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Le supercalcul en appui à une combustion sûre & efficace

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Sept ans déjà …

- En 7 ans Myria a rendu de très bons et loyaux services. Austral va remplacer Myria mais la super équipe du CRIANN reste et ça donne confiance pour la suite.
- En 7 ans, mon équipe-projet a contribué à beaucoup d'études sur la combustion turbulente (ou pas). Une grosse dizaine de doctorants ont été formés au HPC grâce à Myria et après avoir fait avancer la recherche travaillent maintenant pour la plupart dans des centres de R&D ou ont lancé leur propre entreprise.
- Je ne pouvais pas résumer 7 ans de simulations sur Myria en 10 mn et je ne vais donc présenter que deux courtes pastilles :

1. La simulation d'un four industriel avec utilisation de l'apprentissage machine.
2. La rencontre d'une flamme hydrogène/air avec un choc.

Pourquoi étudier la combustion ?

Aspects sécurité

Incendie

- Sites industriels– problématique du stockage conduisant à une dangerosité accrue de feux par contagion (voir Lubrizol)
- Habitat, habitacle (très lié aux matériaux utilisés)
- Végétation (lien avec évènements climatiques : sécheresse, réchauffement)
- Feux de batteries

Conséquences

- Toxicité atmosphérique (dispersion de polluants et de suies, exemple explosion de citerne d'ammoniac à Dakar en 1992, 129 morts)
- Toxicité localisée avec pertes humaines ou animales (exemple incendie de bâtiments, habitats ou étables)
- Explosions facilitées (voir AZF en 2007, 30 morts)

Rôle de la combustion dans la stratégie nationale bas carbone

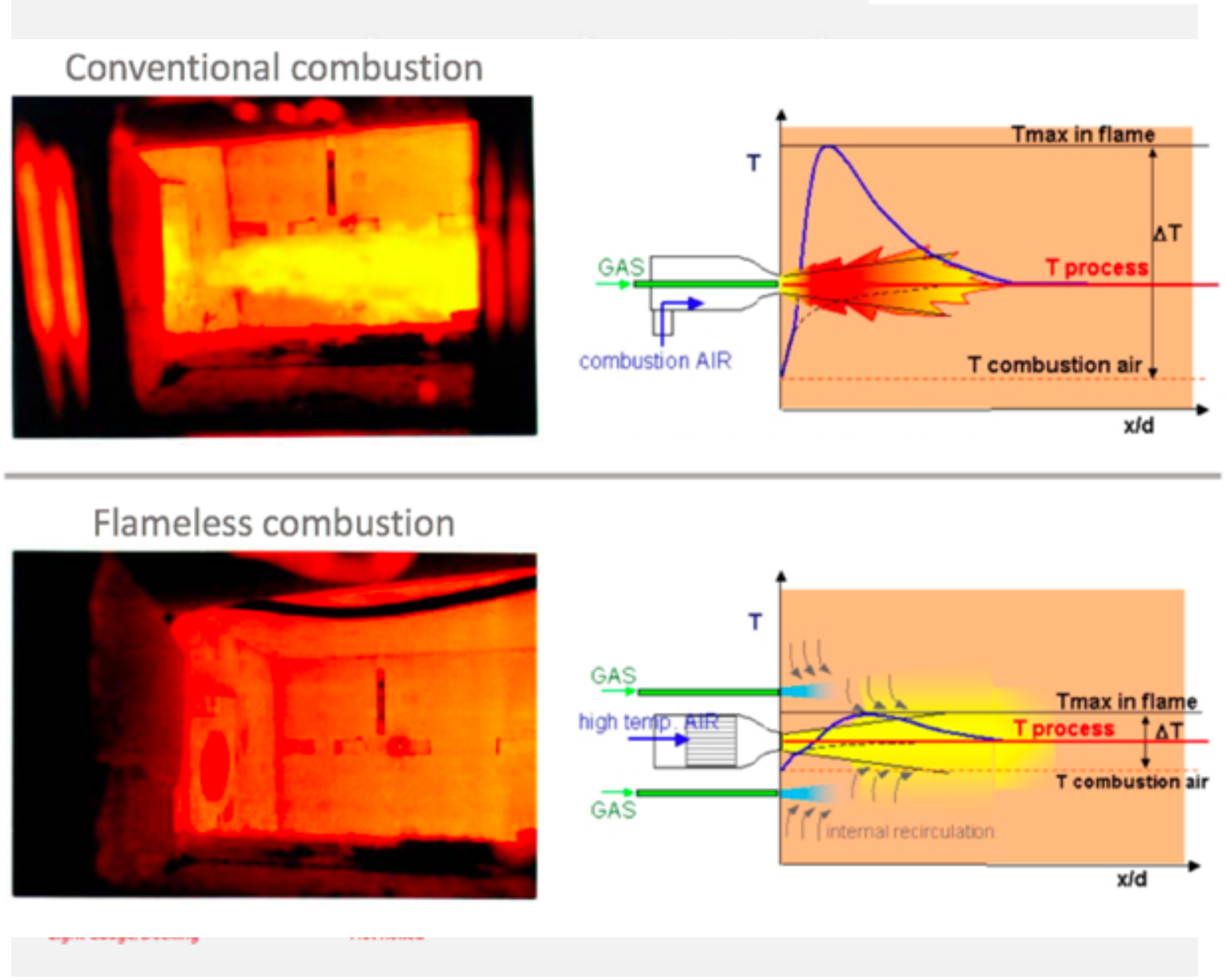
Exemple

- Hydrogène : utilisé seul ou en complément
- Structuration internationale, nationale (FRH2, …), régionale
- Mise en place de nombreux écosystèmes locaux
- Décarbonation de l'industrie, de la mobilité
- Forte augmentation des projets européens, nationaux (PEPR, ANR)
- Nombreux verrous scientifiques associés et aussi dangerosité par risque explosif

Sandvika, Norvège, 2019
Explosion d'une station d'hydrogène

Simulation d’un four industriel avec utilisation de l’apprentissage machine.

- **Context of decarbonization** of the energy production and of the **transformation industries**,
- Combination of fuel efficiency & more stringent regulation on emissions, such as NOx and particulate,
- **Recycling of any type of Low Carbon Fuel (LCF) gases produced on-site or by external parties**,
- Need to revisit many industrial combustion systems,
- **Multi-fuel injection** = promising way to transform recycled gases into additional useful energy,
- In **steel industry**, **LCF includes auto-produced by-product steel gases** (Coke Oven Gas (COG), Blast Furnace Gas (BFG), Basic Oxygen Furnace Gas (BOFG)), biogases and green hydrogen,
- For these applications, **burnt gases diluted combustion and flameless oxidation** seem a good choice,
- Design based on both experimental and numerical studies.



Ambrogio Milani, Alessandro Saponaro, et al. Diluted combustion technologies. IFRF Combustion Journal, 1:1–32, 2001.
Task Force on Techno-Economic Issues. Reduction of NOx emissions.

Simulation d’un four industriel avec utilisation de l’apprentissage machine.

Complex description of combustion chemistry in unsteady simulations using artificial neural networks (ANN) allows for performing multiple simulations to optimise burners and boilers, thanks to a CPU time kept to a minimum.

Objective: reproduce by LES the UMONS flameless furnace

Step 1: Develop a reduced chemistry including the specific high-dilution rates and heat-losses as observed in the UMONS furnace,

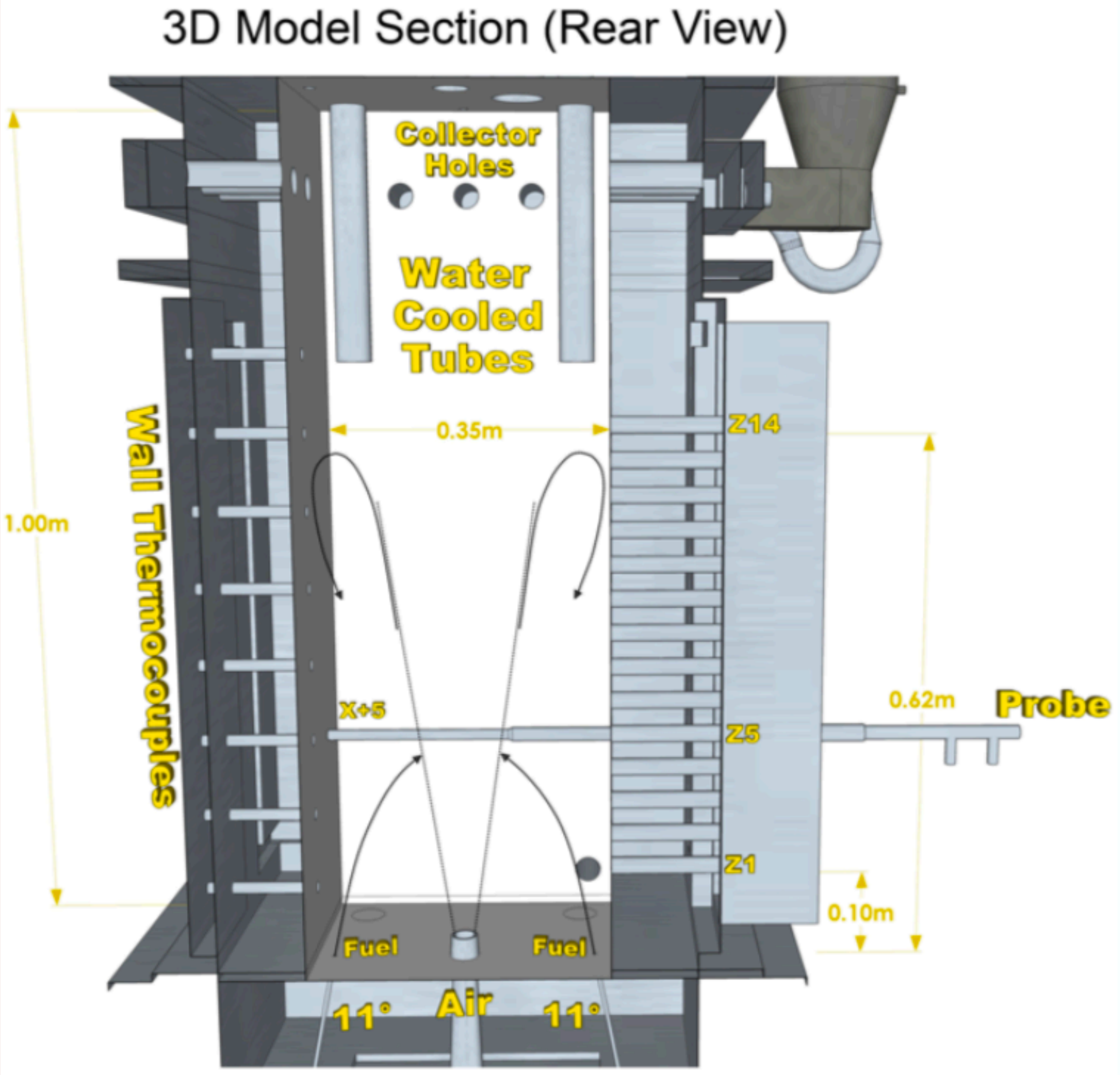
Step 2 : Couple the ANN described chemistry with Code Saturne,

Step 3: Compare the LES results to experimental measurements.

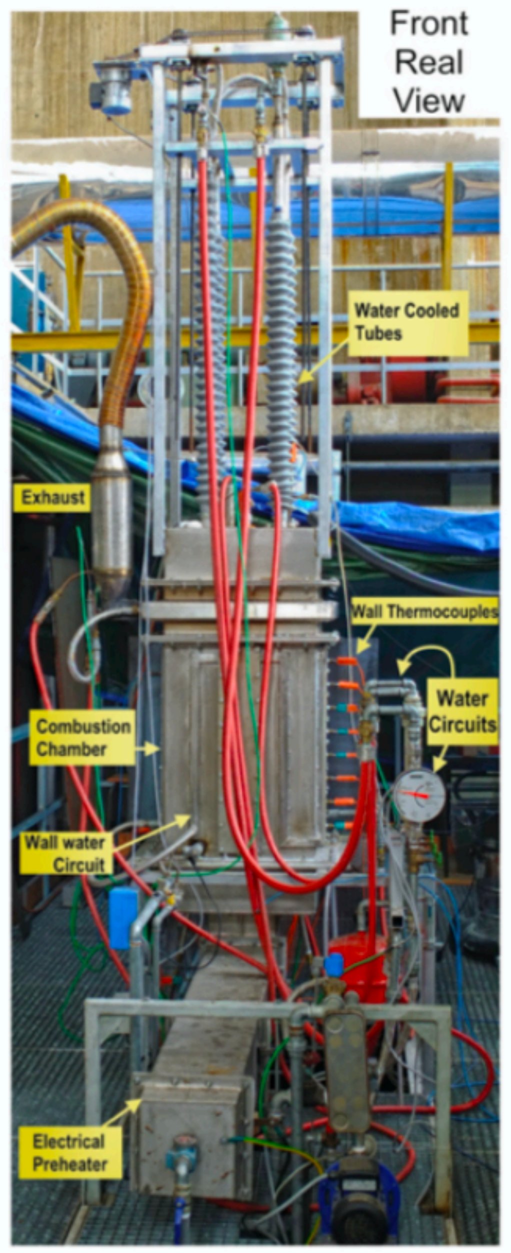
Le four de UMONS : description

Lab-scale furnace designed to mimic some of the main features of industrial furnaces, through the configuration of the injection of the gases, the global geometry of the enclosure, the amount of air preheating and the variable thermal charge.

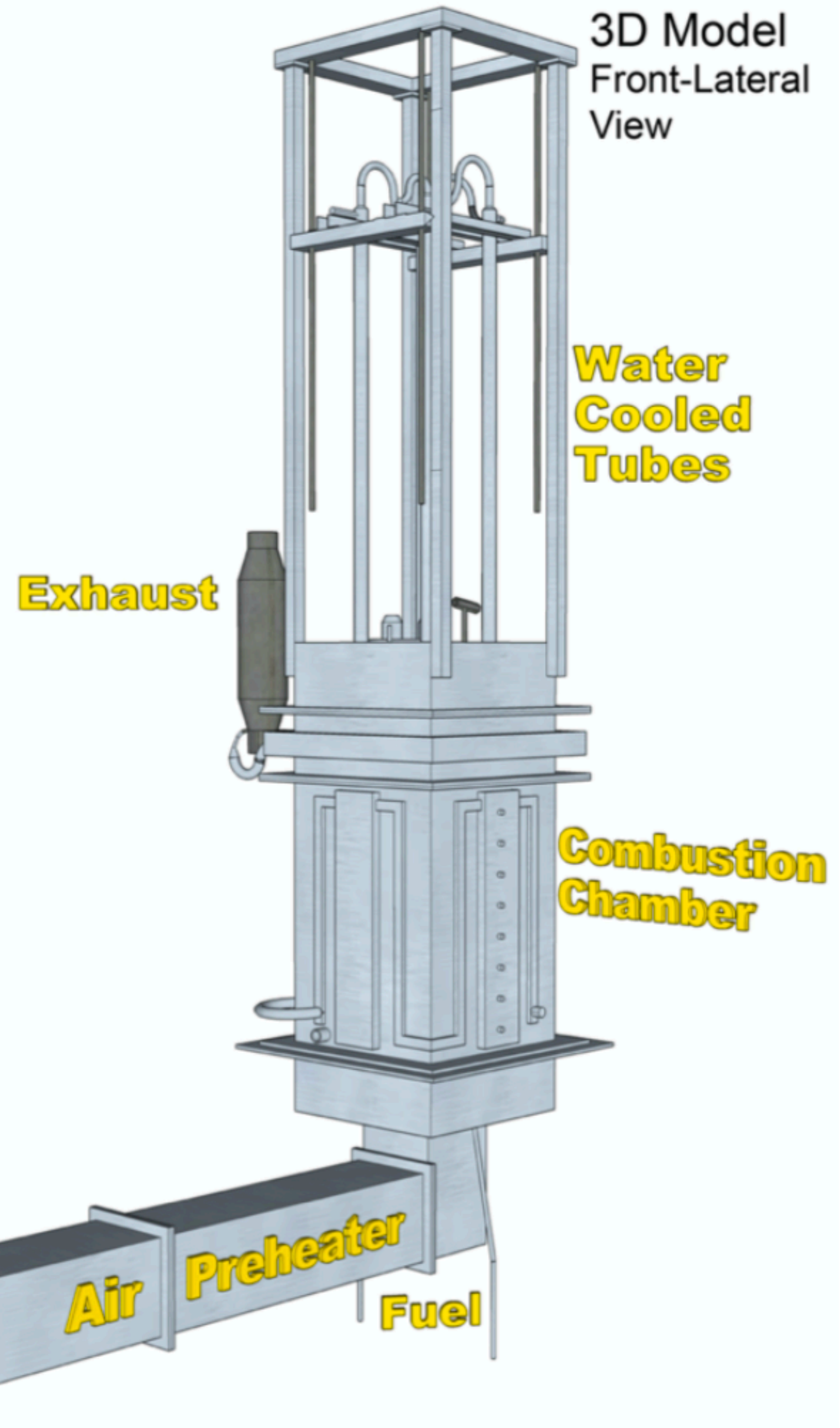
- **30kW pilot experiment: flameless combustion with high dilution of the reactants (air and fuel) by burnt gases and strong heat transfer,**
- Radiative transfer = ~ 80% of the total heat transfer,
- **Square inner section of 0.35m × 0.35m for 1.0m high**
- Air injection (reheated up to 800°C) in the center of the bottom wall surrounded by two gas injectors with 11° tilt angle (fuel: B50),
- **Thermal charge and furnace temperature controlled through four water cooling tubes plus a reduced water circuit along the outer walls,**
- A side wall (on the right) equipped with **eight S-type thermocouples to provide a wall temperature profile** in the vertical symmetry plane containing the air and gas injectors,
- **Fourteen probes** inserted inside the furnace on the wall opposite to the thermocouples wall, to measure the temperature and species concentration of **O_2, CH_4, CO_2 and CO** (on dry basis) by paramagnetic and infrared **gas analysers**. Measurement of **H_2 and N_2** and additional measurements of O_2, CH_4 and CO were realized by a **gas chromatograph**.



3D Model Section (Rear View)



Front Real View



3D Model Front-Lateral View

G. Mosca, Experimental and numerical study on MILD combustion of low LHV fuels, PhD thesis, Polytech de Mons (2017).

G. Mosca, D. Lupant, P. Lybaert, Effect of increasing load on the MILD combustion of COG and its blend in a 30 kW furnace using low air preheating temperature, Energy Procedia 120 (2017) 262–269.

Réduction d'un mécanisme cinétique pour la combustion sans flamme

Build a training data base (stochastic particle evolution) with GRI 3.0:
Each particle carries information on the species mass fraction vector and enthalpy. From this non-premixed initial condition, the stochastic particles evolve in time according to:

$$\begin{aligned}\frac{\partial Y_k^p(t)}{\partial t} &= \mathrm{MIX}^p(\tau_\mathrm{T}) + \dot{\omega}_{Y_k}^p \ , \\ \frac{\partial h_s^p(t)}{\partial t} &= \mathrm{MIX}^p(\tau_\mathrm{T}) + \dot{\omega}_{h_s}^p + \alpha_{loss}(T_p - T_{wall}) \ .\end{aligned}$$

Chosen such that Teq between 1200 and 1500K

Averaged wall temperature from experiment: 1249,4 K

Identification of the species relevant to capture the thermo- chemistry with direct relation graph with error propagation analysis (DRGEP): **14 species** H_2, H, O, O_2, OH, H_2O, HO_2, CH_3, CH_4, CO, CO_2, HCO, CH_2O and N_2.

These species mass fractions and the temperature serve as input to the neural networks, which are trained to return their increments, or source terms, for a given time step. Meaning that 14 scalars will be solved in LES.

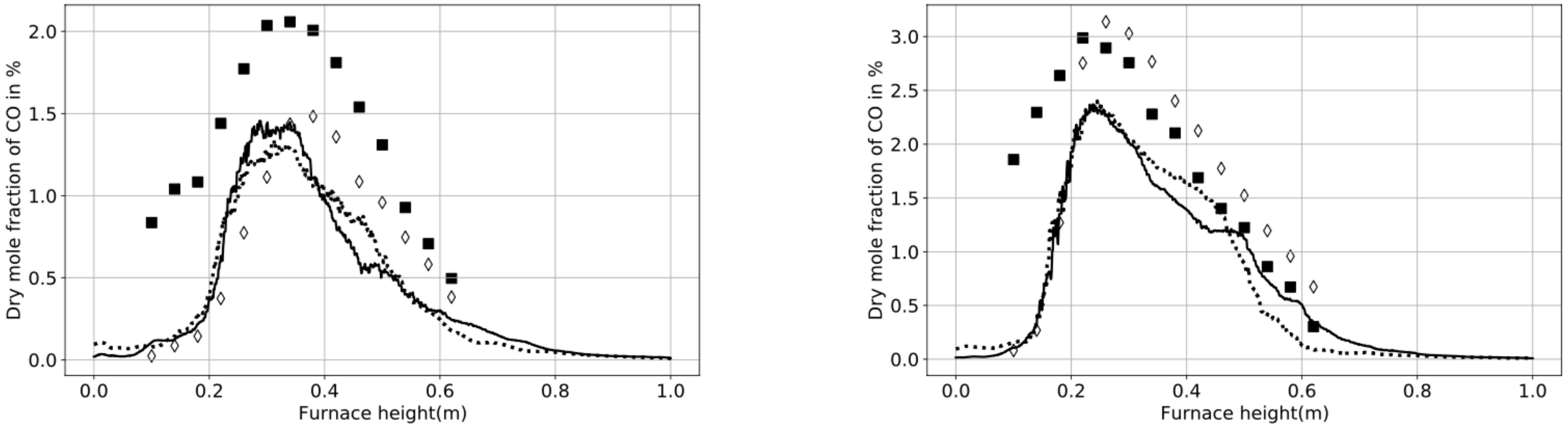
Inlet	B50	Air	Recirculation
$X_{\mathrm{CH_4}}$ (molar fraction)	0.1425	-	-
$X_{\mathrm{H_2}}$	0.325	-	-
$X_{\mathrm{N_2}}$	0.28	0.79	0.696219
$X_{\mathrm{O_2}}$	-	0.21	0.0175578
$X_{\mathrm{CO_2}}$	0.12	-	0.112496
X_{CO}	0.1325	-	-
$X_{\mathrm{H_2O}}$	-	-	0.173727
T(K)	290.65	1075.66	1300
Mass flow rate (kg/s)	0.002572941	0.010293228	0.064330844
Pressure (Pa)	101325	101325	101325

Training of the ANNs with Tensorflow 2 with GPU support (NVIDIA GeForce GTX 1080 Ti)

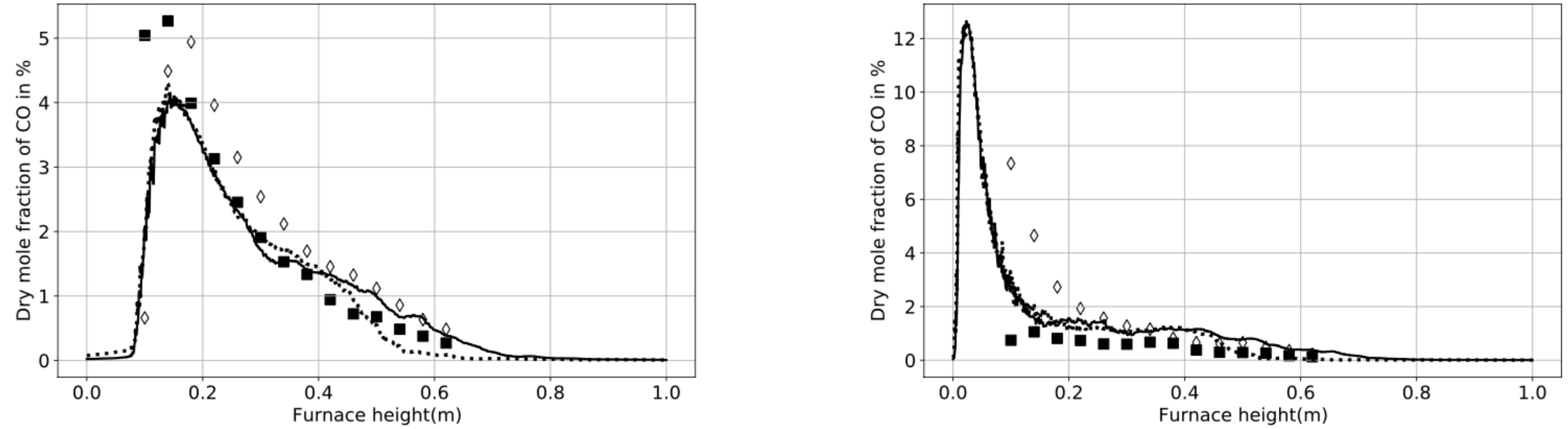
Clustering with K-means (K- means++ algorithm) necessary due to the complexity of the setup (increase the CPU time of the training but not the LES CPU cost)

Comparaison LES / Experiment

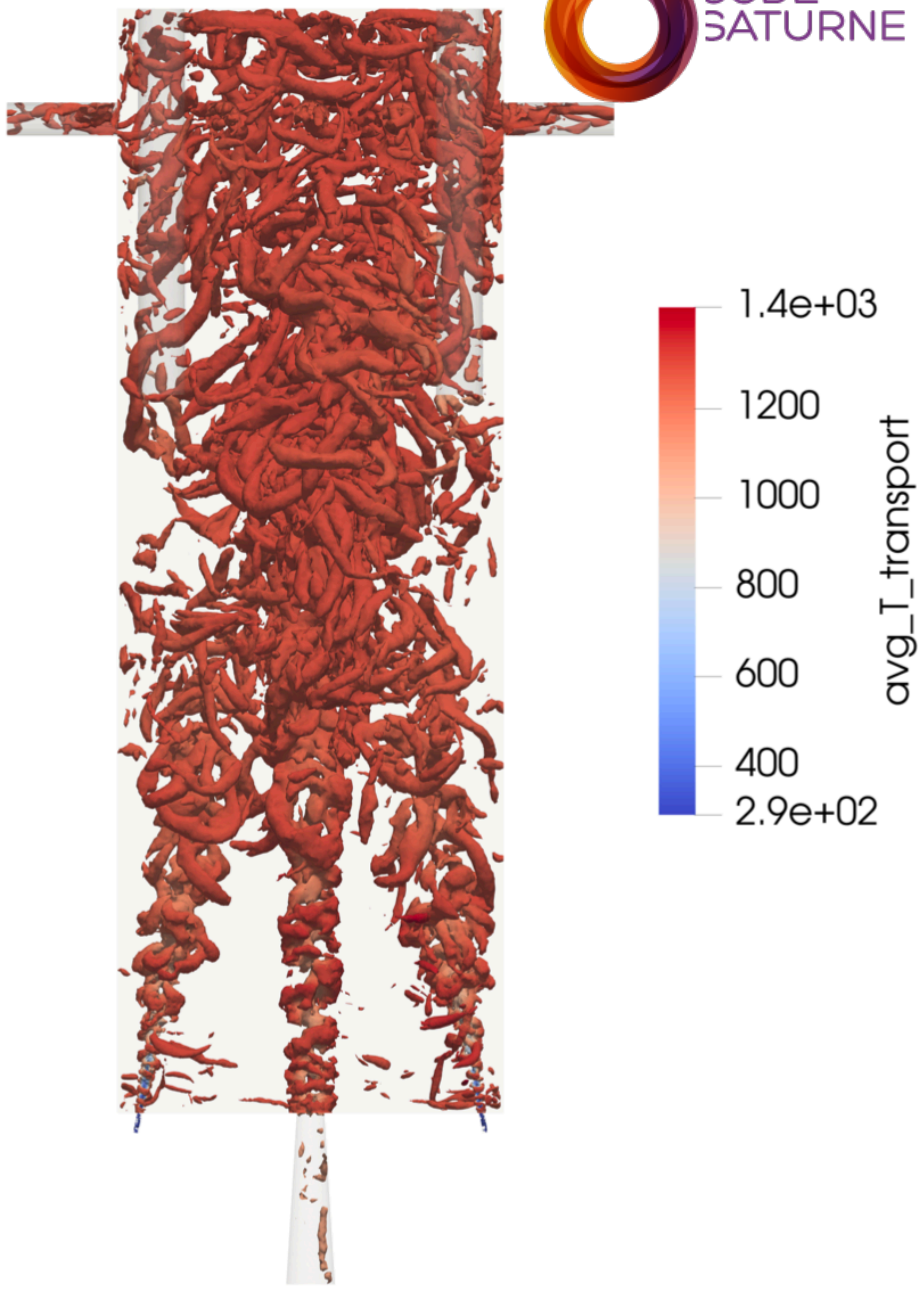
Experimental (symbol) and simulated vertical profiles of mean CO in volume percentage on dry basis. Dashed line and empty symbols: $x < 0$ (left side of furnace). Line and symbols: $x > 0$ (right side). Maximum measurement uncertainty is 0.28%.



(a) x= ±0.06 (b) x= ±0.09



(c) x= ±0.12 (d) x= ±0.15



Instantaneous iso-surface of Q criterion $Q = 6.10^5 s^{-2}$, colored by time-averaged temperature.

Simulation d'un four industriel avec utilisation de l'apprentissage machine / conclusion

- Application of **neural networks** for introducing complex combustion chemistry **in Large Eddy Simulation of flameless combustion.**
- Storing the species mass fraction increments, **the neural networks both reduce and pre- integrate stiff chemical systems**, allowing for performing the **complex chemistry simulations at a very moderate CPU cost (nearly no over-cost compared to a non-reactive simulation).**
- The numerical results compare well with experiments, which is very encouraging considering the low computing cost of these simulations. **However, to fully conclude on the validity and the robustness of this approach, additional test cases need to be considered, also including measurements of emissions such as NOx.**

Large-Eddy Simulation of flameless combustion with neural-network driven chemistry, Huu-Tri Nguyen, Camille Barnaud, Pascale Domingo, Luc Vervisch, Phuc-Danh Nguyen

Applications in Energy and Combustion Sciences (2023)

Interaction entre un choc et une flamme

Hydrogen is a key ingredient to the energy transition:
- Supposing it is produced in an eco-friendly process,
- No green house gases emissions during combustion,
- Can be used to produce electricity (fuel cell),
- Can store surplus of renewable energy from solar or wind farms.

Green Hydrogen

Even produced with an eco-friendly process:
- Highly flammable,
- High susceptibility to leaks resulting in explosion.

Cons


Courtesy of Gangwon Fire HeadQuarter

Hydrogen station, South Korea, 2019

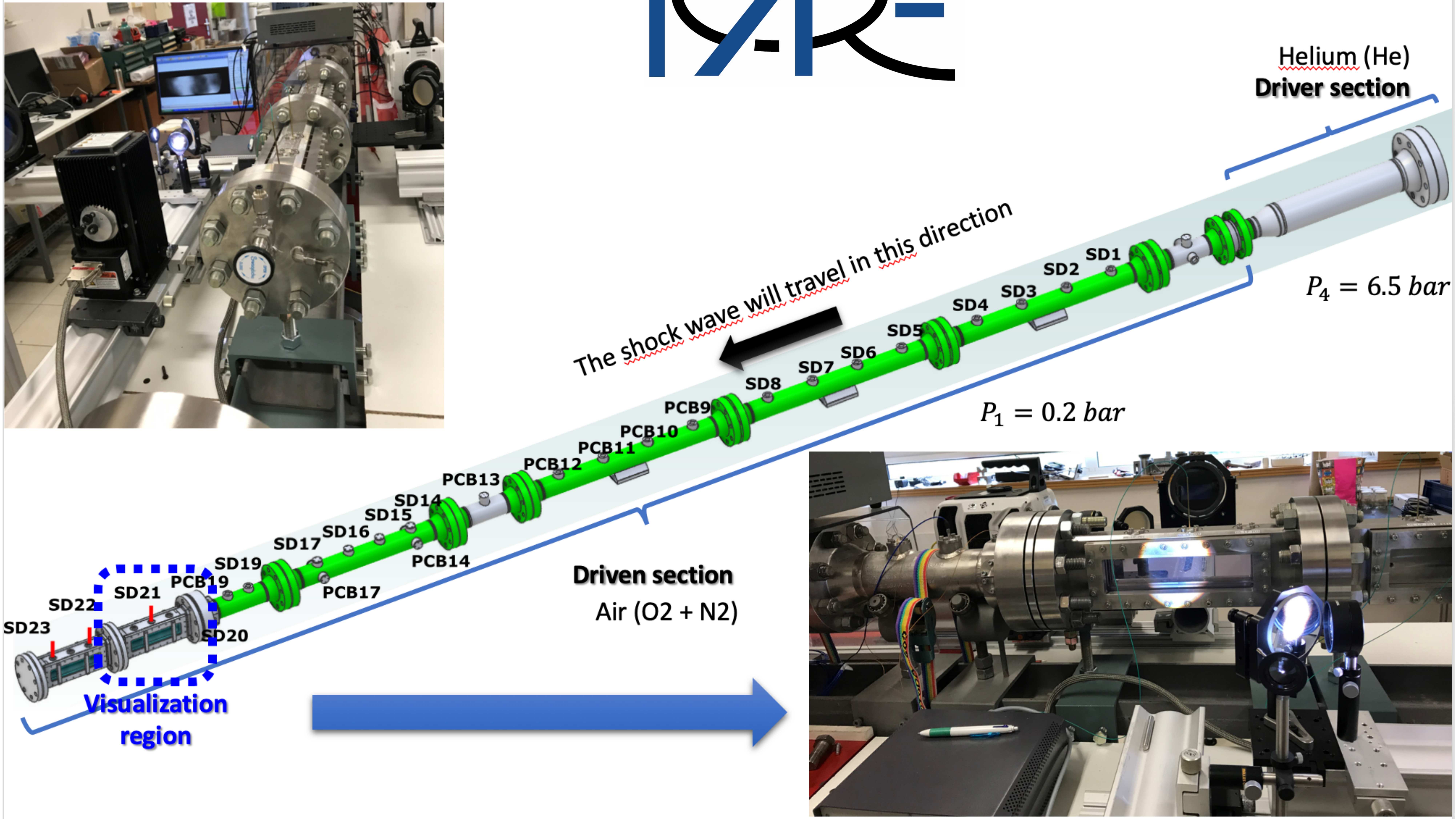
The prediction of such a scenario by numerical simulation is therefore necessary in the prevention of disasters.

Oran E. (2015) Understanding explosions - From catastrophic accidents to creation of the universe. Proc. Combust. Inst. 35(1): 1–35.

[redacted]

E. Yhuel, G. Ribert, P. Domingo, Numerical simulation of laminar premixed hydrogen-air flame flame/shock interaction in a semi-closed channel International Symposium of combustion, Vancouver 2022

FSI in a centimetric shock tube: experimental set-up (ICARE, Orléans)



Helium (He)
Driver section

$P_4 = 6.5\ bar$

The shock wave will travel in this direction

$P_1 = 0.2\ bar$

Driven section
Air (O2 + N2)

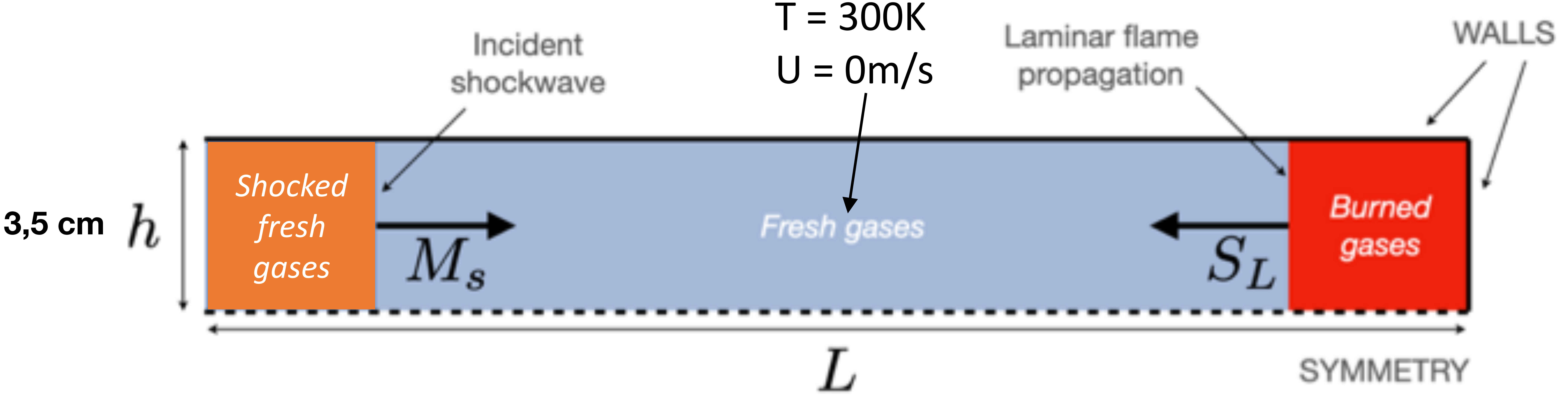
Visualization region

FSI in a centimetric shock tube: numerical set-up

Mach	1.4	1.9
Pressure (kPa)	42.4	80
Temperature (K)	376	483
Velocity (m/s)	227	455

Mixture	H2 - Air
Mechanism	San Diego 9 species, 23 reactions [1]
Equivalence ratio ϕ	0.8
S_L (m/s)	1.77

[1] https://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html



ADIABATIC / ISOTHERMAL (300K) NOSLIP

P = 20kPa
T = 300K
U = 0m/s

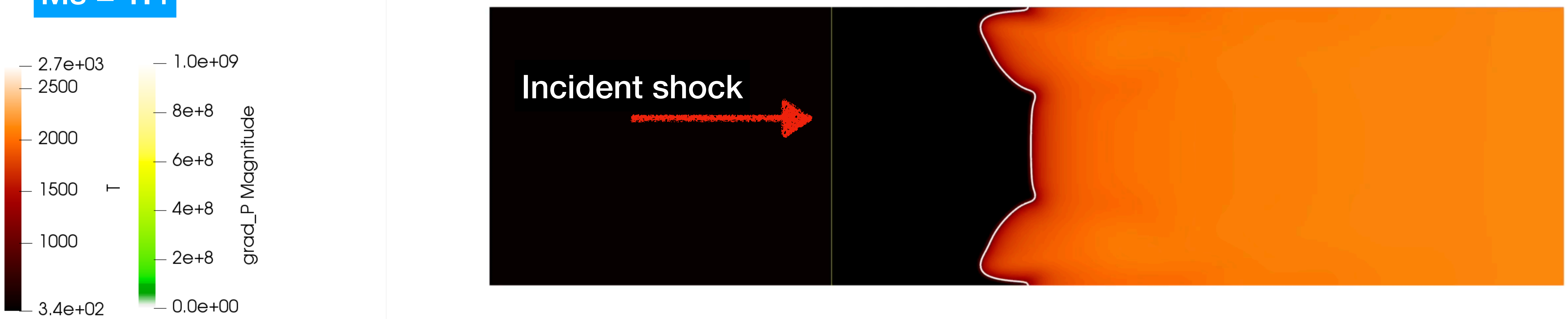
2D Parametric study (16 simulations):

- Two values of the Mach number (1.4 and 1.9) for the incident shock,
- Two initial shapes of the flame (tulip or glove finger) interacting with the incident shock,
- Unity Lewis number for all species versus complex transport properties,
- Cool wall at 300 K versus adiabatic wall condition.

Regular mesh distribution: 31,25 microns
Code: SiTComB

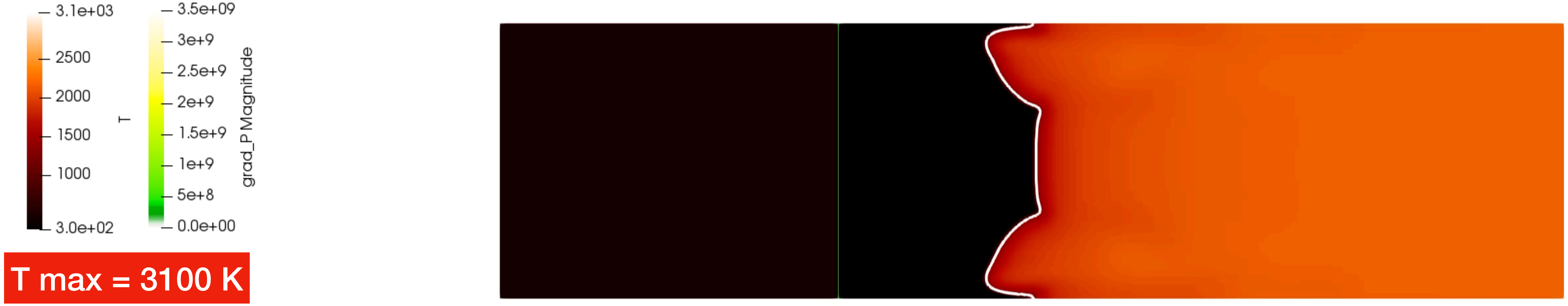
Shock addition: Incident shock Mach number 1.4 & 1.9

Ms = 1.4



T max = 2700 K

Ms = 1.9



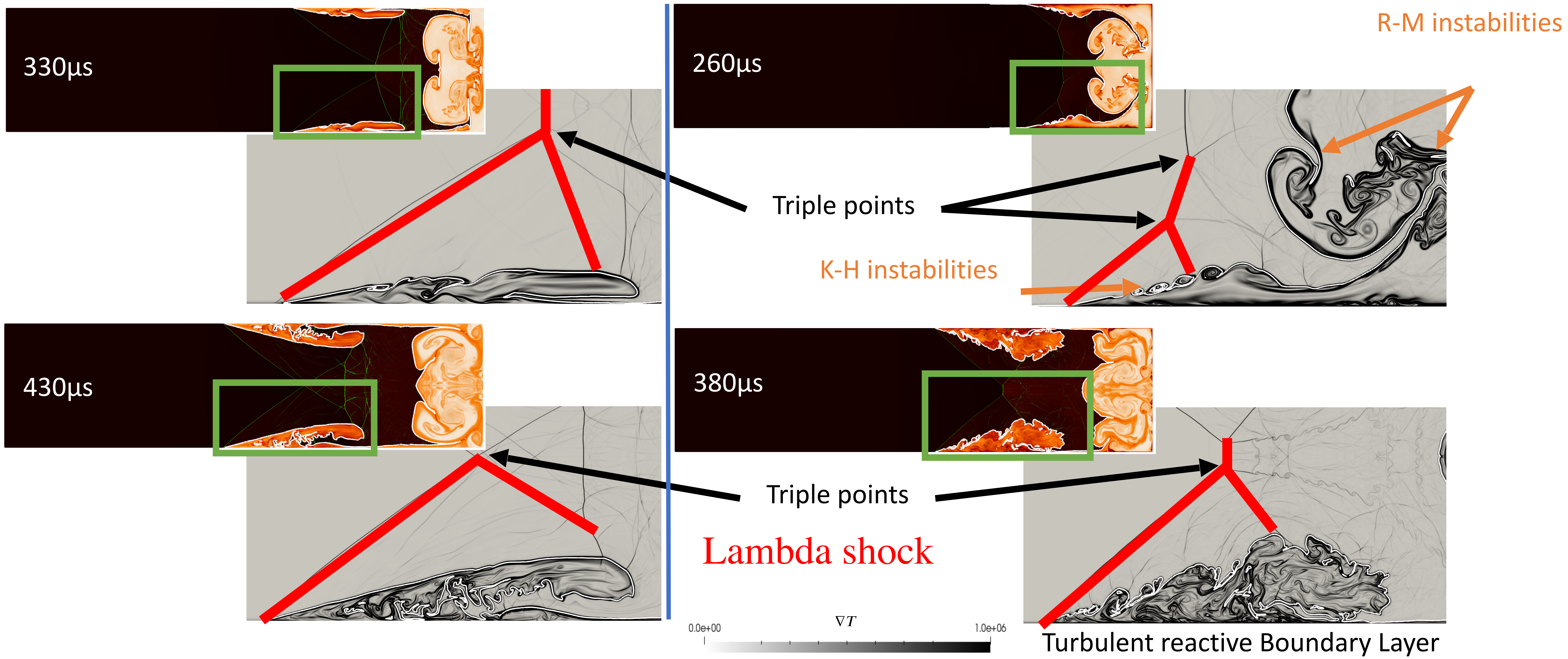
T max = 3100 K

Adiabatic versus isothermal walls (complex transport)

Ms=1.9

ADIABATIC

ISOTHERMAL



R-M instabilities

Triple points

K-H instabilities

Triple points

Lambda shock

Turbulent reactive Boundary Layer

White line : c=0.5

[6] E. Oran et al., Combustion and Flame, Vol 126, 2001

Le futur …

- Flamme/choc : comparaison avec l’expérience et étude détonation
- Apprentissage machine et combustion : Digital twins
- Oxydes d’azote et combustion de l’hydrogène
- Propulsion supersonique
- …..

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