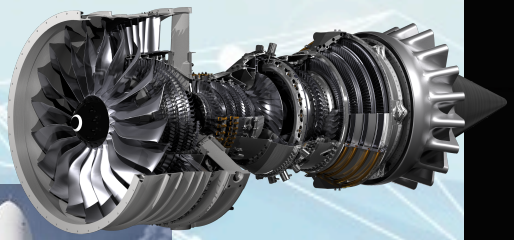
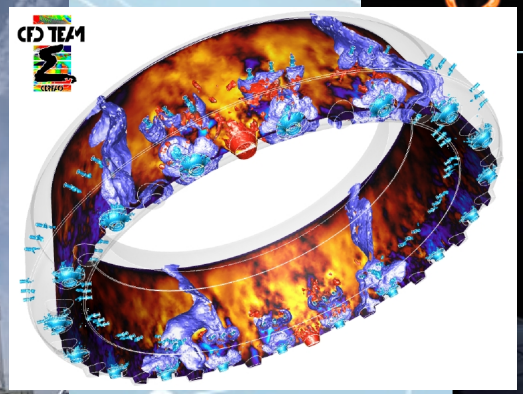
CERFACS

EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Simulation of Turbulent Combustion : Models and Applications

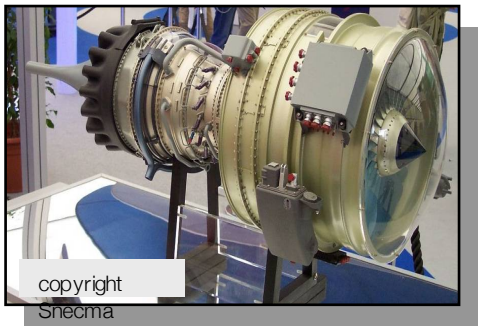




B.Cuenot & the CFD Team

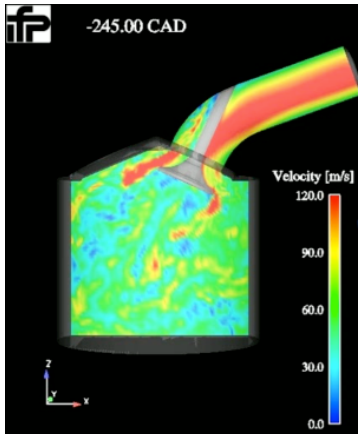
Combustion is (almost) everywhere ...

- Aeronautical engines (planes / helicopters)

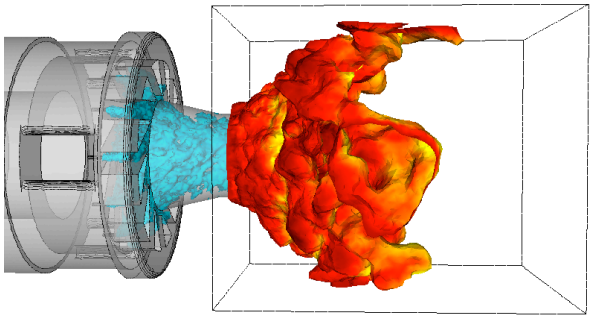


- Spatial launchers (solid and liquid propulsion)

- Piston engines

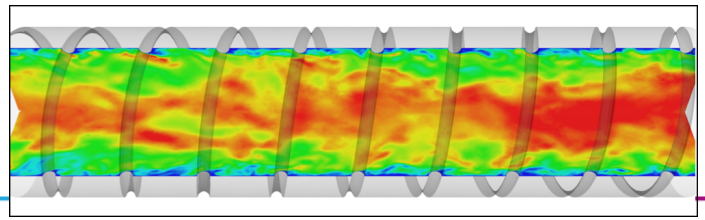


- Gas turbines

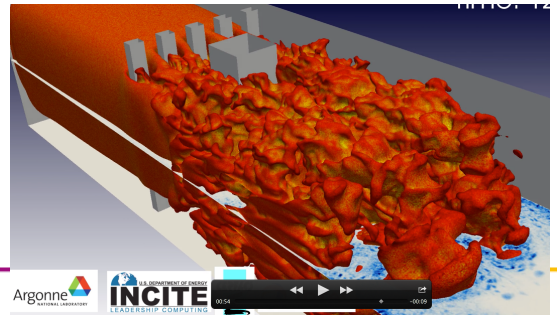


- Fires

- Petrochemistry



- Transition to detonation



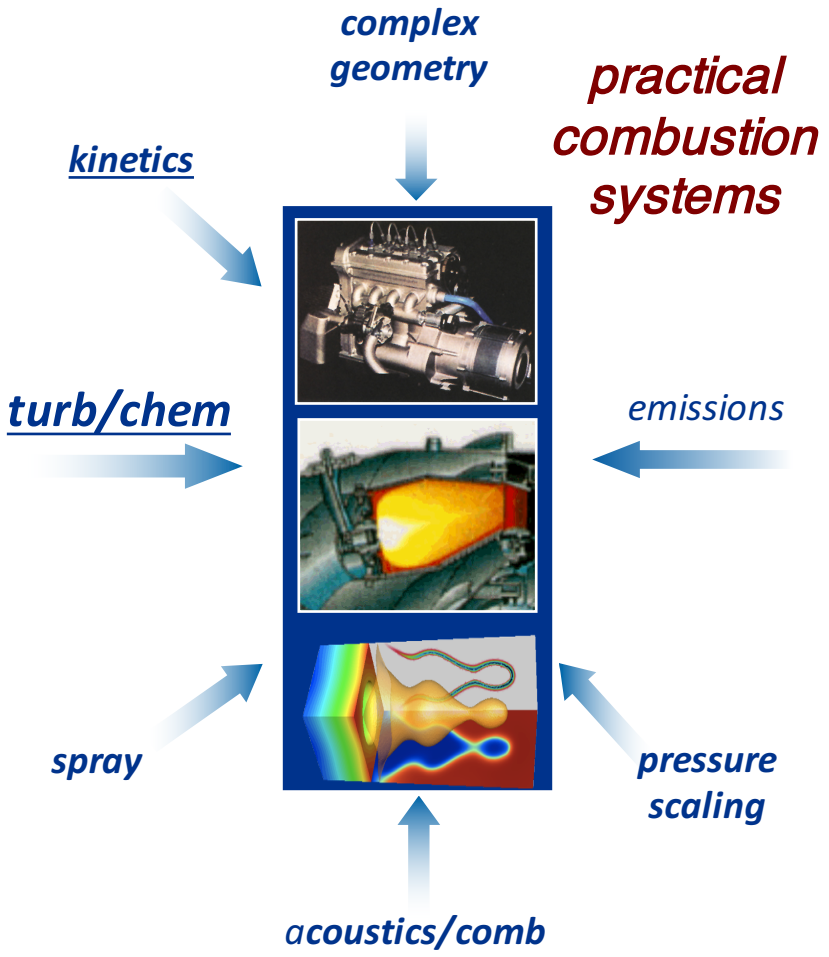
Why study Turbulent Combustion?

Performances

- Temperature field ⟹ Machine life cycle
- Efficiency & Emissions ⟹ NOx, CHx, CO2,CO
- Wall temperature ⟹ Cooling systems
- Stability & ignition

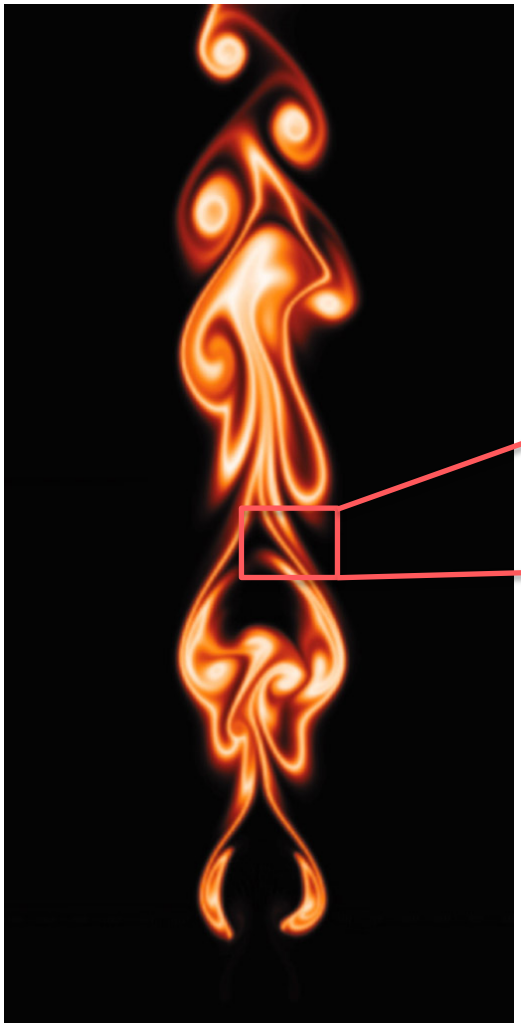
Technical challenges

- Aerodynamics & mixing
  ⟹ swirl, jets in cross-flow, multiperf.
- Turbulence / chemistry interation
  ⟹ kerosene kinetics, pollutants
- Two-phase flow
  ⟹ fuel flow physics & dynamics
- Heat transfer
  ⟹ cooling, thermal radiation

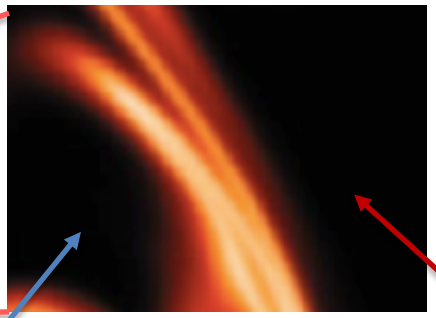


Advanced CFD and ***Massively parallel*** computer architectures offer a clear potential for time and cost reductions of the design process by providing ***accurate predictions***

What is a flame?



A flame is the combination of thermochemical processes and transport (mixing)



Reactants

flame zone

Products + Heat release

Flow model:
- variable density
- multi-species
- chemical source terms

What are the equations?

Navier-Stokes equations:

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

- steady / unsteady
- compressible / low-mach

Species conservation equations

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

- thermodynamic and transport properties
- chemical kinetics

Energy equation

$$\rho\frac{DE}{Dt} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij}u_i) - \frac{\partial}{\partial x_i}(Pu_i) + \dot{\omega}_T + \dot{\mathrm{Q}}$$

4 + Nspec* conservation equations

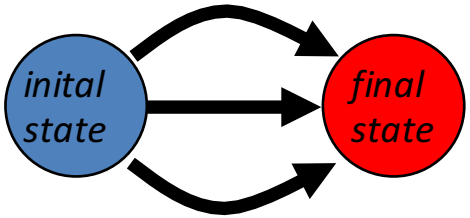
* without continuity equation

Chemical equilibrium

Any chemical reaction is accompanied by an absorption or evolution of energy (heat)

⇒ Thermodynamics of mixtures :

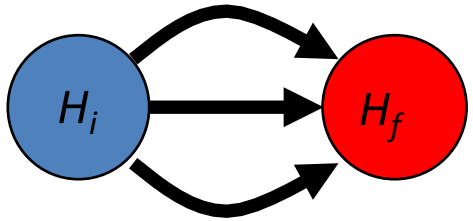
- The *total energy change* of a system is independent of the path taken to change state.



- The *internal energy* essentially depends on *temperature, pressure* and *composition.*

$$E = \sum_k Y_k E_k(T,P)$$

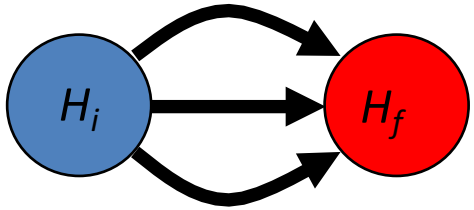
⇒ The heat released by reaction is equal to the change in enthalpy of the (open) system.



$$Q_p = -\Delta H = H_f - H_i$$

⇒ If combustion is complete: $T_2 = T_{ad} = T_1 + Y_F Q_p / C_p$ is the *adiabatic flame temperature*

n_i *reactants* T_1

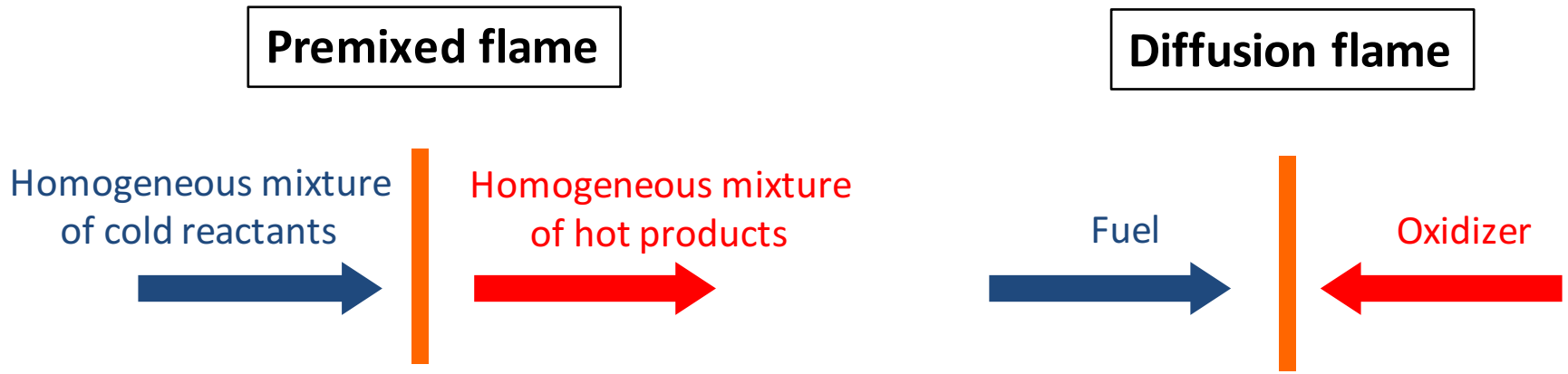


n_j *products* T_2

(isobaric process)

Laminar flame structures

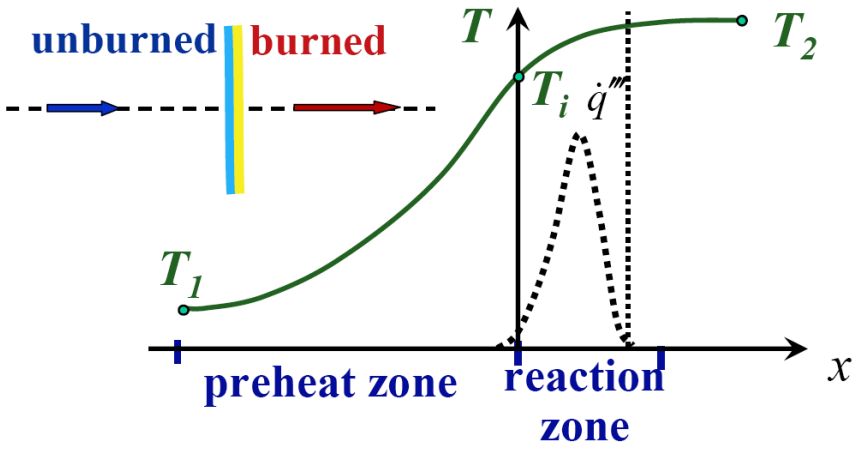
- Laminar flames with detailed measurements are useful to validate combustion chemistry.
- Laminar flames are generic cases at the basis of most turbulent combustion models.
- Laminar flames are reference solutions for complex flame analysis.



Equivalence ratio: $$\phi = s\frac{Y_{Fuel}}{Y_{Oxyd}} = \frac{Y_{Fuel}}{Y_{Oxyd}}\frac{Y_{Oxyd}}{Y_{Fuel}}\bigg|_{st} = s\frac{\dot{m}_{Fuel}}{\dot{m}_{Oxyd}}$$

- Stoichiometry $\phi = 1$
- Fuel rich $\phi > 1$
- Fuel lean $\phi < 1$

Laminar (1D) premixed flame



Simplifying assumptions:

- $W_k = W$, $C_{p,k} = C_p$
- $D_k = D \Rightarrow Le = 1$
- $\dot{\omega}_T = -Q\,\dot{\omega}_F$

$$\rho\, u = Cst = \rho_1\, u_1 = \rho_1\, S_L$$

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

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

$$CL: \quad u(x=-\infty) = u_1, \quad T(x=-\infty) = T_1, \quad Y_F(x=-\infty) = Y_{F,1}$$

After integration: $\int \dot{\omega}_F\, dx = \Omega_F$

$$\rho_1\, S_L\, Y_F^1 = \Omega_F$$

$$\rho_1\, C_p\, S_L\, (T_2 - T_1) = Q\, \Omega_F$$

$$T_2 = T_1 + Q Y_F^1 / C_p$$

Adiabatic flame temperature

Progress variable

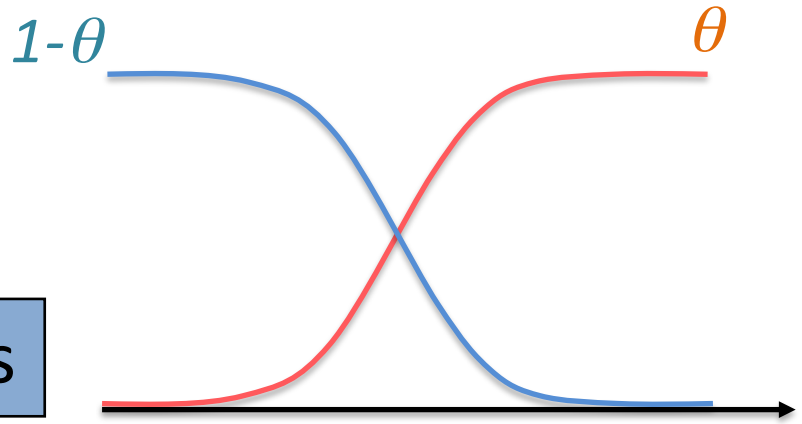
Reduced variables: $$Y = \frac{Y_F}{Y_F^1}, \quad \theta = \frac{T - T_1}{T_2 - T_1} = \frac{C_p\,(T - T_1)}{\mathrm{Q}\,Y_F^1}$$

(1) $$\rho_1\, S_L\, \frac{dY}{dx} = \frac{d}{dx}\left(\rho\, D\, \frac{dY}{dx}\right) + \frac{\dot{\omega}_F}{Y_F^1}, \quad \text{with } Y(-\infty) = 1, Y(+\infty) = 0$$

(2) $$\rho_1\, S_L\, \frac{d\theta}{dx} = \frac{d}{dx}\left(\frac{\lambda}{C_p}\, \frac{d\theta}{dx}\right) - \frac{\dot{\omega}_F}{Y_F^1}, \quad \text{with } \theta(-\infty) = 0, \theta(+\infty) = 1$$

(1)+(2) $$\rho_1\, S_L\, \frac{d}{dx}(Y + \theta) = \frac{d}{dx}\left[\rho\, D\, \frac{d}{dx}(Y + \theta)\right] \quad \text{with } [Y + \theta](-\infty) = 1, [Y + \theta](+\infty) = 1$$

$\Longrightarrow$ $Y+\theta = 1$ everywhere



(1-Y) or θ are called progress variables

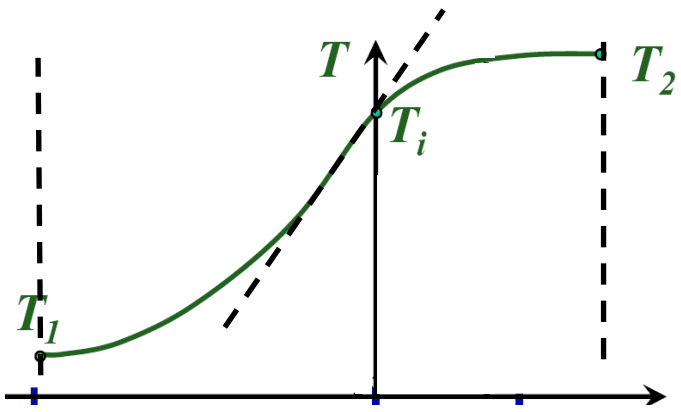
Flame speed and thickness

In premixed lean flames: $$\rho_1 S_L \frac{d\theta}{dx} = \frac{d}{dx}\left(\frac{\lambda}{C_p}\frac{d\theta}{dx}\right) - \frac{\dot{\omega}_F}{Y_F^1}$$

S_L is determined by two competitive phenomena:
- thermal diffusion $D_{th} = \lambda / Cp$
- chemistry

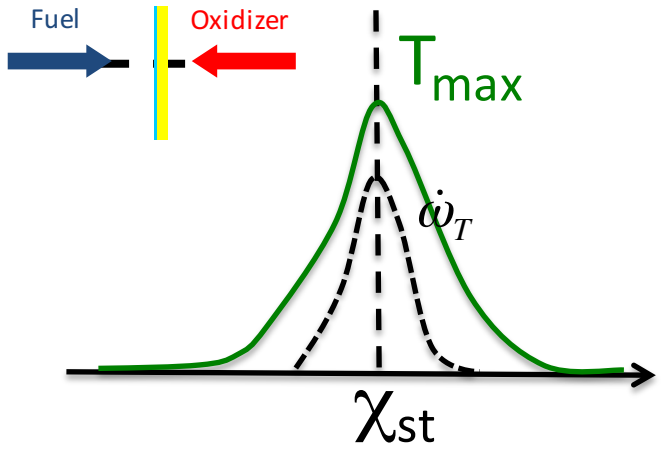
$\Rightarrow$ Asymptotic analysis yields: $S_L \propto \sqrt{D_{th}^1 \, \mathcal{A}}$ ← pre-exponential factor

$\Rightarrow$ The same phenomena control the flame thickness:



- From scaling laws $$\delta_L = \frac{D_{th}^1}{S_L} \propto \sqrt{\frac{D_{th}^1}{\mathcal{A}}}$$
- From temperature profiles $$\delta_L^0 = \frac{T_2 - T_1}{\max\left(\left|\frac{\partial T}{\partial x}\right|\right)}$$

Laminar (1D) diffusion flame



Simplifying assumptions:

- $W_k = W$, $C_{p,k} = C_p$
- $D_k = D \Rightarrow Le = 1$
- $\dot{\omega}_O = s\,\dot{\omega}_F$ with, $s = \dfrac{\nu_O W_O}{\nu_F W_F}$

$\dot{\omega}_T = -\mathrm{Q}\,\dot{\omega}_F$

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

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

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

Reactants diffuse and reaction occurs where they meet, at the optimum mixing conditions (ie., stoichiometry).

Characteristic *flame speed* and *thickness* do not apply in this context.

Define :

$$Z_1 = sY_F - Y_O, \quad Z_2 = \frac{C_P T}{Q} + Y_F, \quad Z_3 = s\frac{C_P T}{Q} + Y_O$$

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

⇒ Passive scalar

⇒ The problem is reduced to *1 variable*:

$Y_k = f_k(Z)$, $T = T(Z)$

In Z-space:

$$\rho D \left(\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}\right)\frac{\partial^2 Y_k}{\partial Z^2} = \dot{\omega}_k$$

Scalar dissipation rate: 1/2 χ

Infinitely fast chemistry

Burke-Schumann solution: reaction occurs only at $Z_{st} = \dfrac{1}{1 + sY_F^0 / Y_O^0}$

$$\Longrightarrow \quad \frac{\partial^2 Y_k}{\partial Z^2} = 0$$

- Fuel side: $Z > Z_{st}$

$$Y_F(Z) = Z\,Y_F^0 + (Z-1)\frac{Y_O^0}{s} = Y_O^0\,\frac{Z - Z_{st}}{1 - Z_{st}},$$

$$Y_O(Z) = 0,$$

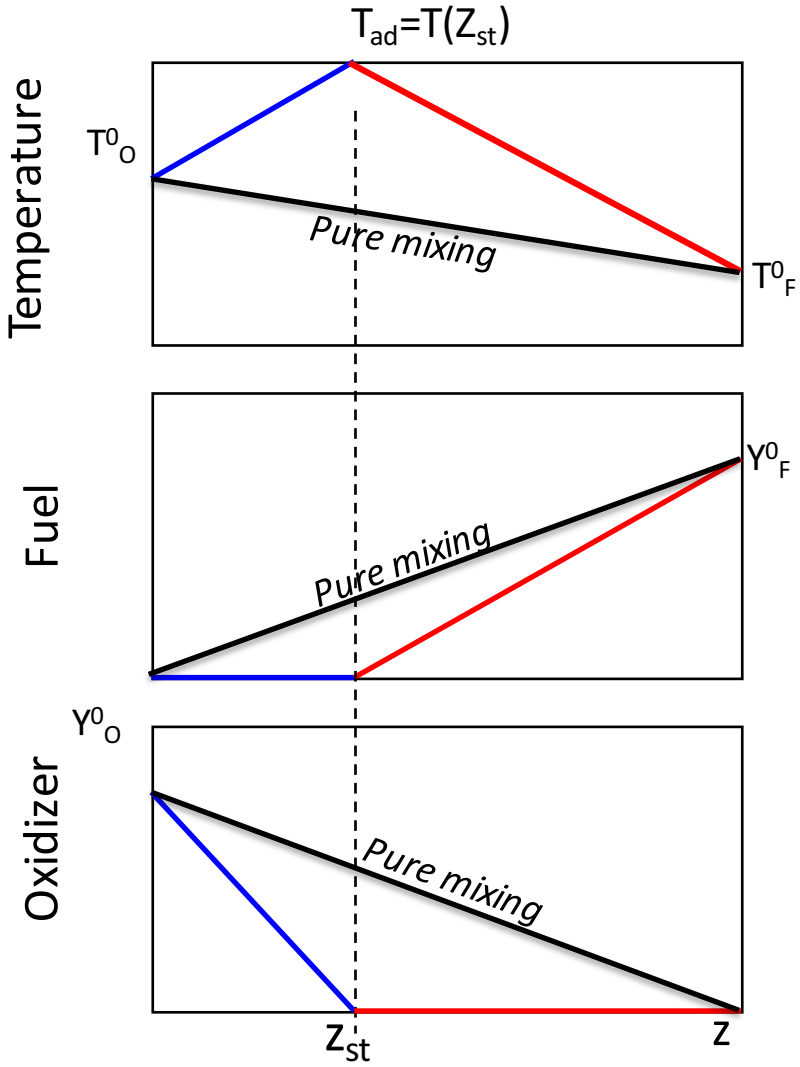
$$T(Z) = Z\,T_F^0 + (1-Z)\,T_O^0 + \frac{QY_F^0}{C_P}\,Z_{st}\,\frac{1-Z}{1-Z_{st}},$$

- Oxidizer side: $Z < Z_{st}$

$$Y_F(Z) = 0,$$

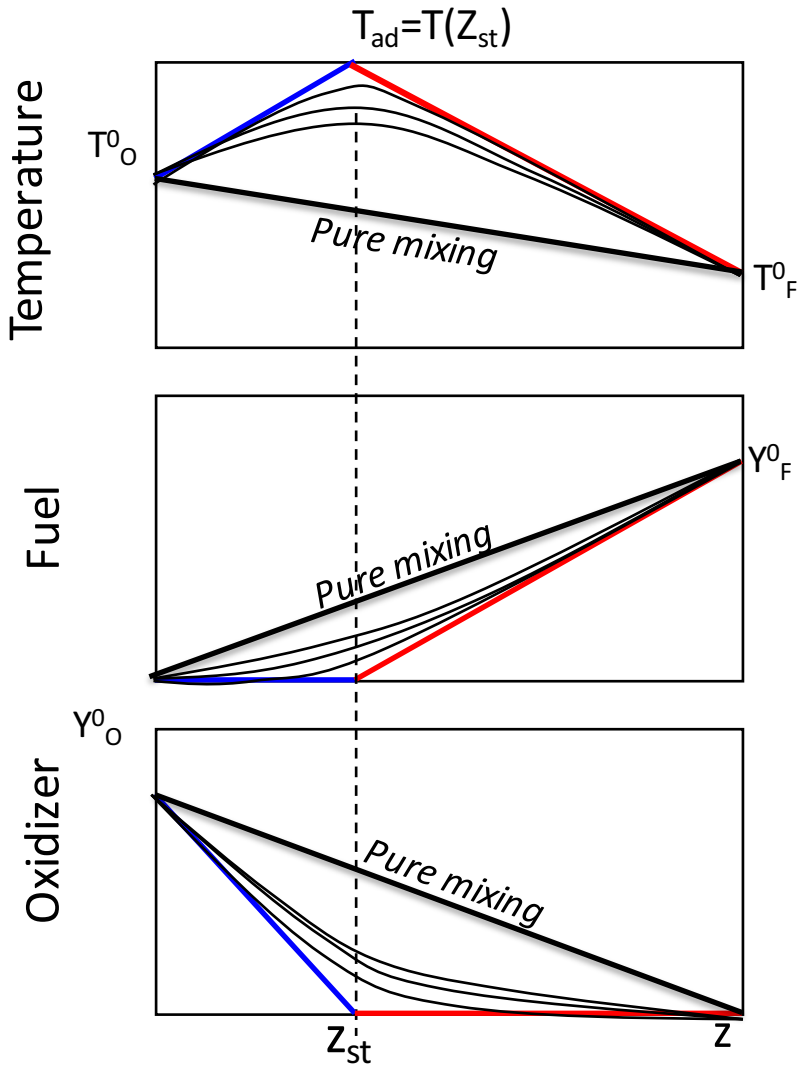
$$Y_O(Z) = Y_O^0\,\left(1 - \frac{Z}{Z_{st}}\right),$$

$$T(Z) = Z\,T_F^0 + (1-Z)\,T_O^0 + \frac{QY_F^0}{C_P}\,Z,$$



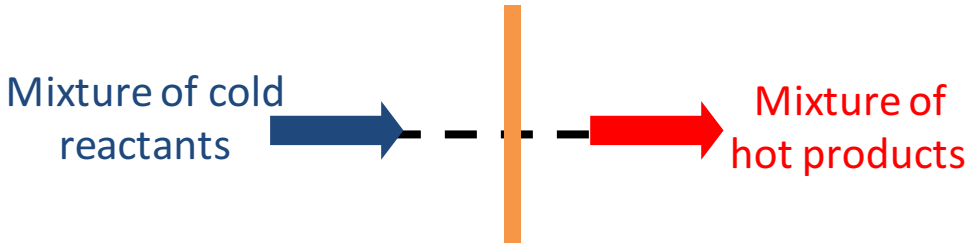
$$\Longrightarrow \quad \rho \frac{\chi}{2} \frac{\partial^2 Y_k}{\partial Z^2} = \dot{\omega}_k$$

- χ controls mixing: if known, the *flamelet equation* can be solved in *Z*-space to provide the flame structure.
- A characteristic length representative of the mixing layer reads: $\sqrt{D/\chi}$
- When flame strain rate increases, χ increases



Laminar flames : synopsis

Premixed flames

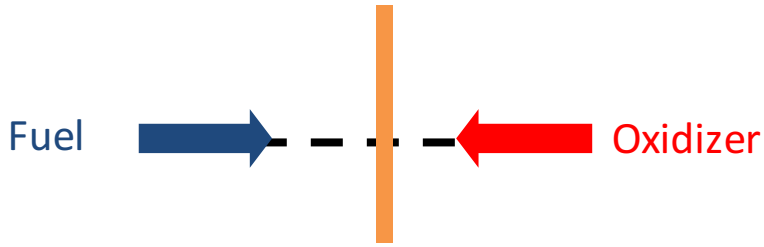


- Chemistry dominated
- Flame speed and thickness:

$$S_L \propto \sqrt{D^1_{th}\,\mathcal{A}} \qquad \delta_L = \frac{D^1_{th}}{S_L} \propto \sqrt{\frac{D^1_{th}}{\mathcal{A}}}$$

- Progress variable: *(1-Y)* or θ
- Influence by stretch: κ

Diffusion flames



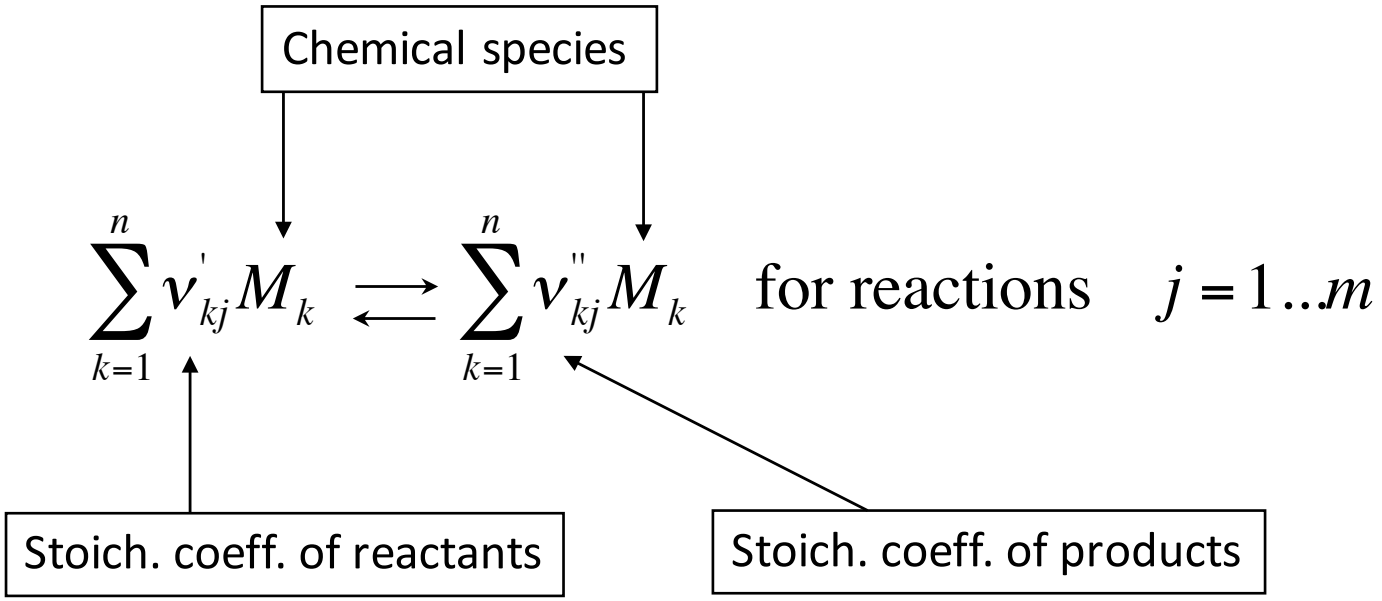
- Diffusion dominated
- Passive / conserved scalar variable: *Z*
- Mixing state provides the flame structure:

  T(Z), Y_k(Z)
- Strongly influenced by flow structures:

$$\chi = 2\,D\left(\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}\right)$$

Real applications are in-between: *partially premixed* configurations
… and *turbulent*

Stoichiometric relationships for an arbitrarily complex set of *m* reactions involving *n* species, may be written:



Nb	Reaction
1	$H_2 + O_2 \rightleftharpoons 2OH$
2	$OH + H_2 \rightleftharpoons H_2O + H$
3	$H + O_2 \rightleftharpoons OH + O$
4	$O + H_2 \rightleftharpoons OH + H$
5[a]	$H + O_2 + M \rightleftharpoons HO_2 + M$
6	$H + O_2 + O_2 \rightleftharpoons HO_2 + O_2$
7	$H + O_2 + N_2 \rightleftharpoons HO_2 + N_2$
8	$OH + HO_2 \rightleftharpoons H_2O + O_2$
9	$H + HO_2 \rightleftharpoons 2OH$
10	$O + HO_2 \rightleftharpoons O_2 + OH$
11	$2OH \rightleftharpoons O + H_2O$
12[b]	$H_2 + M \rightleftharpoons H + H + M$
13	$O_2 + M \rightleftharpoons O + O + M$
14[c]	$H + OH + M \rightleftharpoons H_2O + M$
15	$H + HO_2 \rightleftharpoons H_2 + O_2$
16	$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$
17	$H_2O_2 + M \rightleftharpoons OH + OH + M$
18	$H_2O_2 + H \rightleftharpoons HO_2 + H$
19	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$

Reduced chemical schemes

Accuracy

- Detailed schemes (GRImech~500 reactions) are produced from very large size schemes developed by chemists and are able to accurately describe oxidation of most hydrocarbons
- A first reduction step leads to skeletal mechanisms (~50-100 reactions) that keep most of the performances of detailed schemes
- A second reduction step (QSS) leads to analytical schemes (~10-30 reactions) having reduced but still reasonable performances
- Finally, optimally fitted global or semi-global schemes (1 to 4 steps) often require on-line adjustment of constants with P, Φ, etc

CPU cost

In addition, complex fuels are simplified and described with surrogate fuels

	Surrogate 1		Surrogate 2	
Component	mole [%]	vol. [%]	mole [%]	vol. [%]
n-heptane	22.0	23.5	66.8	74.1
iso-octane	44.8	53.6	0.4	0.5
benzene	13.0	10.0	24.8	20.0
toluene	20.2	12.9	7.9	5.3
Avg. formula	$C_{7.32}H_{14.0}$		$C_{6.75}H_{12.9}$	

The Arrhenius law

The progress rate of the j^{th} reaction is given by:

$$Q_j = K_j^f \prod_{k=1}^{n} \left[\frac{\rho Y_k}{W_k}\right]^{\nu'_{kj}} - K_j^b \prod_{k=1}^{n} \left[\frac{\rho Y_k}{W_k}\right]^{\nu''_{kj}}$$

Reverse rate of reaction

Forward rate of reaction

The essential problem of chemists is to provide these two rates. They usually rely on the Arrhenius law:

$$K_j^f = A_j^f T^{\beta_j} \exp(-E_j / RT)$$

Collision frequency:
- Pre-exponential Cst
- Temp. modulation

Activation energy

and equilibrium constants:

$$K_j^r = \frac{K_j^f}{(P_a/RT)^{\sum_{k=1}^{n}(\nu'_{kj}-\nu''_{kj})}} \exp\left(\frac{\Delta S_j^0}{R} - \frac{\Delta H_j^0}{RT}\right)$$

Entropy and enthalpy changes of j^{th} reaction (from the thermodynamics table)

The Arrhenius law

The progress rate of the j^{th} reaction is given by:

$$Q_j = K_j^f \prod_{k=1}^{n} \left[\frac{\rho Y_k}{W_k}\right]^{\nu'_{kj}} - K_j^b \prod_{k=1}^{n} \left[\frac{\rho Y_k}{W}\right]^{\nu''_{kj}}$$

Reverse rate of reaction

Forward ra

HIGHLY NON-LINEAR !!

The essential pr ue these two rates. They usually rely on the Arrhe and equilibrium constants:

$$K_j^f = A_j^f T^{\beta_j} \exp(-E_j/RT)$$

Collision frequency:
- Pre-exponential Cst
- Temp. modulation

Activation energy

$$K_j^r = \frac{K_j^f}{(P_a/RT)^{\sum_{k=1}^{n}(\nu'_{kj}-\nu''_{kj})}} \exp\left(\frac{\Delta S_j^0}{R} - \frac{\Delta H_j^0}{RT}\right)$$

Entropy and enthalpy changes of j^{th} reaction (from the thermodynamics table)

Turbulence / Combustion interaction

Turbulence enhances combustion thanks to increased mixing:

- between fresh and burnt gas in premixed flames
- between reactants in diffusion flames

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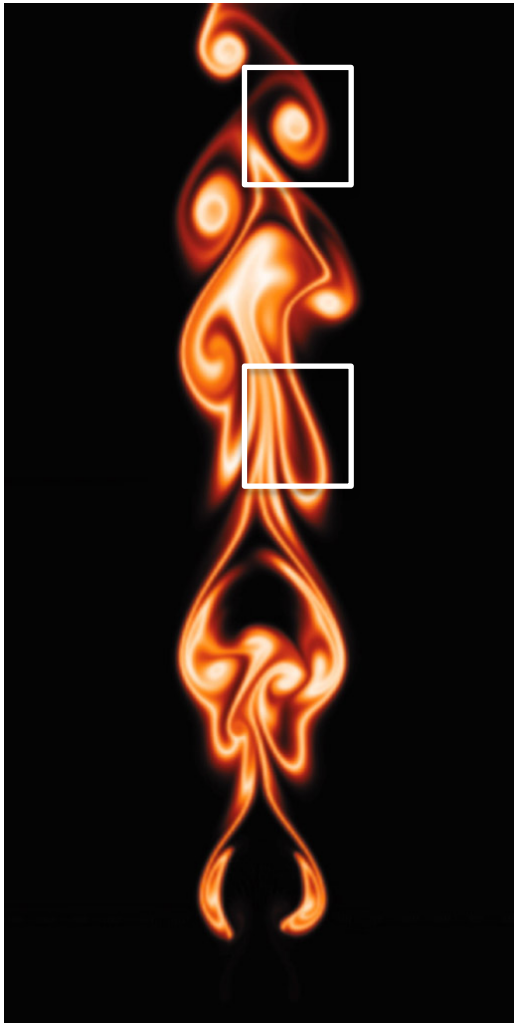
⟹ Flame wrinkling

Turbulence / Combustion interaction



Turbulence enhances combustion thanks to increased mixing:

- between fresh and burnt gas in premixed flames
- between reactants in diffusion flames

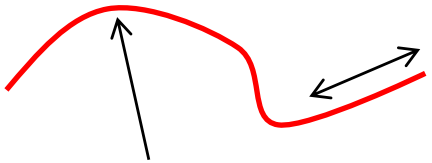
⟹ Flame wrinkling

Turbulence can be detrimental to combustion by altering the inner flame structure, even leading to local quenching

⟹ Strain, curvature

Flames are sensitive to flow perturbations: strain rate and curvature

- premixed flames: stretch
- diffusion flames: scalar dissipation rate



=> **Damköhler number**:
ratio between the turbulent eddy time and the chemical time-scale

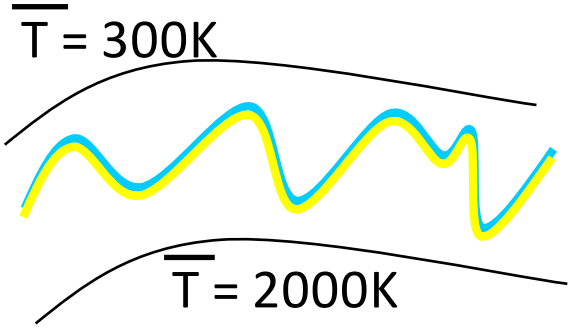
$$Da = \frac{\tau_t}{\tau_c}$$

$$\tau_t = \frac{l_t}{u'}$$

l_t ← Characteristic length of turbulence

u' ← Turbulence intensity

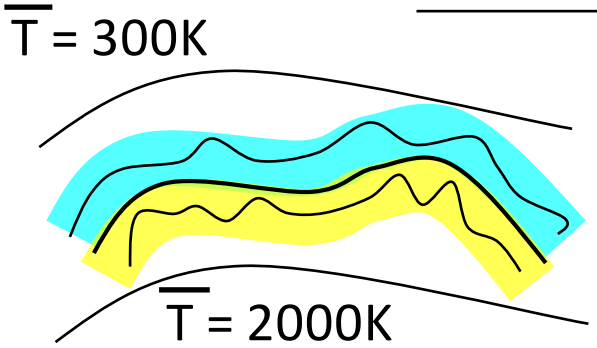
Premixed Turbulent Flames $\tau_c = \frac{\delta_L}{S_L}$



- Chemistry is fast and the reaction zone is thin compared to the intensity and size of the eddies:

$$l_t >> \delta_L \quad \text{or} \quad Da >> 1$$

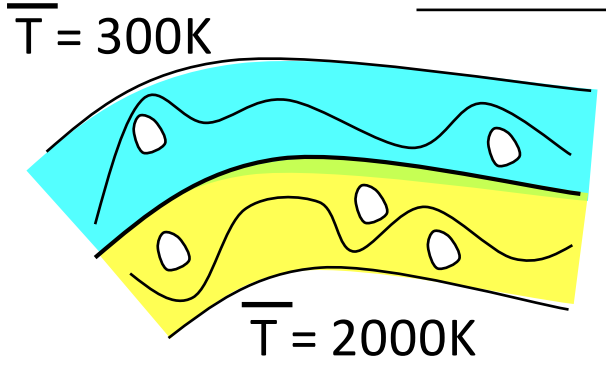
--> **Inner flame structure is unaffected**



- Chemistry and turbulence characteristic sizes are comparable:

$$l_t \approx \delta_L \quad \text{or} \quad Da \approx 1$$

--> **Inner flame structure is affected**

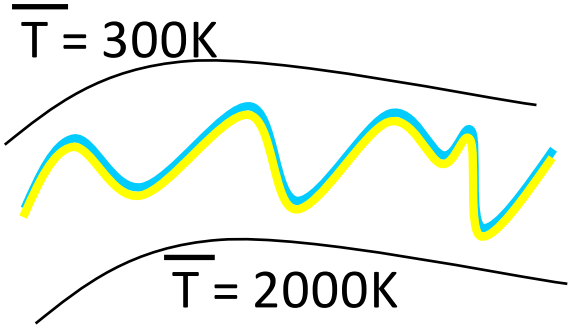


- Chemistry is much slower than turbulence:

$$l_t << \delta_L \quad \text{or} \quad Da << 1$$

--> **Inner flame structure is changed**

Premixed Turbulent Flames $\tau_c = \frac{\delta_L}{S_L}$

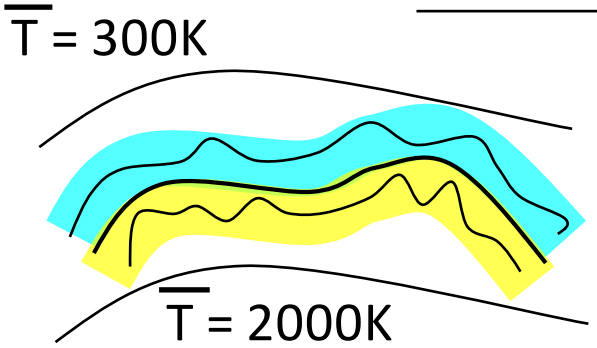


- Chemistry is fast and the reaction zone is thin compared to the intensity and size of the eddies:

Flamelet regime

$$l_t \geq \delta_L \quad \text{or} \quad Da >> 1$$

--> **Inner flame structure is unaffected**



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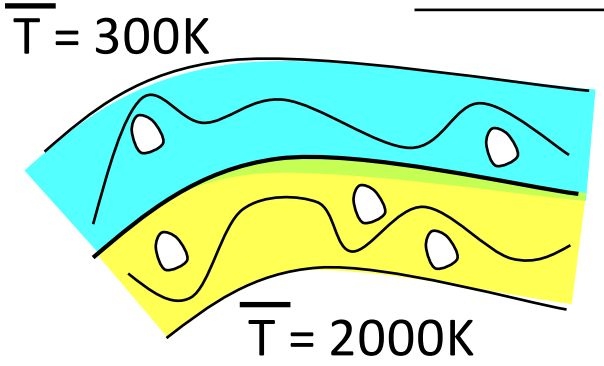
$$l_t \approx \delta_L \quad \text{or} \quad Da \approx 1$$

--> **Inner flame structure is affected**



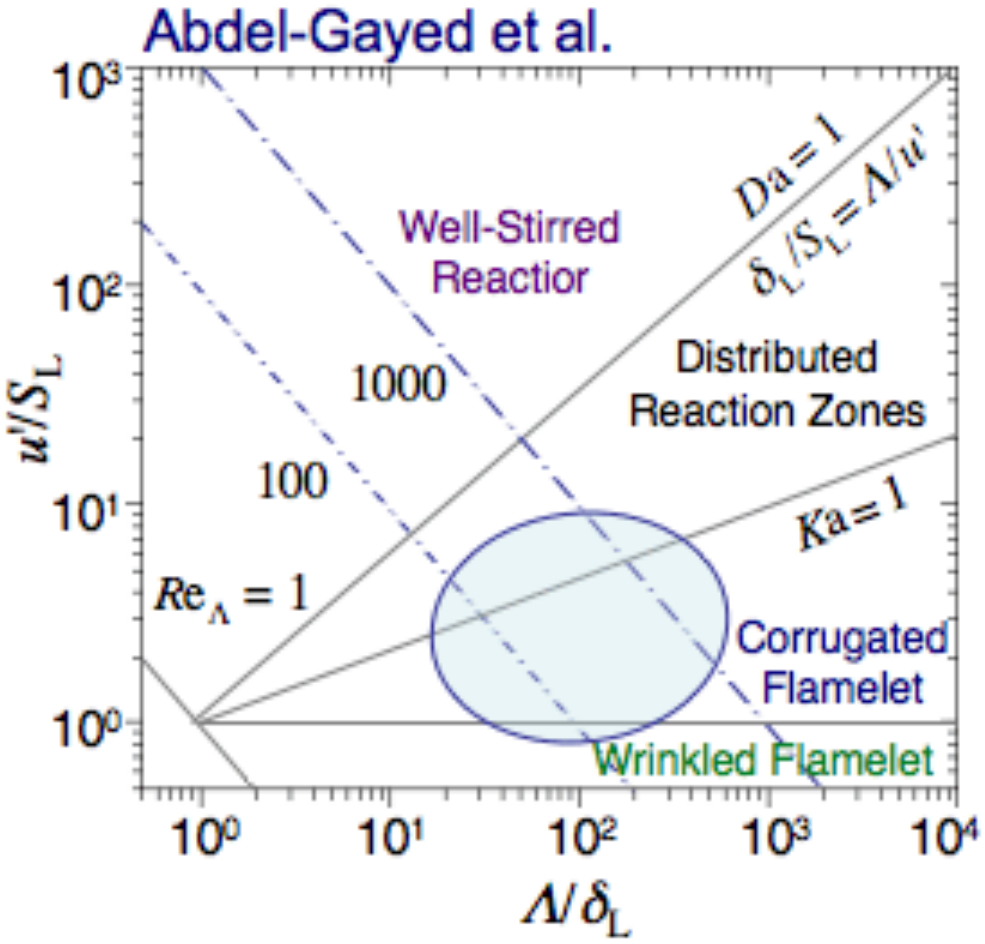
- Chemistry is much slower than turbulence:

Well stirred reactor

$$l_t << \delta_L \quad \text{or} \quad Da << 1$$

--> **Inner flame structure is changed**

Premixed Turbulent Flames: Regime Diagram



Karlovitz number:

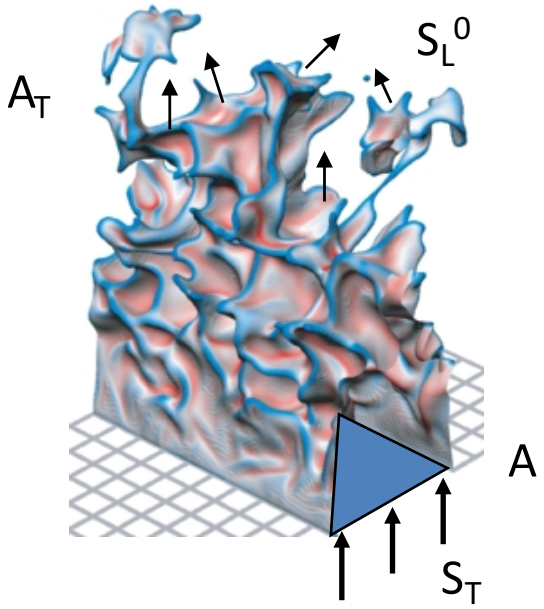
$$Ka = \frac{\tau_c}{\tau_K}$$

Kolmogorov scale

=> Turbulent combustion encompasses a wide realm of physical features which must be captured by turbulent combustion models

Premixed Turbulent Flames: Turbulent Flame Speed

The main impact of turbulence is to increase the heat release rate through flame wrinkling :



$$A_T \ \rho_1 \ Y_F^1 \ S_L^0 = -\int_V \dot{\omega}_F \ dV$$

$$= A \ \rho_1 \ Y_F^1 \ S_T$$

S_T is the turbulent flame speed

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

A_T/A (wrinkling factor) increases with Re

Note: stretch effects are ususally not modelled

!!! Reactants need to mix prior to combustion !!!

⇒ Fast mixing and slow combustion : premixed combustion !
⇒ Fast reactions and slow mixing: flame is controlled by diffusion

Problem: how to define characteristic scales?

$$\tau_f \approx \frac{1}{\chi_{st}}$$

Scalar dissipation rate @ stoich. line

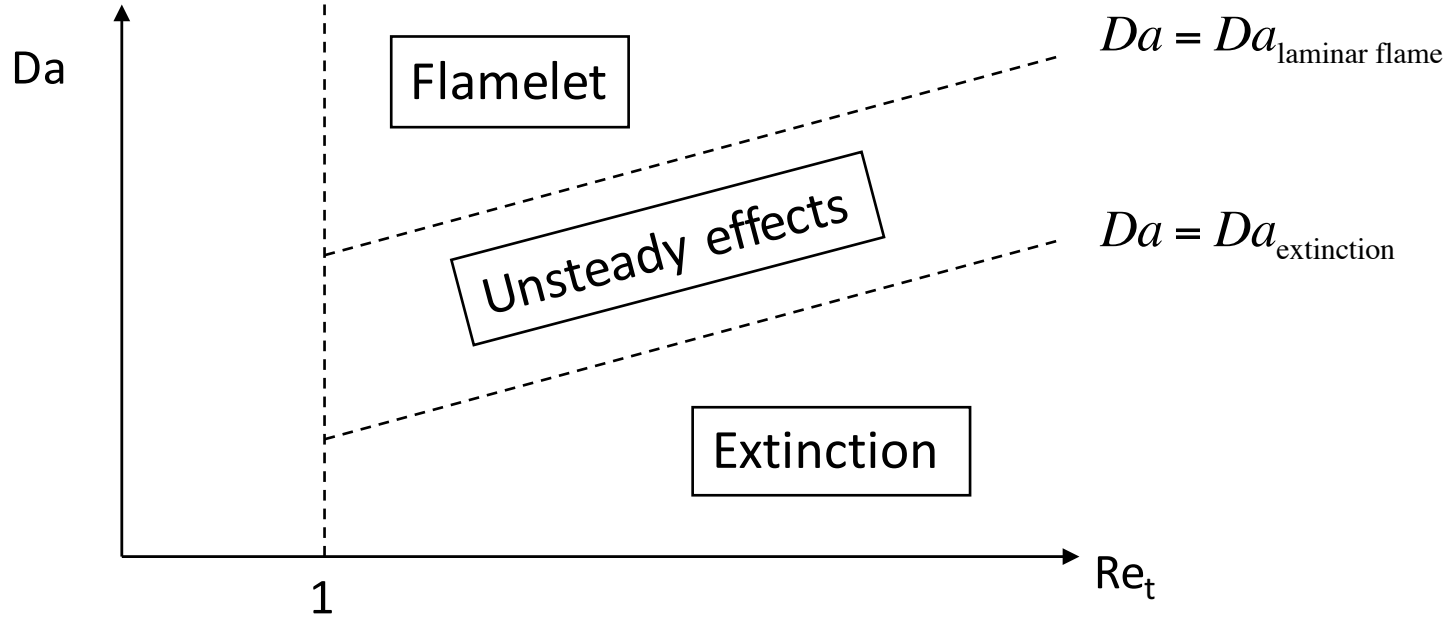
$$D_a = \frac{\tau_f}{\tau_c} \approx \left(\chi_{st}\ \tau_c\right)^{-1}$$

Non-Premixed Turbulent Flames : Regime Diagram

For highly turbulent non-premixed flames:

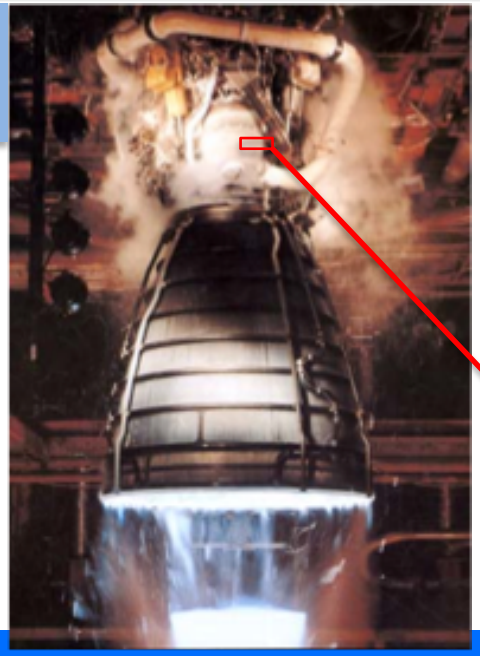
The diffusion / mixing process is supposed to be governed by the Kolmogorov time-scale τ_K which yields:

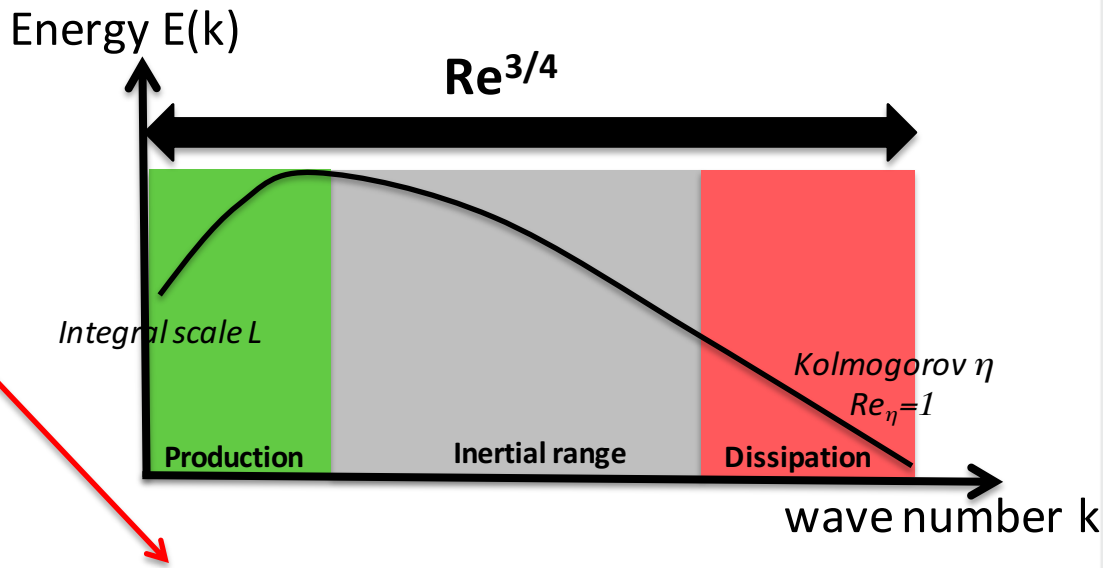
$$Da = \frac{\tau_t}{\tau_c} \approx \frac{\sqrt{\mathrm{Re}_t}}{\chi_K \tau_c}$$



Scales in Turbulent Combustion

Combustion chamber
~m



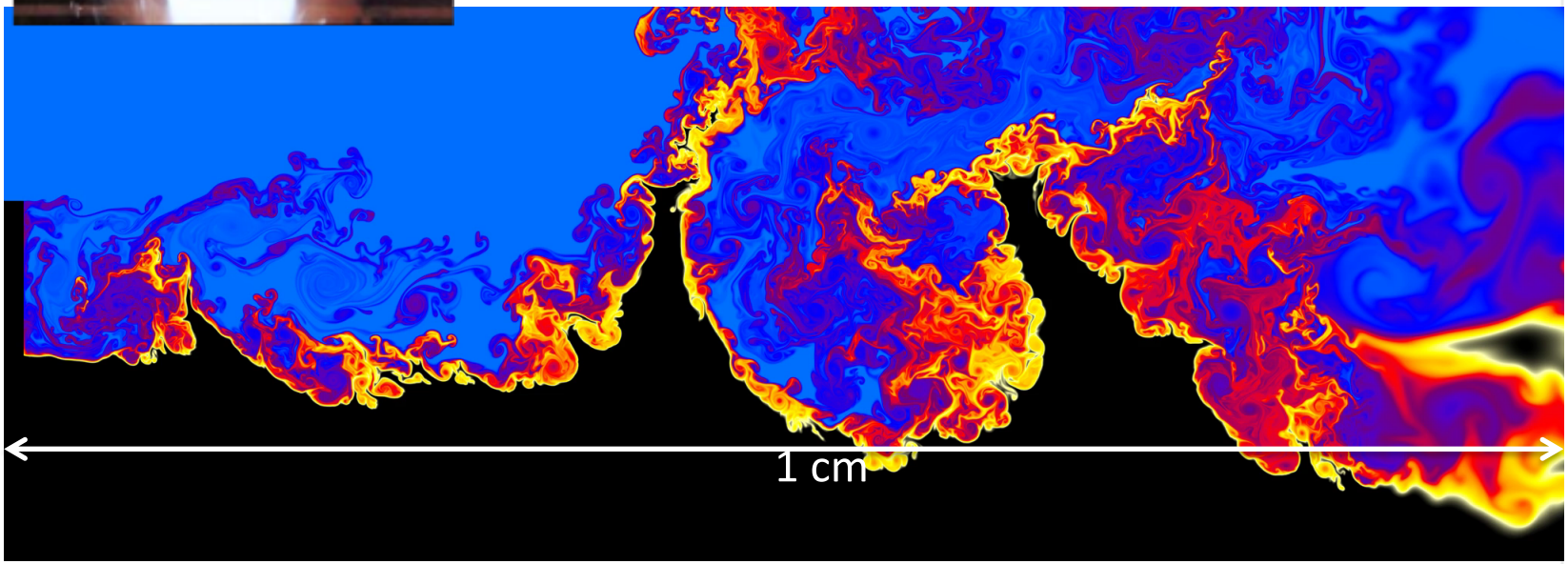


Turbulent scales

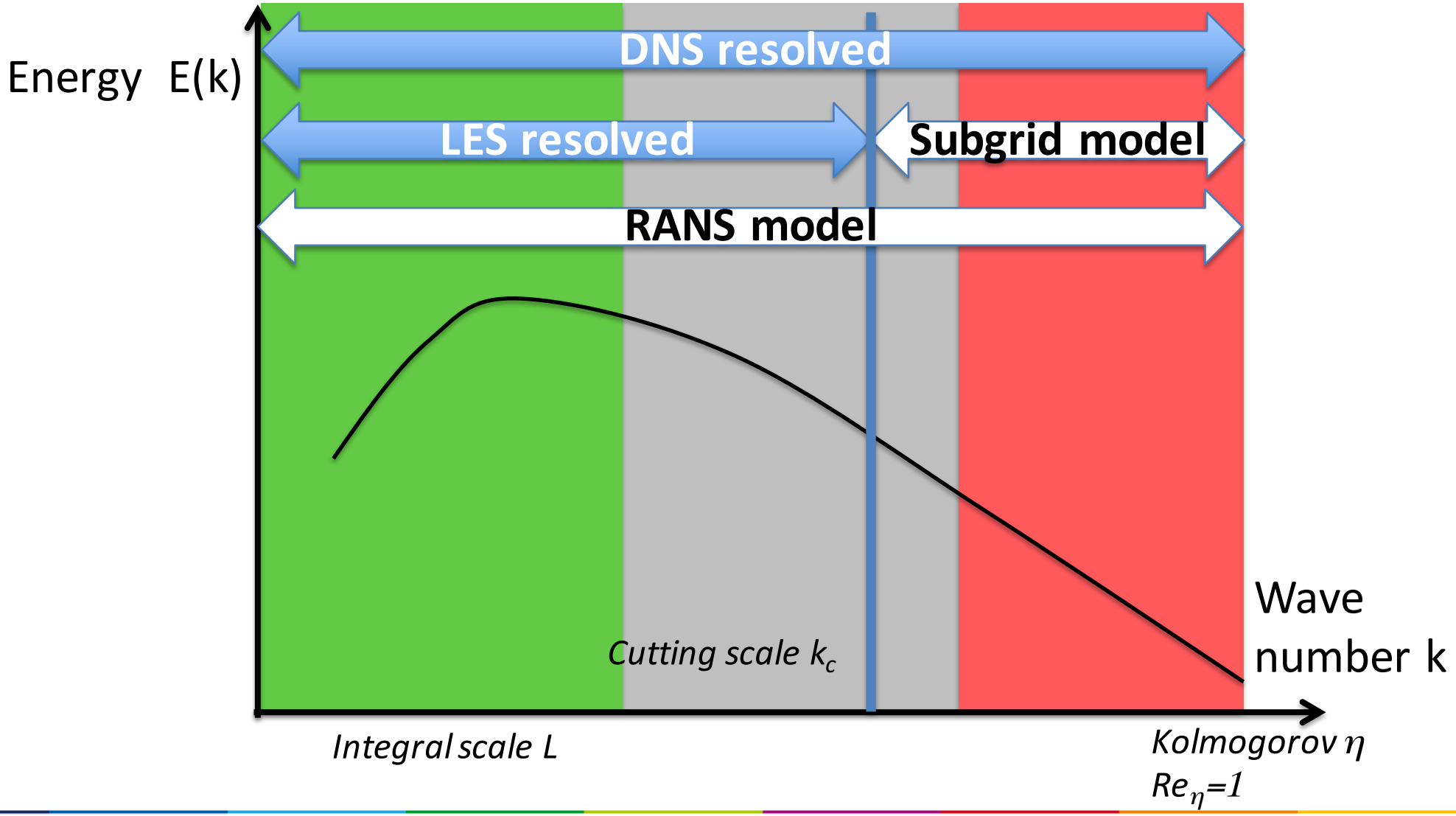
Air flow
- U=50m/s
- L=1m
- $\nu=10^{-5} m^2/s$

→
- $Re = 5\ 10^6$
- $\eta = 10\ \mu m$

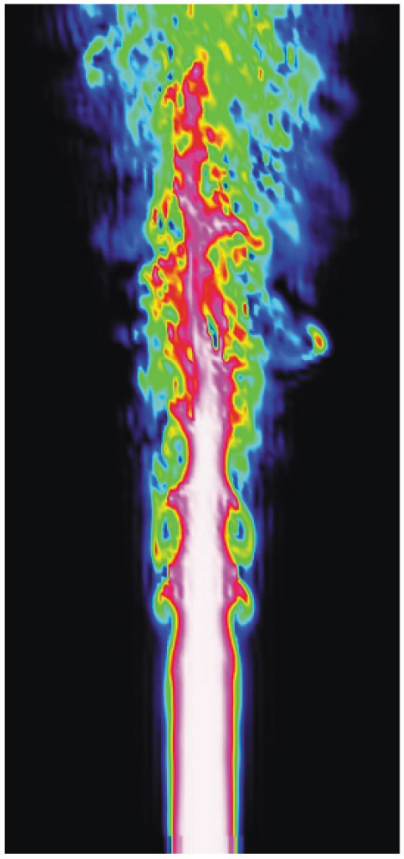
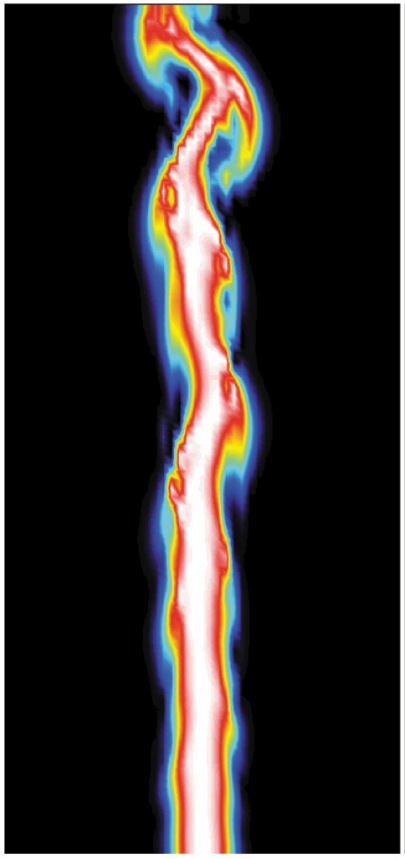
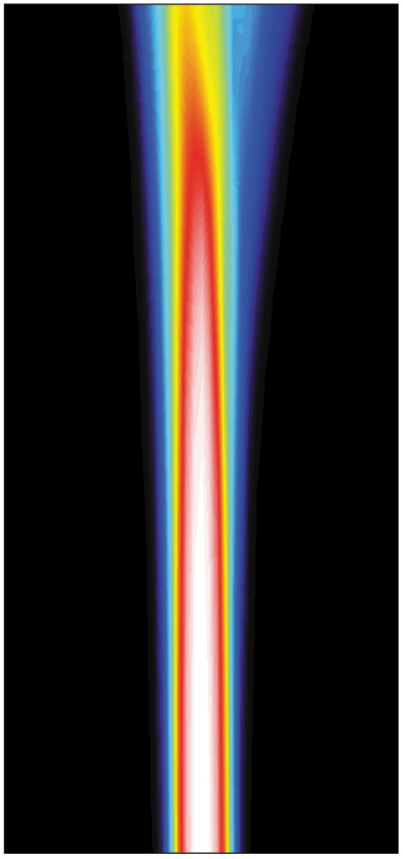
Flame thickness
~mm



Numerical Strategies for Turbulent Combustion



Turbulent Combustion Modeling : RANS vs LES

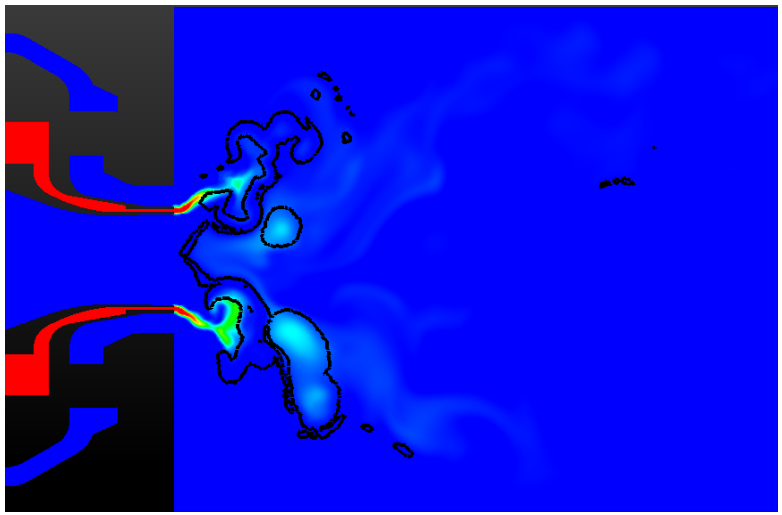
All vortices are resolved	Large scale vortices are kept	All vortices have disappeared
		
Direct Numerical Simulation (DNS) – all scales of fluid's motion are fully resolved	Large Eddy Simulation (LES) – large scales of fluids's motion are resolved, while small scales are modeled	Reynolds Average Simulation (RAS) – all flow scales of fluid's motion are averaged in time

What is different with LES?

- The flame sees a real (filtered) flow:

  Less mixing → more heterogeneity
  (equivalence ratio, stretch)

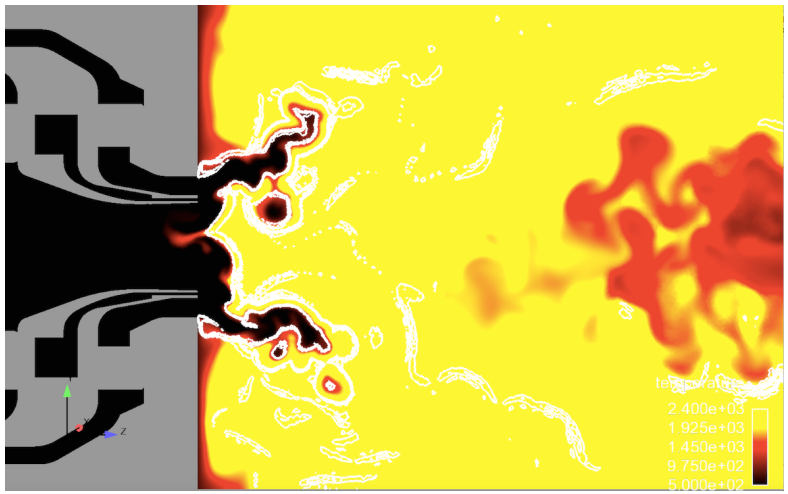
  Both premixed / non premixed flames



- The flame is a real (filtered) flame :

  Flame space / time scales are described

  Turbulence / flame interactions are (partly) resolved



What is different with LES?

CFD for combustion has massively moved to LES

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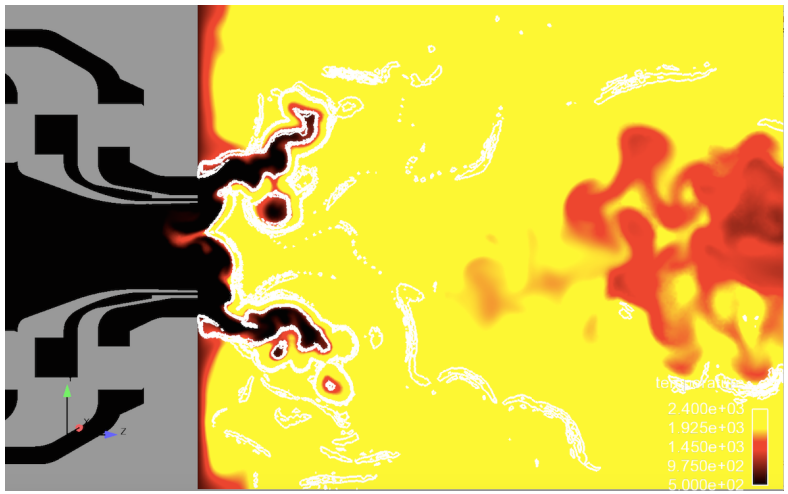
  Both premixed / non premixed fla



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Subgrid scale modelling of turbulent combustion

Filtering leads to unclosed terms:

- transport (convection / diffusion) → classical "gradient" – type closures
- chemical source terms for species and energy are highly non-linear, mostly at the sub-grid scale
- premixed flame are unresolved on LES grids → numerical instabilities (and crash!)
- "gradient" – type closures are not adapted

Two classes of approaches:

Mathematical approach: PFD methods

$$\widetilde{\Phi} = \int_{c*}^{\cdot} \int_{Z*}^{\cdot} \Phi(c^*, Z^*) P(c^*) P(Z^*) dc^* dZ^*$$

- Presumed / transported Pdf
- Direct / tabulated chemistry description

The issue is to determine the Pdf!

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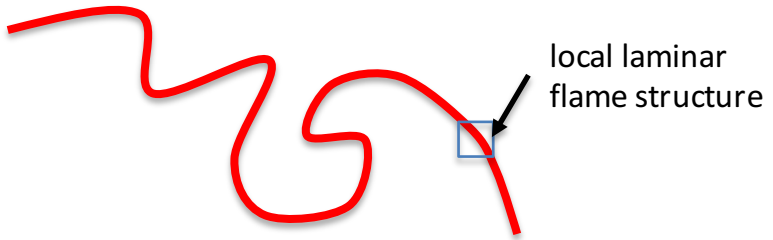
- Direct / tabulated chemistry description

The issue is to determine the Pdf!

Phenomenological approach: flame surface



- Surface area Σ → wrinkling
- Local flame structure: tabulated Ω

$$\widetilde{\Omega} = \widetilde{\Sigma} \, . \, \Omega$$

The issue is to freeze the local flame structure!

The property derived for laminar flame also holds for turbulent flames :
a premixed flame front can be thickened and still travel at the same speed.

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right) + \dot{\omega}_k \qquad \delta = \frac{D_{th}^1}{s_L}$$

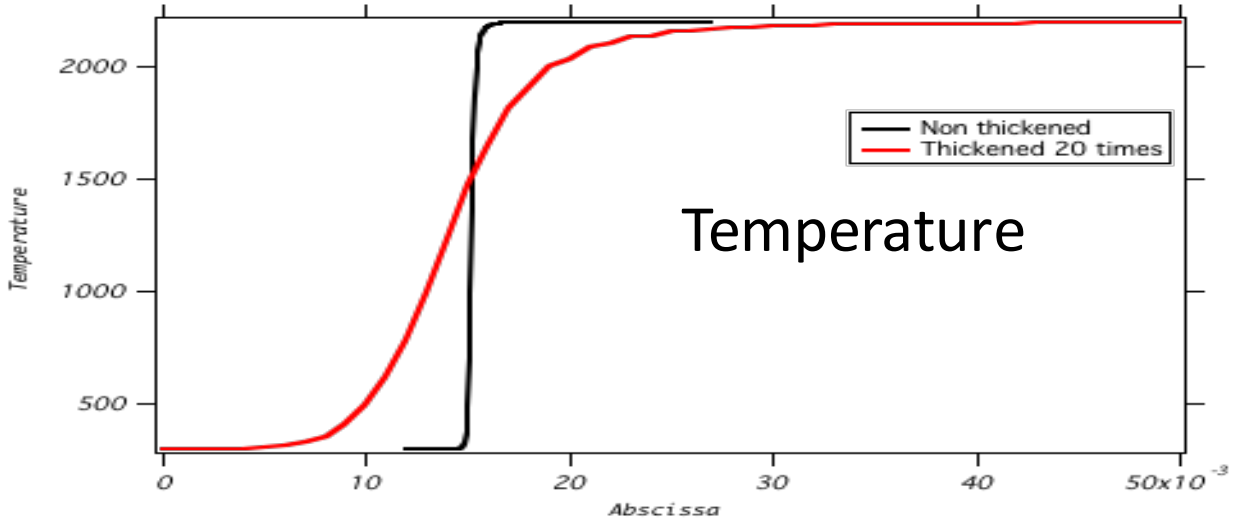
$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left(\rho \mathbf{F} D_k \frac{\partial Y_k}{\partial x_i}\right) + \frac{1}{\mathbf{F}}\dot{\omega}_k \qquad \delta = \frac{\mathbf{F} D_{th}^1}{s_L}$$

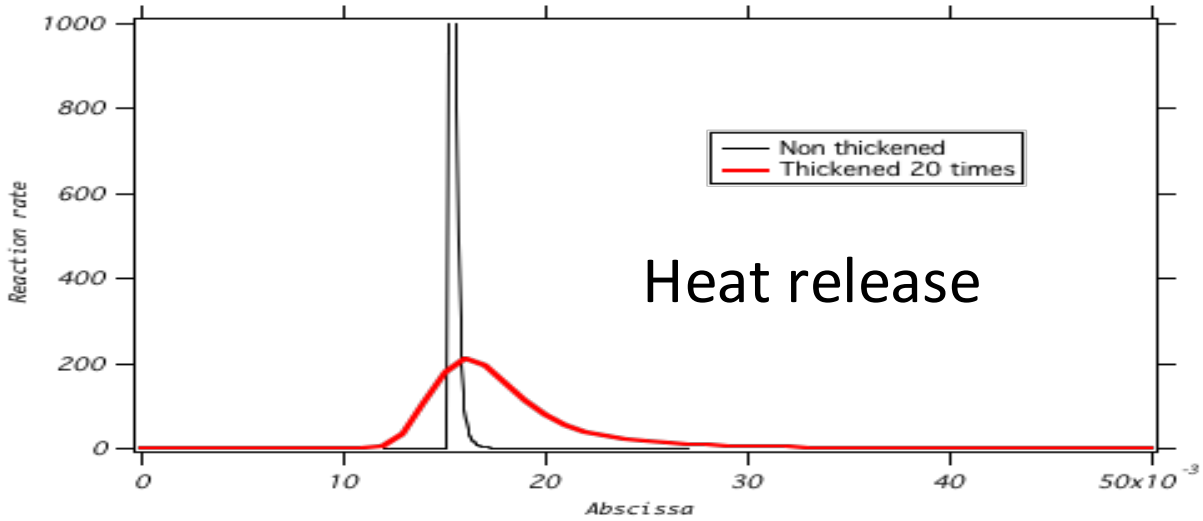
- Both equations propagate flames at the same speed s_L
- But the flame thickness is increased by a factor F in the second case ==> the flame front can be adjusted to any thickness

LES turbulent combustion model : TFLES

Thickened and non-thickened flames

- CH4- air
- simple chemistry
- F=20





Heat release

The thickened flame does not respond to turbulence like the initial unthickened flame.

This can be parametrized (subgrid scale wrinkling) and turbulent effects are included using an efficiency function **E** (*Colin et al, Phys. Fluids 2000*) derived from DNS of flame vortex interactions:

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left(\rho \mathbf{F} D_k \frac{\partial Y_k}{\partial x_i}\right) + \frac{\mathbf{E}}{\mathbf{F}}\dot{\omega}_k$$

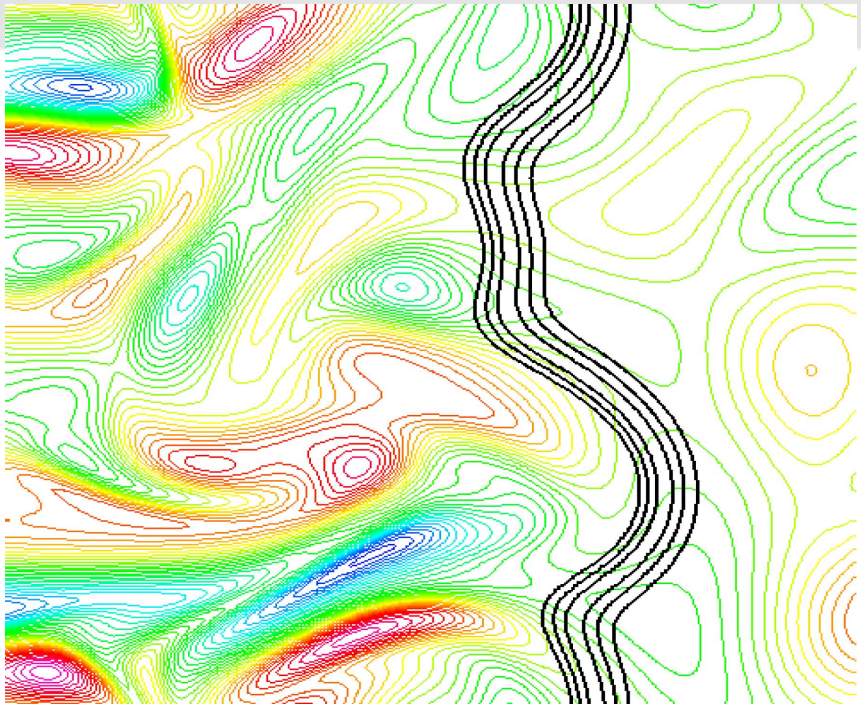
where **E** is a function of the local turbulence and of the premixed flame characteristics (speed and thickness).

E measures the subgrid scale wrinkling

LES turbulent combustion model : TFLES

F = 1

Non thickened DNS:
Total reaction rate R1



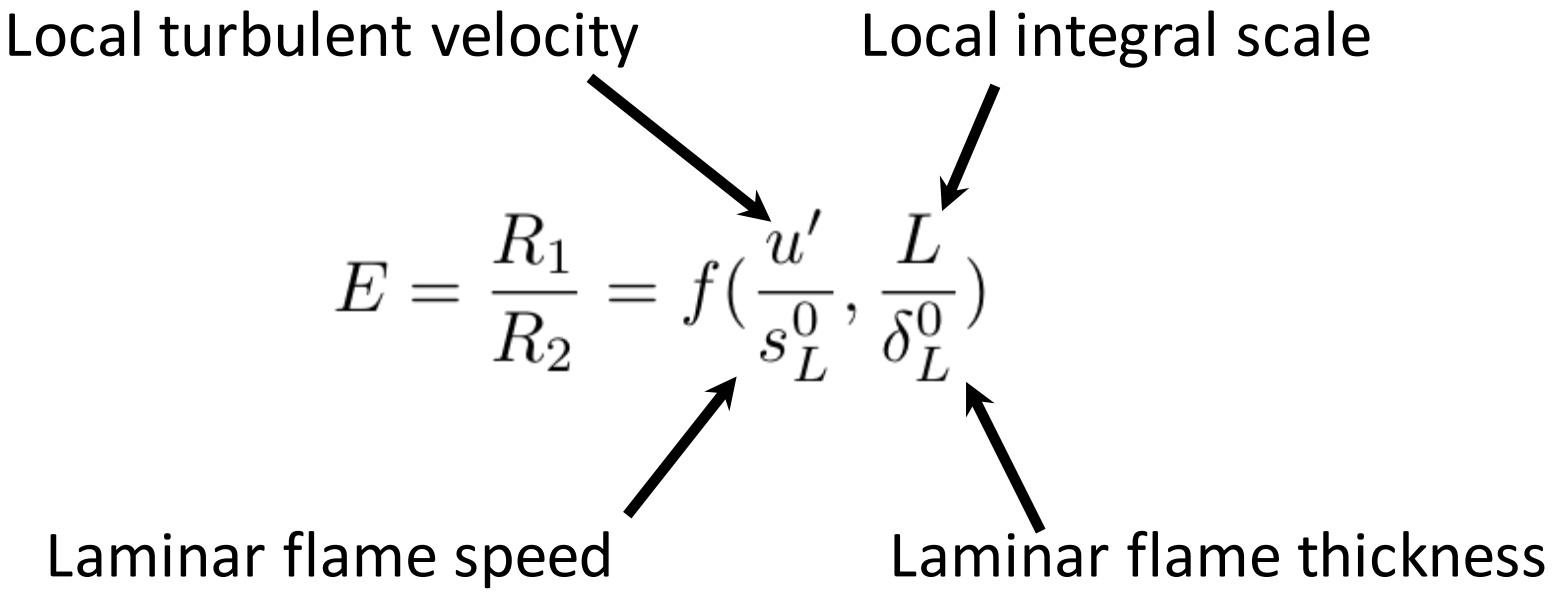
F = 5

Thickened DNS:
Total reaction rate R2

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

Colin et al, Phys Fluids 2000, Poinsot Veynante, Chapter 5

LES turbulent combustion model : TFLES



- Simple to implement: algebraic expressions given in the initial paper of Colin et al (Phys Fluids 2000).
- Extensions in papers by Charlette et al, Comb Flame 2002
- Dynamic versions by Wang et al Comb. Flame 2012
- The whole question of flame / turbulence interactions is hidden in the E function. Careful…

Colin's model (Phys. Fluids 2000)

$$E\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_l\right)=1+\beta\frac{2\ln(2)}{3c_{ms}(\mathrm{Re}_l^{1/2}-1)}\Gamma\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0}\right)\frac{u'_\Delta}{s_l^0}$$

with $$\Gamma\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0}\right)=0.75\exp\left[-\frac{1.2}{(u'_\Delta/s_l^0)^{0.3}}\right]\left(\frac{\Delta}{\delta_l^0}\right)^{2/3}$$

Charlette / Meneveau model (Comb Flame 2002)

$$E\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_\Delta\right)=\left(1+\min\left(\frac{\Delta}{\delta_l^0},\Gamma\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_\Delta\right)\frac{u'_\Delta}{s_l^0}\right)\right)^\beta$$

with $$\Gamma\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_\Delta\right)=fit\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_\Delta\right)$$

EXTENSION TO ALL REGIMES: the basic idea of the DTF model

1/ Thicken only where reaction takes place: the flame zone. Detect it using a sensor *S* (based on reaction rate for example):
S=1 in the flame reaction zone. *S=0* elswhere

2/ In other regions (*S=0*), simply return to normal LES model:

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left[\rho\left(\mathbf{F}D_k S + D_t(1-S)\right)\frac{\partial Y_k}{\partial x_i}\right] + \frac{\mathbf{E}}{\mathbf{F}}_k$$

This formulation actually allows to compute all regimes with only one single equation.

LES turbulent combustion model : TFLES

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left[\rho\left(\mathbf{F}D_k S + D_t(1-S)\right)\frac{\partial Y_k}{\partial x_i}\right] + \frac{\mathbf{E}}{\mathbf{F}}\dot{\omega}_k$$

It degenerates to:

In reaction zones: *S=1*

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left[\rho\mathbf{F}D_k\frac{\partial Y_k}{\partial x_i}\right] + \frac{\mathbf{E}}{\mathbf{F}}\dot{\omega}_k$$

Standard thickened flame equation

Pure mixing zones : *S=0*

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left(\rho D_t\frac{\partial Y_k}{\partial x_i}\right)$$

LES mixing model

LES turbulent combustion model : TFLES

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left[\rho\left(\mathbf{F}D_k S + D_t(1-S)\right)\frac{\partial Y_k}{\partial x_i}\right] + \frac{\mathbf{E}}{\mathbf{F}}\dot{\omega}_k$$

For small domain size or large computers: Go to F=1, E=1 and DNS	$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left[\rho D_k \frac{\partial Y_k}{\partial x_i}\right] + \dot{\omega}_k$ Resolved laminar premixed flame
In ignition regions	$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\mathbf{E}}{\mathbf{F}}\dot{\omega}_k$ Usual perfectly stirred reactor
Diffusion flames	Only the reaction zone is thickened
Near walls	No ad-hoc correction : quenching is obtained thanks to Arrhenius expression

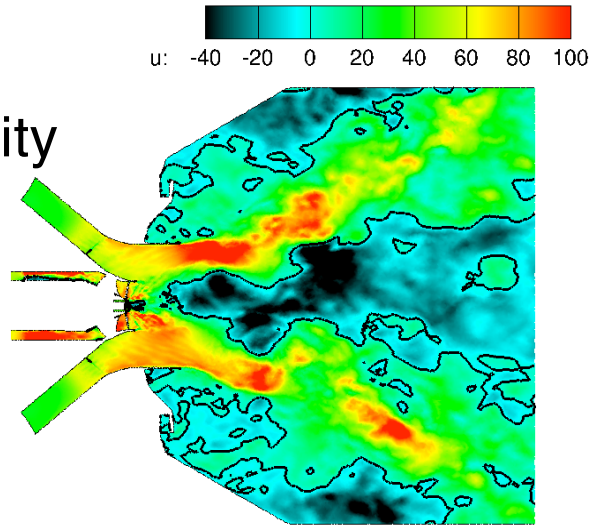
Major advantages of DTFLES

- Today for very large chambers, the typical values of F (the thickening factor) is 100 to 200. For small chambers, F is of the order of 10
- But when the computer resources increase, F goes down.
- Ultimately, F will go to 1. This is DNS (in the flame sense)...
- Kinetics are directly introduced. No need for models

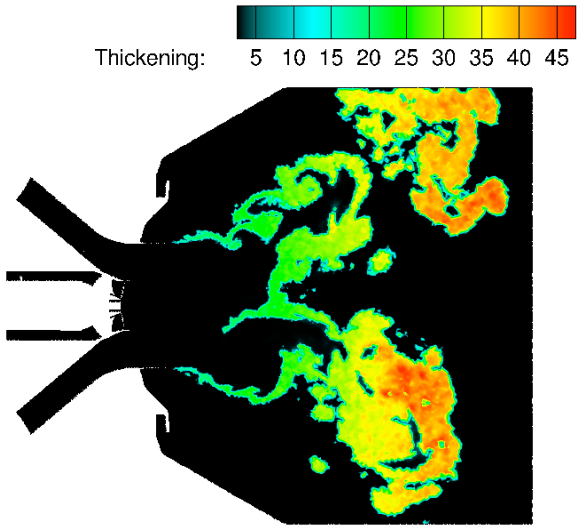
LES turbulent combustion model : TFLES

Example of thickened flames in an industrial gas turbine

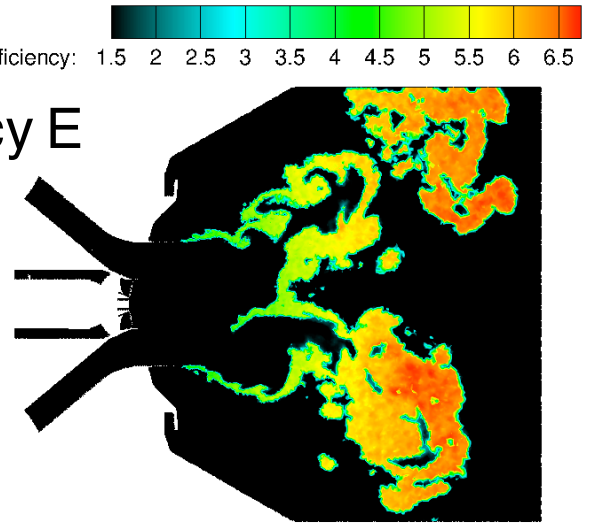
Axial velocity



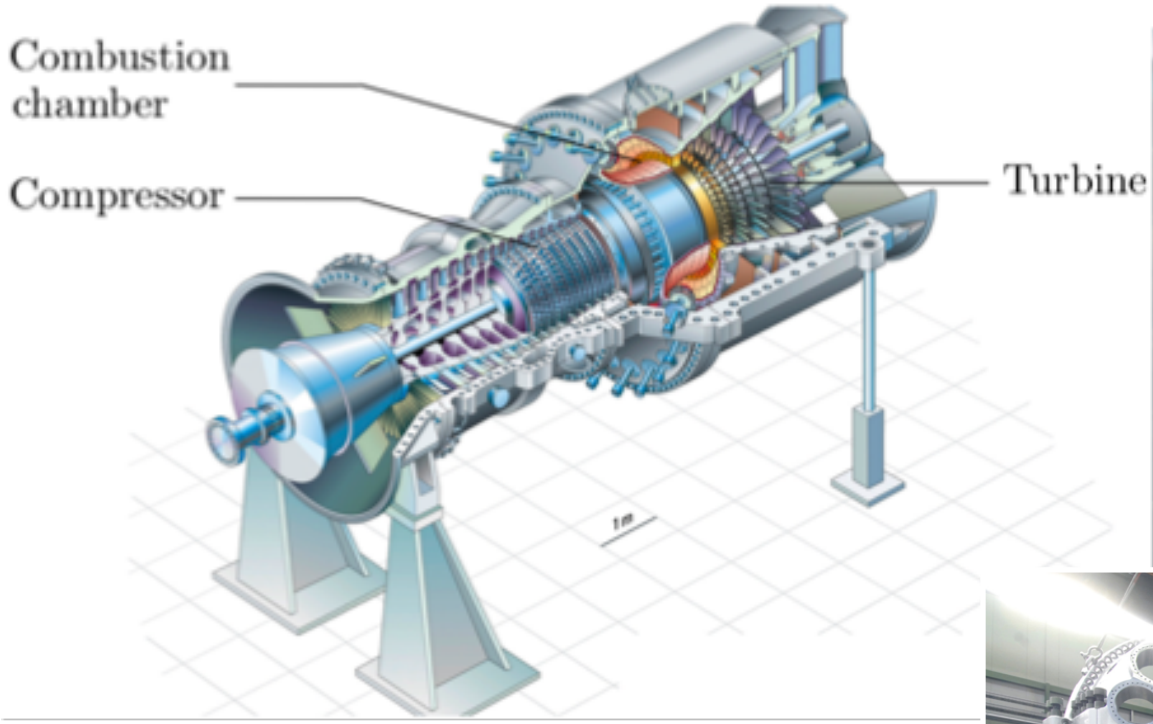
Thickening factor F



Efficiency E

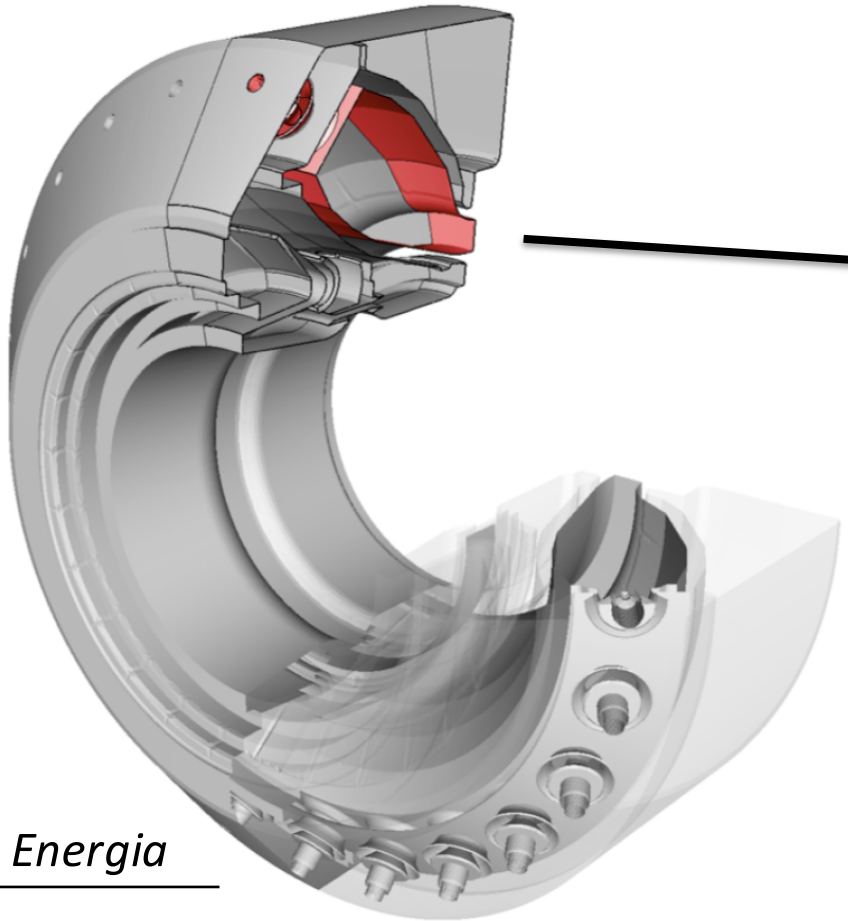


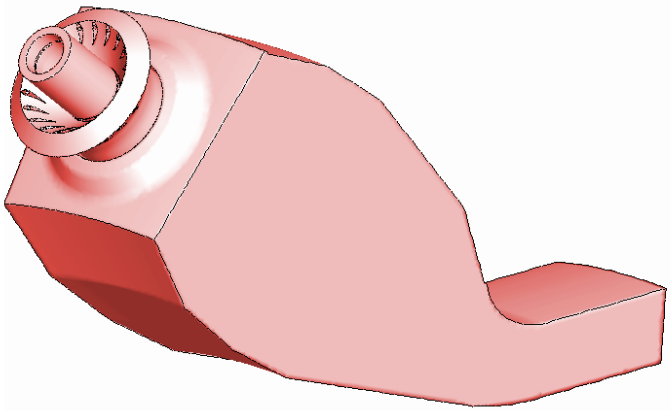
Example: an industrial gas turbine



Annular combustion chamber [35]

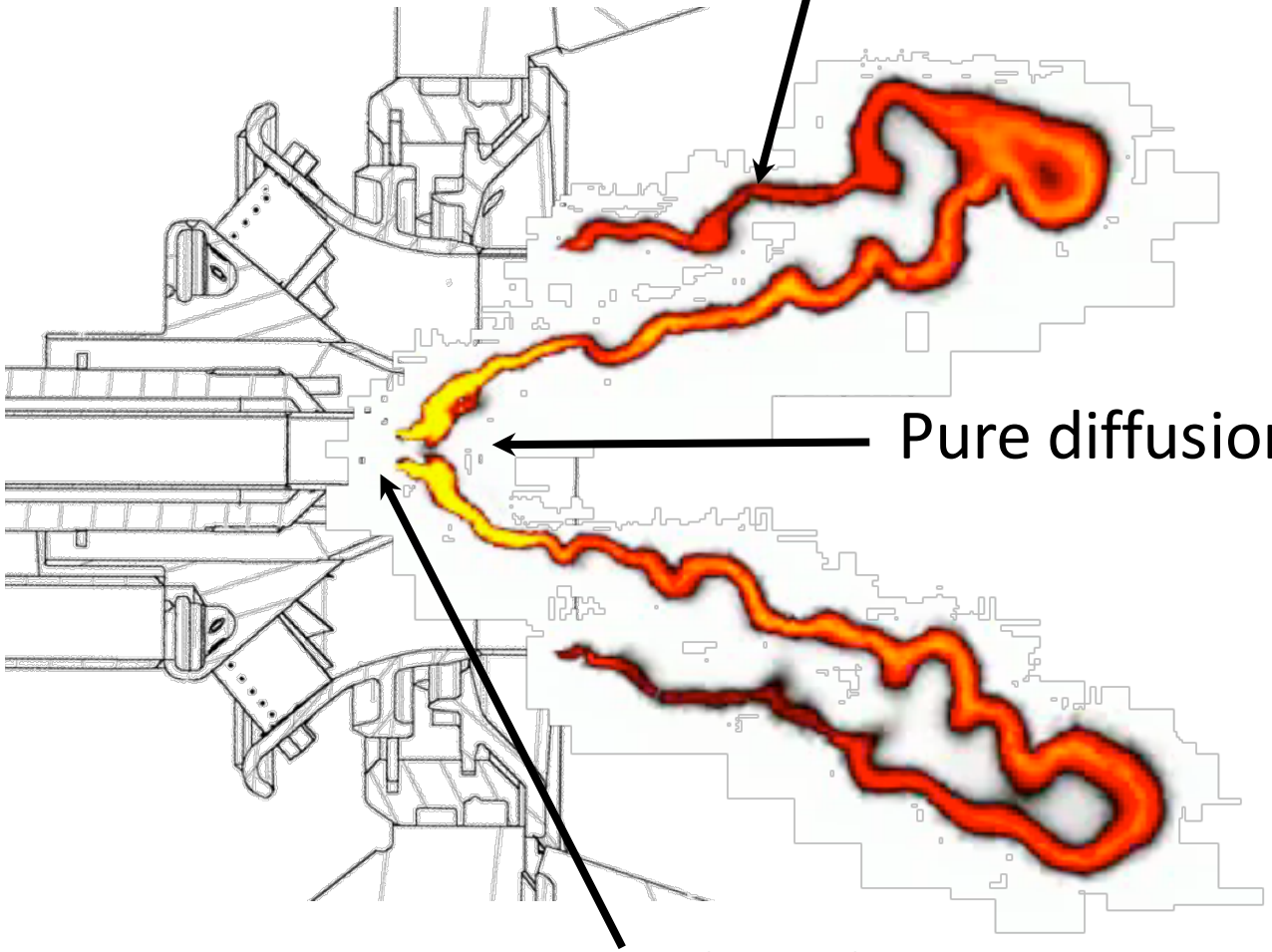
LES of one sector





[35] Ansaldo Energia

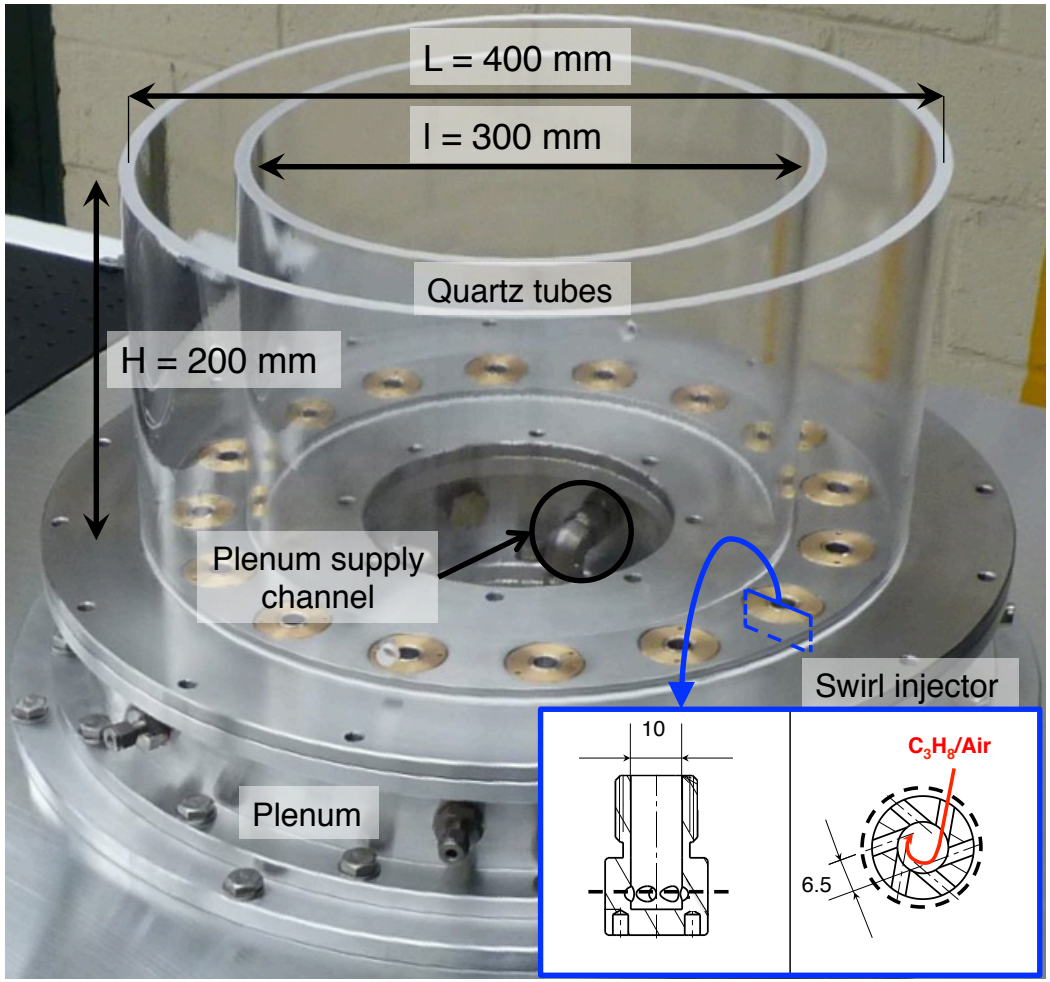
Six inlets ! Difficult to define a mixture fraction *z !*



Model must handle both regimes

Model must handle non adiabatic flames

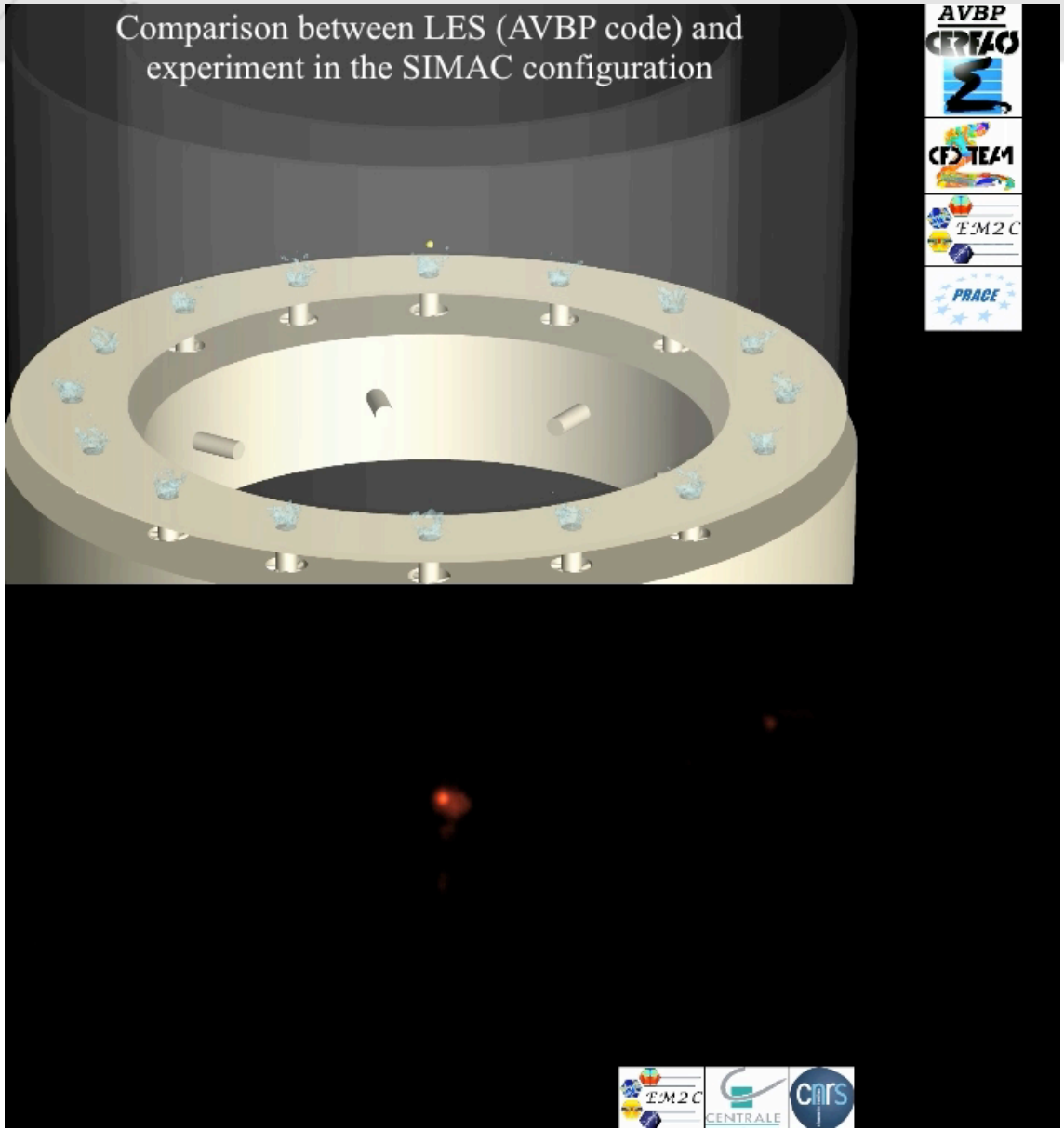
Ignition of the MICCA burner of EM2C



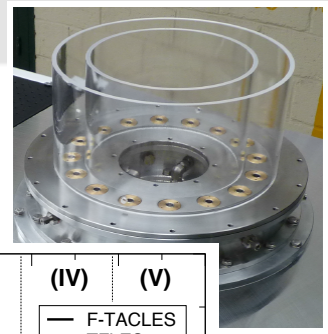
MICCA (EM2C) (*Durox et al*)

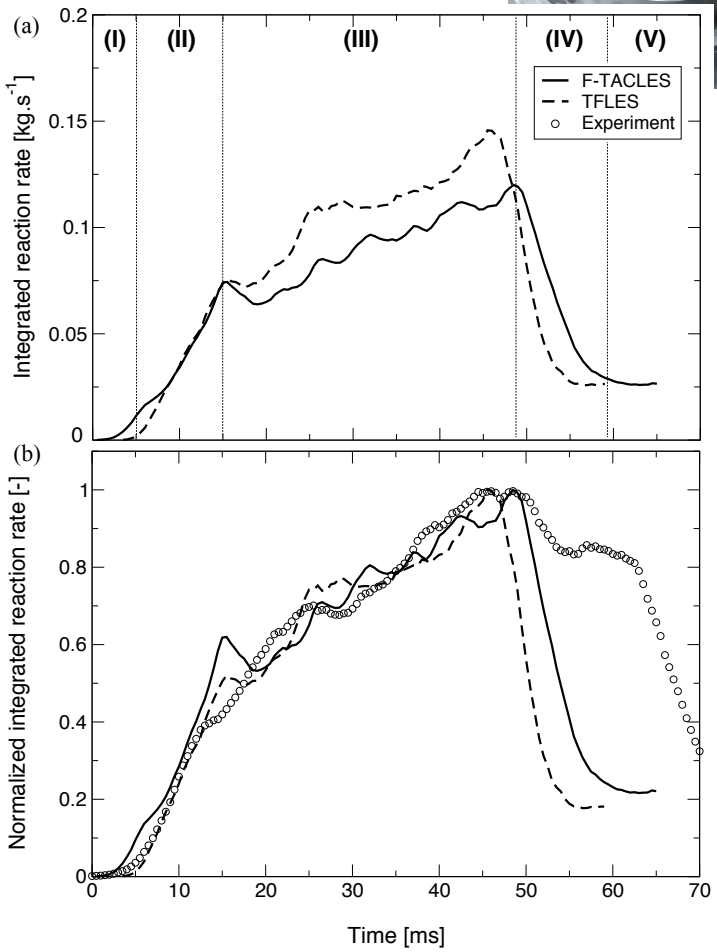
- Annular chamber
- 16 swirled injectors
- propane
- transparent walls

Ignition of the MICCA burner of EM2C



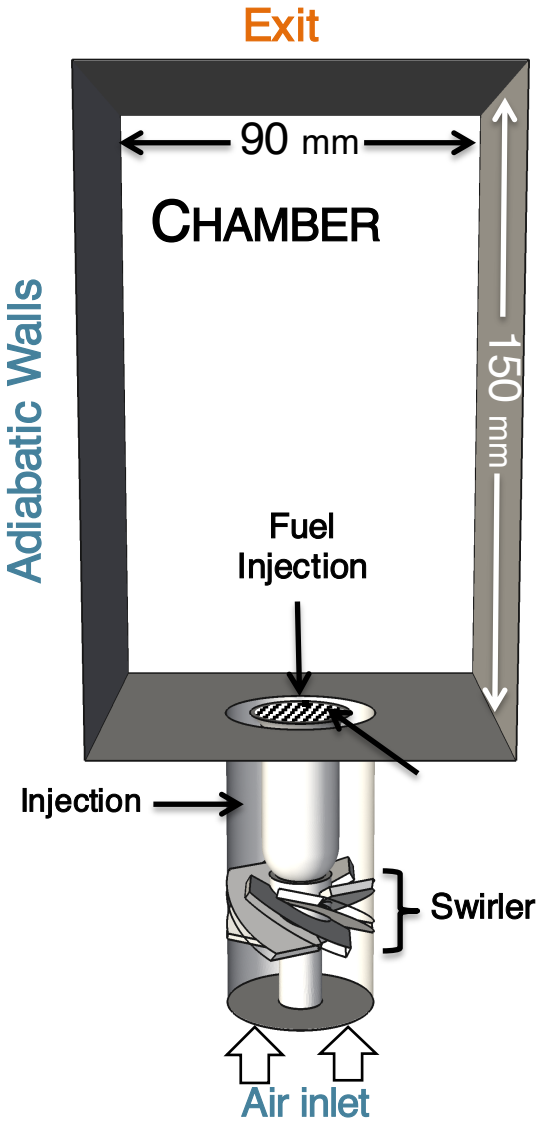
Philip et al, ASME 2013

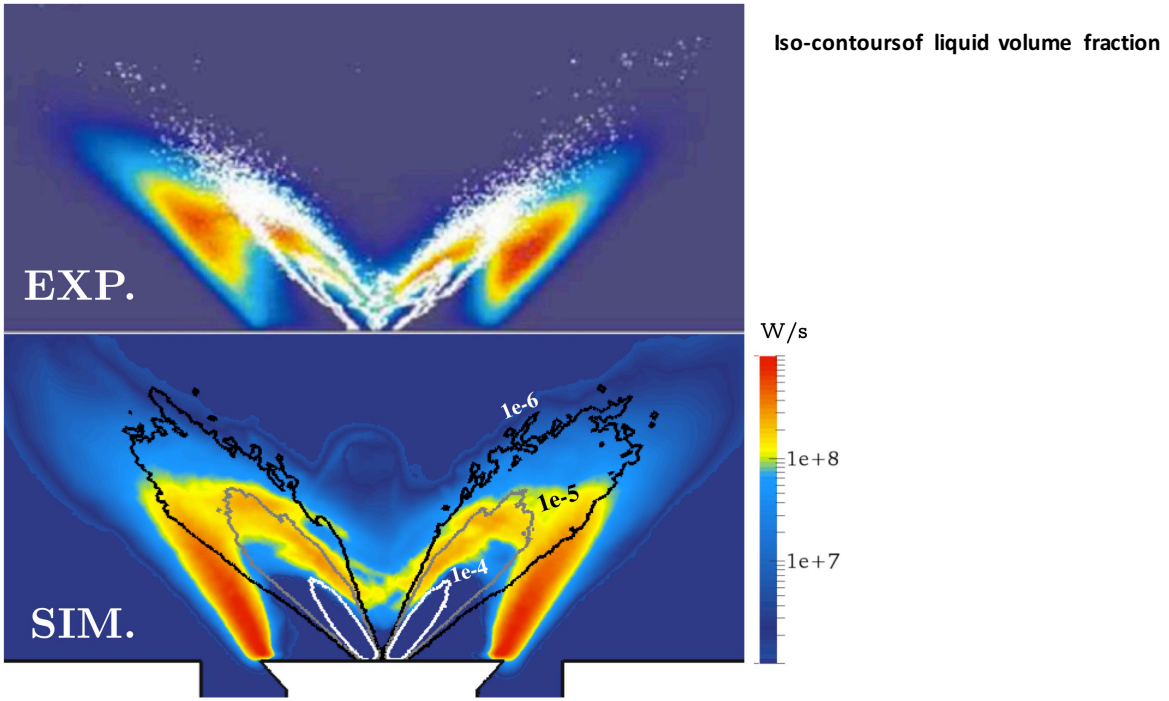


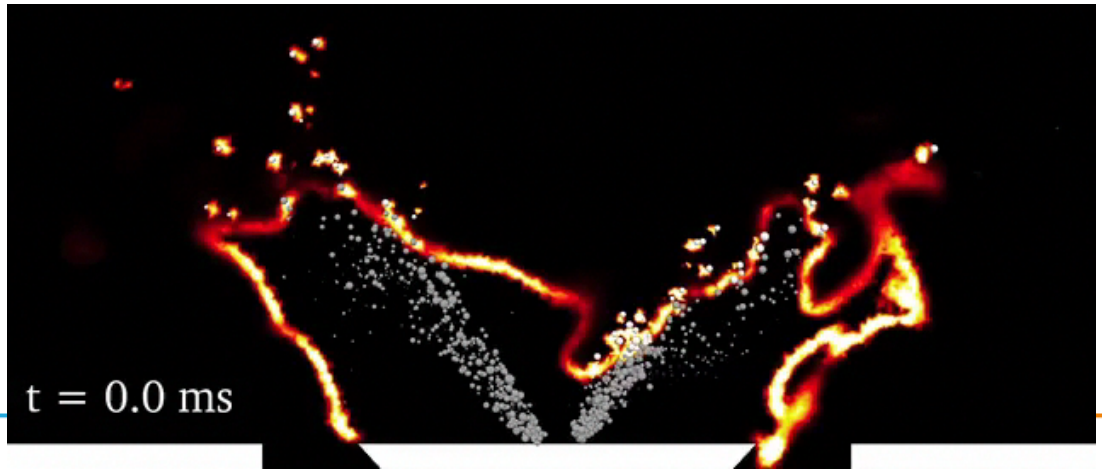


Adding two-phase flow : liquid fuel

Experiment of Cambridge university

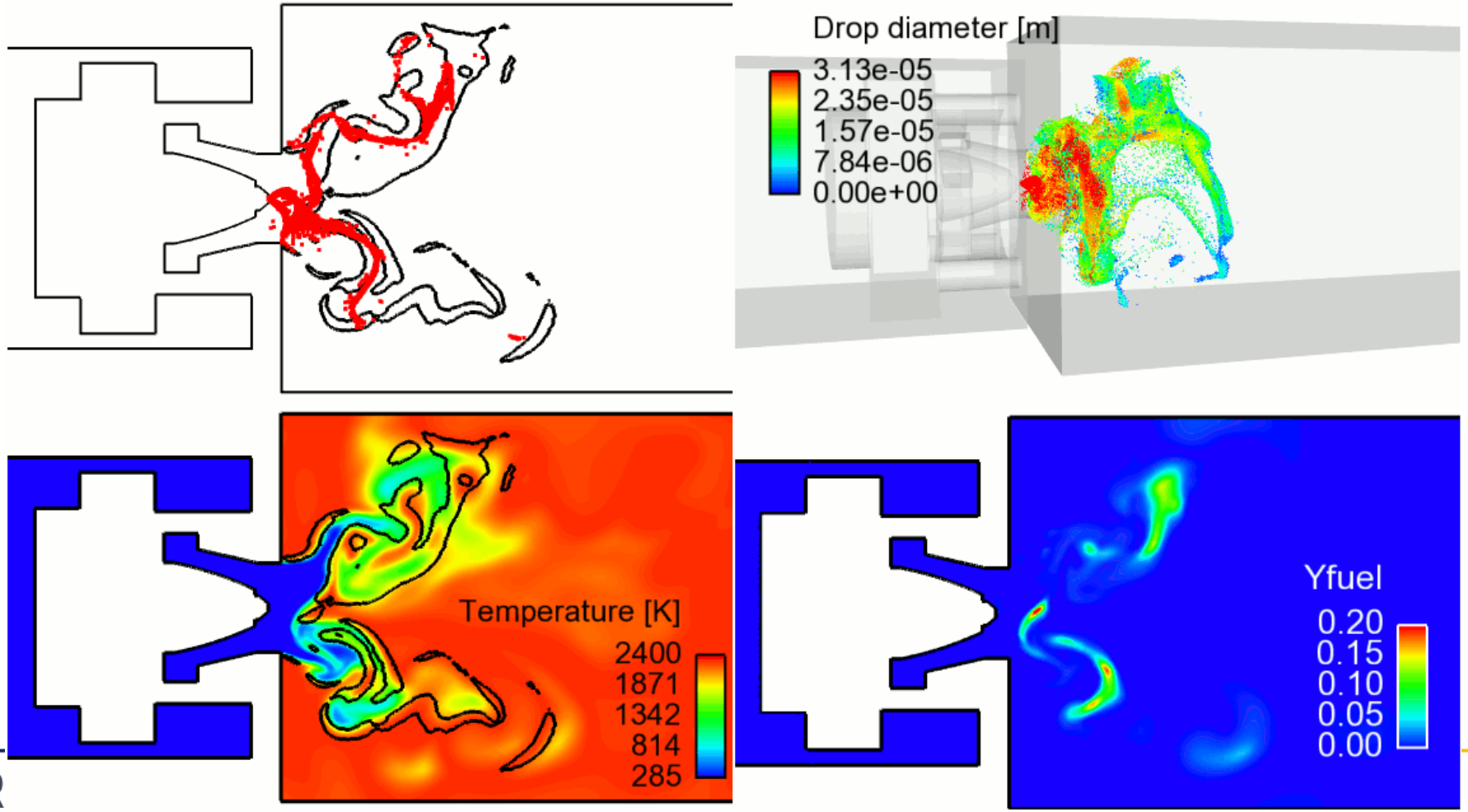






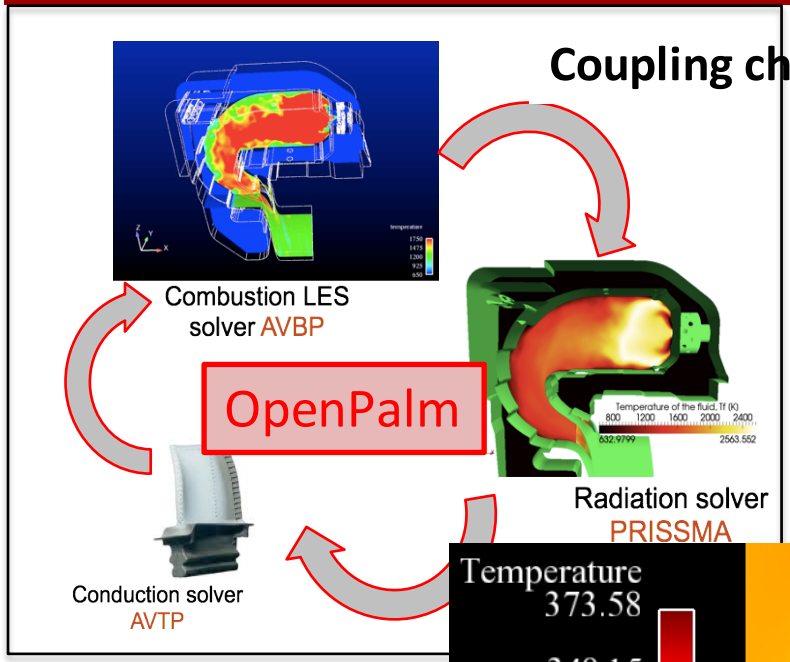
Application to MERCATO combustion chamber

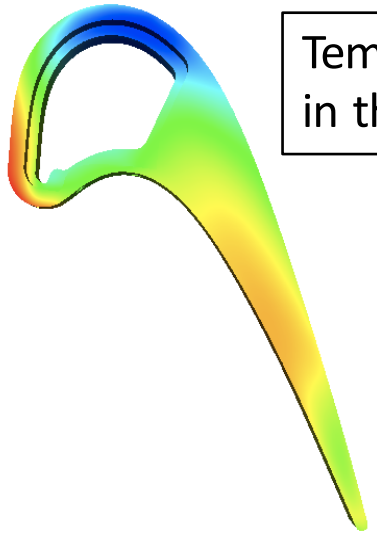
(a) Drop and Heat release isoline, (b) Drop diameter, (c) Gaseous temperature in the median cut plane and (d) Kerosene field in the median cut plane



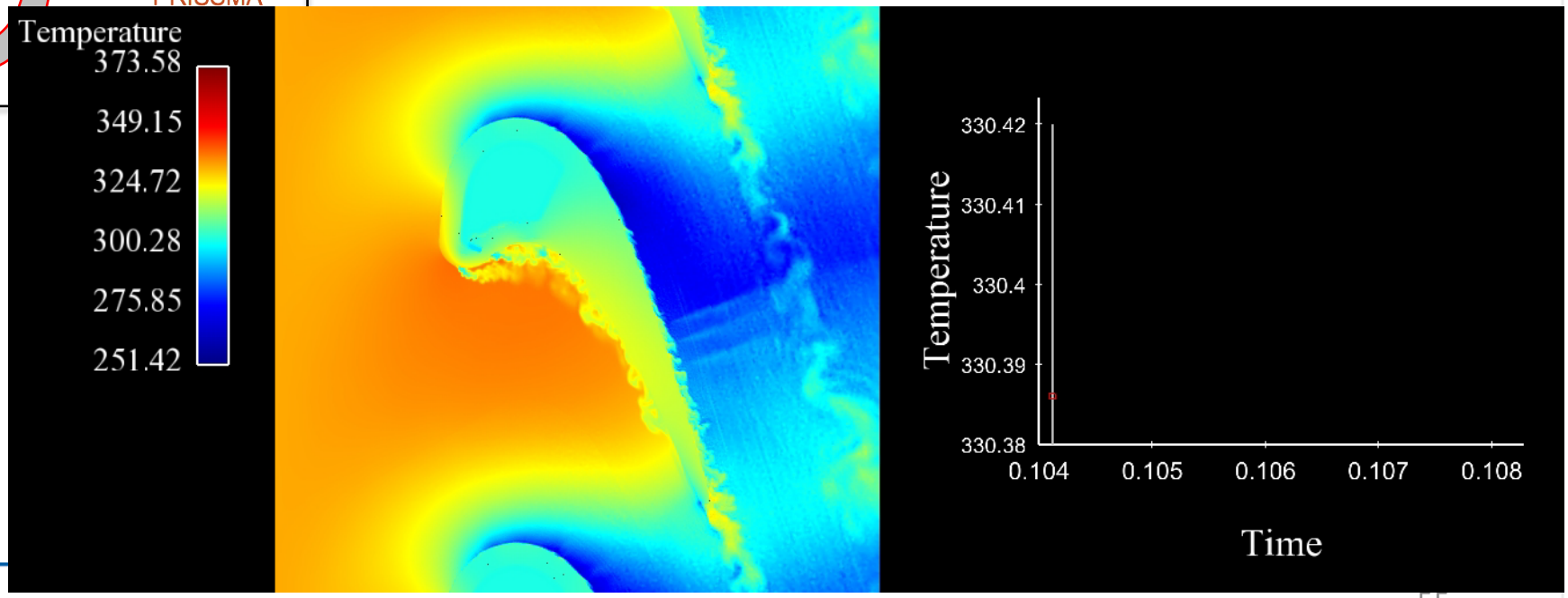
Adding heat transfer

Turbine blade cooling





Temperature
in the solid

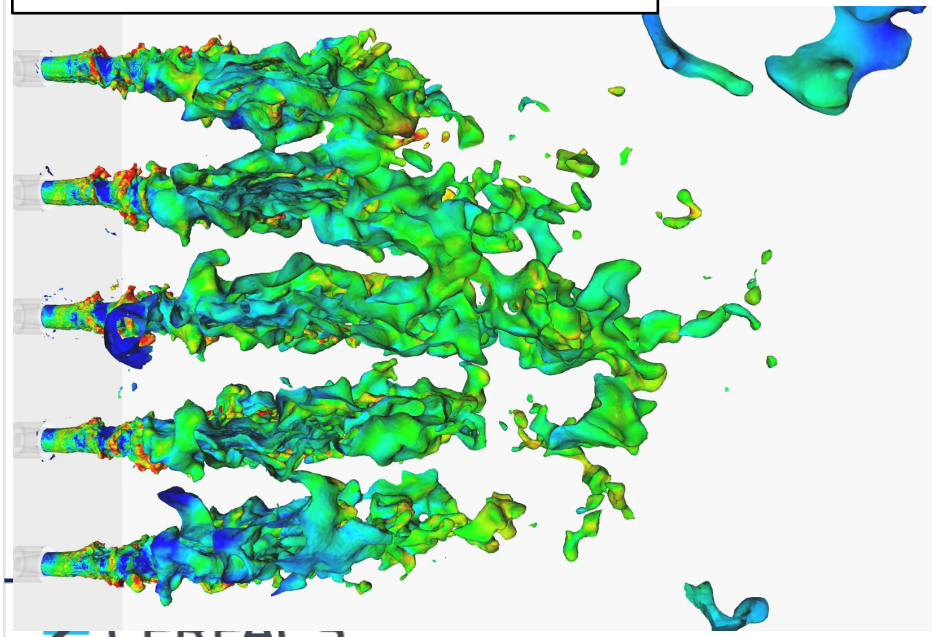


Other applications : cryotechnic combustion

Instabilities

A. Urbano, 2015
Hakim et al., 2014

H2/O2 cryogenic, 100 bar
8,5 Millions hours CPU



H2/O2 cryogenic, 75 bar, 80 MW
80 Millions hours CPU