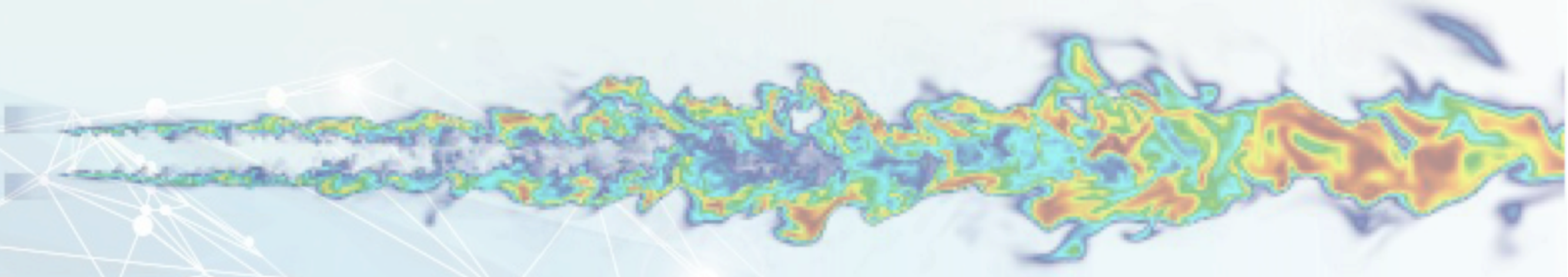
CERFACS

EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Large Eddy Simulation of turbulent reacting flows: methods & applications



B. Cuenot & the CFD team*, *Cerfacs*

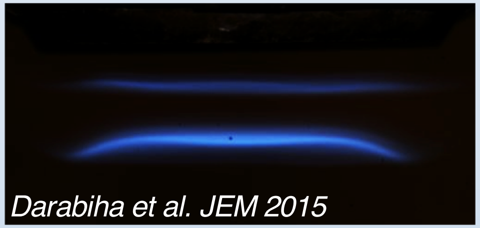
* T. Poinsot, L. Gicquel, O. Vermorel, F. Duchaine, E. Riber, A. Dauptain, G. Staffelbach, J. Dombard, A. Misdariis, C. Lapeyre

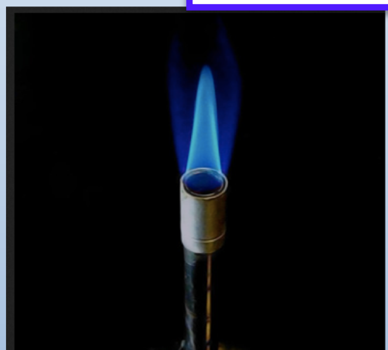
Objectives & methodology

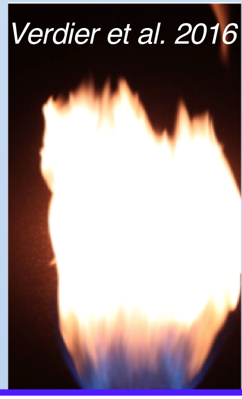
The objective is to provide accurate and reliable predictions of combustion in real conditions

Safran Silvercrest

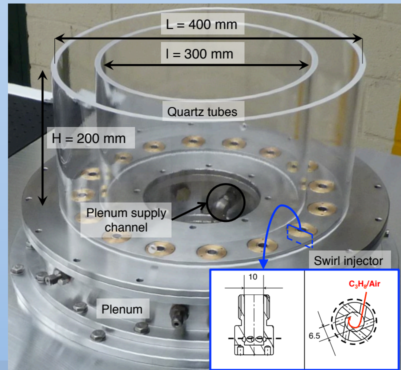
Objectives & methodology


Darabiha et al. JEM 2015

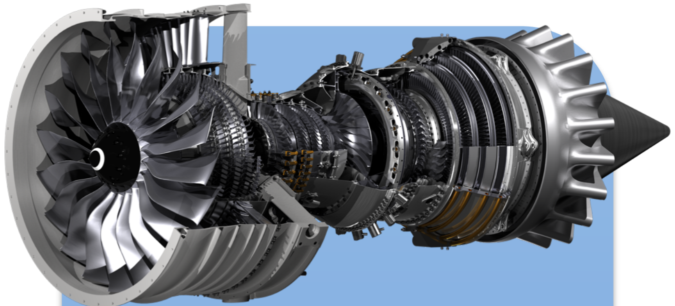


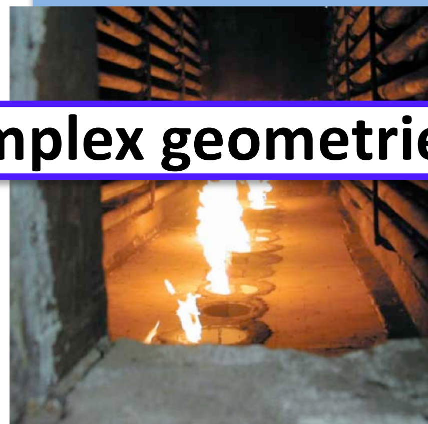

Verdier et al. 2016

From simple laminar flames to complex geometries



J-F. Bourgouin et al., C&F (2013)
M. Philip et al., PCI (2014)



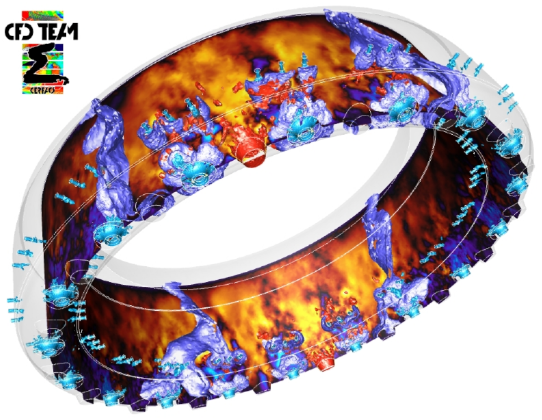


Involved physics

Complex burner geometries

Multiple combustion regimes

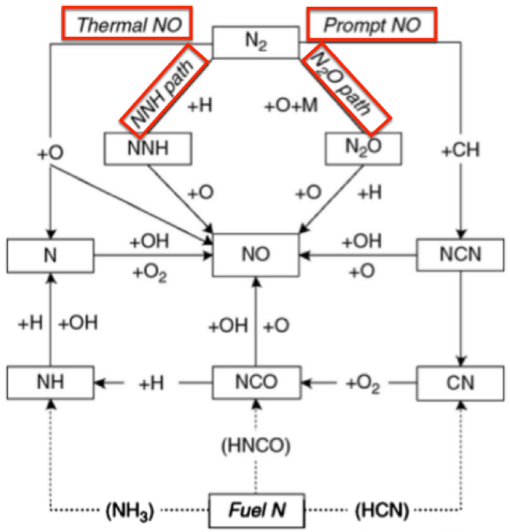
Turbulence and turbulent flame structure



Flame and Pollutant chemistry

Complex chemical processes

Multiple Timescales

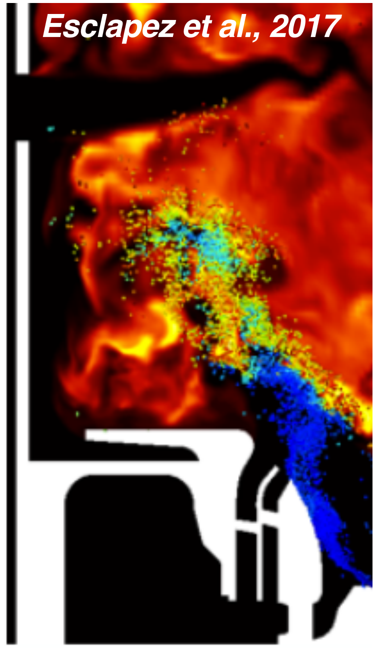


From Gas Turbine Emissions, 2013

Two-phase flow

Spray physics

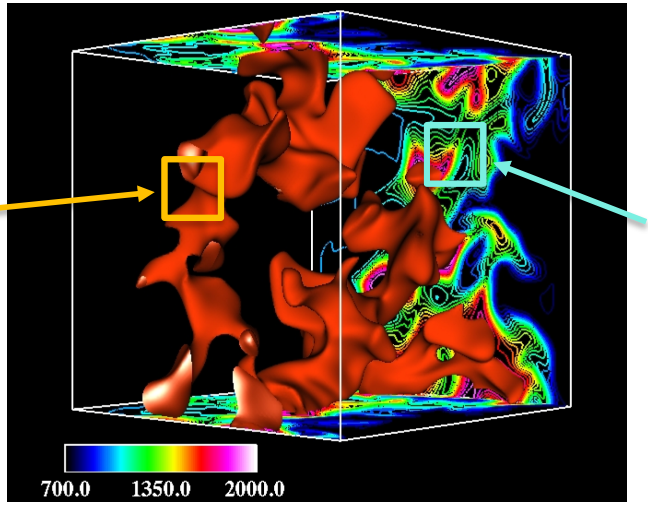
Spray flame



Turbulent combustion modeling

Flame front scales

- Thickness δ
- Laminar speed S_L



Turbulence scales

- Integral scales : L , u'
- Komogorov scales : η, u'_η

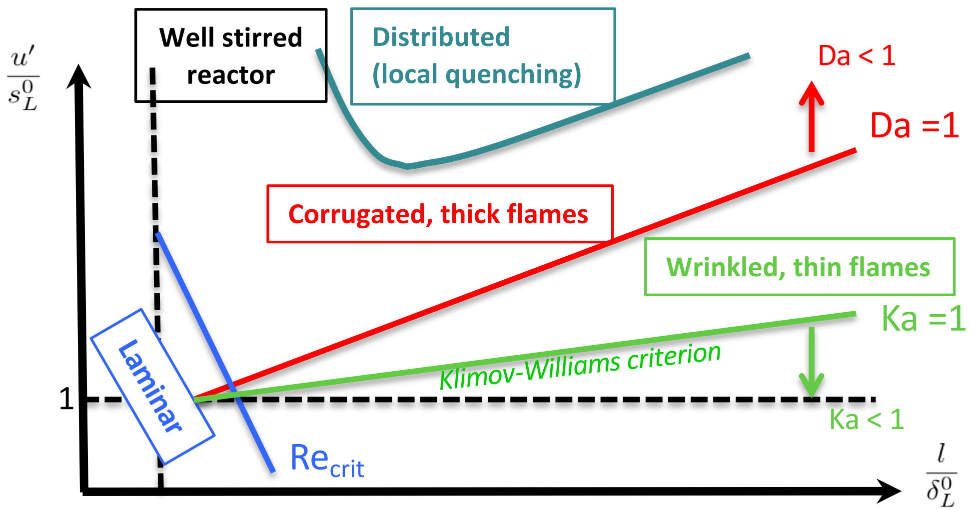
Flame-turbulence interaction

+ wrinkling

$$\boxed{\frac{S_T}{S_L^0} = \frac{A_T}{A}}$$

+/- stretching

- quenching



Combustion regime diagram

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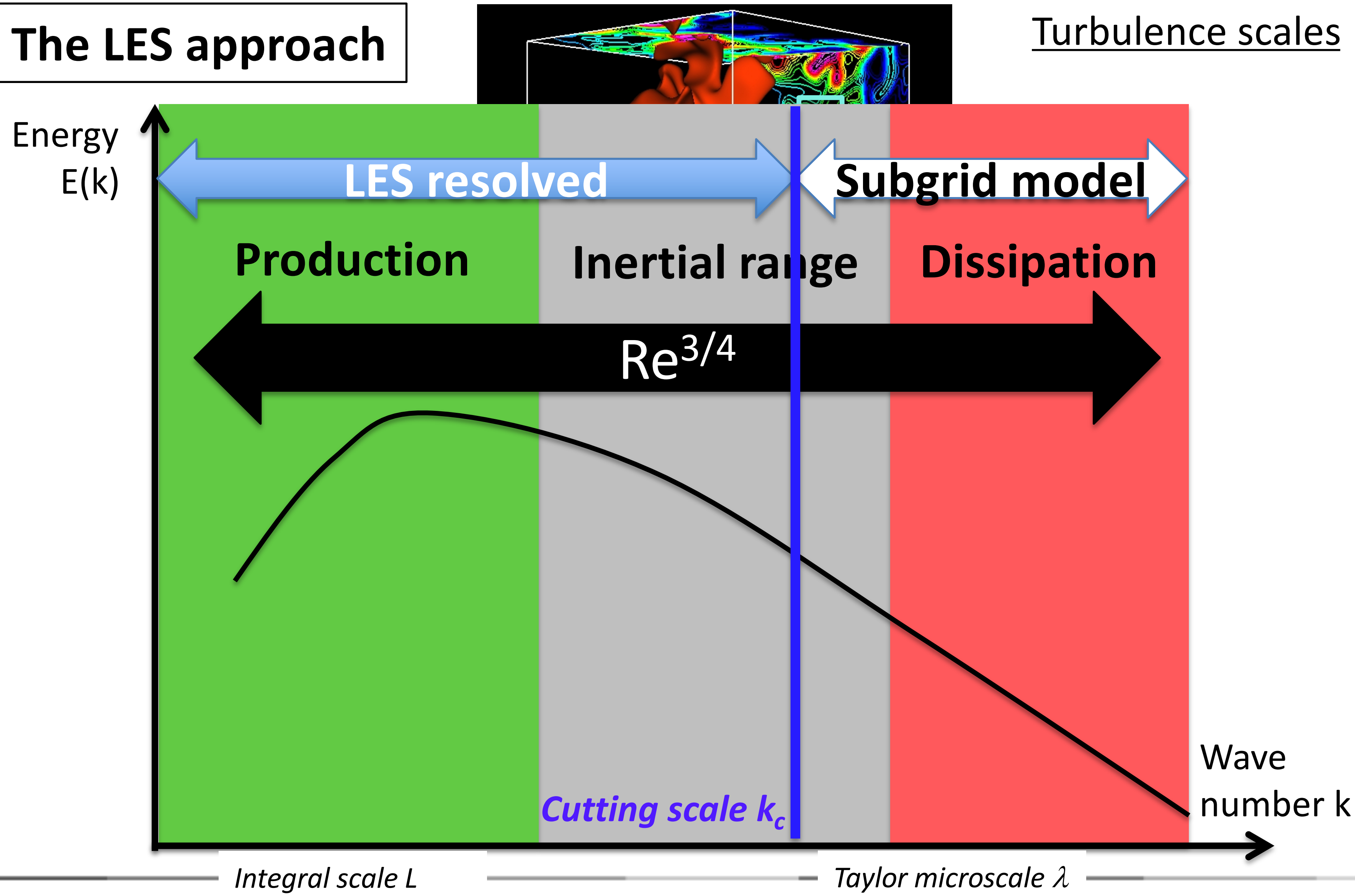
Turbulent combustion modeling

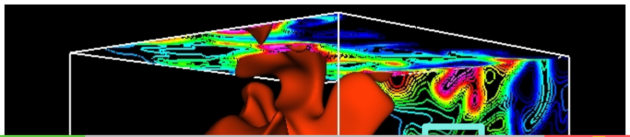
The LES approach

<u>Turbulence scales</u>

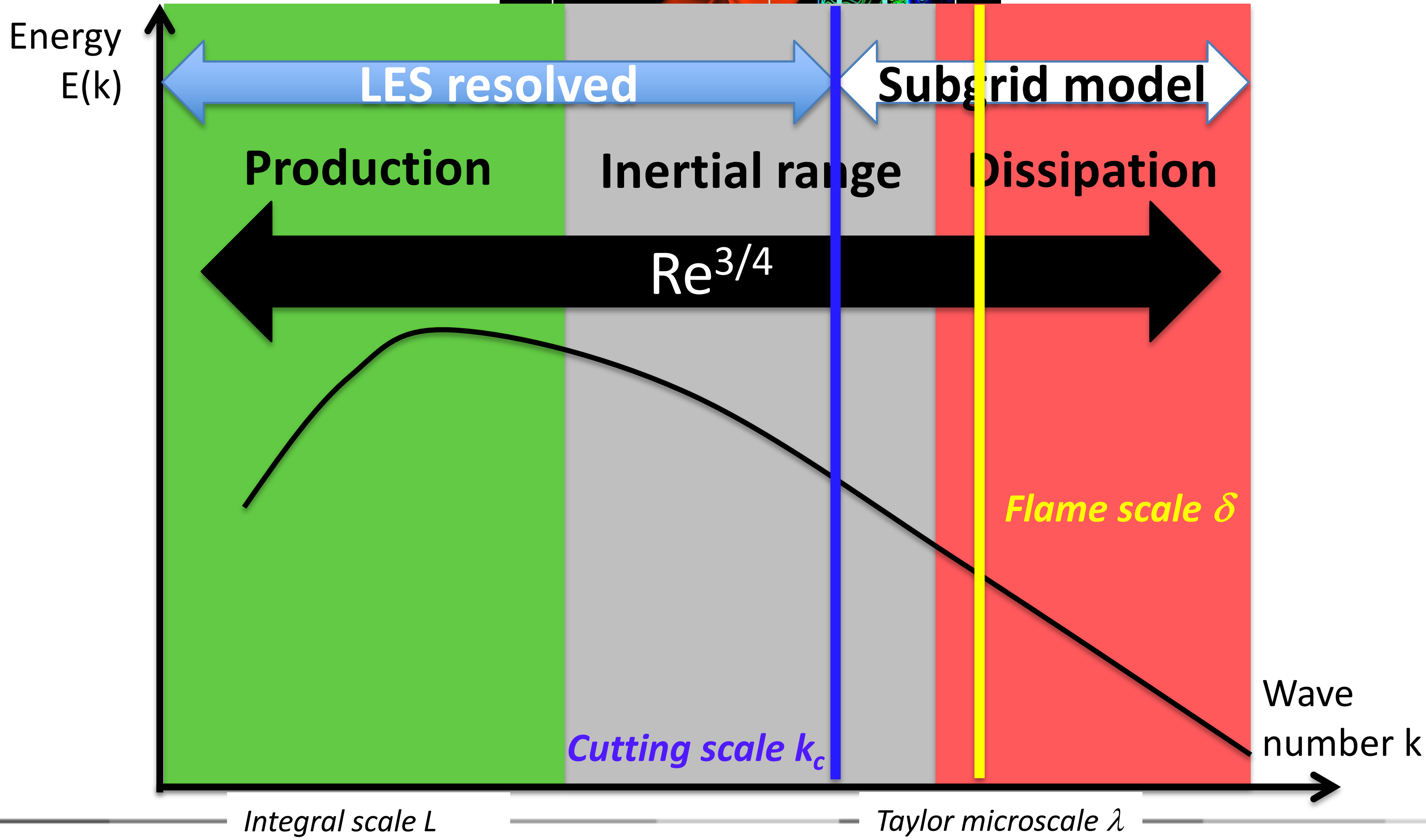


Turbulent combustion modeling

The LES approach

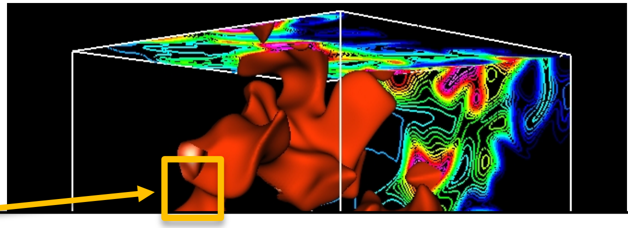


__Turbulence scales__



Turbulent combustion modeling

Flame front scales



The Thickened Flame approach

Premixed flame

- *Thickness* $\delta = \sqrt{D/A}$
- *Speed* $S_L = \sqrt{DA}$

$\Rightarrow$

$D \dashrightarrow DF$

$A \dashrightarrow A/F$

$\Rightarrow$

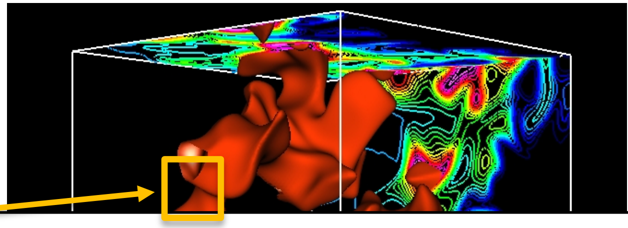
$\delta^* = F\sqrt{D/A} = F\delta$

$S_L^* = \sqrt{DA} = S_L$

- Both equations propagate 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 resolved on any mesh

Turbulent combustion modeling

Flame front scales



The Thickened Flame approach

Premixed flame

- *Thickness* $\delta = \sqrt{D/A}$ $D \longrightarrow DF$ $\delta^* = F\sqrt{D/A} = F\delta$

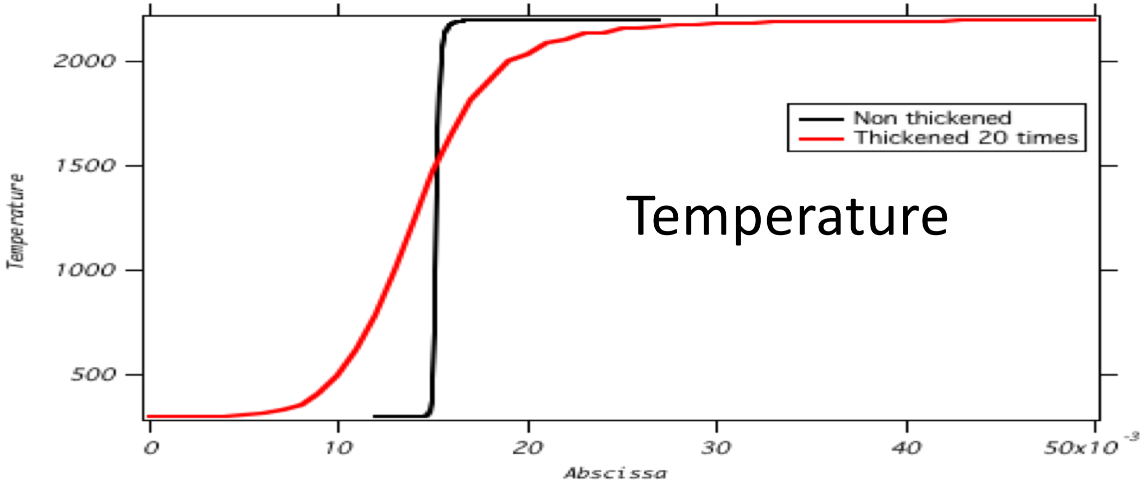
Allows to resolve the flame front, even if $\delta < k_c$

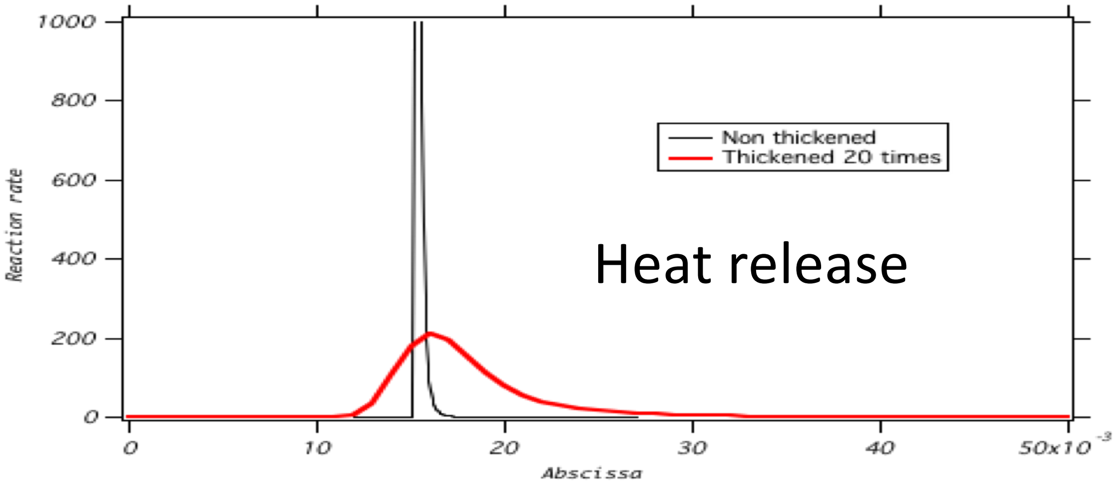
- Both equations propagate flames at the same speed s_L
- But the flame thickness is increased by a factor F in the second case ==> the flame front can be resolved on any mesh

The Thickened Flame approach

Thickened and non-thickened laminar flames

- CH4- air
- simple chemistry
- F=20



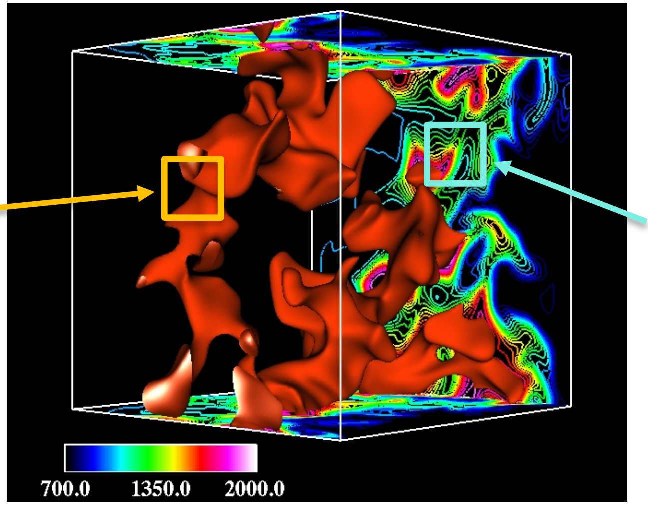


Turbulent combustion modeling

Flame front scales

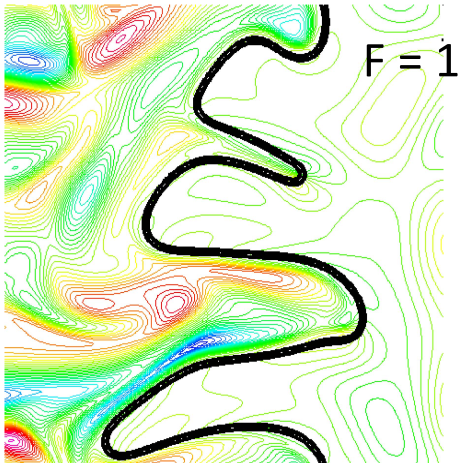
Turbulence scales

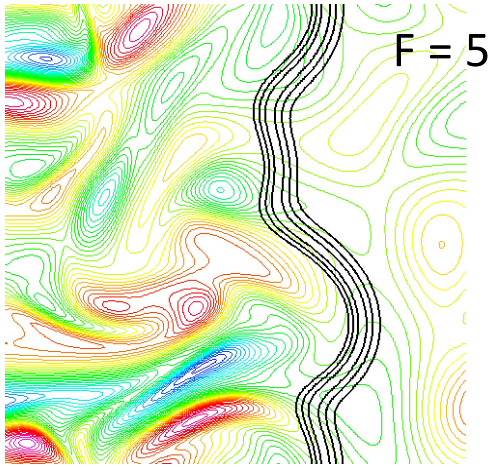
Thickened Flame



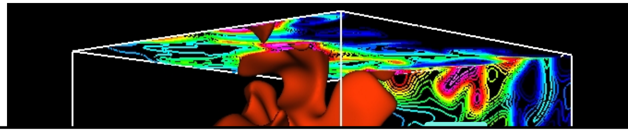
LES

Flame-turbulence interaction





Flame-turbulence interaction



The efficiency function E[1-3]

Local turbulent velocity

Local integral scale

$$E = \frac{R_1}{R_2} = f\left(\frac{u'}{s_L^0}, \frac{L}{\delta_L^0}\right)$$

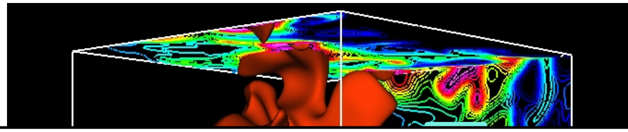
Laminar flame speed

Laminar flame thickness

[1] *Colin et al, Phys. Fluids 2000*
[2] *Charlette et al, C&F 2002*
[3] *Schmitt et al., Flow. Turb. Comb. 2014*

Turbulent combustion modeling

Flame-turbulence interaction



The efficiency function E

$$D \longrightarrow DEF$$

$$A \longrightarrow AE/F$$

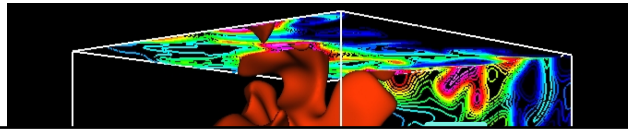
$$\Longrightarrow$$

$$\delta \longrightarrow \delta^* = F\delta$$

$$S_L \longrightarrow S_L^* = ES_L \approx S_T$$

Turbulent combustion modeling

Flame-turbulence interaction



The Dynamic Thickened Flame model (DTF):

A sensor (S) is introduced to identify burning vs mixing regions

$$F = 1 + (F_{\max} - 1)S$$

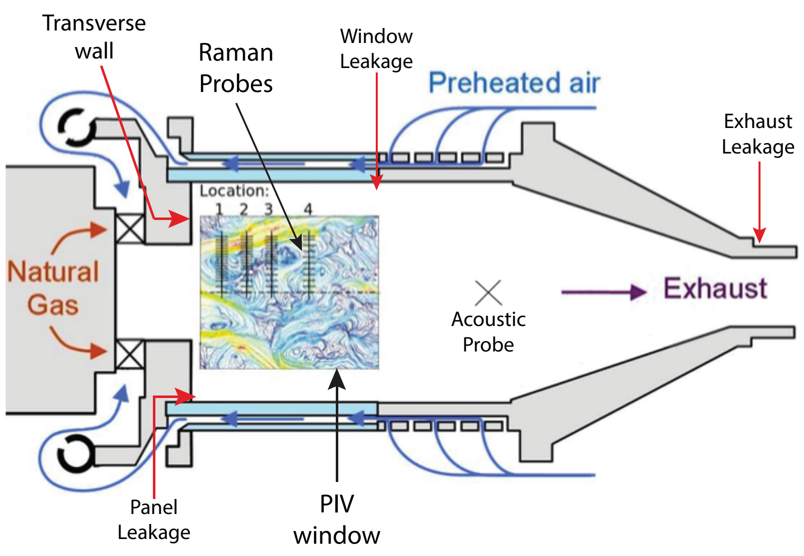
- Thicken only where reaction takes place:

$$\frac{d}{dt}(\rho Y_k) = \frac{\partial}{\partial x_i}\left[\rho(EDF + (1-S)D_t)\frac{\partial Y_k}{\partial x_i}\right] + E\frac{A}{F}\rho Y_1..Y_n \exp\left(-\frac{T_a}{T}\right)$$

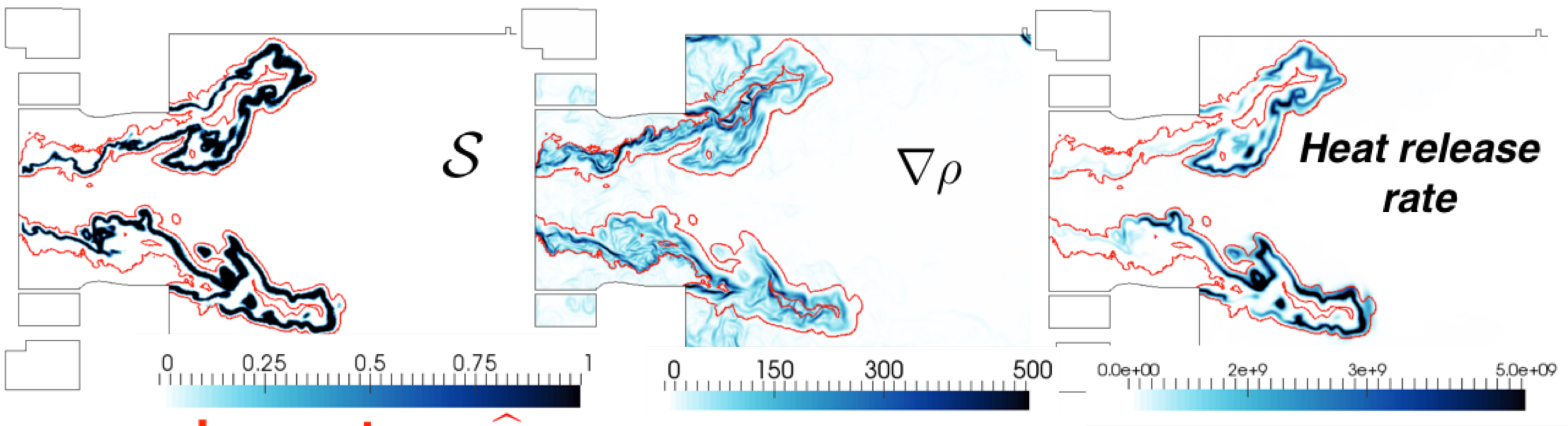
- Standard LES equation outside reaction zones :

$$\frac{d}{dt}(\rho Y_k) = \frac{\partial}{\partial x_i}\left(\rho(D + D_t)\frac{\partial Y_k}{\partial x_i}\right)$$

Turbulent combustion modeling : validation



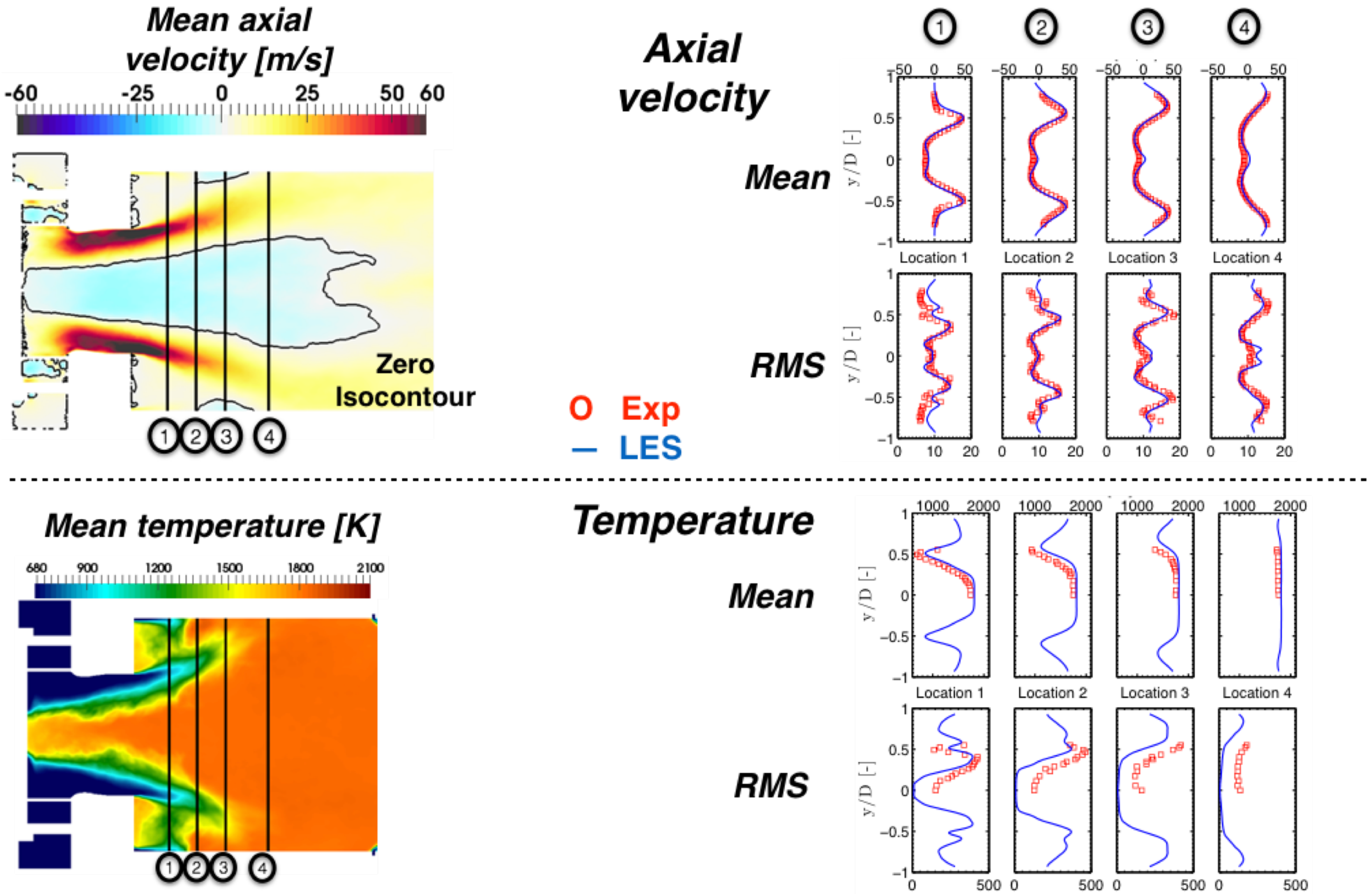
Siemens SGT-100[1-3]



Isocontour $\widehat{S} = 0.5$

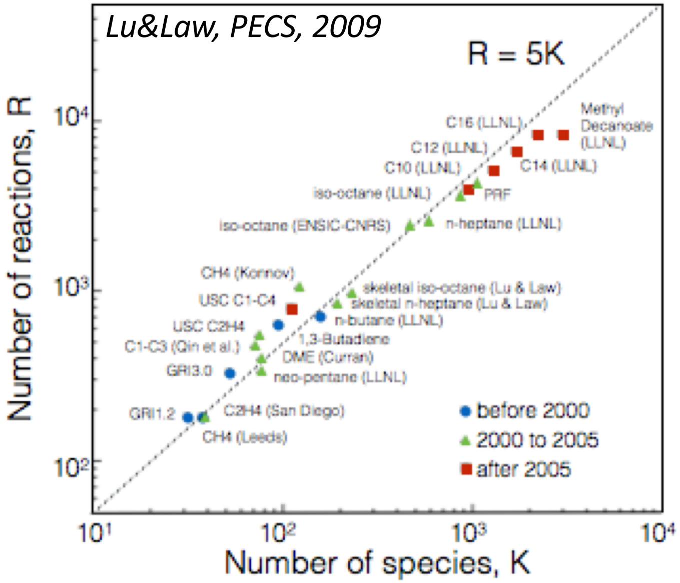
[1] *Stopper et al C&F 2013*
[2] *Bulat et al C&F 2014*
[3]*Jaravel et al. PCI 2017)*

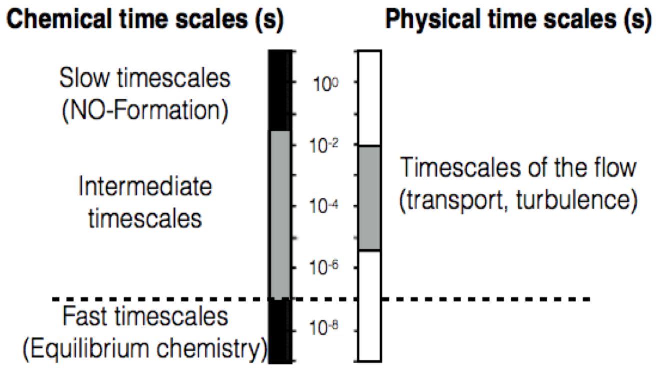
Turbulent combustion modeling : validation



Challenges of chemistry in combustion LES

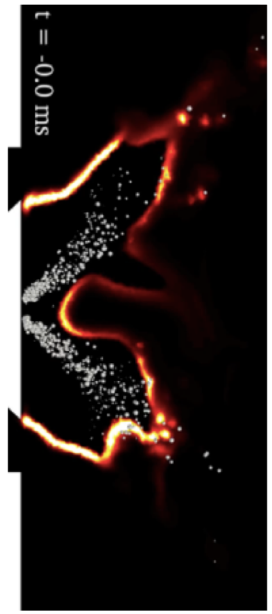
Large size, non-linear, **stiff** system





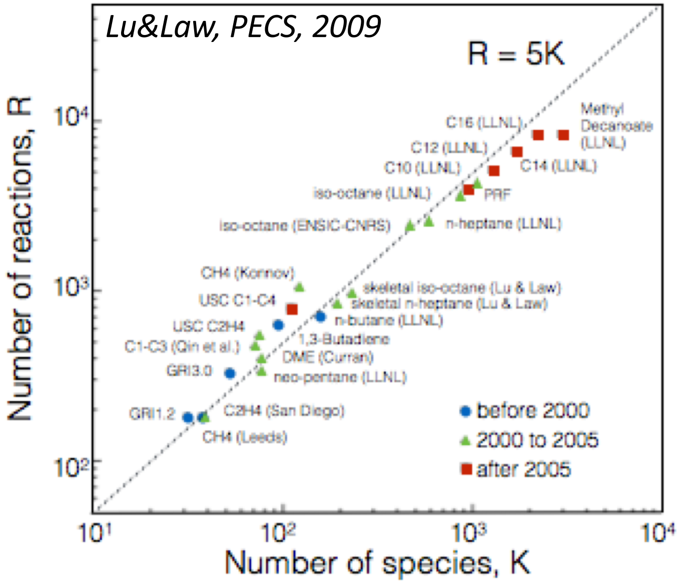
Coupling with the flow

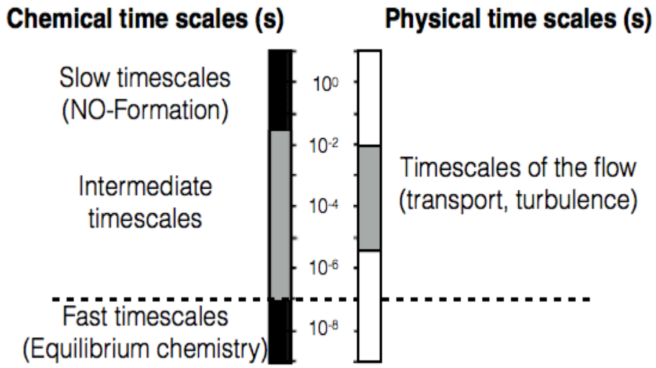
- Heat losses
- Dilution
- Spray flames



Challenges of chemistry in combustion LES

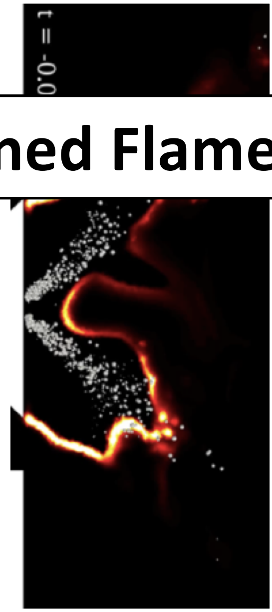
<u>Large size, non-linear, **stiff** system</u>





<u>Coupling with the flow</u>

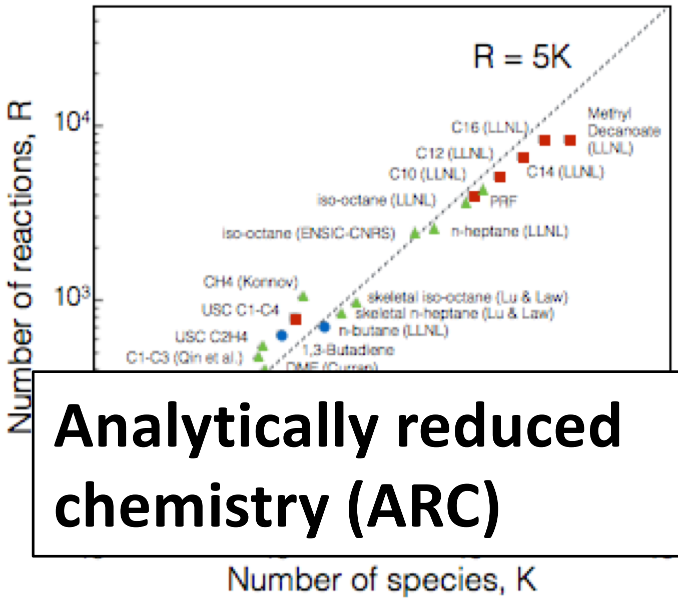
- Heat losses
- Dilution
- Spray flames



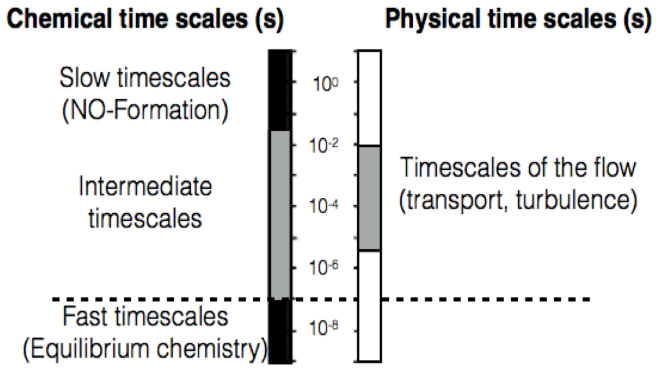
Thickened Flame model

Challenges of chemistry in combustion LES

Large size, non-linear, **stiff** system

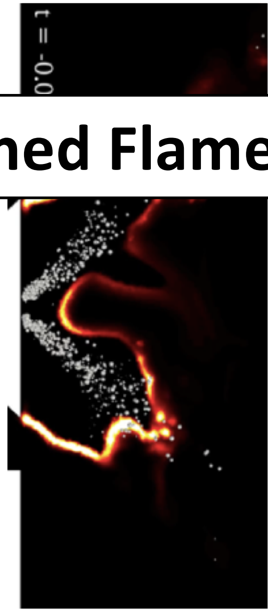


Analytically reduced chemistry (ARC)



Coupling with the flow

- Heat losses
- Dilution
- Spray flames



Thickened Flame model

Analytically Reduced Chemistry

- Derives from a detailed mechanism
- Keeps relevant chemical pathways <u>without</u> constant fitting
- Reduction in two steps:

Detailed mechanism —1→ Skeletal mechanism —2→ ARC

Many reactions
Many species

~300 reactions
~75 species

~20-30 species

1. Skeletal reduction = Elimination of unimportant species and reactions
- DRGEP [Pepiot, C&F, 2008]

2. Analytical reduction = Quasi Steady State (QSS) assumption → elimination of species
- Level Of Importance [Lovas, PCI, 2000)

Reduce CPU (number of species)

Reduce stiffness

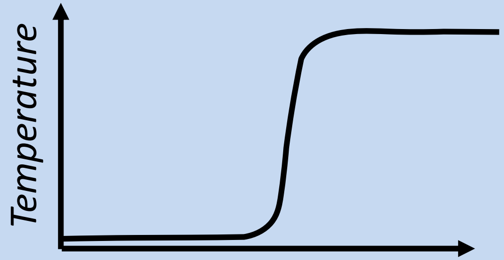
ARC can be derived automatically

INPUT

Detailed Mechanism

Reaction	A^a	n	E^a
$H + O_2 \rightleftharpoons OH + O$	3.52×10^{16}	-0.7	71.42
$H_2 + O \rightleftharpoons OH + H$	5.06×10^{4}	2.67	26.32
$H_2 + OH \rightleftharpoons H_2O + H$	1.17×10^{9}	1.3	15.21
$H_2O + O \rightleftharpoons 2OH$	7.06×10^{0}	3.84	53.47
$2H + M \rightleftharpoons H_2 + M^b$	1.30×10^{18}	-1.0	0.0
$H + OH + M \rightleftharpoons H_2O + M^b$	4.00×10^{22}	-2.0	0.0
$2O + M \rightleftharpoons O_2 + M^b$	6.17×10^{15}	-0.5	0.0
$H + O + M \rightleftharpoons OH + M^b$	4.71×10^{18}	-1.0	0.0
$O + OH + M \rightleftharpoons HO_2 + M^b$	8.30×10^{14}	0.0	0.0

Target canonical cases



Target quantities
- SL
- T° profile
- Species profiles
- etc.

Apply reduction techniques

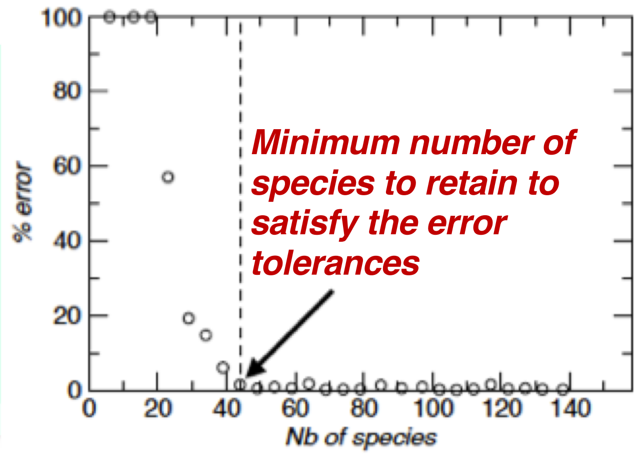
ARCANE[1]

CANTERA

Computes test cases

OUTPUT

- List of ARC schemes : CHEMKIN/CANTERA format + .f90 routine for source terms
- Ordered list of QSS species
- Errors on the targeted quantities



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[1] *In collab. with Cornell Univ. (P. Pepiot)*

Example of ARC derivation for methane-air flames

Objective: build a scheme for methane-air able to accurately reproduce **NO and CO formation**

- 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

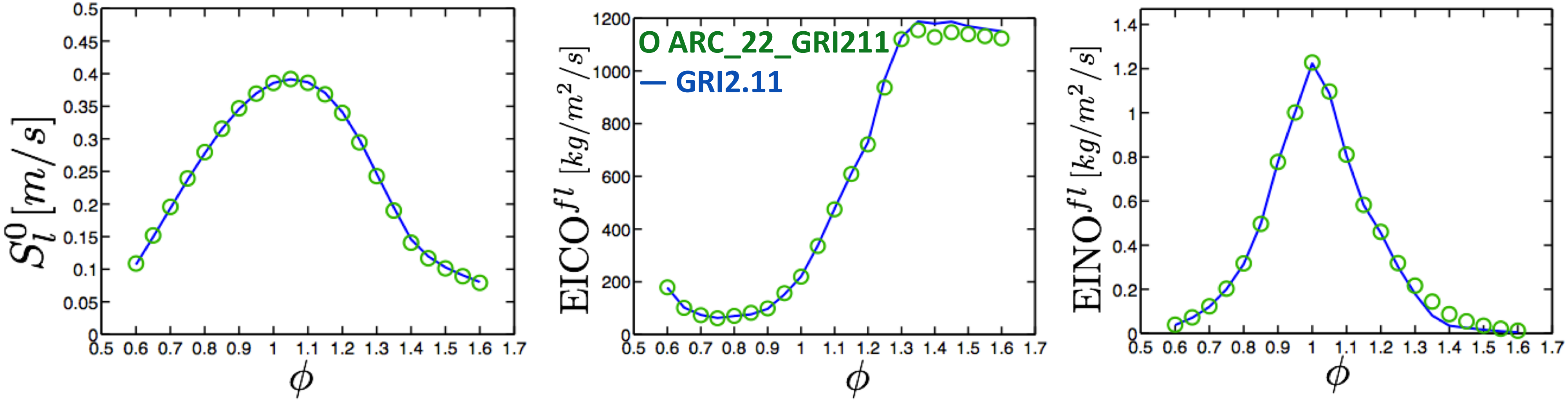
Detailed Chemistry
GRI-2.11

ARCANE

ARC_22_GRI211
(22 transported species)

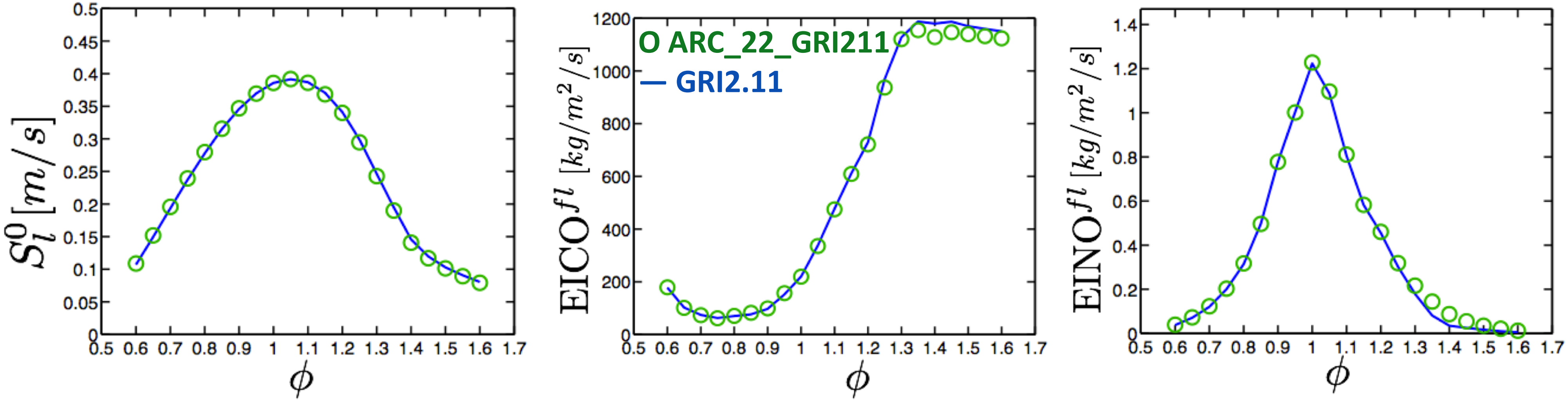
Example of ARC derivation for methane-air flames

300 K, 1 bar (Scheme derivation conditions)



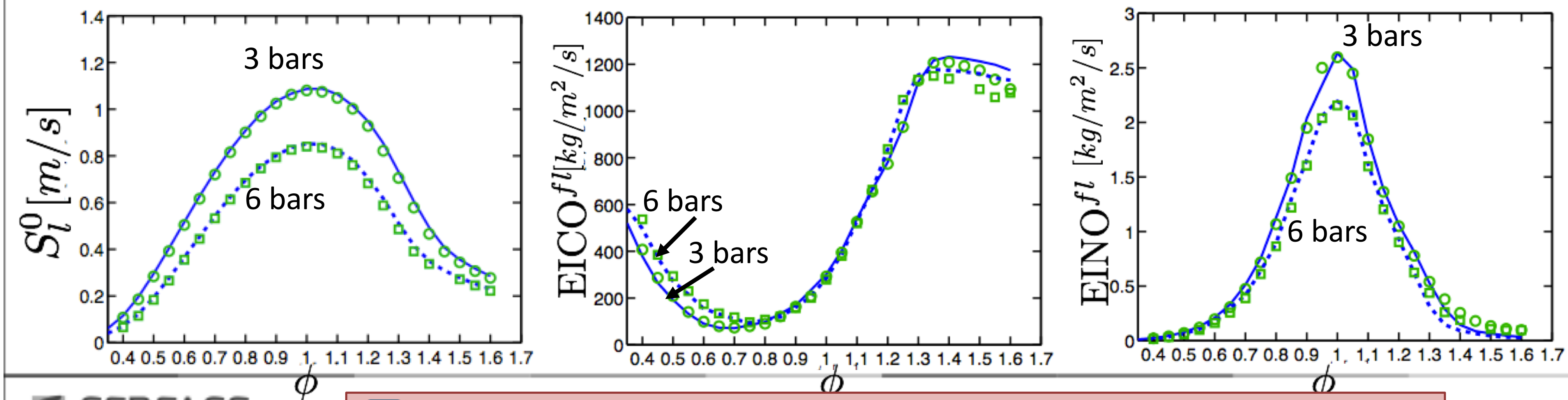
Example of ARC derivation for methane-air flames

300 K, 1 bar (Scheme derivation conditions)



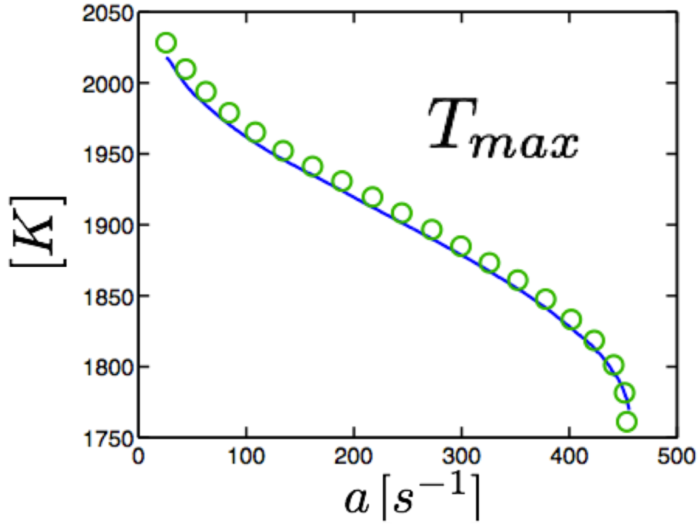
680 K, 3-6 bars (Gas turbine conditions)

GRI2.11: 3 bars (—) and 6 bars (- - -)
ARC_22_GRI211: 3 bars (O) and 6 bars (☐)

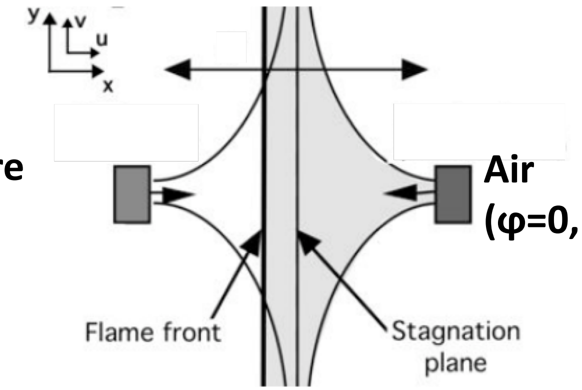


➡️ Accurate description far beyond the range of derivation

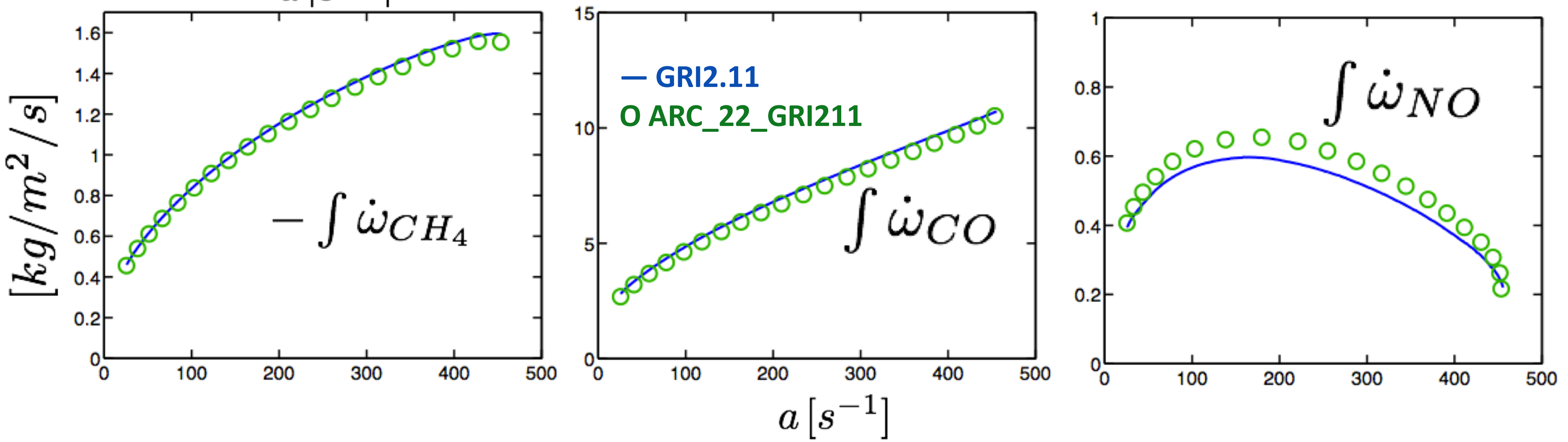
Example of ARC derivation for methane-air flames



Rich air-fuel mixture
(φ=3.2, T=300 K)



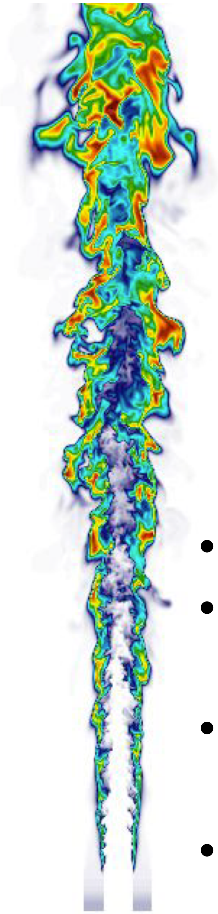
Air
(φ=0, T=300 K)

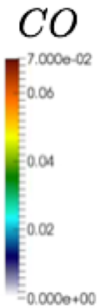


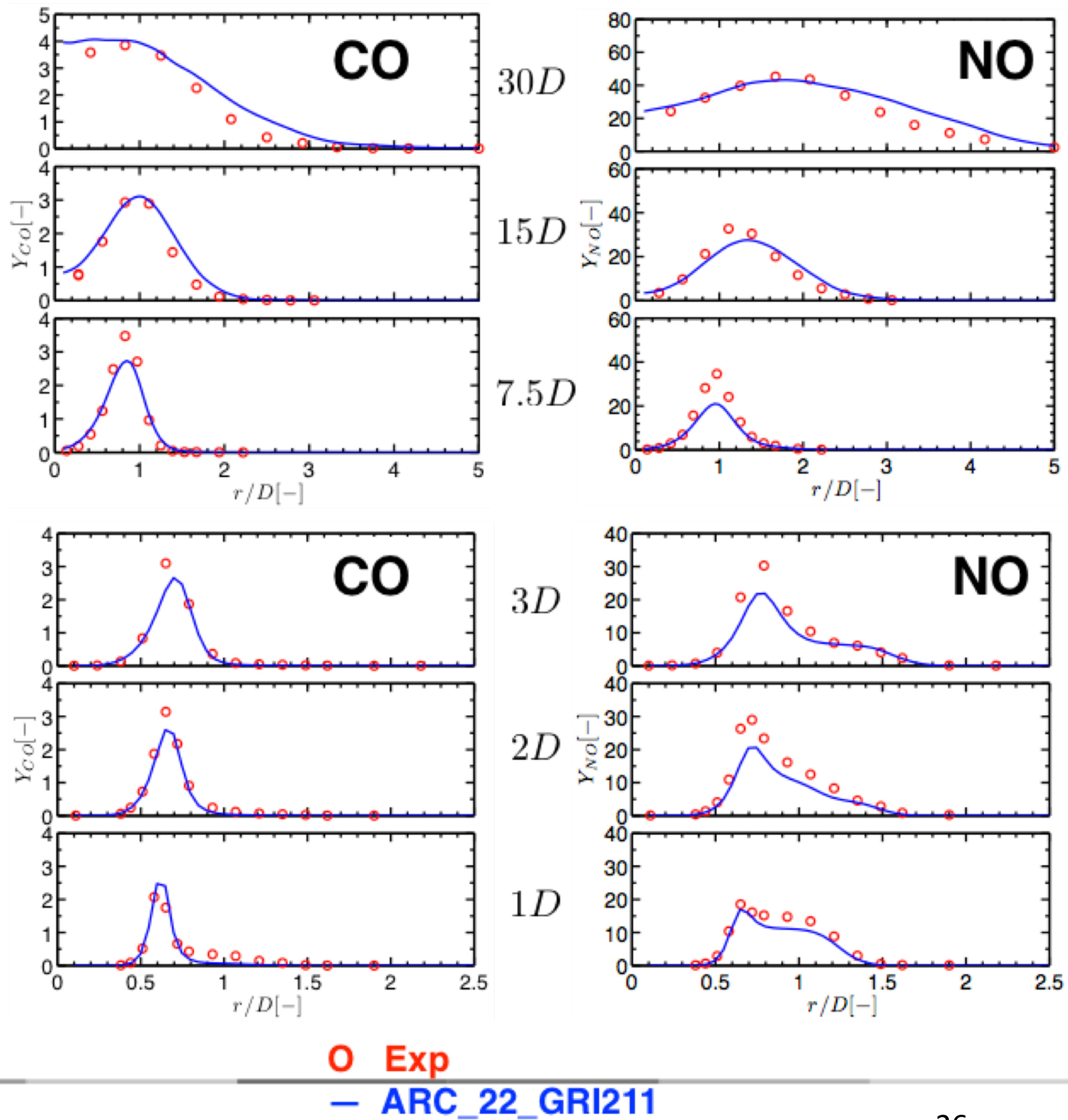
➡️ Accurate response to strain although it is not part of the target canonical case

Validation : the turbulent SANDIA-D jet flame[1]

- Highly resolved LES
- Direct resolution of the chemistry on the grid







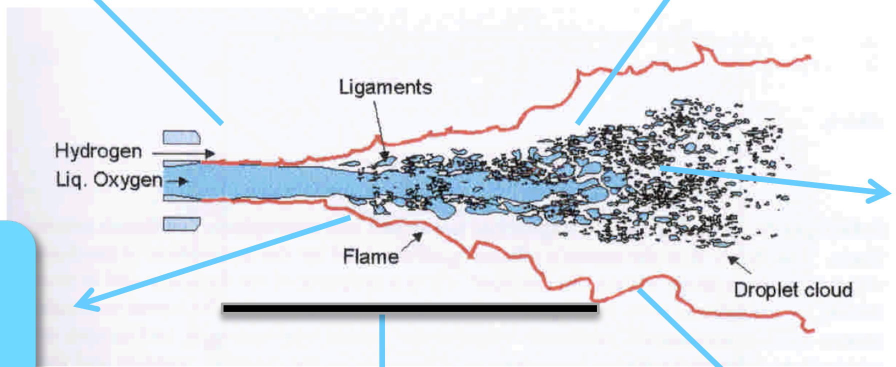
- 3 coaxial jets :
- **Main**: methane-air mixture, φ=3.2, T=300 K
- **Pilot**: burnt gases, φ=0.77, T = 1900 K
- Co-Flow: fresh air , T= 300 K

[1]*Jaravel et al. C.&F. 2018*

Turbulent spray flames

Injection

Turbulent dispersion



Evaporation

Atomisation
1. Primary atomisation
2. Secondary breakup

Drop/drop & drop/wall interactions

Combustion

Turbulent spray flames

Thickened Flame model

+

Lagrangian particle tracking

Injection

Turbulent dispersion

Evaporation

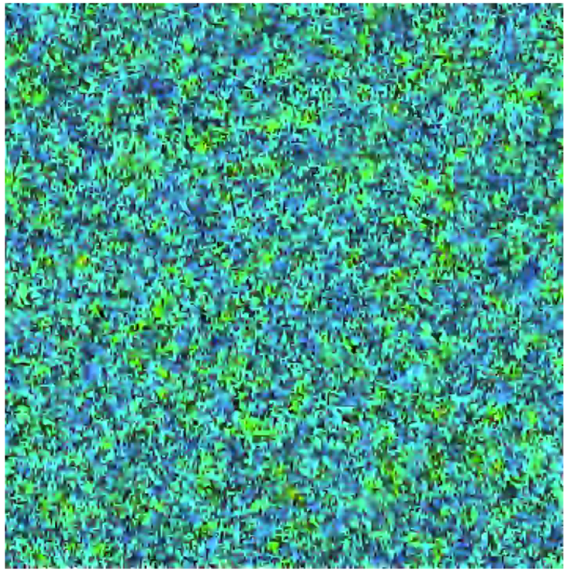
Atomisation
1. Primary atomisation
2. Secondary breakup

Drop/drop & drop/wall interactions

Combustion

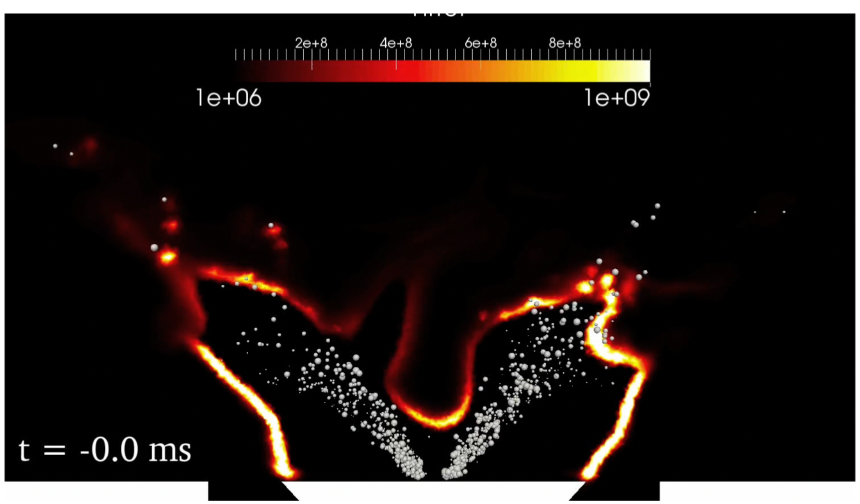
Turbulent spray flames

Turbulence – spray interaction



Droplets at moderate Stokes number in decaying HIT

Spray – flame interaction

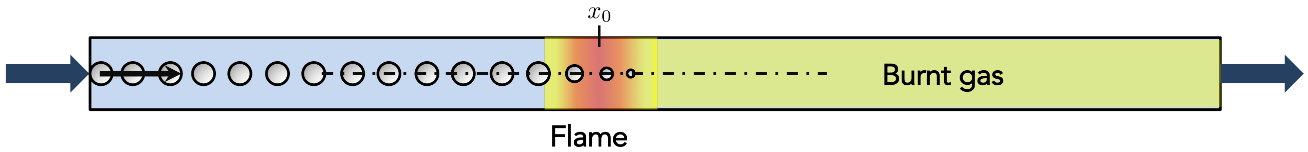


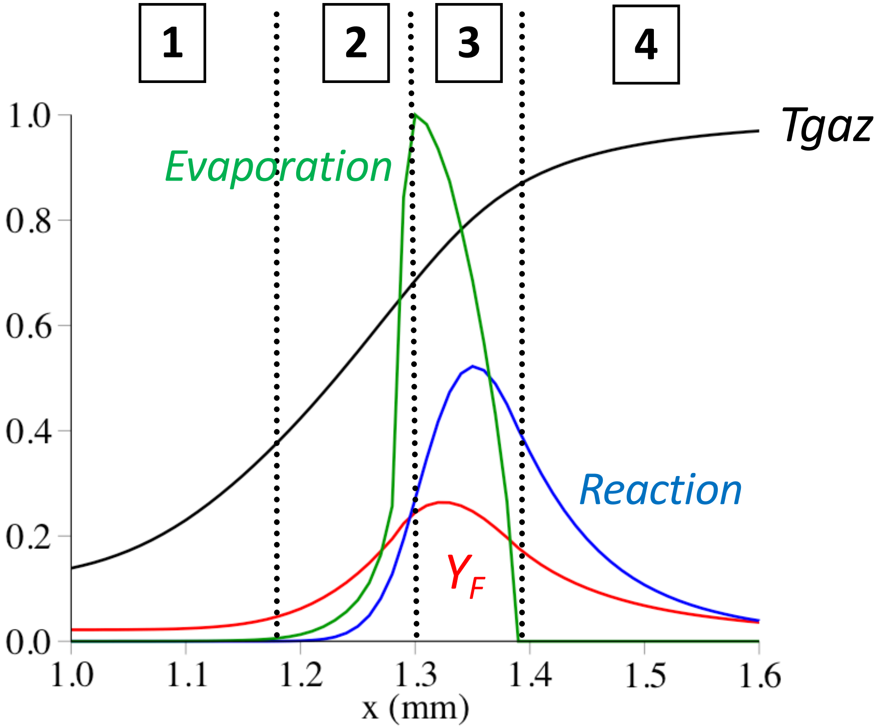
Swirled spray flame[1]

[1] *Paulhiac PhD, 2016*

How to combine droplets with the TFLES model?

Premixed flame burning a saturated mixture of air, fuel vapor and droplets.

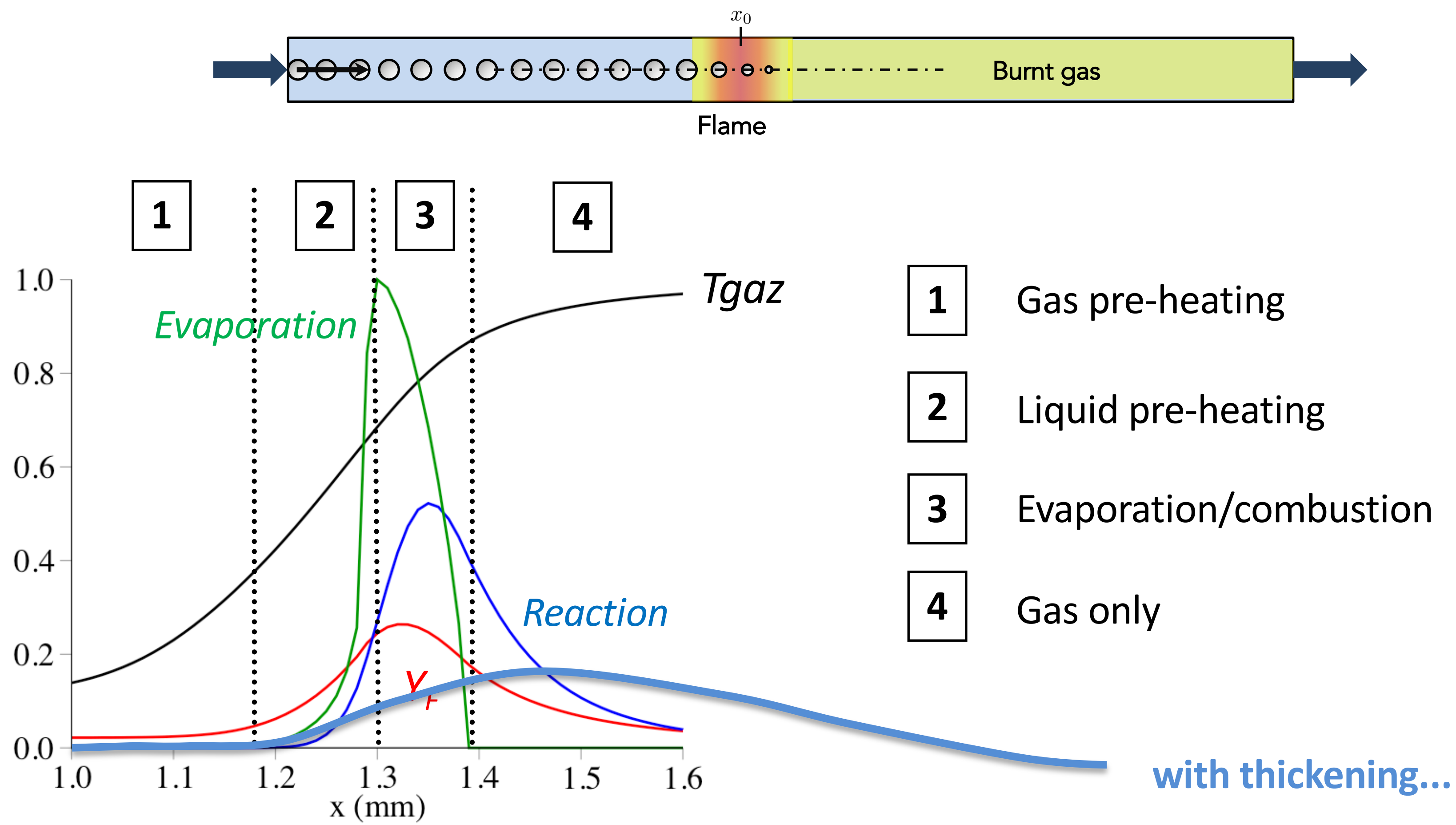




- **1** Gas pre-heating
- **2** Liquid pre-heating
- **3** Evaporation/combustion
- **4** Gas only

How to combine droplets with the TFLES model?

Premixed flame burning a saturated mixture of air, fuel vapor and droplets.



1 Gas pre-heating

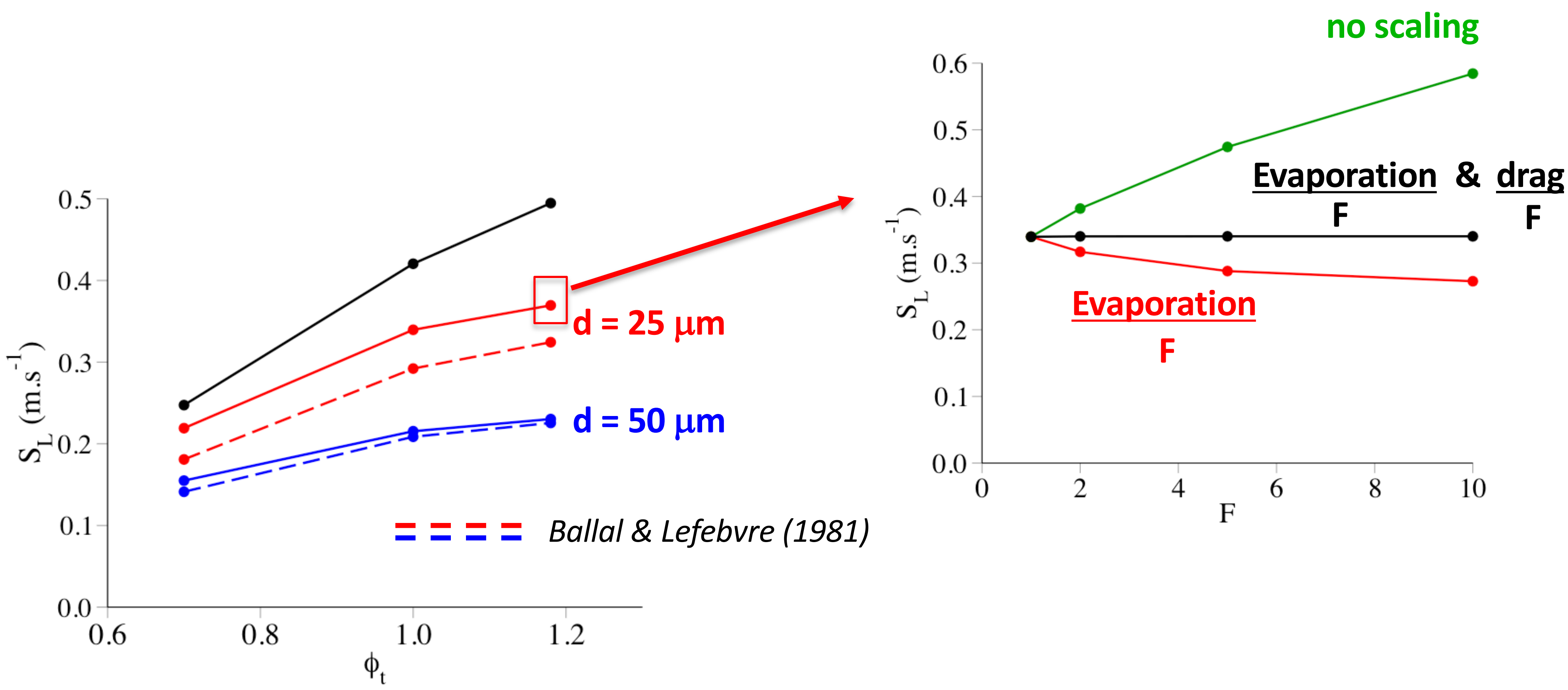
2 Liquid pre-heating

3 Evaporation/combustion

4 Gas only

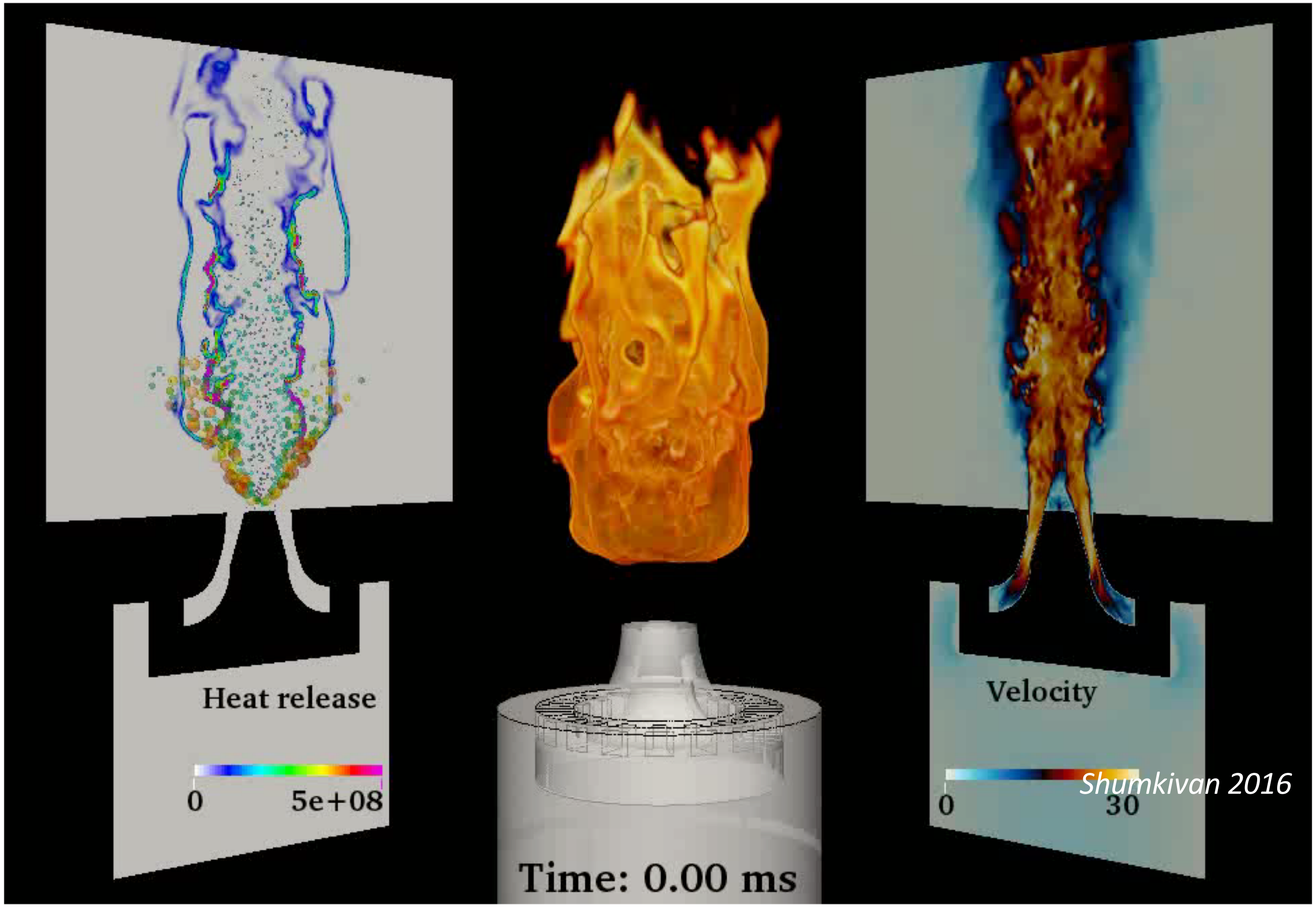
How to combine droplets with the TFLES model?

Laminar flame speed as a function of the droplet diameter



Turbulent spray flames : validation

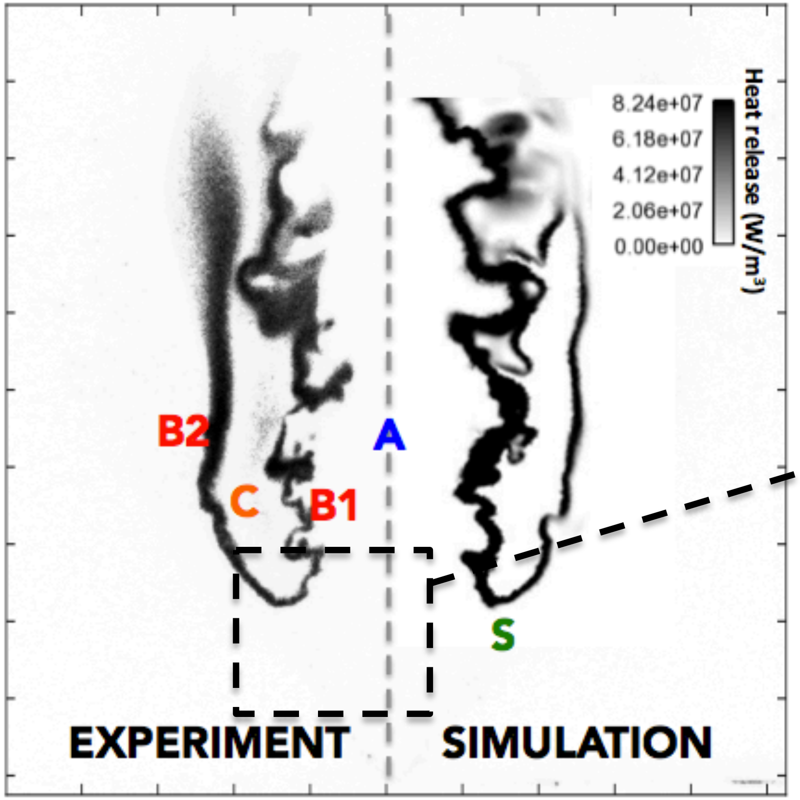
LES of the unswirled burner of CORIA[1,2]



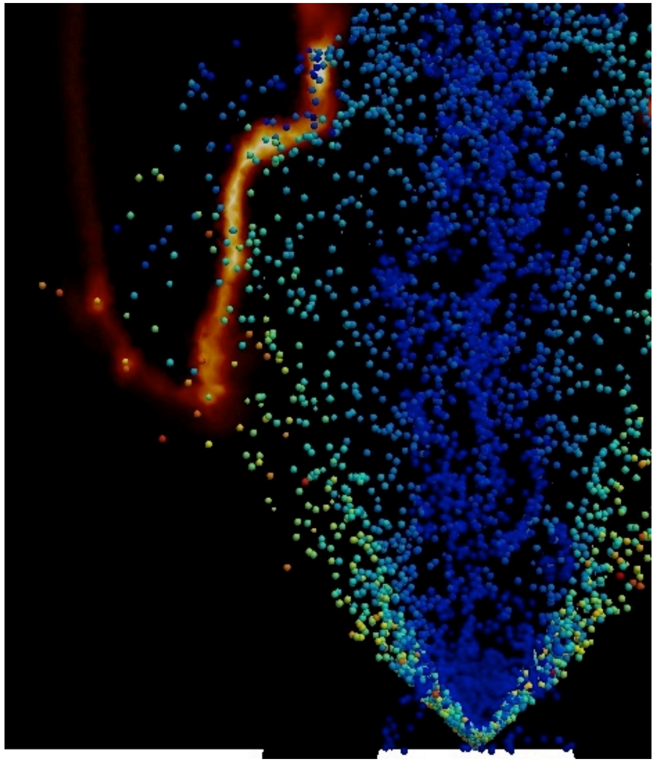
Photographie Exp.

[1]Verdier et al. 2016 [2]Shum-Kivan et al., PCI 2017

LES of the unswirled burner of CORIA[1,2]



Heat release with droplets colored with their size



(A) Fresh air (+ small droplets)

(B1) Internal reaction zone

(B2) External reaction zone

(C) Hot gas + fuel vapor

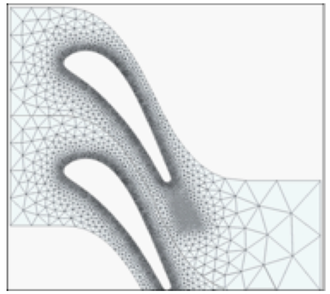
(S) Flame stabilization

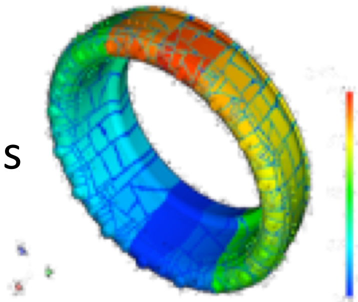
[1]Verdier et al. 2016 [2]Shum-Kivan et al., PCI 2017

AVBP – An unstructured LES solver

Jointly developed by IFPEN and CERFACS

- External, internal flows
- Fully compressible turbulent reacting flows (ideal & real gas thermo.)
- DNS / LES approach





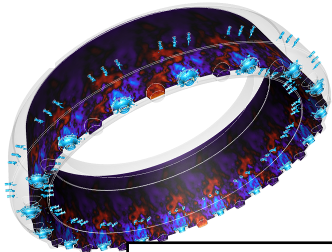
- Unstructured hexaedral, tetraedral, prisms & hybrid meshes
- Massively parallel, SPMD approach
- Explicit in time
- Centered schemes

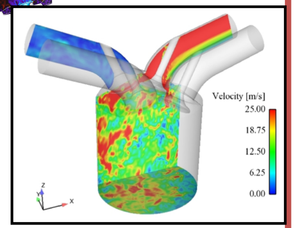
  Finite Volumes / Finite Elements (2nd/3rd order[a])

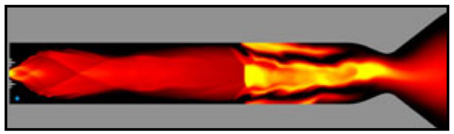
- SGS models : Smagorinsky(dynamic)/WALE[b]
- NSCBC[c] boundary cond. + wall laws
- Reduced[d] or tabulated[e] chemical kinetics
- Thickened flame turb. combustion model (TFLES)[f]
- Multi-phase solvers (Lagrangian & Eulerian)

Applications

- Gas turbines
- Aeronautical engines
- Piston engines
- Statoreactor
- Rocket engines
- Furnaces
- Heat exchangers

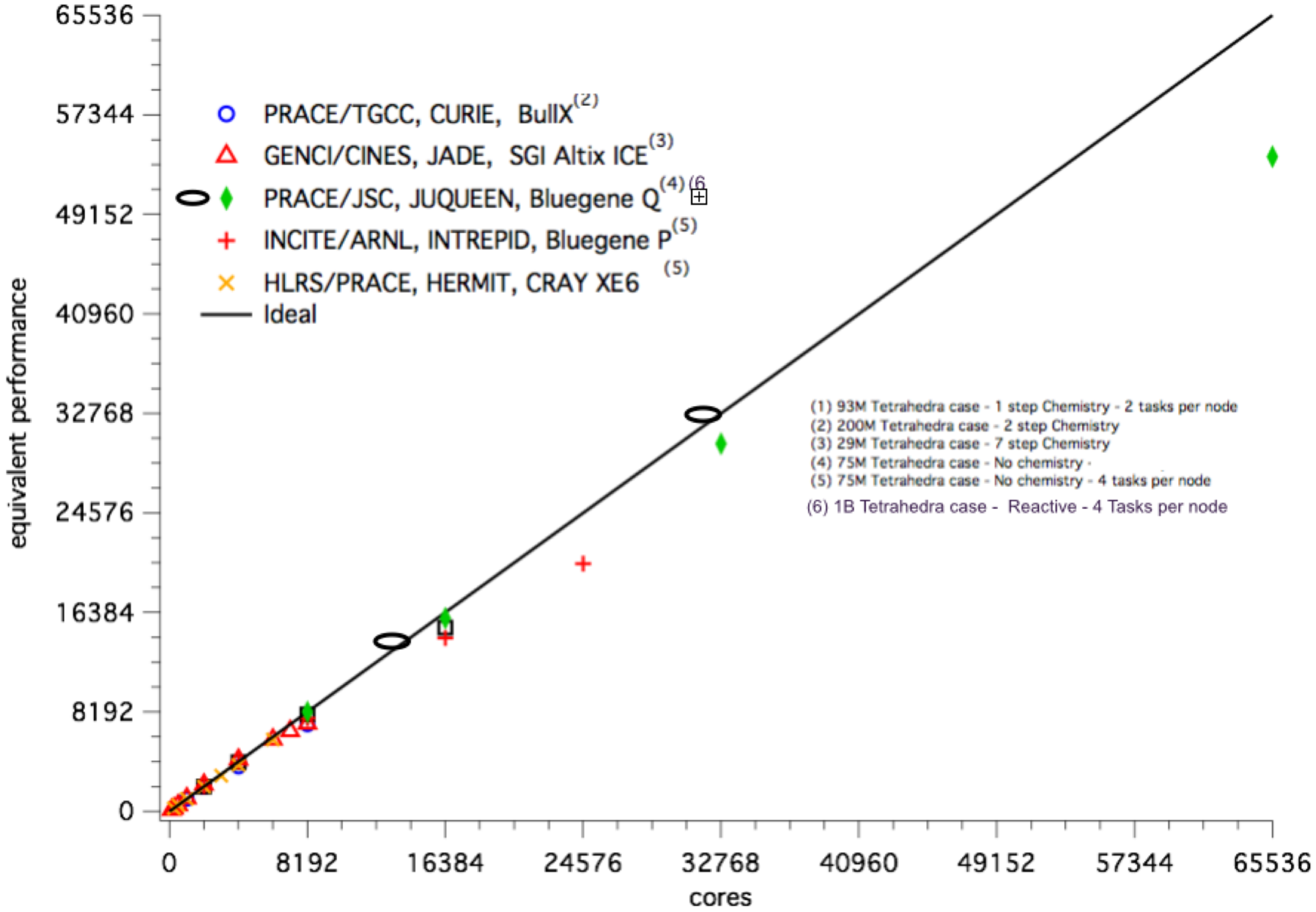






[a]Colin 2000 [b]Nicoud 1999 [c]Poinsot 1992
[d]Franzelli 2010 [e]Fiorina 2010 [f]Colin 2000

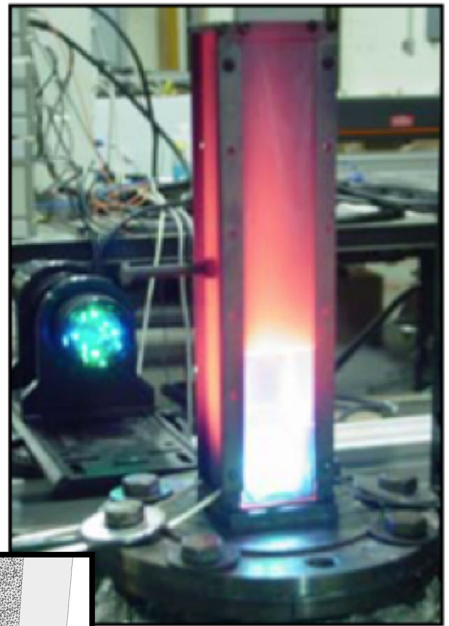
MPI strong scaling of AVBP for REAL industry type configurations

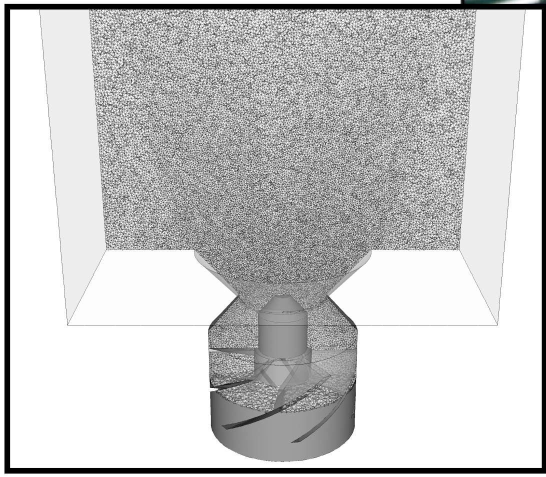


Application to a two-phase kerosene-air burner[3]

NASA-LDI configuration[1-3]

- 6 blades axial swirler
- Kerosene (Jet-A) combustion
- Pressure-swirl atomizer
- Large quartz optical access
- Ambient conditions, 8.16 g/s air, 0.415 g/s Jet-A2 -> ϕ = 0.75





- Experimental data

PIV, PDPA, T, CO, CO_2, H_2O, NO

[1] *Cai et al., AIAA, 2005*
[2] *Iannetti et al., 2008, NASA Report*

[3]*Felden et al. C. & F. 2018)*

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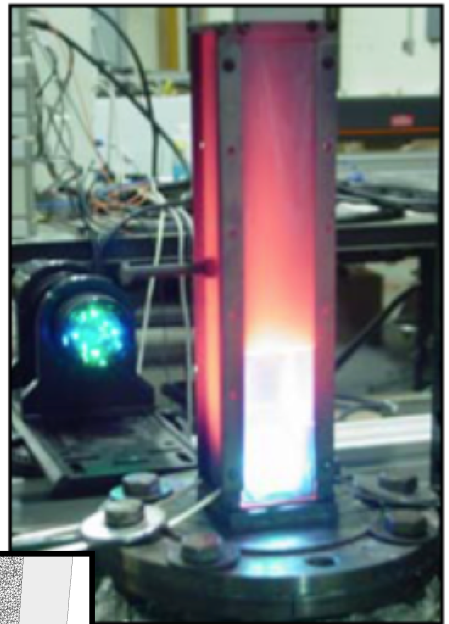
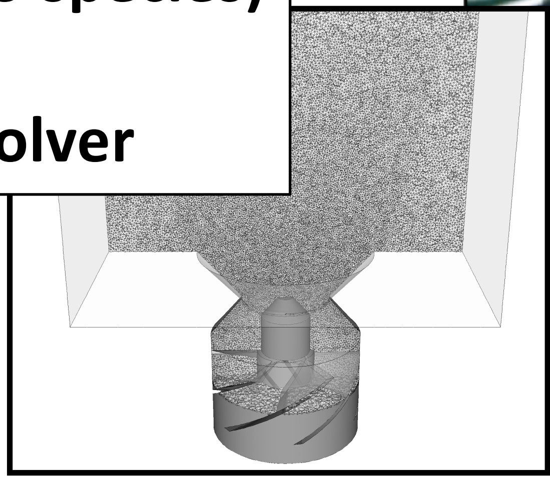
Thickened Flame model
+
ARC chemistry (29 species)
+
Lagrangian solver





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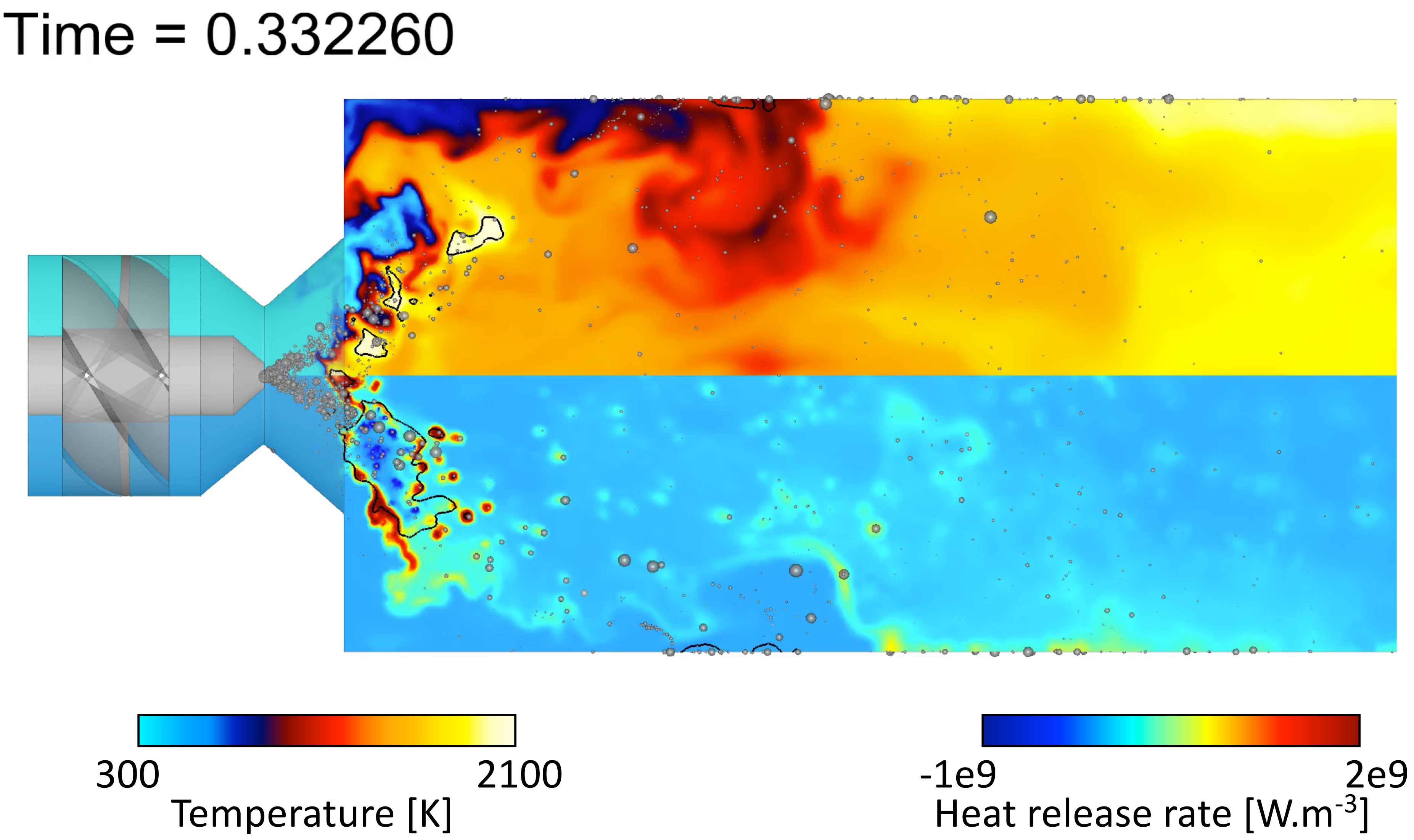
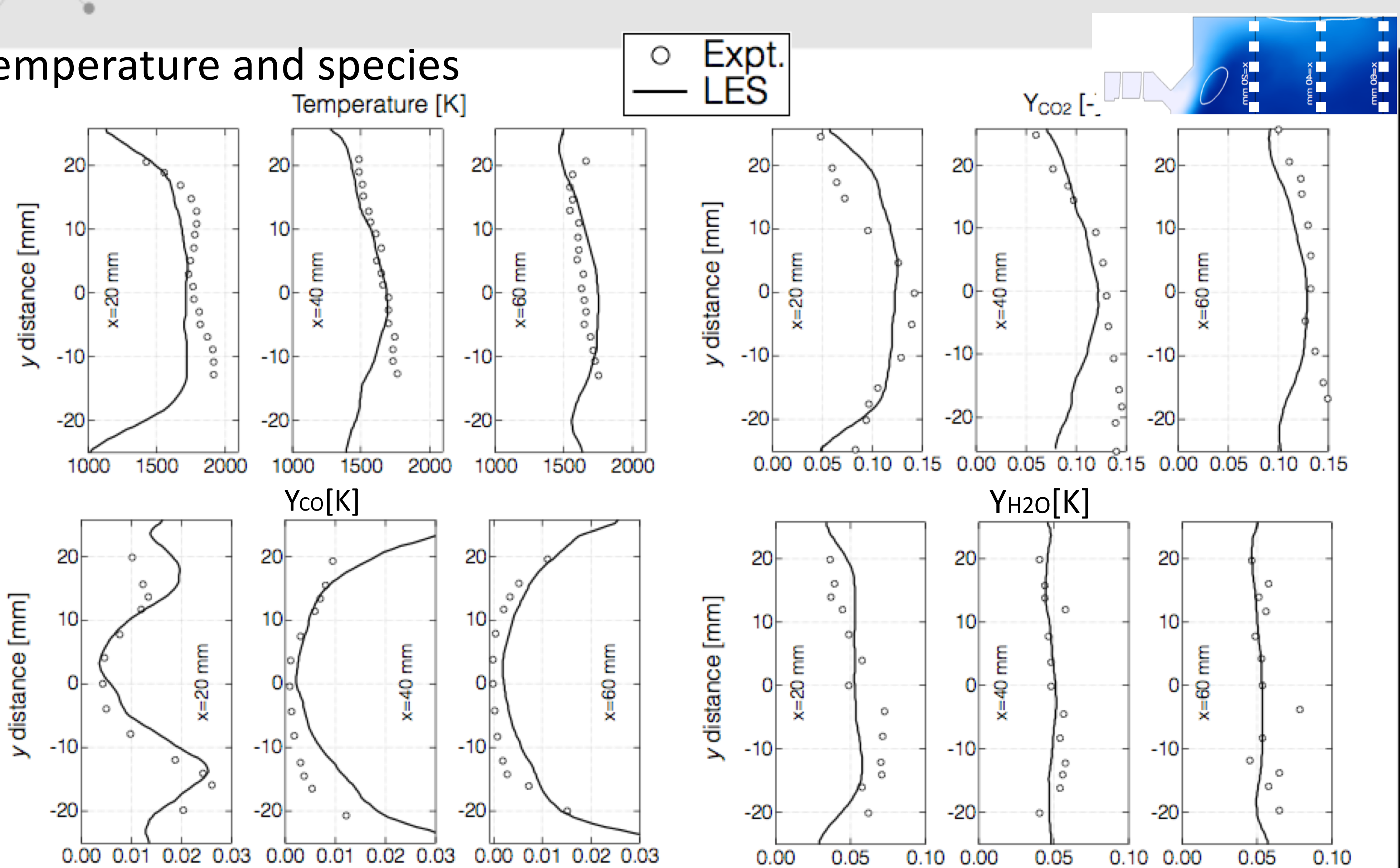
The two-phase flow and flame

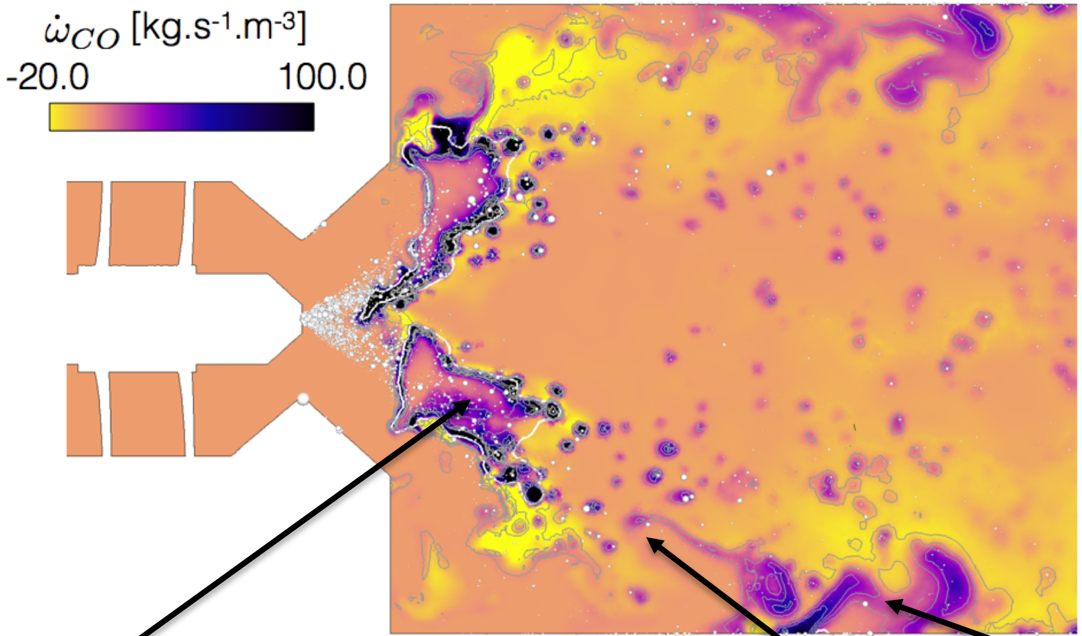


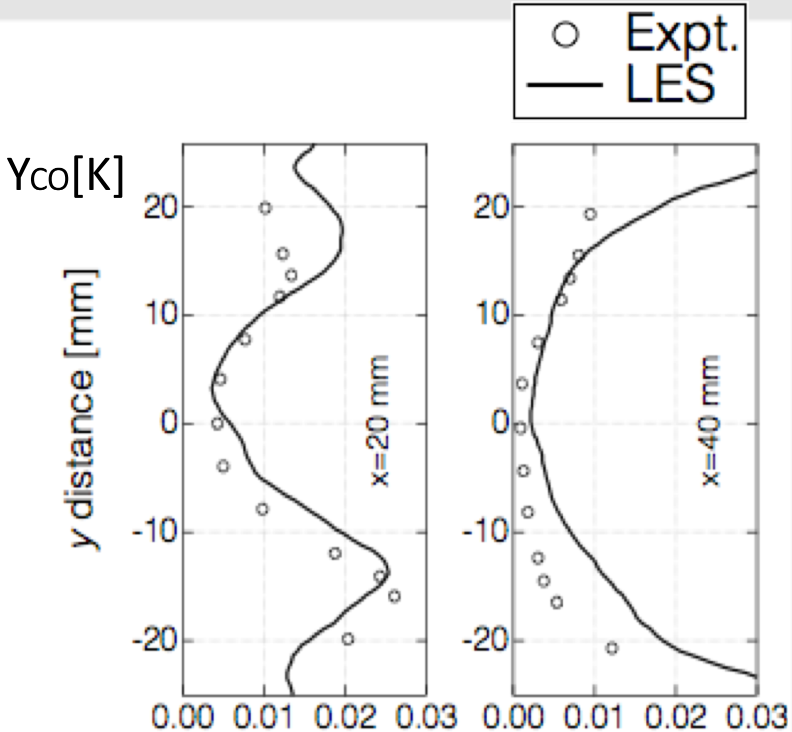
Comparison with experiment

Temperature and species

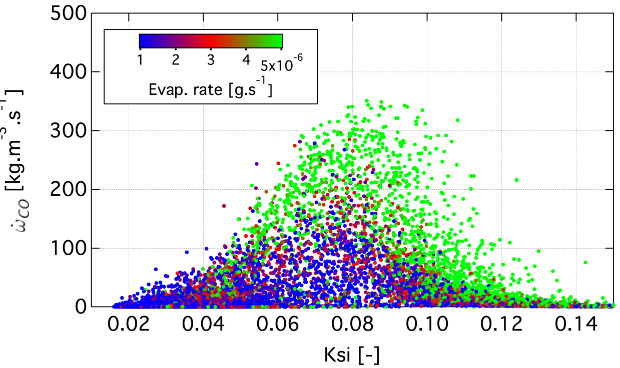


Analysis of CO formation





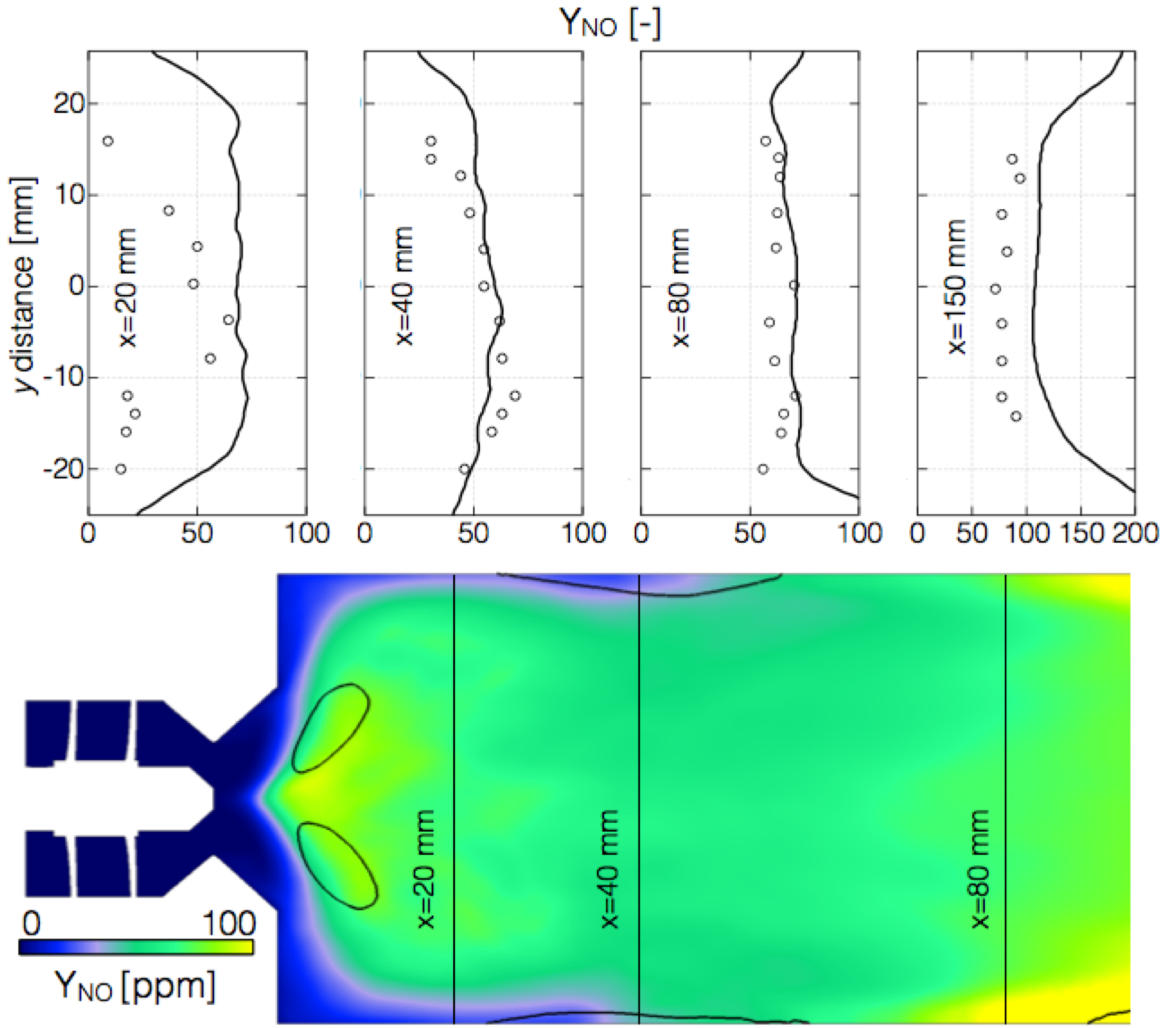
CO produced in the back diffusion flame, enhanced by evaporation



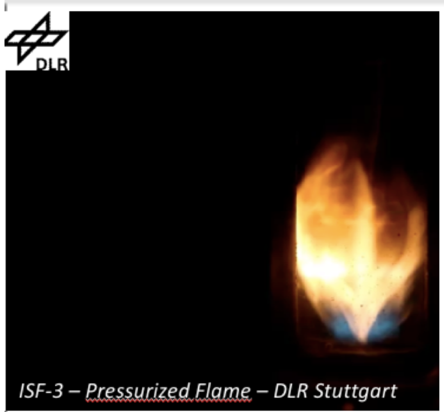
CO consumed in the lean premixed flame

CO produced along the walls

What about NO?

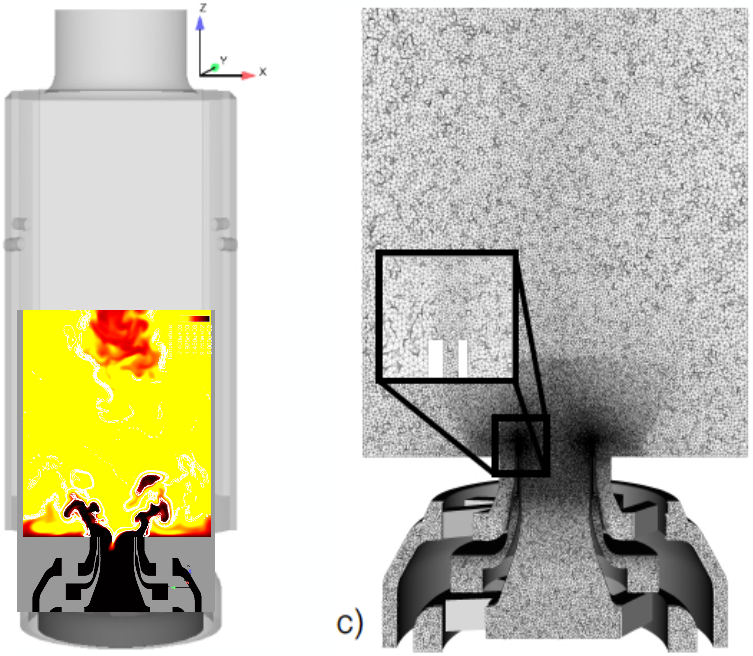


Application to soot production[1]



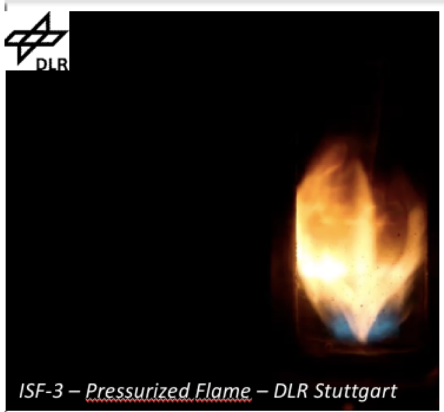
Soot modelling applied to a gas turbine combustor[2]

- Sooting turbulent swirled non-premixed C_2H_4 – Air flame
- Three concentric swirled nozzles providing air and fuel
- secondary air injection

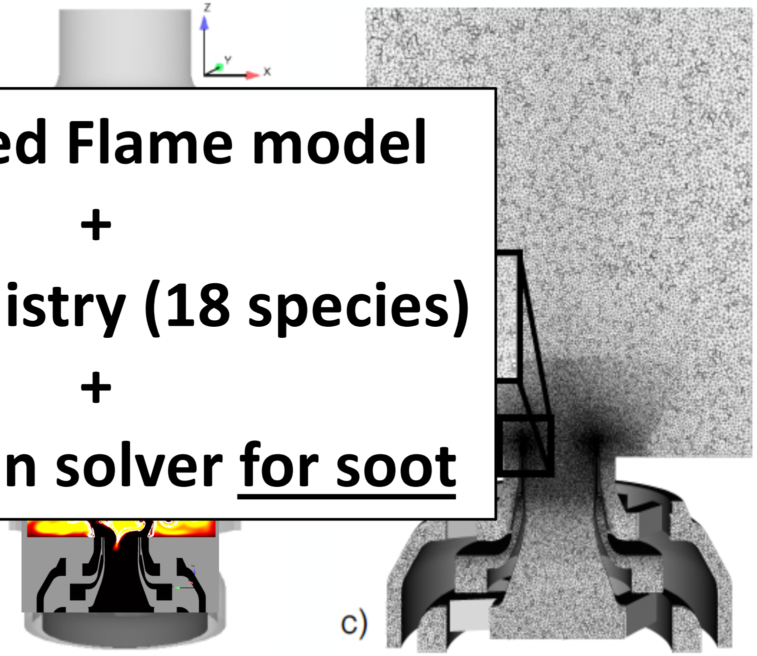


[1]Gallen et al. PCI 2019

[2]Geigle et al. PCI 2015



Soot modelling applied to a gas turbine combustor[2]



Thickened Flame model

+

ARC chemistry (18 species)

+

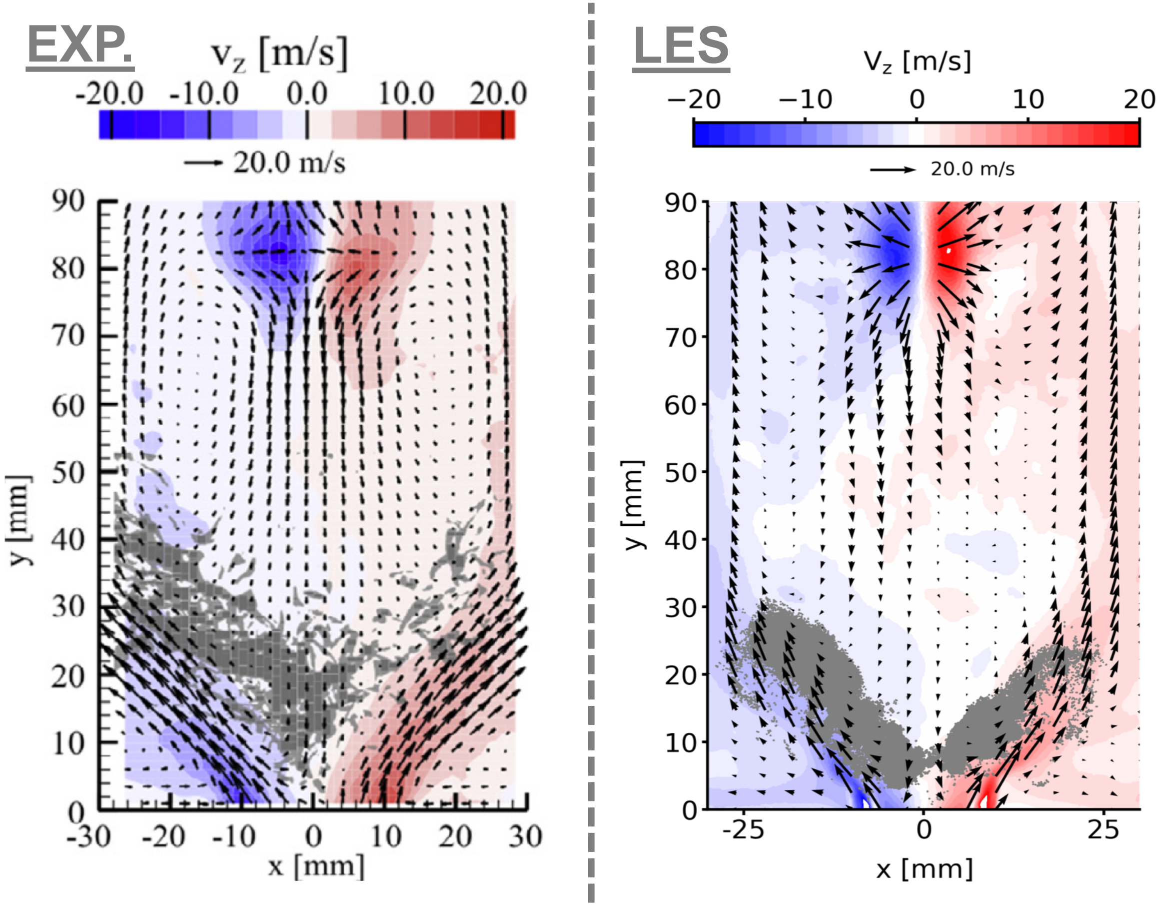
Lagrangian solver <u>for soot</u>

- Sooting turbulent swi
  non-premixed C_2H_4 –
  flame
- Three concentric swir
  nozzles providing air and
  fuel
- secondary air injection

Application to soot production[1]

Mean soot presence

~ 30 Millions of numerical particles

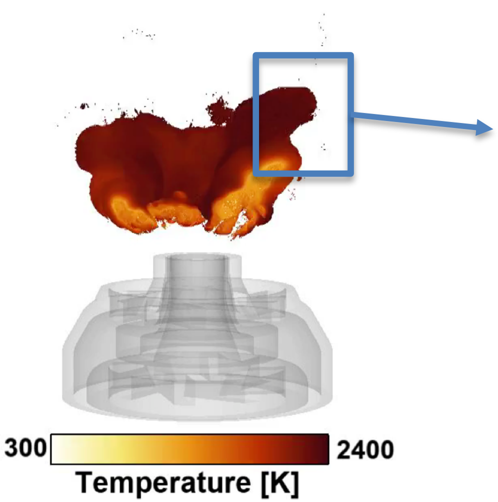


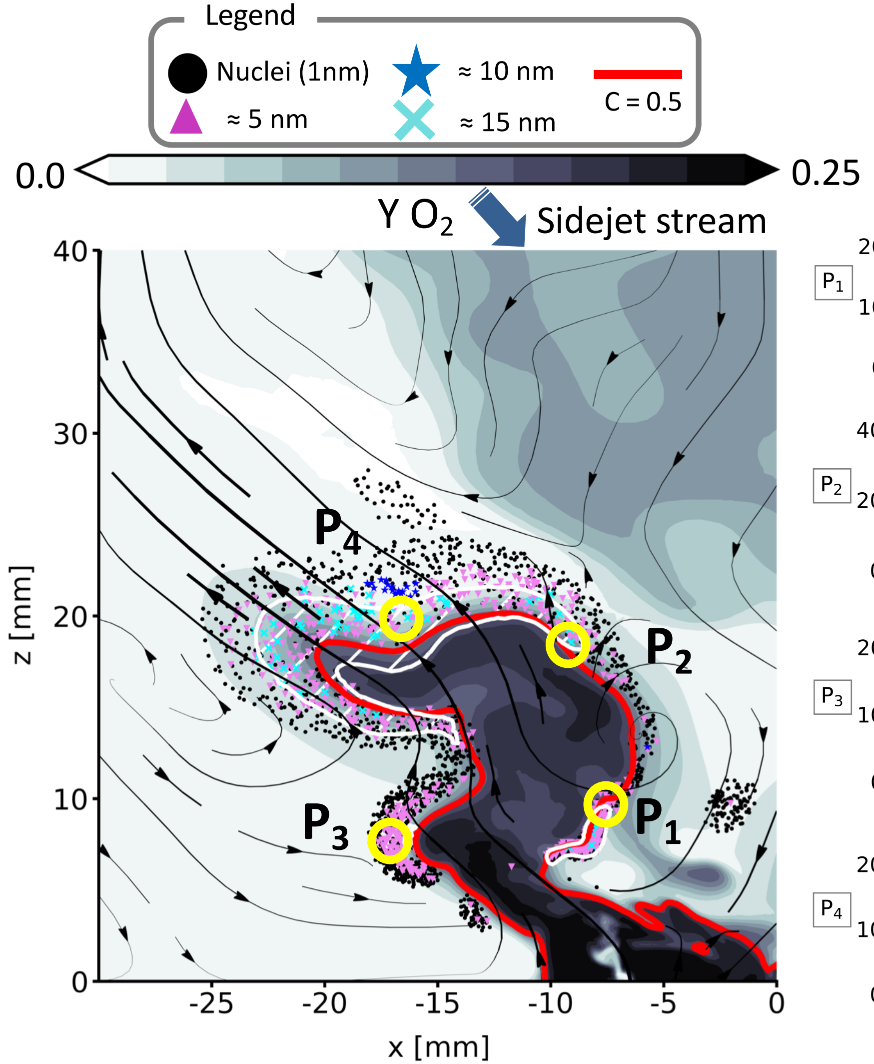
Soot presence superimposed on mean tangential velocity

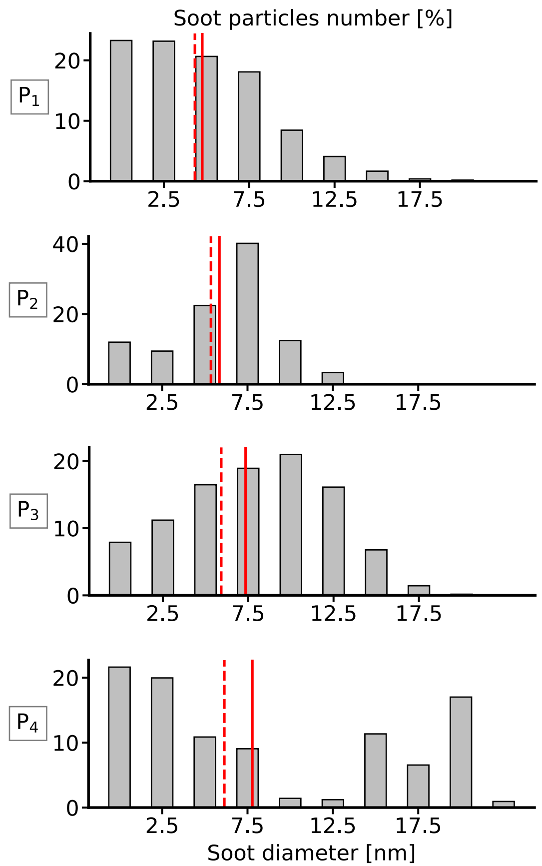
[1]*Gallen et al. PCI 2019*

Application to soot production[1]

Direct access to soot particle size distribution

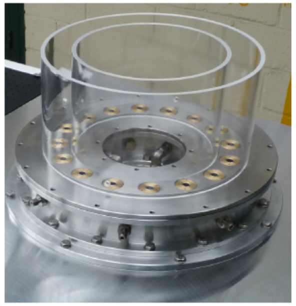






[1]*Gallen et al. PCI 2019*

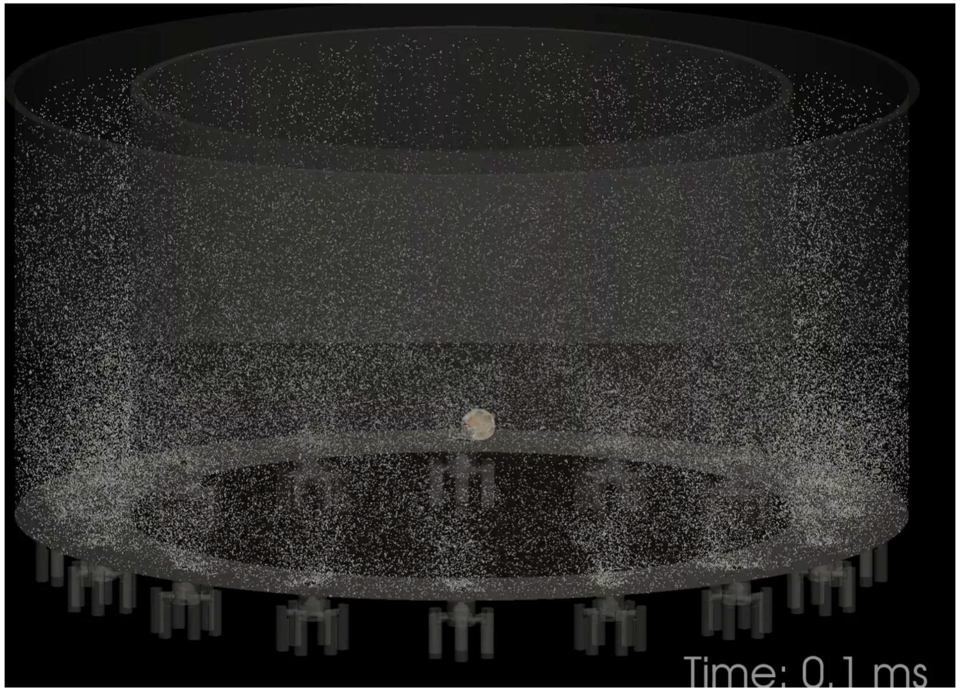
Ignition of the MICCA-Spray burner of EM2C[1,2]



Philip et al, ASME 2013
Prieur et al, PCI 2017

- 16 swirled injectors
- n-heptane – air

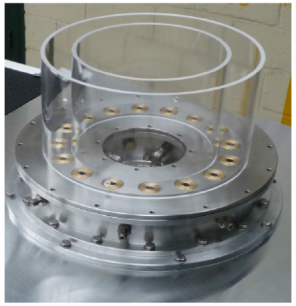
- 320 Million cells
- 50 Million droplets



CERFACS

[1]*Lancien PhD, 2018*
[2]*Collin PhD, 2019*

Ignition of the MICCA-Spray burner of EM2C[1,2]



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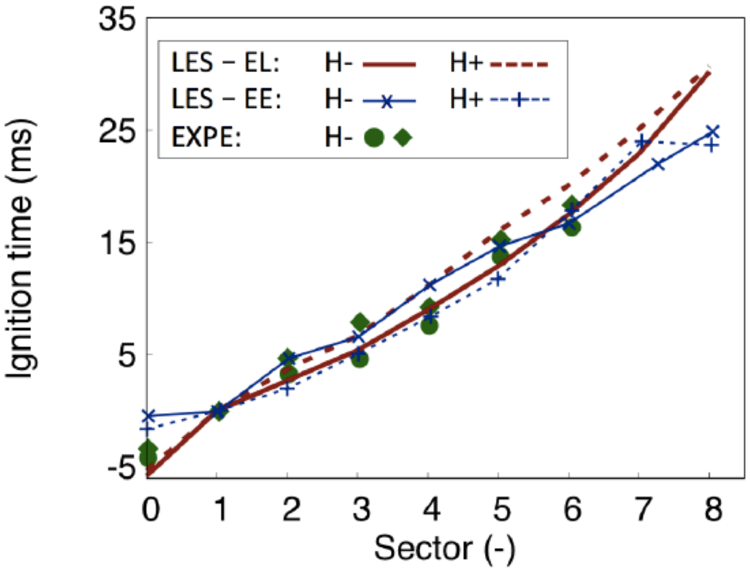
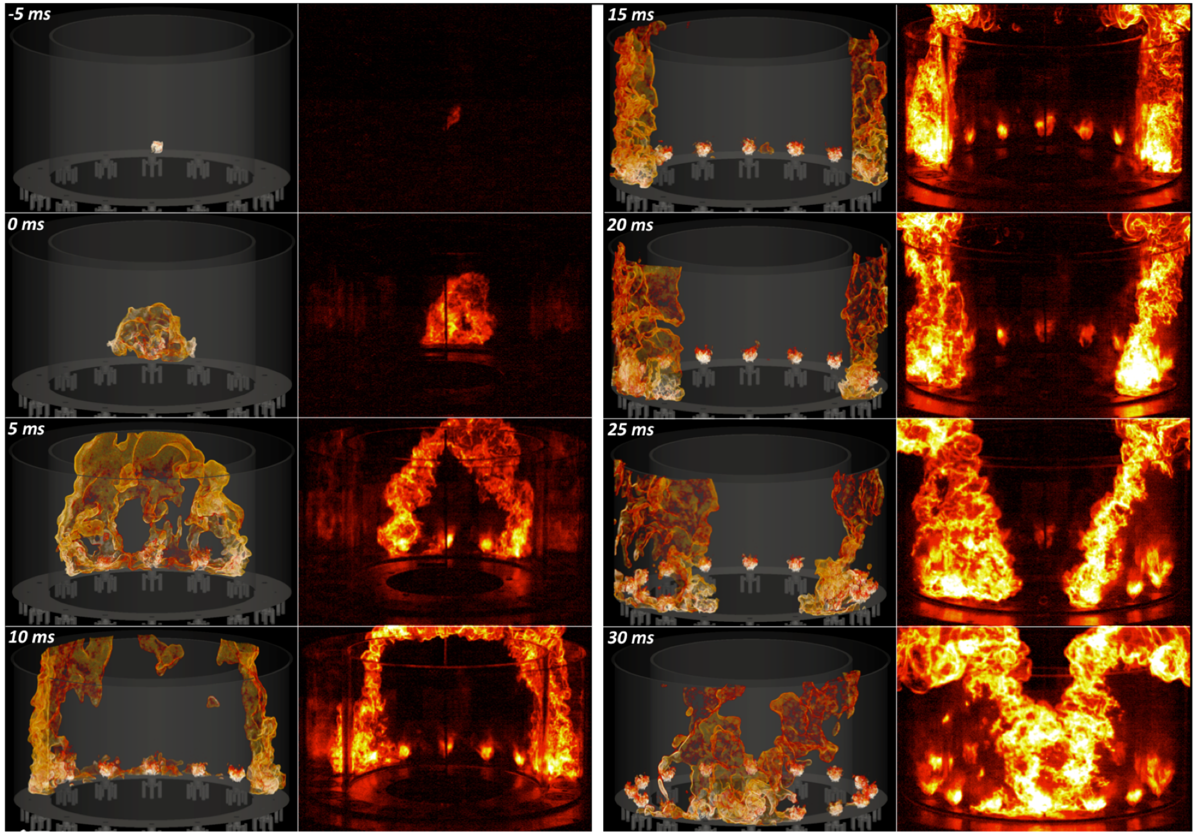
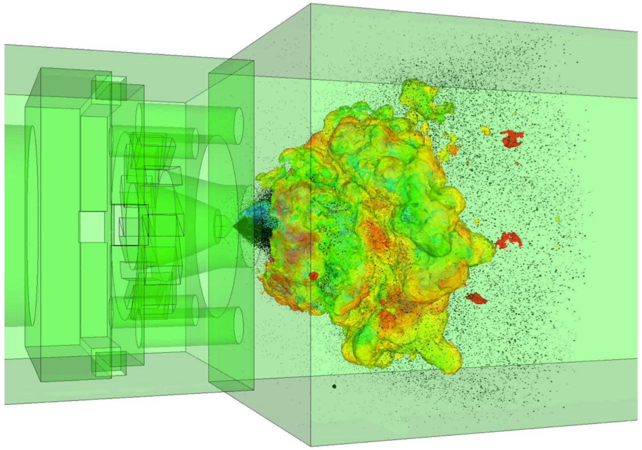
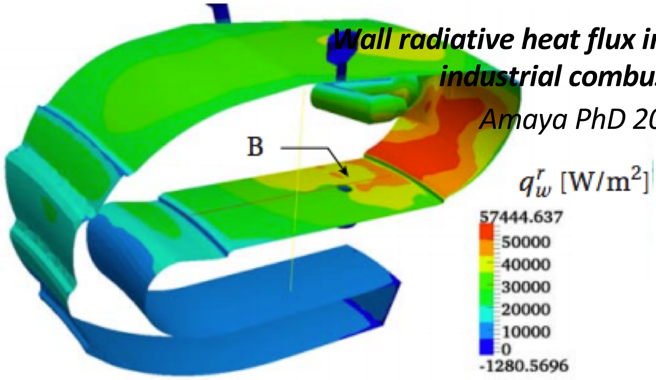




Conclusions

✓ **LES** with **DTFLES**, **ARC** chemistry and **Lagrangian** solver is able to describe turbulent gaseous and spray flames, their pollutant emissions, and transient behaviors with good accuracy in complex geometries.





Wall radiative heat flux in an industrial combustor
Amaya PhD 2010

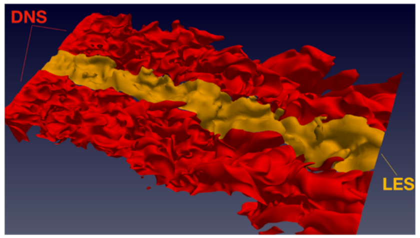
✓ LES may be coupled to other physics (thermal radiation, conduction, etc)

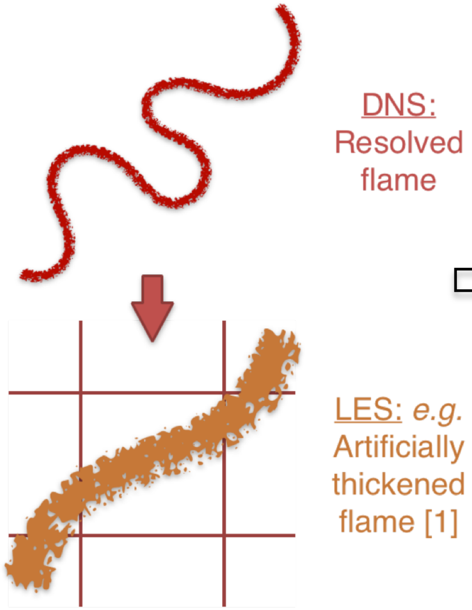
✓ Improvements are still necessary:
- Soot chemistry
- Multi-component liquid fuel
- ARC for fuel blends
- Turbulent combustion model

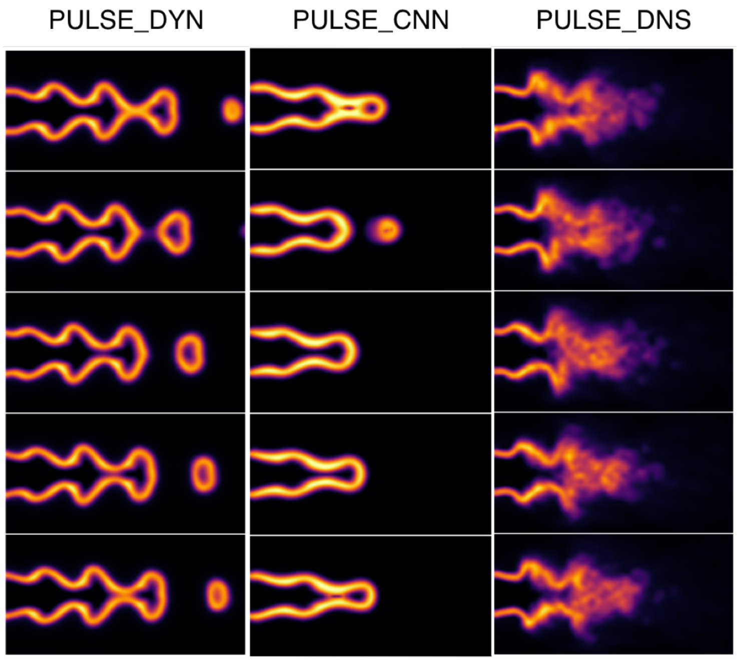
Can Machine Learning help?

Training convolutional neural networks to estimate turbulent sub-grid scale reaction rates.

Lapeyre et al, C. & F. 2019







Special thanks to

Thomas Jaravel

Damien Paulhiac

Lucas Esclapez

Francis Shum-Kivan

Anne Felden

Félix Collin-Bastiani

Lucien Gallen