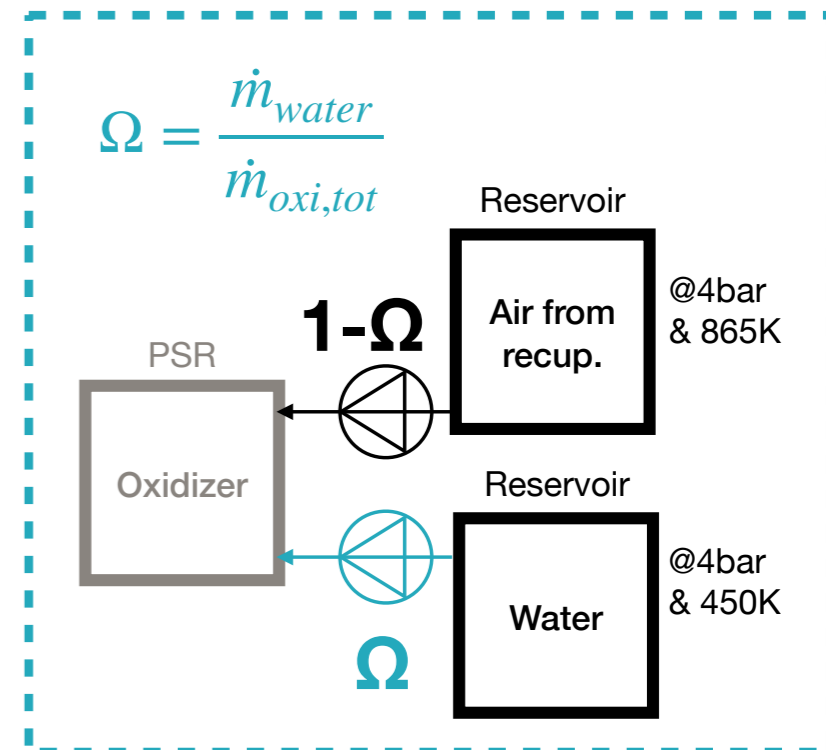
$\Omega?$ *EGR?*

$$S_{l,X_{H_2}} \simeq S_{l,ref}$$

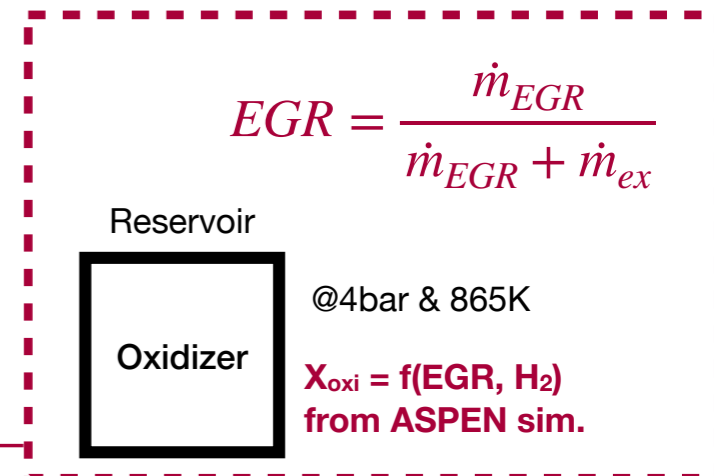
Turbec T100 combustor



Humidification

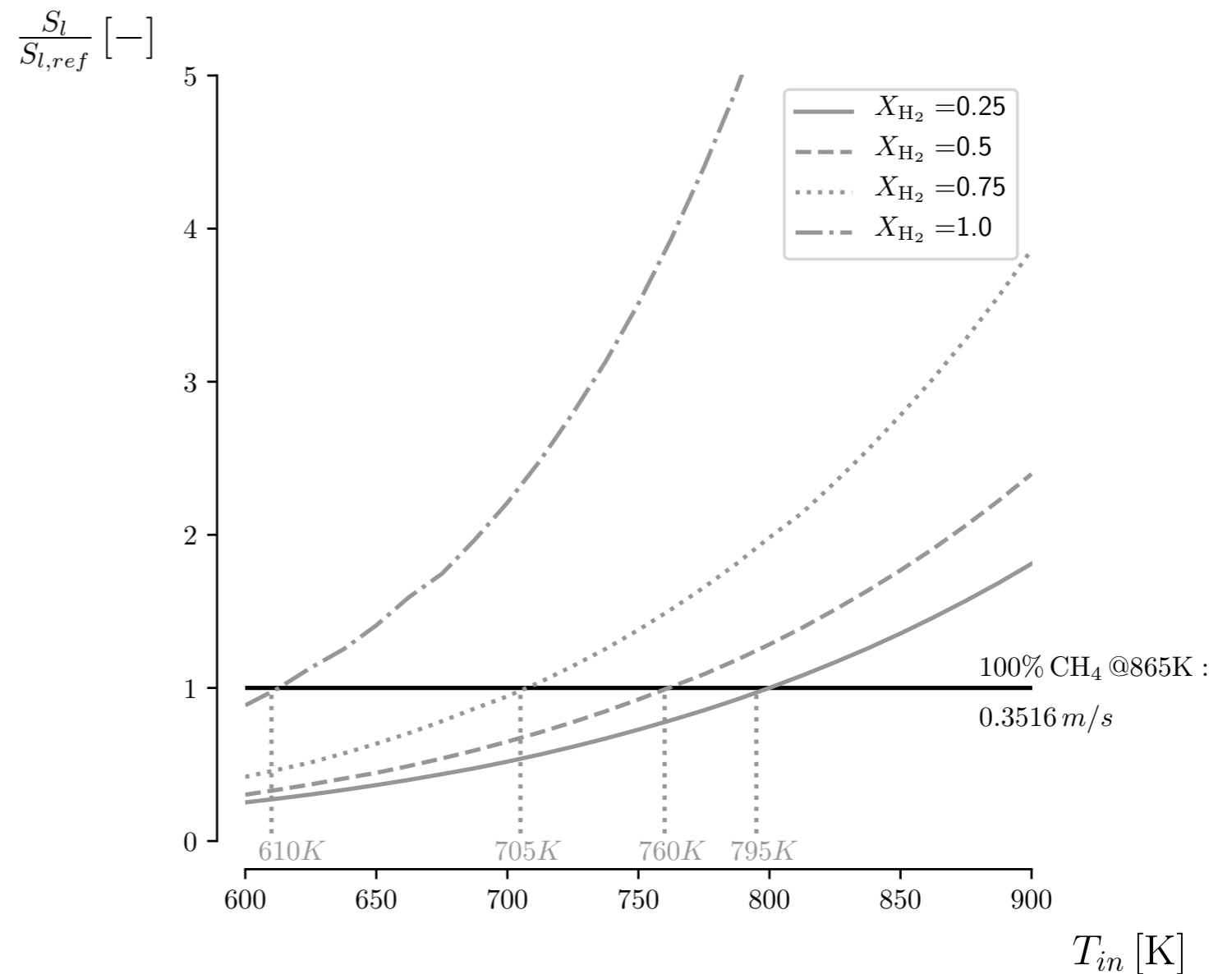


Exhaust Gas Recirculation

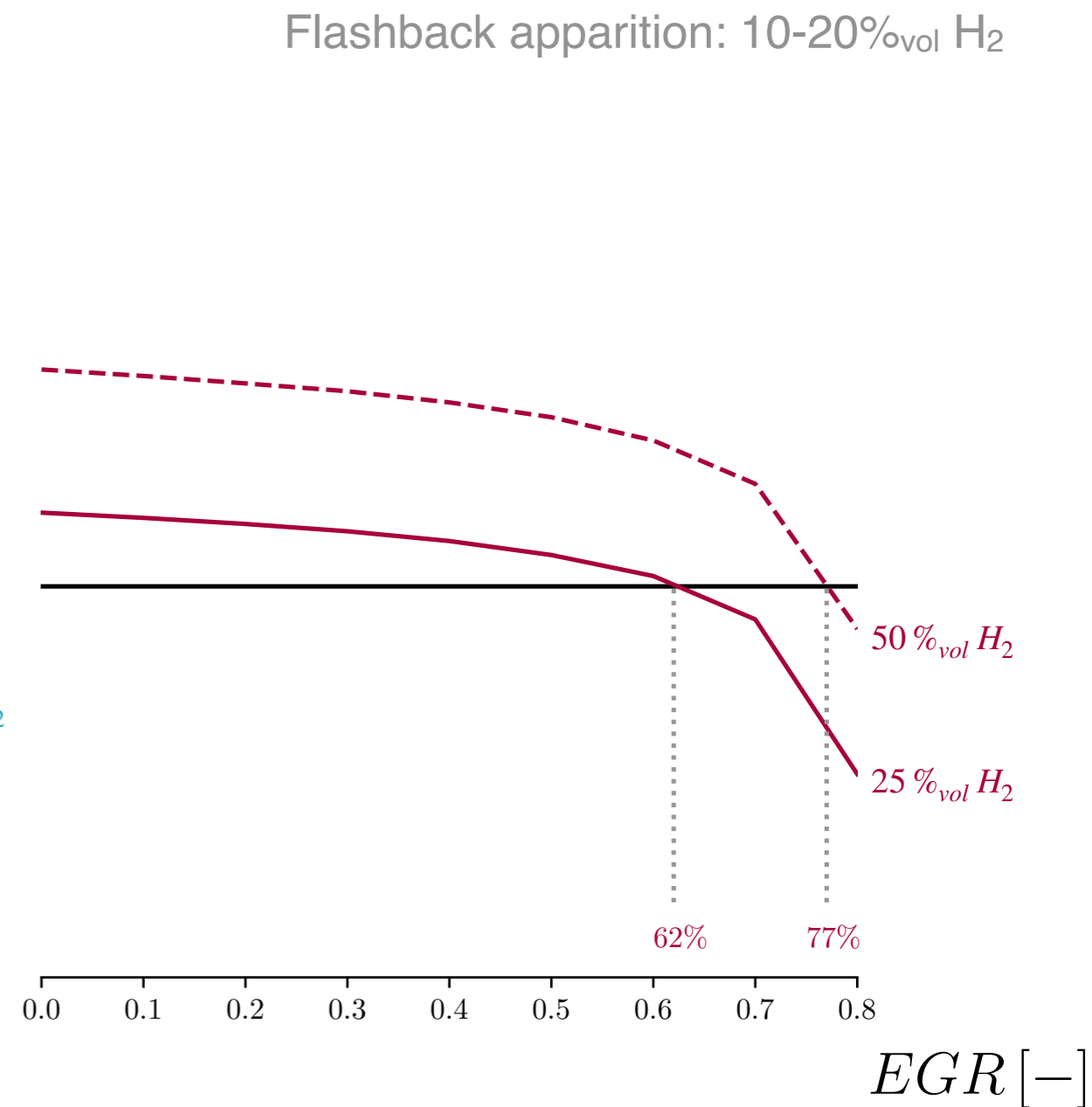
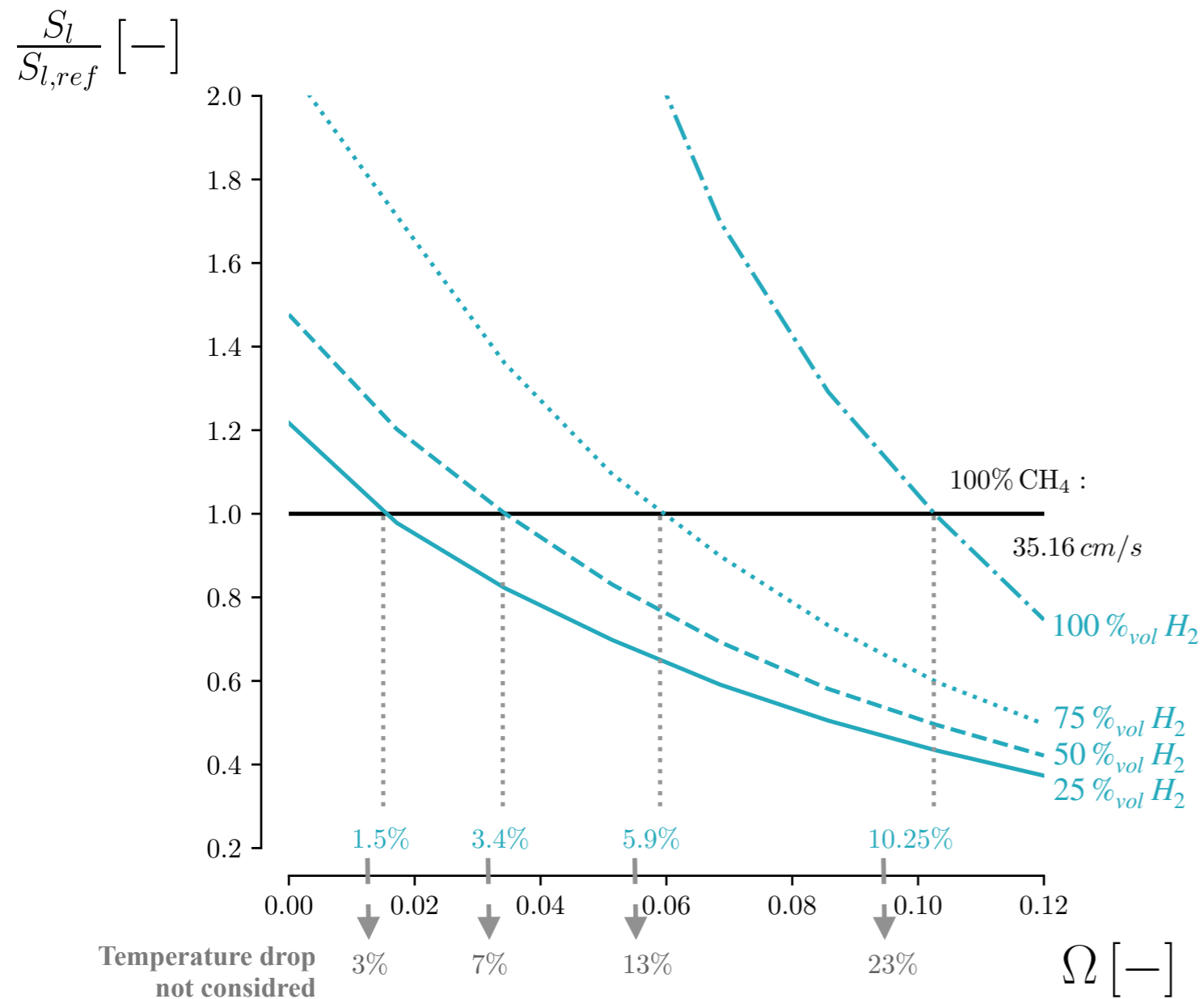


Inlet temperature has an important impact on the laminar flame speed

Burning up to **100% H₂** requires to **decrease** the inlet temperature **down to 610K**.



0D CRN/1D Flame on various H₂ blends: comparison humidification & EGR



Considered cases for the LES simulations

Case	Fuel composition	Dilution	Operating conditions
Ref	100 % _{vol} CH ₄	-	Turbec T100 nom. cdt
FB	50 % _{vol} CH ₄ / 50 % _{vol} H ₂	-	Turbec T100 nom. cdt
50H ₂ LT	50 % _{vol} CH ₄ / 50 % _{vol} H ₂	-	Lower premix temp. (760K)
50H ₂ Ω	50 % _{vol} CH ₄ / 50 % _{vol} H ₂	Ω = 3.4 %	Turbec T100 nom. cdt
50H ₂ EGR	50 % _{vol} CH ₄ / 50 % _{vol} H ₂	EGR = 77 %	Turbec T100 nom. cdt
100H ₂ Ω	100 % _{vol} H ₂	Ω = 10.25 %	Turbec T100 nom. cdt

Target

Flashback prevention for various H₂ blends without any redesign of a mGT combustor.

Considering humidification & EGR as solution.

Outline

**Burner layout &
operating conditions**

Large-Eddy Simulations

- Numerical set-up
- Flashback phenomenology
- Stability analysis

Conclusions

Numerical set-up of the LES

CFD code: YALES2

Solver: Variable Density (Low-Mach N-S eq.)

Sub-grid scale stresses model:

Dynamic Smagorinsky

$Re = 37500$ $y^+ = 38$ (in the main swirler)

Wall model: Classical log-law

Heat losses: Adiabatic wall condition

Complex chemistry

+ reduced kinetic scheme: DRM19

21 species - 84 reactions

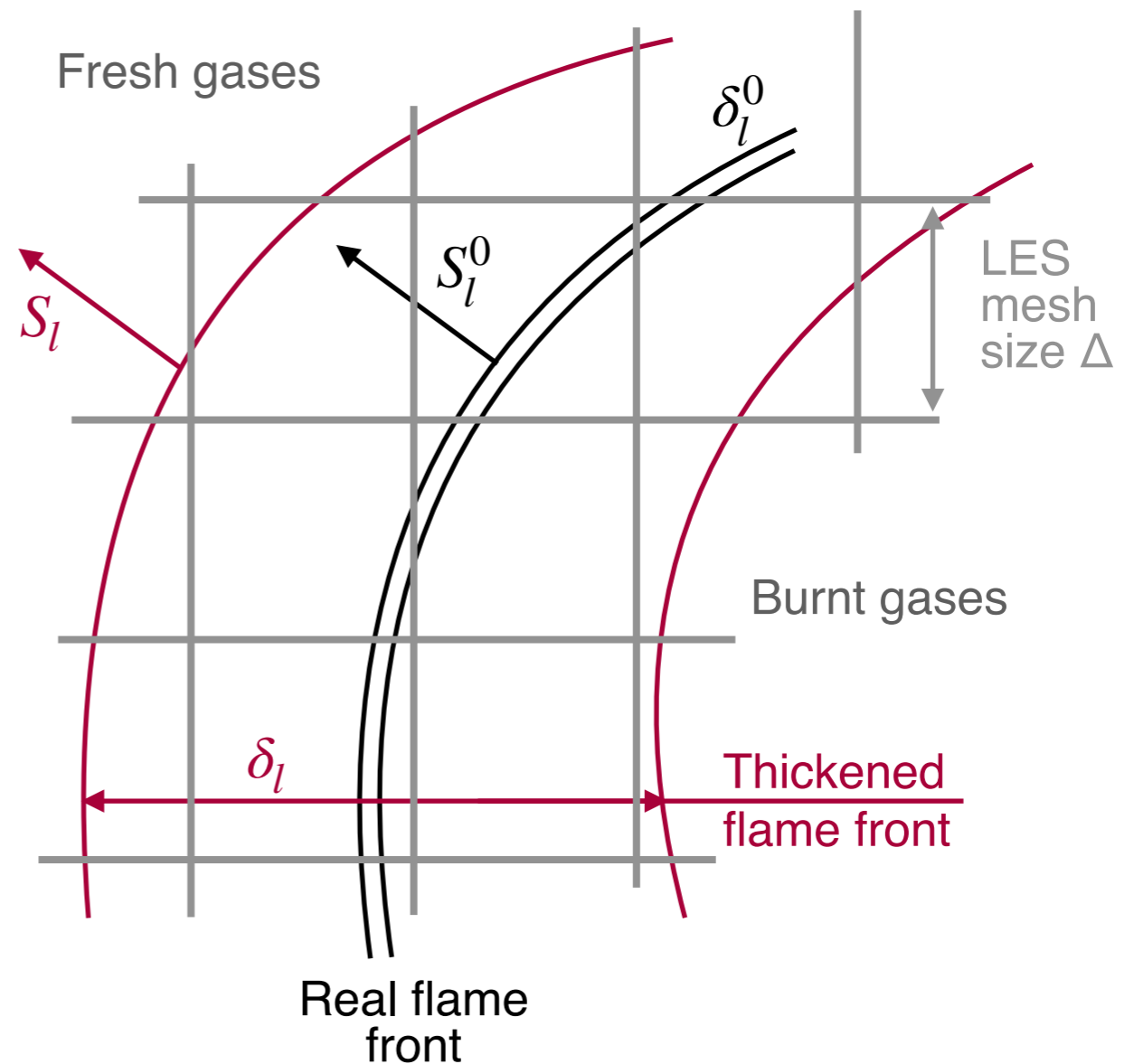
Combustion model: DTFLES

The DTFLES model artificially thicken the flame front without modifying the flow dynamic

$$\Delta > \delta_l^0$$

Flame front thickened of a factor F

Efficiency E function to compensate the surface reduction & avoid wrinkling issues

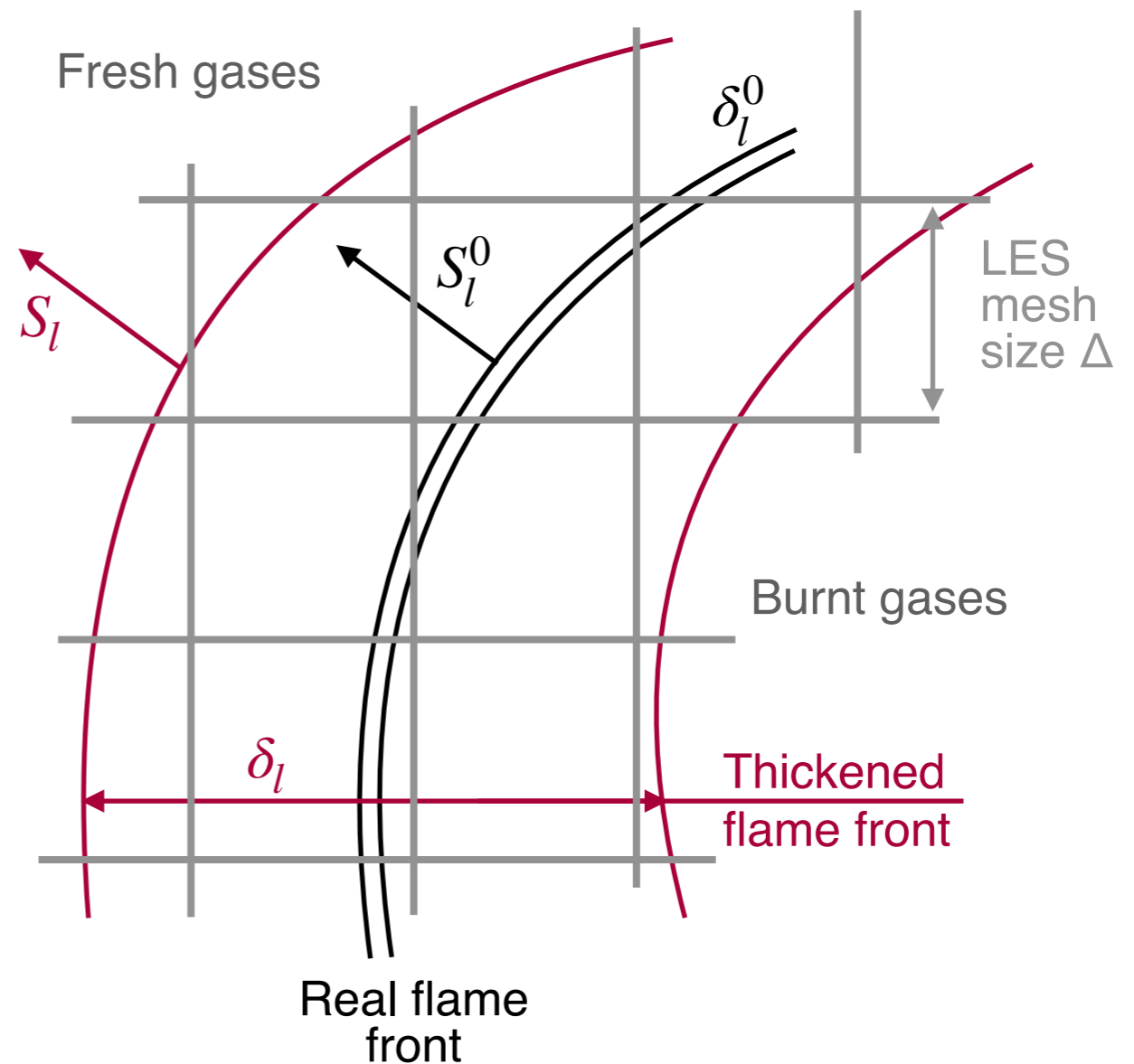


The DTFLES model artificially thicken the flame front without modifying the flow dynamic

Dynamic formulation of the TFLES model to handle **premixed** and **non-premixed** flames:

F is not constant on the domain.

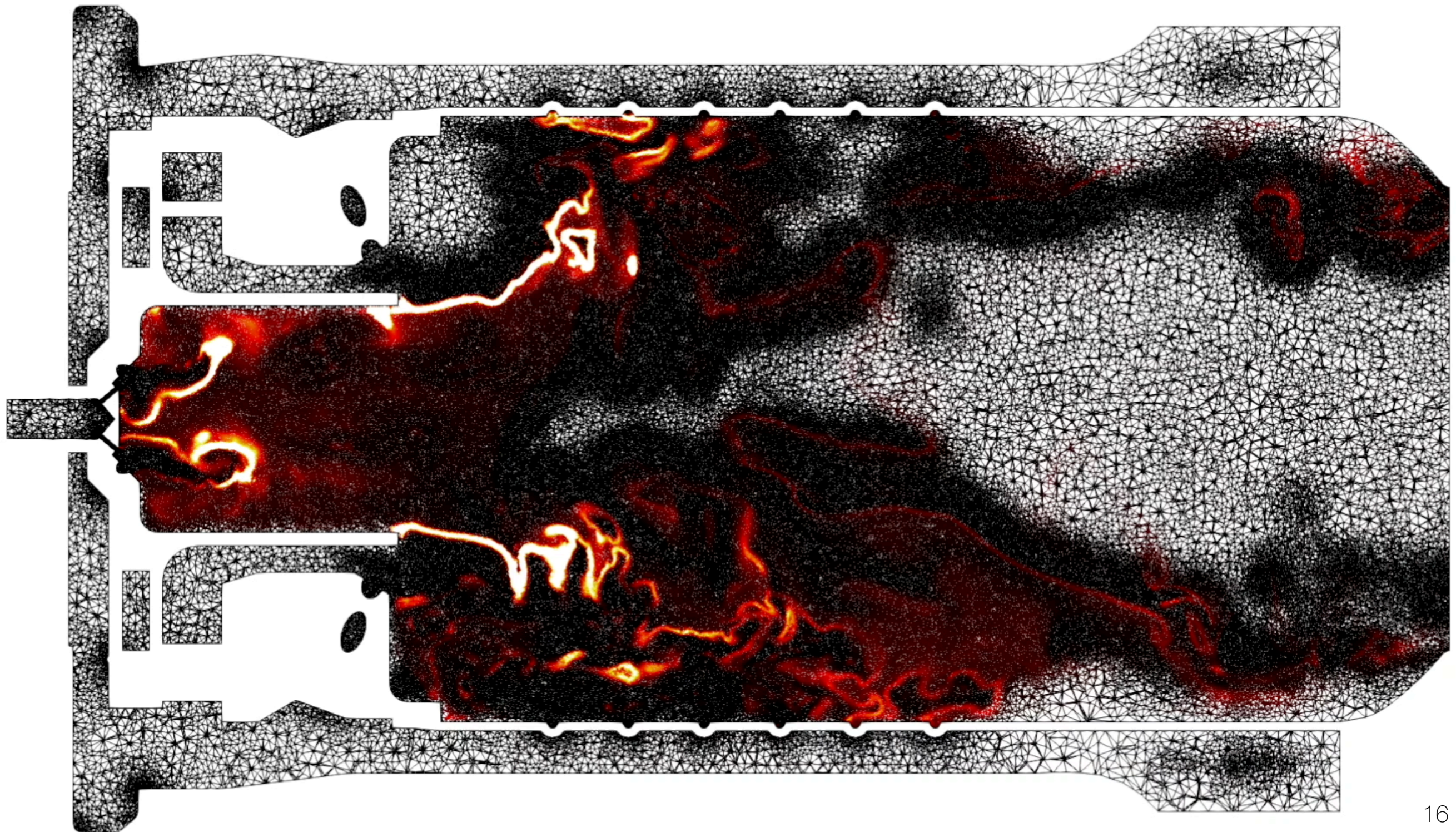
Flame sensor (reaction rate) to detect where the reaction takes place.



Dynamic Adaptive Mesh Refinement performed to capture the flame front

Dynamic AMR
 $\pm 80 \cdot 10^6$ cells
 $\Delta_{\min} = 0.7\text{mm}$
 $\Delta_{\max} = 3\text{mm}$

Cost: 1-10% total CPU load



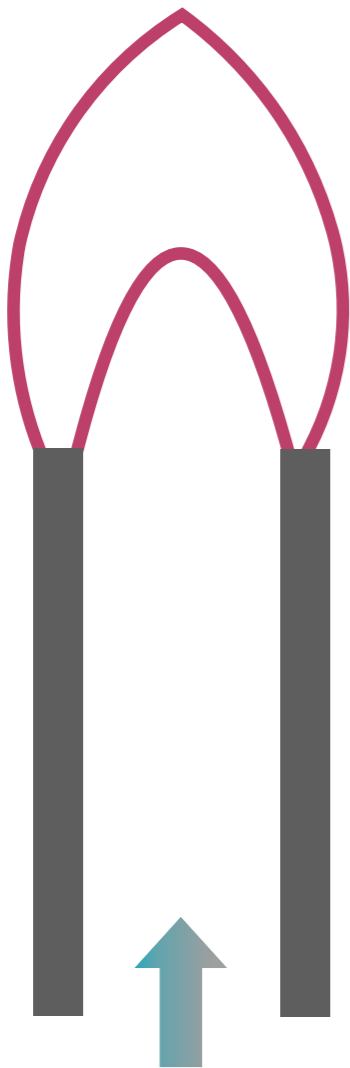
Stability analysis, allowed by LES, shows
no flashback for 50%_{vol} H₂ — $\Omega=3.4\%$

CPU cost: ~ 576k CPUh
(~ 25sim x 24h x 960CPU)
on Zenobe



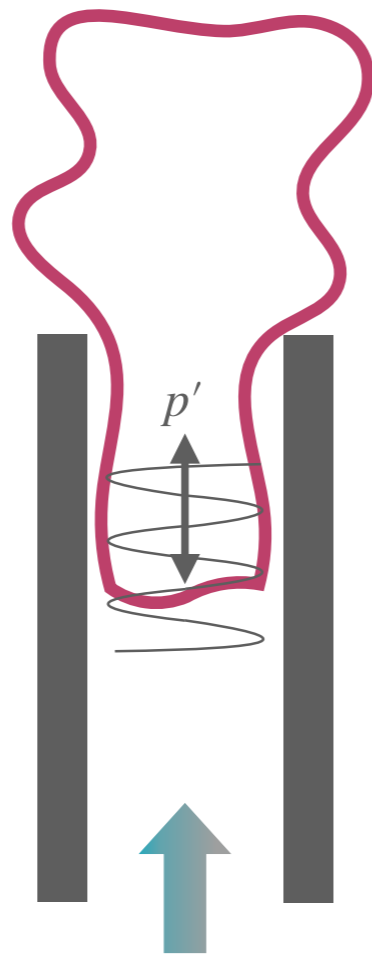
Flashback phenomenology: three distinctive mechanisms of fast upstream traveling of the flame front

Normal combustion



Air-fuel premix

Thermo-acoustic
flashback



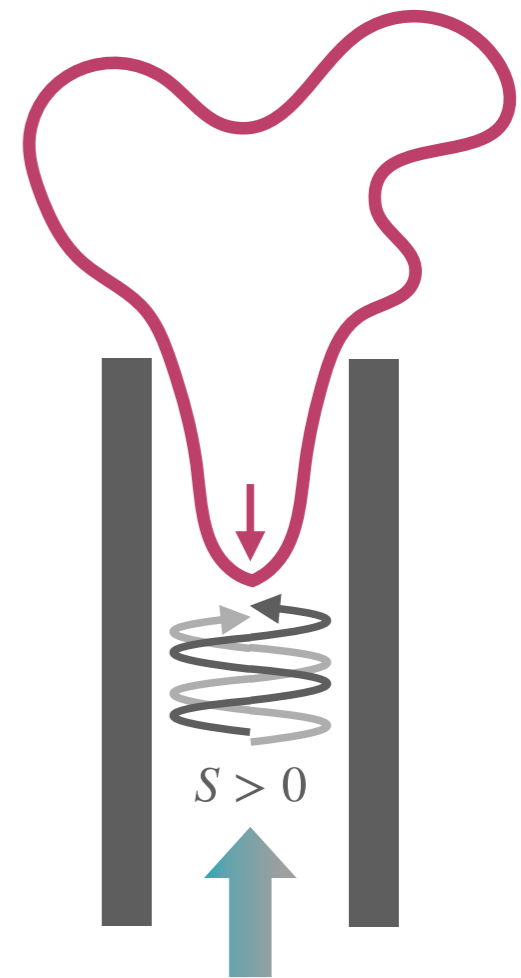
Air-fuel premix

Boundary layer
flashback



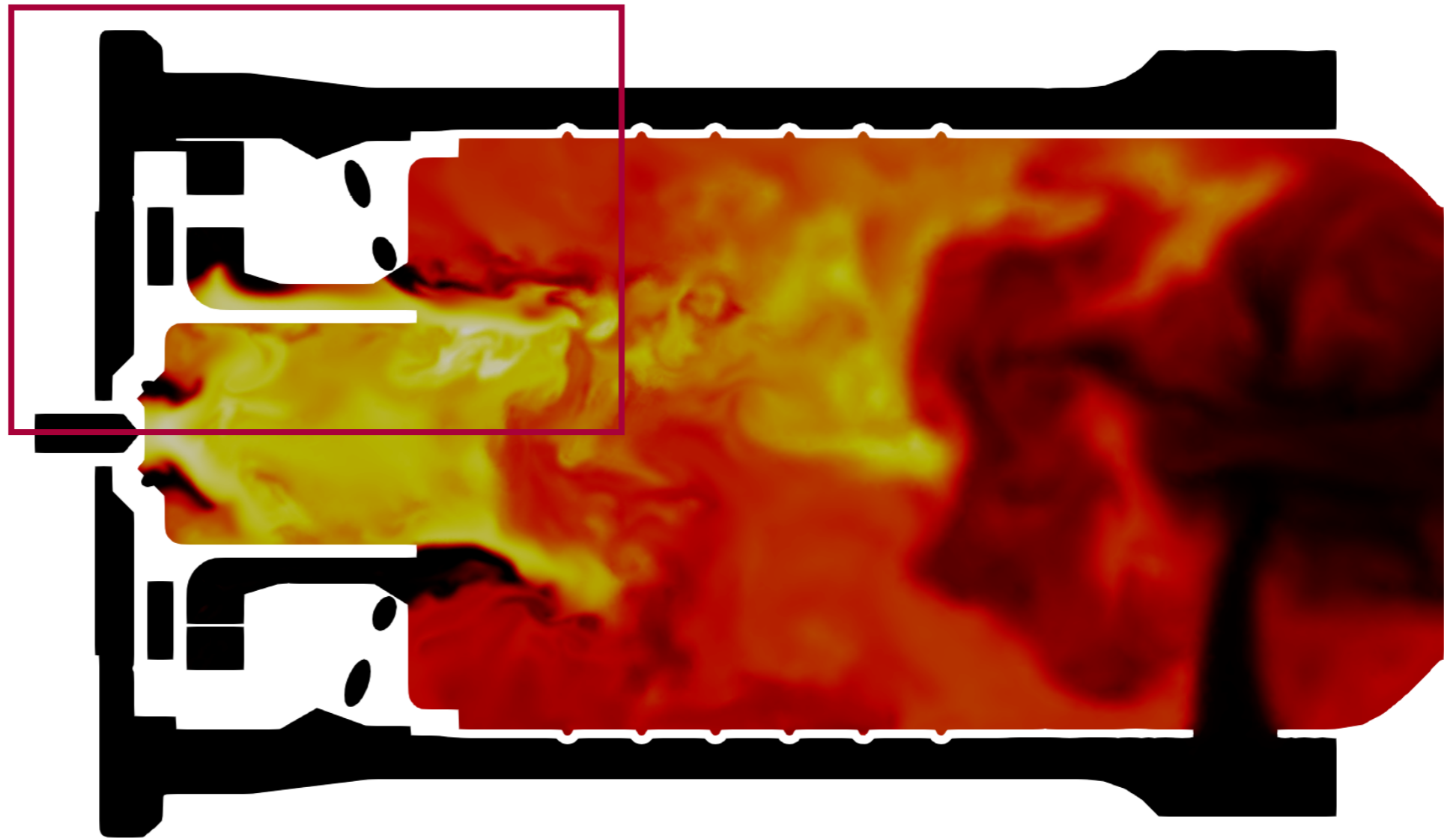
Air-fuel premix

Core flow
flashback

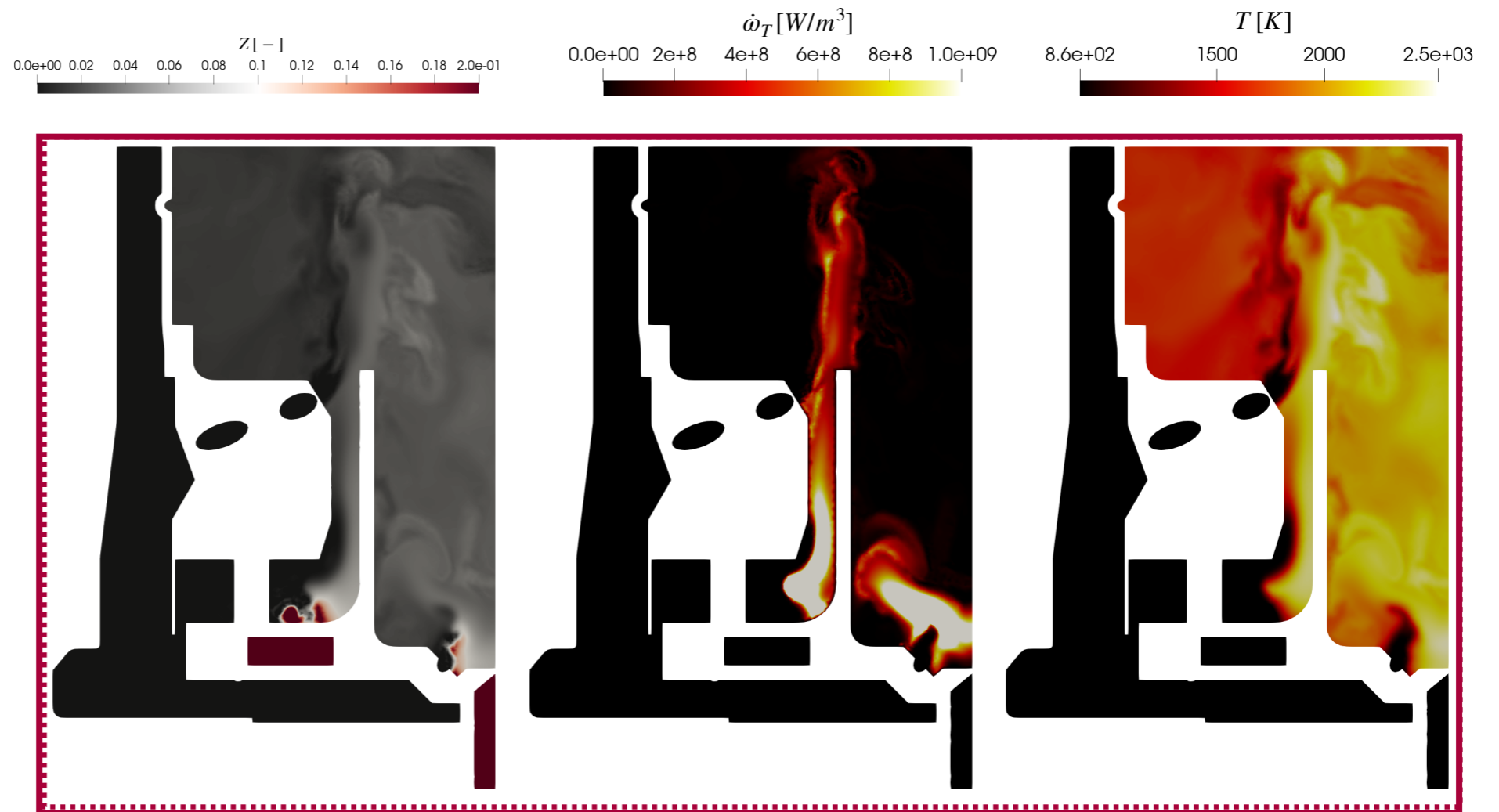


Air-fuel premix

Flashback phenomenology: boundary flashback



Flashback phenomenology: boundary flashback

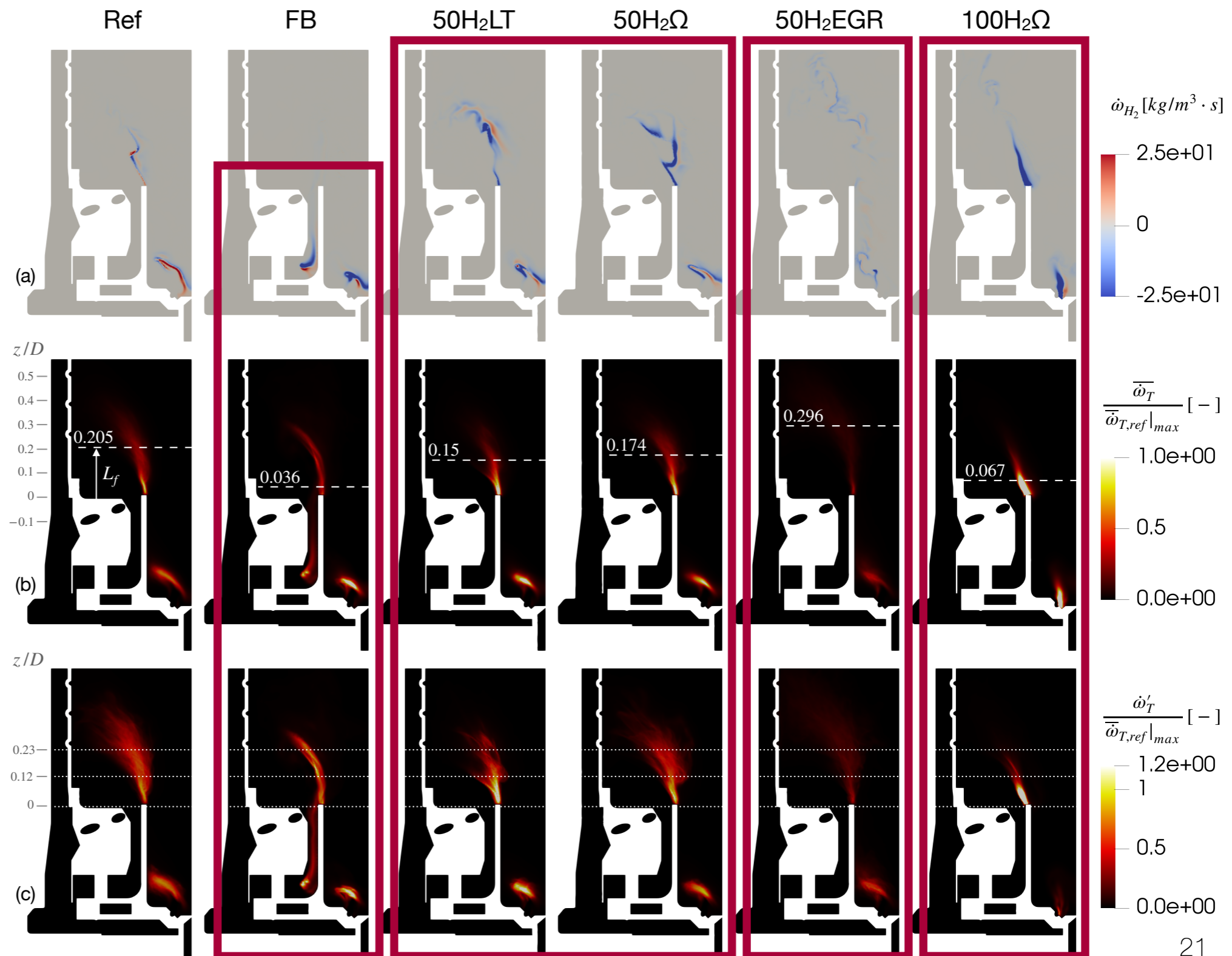


FB case
50%_{vol} H₂

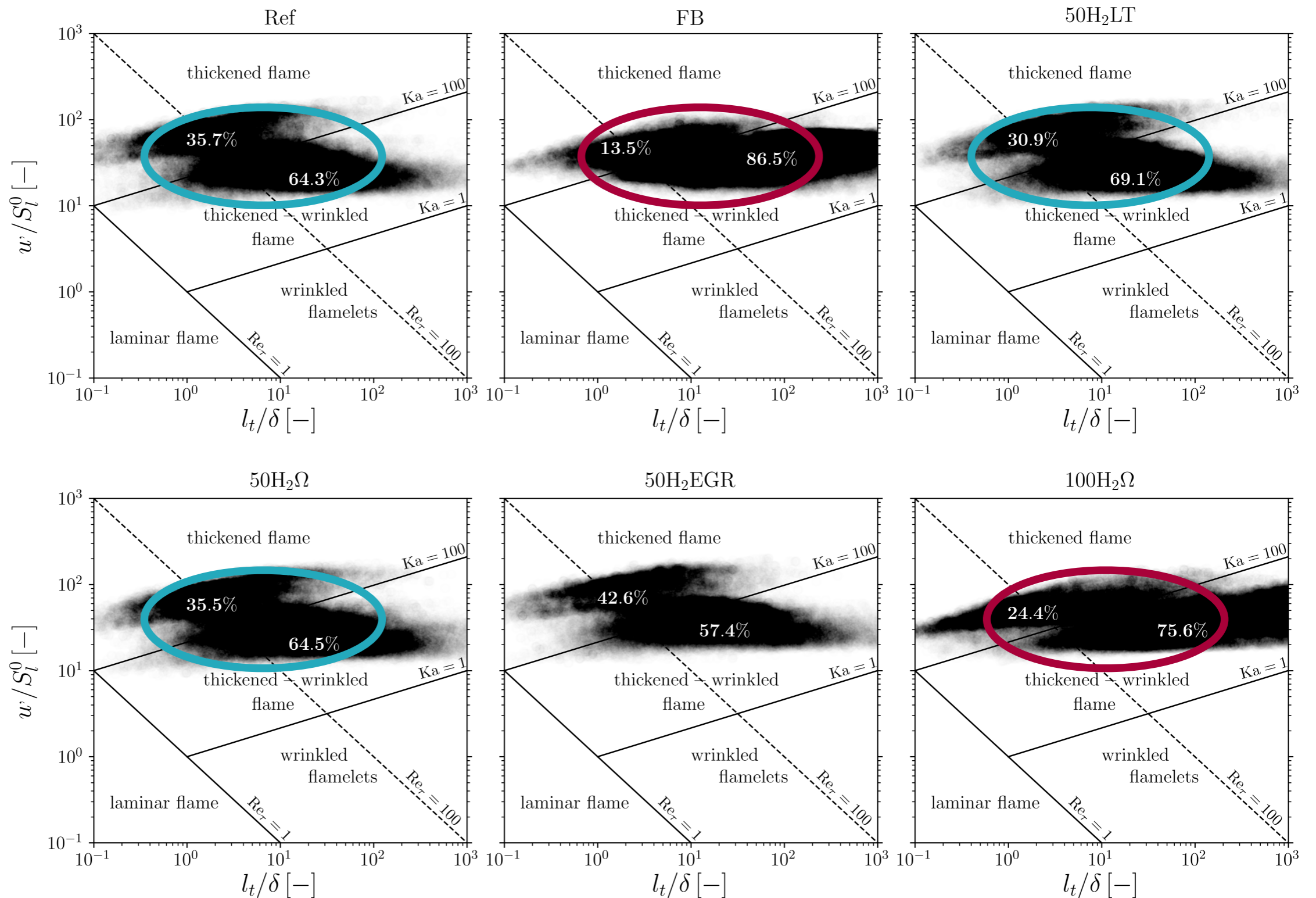
All solution cases are not showing any flashback

H₂ source term shows the production and consumption rates.

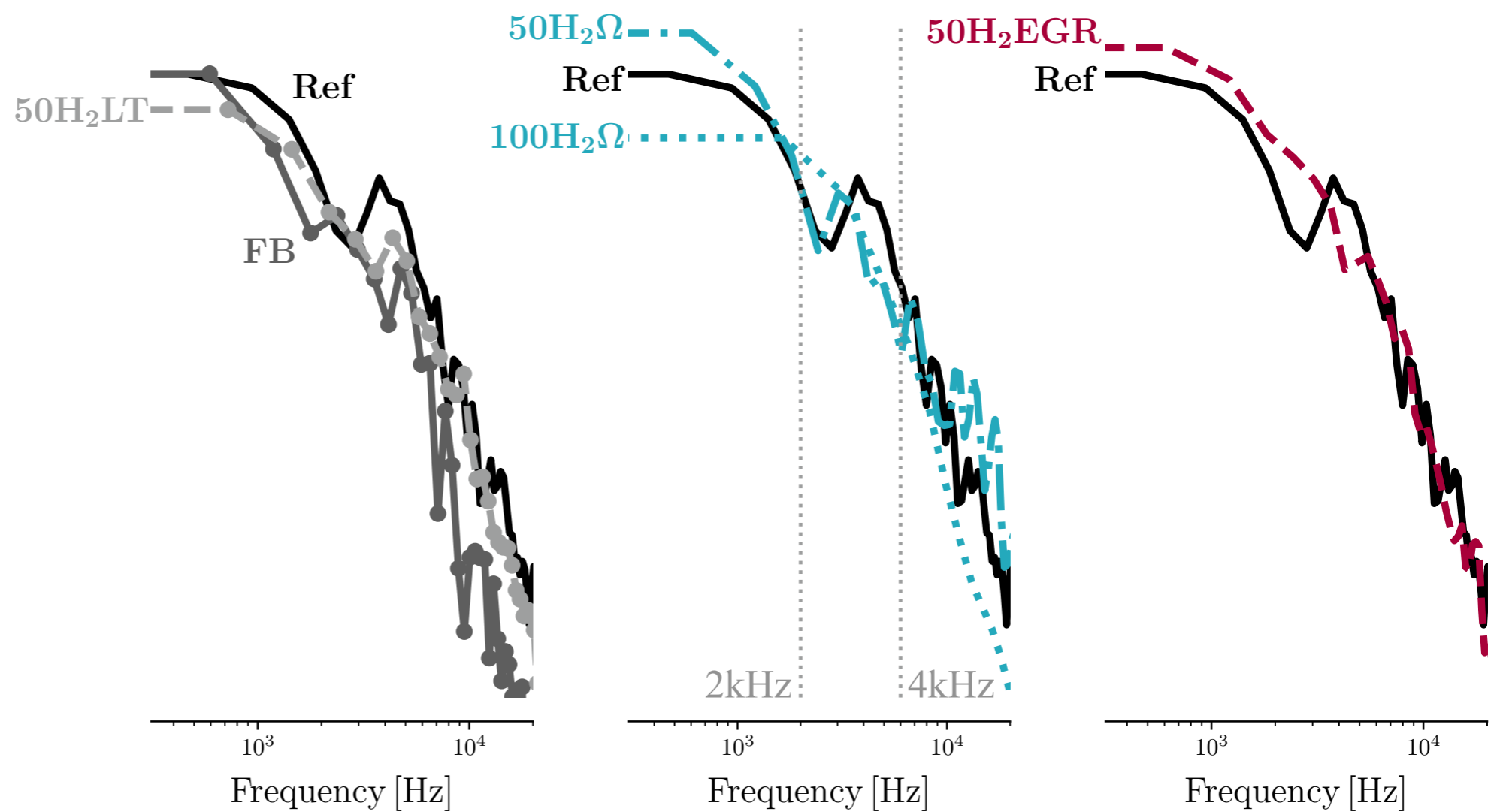
$$L_f = \frac{\int z \bar{\dot{\omega}}_{T,xy} dz}{\int \bar{\dot{\omega}}_{T,xy} dz}$$



Combustion regime diagrams showing scatter plots of injector fresh gases



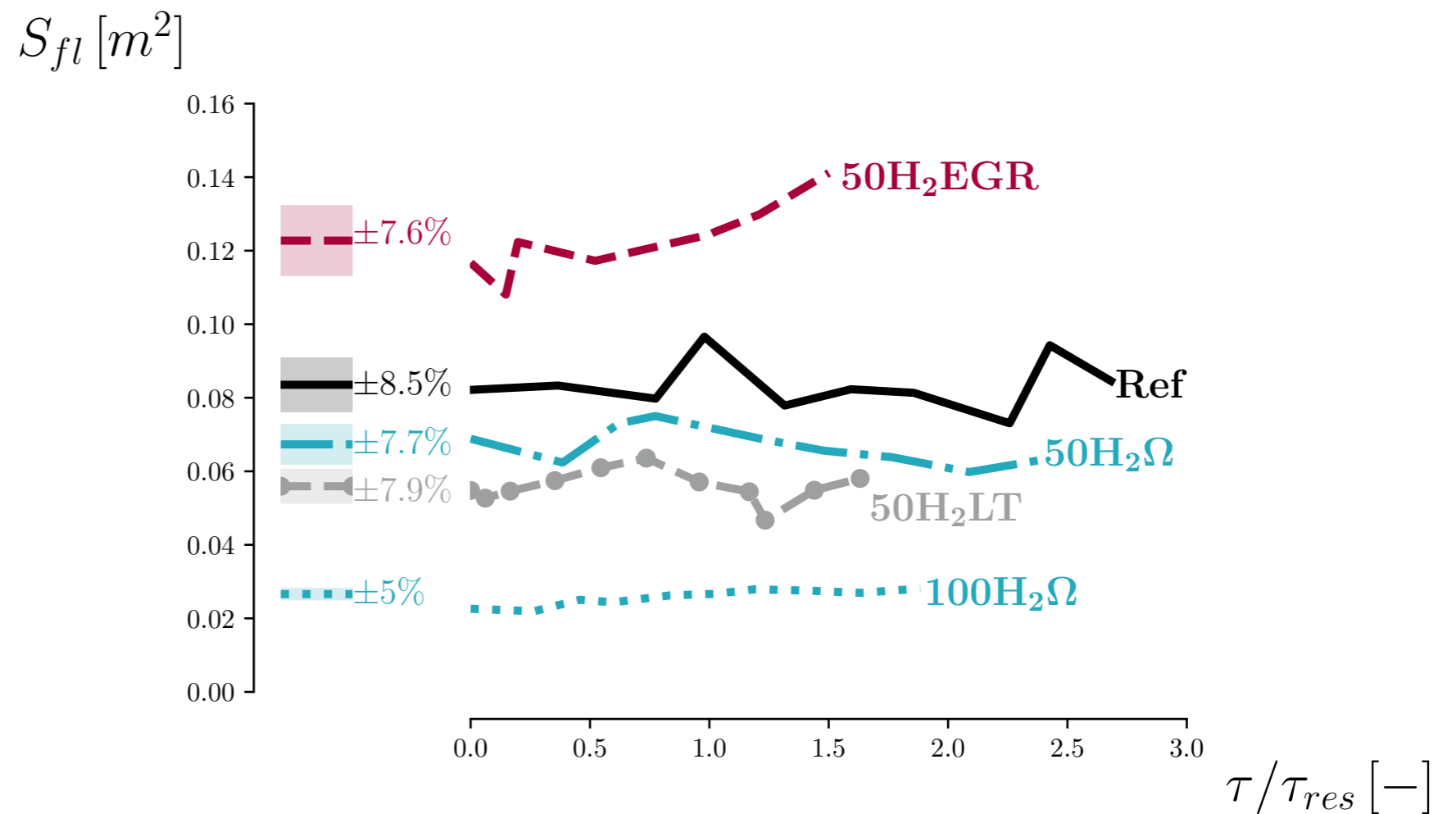
Normalized PSD of the axial velocity: Ref mode only reproduced by 50%_{vol} H₂ — $\Omega=3.4\%$



Comparison of the flame surface gives a clue on the flame ability to sustain perturbations

Fluctuations
= flame able to sustain perturbations

Increasing surface
= sign of thermo-diffusive instabilities or blow-out issues



Target

**Flashback prevention for various H₂ blends
without any redesign of a mGT combustor.**

Considering humidification & EGR as solution.

Outline

**Burner layout &
operating conditions**

Computational Fluid Dynamics

Conclusions

Flashback prevention without any redesign of the mGT combustor

Low computational
cost predictions
using 0D CRN / 1D Flame

100% H₂ can be reached when performing humidification while only 50%_{vol} H₂ with EGR.

No flashback was observed for all considered cases.

However, potential **risk of flashback** apparition for the **100%H₂Ω**.

- ▶ Advanced simulations are required, including wall heat transfer.

Risk of **less stable** flame observed for the **50%H₂EGR**.

Flashback prevention in a micro Gas Turbine fueled by hydrogen without any combustor redesign

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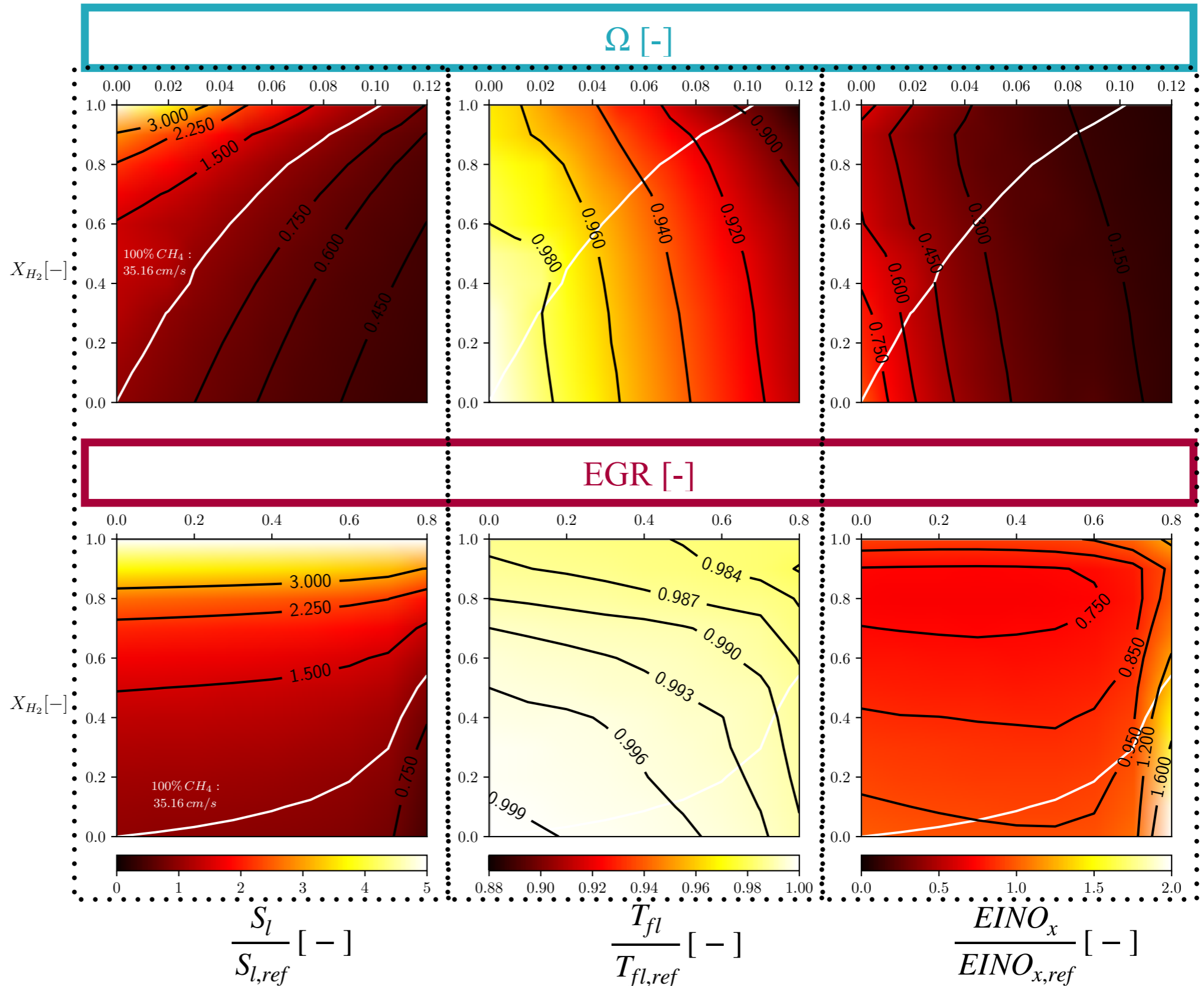
Ward De Paepe

ERCOFTAC Autumn Festival 2023

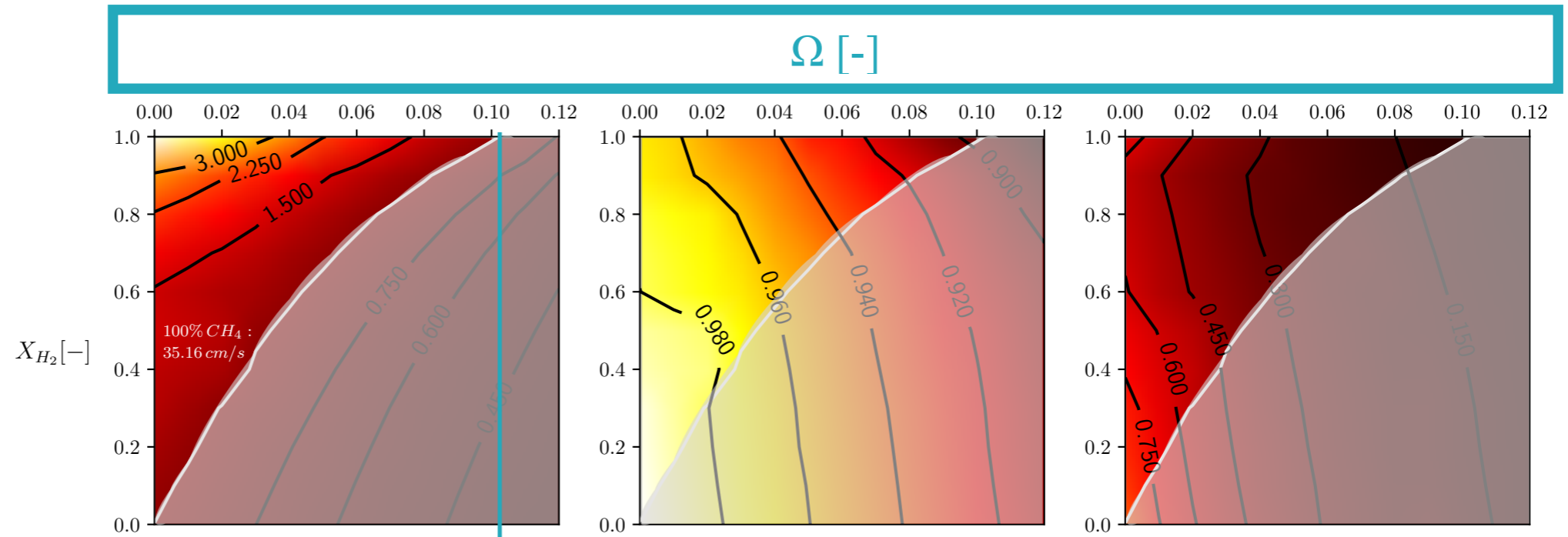
12th October 2023

0D CRN/1D Flame on various H₂ blends: comparison humidification & EGR

$$EINO_x = \frac{X_{NO_x} \cdot \dot{m}_{oxi}}{P_{el}}$$

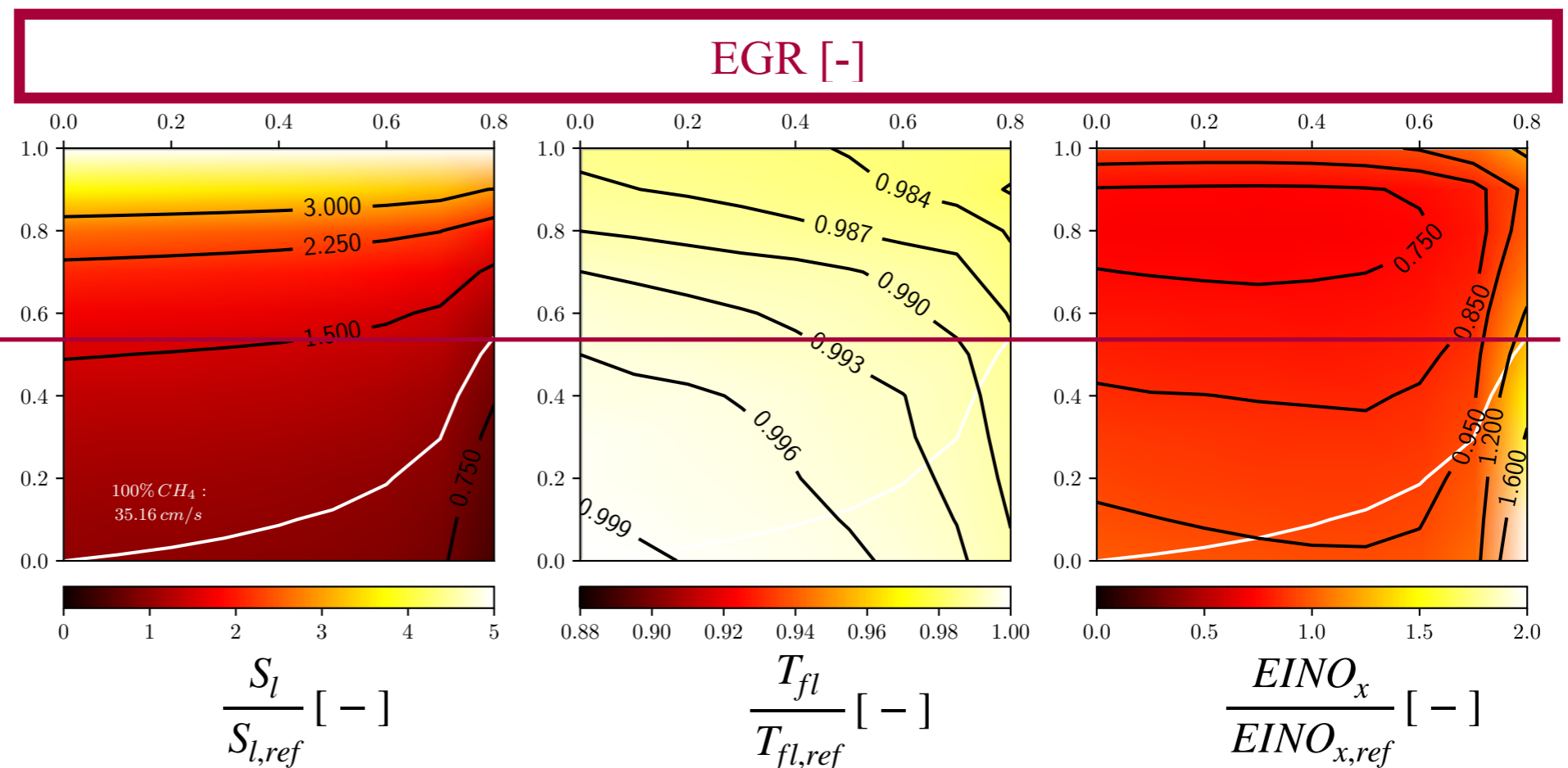


0D CRN/1D Flame on various H₂ blends: 100% H₂ requires only $\Omega=10.3\%$



$S_l < S_{l,ref} \quad \forall X_{H_2}$ ✓

$\Omega = 10.3\%$



$S_l > S_{l,ref}$ ✗

$X_{H_2} > 55\%$

X_{H_2} [-]

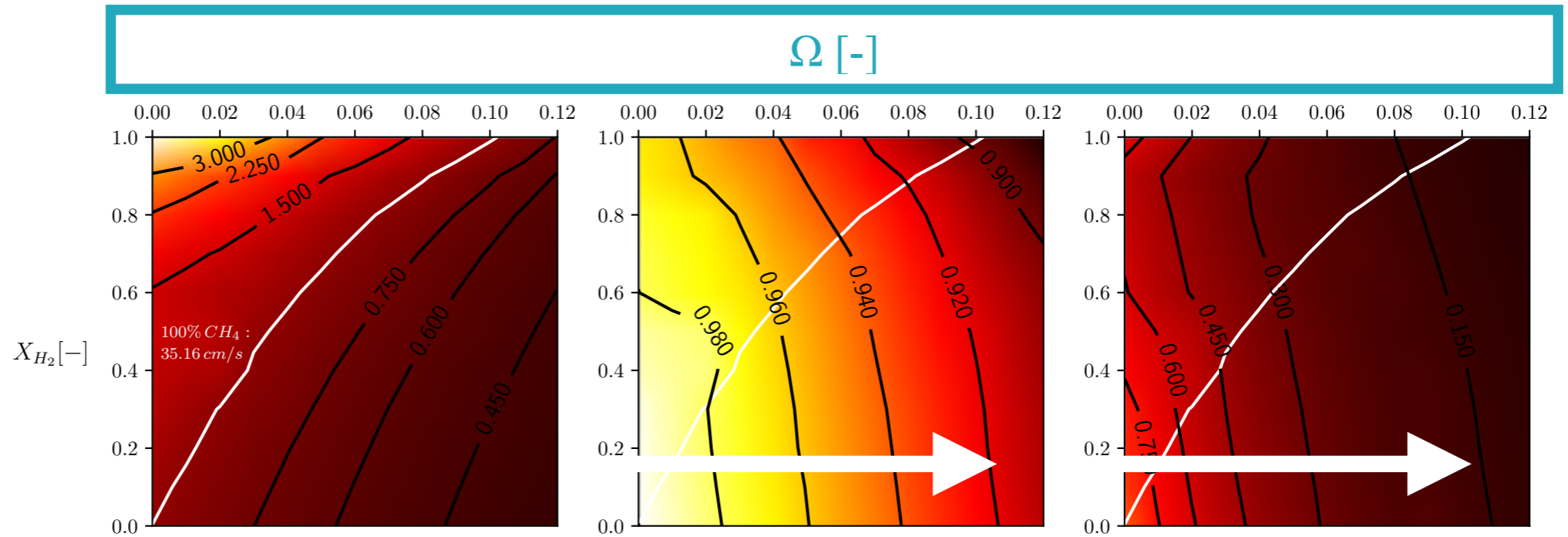
$\frac{S_l}{S_{l,ref}}$ [-]

$\frac{T_{fl}}{T_{fl,ref}}$ [-]

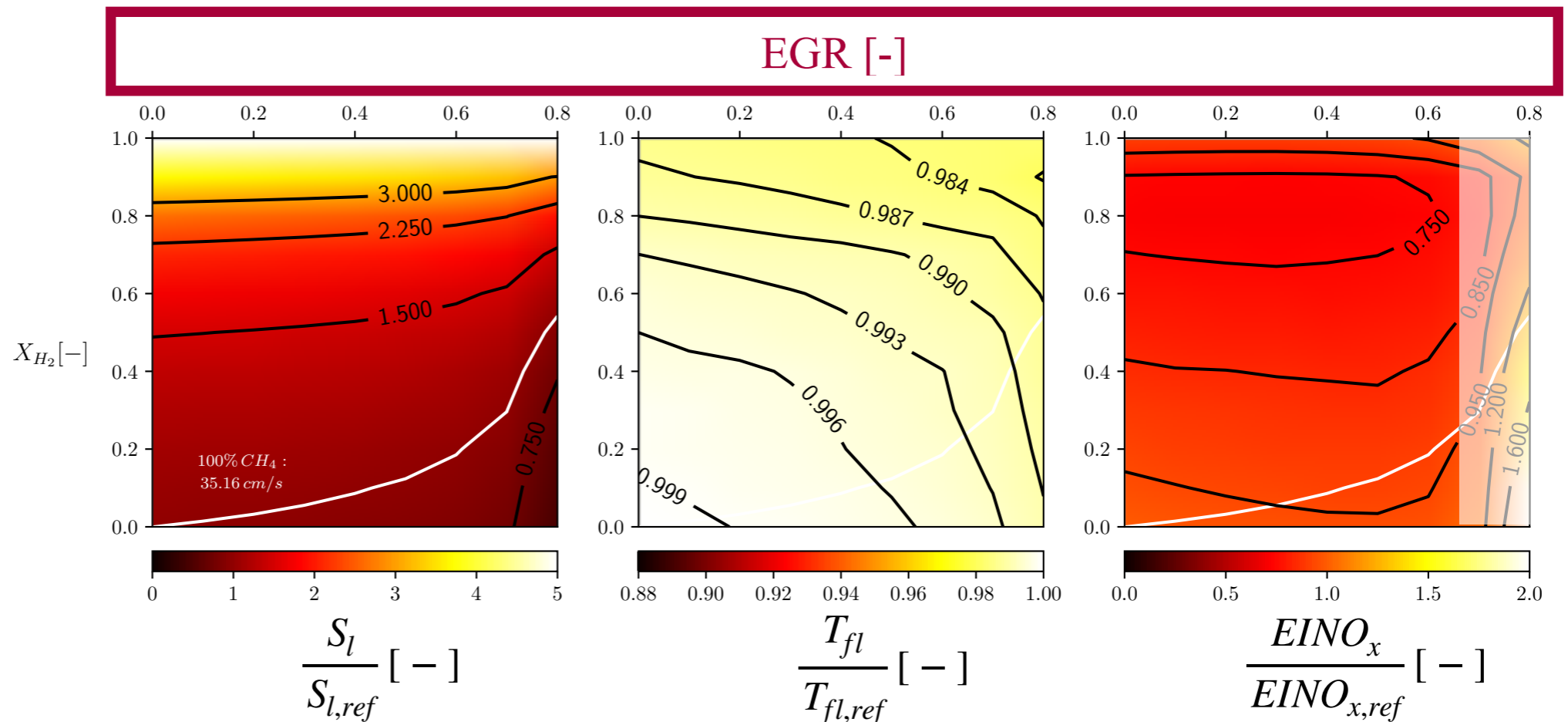
$\frac{EINO_x}{EINO_{x,ref}}$ [-]

0D CRN/1D Flame on various H₂ blends: decrease of T and NO_x with humidification

Temperature decrease of ~10% with water addition, inducing a decrease in the NO_x levels.



No significant temperature decrease (~0.2%), while the NO_x levels actually increase (~30-60%).



N₂ ↑ with EGR

Evolution of T_{fl} with $X_{H_2} \uparrow$ & fixed Ω : $T_{fl} \downarrow$

@ fixed thermal power and oxidizer flow rate

$X_{H_2} \uparrow$
($\phi \downarrow$)

REF:
 $f = CH_4$

100% H₂:
 $f = H_2$

$\sim 2.2 \text{ kJ/kgK}$

$$\dot{m}_f \cdot C_{p_f} \cdot T_f + \dot{m}_{oxi} \cdot C_{p_{oxi}} \cdot T_{oxi} = \dot{m}_{mix} \cdot C_{p_{mix}} \cdot T_{mix}$$

$\downarrow \quad \uparrow \quad \parallel \quad \parallel \quad \downarrow$

$\uparrow \quad \uparrow \quad 300K \quad \parallel^* \quad \uparrow \quad \downarrow$

$$\dot{m}_f \cdot C_{p_f} \cdot T_f + \dot{m}_{oxi} \cdot C_{p_{oxi}} \cdot T_{oxi} = \dot{m}_{mix} \cdot C_{p_{mix}} \cdot T_{mix}$$

$\sim 14.3 \text{ kJ/kgK}$

$\uparrow \quad \downarrow$

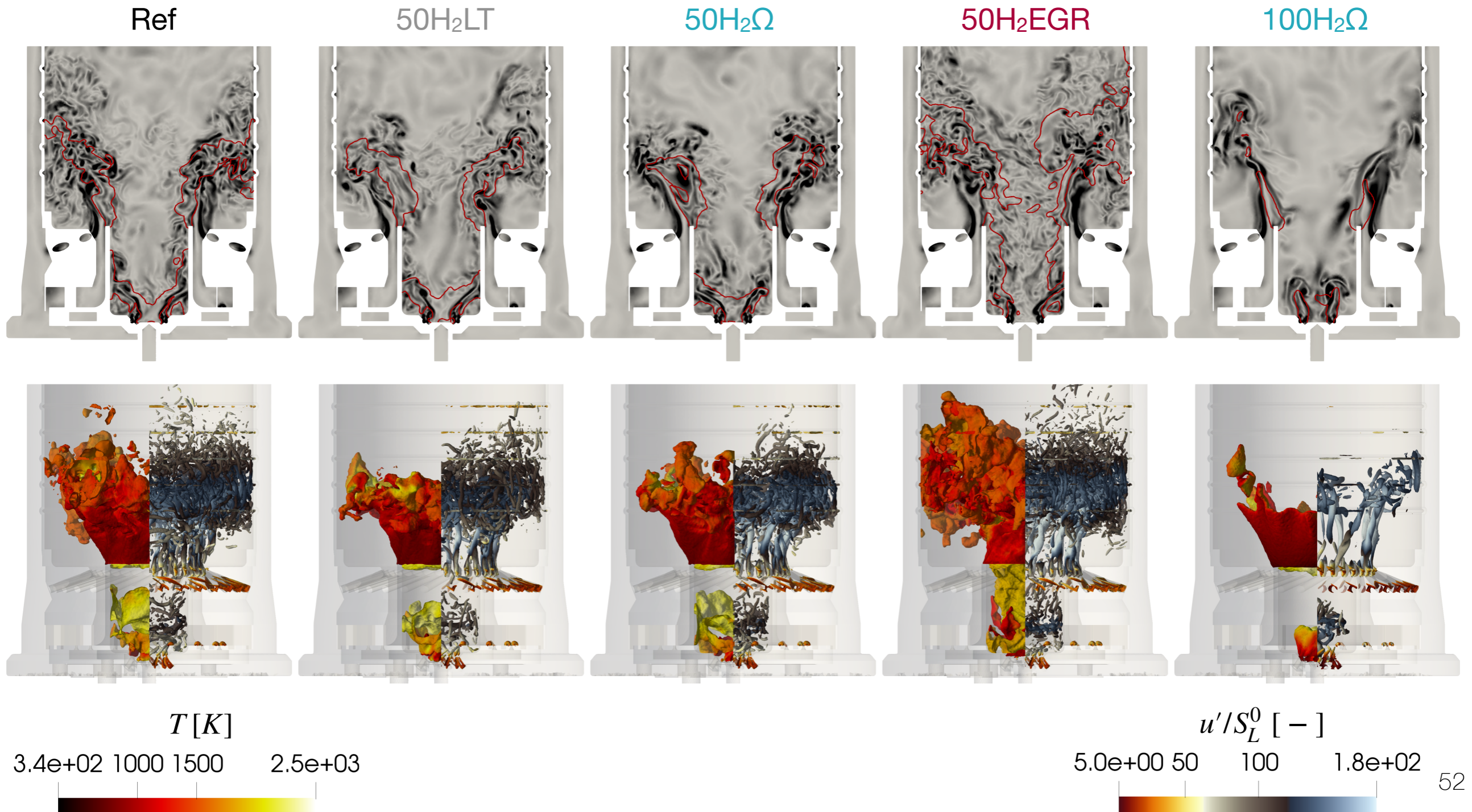
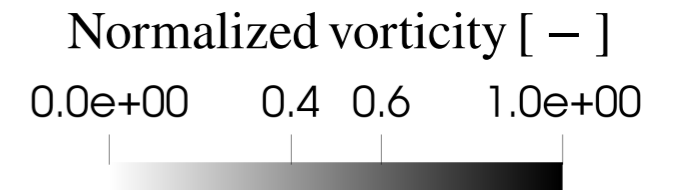
* $\dot{m}_f \ll \ll \dot{m}_{oxi}$

$$T_{mix} \downarrow \quad \longrightarrow \quad T_{fl} \downarrow$$

Dilution impact on the flame-turbulence interaction

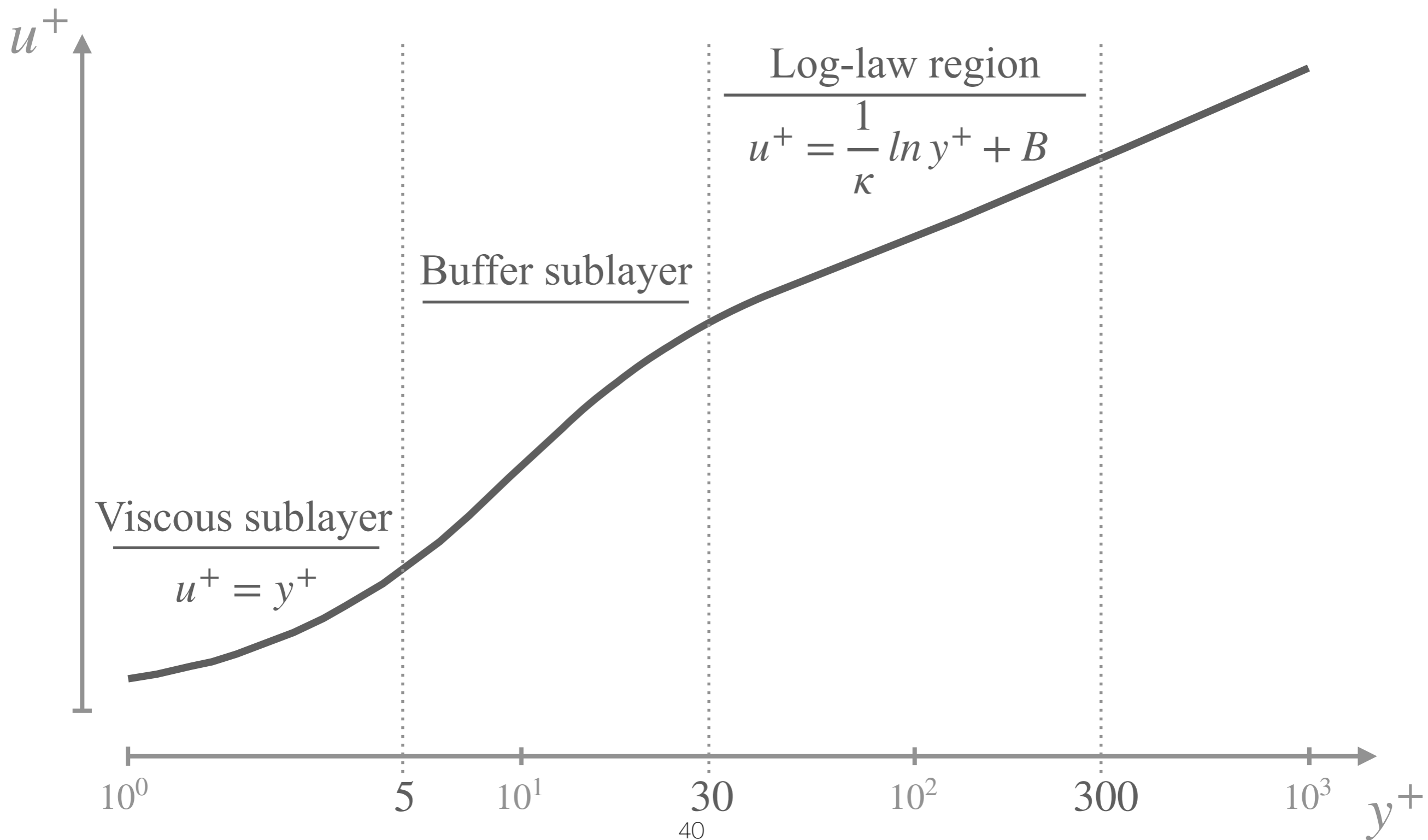
Thickened-wrinkled flame regime = Turbulence thickens the flame preheat zone, but not the reaction zone (only wrinkled)

Thickened flame regime = Turbulence penetrates the inner flame structure & affects both diffusion & reaction zones

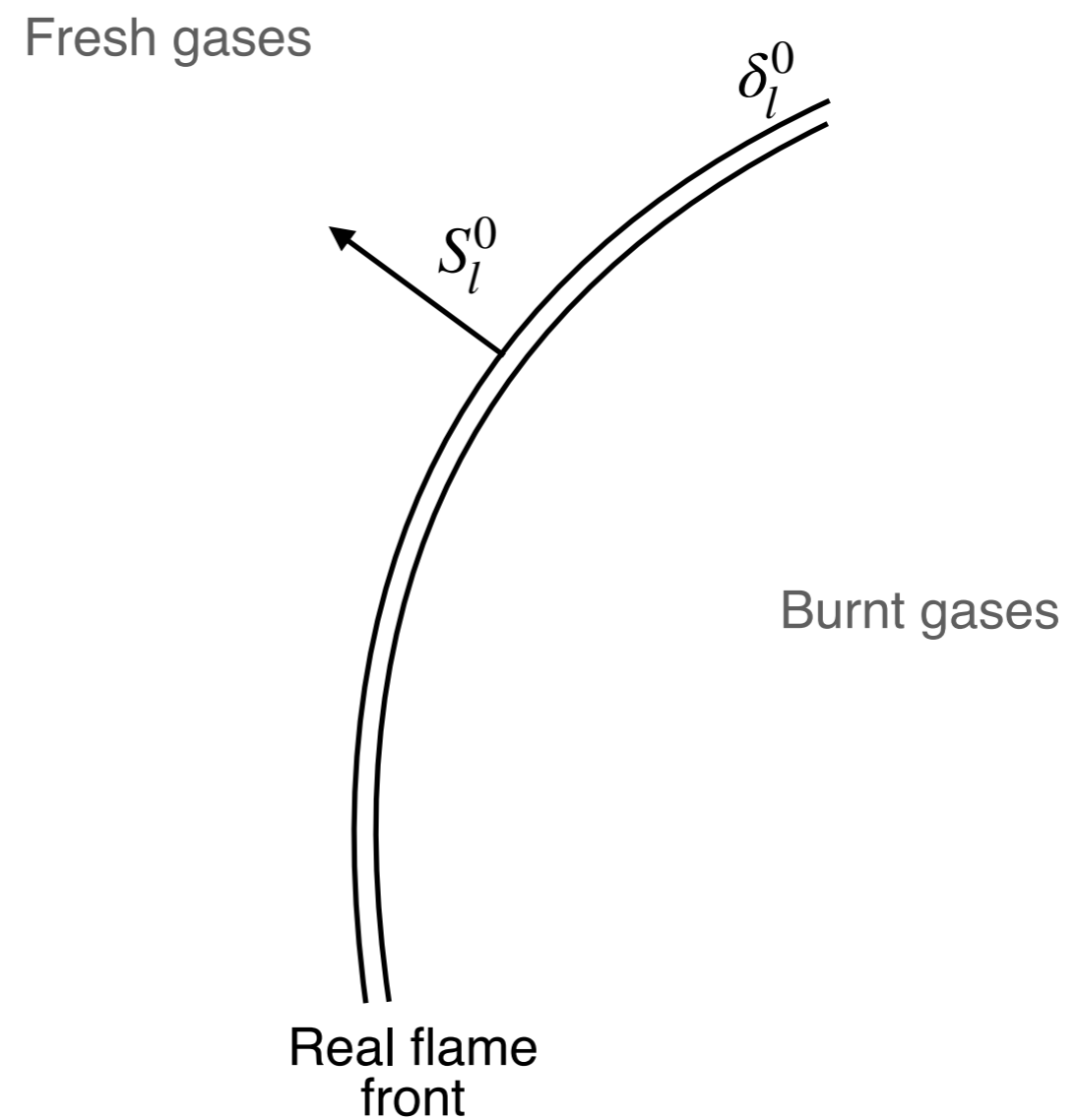


Thickened Flame Model

Near-wall flows

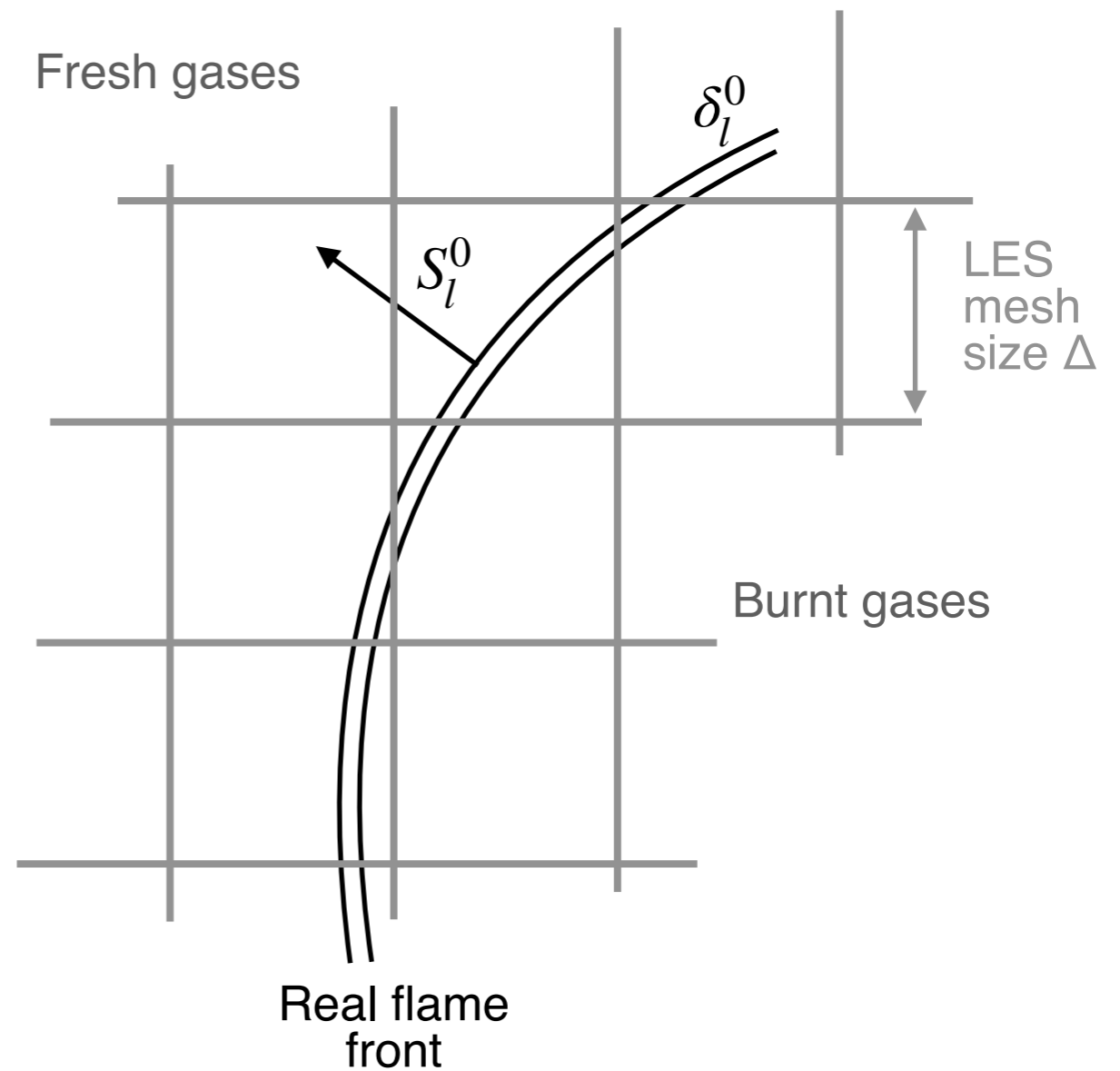


The DTFLES model artificially thickens the flame front without modifying the flow dynamic



The DTFLES model artificially thicken the flame front without modifying the flow dynamic

$$\Delta > \delta_l^0$$

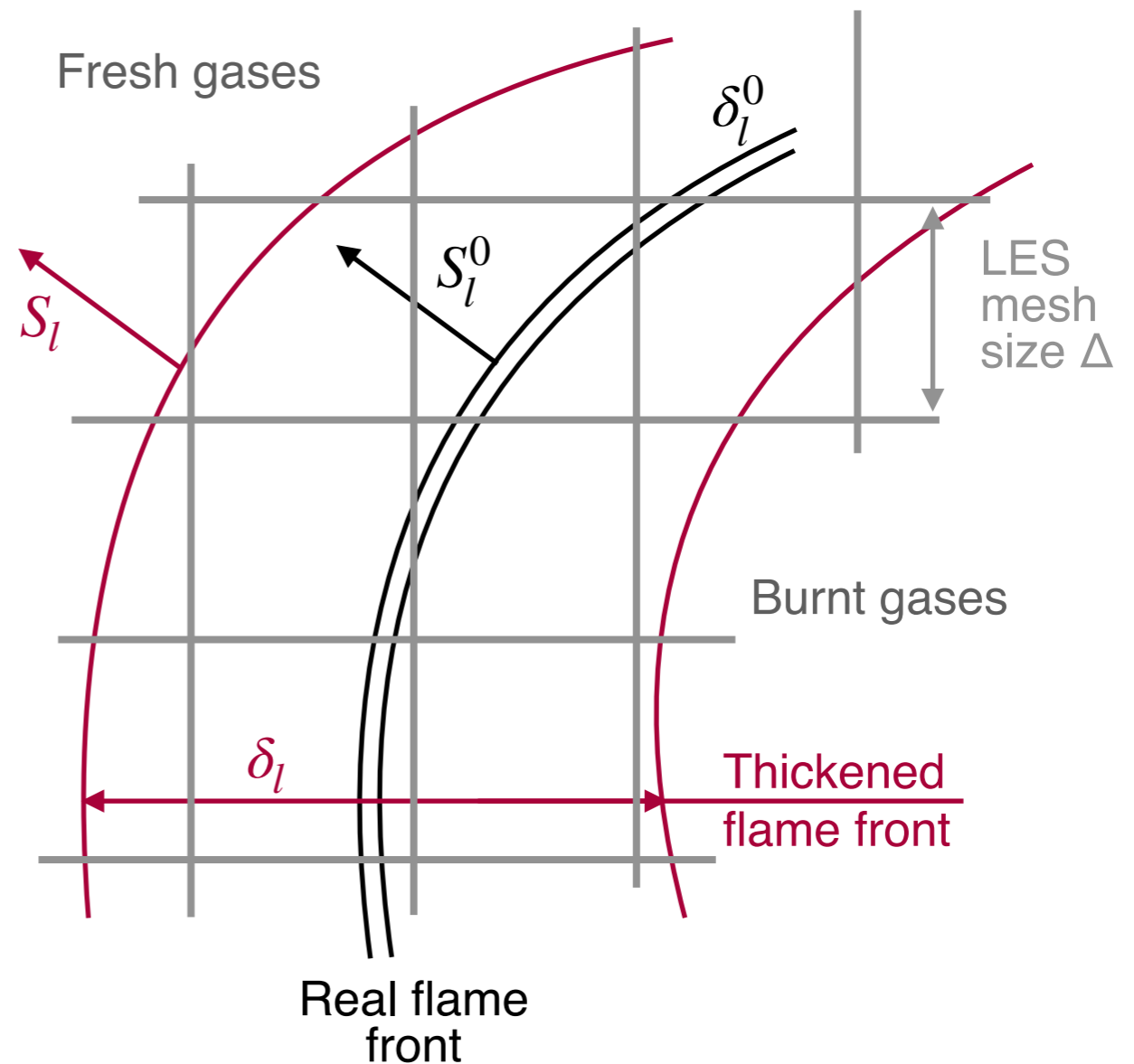


The DTFLES model artificially thicken the flame front without modifying the flow dynamic

$$\Delta > \delta_l^0$$

Flame front thickened of a factor F

Efficiency E function to compensate the surface reduction & avoid wrinkling issues

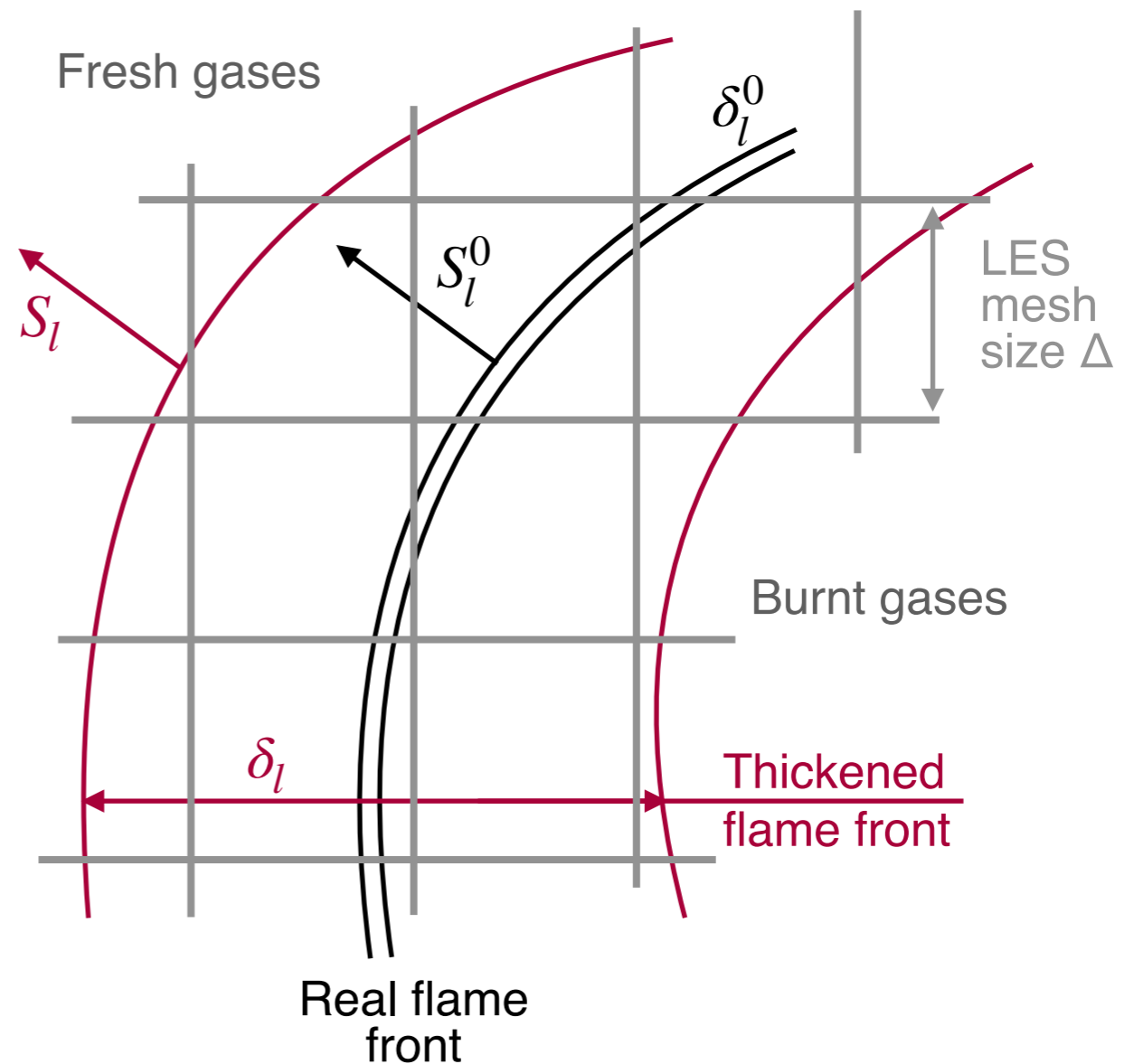


The DTFLES model artificially thicken the flame front without modifying the flow dynamic

Dynamic formulation of the TFLES model to handle **premixed** and **non-premixed** flames:

F is not constant on the domain.

Flame sensor (reaction rate) to detect where the reaction takes place.



The flame is artificially thickened to predict correctly the combustion

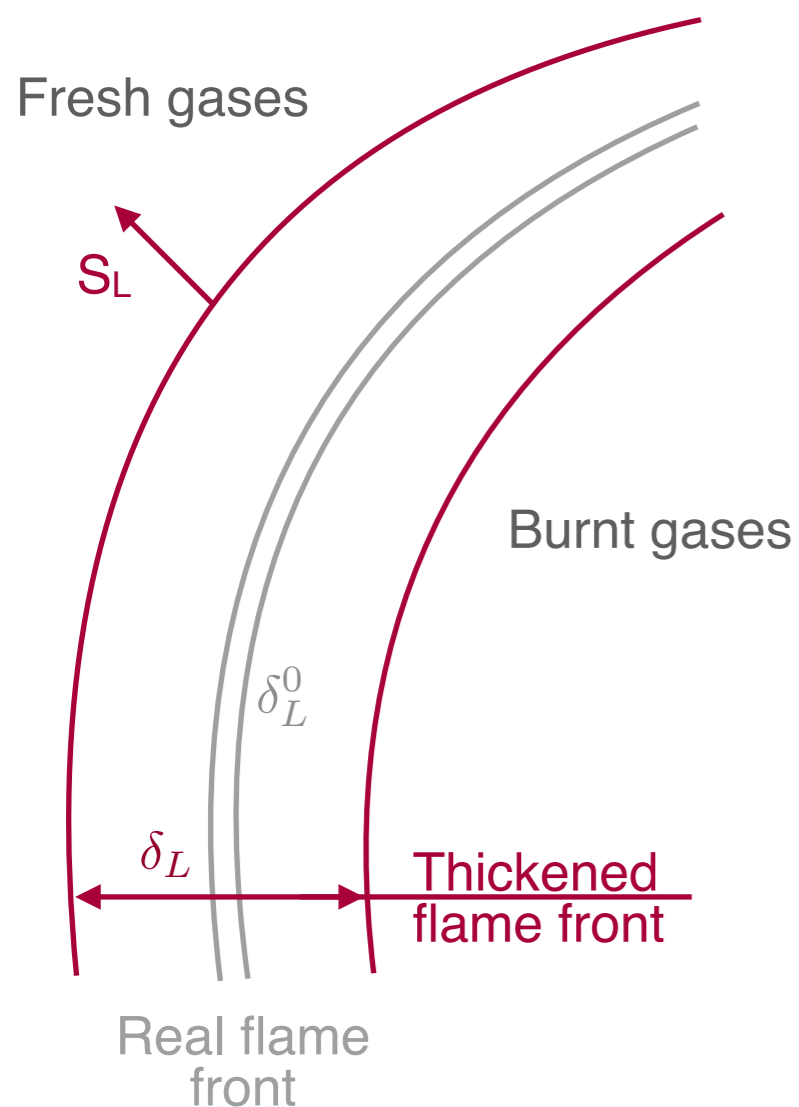
Theoretical unstrained 1D laminar flame simulated in the same operating conditions than the considered case.

The cells size is not refined enough in the region of the flame front:

- ▶ The thermal flame thickness $\delta_L^0 = 102\mu m$
- ▶ $250\mu m \leq \Delta \leq 1000\mu m$

➡ The source terms of the species could be under-resolved

The flame is artificially thickened to predict correctly the combustion



TFLES model modifies the conservation equations with a thickening factor F :

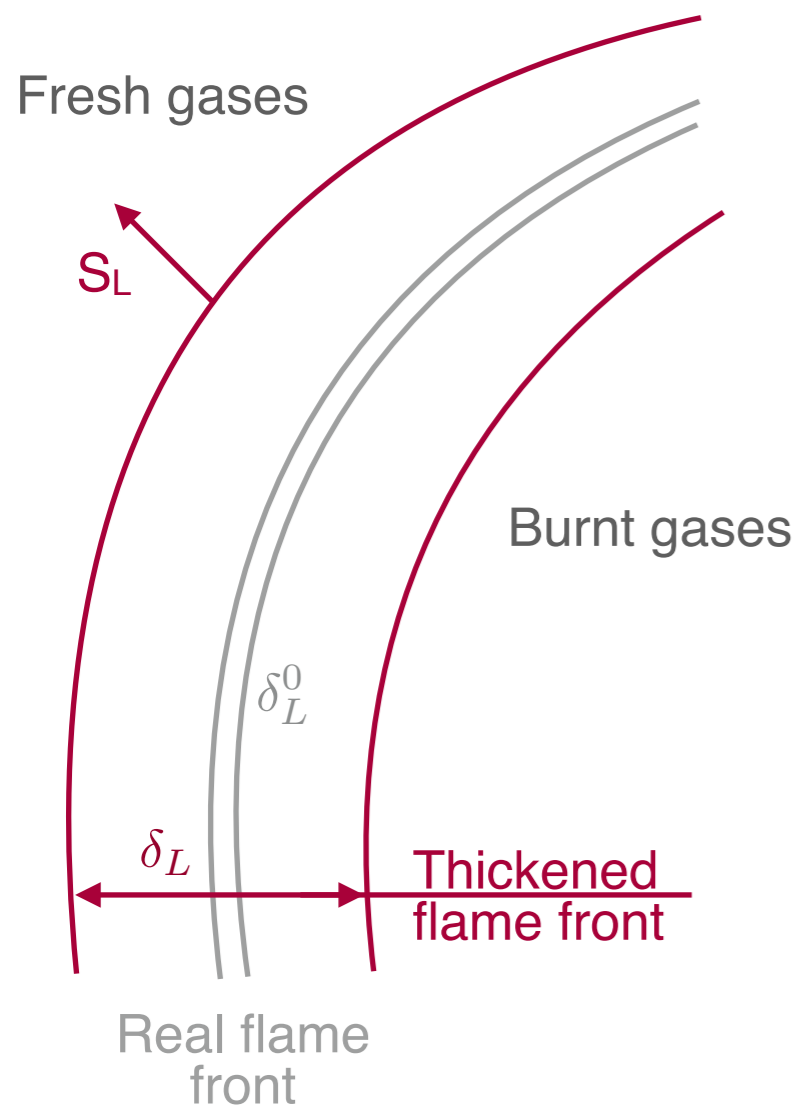
$$\triangleright \delta_L = F \cdot \delta_L^0$$

Thicken only the zone where reactions take place, identified by a flame sensor, and $F=1$ where $\dot{\omega}_k = 0$.

In the reaction zones, F depends on the ratio of the mesh size to the flame thickness, adjusted to have typically 3 to 5 points.

The flame is thickened but the laminar flame speed S_L is constant.

The flame is artificially thickened to predict correctly the combustion



TFLES model modifies the conservation equations with:

- ▶ a thickening factor F
- ▶ an efficiency function E of Charlette considering a static formulation with $\beta=0.5$

In reaction zones, both diffusivity and reaction rate are modified to ensure the flame thickening.

The flame is artificially thickened to predict correctly the combustion

$$\delta_L^0 = \frac{\Delta T}{\nabla T|_{max}}$$

$$S_L^0 = \frac{\int_V \dot{\omega}_k dV}{Y_k^{out} - Y_k^{in}}$$

$$\delta_T^0 = F \cdot \delta_L^0$$

$$S_T^0 = E \cdot S_L^0$$

$$\delta_L^0 \propto \frac{D_{th}}{S_L^0} = \sqrt{\frac{D_{th}}{B}}$$

$$S_L^0 \propto \sqrt{D_{th} B}$$

Thermal diffusivity:

$$D_{th} \longrightarrow F \cdot D_{th} \longrightarrow E \cdot F \cdot D_{th}$$

Preexponential constant:

$$B \longrightarrow \frac{B}{F} \longrightarrow E \cdot \frac{B}{F}$$

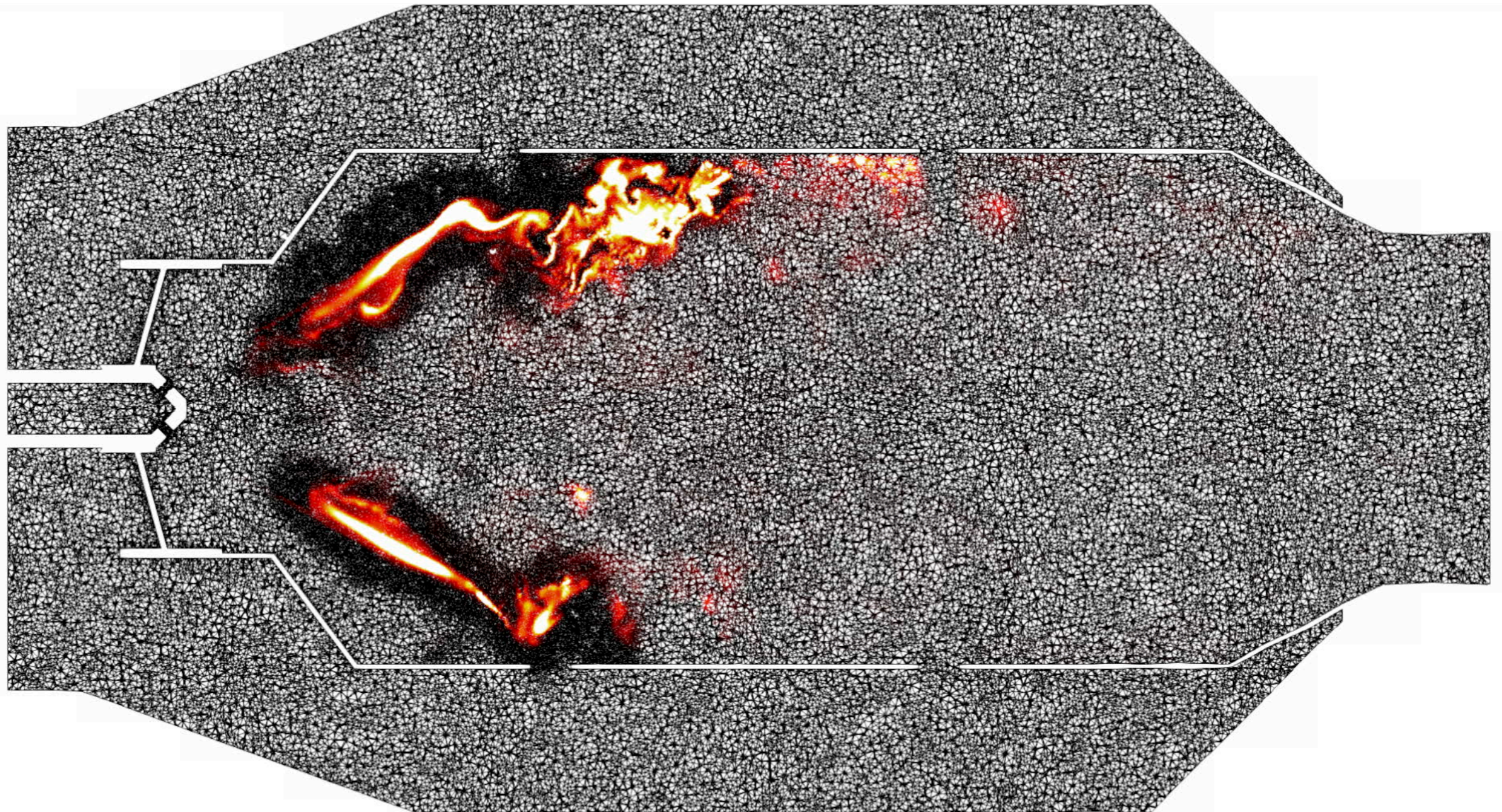
Adaptive Mesh Refinement

Appendix A

Appendix B

Flame front evolution followed by the Adaptive Mesh Refinement

Adaptation criterion based on the heat release using the flame sensor of the TFLES model.



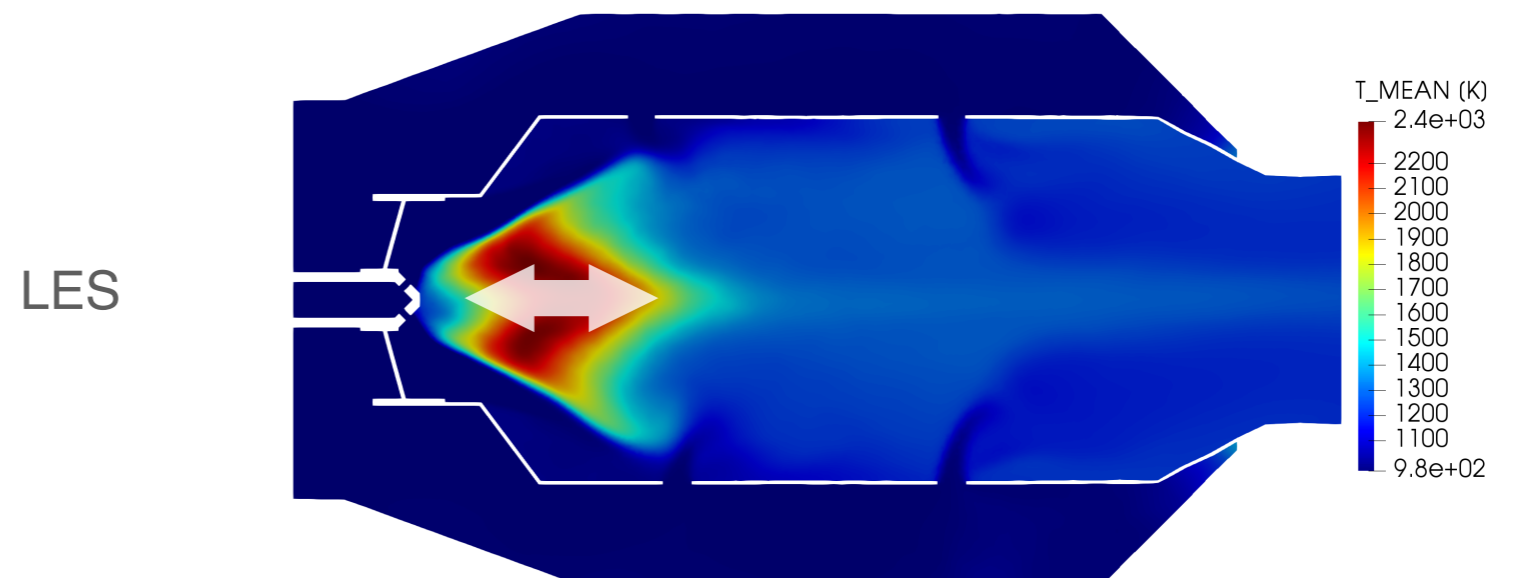
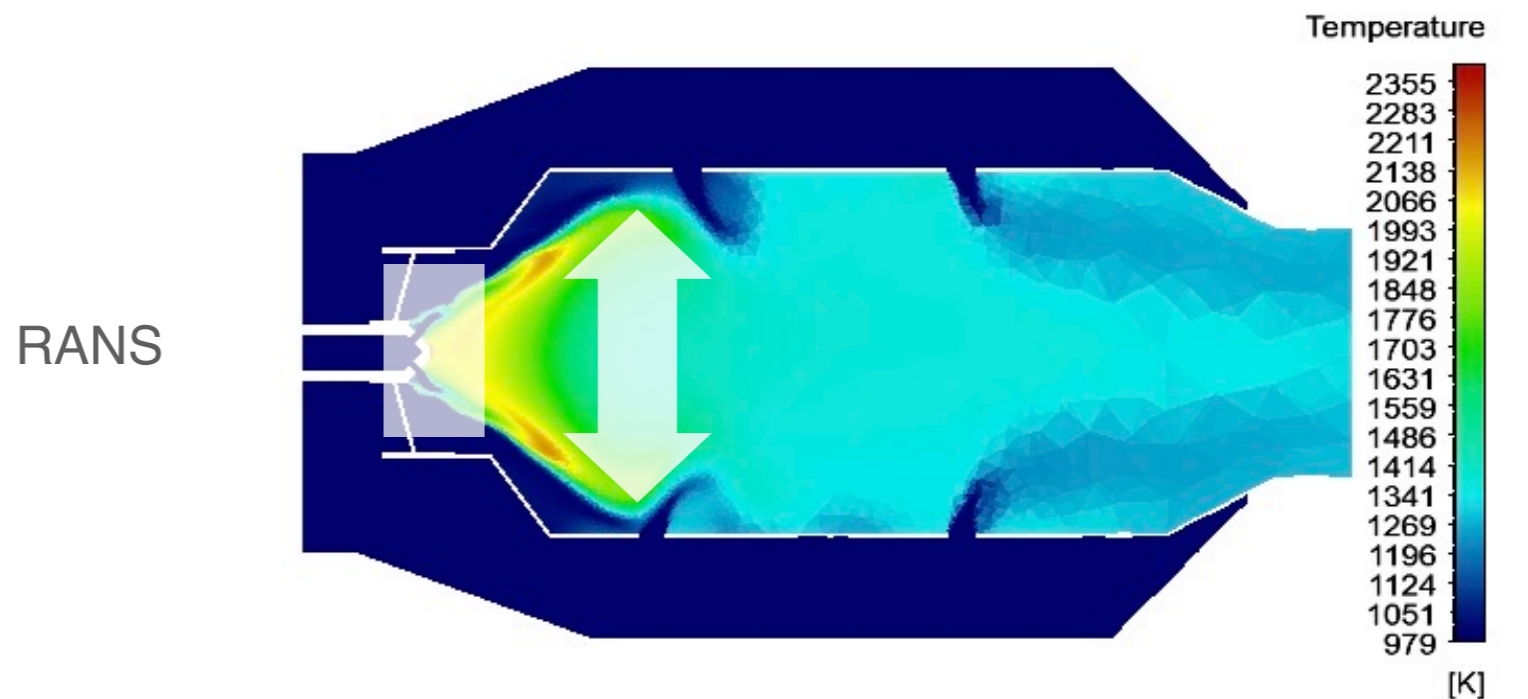
Color maps of the time-averaged temperature show higher temperature range and axial shift of the reaction area with LES

RANS predicts a larger flame with a **higher radial expansion** of the front spreading beyond the first row of dilution holes.

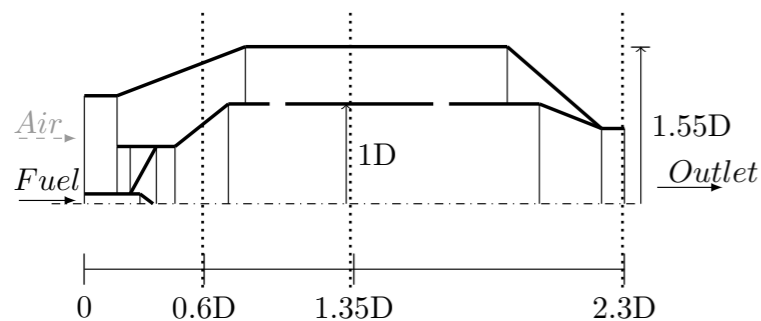
LES results show a more **centered peak** where this front is expanding along the centerline.

RANS shows also a more **attached** reacting region to the **fuel injector**.

REF case



LES shows higher temperature variation for the REF case while both approaches provide similar trends for the Syngas case

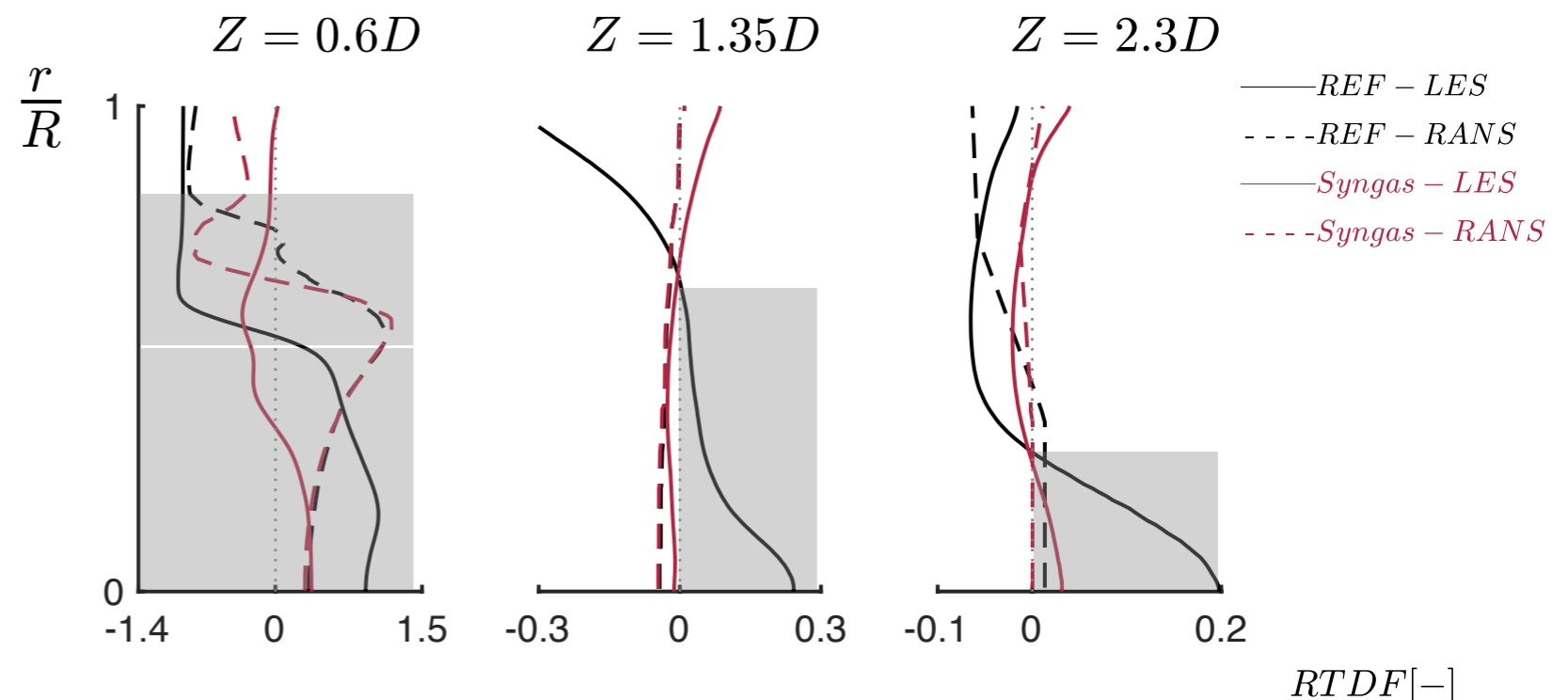


Aim of the Radial Temperature Distribution Function:
quantify the radial evolution of the mean azimuthal temperature variation from the mean planar value.

Differences essentially appear for high radial positions. The peak of temperature is located closer to the centerline in LES.

- ▶ As an effect of different resolution of the swirled air injection.

Less penetrating air jet in RANS involves a radial expansion of hot products (higher temp. located at higher radial position).



RTDF[-]

Combustor outlet conditions and emissions comparison shows a slight overestimation of CO fraction with LES

	REF			Syngas	
	RANS	LES	Literature	RANS	LES
Outlet temperature $\langle \bar{T} \rangle$ [K]	1273	1268	1250 ⁽¹⁾	1224	1228
Y_{O_2} [%mass]	20.2	20.2	-	19.4	19
Y_{CO_2} [%mass]	2	2	-	4.6	4.6
Y_{CO} [ppm _{mass}]	75	94	50 ⁽²⁾	37	65
Y_{NO_x} [ppm _{mass}]	5.5	-	1 ⁽²⁾	2	-

(1) Visser et al., J.of Eng. for Gas Turbines and Power, 2011, 133 (pp. 042301-1-8)

(2) MTT Enertwin CHP system: specifications

Adaptive Mesh Refinement implemented and adapted to combustion cases

Dynamic adaptation **in the flame region**
all along the simulation.

Refinement **criterion** based on the flame
sensor (**reaction rate**) of the DTFLES model.

Metric size defined in the flame and
the background

Triggering adaptation: **Error metric-based**
(from the defined interface and background
metrics).

$$\epsilon = \max \left(\left| \frac{M_{current} - M_{target}}{M_{target}} \right| \right)$$

Dynamic mesh adaptation aims to automatically refine flame region over time

Refinement criteria based on Flame sensor

S=1 into flame front (stiff reaction zone)

S=0 downstream (slow reactions) and upstream the flame (thermal diffusion zone)

$$\dot{\omega}_c = \dot{\omega}_{CO_2} + \dot{\omega}_{CO} + \dot{\omega}_{H_2O}$$
$$S = 1 \text{ if } \dot{\omega}_c > 0.1 \max(\dot{\omega}_c)$$
$$S = 0 \text{ else}$$

Target Metrics

Interface metric = 1mm

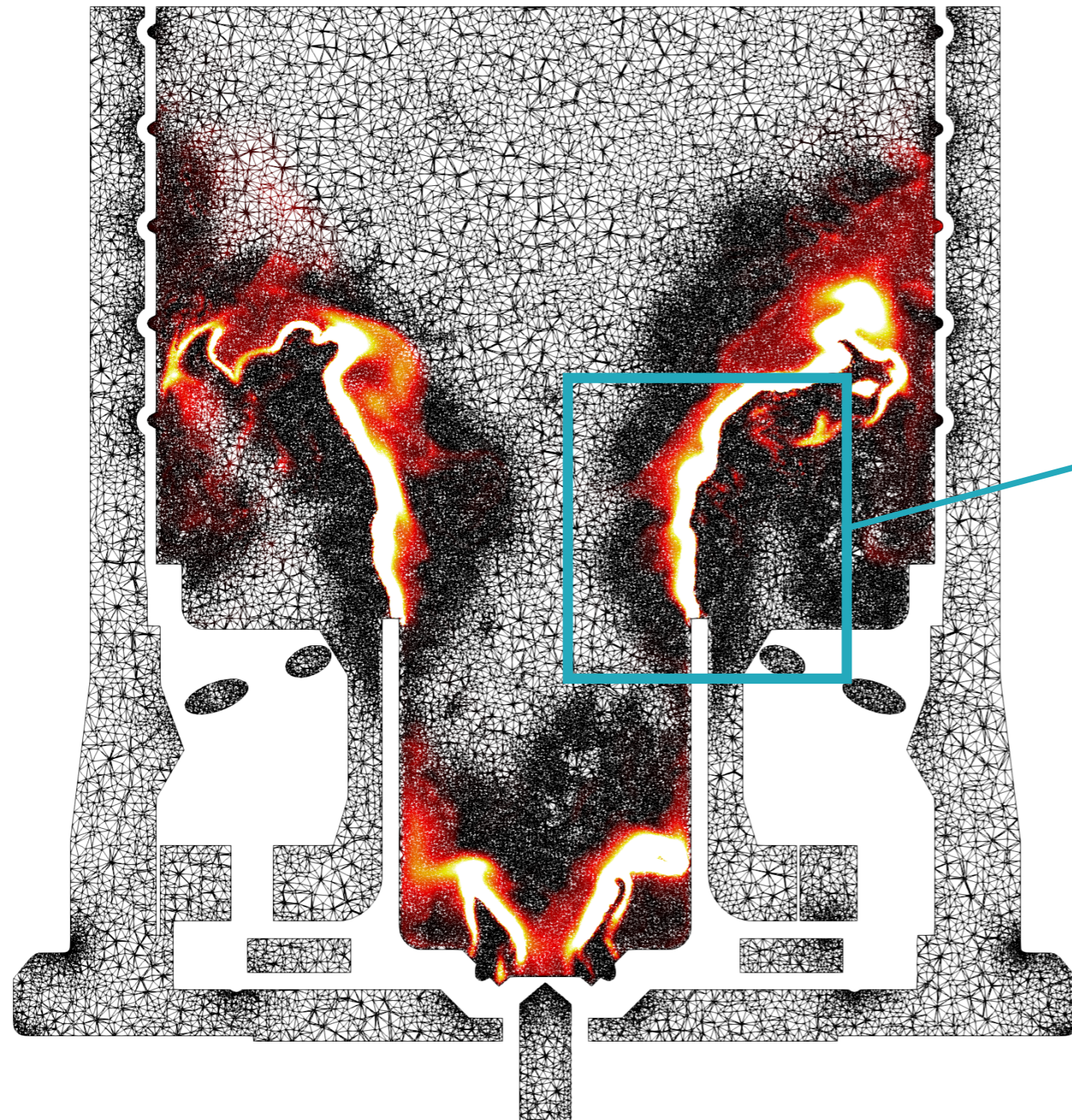
Background metric = 5mm

Triggering adaptation

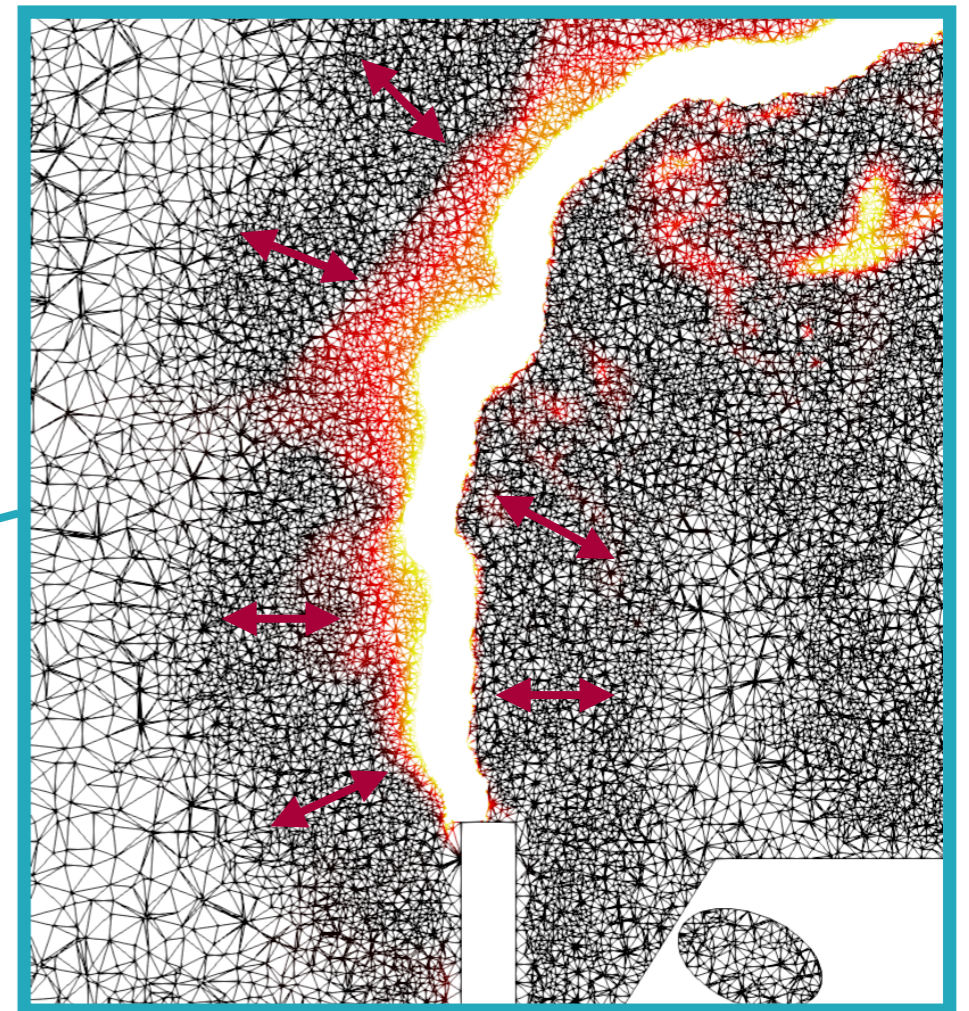
Depend on flow dynamics ← ~~Time period based (triggered at each Δt)~~

Error metric-based (triggered at each $\varepsilon > \varepsilon_{\max}$)

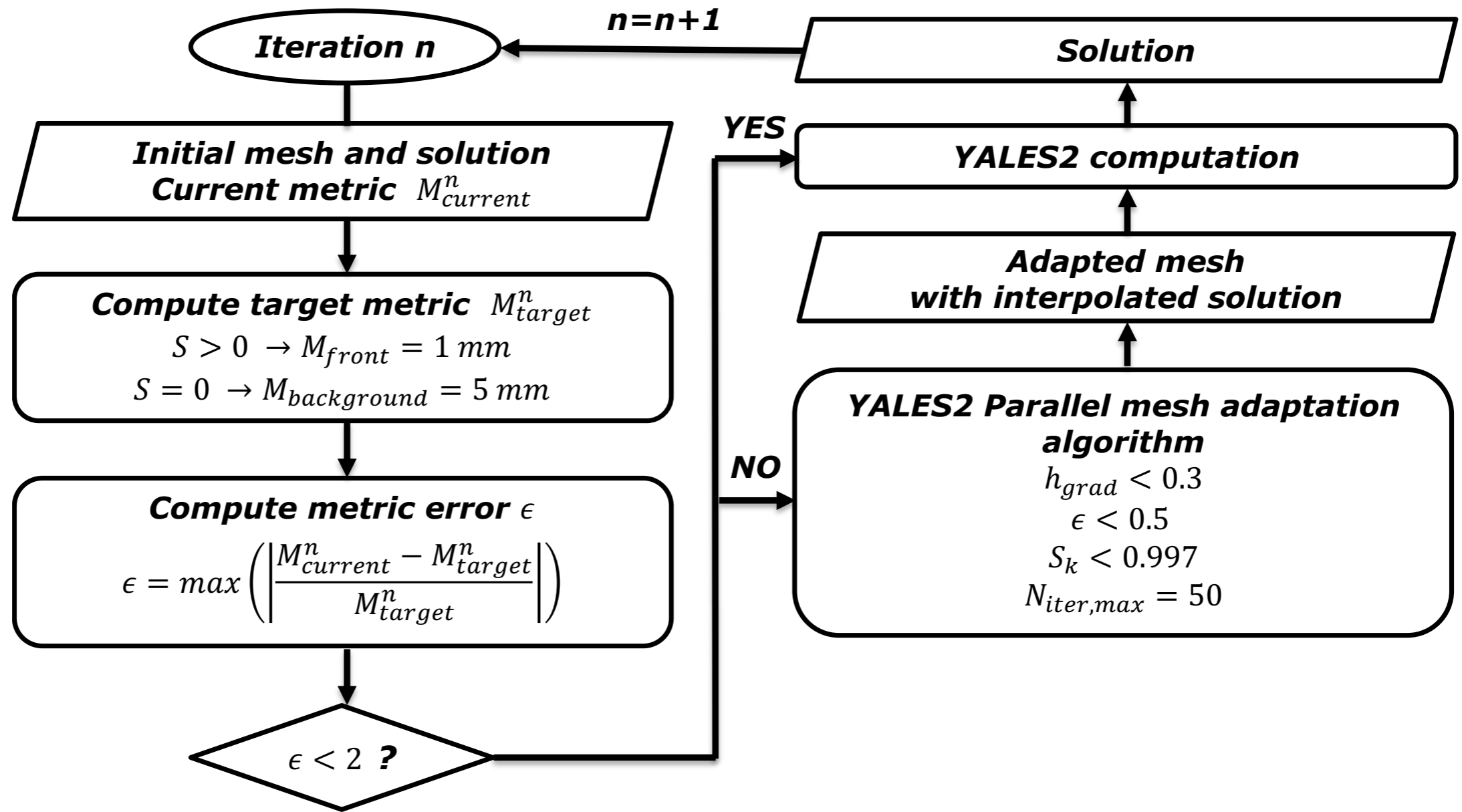
Propagation cells to prevent fluctuations and avoid unnecessary re-meshing



Propagation cells



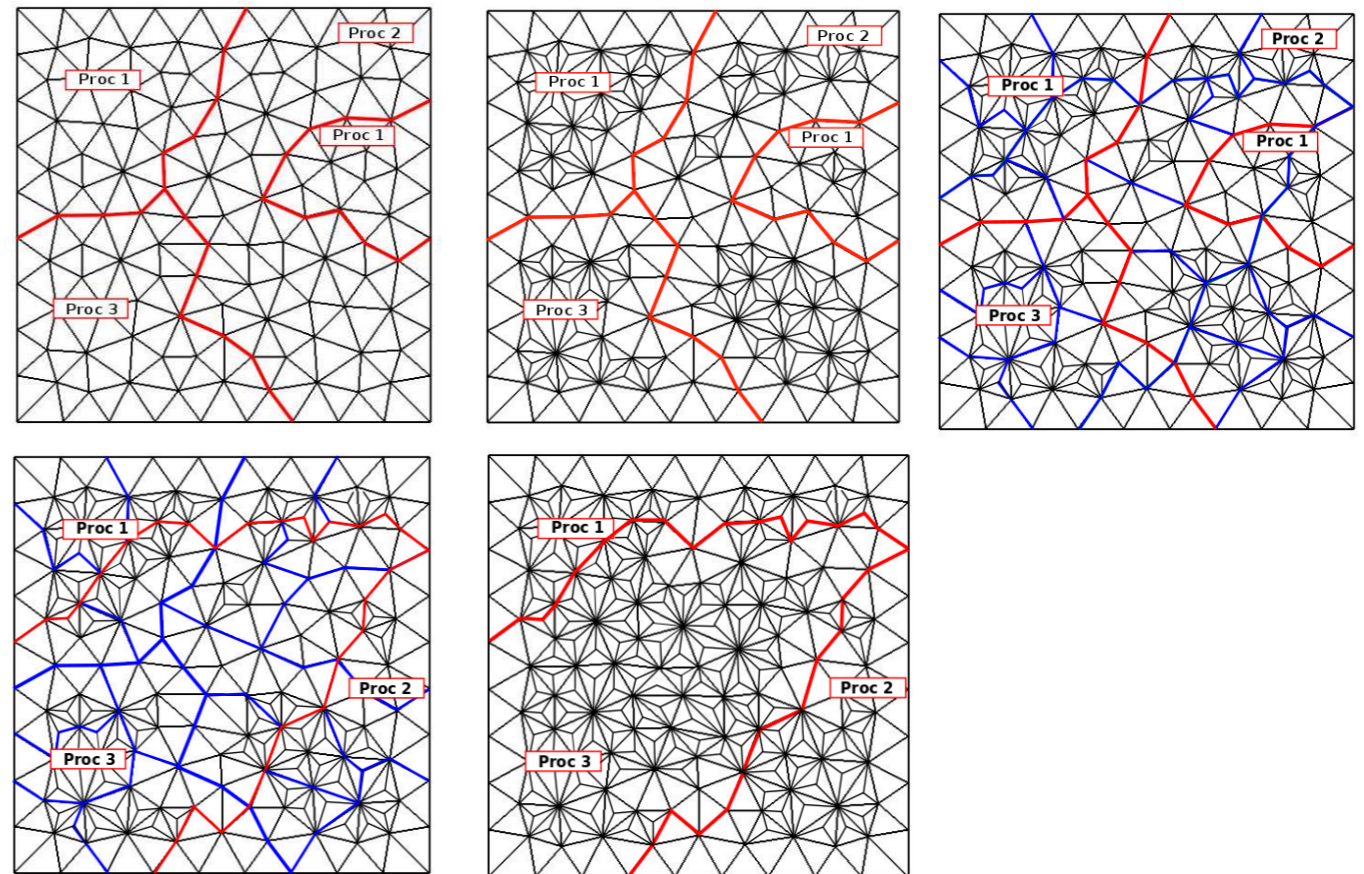
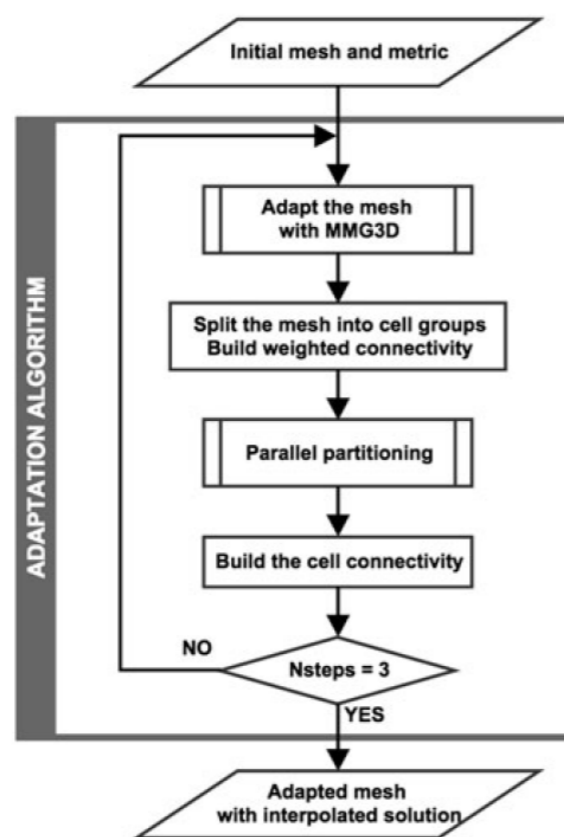
Mesh adaptation procedure ensures a refined mesh in flame region before computation at each iteration



The coupling between YALES2 and MMG3D allows the mesh to be adapted over the entire domain

MMG3D library: adaptation and optimisation of tetrahedral meshes

Problem : MMG3D does not allow remeshing on boundaries



Operational flexibility

Fuel flexibility

Simplified mGT layout

mHAT

Dry EGR

Wet EGR

3 diluted cases compared to

Typical NG combustion

50%_{vol} H₂ + $\Omega = 10\%$

\approx

100% CH₄

Energy (2022), EGY-123446

J. of Eng. for Gas Turbines and Power (2021), GTP20-1620

Tool developments

Adaptive Mesh Refinement

LES \times RANS (justify LES)

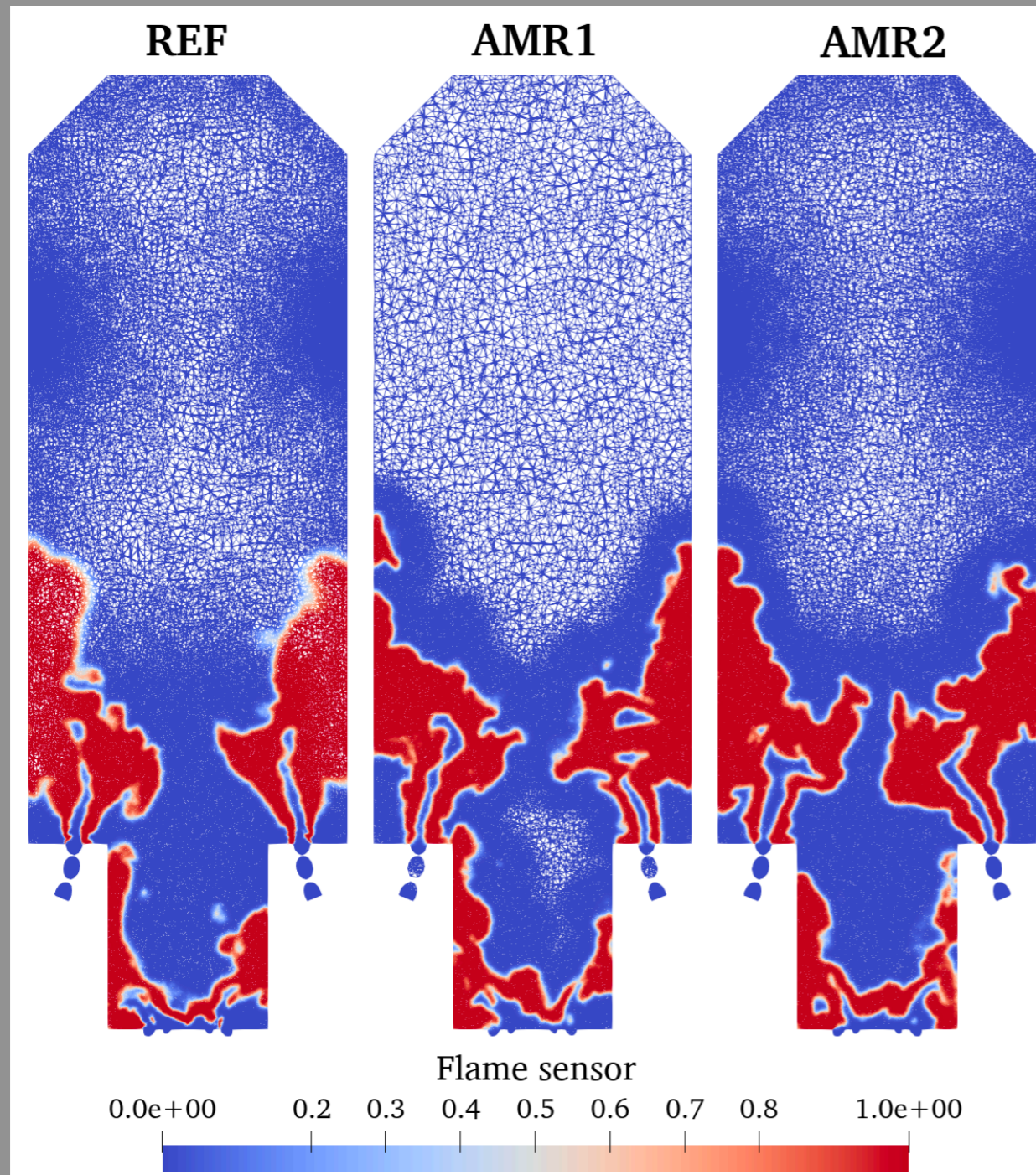
0D CRN / 1D Flame predet.



Adaptive Mesh Refinement

LES \times RANS (justify LES)

0D CRN / 1D Flame predet.



Dynamic adaptation in the flame region all along the simulation.

Refinement **criterium** based on the flame sensor (**reaction rate**) of the TFLES model.

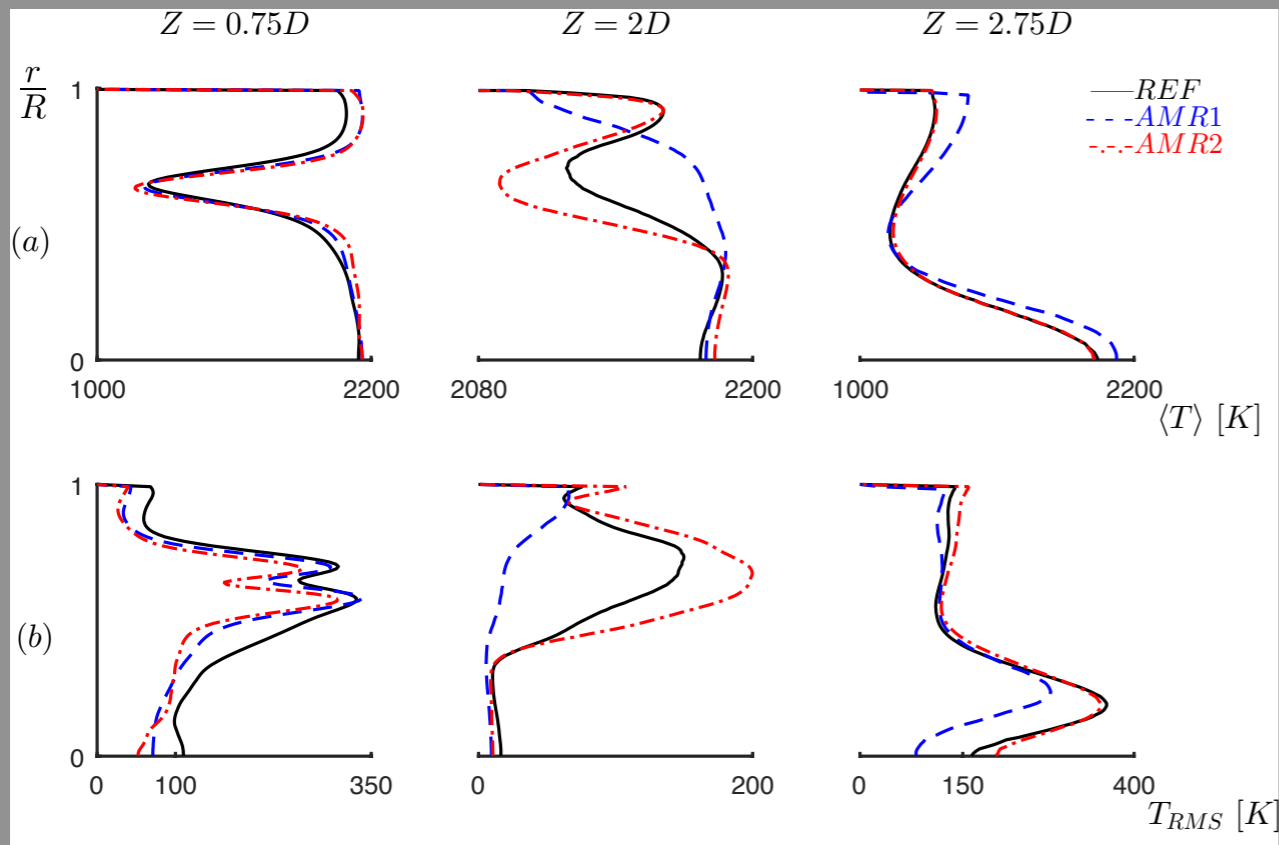
Triggering adaptation: **Error metric-based** (from the defined interface and background metrics).

REF: Initial mesh with a typical distribution - $33 \cdot 10^6$ cells

AMR1: Flame region refinement only - $19.6 \cdot 10^6$ cells

AMR2: Initial mesh + flame region refinement - $34.5 \cdot 10^6$ cells

Adaptive Mesh Refinement



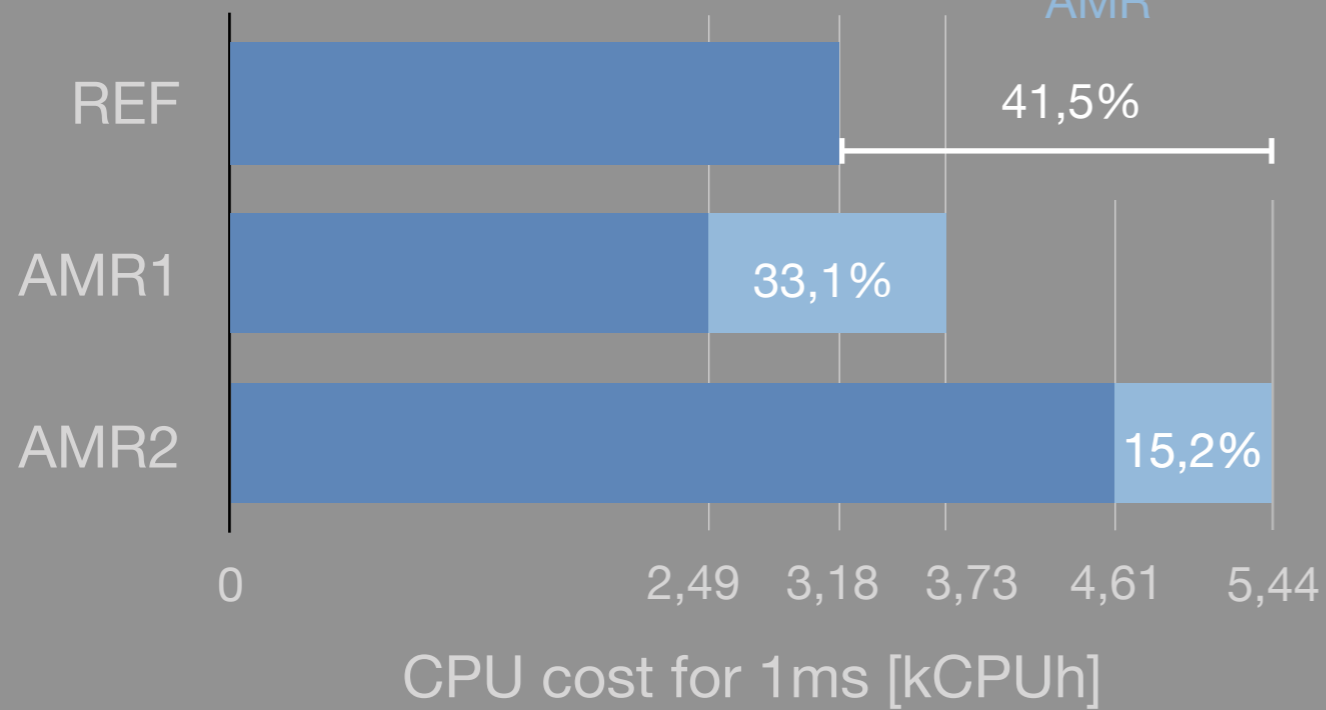
Main conclusions:

- Finer resolution of the flame for both AMR cases.
- AMR1 loses information after the flame.

	REF	AMR1	AMR2
$Y_{CO} [ppm]$	34	48	35

Adaptive Mesh Refinement

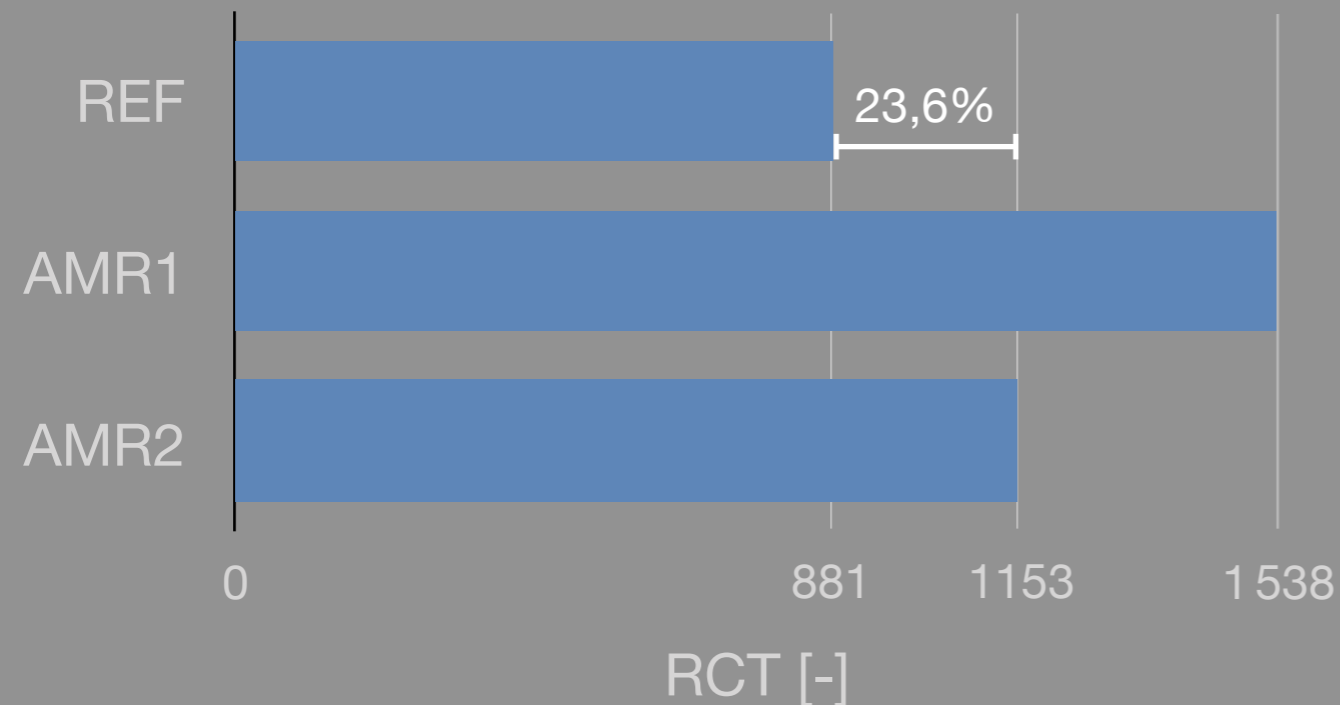
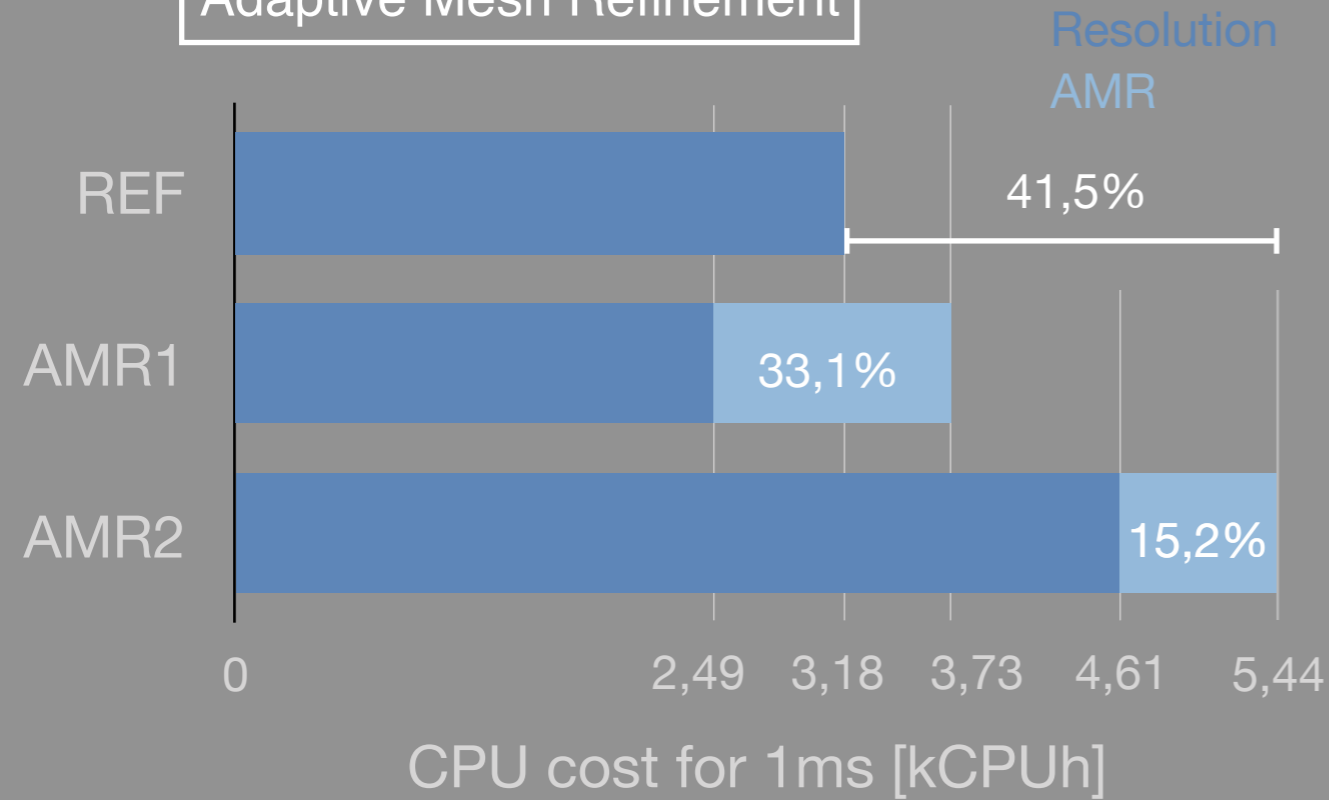
Resolution
AMR



Main conclusions:

- Finer resolution of the flame for both AMR cases
- AMR1 shows a lost of information after the flame
- **Adaption** for AMR2 costs only **15.2%** of the total cost.
- AMR2 case requires **41.5%** more than the REF case.

Adaptive Mesh Refinement



Main conclusions:

- Finer resolution of the flame for both AMR cases
- AMR1 shows a lost of information after the flame
- **Adaption** for AMR2 costs only **15.2%** of the total cost.
- AMR2 case requires **41.5%** more than the REF case.

Reduced Computational Time,

$$RCT = \frac{WCT \cdot N_{CPU}}{N_{iter} \cdot N_{node}}$$

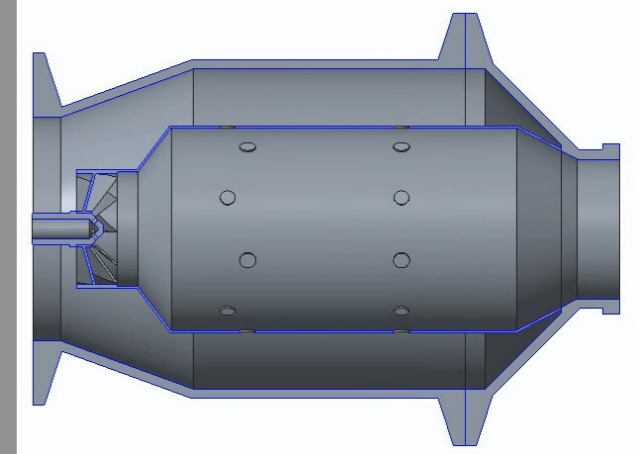
Tool developments

LES \times RANS (justify LES)

Aim: Justify LES in an industrial context (**RANS vs LES**).

Comparison RANS \times LES on **Enertwin MTT** (3kW mGT).

From collaboration with
University of Bolzano.



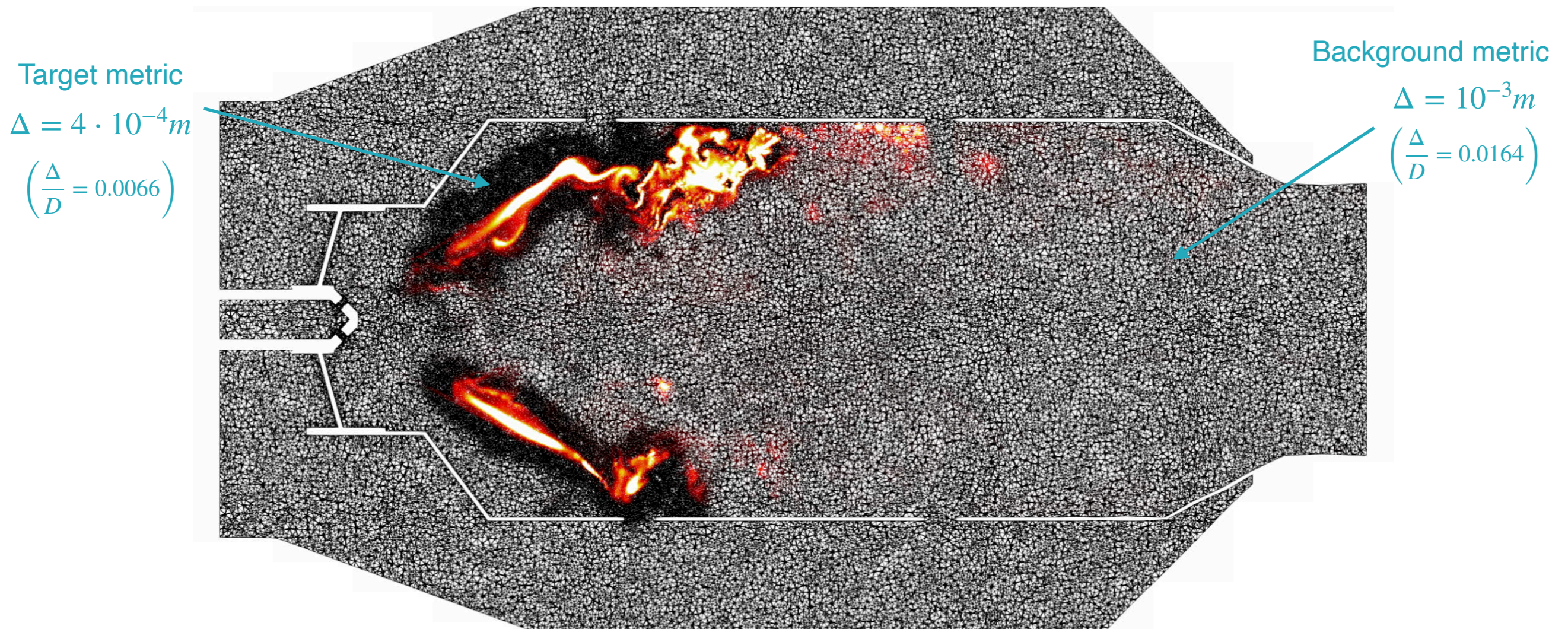
Tool developments

LES \times RANS (justify LES)

Aim: Justify LES in an industrial context (**RANS vs LES**).

Comparison RANS \times LES on **Enertwin MTT** (3kW mGT).

AMR implemented for the LES.



Numerical set-up summary to compare both methods

	RANS	LES
Mesh cell number ($\times 10^6$)	6.3	25
CFD code	ANSYS Fluent 19.1	YALES2
Turbulence model	k- ϵ Realizable	Sub-grid scale stresses model: Dynamic Smagorinsky
Combustion model	Partially Premixed with diffusion FGM	Complex chemistry + TFLES model
Kinetic scheme	DRM19	DRM19
Heat losses	Adiabatic condition	Adiabatic condition
Total CPU cost	480 CPUh for REF 1200 CPUh for Syngas	70560 CPUh for each case

Flame fronts of the reference case highlighted by the reaction rate iso-surface

