“Modelling of turbulent flames with tabulated chemistry based on mixture fraction and progress variable”

Bertrand Naud

25 May 2011

Workshop on Mathematical Modelling of Combustion

Santiago de Compostela

Introduction

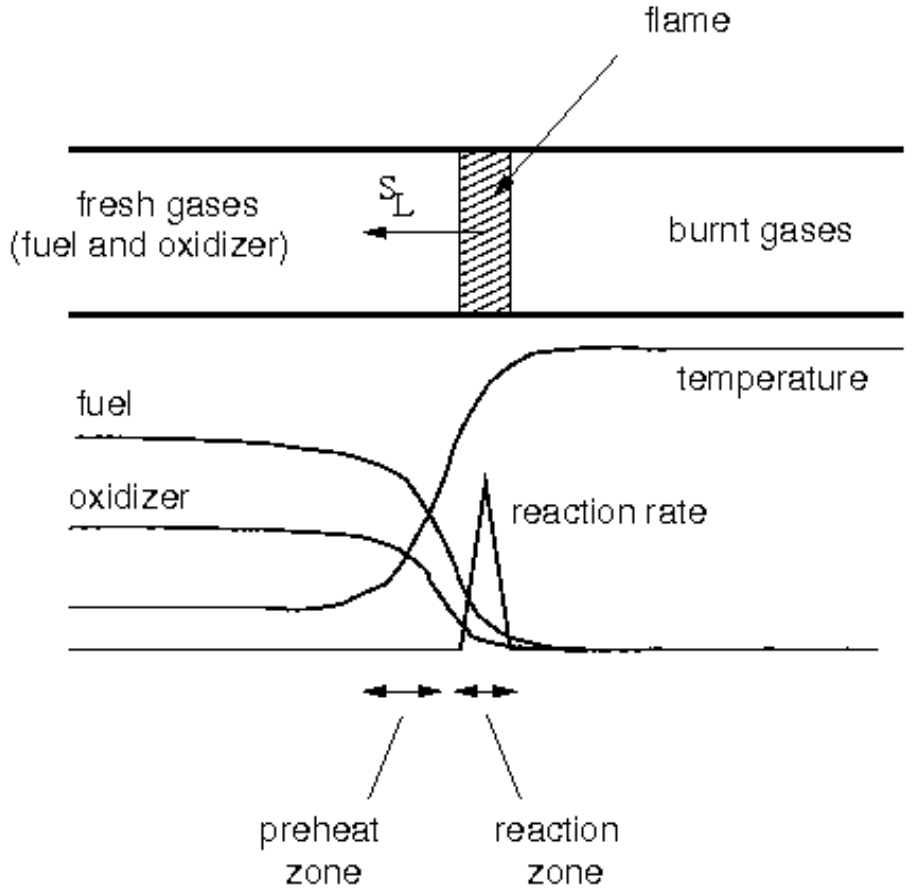
- laminar flames
- reduced chemistry
- turbulent flames (RANS and LES approaches)
- flamelets + PDF

Mixture fraction (Z) + progress variable (c)

- FPI/FGM or REDIM
- Comparison to experimental data:
    - a priori validation of the 2D-manifold
    - underlying flame structures from data
    - independence of marginal Z- and c-PDF
- Some considerations on the choice of c

Laminar premixed flames

Laminar premixed flames



Thin reaction zone

Strong temperature gradient

Propagation towards the fresh gases (preheating, reaction)

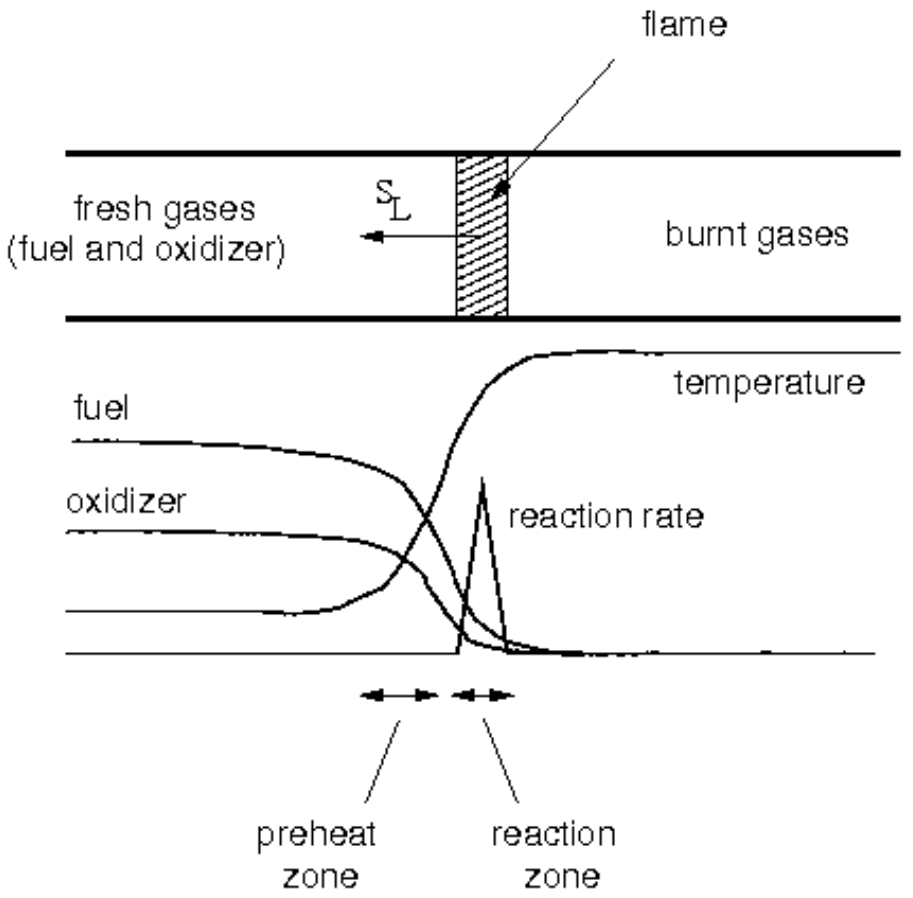
→ heat diffusion + reaction

Laminar premixed flames

Conditions:

- Temperature
- “Equivalence ratio” ϕ

$$\phi = \frac{m_F / m_O}{\left(m_F / m_O\right)_{st}}$$

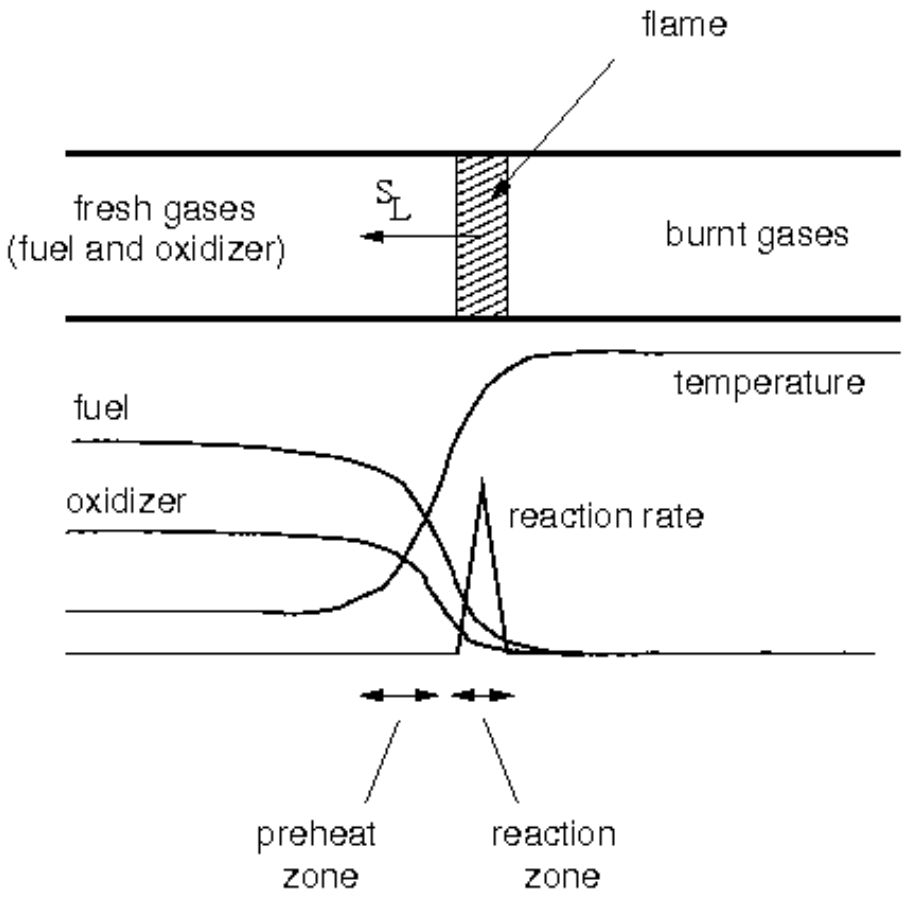


Laminar premixed flames

Conditions:

- Temperature
- “Equivalence ratio” ϕ

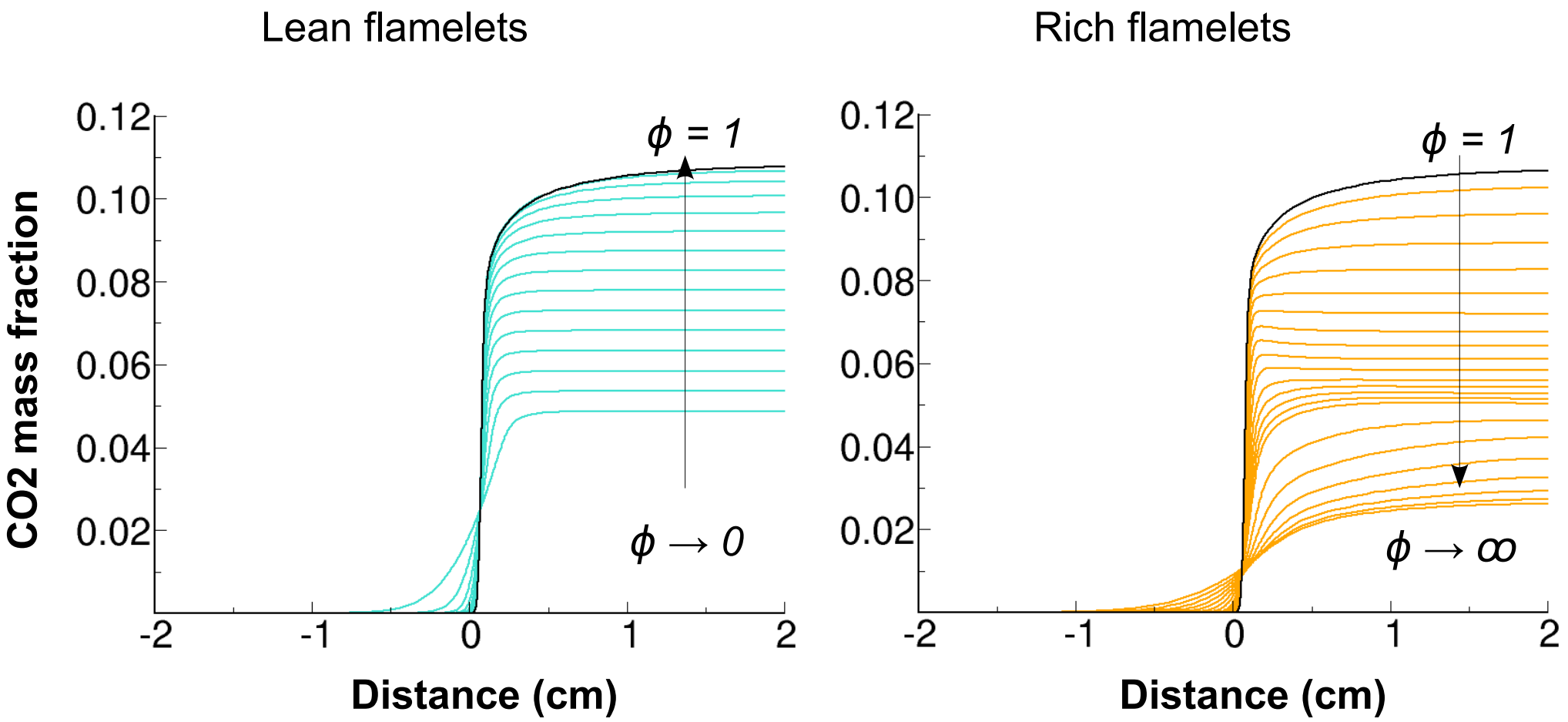
$$\phi = \frac{m_F / m_O}{\left(m_F / m_O\right)_{st}}$$



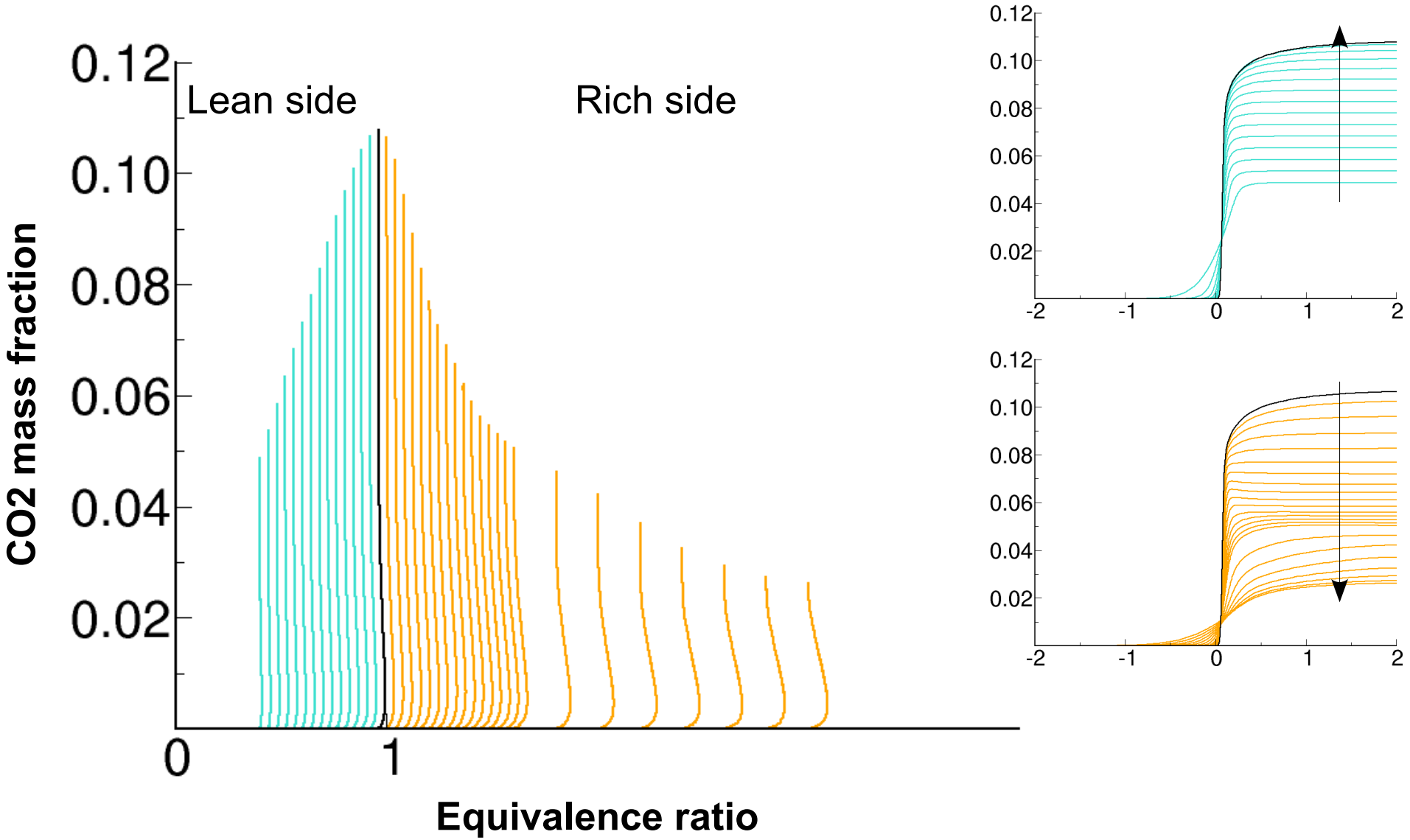
One progress variable *c* (temperature, product mass fraction, ...) allows to describe a premixed flame.

One value c_{fl} locates the flame front.

Premixed flames: different "equivalence ratio"

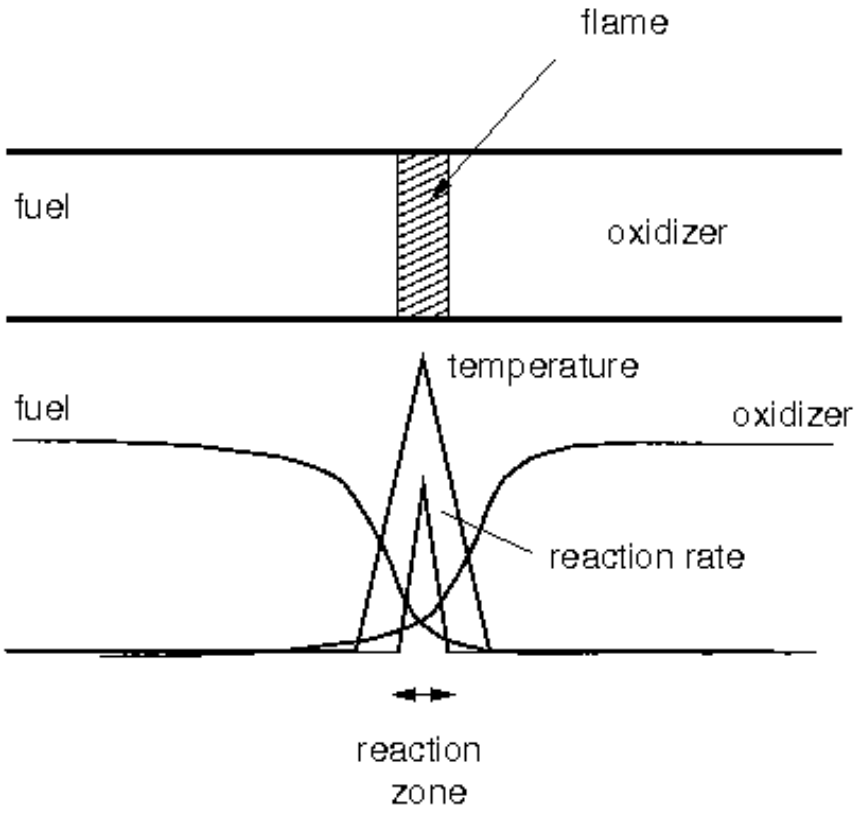


As a function of the “equivalence ratio”



Laminar diffusion flames

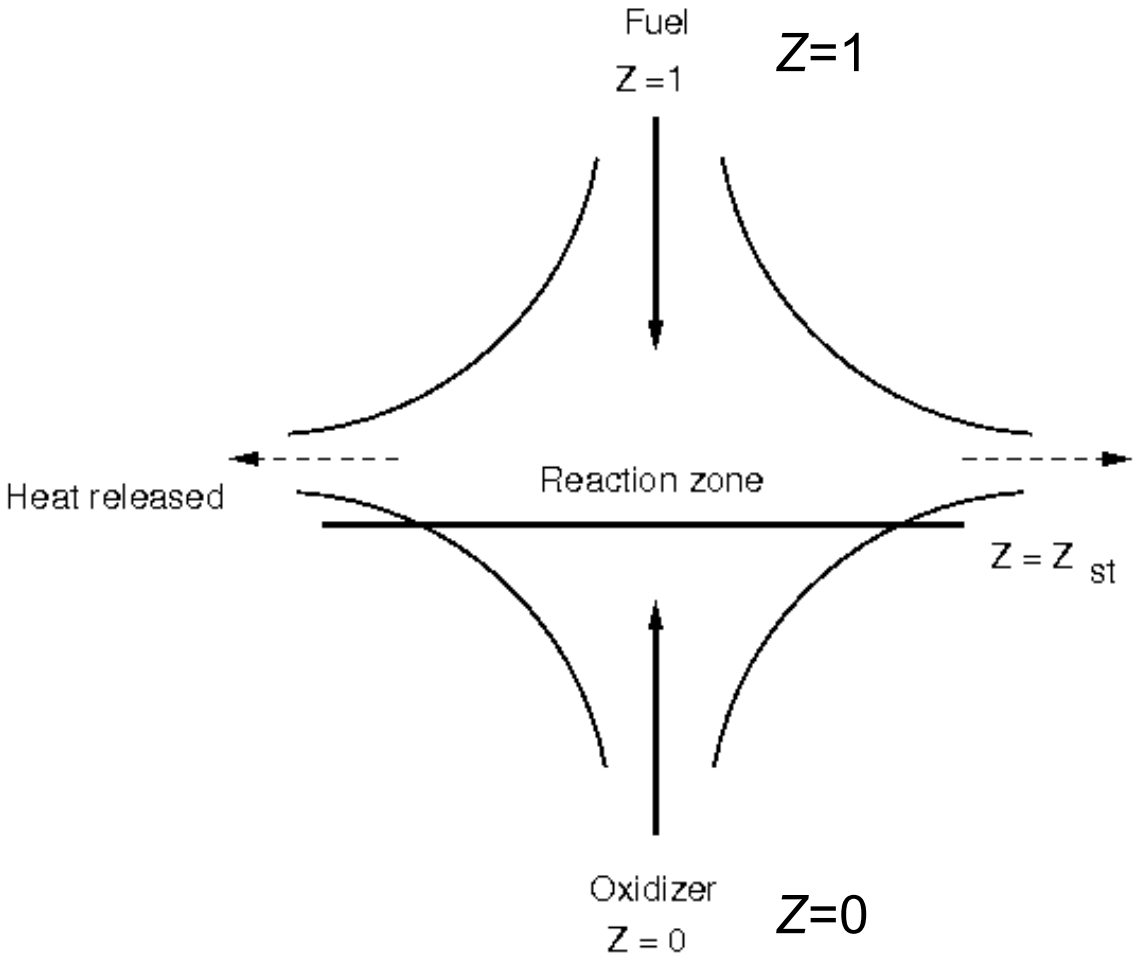
Laminar diffusion flames



(for example: mixing layer)

Reaction limited by mixing of reactants (heat loss by convection + diffusion)

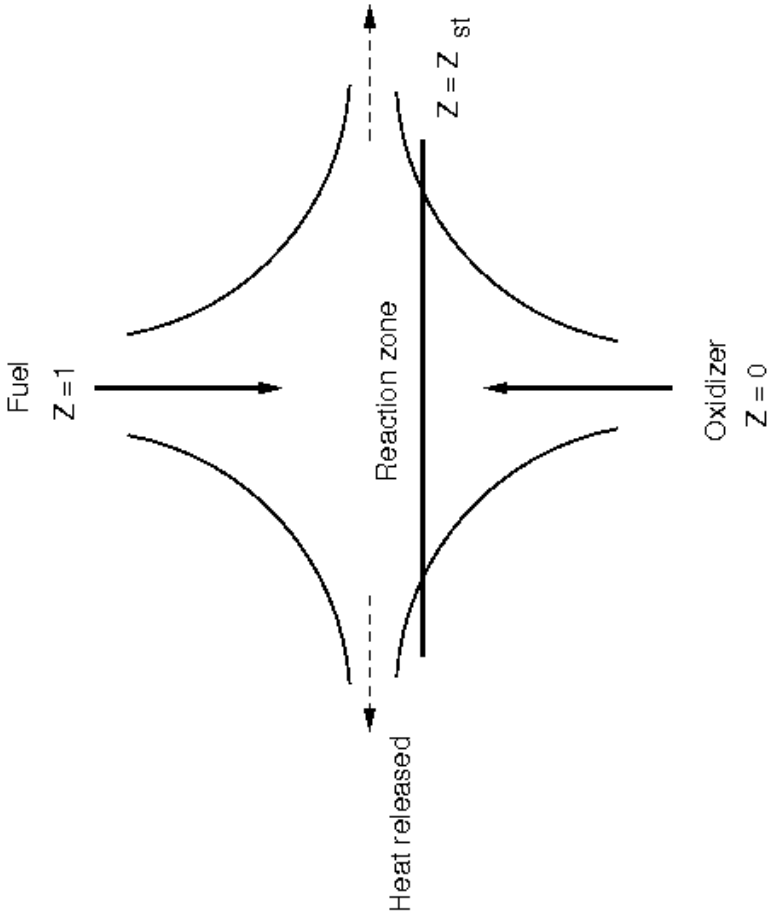
Diffusion flame configuration

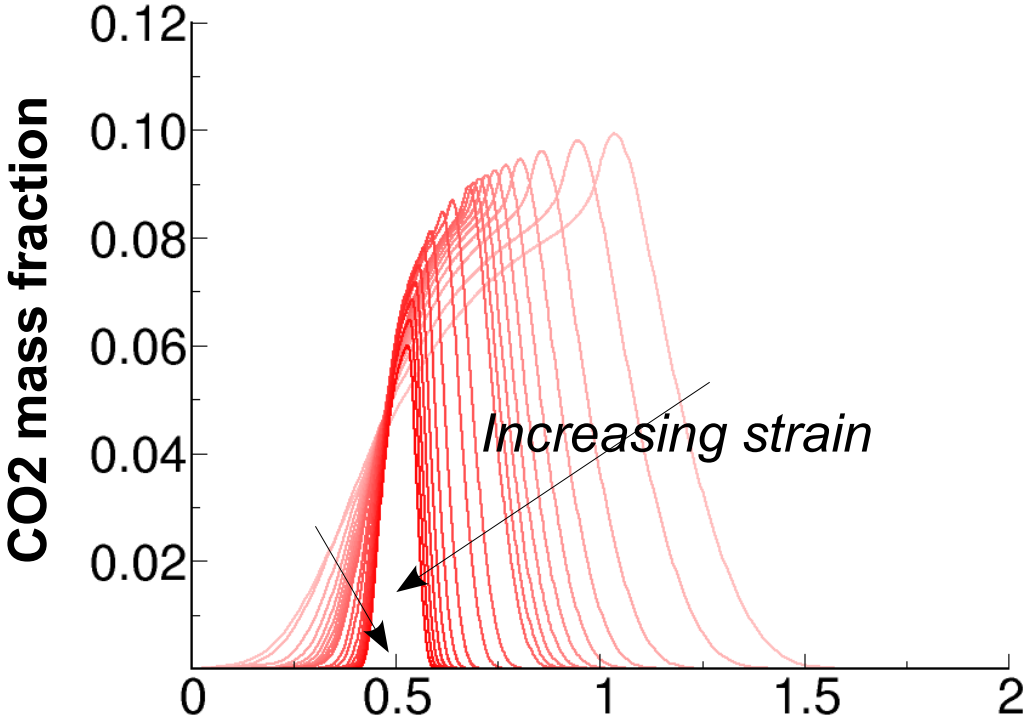


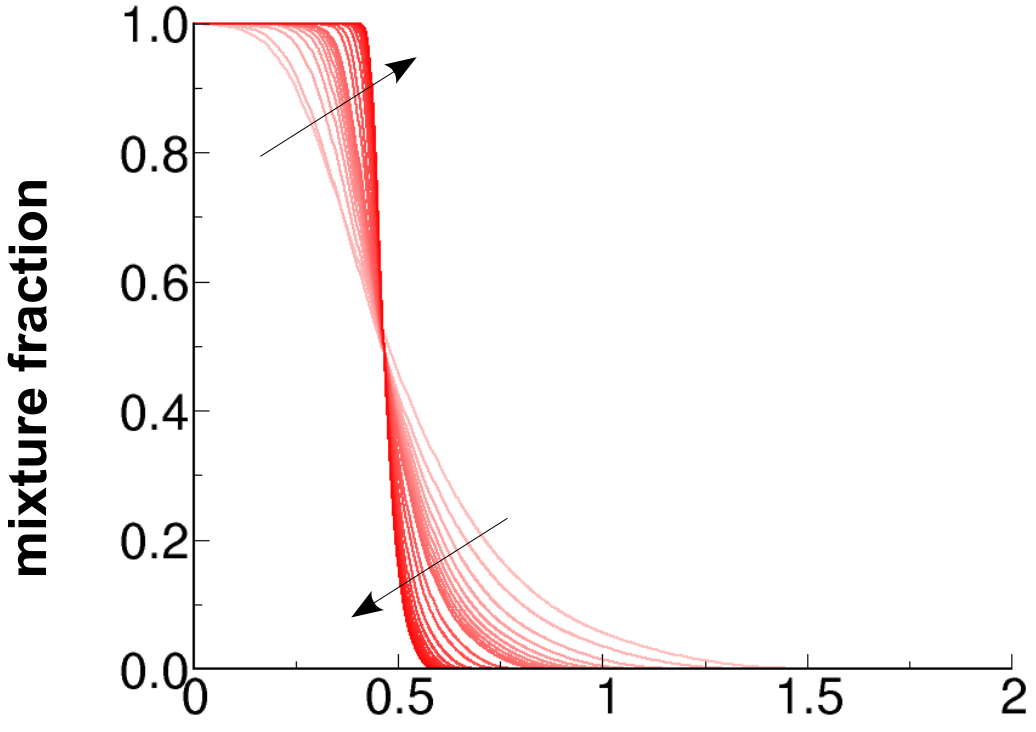
Velocity gradient → "Strain rate"

The flame extinguishes if heat loss larger than heat generated by reaction

Diffusion flames







Scalar dissipation

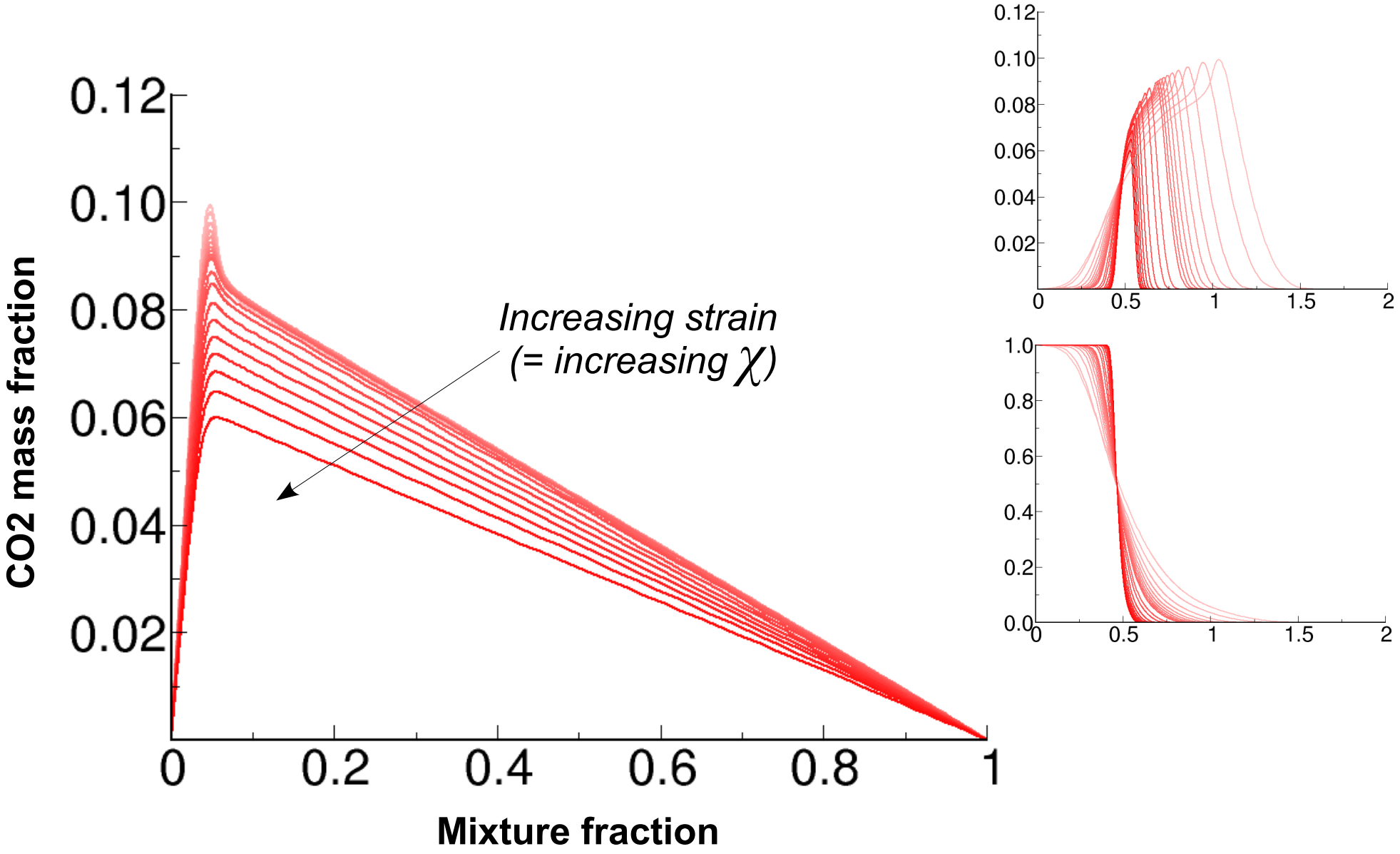
$$\frac{\partial \rho Y}{\partial t}+\frac{\partial \rho U_j Y}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\rho D_Y \frac{\partial Y}{\partial x_j}\right]+\dot{\omega}_Y$$

Diffusion flame: “scalar dissipation rate”

$$\frac{\partial \rho Y}{\partial t}+\frac{\partial \rho U_j Y}{\partial x_j}=\rho \chi \frac{\partial^2 Y}{\partial Z^2}+\dot{\omega}_Y$$

$$\chi = D_Y \frac{\partial Z}{\partial x_j}\frac{\partial Z}{\partial x_j}$$

As a function of mixture fraction



Equations

Reaction rates

Equations (low Mach)

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} = 0$$

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

$$\tau_{ij} = \nu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \nu \frac{\partial U_k}{\partial x_k} \delta_{ij}$$

"Low Mach": $p = p_0(t) + \Delta p$

$$\rho = p_0(t) / rT$$

r : function of composition (e.g. mass fractions *Y*)

T : function of *Y,* and total enthalpy *h*

Equations (composition)

Mass fractions (How many species?)

$$\frac{\partial \rho Y}{\partial t} + \frac{\partial \rho U_j Y}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\rho D_Y \frac{\partial Y}{\partial x_j}\right] + \dot{\omega}_Y$$

Convection | Diffusion (Fick law) | Reaction

Total enthalpy:

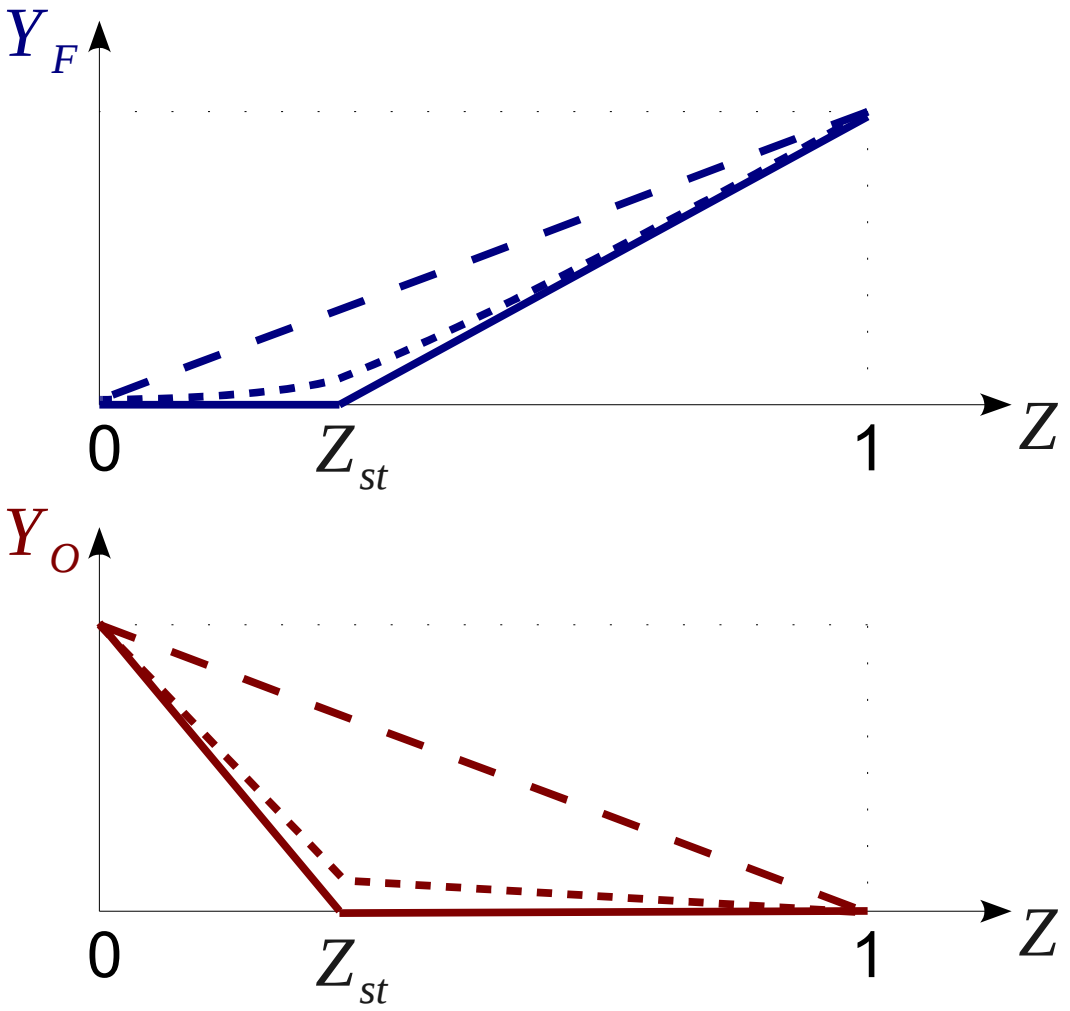
$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho U_j h}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\rho D_h \frac{\partial h}{\partial x_j}\right] + S_h$$

Convection | Diffusion (Fick law) | Radiation

Diffusion flames: 1 step / ω→∞ / Le=1

$\nu_F F + \nu_O O \rightarrow \nu_P P$

Burke & Schumann / “Mixed is burnt”



H_2: detailed mechanism

1. $H + O_2 \rightleftarrows OH + O$
2. $H_2 + O \rightleftarrows OH + H$
3. $H_2 + OH \rightleftarrows H_2O + H$
4. $H_2O + O \rightleftarrows 2OH$
5. $2H + M \rightleftarrows H_2 + M$
6. $H + OH + M \rightleftarrows H_2O + M$
7. $2O + M \rightleftarrows O_2 + M$
8. $H + O + M \rightleftarrows OH + M$
9. $O + OH + M \rightleftarrows HO_2 + M$
10. $H + O_2 + M \rightleftarrows HO_2 + M$
11. $HO_2 + H \rightleftarrows 2OH$
12. $HO_2 + H \rightleftarrows H_2 + O_2$
13. $HO_2 + H \rightleftarrows H_2O + O$
14. $HO_2 + O \rightleftarrows OH + O_2$
15. $HO_2 + OH \rightleftarrows H_2O + O_2$
16. $2OH + M \rightleftarrows H_2O_2 + M$
17. $2HO_2 \rightleftarrows H_2O_2 + O_2$
18. $H_2O_2 + H \rightleftarrows HO_2 + H_2$
19. $H_2O_2 + H \rightleftarrows H_2O + OH$
20. $H_2O_2 + OH \rightleftarrows H_2O + HO_2$
21. $H_2O_2 + O \rightleftarrows HO_2 + OH$

8 species / 21 reactions (University of California, San Diego)

H_2: skeletal mechanism

1. $H + O_2 \rightleftarrows OH + O$
2. $H_2 + O \rightleftarrows OH + H$
3. $H_2 + OH \rightleftarrows H_2O + H$
4.
5. $2H + M \rightleftarrows H_2 + M$
6. $H + OH + M \rightleftarrows H_2O + M$
7.
8.
9.
10. $H + O_2 + M \rightarrow HO_2 + M$
11. $HO_2 + H \rightarrow 2OH$
12. $HO_2 + H \rightleftarrows H_2 + O_2$
13.
14.
15. $HO_2 + OH \rightarrow H_2O + O_2$
16. $H_2O_2 + M \rightarrow 2OH + M$
17. $2HO_2 \rightarrow H_2O_2 + O_2$
18. $HO_2 + H_2 \rightarrow H_2O_2 + H$
19.
20.
21.

8 species / 12 reactions

H_2: reduced mechanism

5 species / 3 steps (Boivin *et al.*)

"Steady state" approximations for OH, O and H_2O_2

I. $3H_2 + O_2 \rightleftarrows 2H_2O + 2H$
II. $H + H + M \rightleftarrows H_2 + M$
III. $HO_2 + H \rightleftarrows H_2 + O_2$ (for autoignition)

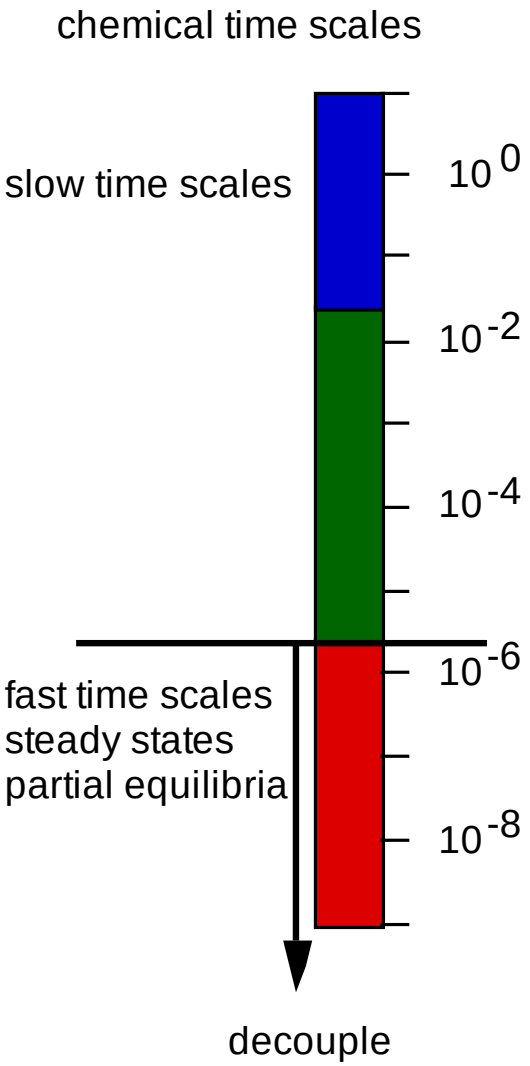
Global reaction rates:

$$\dot{\omega}_I = \dot{\omega}_1 + \dot{\omega}_{11} + \dot{\omega}_{17} + \dot{\omega}_{18}$$

$$\dot{\omega}_{II} = \dot{\omega}_{10} + \dot{\omega}_6 + \dot{\omega}_5 - \dot{\omega}_{17} - \dot{\omega}_{18}$$

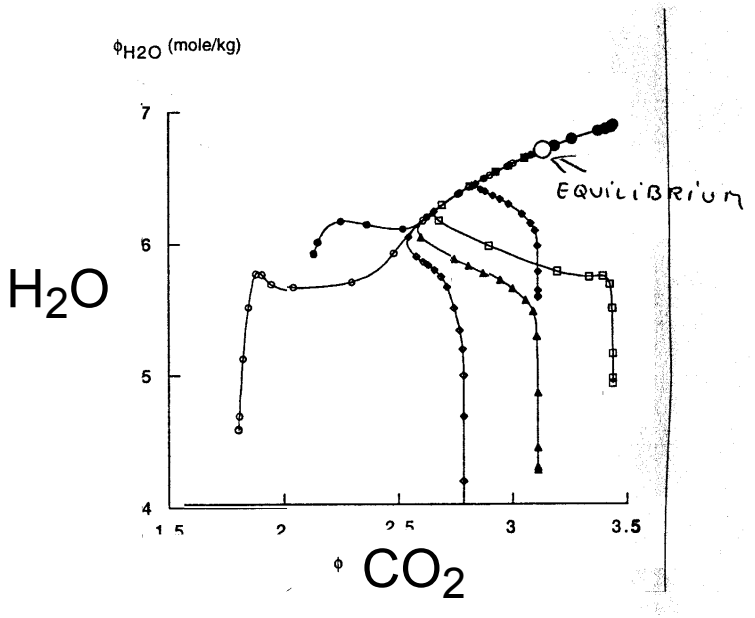
$$\dot{\omega}_{III} = -\dot{\omega}_{10} + \dot{\omega}_{11} + \dot{\omega}_{12} + \dot{\omega}_{15} + 2\,\dot{\omega}_{17} + \dot{\omega}_{18}$$

ILDM (Maas & Pope)



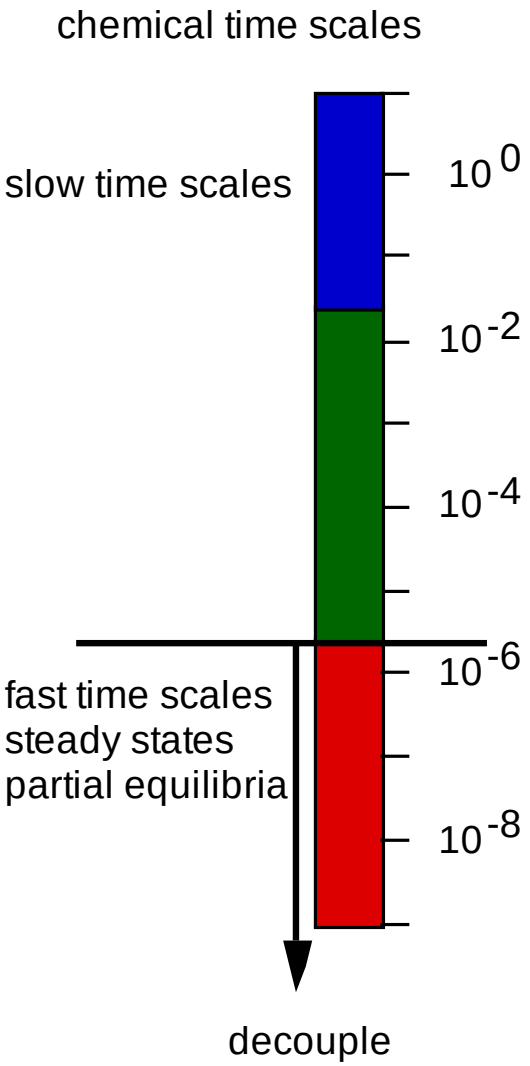
ILDM decouples the fast time scales

Methane oxidation



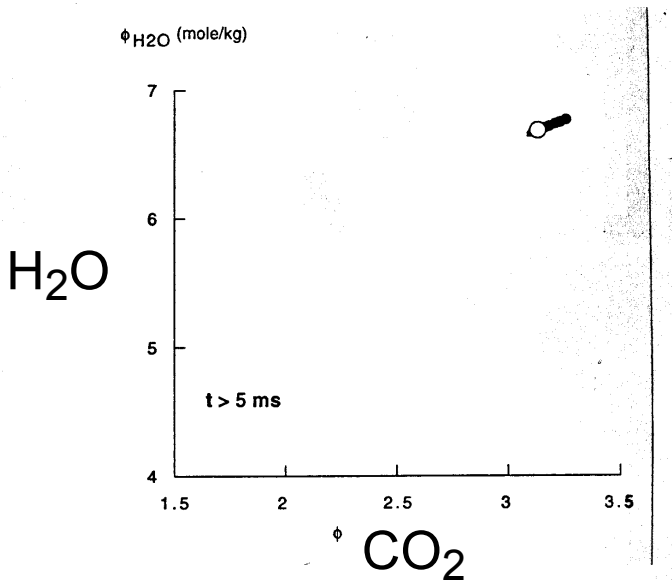
Evolution described by detailed chemical mechanism (showing only H2O and CO2, not the many other species)

ILDM (Maas & Pope)



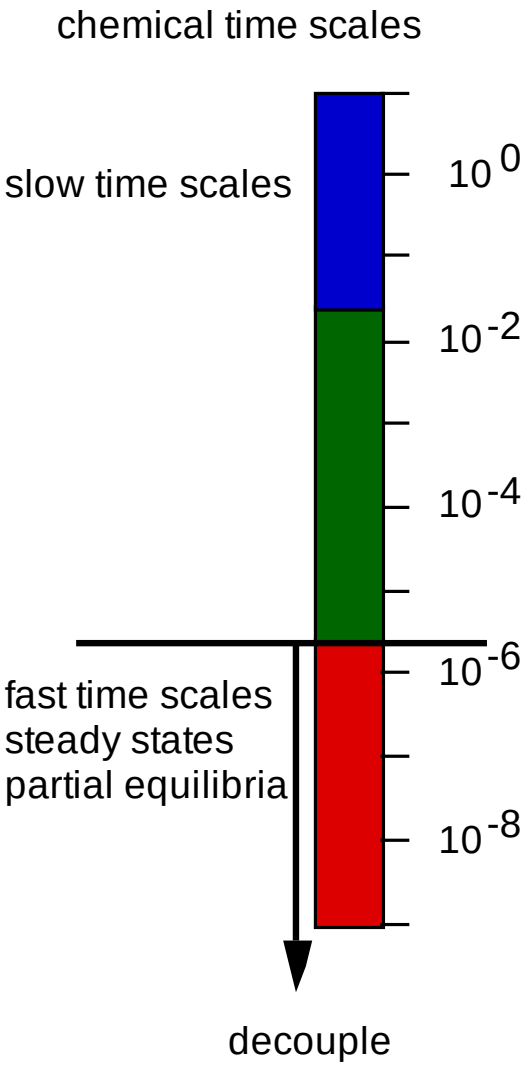
ILDM decouples the fast time scales

Methane oxidation



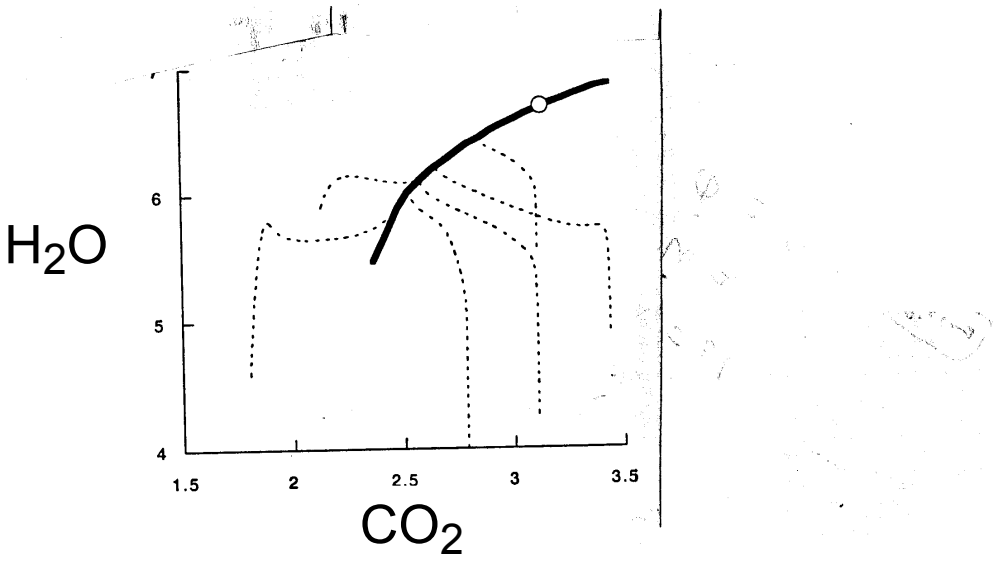
Evolution described by detailed kinetic mechanism **with the first 5 ms omitted**

ILDM (Maas & Pope)



ILDM decouples the fast time scales

Methane oxidation



Dotted: Evolution by detailed mechanism

Line: intrinsic low-dimensional manifold

Reduced chemistries

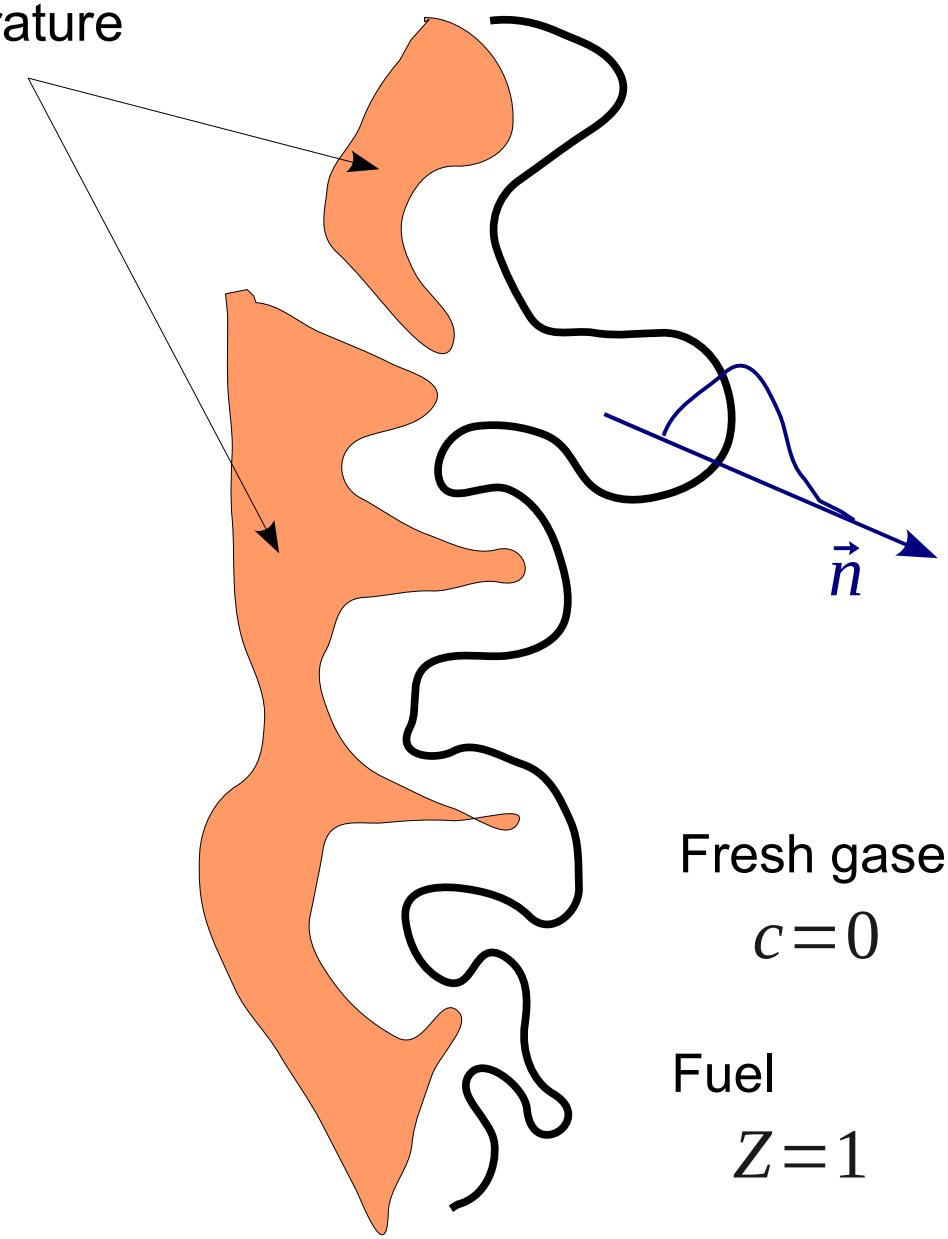
Detailed chemical mechanisms can be reduced:

→ conditions of validity (pressure, temperature, equivalence ratio)

→ what do we expect:

- Temperature
- Minor species
- Autoignition delay
- ...

Flamelets: “flame structure”

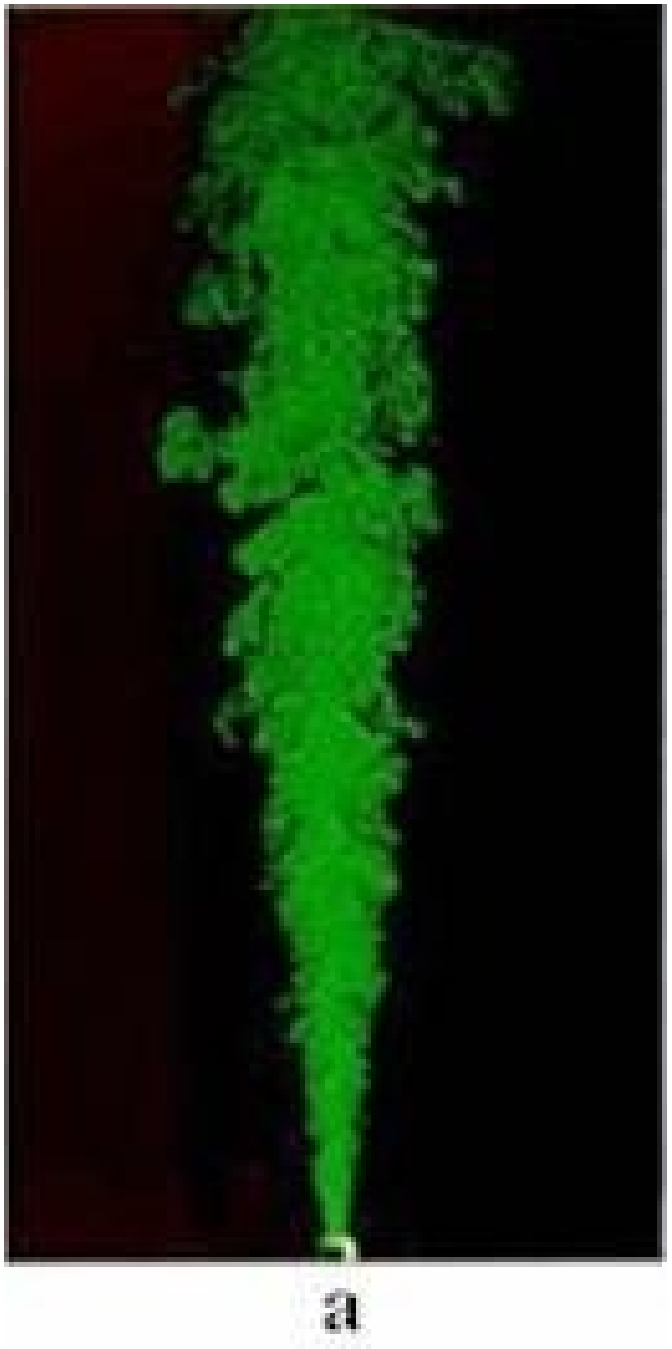


Turbulence

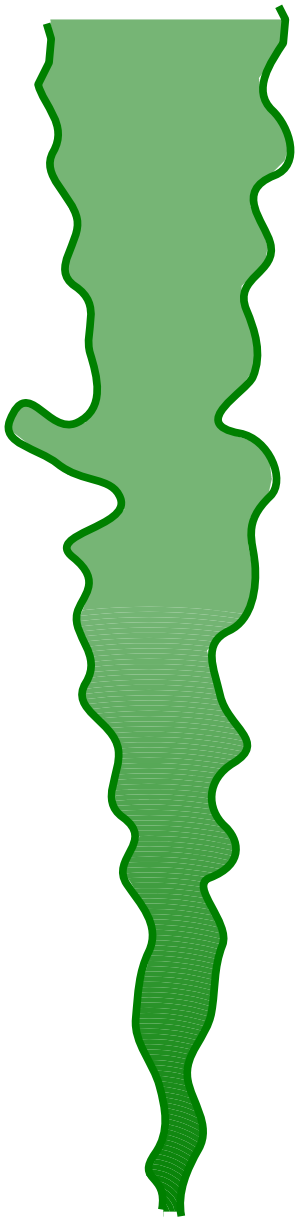
RANS modelling

LES modelling

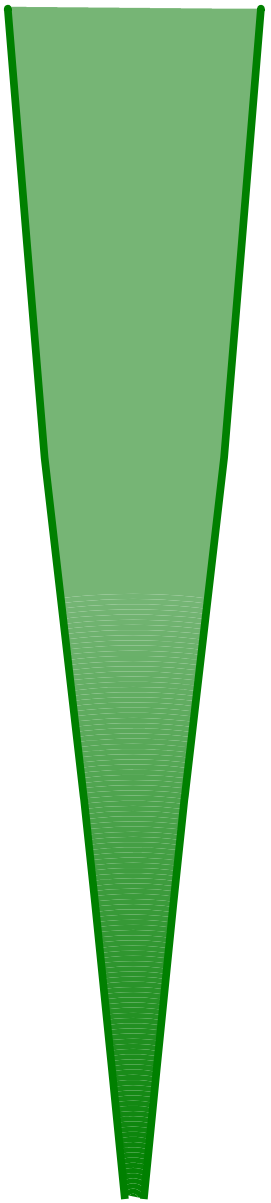
RANS / LES



a

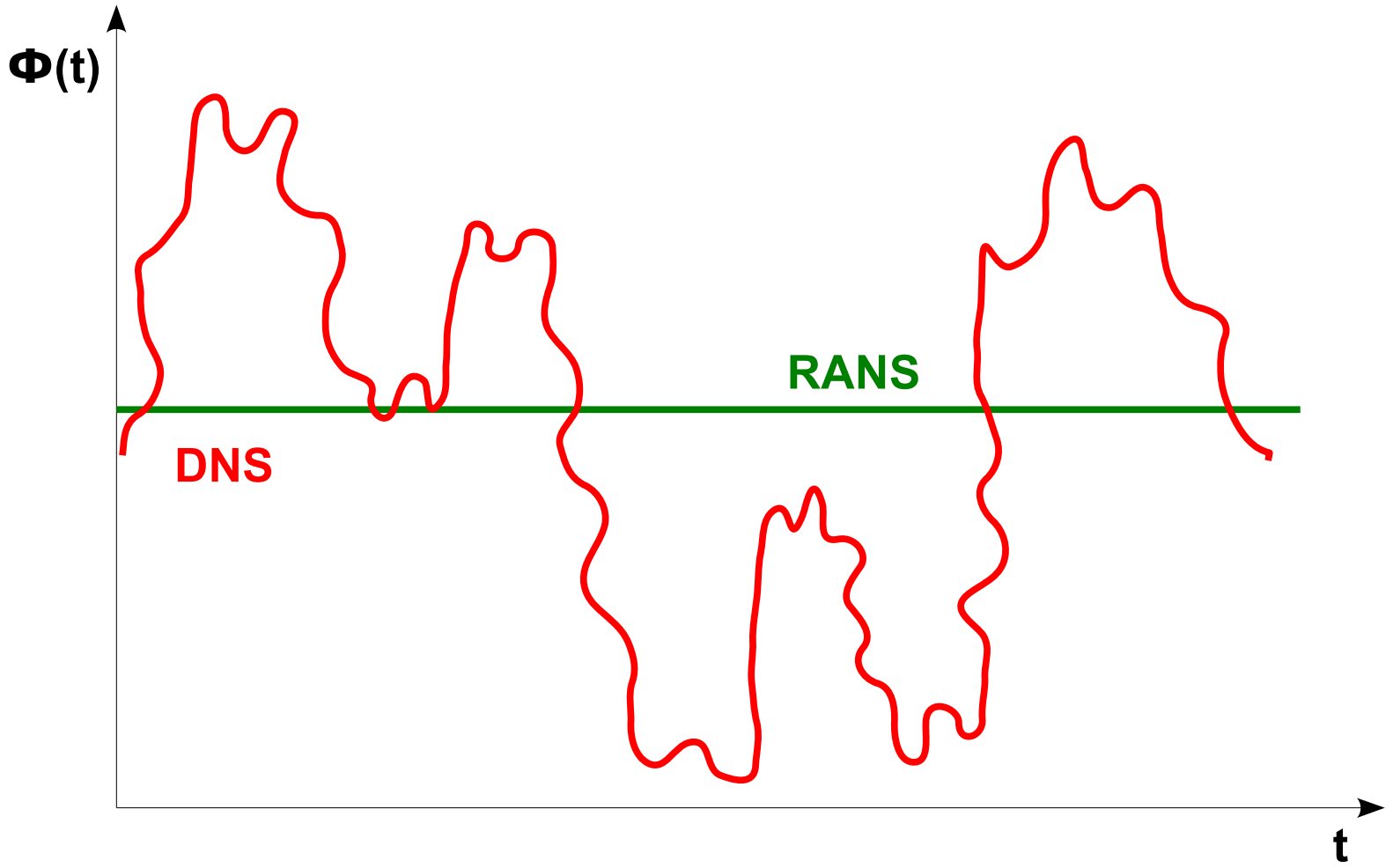


LES

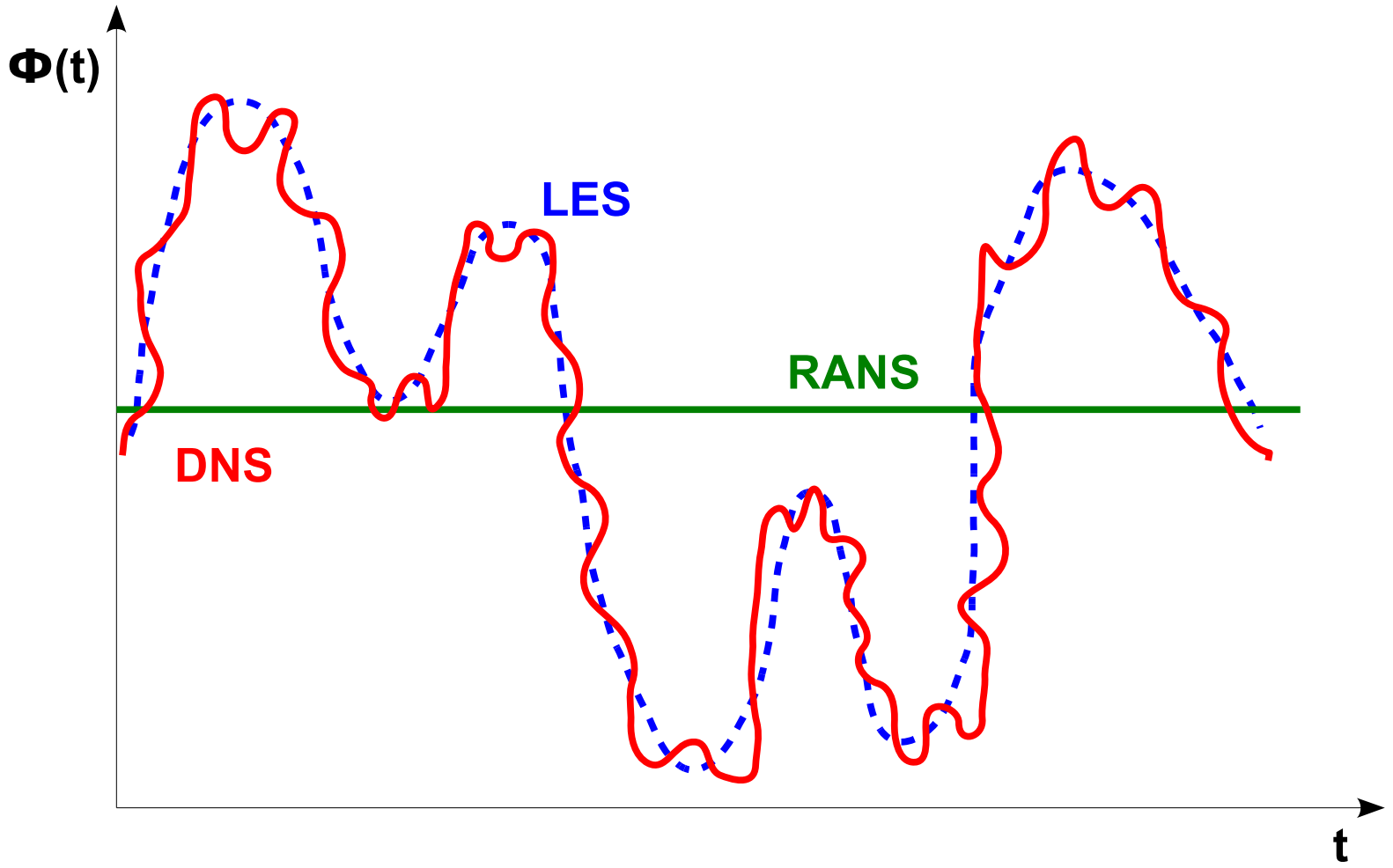


RANS

RANS



LES



Reynolds decomposition / Filtering

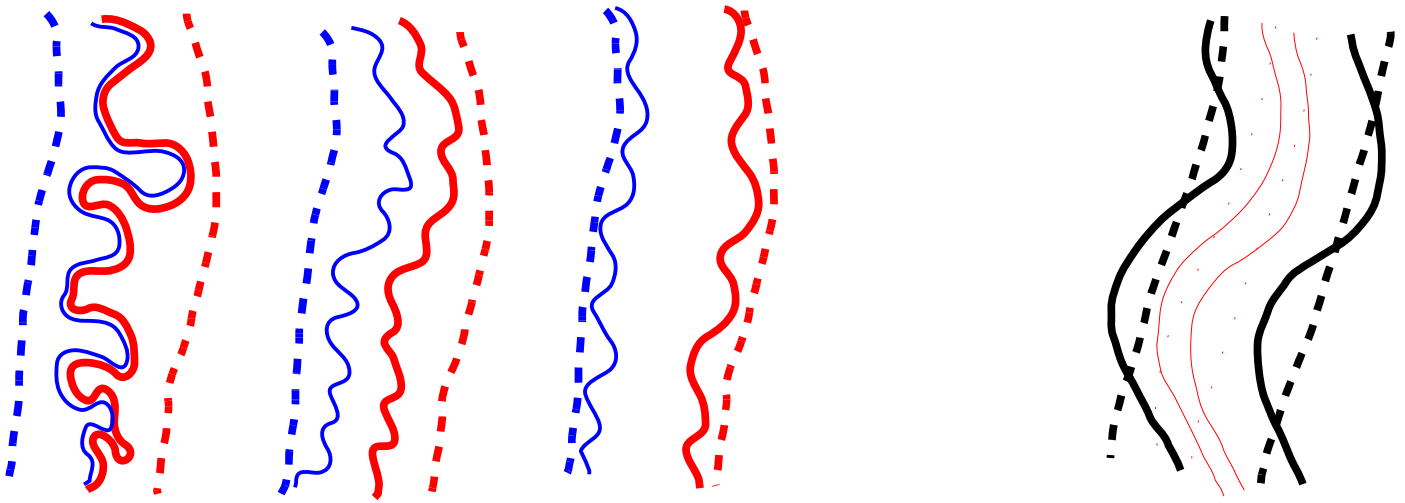
$$\frac{\partial \rho Y}{\partial t} + \frac{\partial \rho U_j Y}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\rho D \frac{\partial Y}{\partial x_j}\right] + \dot{\omega}_Y$$

$$\frac{\partial \overline{\rho Y}}{\partial t} + \frac{\partial \overline{\rho U_j Y}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\overline{\rho D \frac{\partial Y}{\partial x_j}}\right] + \overline{\dot{\omega}_Y}$$

What do we model?

Depending on the type of turbulent flame, hypothesis on the instantaneous reaction rate:

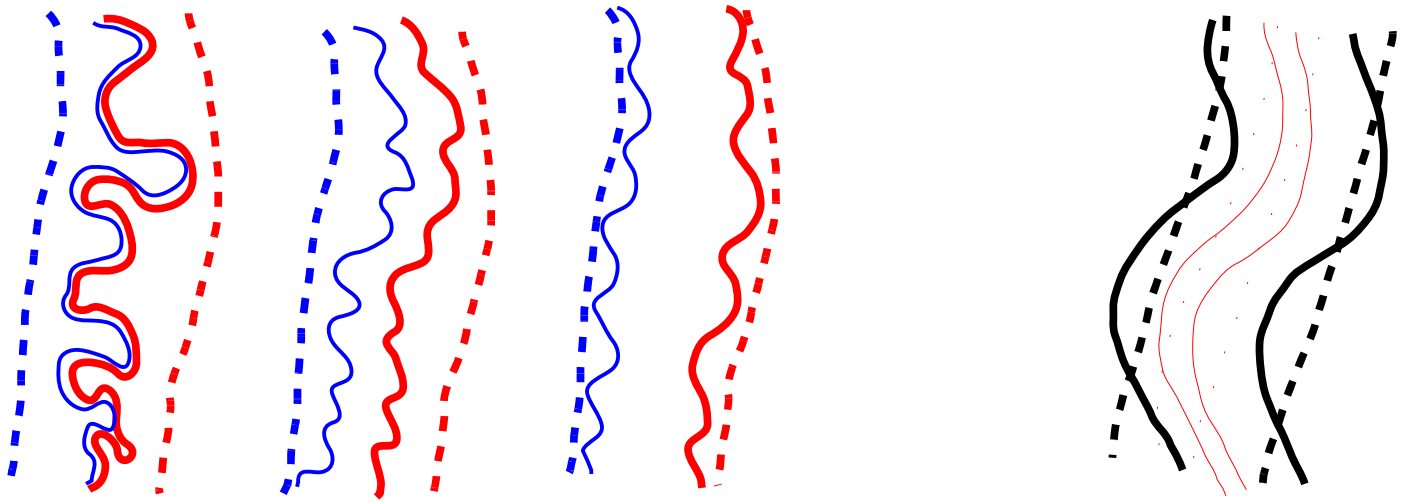
- infinitely fast reaction
- flamelet (the flame is thin and burns like a laminar flamelet)
- simplified kinetics
- complete kinetics (Arrhenius)



Turbulent flames: “wrinkled” = “fluctuacions” / RANS: “thick” flames

What do we model?

Problem: How to obtain the mean reaction rate? $\dot{\omega}_\alpha \rightarrow \overline{\dot{\omega}_\alpha}$?



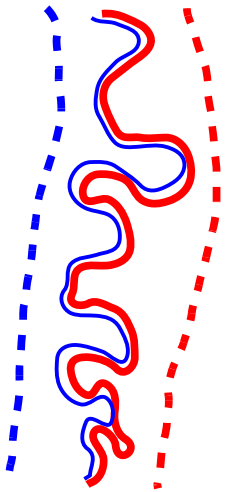
Turbulent flames: “wrinkled” = “fluctuations” / RANS: “thick” flames

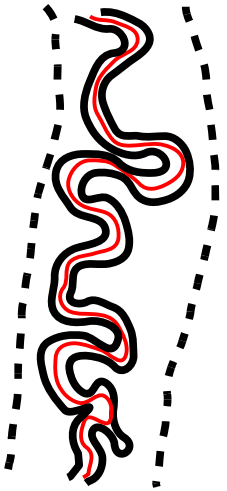
→ Geometrical analysis: include the effect of the wrinkling of the flame (propagation speed, “flame surface density”) / model on the flame structure (Eddy Dissipation Concept)

→ Statistical point of view: probability density function

Flamelets

$$Da = \frac{\tau_t}{\tau_c} \gg 1$$

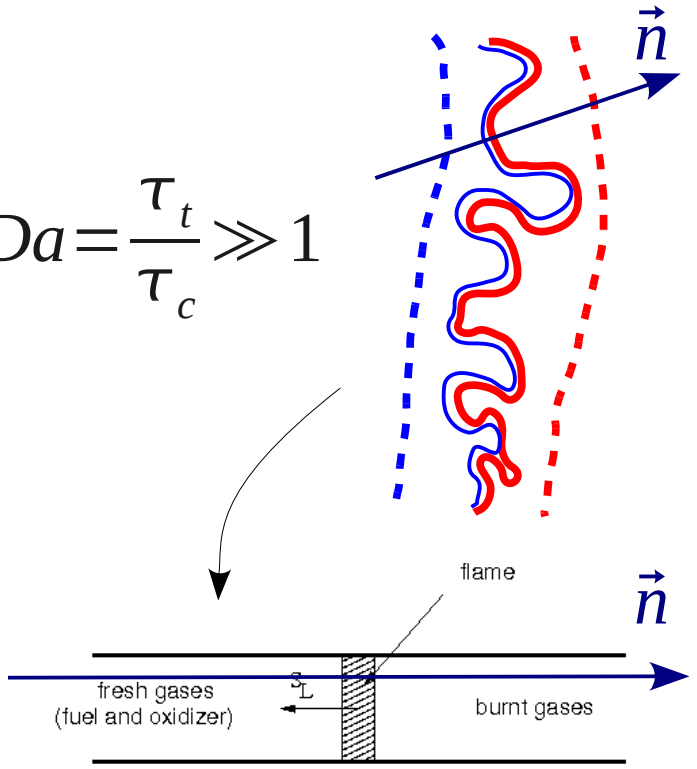


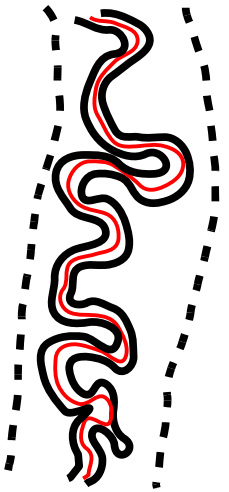


$$Da = \frac{\tau_\chi}{\tau_c} \gg 1$$

Flamelets

$$Da = \frac{\tau_t}{\tau_c} \gg 1$$

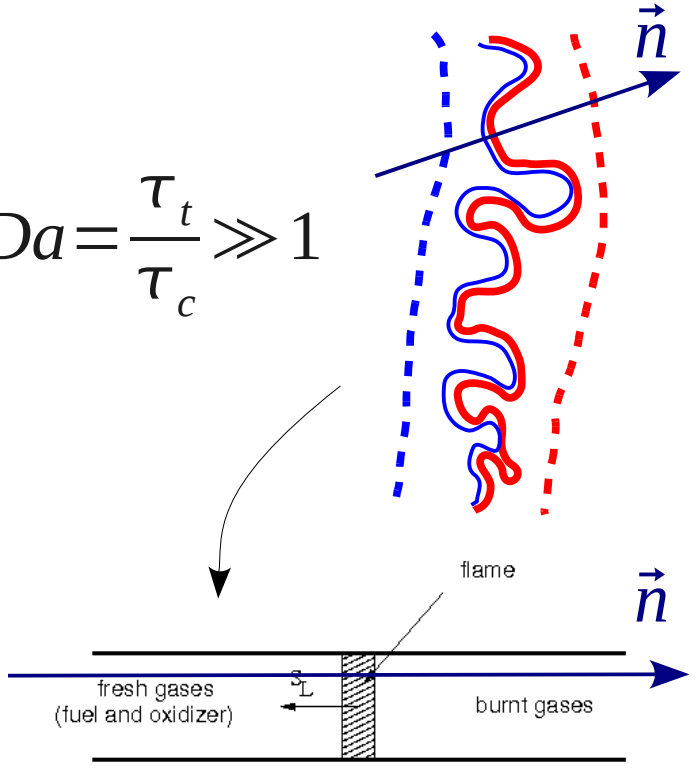




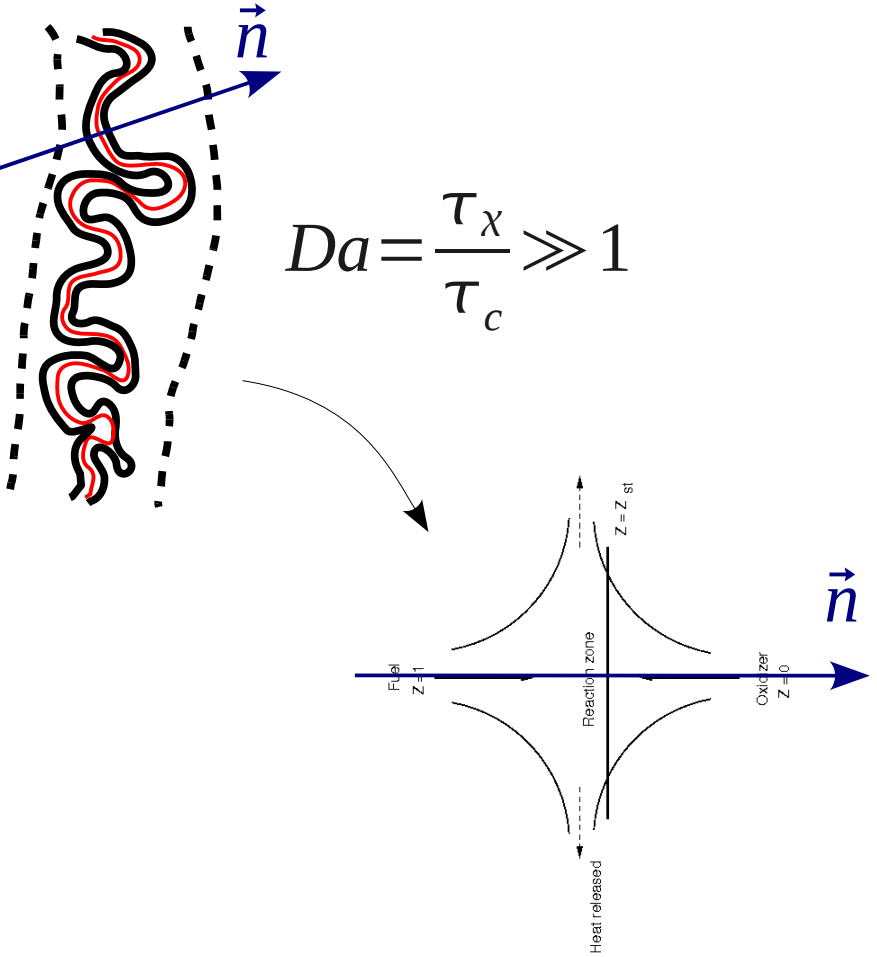
$$Da = \frac{\tau_\chi}{\tau_c} \gg 1$$

Flamelets

$$Da = \frac{\tau_t}{\tau_c} \gg 1$$

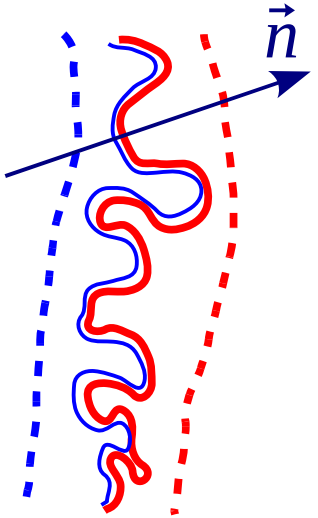


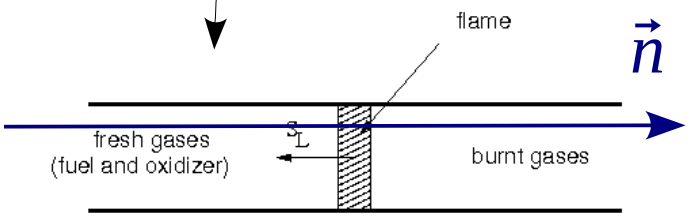
$$Da = \frac{\tau_\chi}{\tau_c} \gg 1$$

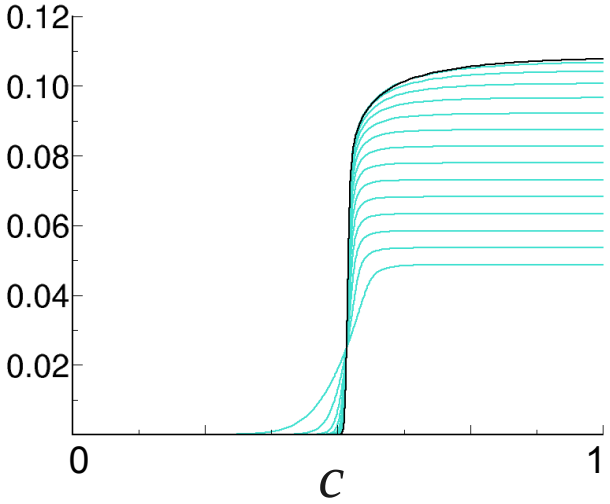


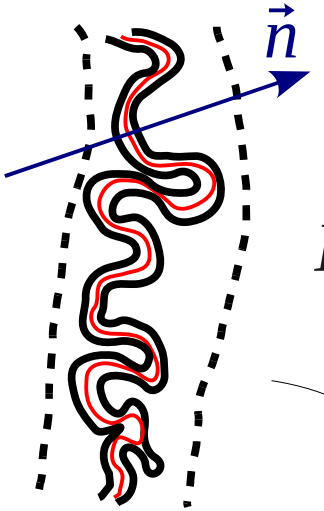
Flamelets

$$Da = \frac{\tau_t}{\tau_c} \gg 1$$

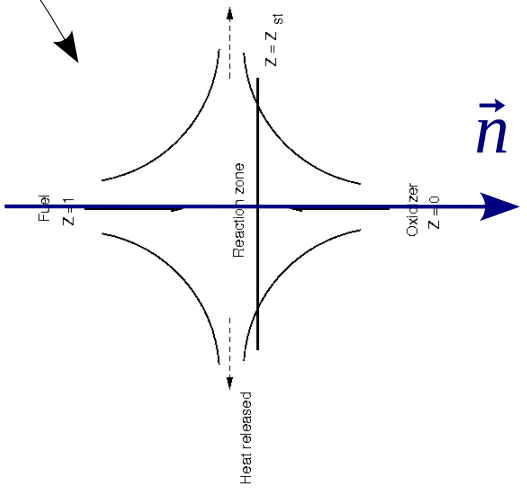






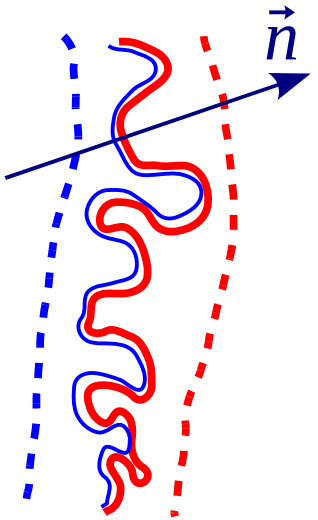


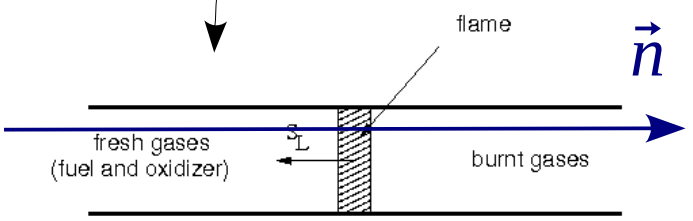
$$Da = \frac{\tau_\chi}{\tau_c} \gg 1$$

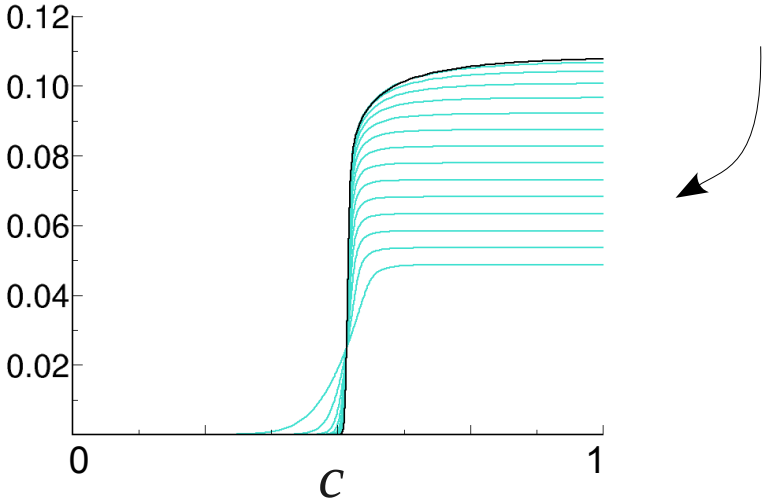


Flamelets

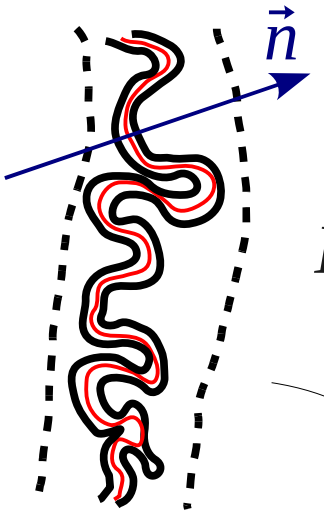
$$Da = \frac{\tau_t}{\tau_c} \gg 1$$

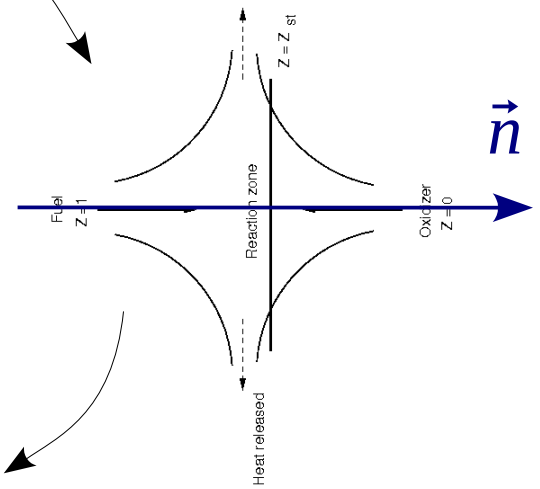


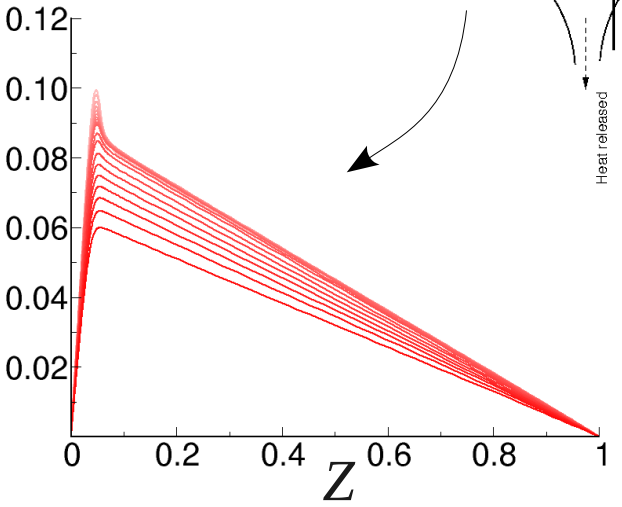




$$Da = \frac{\tau_\chi}{\tau_c} \gg 1$$

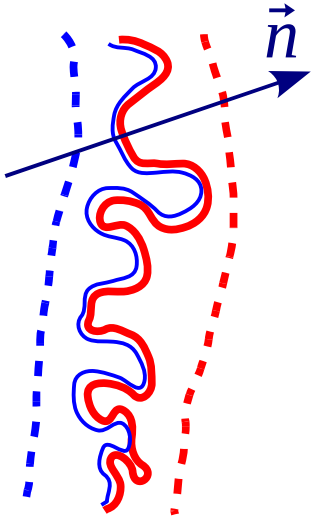


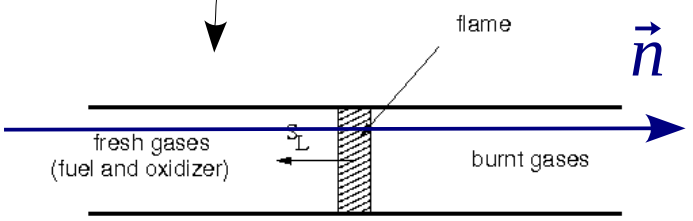


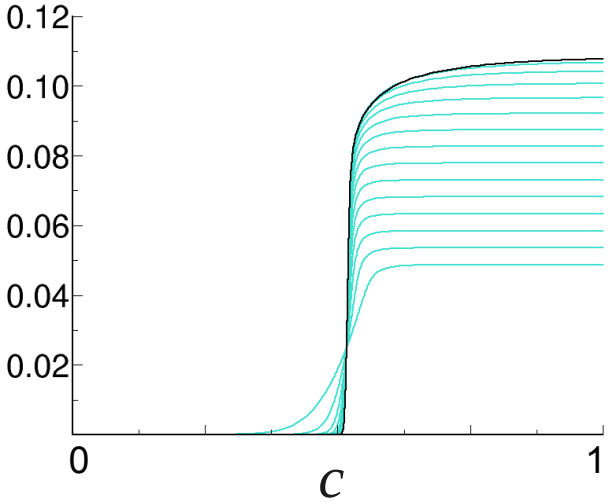


Flamelets

$$Da = \frac{\tau_t}{\tau_c} \gg 1$$

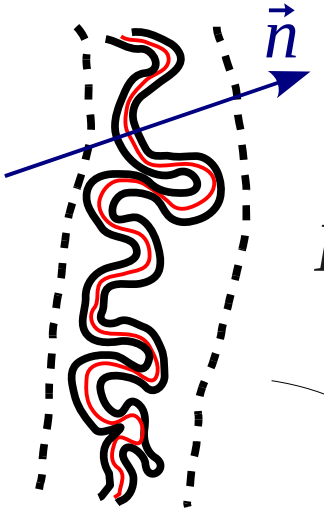


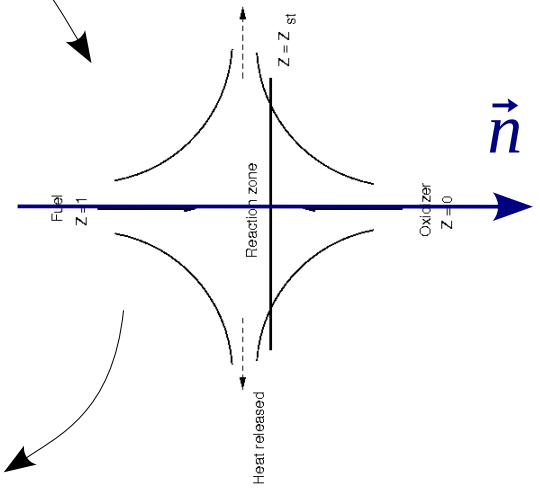


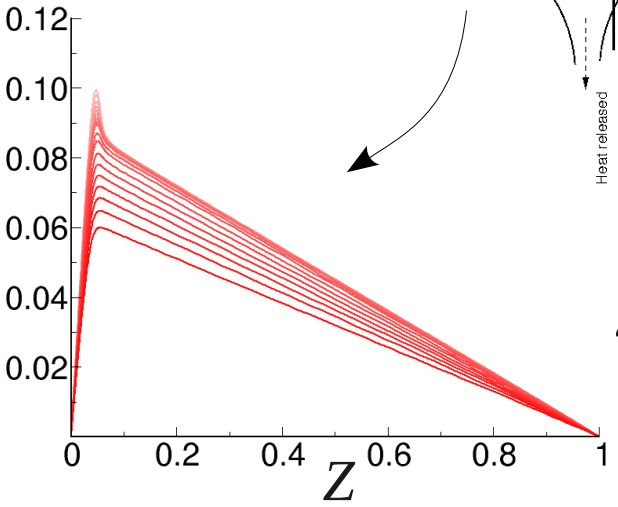


ϕ ?

$$Da = \frac{\tau_\chi}{\tau_c} \gg 1$$



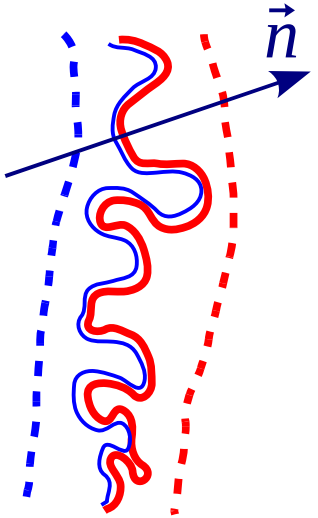




χ ?

Flamelets

$$Da = \frac{\tau_t}{\tau_c} \gg 1$$

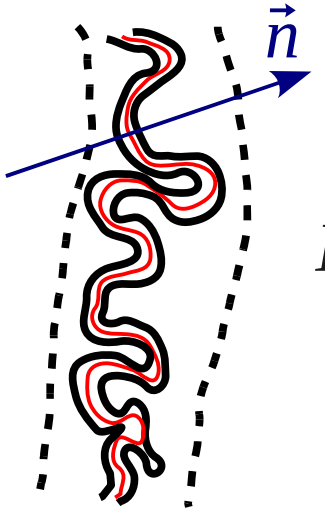


$$T(c, \phi)$$

Turbulent premixed flame:

→ simplification, one single ϕ

$$T(c)$$



$$Da = \frac{\tau_\chi}{\tau_c} \gg 1$$

$$T(Z, \chi)$$

Turbulent diffusion flame:

→ simplification, one single χ

$$T(Z)$$

Flamelets

RANS: we solve mean values... (or in LES, filtered values)

$$\frac{\partial \overline{\rho}\tilde{Z}}{\partial t}+\frac{\partial \overline{\rho}\widetilde{U}_j\tilde{Z}}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\overline{\rho D_Z \frac{\partial Z}{\partial x_j}}\right]-\frac{\partial \overline{\rho}\widetilde{u_j Z''}}{\partial x_j}$$

$$\frac{\partial \overline{\rho}\tilde{c}}{\partial t}+\frac{\partial \overline{\rho}\widetilde{U}_j\tilde{c}}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\overline{\rho D_c \frac{\partial c}{\partial x_j}}\right]-\frac{\partial \overline{\rho}\widetilde{u_j c''}}{\partial x_j}+\overline{\dot{\omega}_c}$$

$\widetilde{T(Z)}$? $\widetilde{T(c)}$?

→ Probability Density Function

= statistical point of view on the wrinkling of iso-*Z* or iso-*c* surfaces

Flamelets + PDF

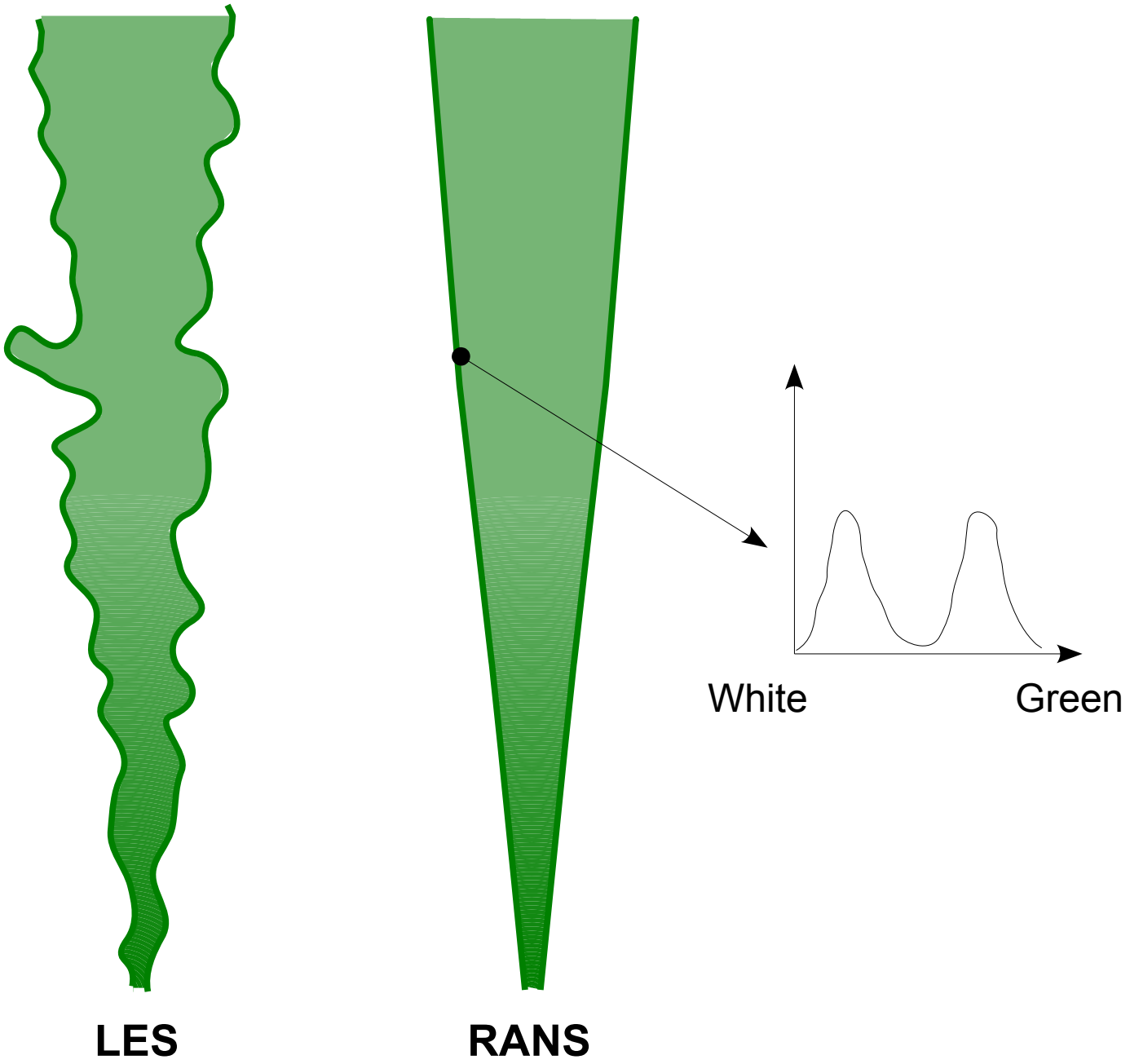
$$T = \overline{T} + T'$$

$$\overline{T} = \overline{T[Z(x,t)]} = \int T(\eta) P_Z(\eta; x, t) . d\eta$$

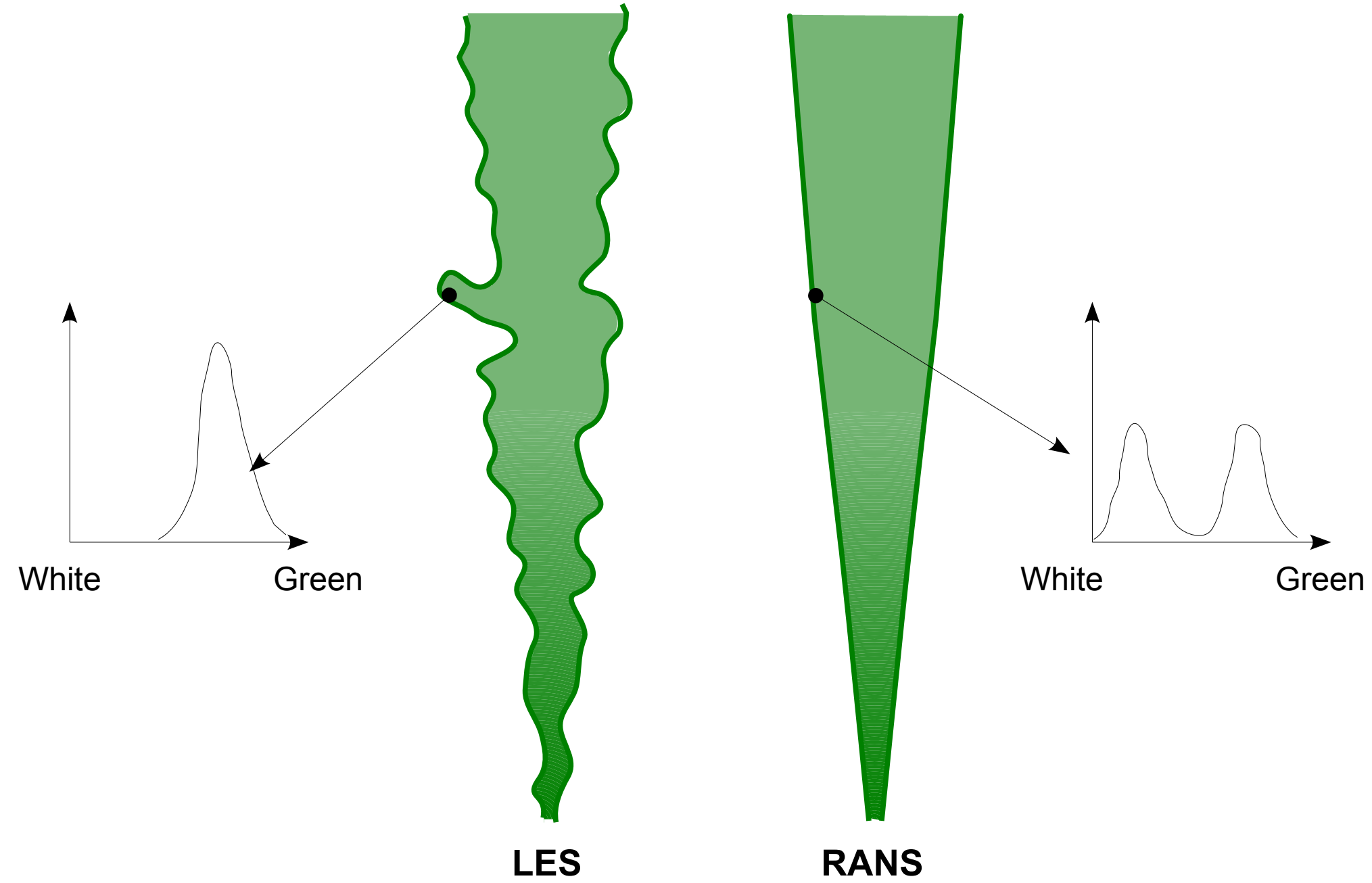
PDF of Z = distribution of the probable values of $Z(x,t)$ over the space of possible values η

Ideas on PDF's

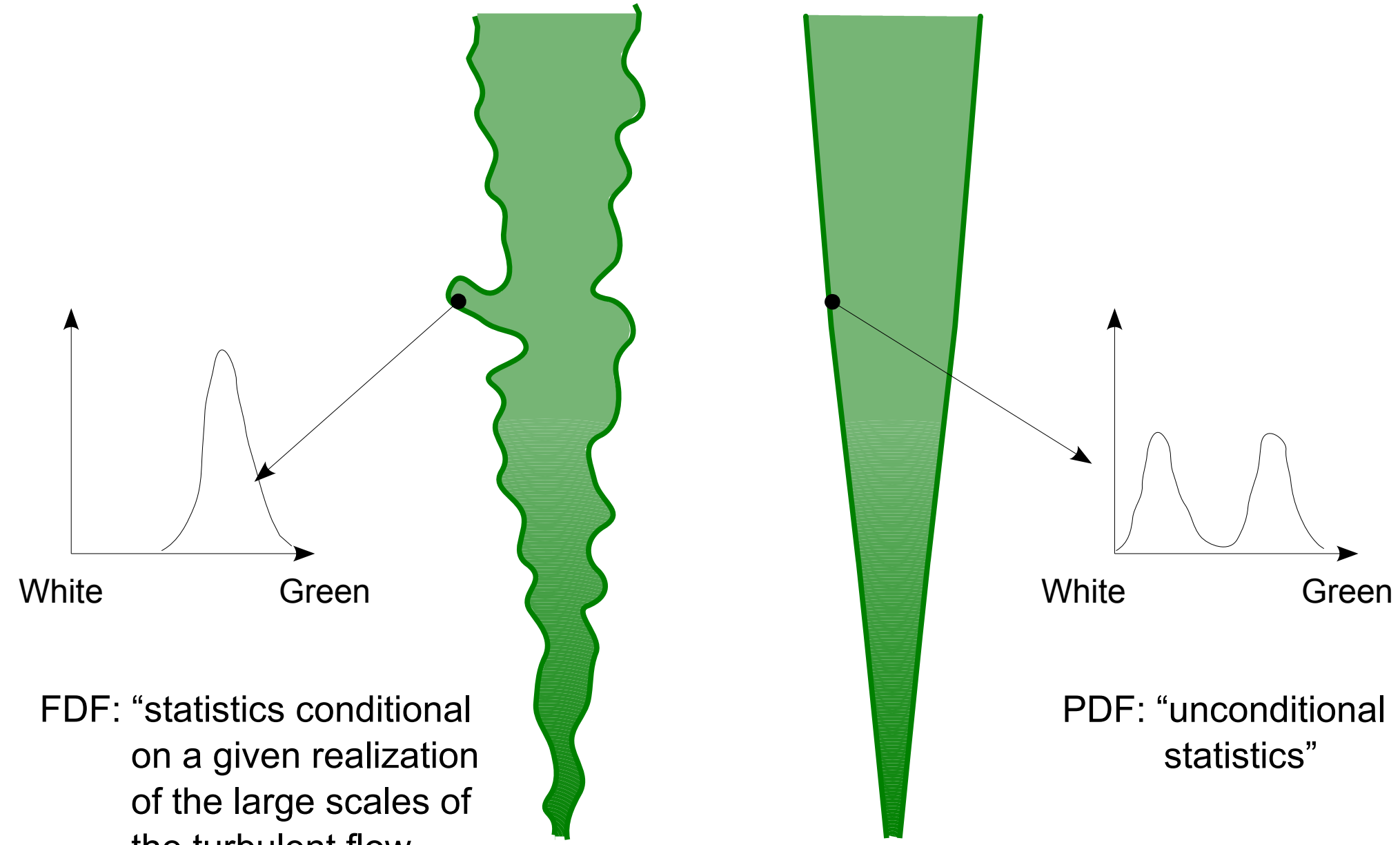
RANS: PDF / LES: FDF



RANS: PDF / LES: FDF



RANS: PDF / LES: FDF



FDF: “statistics conditional on a given realization of the large scales of the turbulent flow.

PDF: “unconditional statistics”

Flamelets + PDF

$$T = \overline{T} + T'$$

$$\overline{T} = \overline{T[Z(x,t)]} = \int T(\eta) P_Z(\eta; x, t) . d\eta$$

PDF of Z = distribution of the probable values of $Z(x,t)$
over the space of possible values η

"Presumed-PDF":

→ approximation based on: the mean value $\overline{Z(x,t)}$

and variance $\overline{Z'^2(x,t)}$

Flamelets + PDF

$$T = \overline{T} + T'$$

$$\overline{T} = \overline{T[Z(x,t)]} = \int T(\eta) P_Z(\eta; x, t) . d\eta$$

PDF of Z = distribution of the probable values of $Z(x,t)$
over the space of possible values η

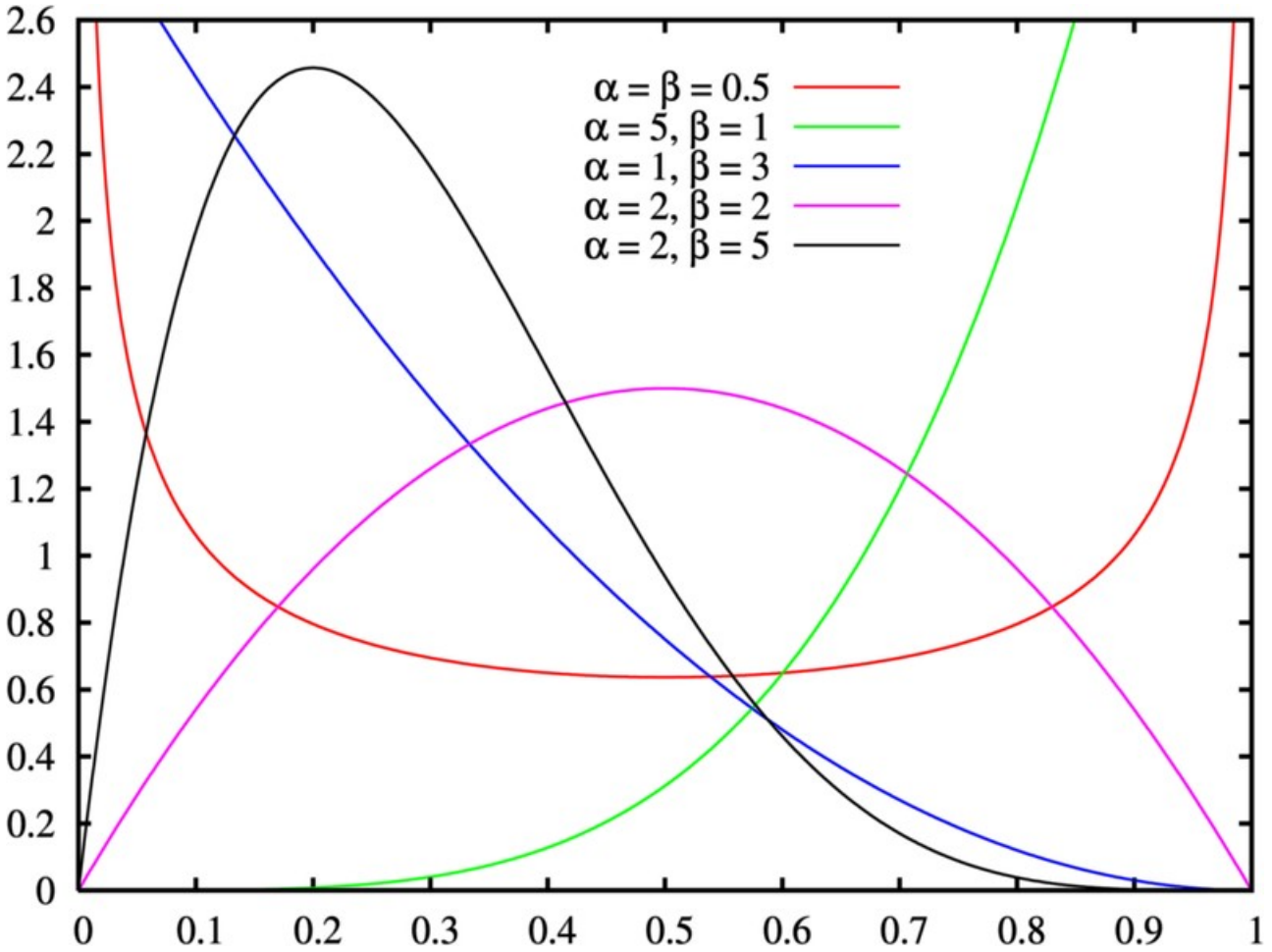
"Presumed-PDF":

→ approximation based on: the mean value $\overline{Z(x,t)}$

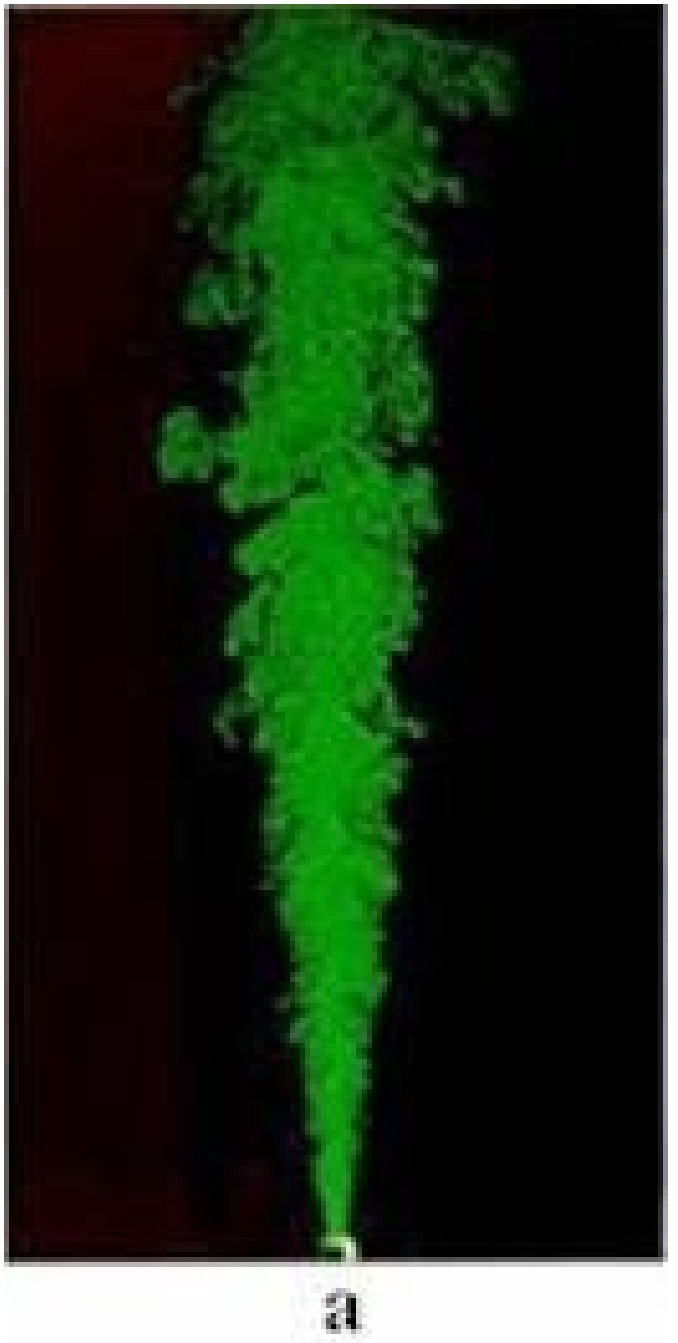
and variance $\overline{Z'^2(x,t)}$

$$\overline{T[Z(x,t)]} = \int T(\eta) P_{\overline{Z}, \overline{Z'^2}}(\eta; x, t) . d\eta = \overline{T}\left[\overline{Z}, \overline{Z'^2}\right]$$

Beta-PDF



$$f^{\beta}_{\tilde{Z},\widetilde{Z''^2}}(\eta;x,t)=\frac{\eta^{a-1}(1-\eta)^{b-1}}{\int \eta^{a-1}(1-\eta)^{b-1}\,d\eta}$$



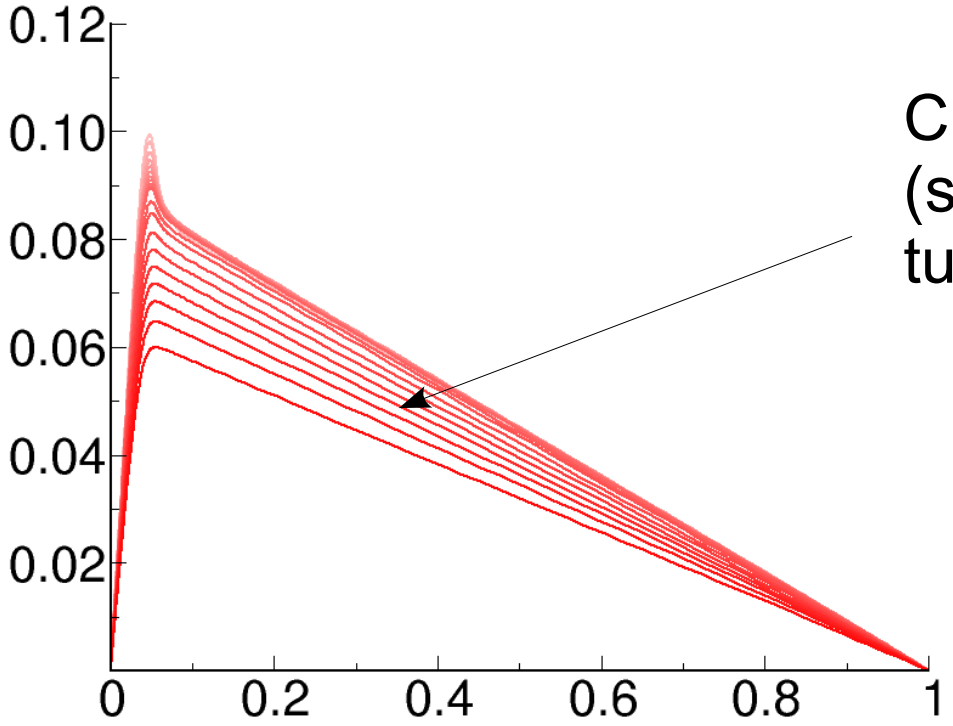
Beta-PDF

$$f^{\beta}_{\tilde{Z},\widetilde{Z''^2}}(Z;x,t)=\frac{(Z-Z_{min})^{a-1}(Z_{max}-Z)^{b-1}}{(Z_{max}-Z_{min})^{a+b-1}\int z^{a-1}(1-z)^{b-1}dz}$$

$$a=\frac{\tilde{Z}-Z_{min}}{Z_{max}-Z_{min}}\left[\frac{(\tilde{Z}-Z_{min})(Z_{max}-\tilde{Z})}{\widetilde{Z''^2}}-1\right]$$

$$b=a\left[\frac{Z_{max}-\tilde{Z}}{\tilde{Z}-Z_{min}}\right]$$

Flamelet + beta-PDF



Choose one flamelet
(strain rate typical of the
turbulent flame to be modelled)

$$\rho(Z), T(Z), Y_\alpha(Z), \ldots$$

$$f^{\beta}_{\tilde{Z},\widetilde{Z''^2}}(\eta; x, t) = \frac{\eta^{a-1}(1-\eta)^{b-1}}{\int \eta^{a-1}(1-\eta)^{b-1} d\eta}$$

$$\tilde{T}(\tilde{Z}, \widetilde{Z''^2}) = \int T(\eta) f^{\beta}_{\tilde{Z},\widetilde{Z''^2}}(\eta; x, t) . d\eta$$

Practical CFD calculation

Store 2-dimensional table:

$$\tilde{T}(\tilde{Z},\widetilde{Z''^2})=\int T(\eta) f^{\beta}_{\tilde{Z},\widetilde{Z''^2}}(\eta;x,t).d\eta$$

one flamelet (given strain rate)

beta-PDF

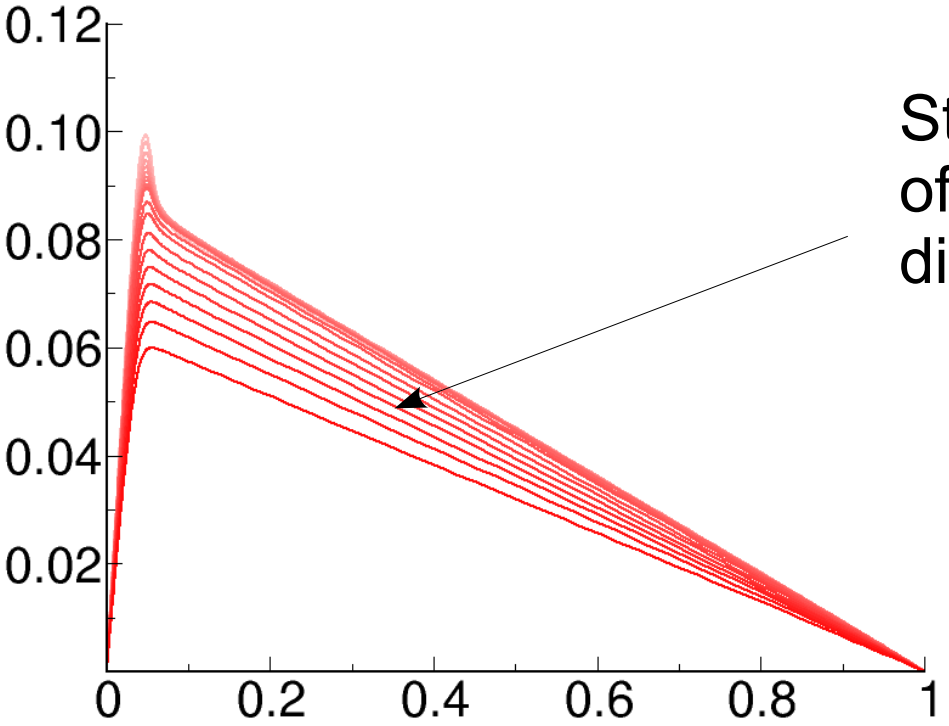
Solve mean and variance:

$$\frac{\partial\langle\rho\rangle\tilde{Z}}{\partial t}+\frac{\partial\langle\rho\rangle\widetilde{U}_j\tilde{Z}}{\partial x_j}=-\frac{\partial\langle\rho\rangle\widetilde{u_j Z''}}{\partial x_j}$$

$$\frac{\partial\langle\rho\rangle\widetilde{Z''^2}}{\partial t}+\frac{\partial\langle\rho\rangle\widetilde{U}_j\widetilde{Z''^2}}{\partial x_j}+2\langle\rho\rangle\widetilde{u_j Z''}\frac{\partial\tilde{Z}}{\partial x_j}=-\frac{\partial\langle\rho\rangle\widetilde{u_j Z''^2}}{\partial x_j}-\tilde{\chi}$$

Presumed PDF of two scalars...

Flamelets + presumed PDF



Store the flamelets as functions of mixture fraction and scalar dissipation rate:

$$\rho(Z,\chi), T(Z,\chi), Y_\alpha(Z,\chi), \ldots$$

How do we assume the shape of the joint PDF of Z and χ?

$$f_{Z,\chi}?$$

$$\rightarrow \tilde{T} = \int T(Z,\chi) f_{Z,\chi} . dZ . d\chi$$

Flamelets + presumed PDF

Z and χ are statistically independent:

$$f_{Z,\chi}(\eta,\hat{\chi}) = f_Z(\eta) f_\chi(\hat{\chi})$$

$$f_Z(\eta) = f^{\beta}_{\tilde{Z},\widetilde{Z''^2}}(\eta)$$

$$f_\chi(\hat{\chi})$$

$$\rightarrow \tilde{T} = \int T(\eta,\hat{\chi}) f^{\beta}_{\tilde{Z},\widetilde{Z''^2}}(\eta) f_\chi(\hat{\chi}) . d\eta . d\hat{\chi}$$

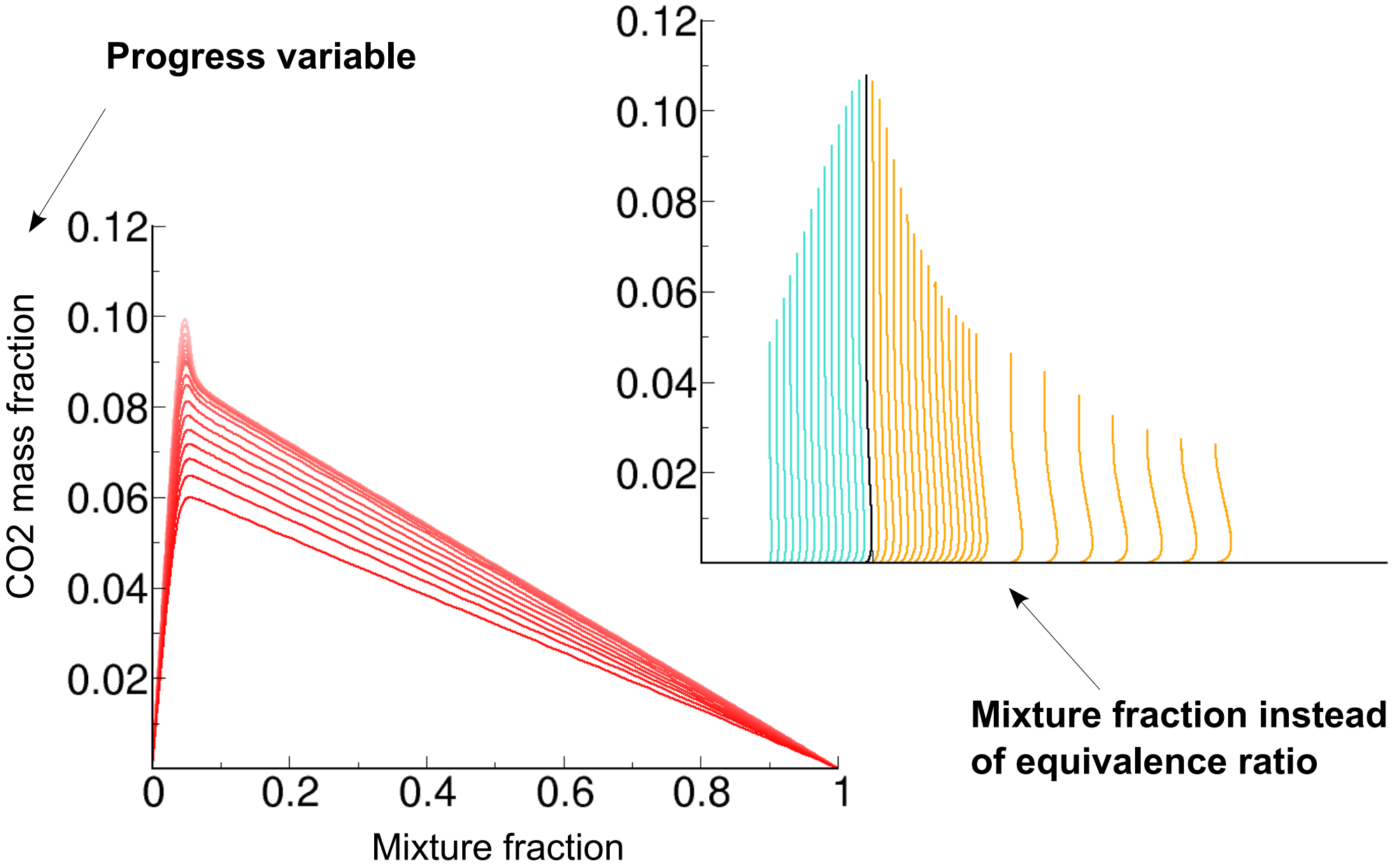
For any value of mixture fraction, same probability of the values of the gradient.

$$f_{\chi|Z} = f_\chi$$

mixture fraction + progress variable

(FPI/FGM REDIM)

Diffusion or premixed flamelets

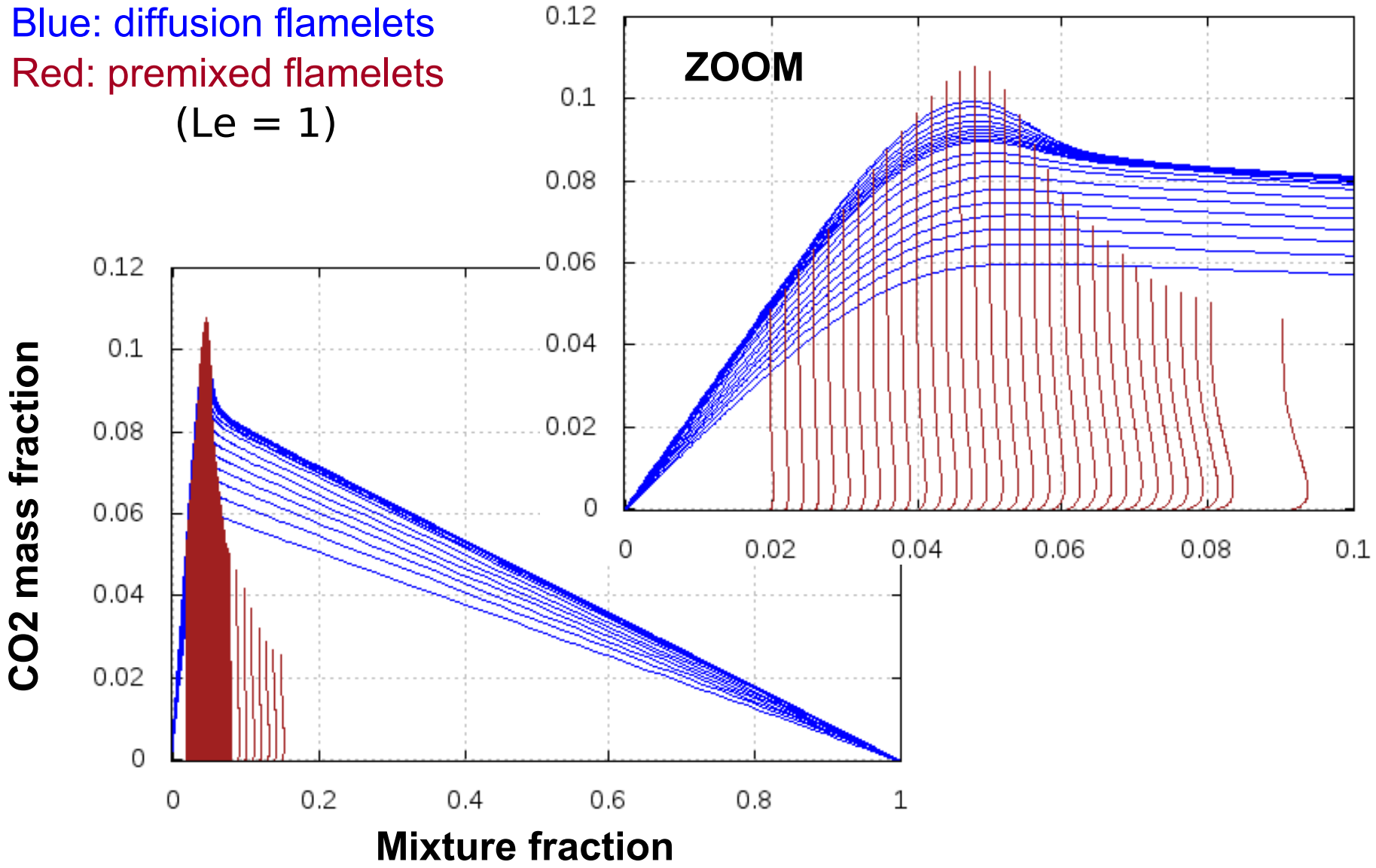


FPI / FGM

Blue: diffusion flamelets

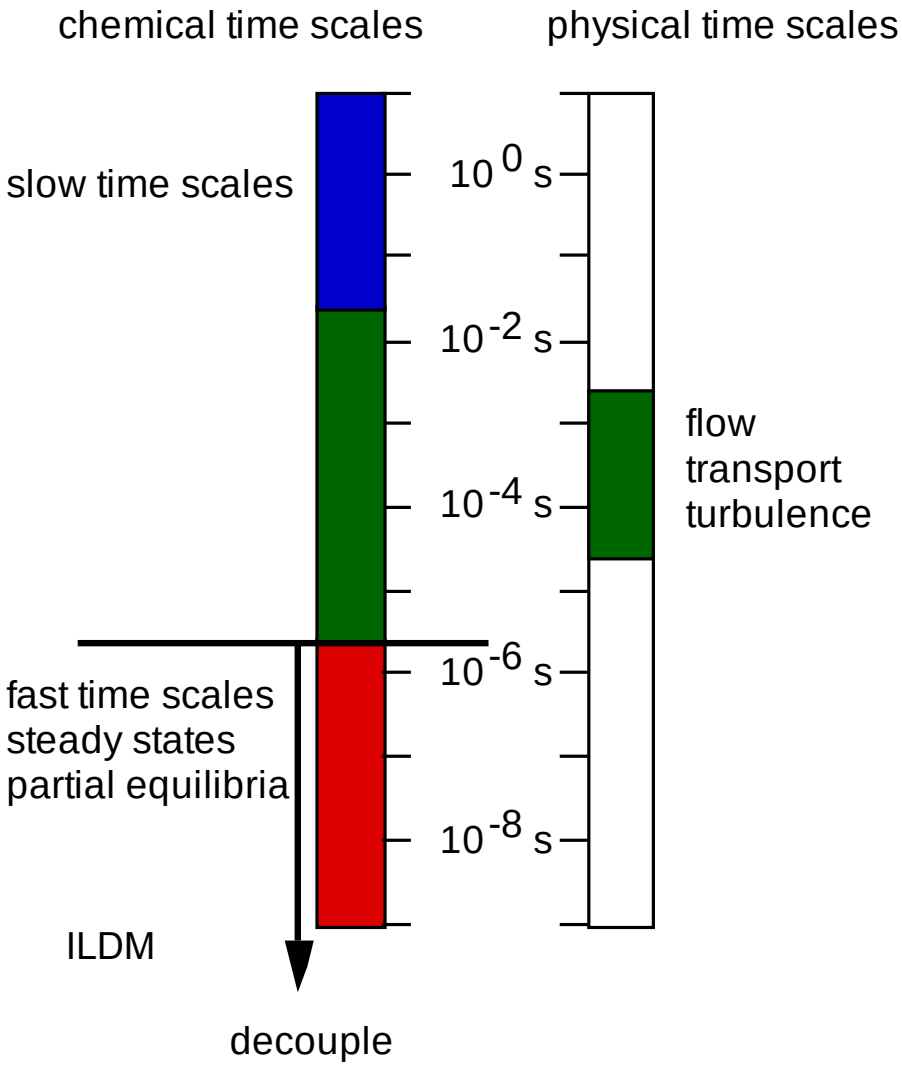
Red: premixed flamelets

(Le = 1)



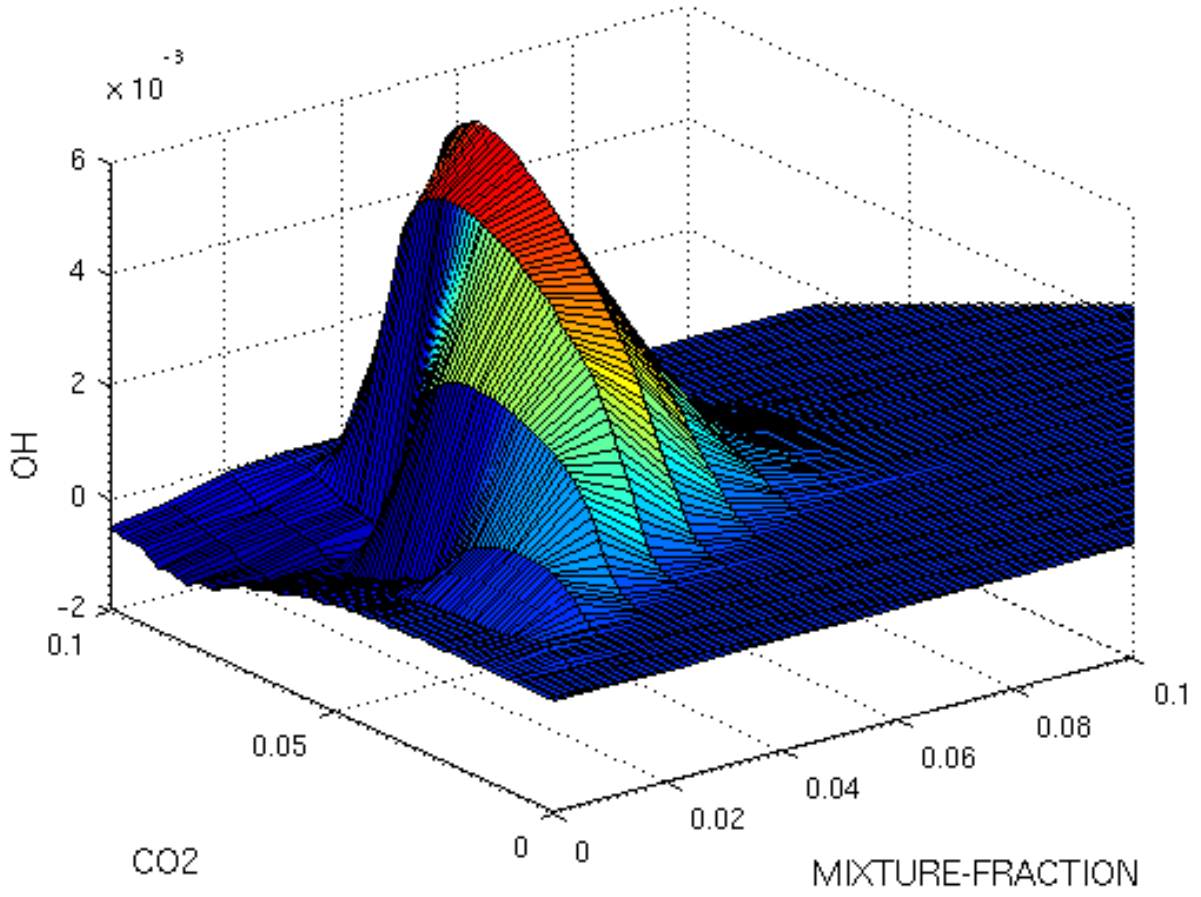
REDIM concept

(Maas and Bykov)

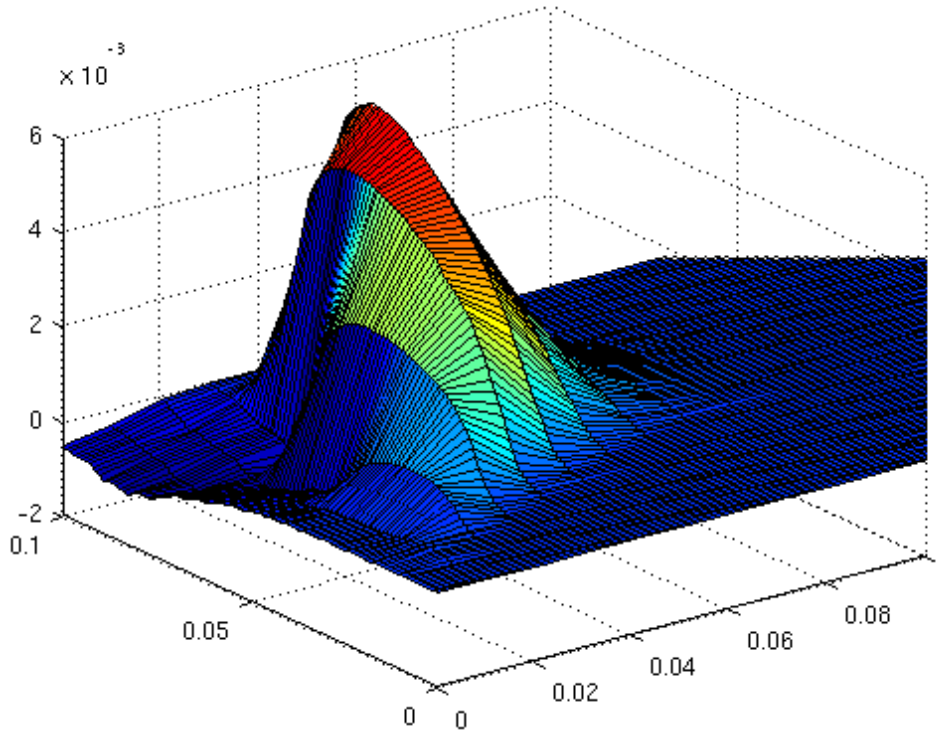


- ILDM decouples only the fast chemical time scales
- REDIM allows in addition to decouple slow chemical processes
  - Domain of slow chemistry: REDIM identifies in principle minimal surfaces caused by diffusion processes
  - Domain of fast chemistry: REDIM is close to ILDM
  - Intermediate range: REDIM accounts for the coupling of reaction and diffusion

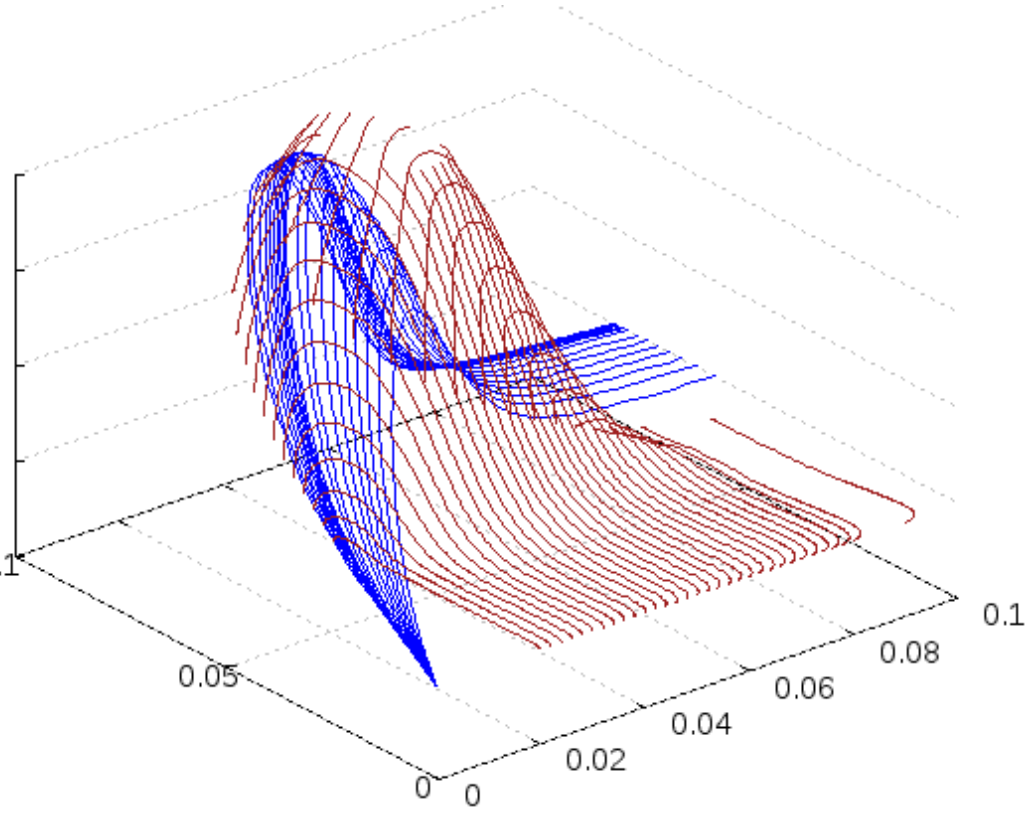
OH profile on REDIM



OH profile on REDIM and FPI



REDIM



FPI / FGM
(Le=1)

REDIM and FPI/FGM

Hidden assumptions on the underlying flame structure: on the gradients in physical space (scalar dissipation).

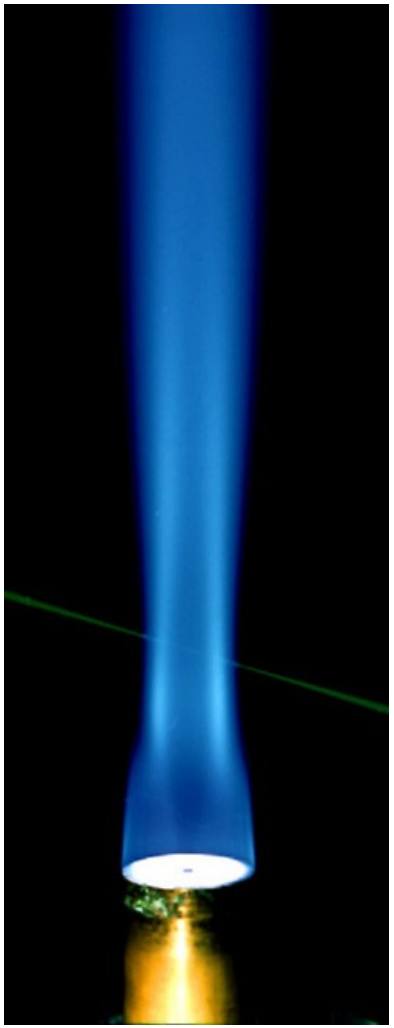
A priori validation by comparing with experimental results:

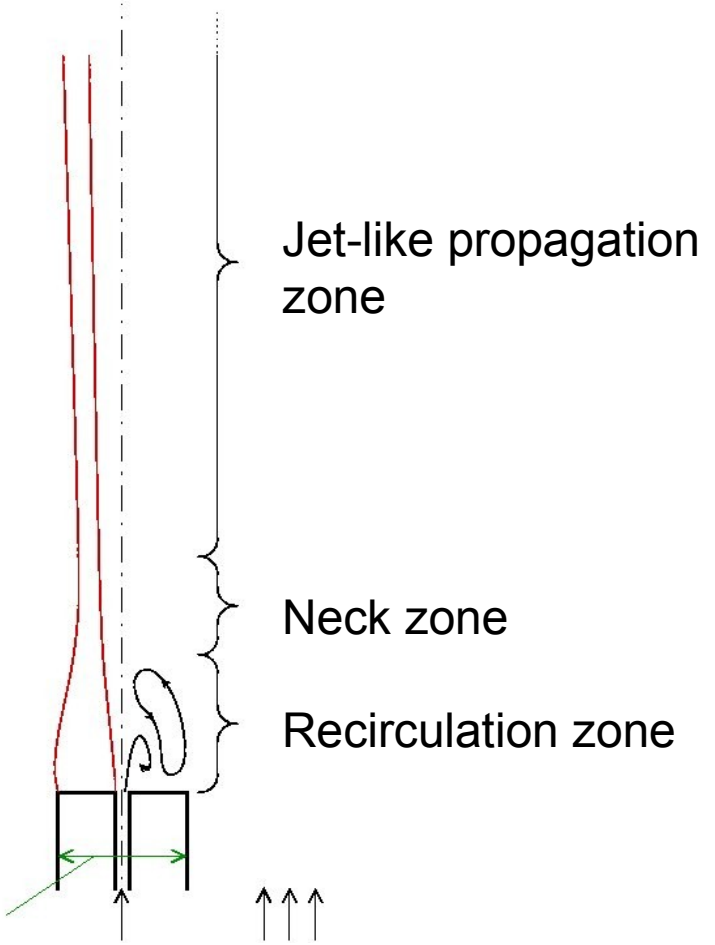
- a priori validation of the 2D-manifold
- a priori study of the possible independence of the marginal PDFs:

$$f_{Z,c} = f_Z \cdot f_c \, ?$$

HM1/HM3 Sydney bluff-body flames

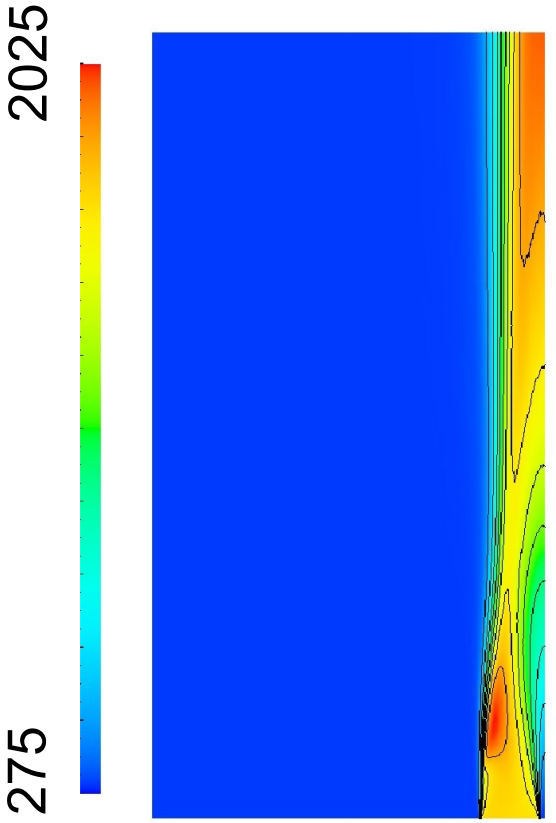
(together with B. Merci, D. Roekerts and U. Maas)





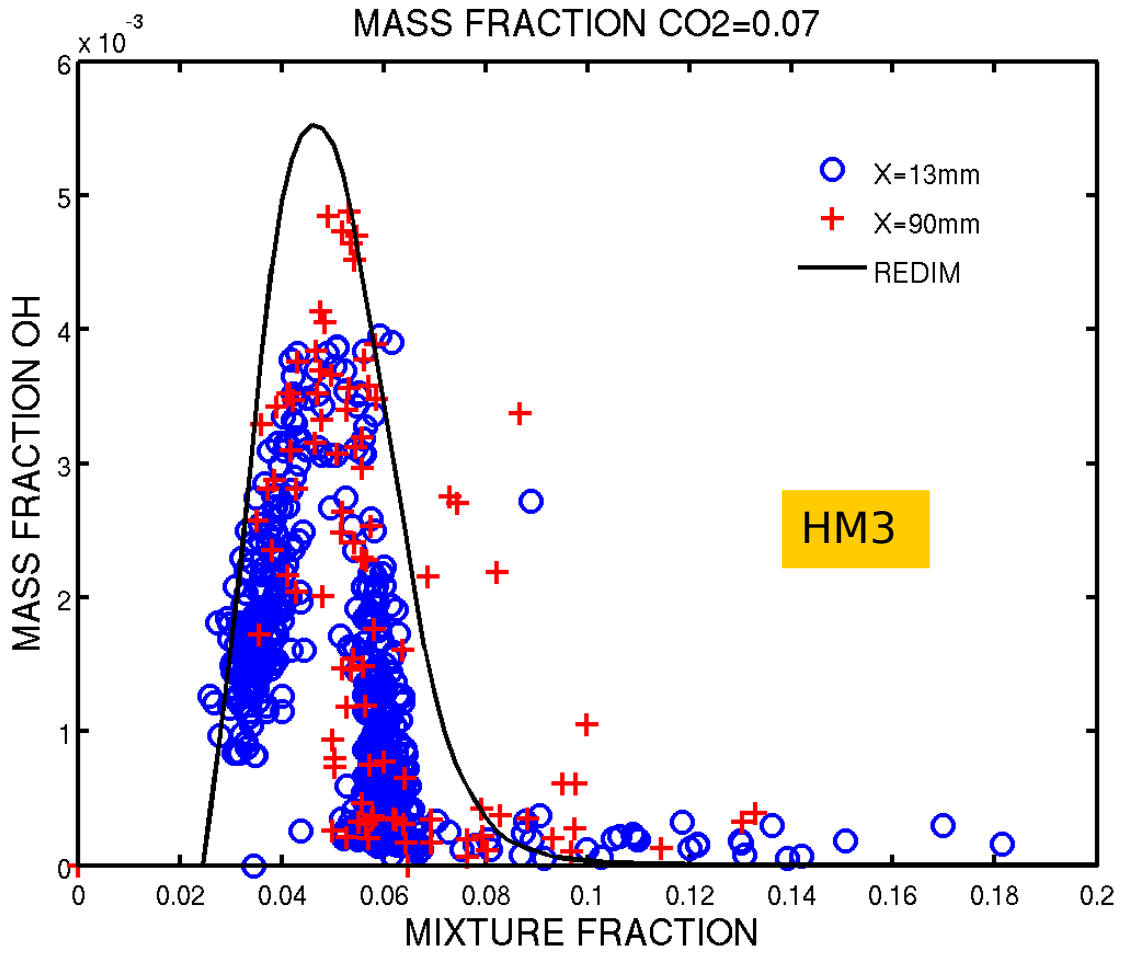
HM1 → 118m/s 40m/s

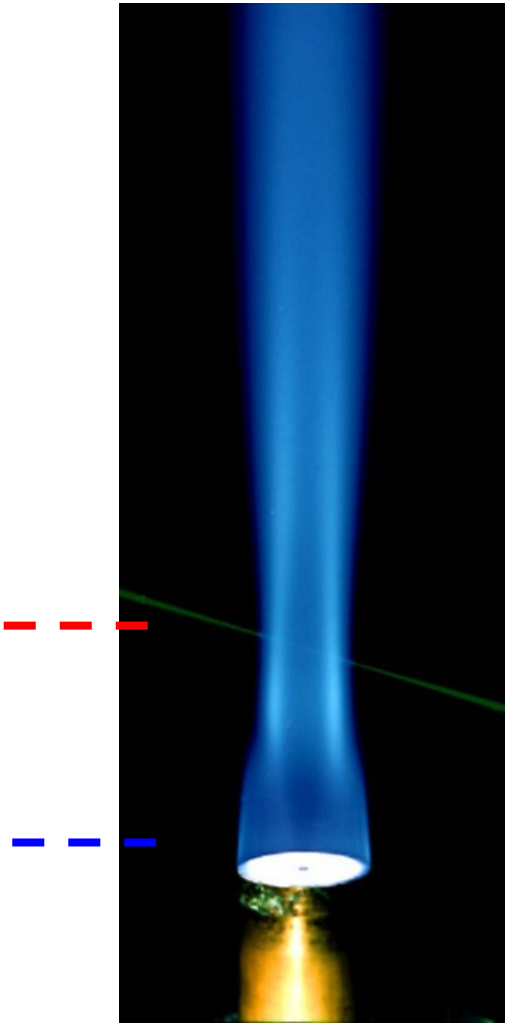
HM3 → 214m/s



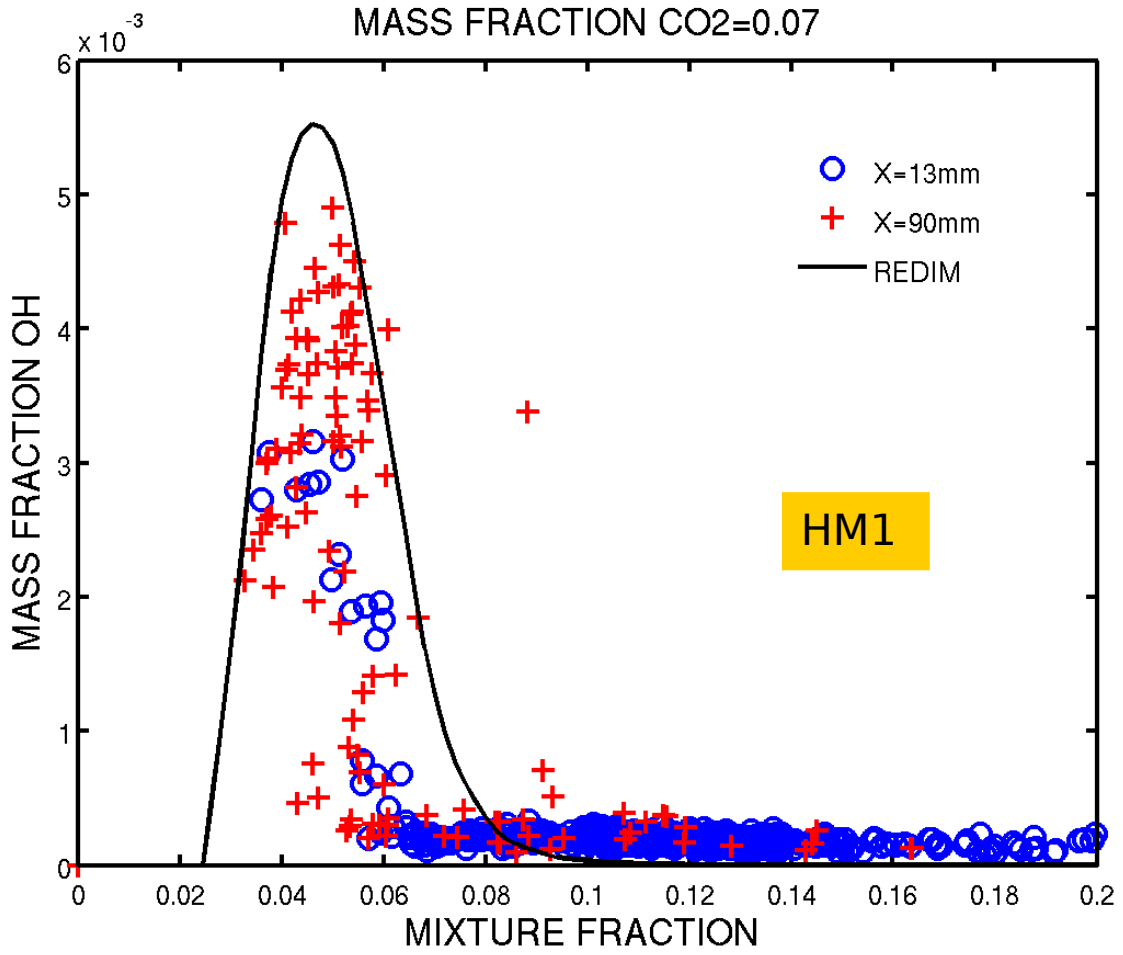
Mean temperature from the ensemble of particles

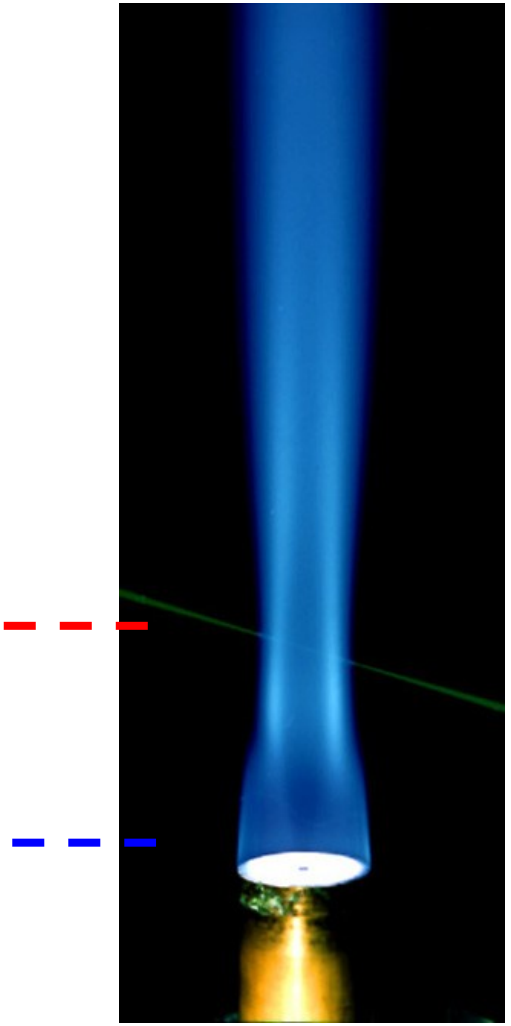
A priori analysis: are the single shot experimental data lying on the calculated REDIM?



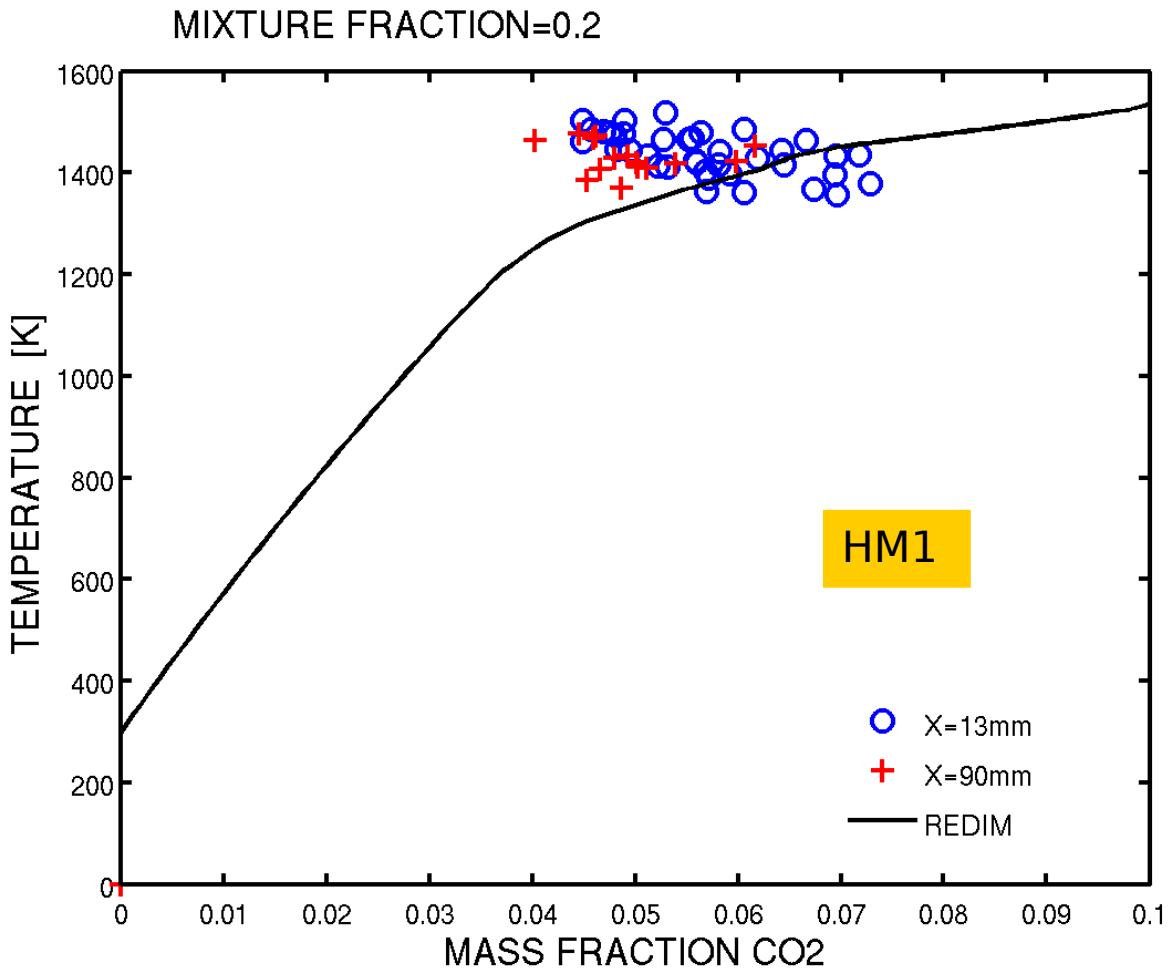


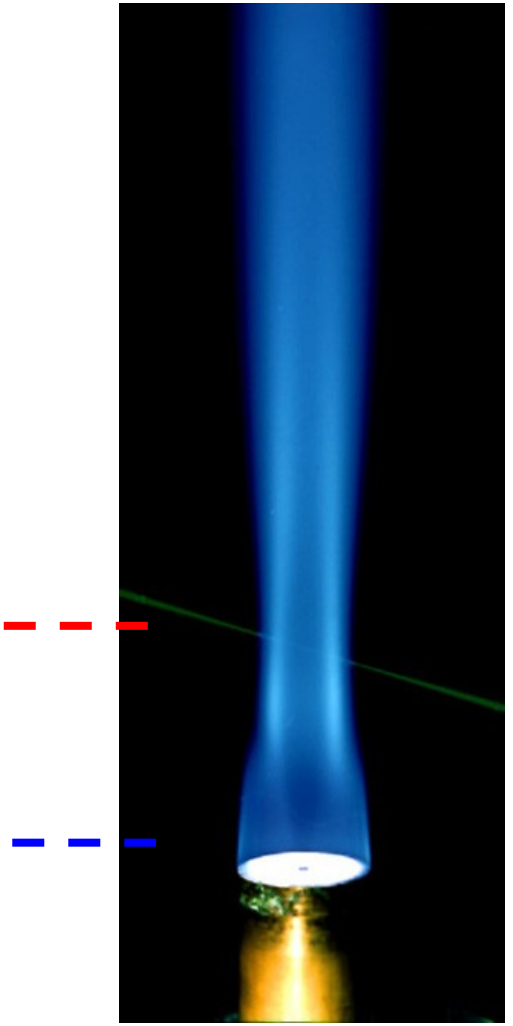
A priori analysis : OH in HM1



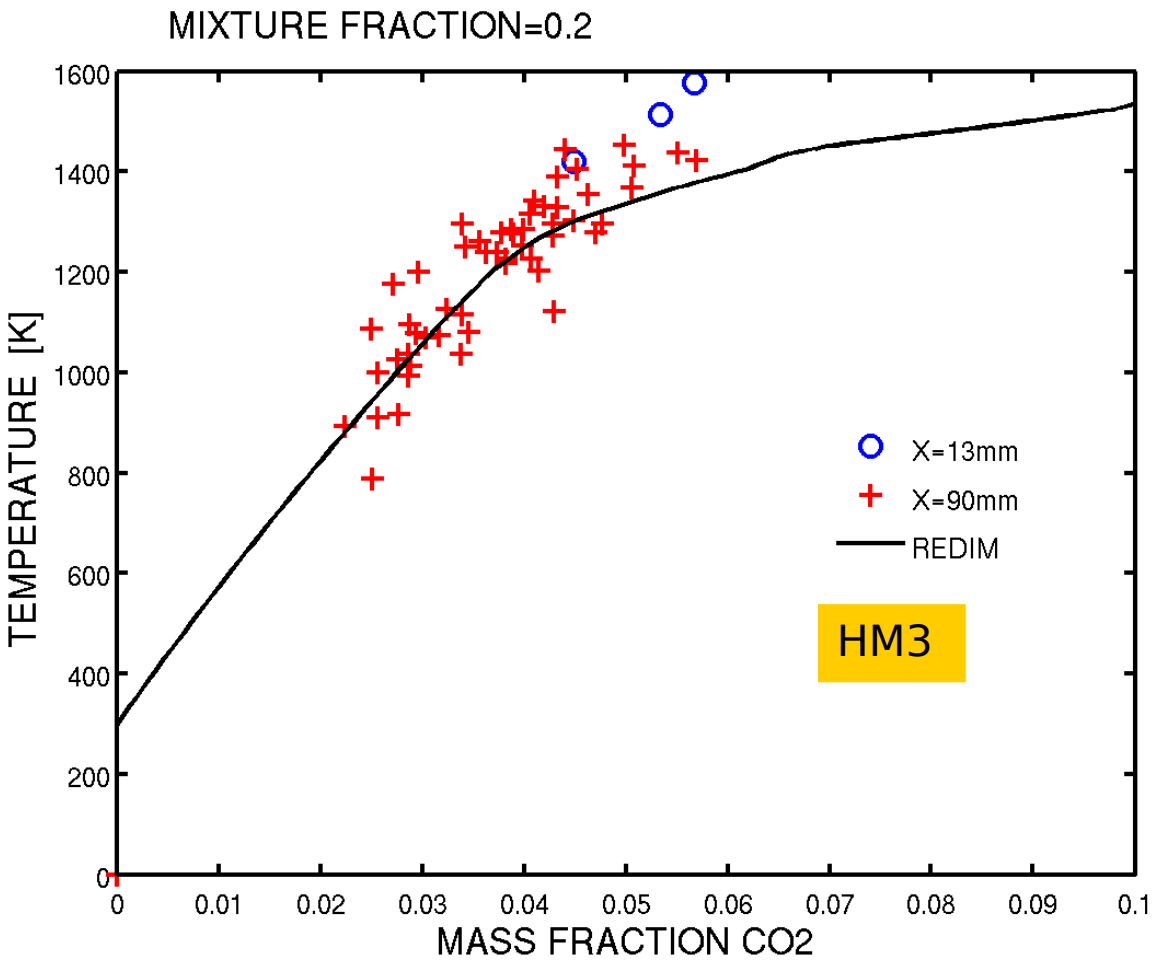


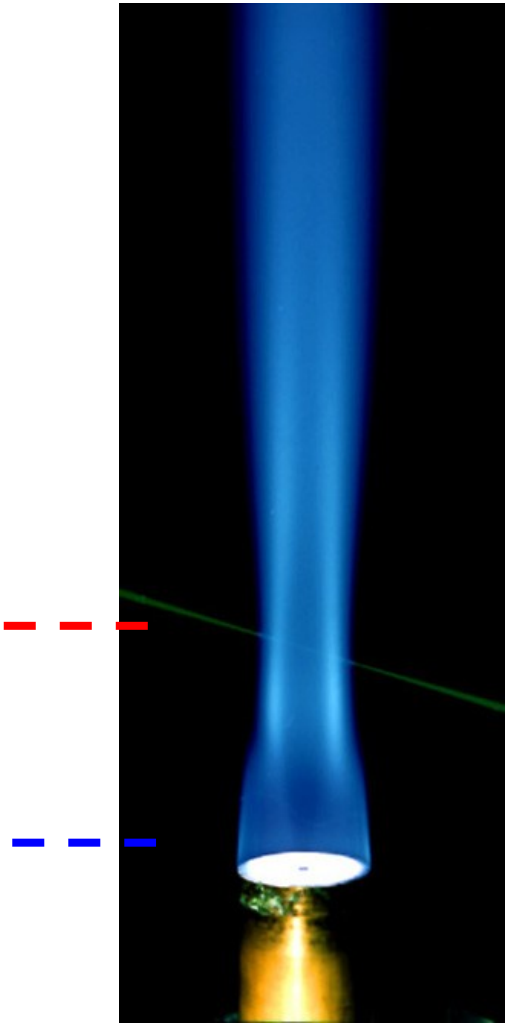
A priori analysis: temperature in HM1





A priori analysis: temperature in HM3



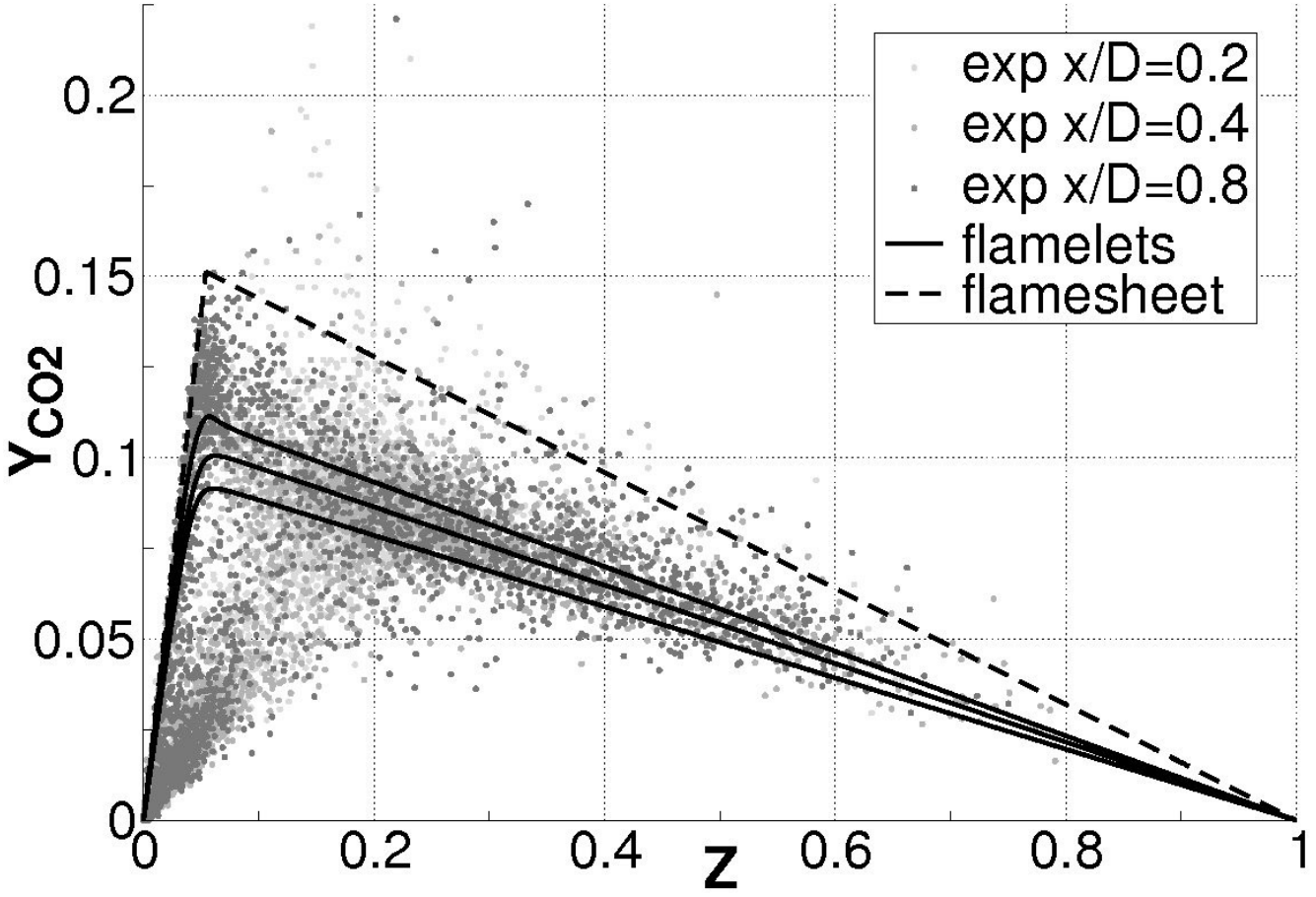


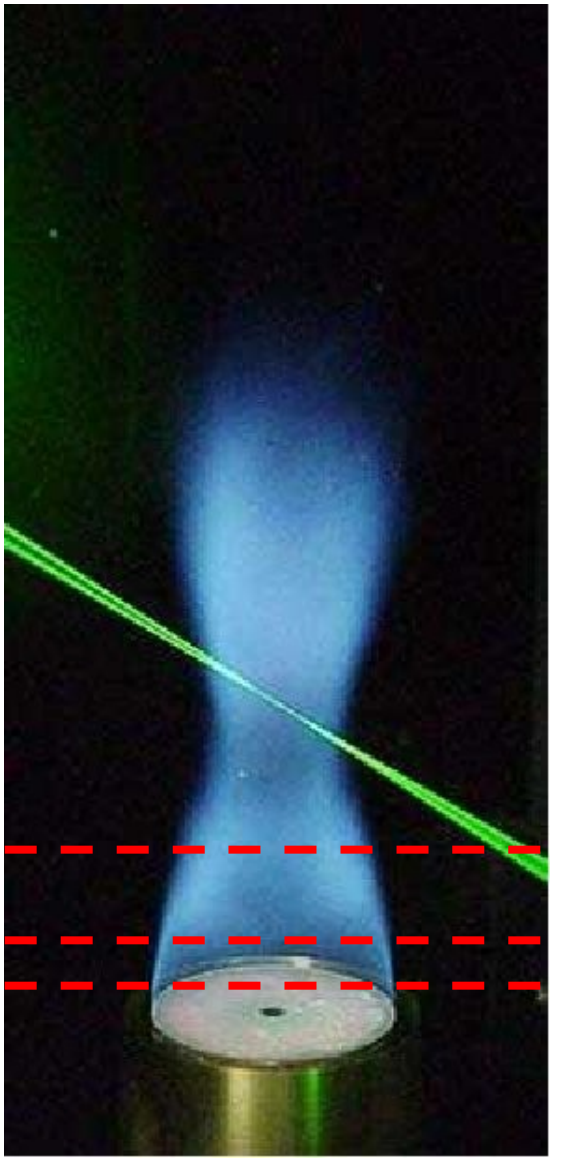
REDIM

- REDIM technique allows to eliminate fast modes in the joint process of chemistry and diffusion.
- *A priori* analysis: experimental data show more complexity than described by the current two-dimensional REDIM
- Under-prediction and over-prediction of mean temperature comes together with under- and over-prediction of CO_2 mass fraction
- For HM3 less good results than for HM1, due to stronger local extinction (i.e. stronger turbulence-chemistry interaction)
- Next steps: include effects of differential diffusion in manifold and/or increase manifold dimension to three

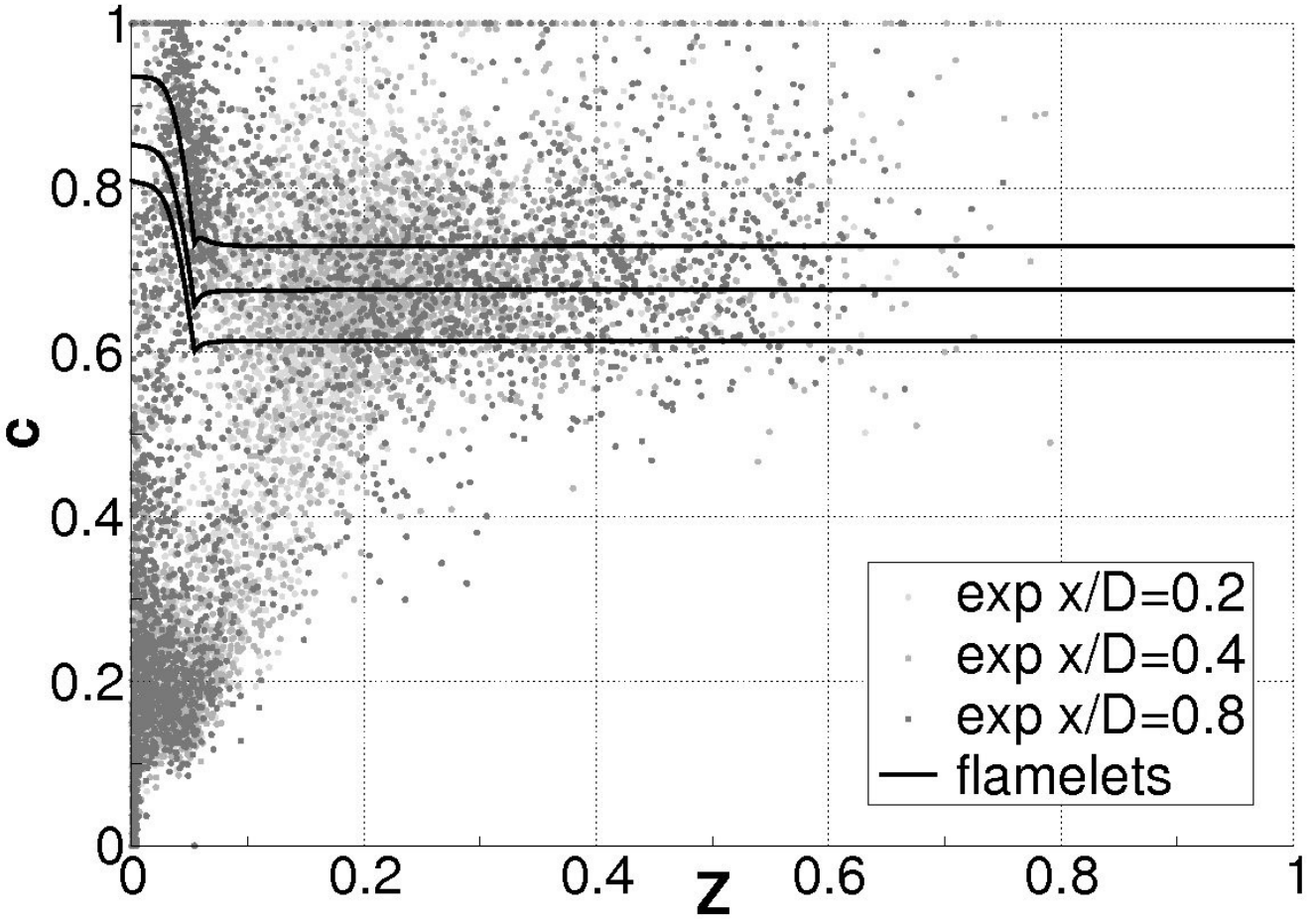
Sydney swirling flame SM1

(together with R. De Meester and B. Merci)



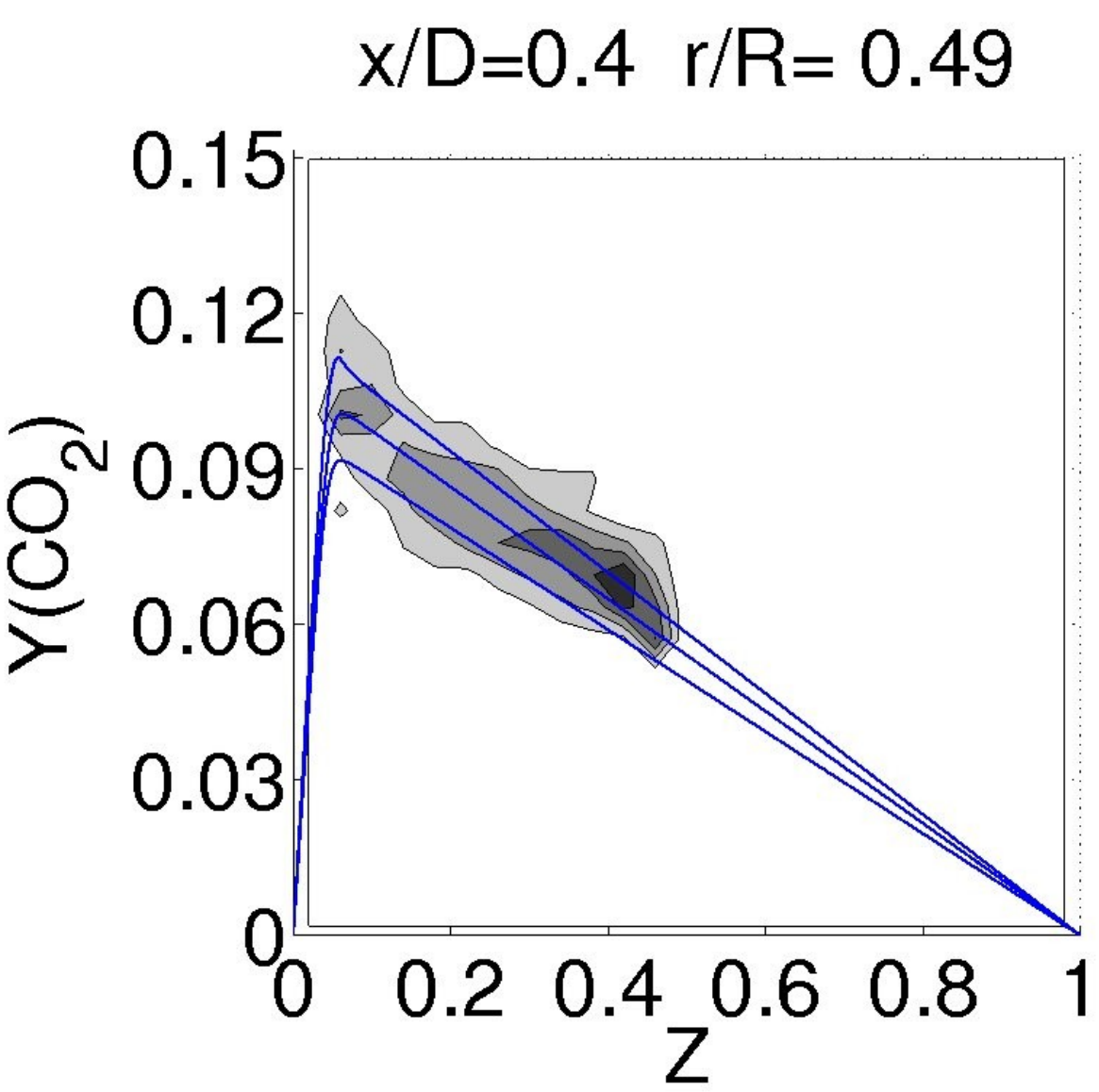


$$c(Z, Y_{CO2}) = \frac{Y_{CO2}}{Y_{CO2}^{fs}(Z)}$$



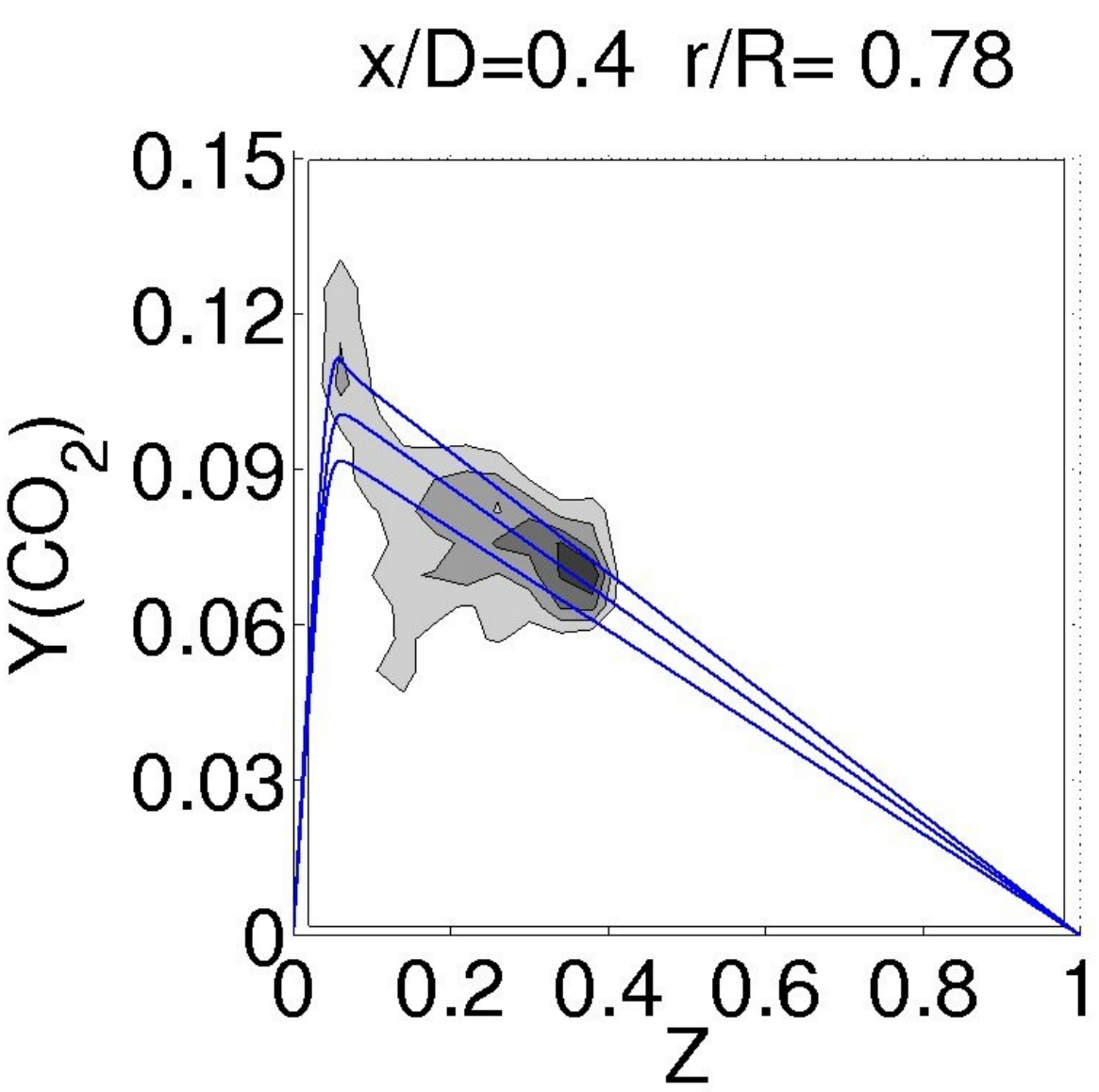
$$P(Z, Y_{CO2}) = P(Z).P(Y_{CO2}|Z)$$

$P(Y_{CO2}|Z)$



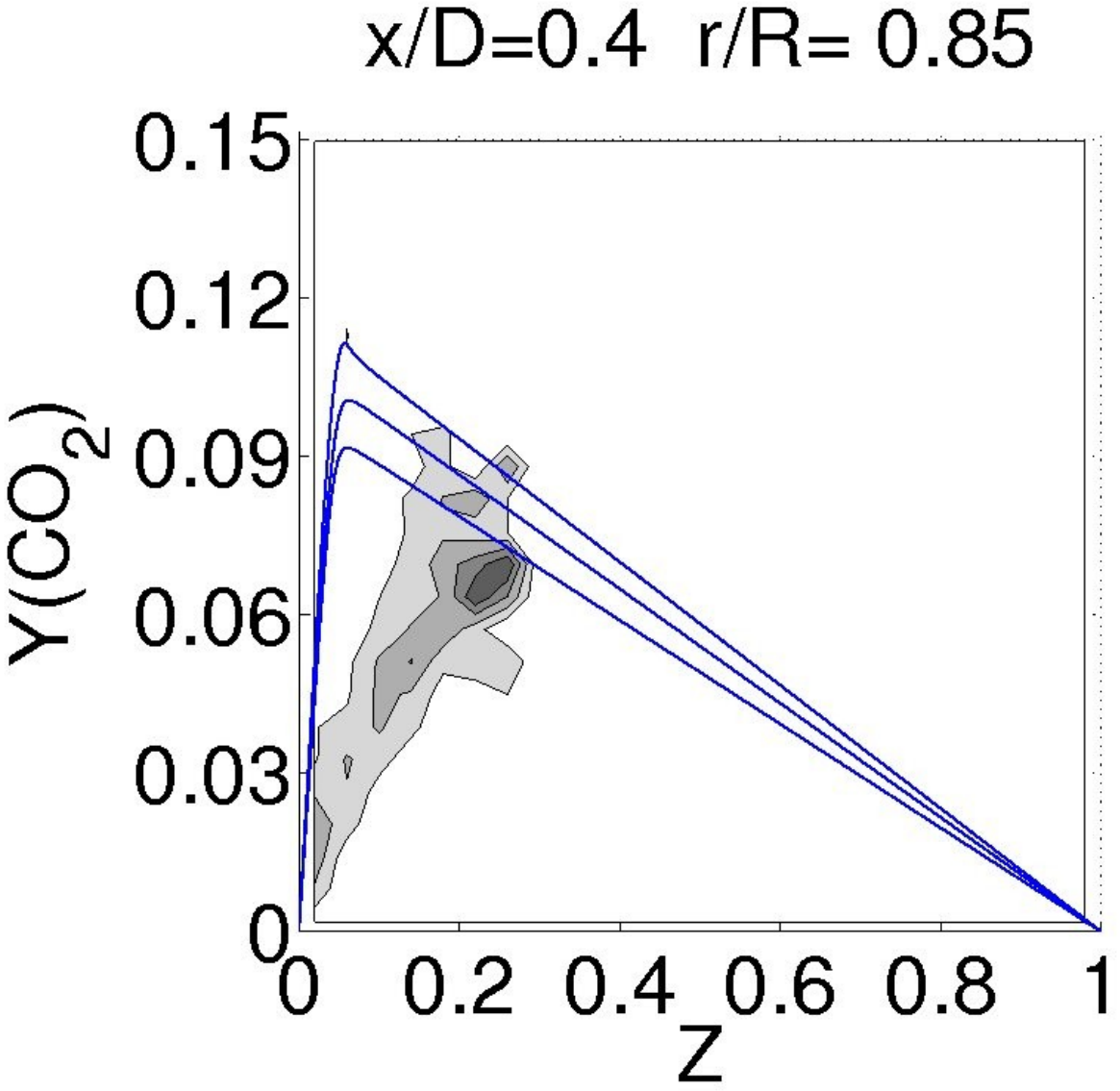
$$P(Z, Y_{CO2}) = P(Z) . P(Y_{CO2}|Z)$$

$P(Y_{CO2}|Z)$



$$P(Z, Y_{CO2}) = P(Z).P(Y_{CO2}|Z)$$

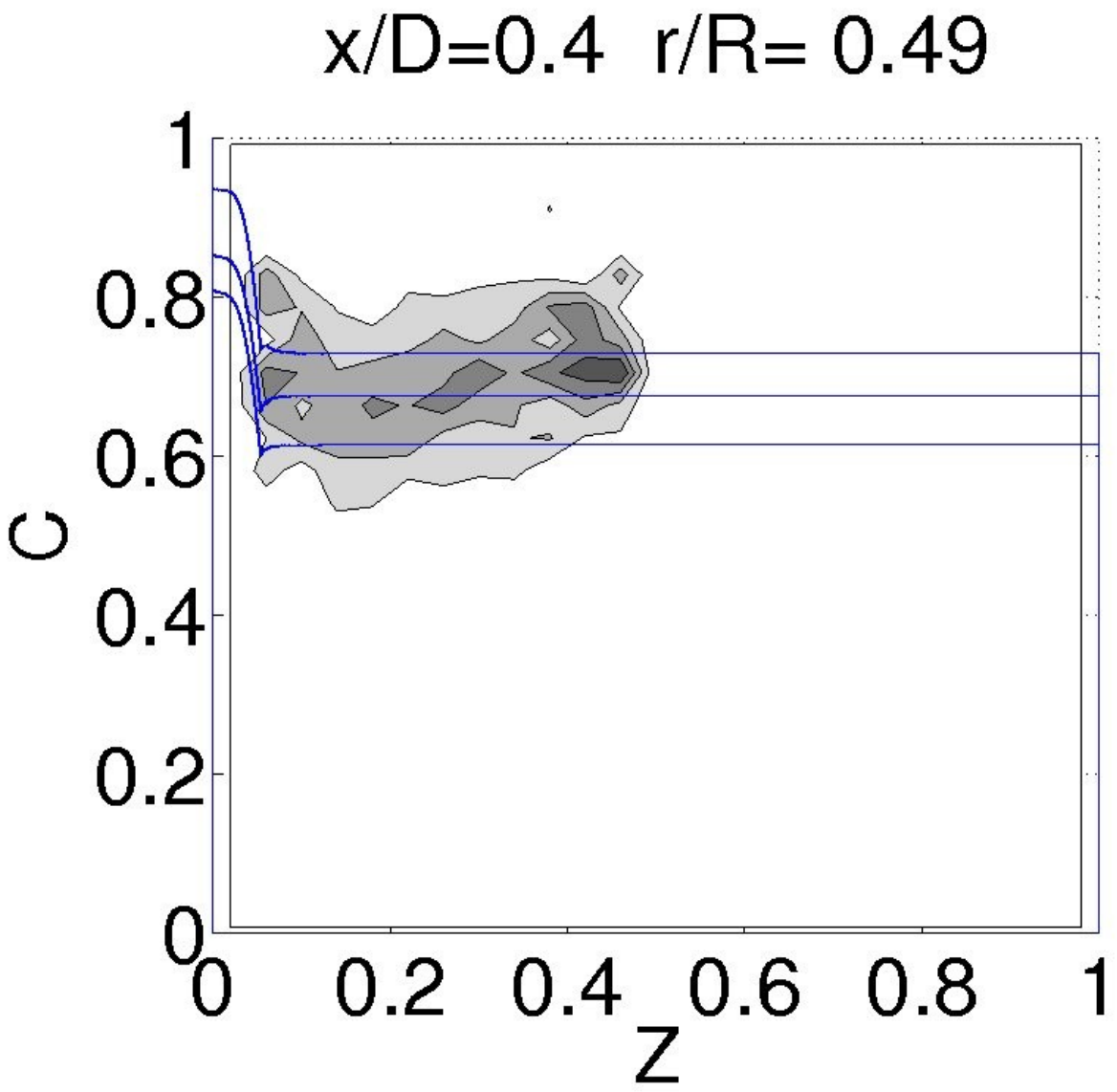
$P(Y_{CO2}|Z)$



$$c(Z, Y_{CO2}) = \frac{Y_{CO2}}{Y_{CO2}^{fs}(Z)}$$

$$P(Z, c) = P(Z) . P(c|Z)$$

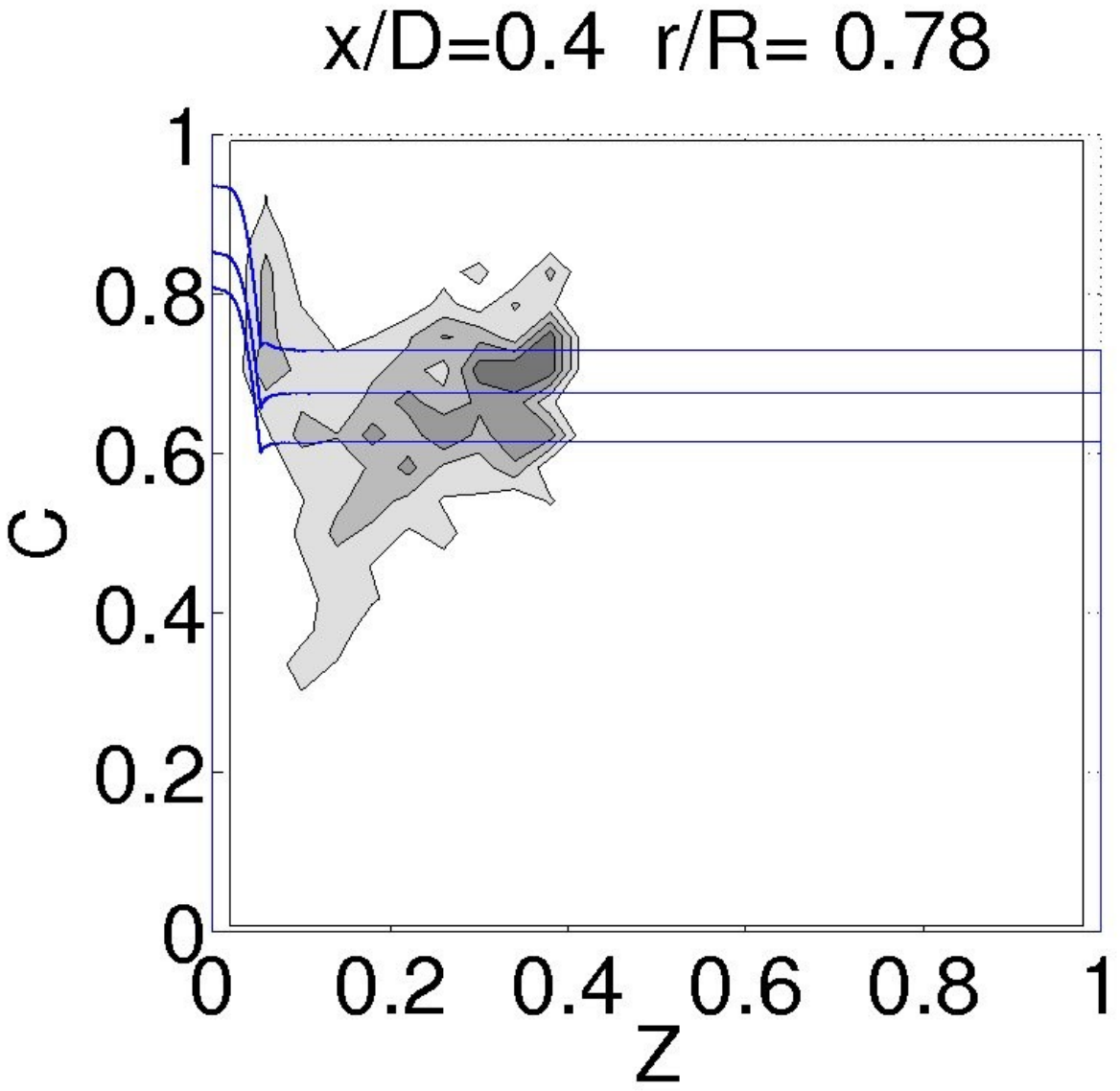
$P(c|Z)$



$$c(Z, Y_{CO2}) = \frac{Y_{CO2}}{Y_{CO2}^{fs}(Z)}$$

$$P(Z, c) = P(Z) . P(c|Z)$$

$P(c|Z)$

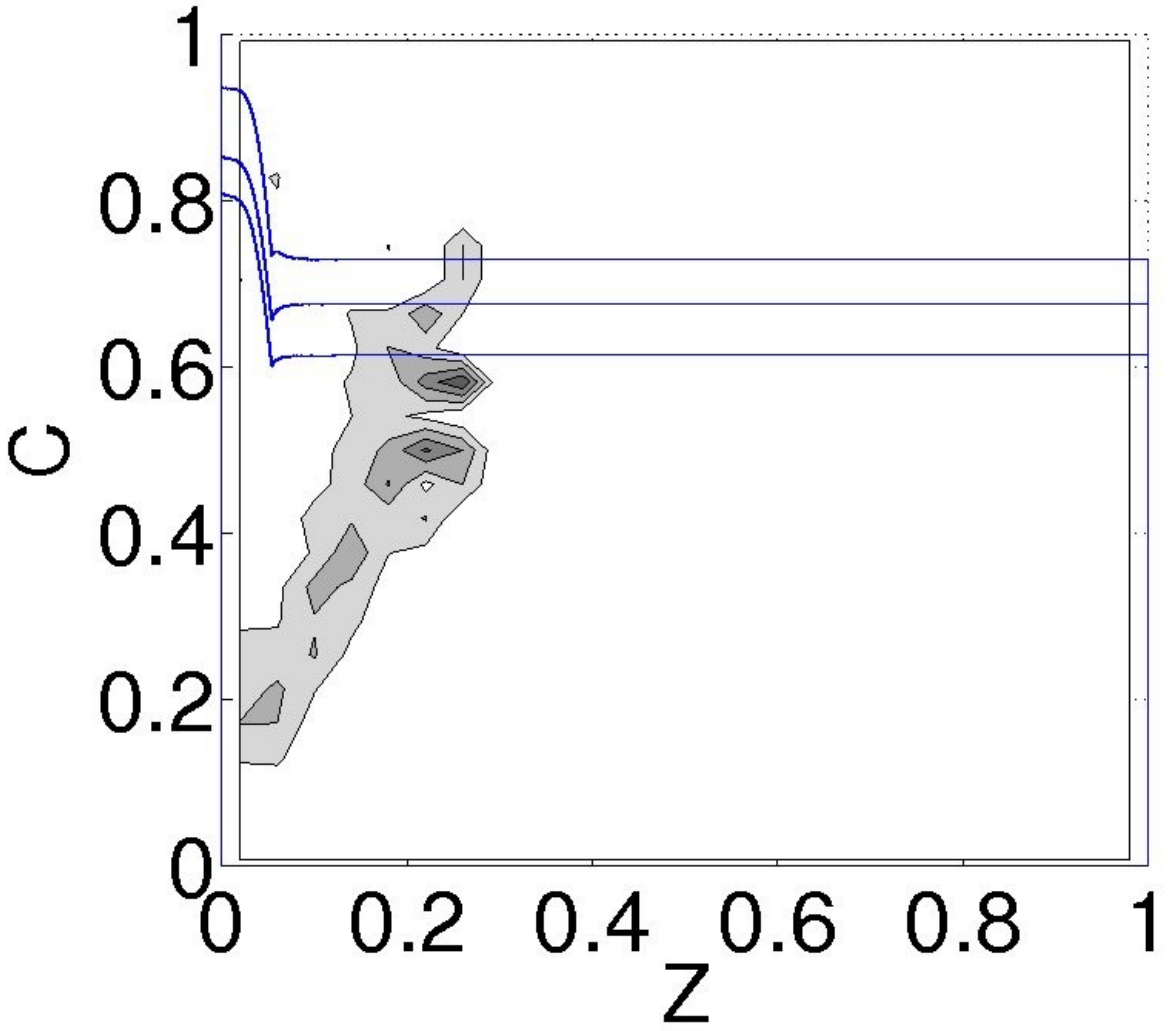


$$c(Z, Y_{CO2}) = \frac{Y_{CO2}}{Y_{CO2}^{fs}(Z)}$$

$$P(Z, c) = P(Z) . P(c|Z)$$

$P(c|Z)$

x/D=0.4 r/R= 0.85



Sydney swirling flame SM1

A priori study of experimental data:

- we identified “flamelet structures”
 → useful to think of what kind of 2D-manifold to use

- at some points: statistical independence of Z and the chosen c... but in general not the case
 → problem with presumed PDF in RANS
 → less problematic in well-resolved LES when subgrid fluctuations of Z are small

- other issue about c in presumed-PDF methods:
 → can we write the transport equations of the mean and variance of c?

Conclusions

Mixture fraction + progress variable
= “minimum” representation of general practical flames

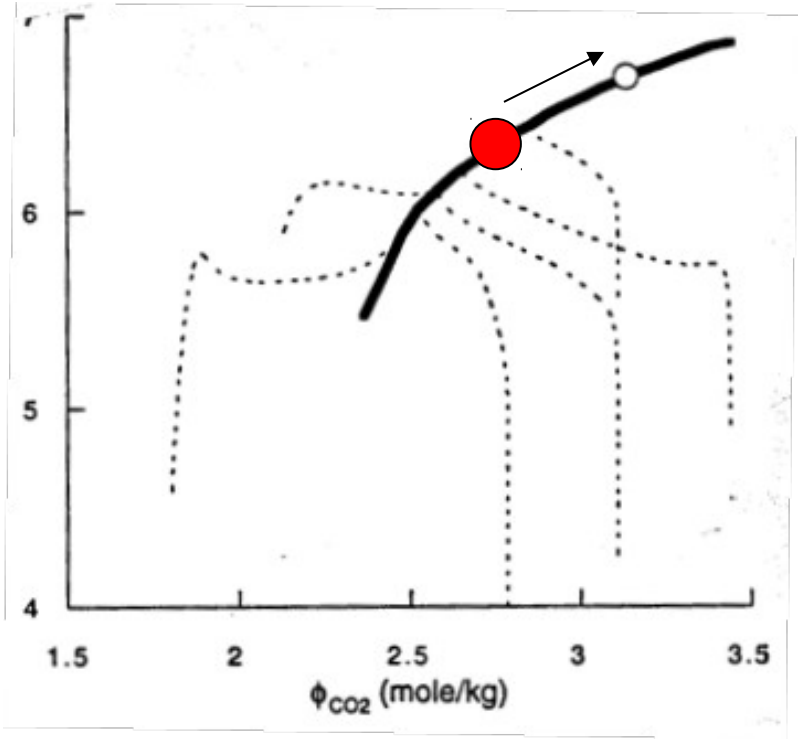
Assumption on the underlying flame structure of the turbulent flame
→ there is an underlying scalar dissipation

Need the joint PDF of Z and c.
→ presumed PDF:
- Can we write and solve equations for the mean and variance of c?
- Is it correct to assume statistical independence? (not really problematic in well resolved LES)

Two variables enough?..
→ radiation, auto-ignition, differential diffusion, ...

REDIM

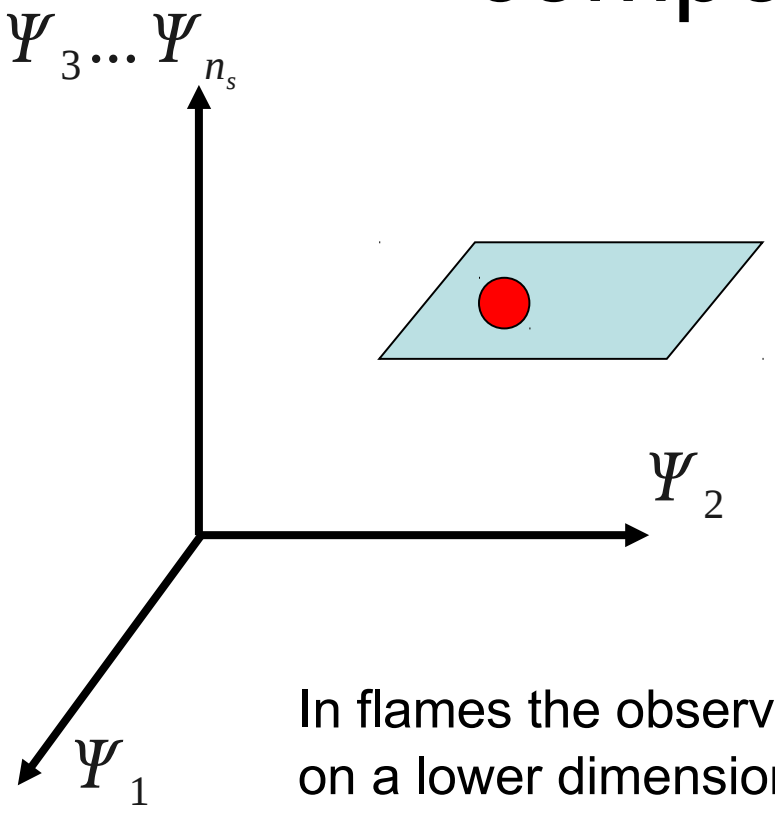
Methane oxidation: ILDM



Dotted: evolution by detailed mechanism

Line: Intrinsic Low-Dimensional Manifold

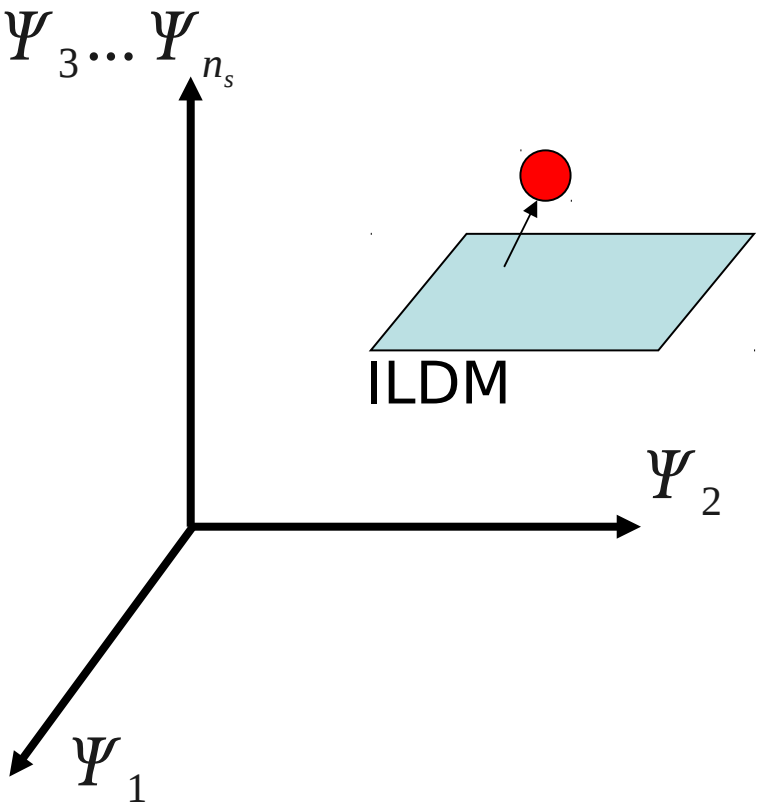
Low-Dimensional Manifolds in composition space

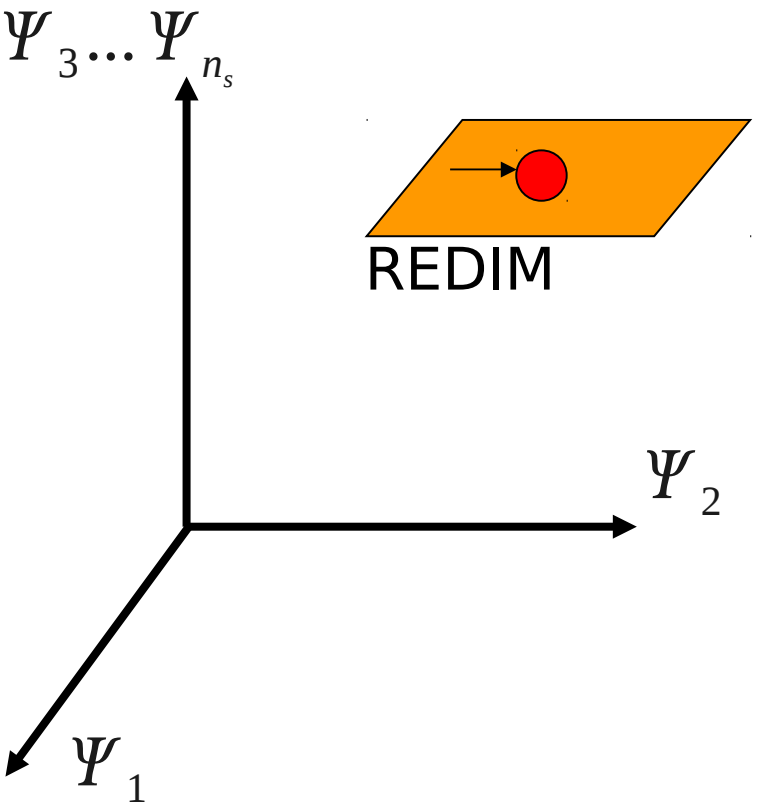


In flames the observed compositions in many cases are located on a lower dimensional subspace of the composition space (confirmed by experiment and by DNS).

This is caused by rapid relaxation of fast chemical processes. Intrinsic low-dimensional manifolds (ILDM) can be determined from the (linearized) chemical rate equations (Maas & Pope 1992)

REDIM



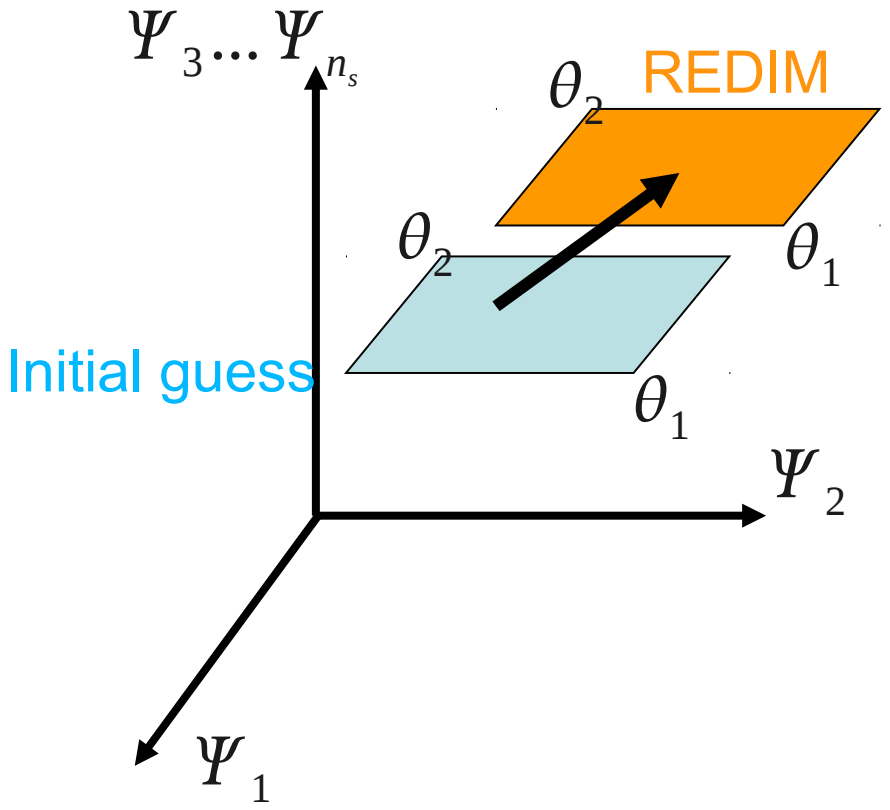


Diffusive processes (in physical space) having similar time scale as the slow chemical processes will move the system away from the states on the ILDM

Is it possible to describe this as a shift of the invariant manifold in composition space, to another manifold called “Reaction-diffusion-manifold” ?

REDIM obtained as steady state of an evolution equation for the manifold

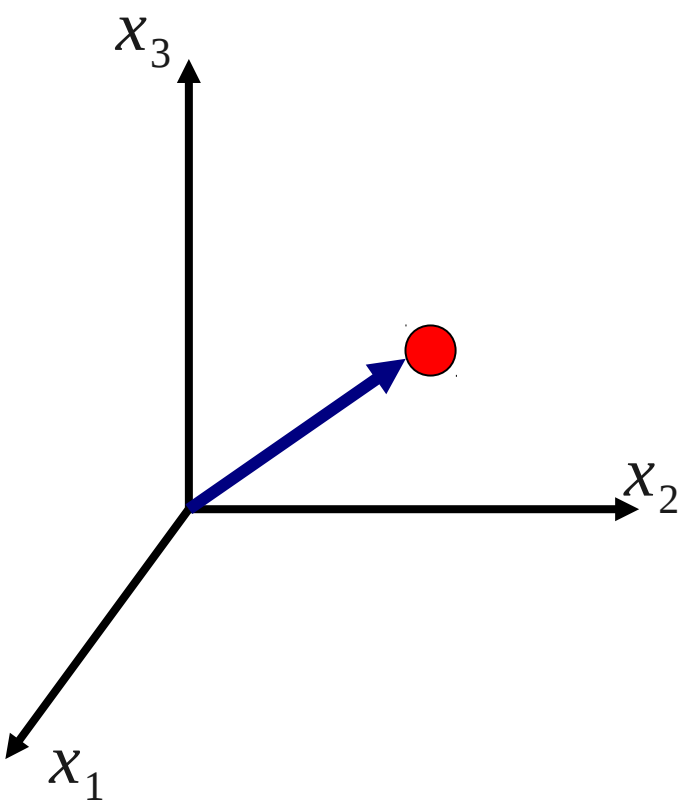
(Bykov & Maas, CTM 2007)



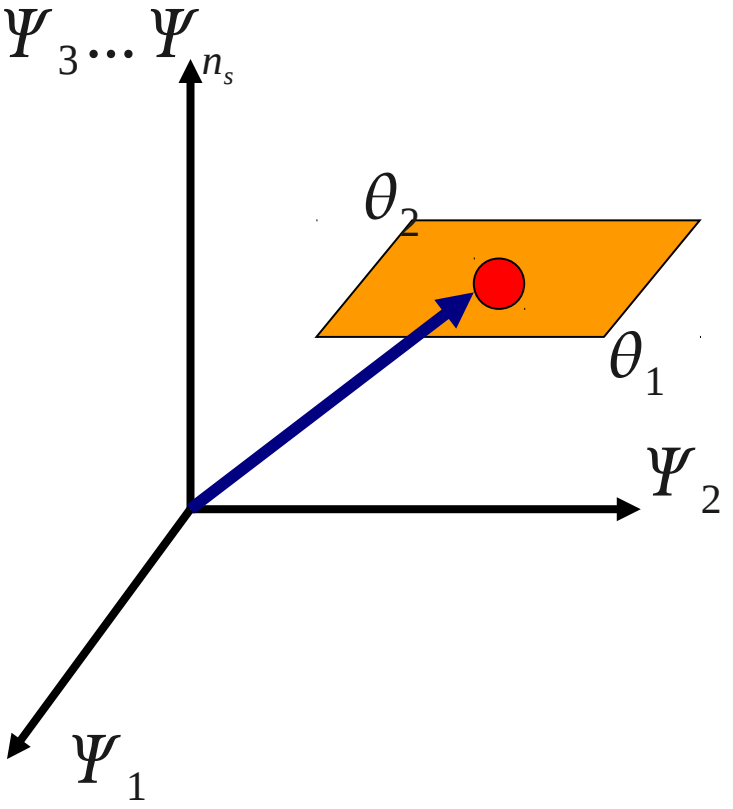
Position of manifold in composition space given by $\Psi(\vec{\theta})$

Where $\vec{\theta}$ is a coordinate system on the manifold

Two points of view on scalar fields



$\Psi(\vec{x},t)$



$\Psi(\vec{\theta})$

REDIM

Scalar transport equation in physical space (Fick with constant D)

$$\Psi(\vec{x},t) \qquad \frac{\partial \Psi}{\partial t} = -U.\nabla\Psi + \frac{D}{\rho}\nabla.\nabla\Psi + S(\Psi)$$

Scalar transport equation as movement of manifold in composition space (manifold points still connected to physical points):

$$\Psi\left[\theta(\vec{x}),\tau\right]$$

$$\frac{\partial \Psi}{\partial \tau} = -U\frac{\partial \theta_l}{\partial x}\frac{\partial \Psi}{\partial \theta_l} + \frac{D}{\rho}\frac{\partial \theta_l}{\partial x}\frac{\partial^2 \Psi}{\partial \theta_l \partial \theta_m}\frac{\partial \theta_m}{\partial x} + S(\Psi) + \ldots$$

convection (crossed out) diffusion reaction

An initial estimate $\Psi^0 = \Psi^0(\theta)$ is needed, e.g. an extended ILDM.

Pessimist: seems case-dependent ← gradient in physical space
Optimist: let us hope for a weak sensitivity to the value of this gradient estimate from typical laminar flamelet results

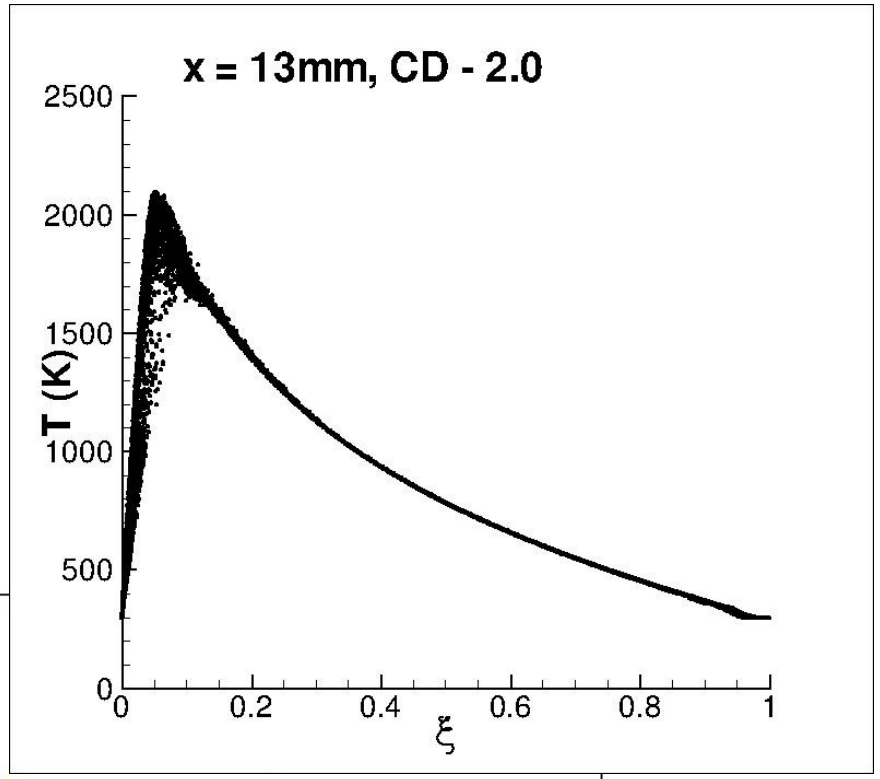
HM1/HM3: construction of a REDIM

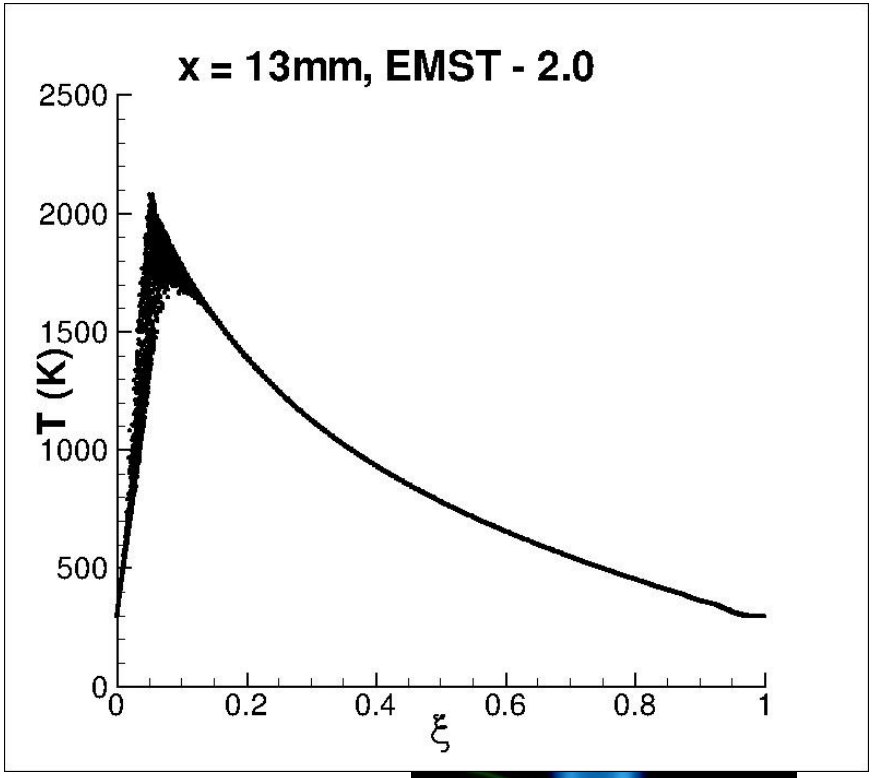
- use detailed reaction mechanism of (Warnatz et al. (1996)), with 34 species and 302 reactions
- choose to solve for two-dimensional REDIM
- solve for case of a 50/50 mixture of CH_4/H_2 burning in air at p = 1 atm
- coordinates on the manifold θ : mass fractions of N_2 and of CO_2
- CO_2 describes progress of chemical reaction
- N_2 describes progress of mixing between fuel and air
  Alternatively 'mixture fraction' Z is used.

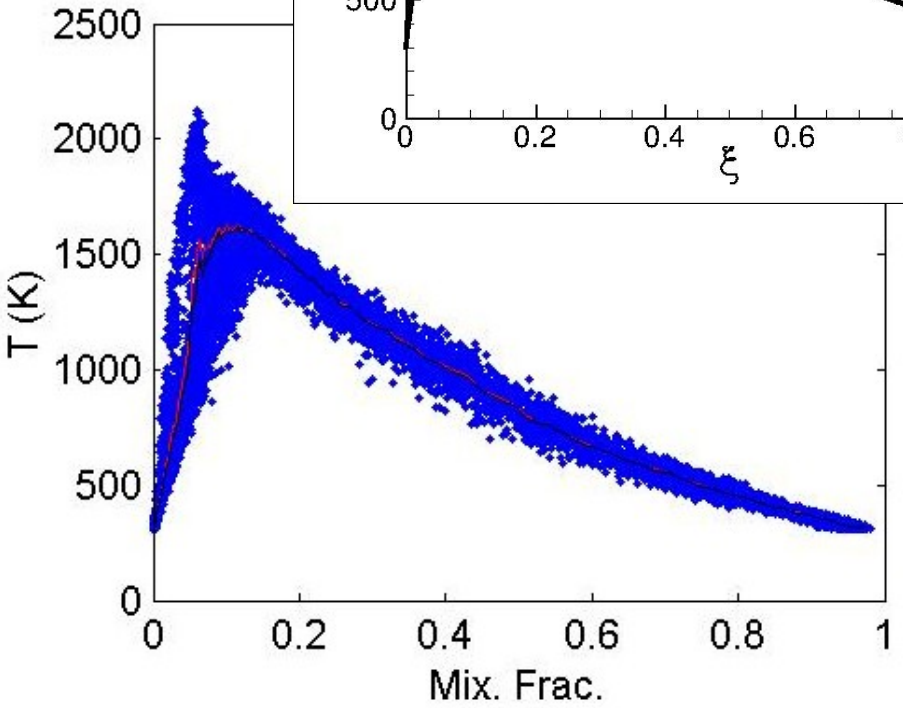
$$Z = 1 - \frac{Y_{N_2}}{Y_{N_2,air}}$$

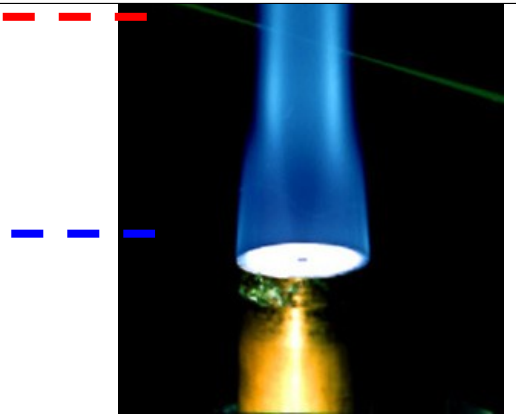
Important special Z-value: 0.05 (stoichiometric mixture)

TPDF results: scatter plots HM1, x=13mm

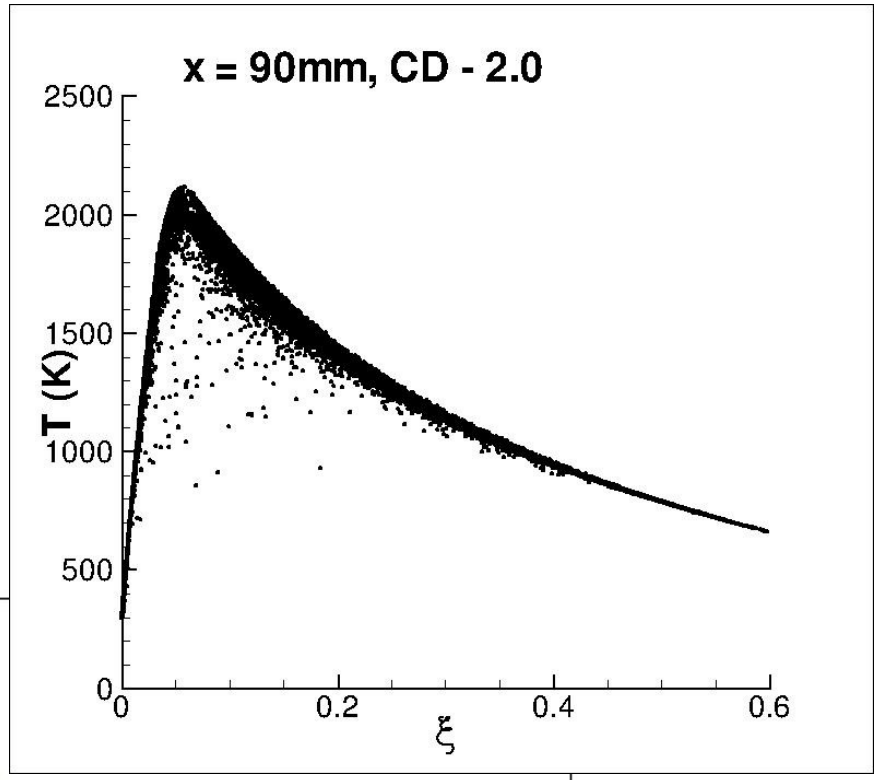


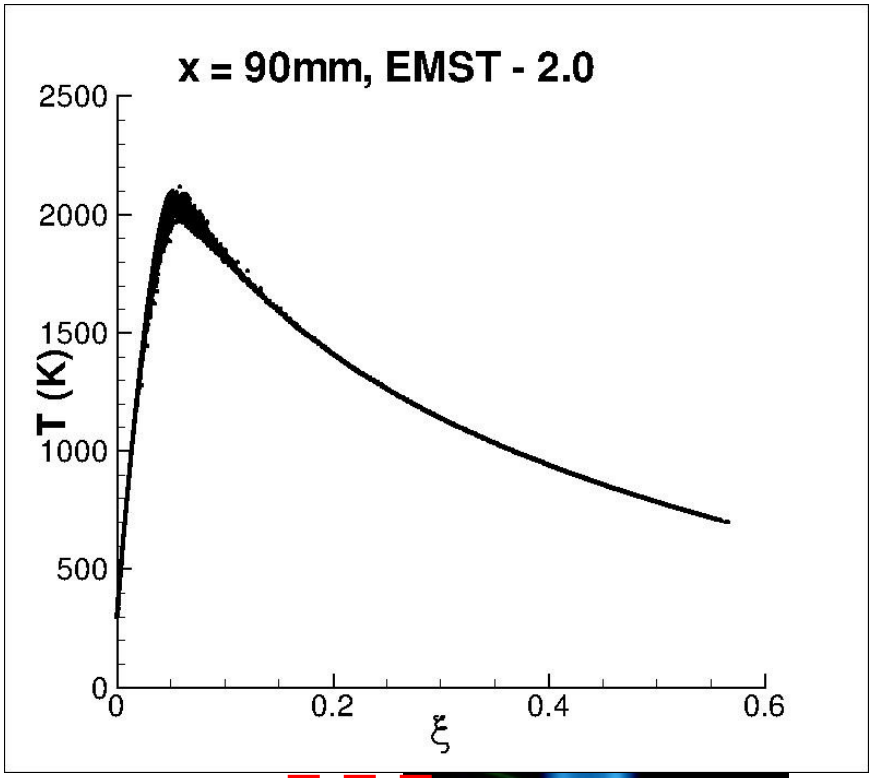


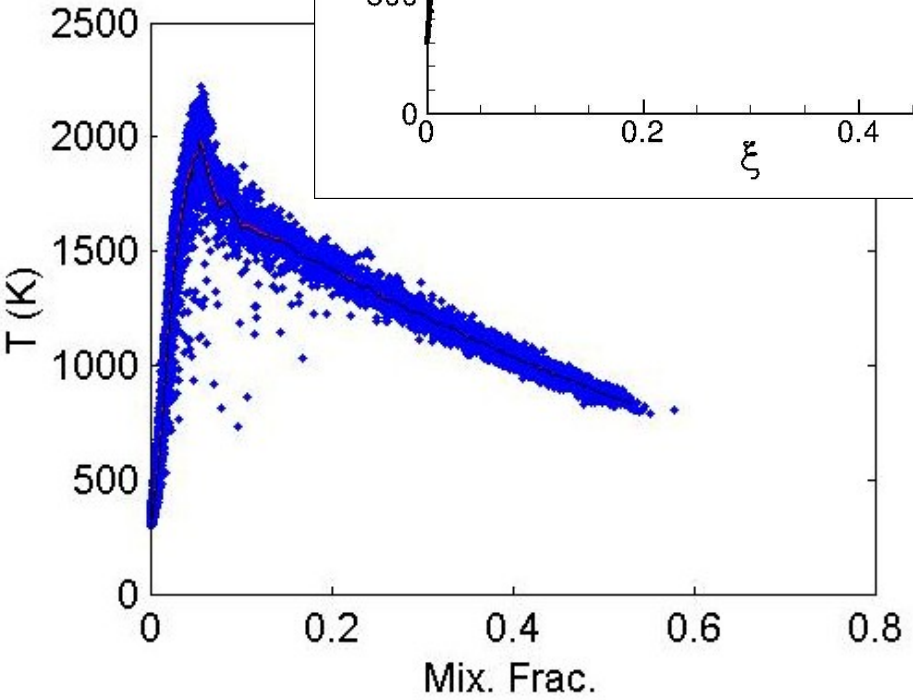


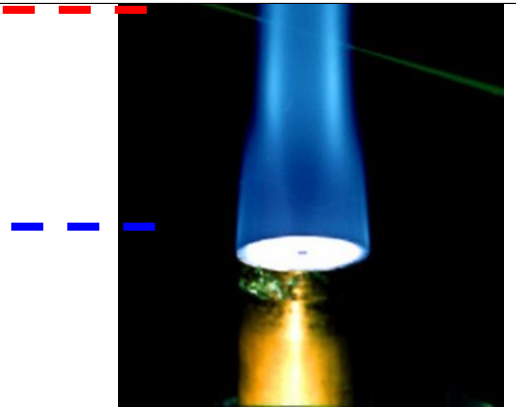


TPDF results: scatter plots HM1, x=90mm

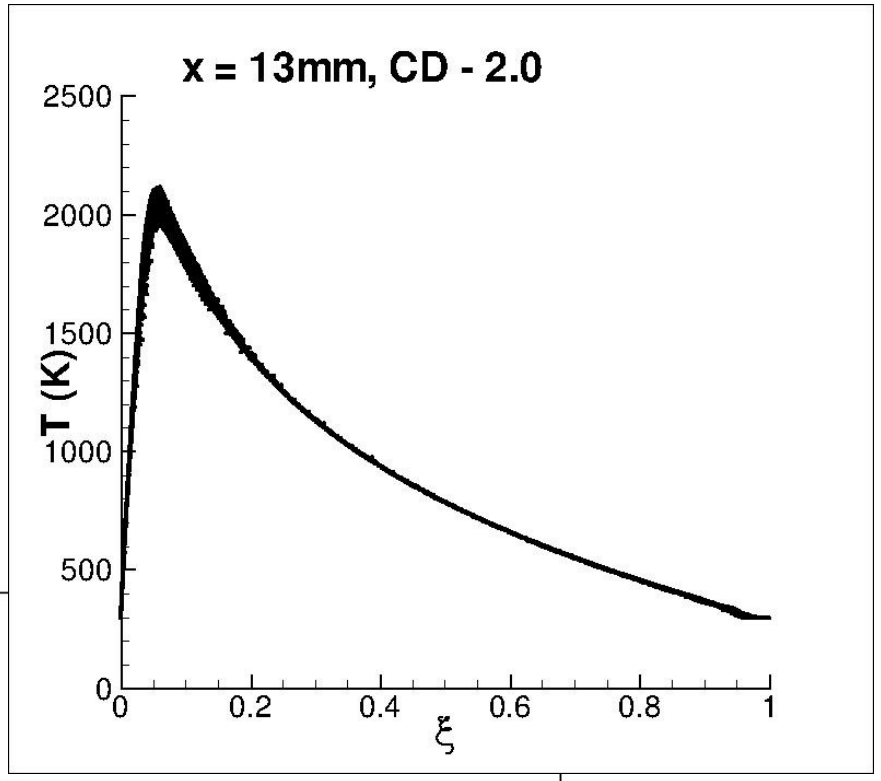


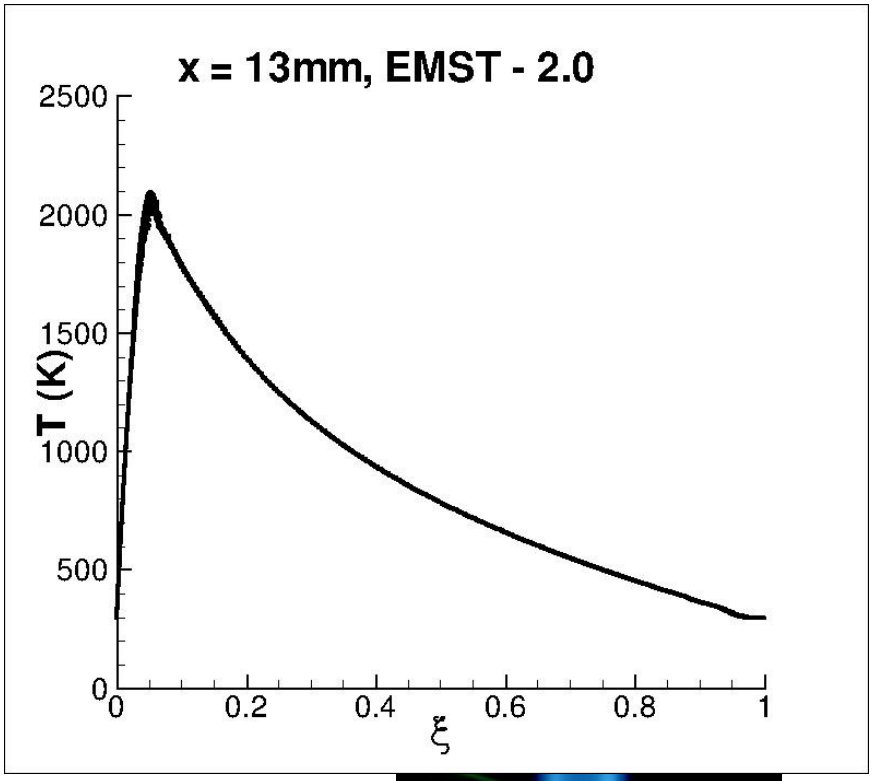


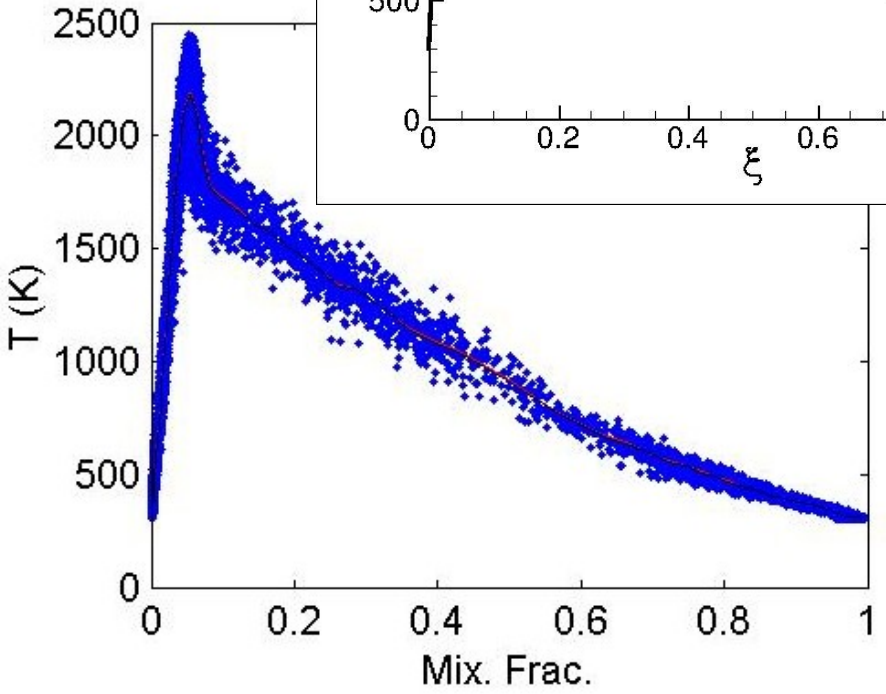


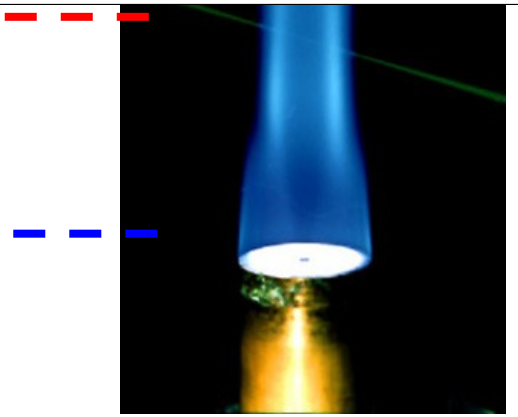


TPDF results: scatter plots HM3, x=13mm

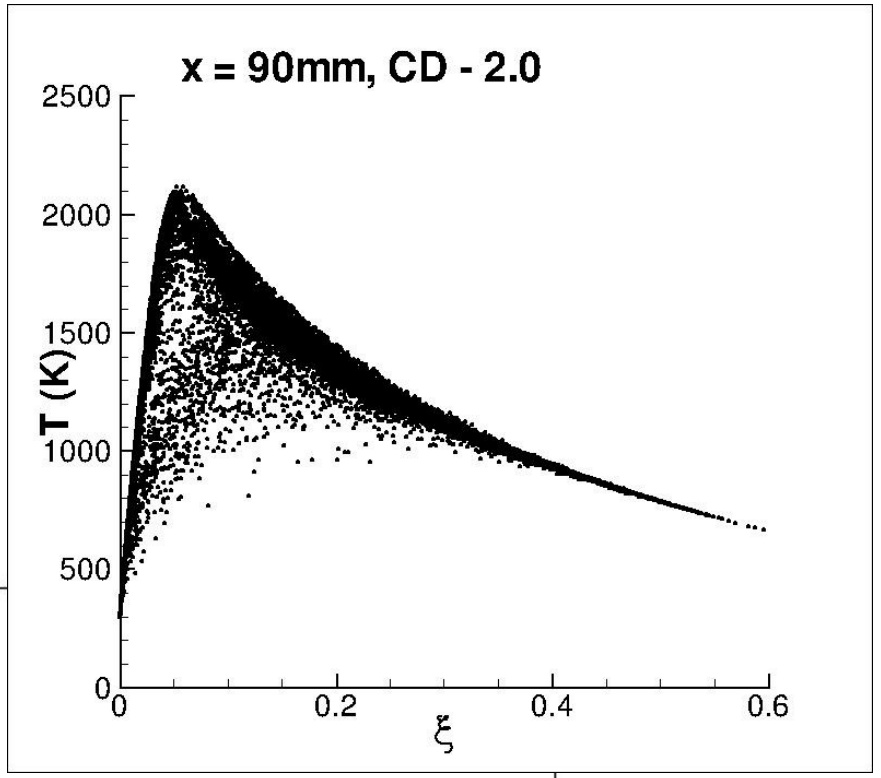


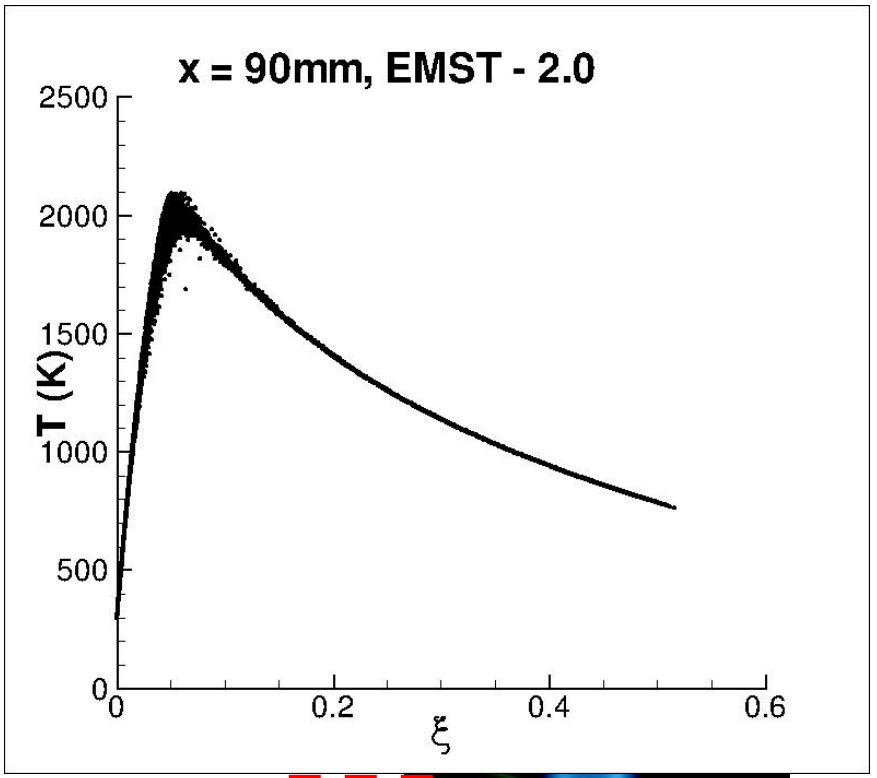


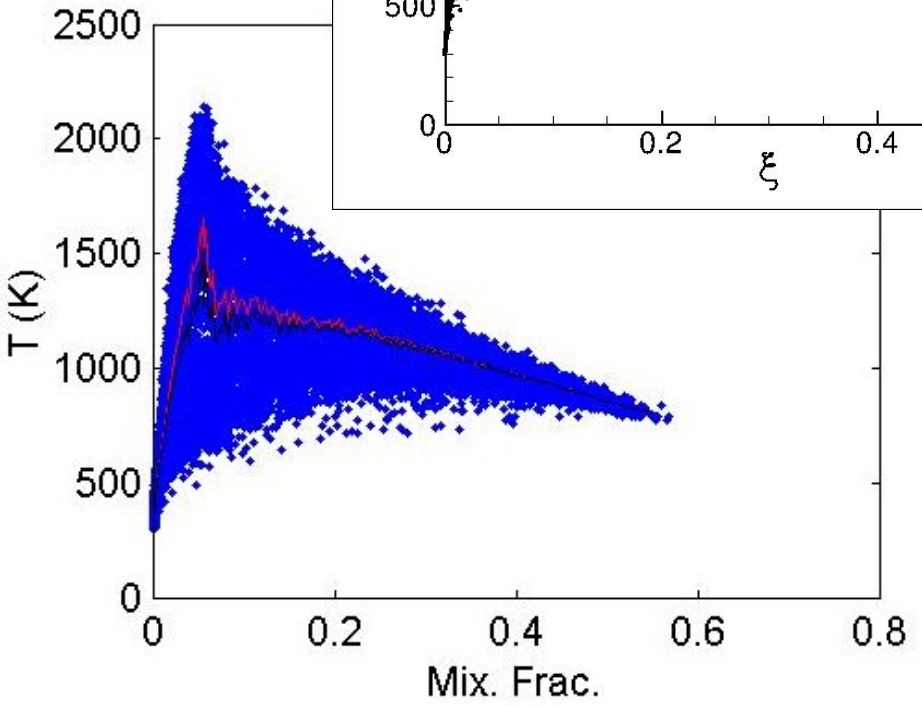


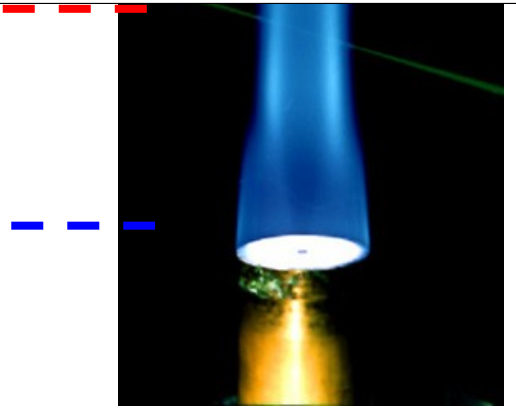


TPDF results: scatter plots HM3, x=90mm









REDIM / FPI

- *A priori* analysis: is the composition manifold in good correspondence with experimental data?
  - REDIM: not completely → add a dimension?
  - FPI: to be tested → combine different types of flamelets?

- A priori analysis (2D DNS): is the progress variable reaction rate in good correspondence with DNS data?
  - No for FPI tables based on premixed or diffusion flamelets
  - To be tested for REDIM

- Should the progress variable reaction rate be dependent on the gradients in physical space (scalar dissipation rate)?
  - Solve the joint PDF of mixture fraction / progress variable(s) / scalar dissipation rate?