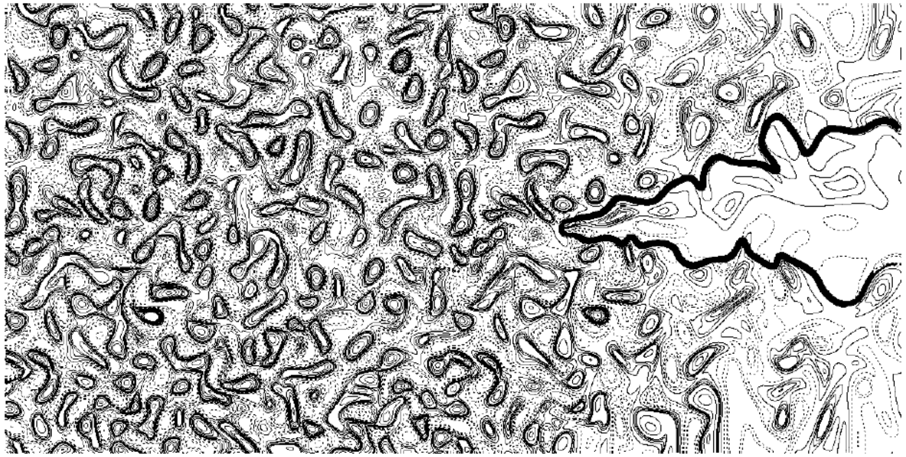
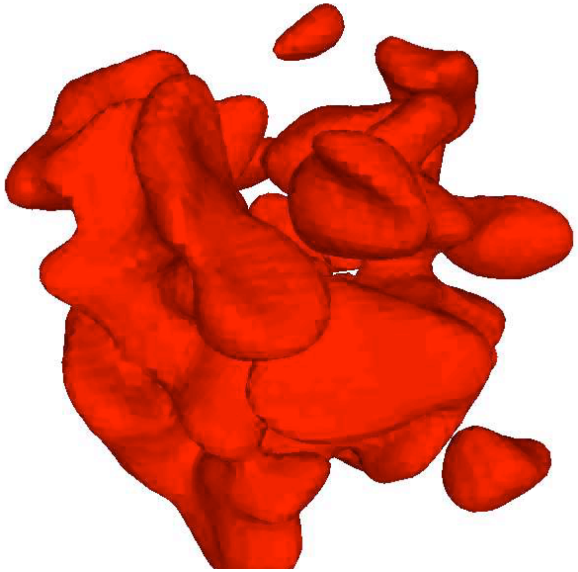


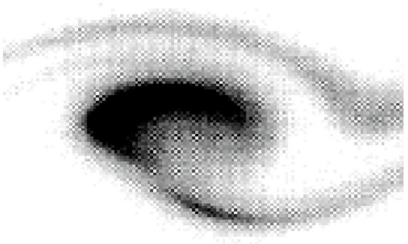
"Computational Fluid Dynamics
Chemical Reaction Engineering IV"
June 19-24, 2005
Barga, Italy

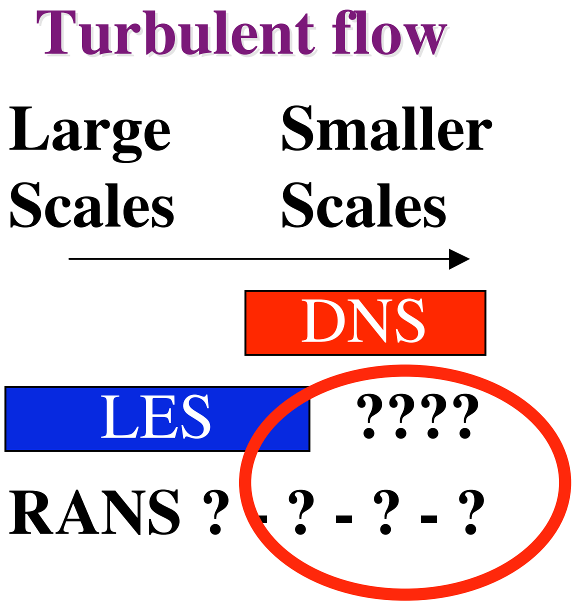
DNS and LES of Turbulent Combustion

Luc Vervisch
INSA de Rouen, IUF, CORIA-CNRS
Pascale Domingo, Julien Réveillon
Sandra Payet, Cécile Péra & Raphael Hauguel



Combustion system:





Turbulent flow

Large Scales

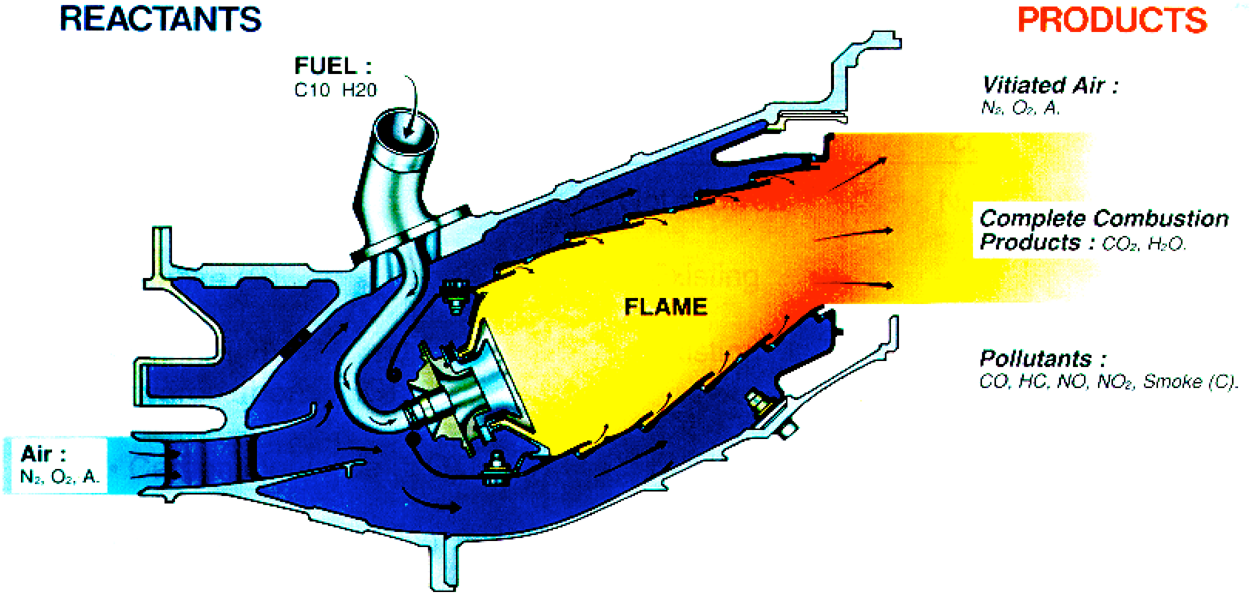
Smaller Scales

DNS

LES

????

RANS ? - ? - ? - ?



- **Unsteady large scales lead to an imperfect mixing in the system. Those scales are geometry dependent and feature a long life time.**
- **Micro-mixing mechanisms bring reactants in contact within thin reaction zones.**

OUTLINE

- ✓ DNS of turbulent combustion.
- ✓ Overview of turbulent combustion modeling.
- ✓ One example of SGS modeling in LES of premixed turbulent combustion.
- ✓ SGS modeling of partially premixed combustion.

Resolution needed for full simulation:

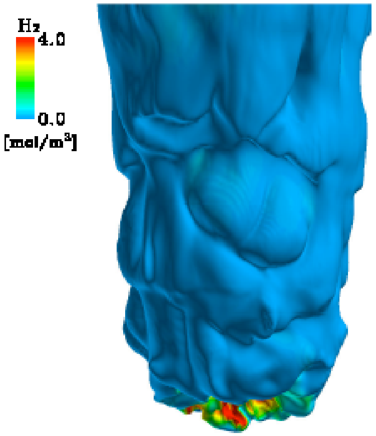
- **Flow:**

$$10^{-6}\,\mathrm{m} < \eta_k < 10^{-4}\,\mathrm{m}$$

$$\eta_k \approx \frac{l_t}{Re_\lambda^{3/2}}$$

Re_λ	Memory	Speed	Year
70	50 Gbytes	50 Gflops	1993
300	50 Tbytes	50 Tflops	2002
1500	50 Pbytes	50 Pflops	2015?

J. Jiménez, Eng. Turbulence Modelling and Experiments-5, 2002



Mizobuchi et al, Proc. Combust. Inst. 2002

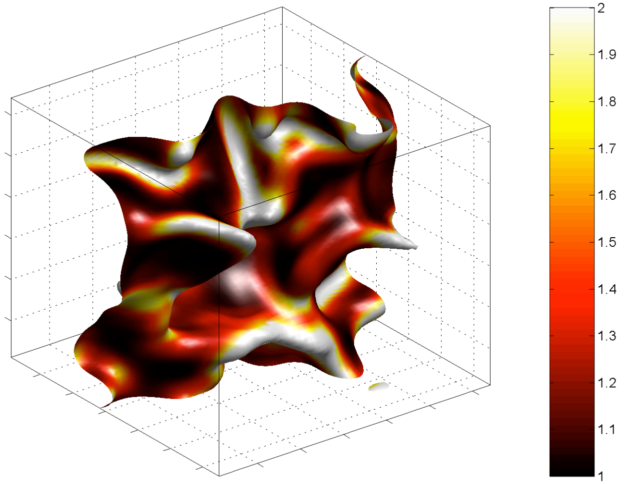
- **Flame (CH4/AIR) :**

$$h \approx 5.\,10^{-6}\mathrm{m}$$

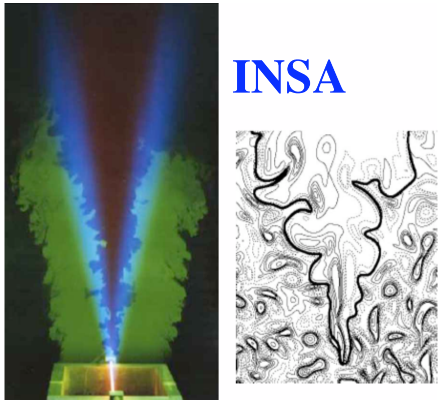
$$\Delta t \approx 1.\,10^{-6}\mathrm{s}$$

So far, three types of ‘full solutions’ (DNS):

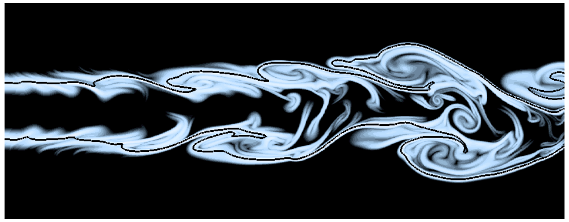
- DNS of synthetic model problem (freely decaying turbulence).
- DNS of laboratory flame, but at much lower Re.
- DNS of laboratory flame.



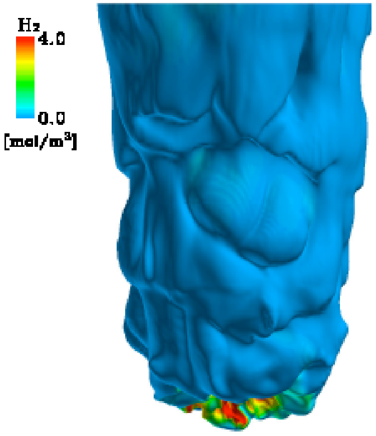
Cambridge



INSA



Sandia, Livermore



JAXA

Synthetic problem **Laboratory flame at lower Re** **Real jet-flame**

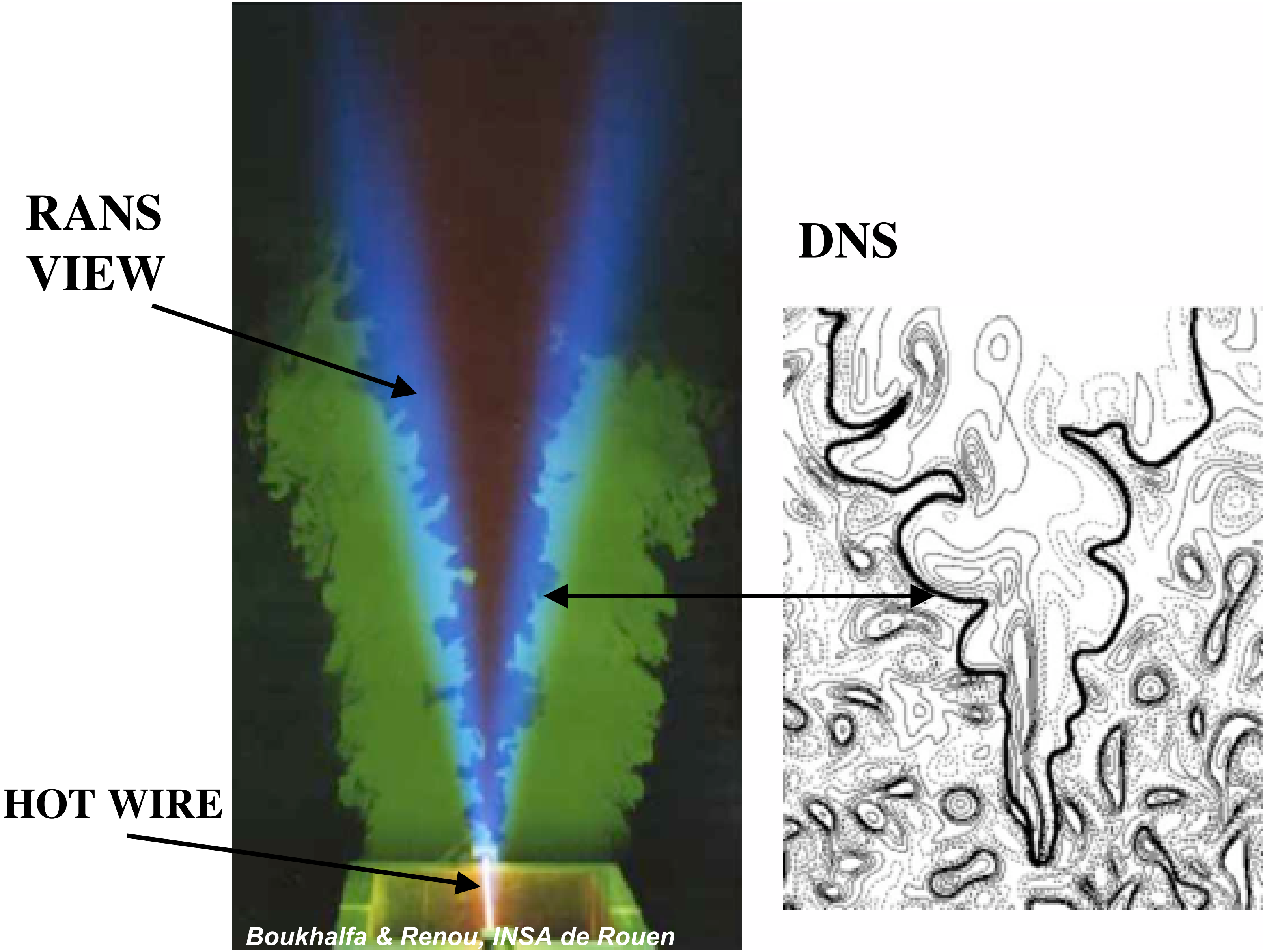
Chemistry:

- Single-step
- Reduced
- Tabulated
- Detailed

Transport:

- Fixed Lewis and Schmidt
- Variable Lewis & Schmidt
- Complex

Premixed Turbulent V-Flame



RANS VIEW

DNS

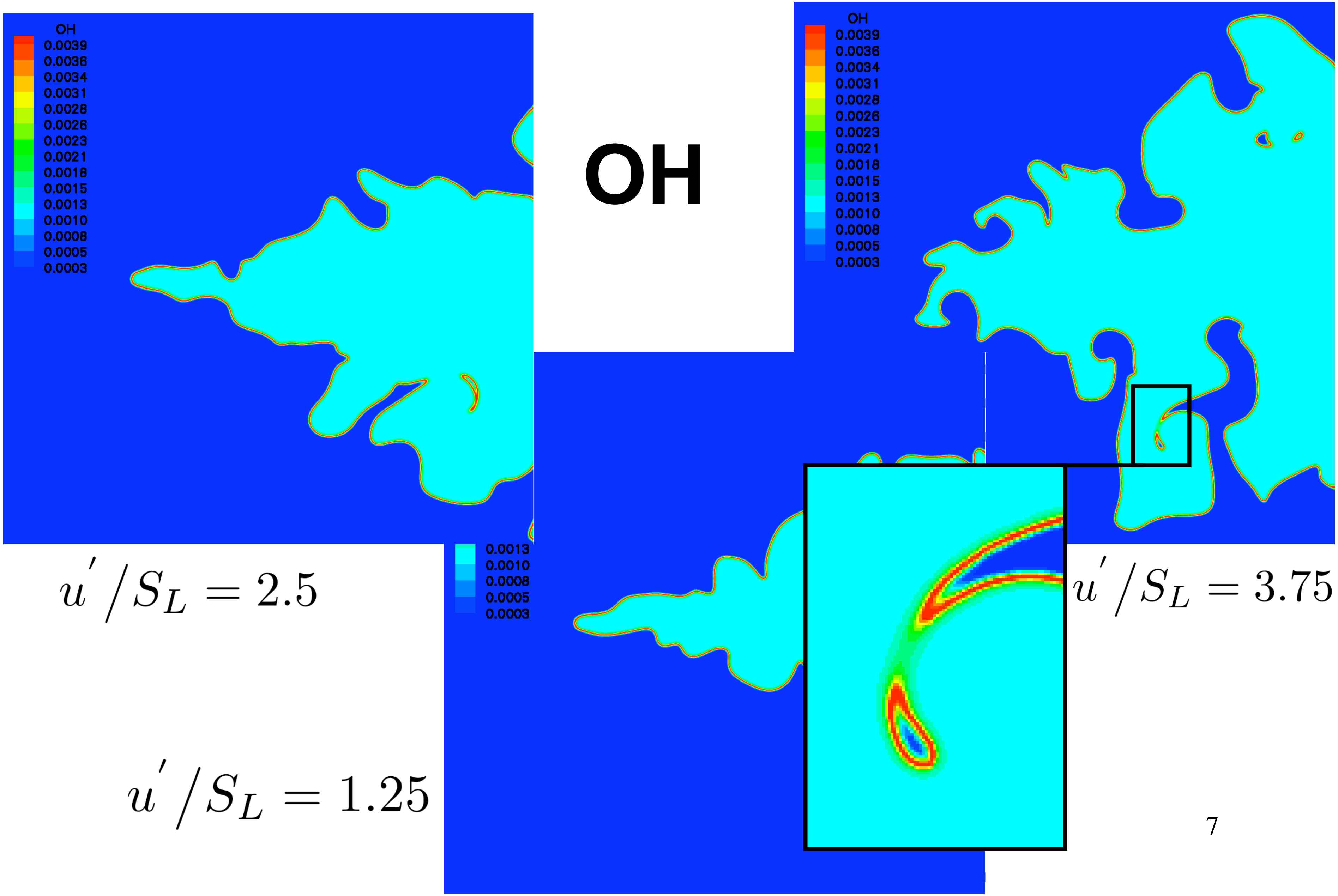
HOT WIRE

Boukhalfa & Renou, INSA de Rouen

Complex chemistry FPI-FGM:

Gicquel et al Proc. Combust. Inst.Vol. 28, 1901-1908, 2000.
Oijen et al Combust. Flame, 127(3):2124-2134, 2001.

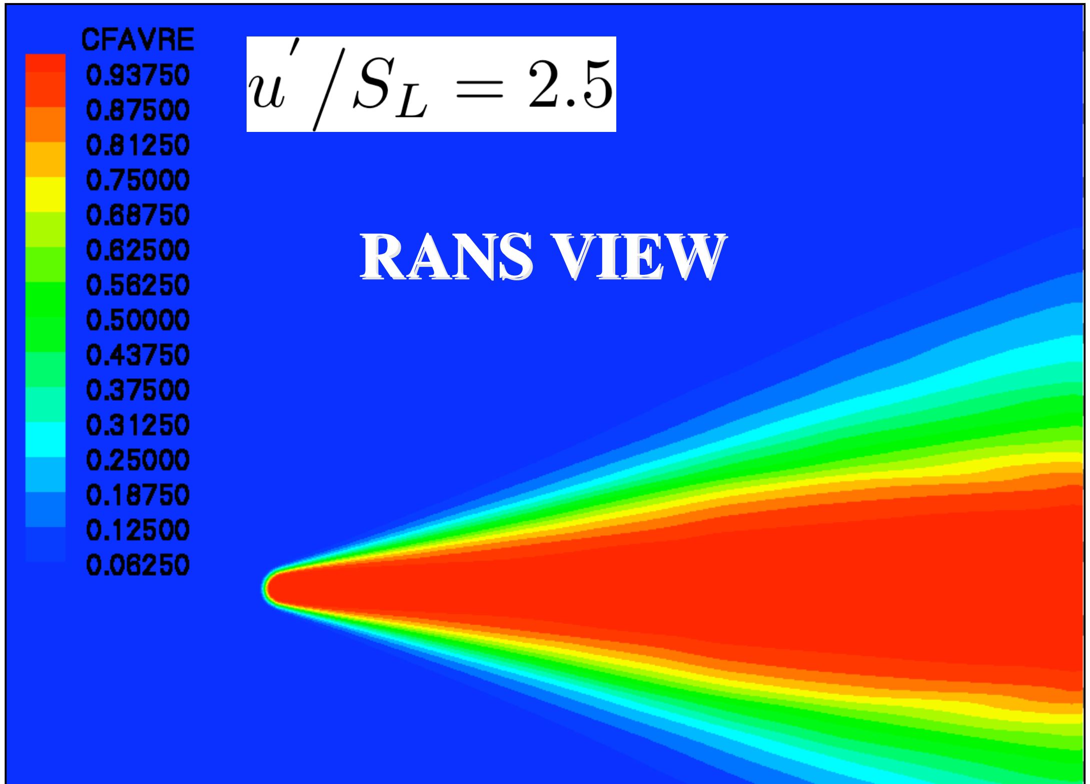
OH



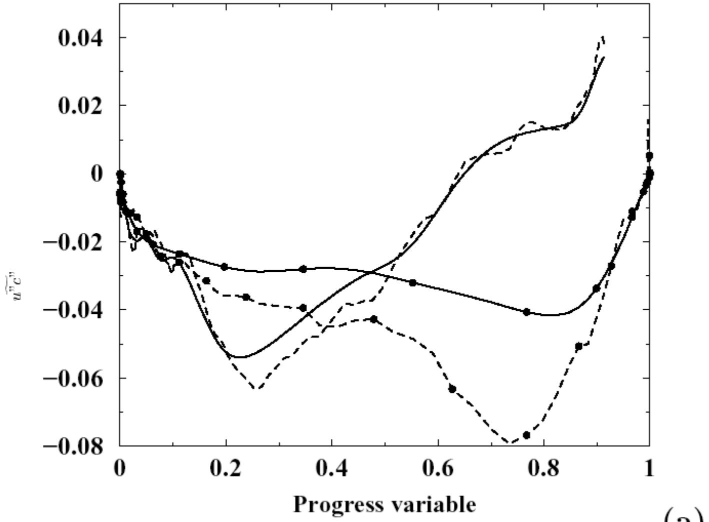
$u'/S_L = 2.5$

$u'/S_L = 3.75$

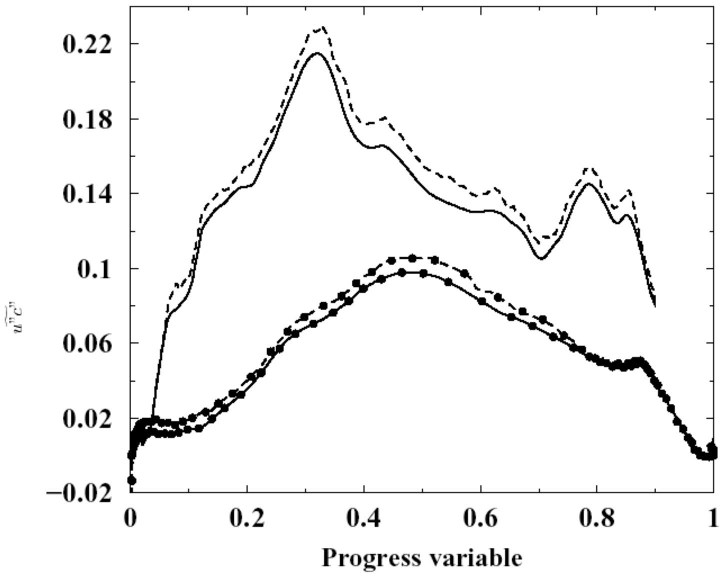
$u'/S_L = 1.25$



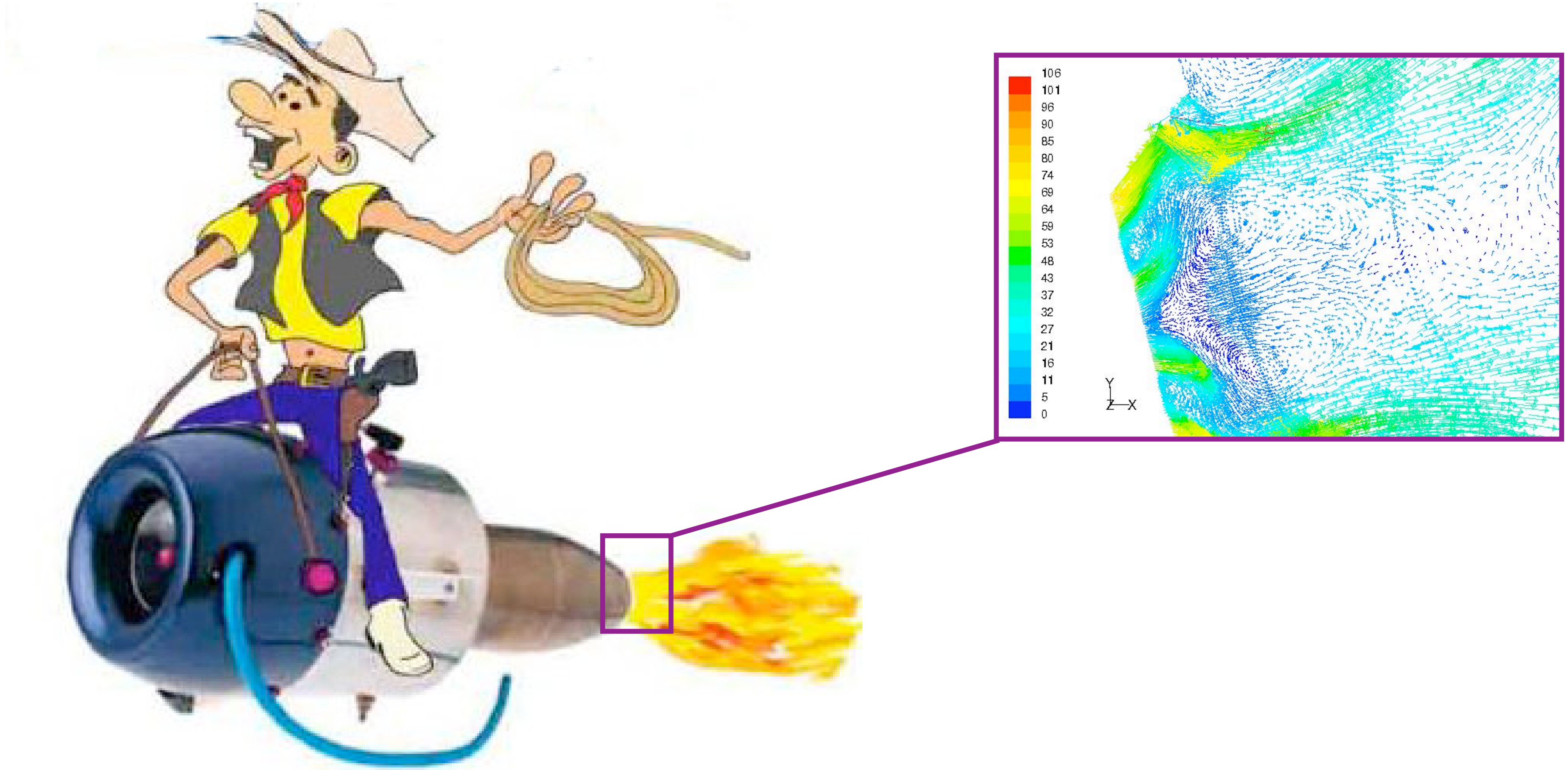
$$\widetilde{u_i'' c''}$$



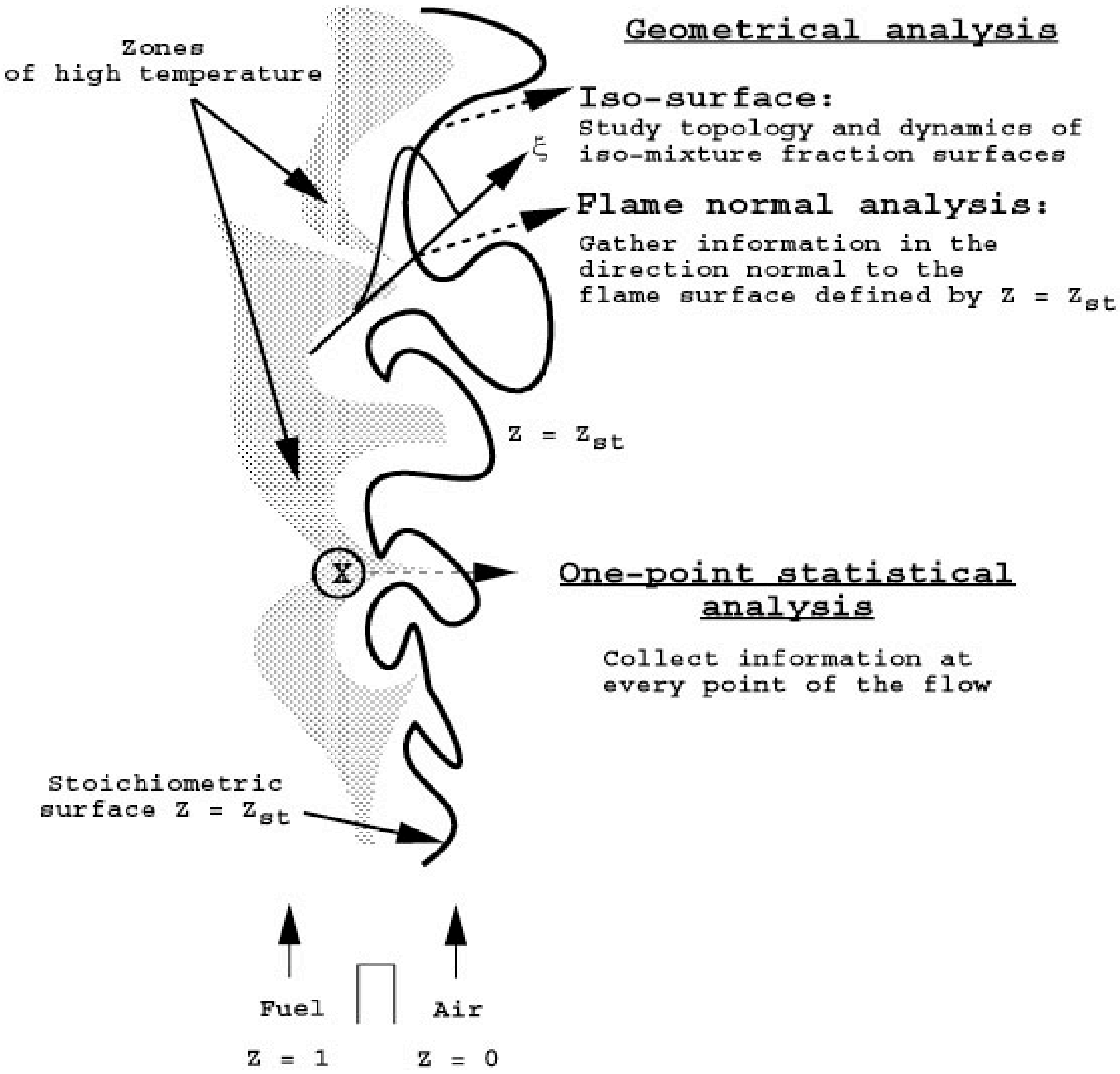
(a)



(c)



Overview of turbulent combustion modeling tools



Geometrical analysis

Iso-surface:
Study topology and dynamics of iso-mixture fraction surfaces

Flame normal analysis:
Gather information in the direction normal to the flame surface defined by Z = Z_{st}

One-point statistical analysis

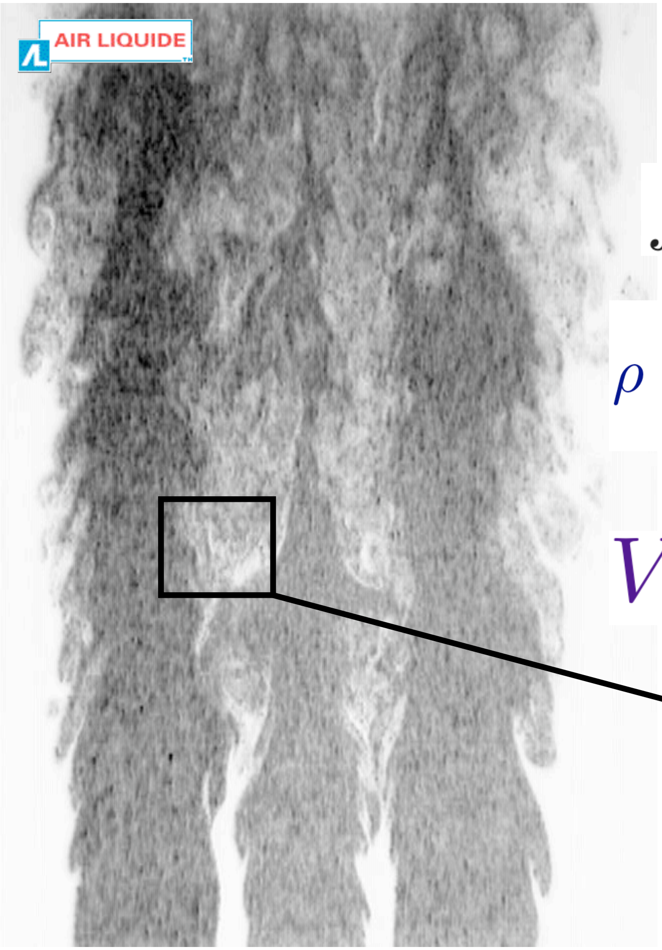
Collect information at every point of the flow

Flame surface density
G-Eq or c-Eq

Flamelet modeling

CMC
PDF transport

Control parameter of molecular mixing?



Oxi **Fuel** **Oxi**

$Z = 0 \quad Z = 1 \quad Z = 0$

$f = 0 \quad f = 0 \quad f = 0$

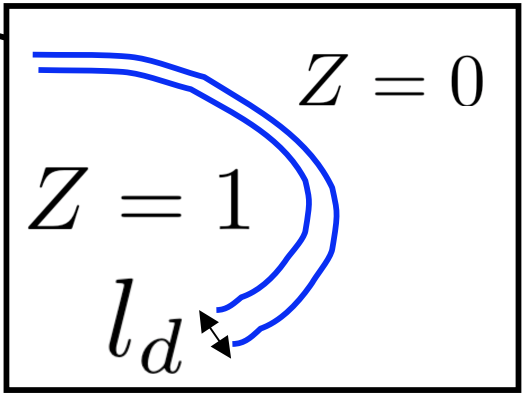
$$\rho\left(\frac{\partial Z}{\partial t} + u \cdot \nabla Z\right) = \nabla \cdot (\rho D \nabla Z)$$

$$f = Z(1 - Z)$$

$$\rho\left(\frac{\partial f}{\partial t} + u \cdot \nabla f\right) = \nabla \cdot (\rho D \nabla f) + \boxed{2\rho D \left|\nabla Z\right|^2}$$

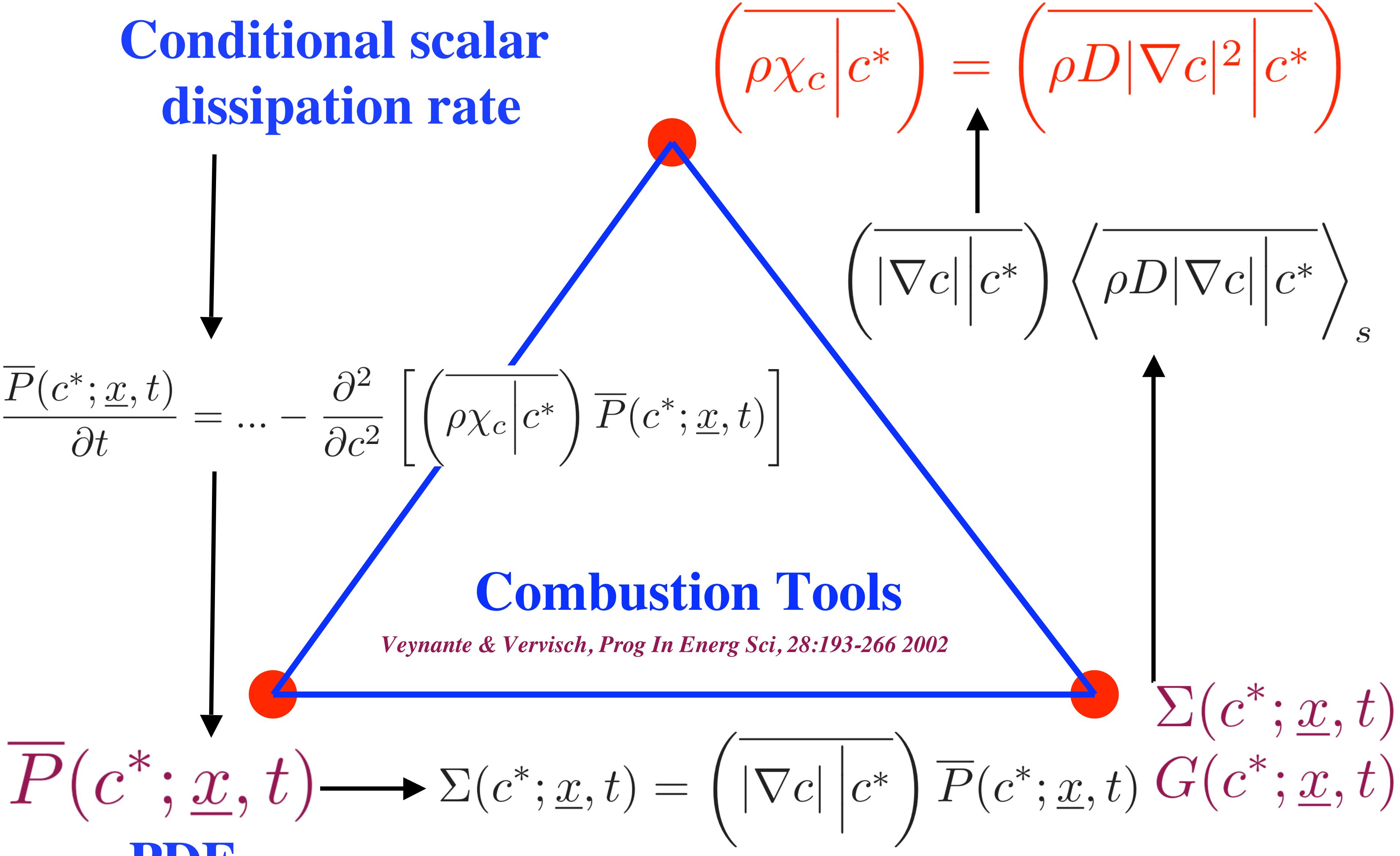
$$V_d = D\left|\nabla Z\right|$$

$$l_d = \left|\nabla Z\right|^{-1}$$



$$\boxed{\tau_{\chi_Z}^{-1} = V_d \big/ l_d = D\left|\nabla Z\right|^2 = \chi_Z}$$

Micromixing



Conditional scalar dissipation rate

$$\left(\overline{\rho\chi_c \,\Big|\, c^*}\right) = \left(\overline{\rho D|\nabla c|^2 \,\Big|\, c^*}\right)$$

$$\left(\overline{|\nabla c| \,\Big|\, c^*}\right) \left\langle \overline{\rho D|\nabla c| \,\Big|\, c^*} \right\rangle_s$$

$$\frac{\overline{P}(c^*;\underline{x},t)}{\partial t} = \ldots - \frac{\partial^2}{\partial c^2}\left[\left(\overline{\rho\chi_c \,\Big|\, c^*}\right)\overline{P}(c^*;\underline{x},t)\right]$$

Combustion Tools

Veynante & Vervisch, Prog In Energ Sci, 28:193-266 2002

$\Sigma(c^*;\underline{x},t)$

$G(c^*;\underline{x},t)$

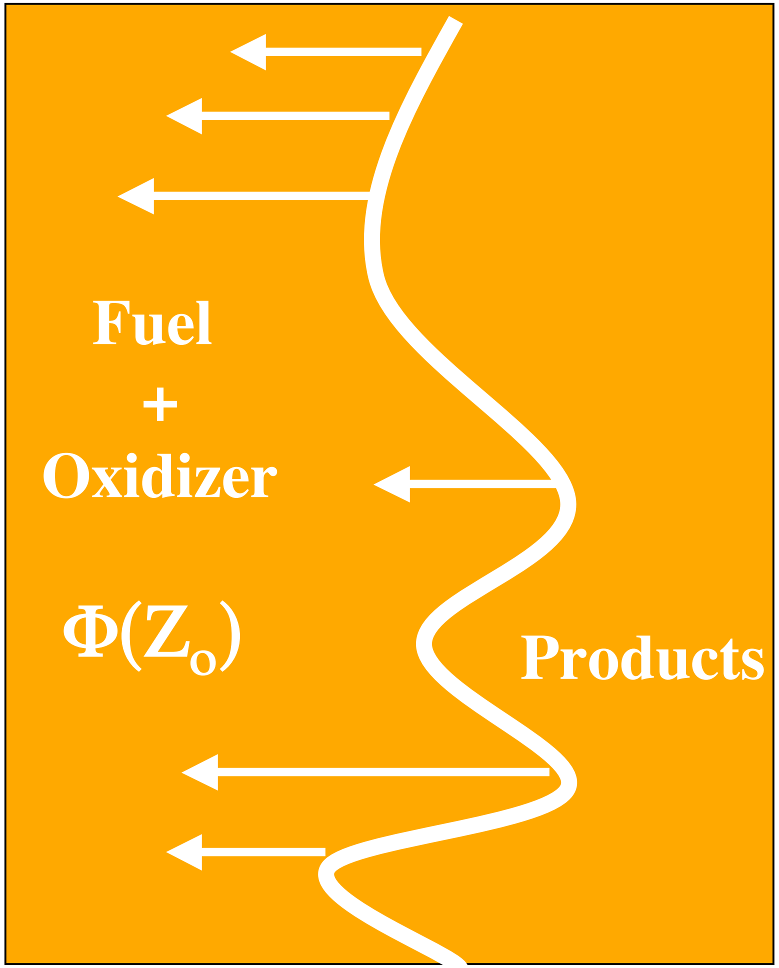
$$\overline{P}(c^*;\underline{x},t) \longrightarrow \Sigma(c^*;\underline{x},t) = \left(\overline{|\nabla c| \,\Big|\, c^*}\right)\overline{P}(c^*;\underline{x},t)$$

PDF

Surface or G-field

“Academic” combustion regimes

Prémélange



Fuel

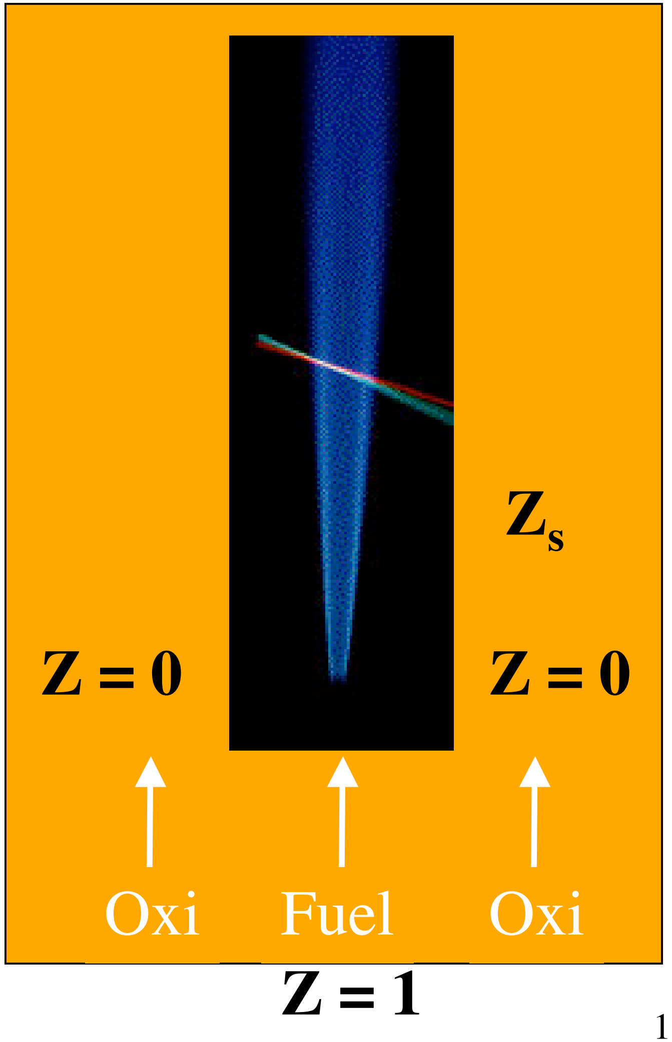
+

Oxidizer

$\Phi(Z_o)$

Products

Diffusion



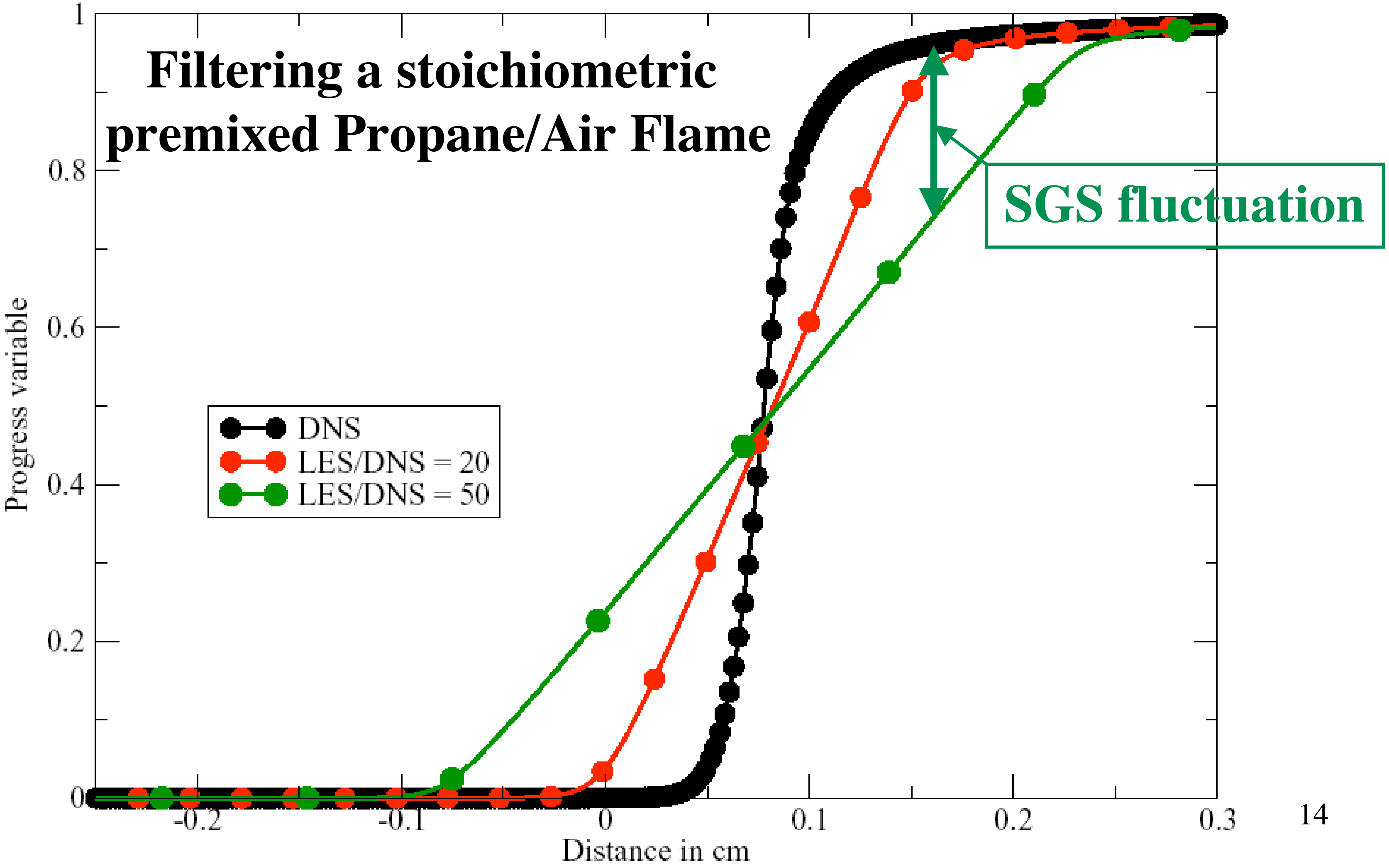
Z_s

$Z = 0$ $Z = 0$

Oxi Fuel Oxi

$Z = 1$

Premixed flame LES filtering



SGS Probability Density Function in premixed flames:

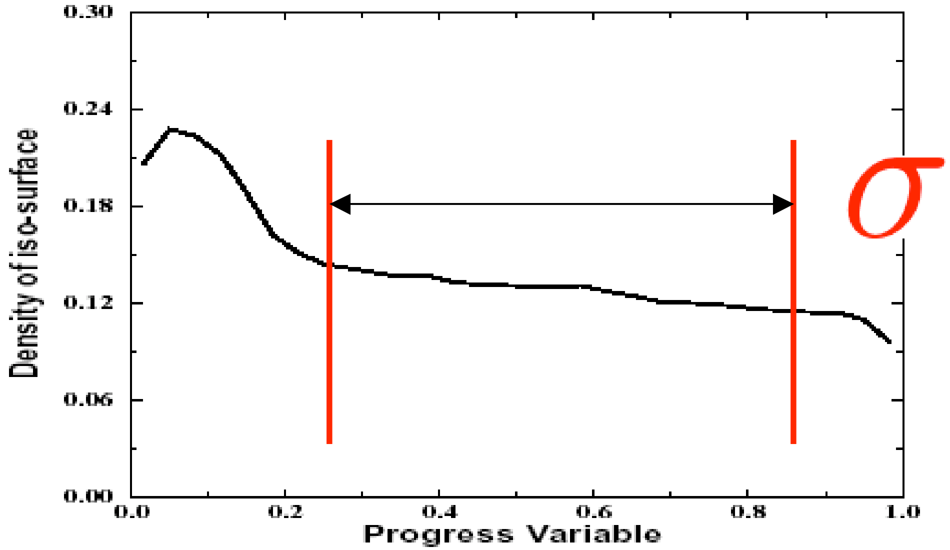
- **The thin flame front has a characteristic scale within the subgrid.**
- **The thin flame is seen at the grid scale Δ.**

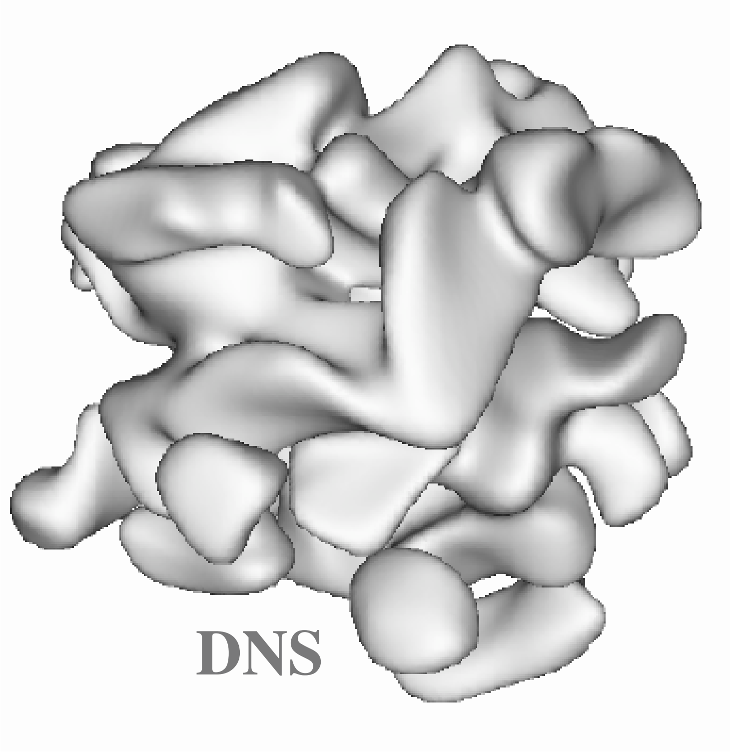
EFFECTS

1. **Thickening by the filter of the thin flame front over the coarse LES grid.**
2. **Wrinkling of the flame within the subgrid that results from interaction with subgrid vortices.**

Flame surface density contains information on the flame characteristic length:

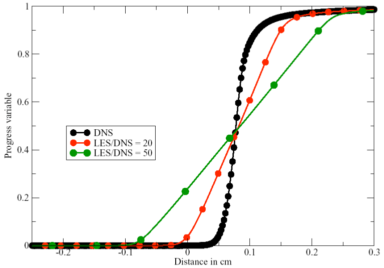
$$\Sigma(c^*;\underline{x},t) = \left(\overline{|\nabla c||c^*}\right)\widetilde{P}(c^*;\underline{x},t)$$

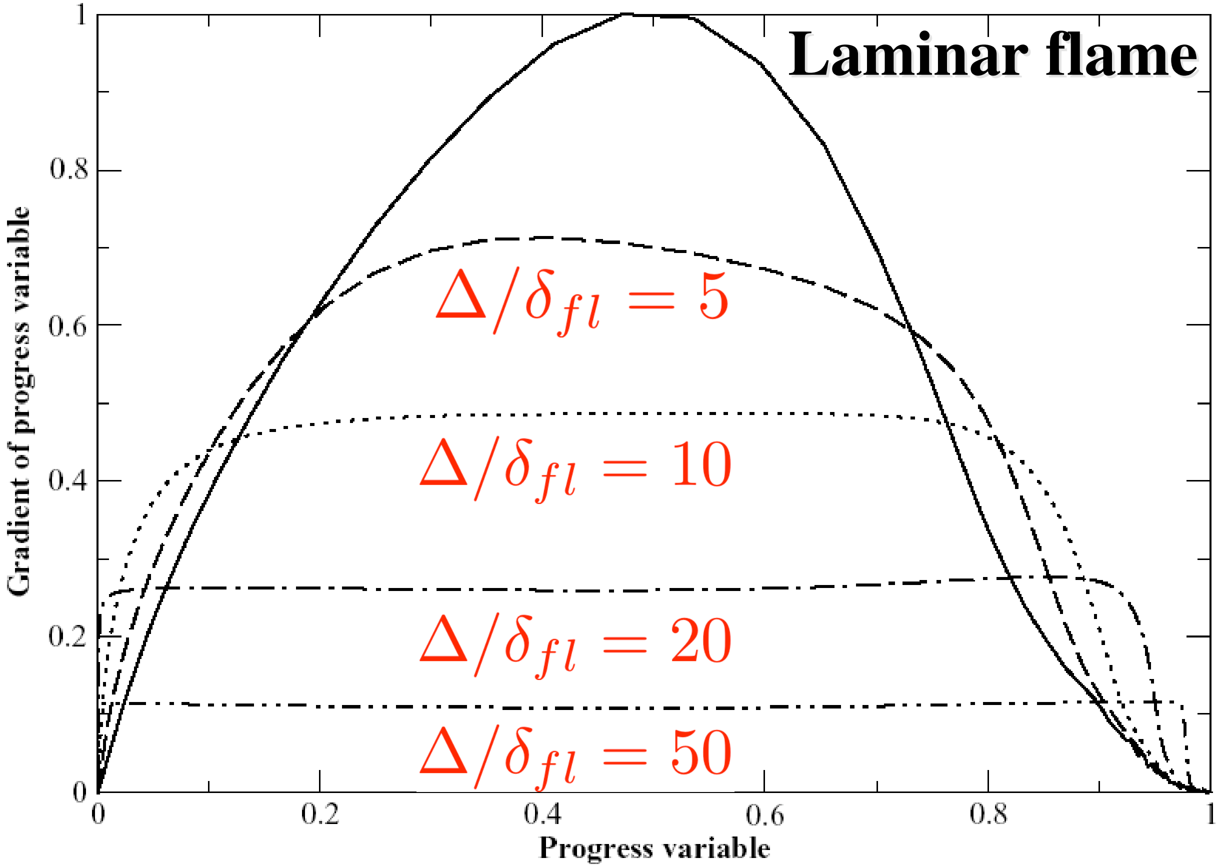




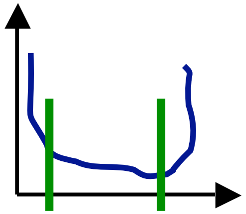
Filtered gradient contains two points information

$$\overline{G}_{\Delta}(c(x)) = \int^{+\infty} |\nabla c|^{FPI} \mathcal{G}_{\Delta}(x - x')dx'$$





Get the PDF from the Flame Surface Density inside the flame:



$$\widetilde{P}(c^*;\underline{x},t) = \frac{\Sigma(c^*;\underline{x},t)}{\left(\overline{|\nabla c||c^*}\right)}$$

$$\boxed{\begin{aligned}\widetilde{P}(c^*;\underline{x},t) &= \alpha(\underline{x},t)\delta(c^*) + \beta(\underline{x},t)\delta(1-c^*)\\ &+ \frac{\sigma(\underline{x},t)}{\overline{G}_\Delta(c^*)}H(c^*)H(1-c^*)\end{aligned}}$$

$$\overline{G}_\Delta(c(x)) = \int_{-\infty}^{+\infty} |\nabla c|^{FPI}\mathcal{G}_\Delta(x-x')dx'$$

Describing SGS variance of progress variable:

$$\widetilde{c}_v = \widetilde{cc} - \widetilde{c}\,\widetilde{c}$$

Energy that is not resolved by the coarse LES grid.

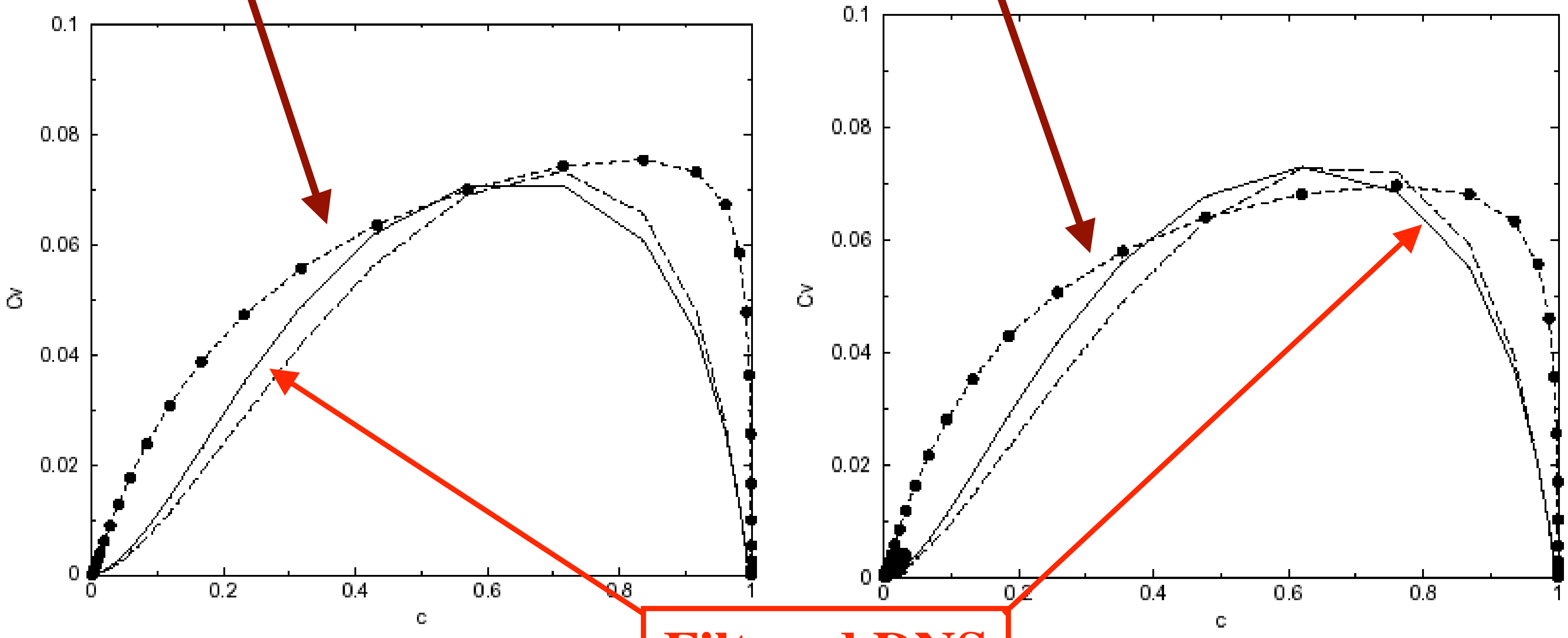
- Try to get it from resolved scales:
  - Scale similarity hypothesis.
  - Equilibrium hypothesis.

- Solve a balance equation to get SGS variance:
  - Which balance equation is the best?
  - Close unknown terms.

$$\widetilde{c_v} = \widetilde{cc} - \tilde{c}\,\tilde{c}$$

Scale similarity assumption:

$$\boxed{\tilde{c}_v = C_c\left(\widehat{\tilde{c}\tilde{c}} - \hat{\tilde{c}}\hat{\tilde{c}}\right)} \qquad \hat{\Delta} > \Delta$$



Filtered DNS

$$\widetilde{c}_v = \widetilde{cc} - \widetilde{c}\,\widetilde{c}$$

Equation for SGS variance:

$$\begin{aligned}
\frac{\partial \overline{\rho}\widetilde{c}_v}{\partial t} + \nabla\cdot(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{c}_v) &= -\nabla\cdot\overline{\tau}_{c_v} + \nabla\cdot(\overline{\rho}D\nabla\widetilde{c}_v)\\
&\boxed{\begin{aligned} -&\quad 2\overline{\tau}_c\cdot\nabla\widetilde{c} + 2\overline{\rho}D|\nabla\widetilde{c}|^2 - 2\overline{\rho D|\nabla c|^2}\\ +&\quad 2\overline{\rho}\left(\widetilde{\dot{\omega}_c c} - \widetilde{\dot{\omega}}_c\widetilde{c}\right)\end{aligned}}
\end{aligned}$$

Production - Dissipation and Source

Dissipation: $\overline{\rho}D|\nabla\widetilde{c}|^2 - \overline{\rho D|\nabla c|^2} \approx -\overline{\rho}\widetilde{c}_v/\tau_t$

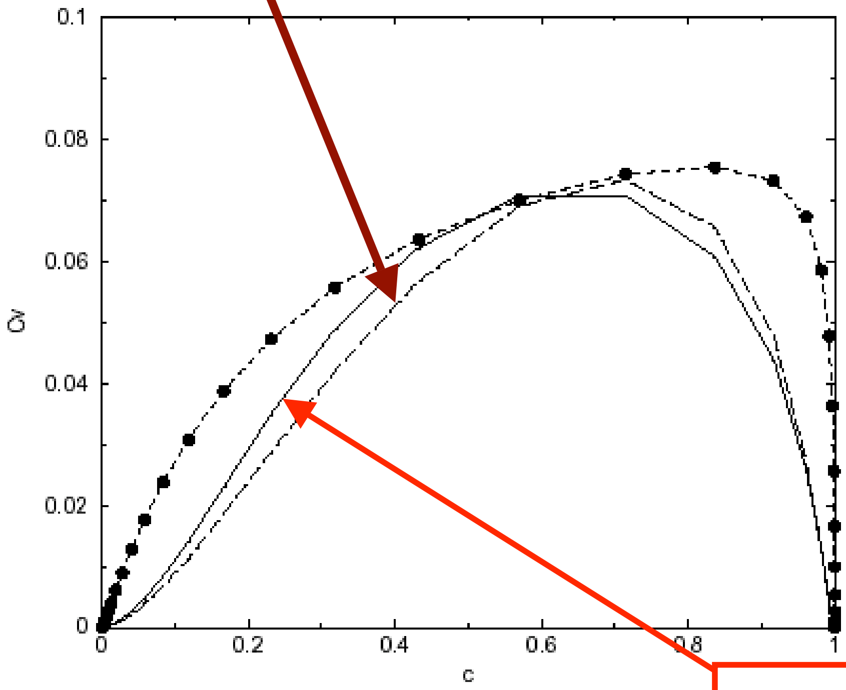
$$\nu_T = (C_s\Delta)^2|\widetilde{S}| \qquad |\widetilde{S}| = (2\widetilde{S}\cdot\widetilde{S})^{1/2}$$

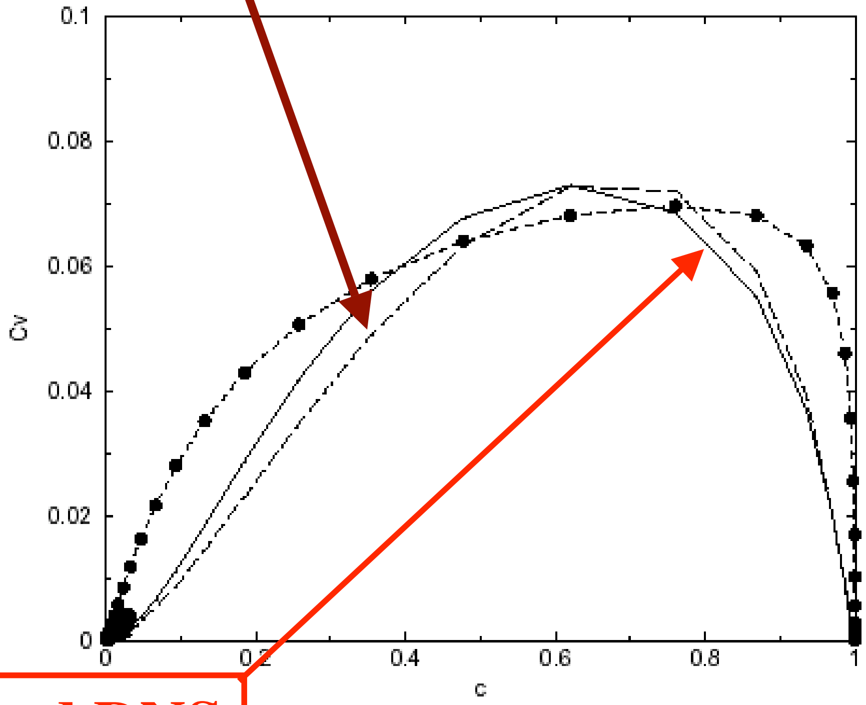
$$\tau_t \approx \Delta^2/(\nu_T/Sc_T) \qquad \widetilde{S} = (1/2)(\nabla\widetilde{u} + \nabla^T\widetilde{u})$$

Equilibrium hypothesis:

Depends on geometry and chemistry…

$$\widetilde{c_v} = C_v \left(\Delta^2 |\nabla \widetilde{c}|^2 + \left(\widetilde{\dot{\omega}_c c} - \widetilde{\dot{\omega}}_c \widetilde{c} \right) \frac{\Delta^2}{(\nu_T / Sc_T)} \right)$$





Filtered DNS

Chose the appropriate variable to be transported
(the one that minimizes LES numerical problems…)

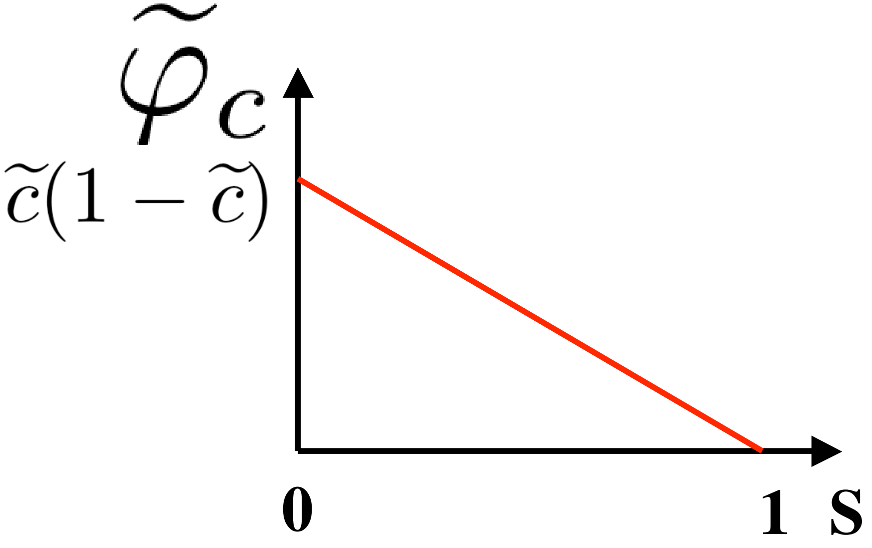
- **Solve for the departure from maximum variance:**

$$\widetilde{c}_v = \widetilde{c\,c} - \widetilde{c}\,\widetilde{c} = \widetilde{c}(1-\widetilde{c}) - \boxed{\widetilde{\varphi}_c}$$

$$\overline{\rho\varphi}_c = \overline{\rho c(1-c)} = \overline{\rho}\,\widetilde{c}(1-\widetilde{c})\,(1-S)$$

Unmixedness:

$$S = \frac{\widetilde{c}_v}{\widetilde{c}(1-\widetilde{c})}$$



The modeled balance equations to be solved for presuming the PDF then reads:

$$\frac{\partial \overline{\rho}\widetilde{c}}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}\widetilde{c}) = \nabla \cdot (\overline{\rho}(D + (\nu_T / Sc_T))\nabla \widetilde{c}) + \overline{\rho}\widetilde{\dot{\omega}}_c$$

$$\frac{\partial \overline{\rho}\widetilde{\varphi}_c}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}\widetilde{\varphi}_c) = \nabla \cdot (\overline{\rho}(D + (\nu_T / Sc_T))\nabla \widetilde{\varphi}_c)$$

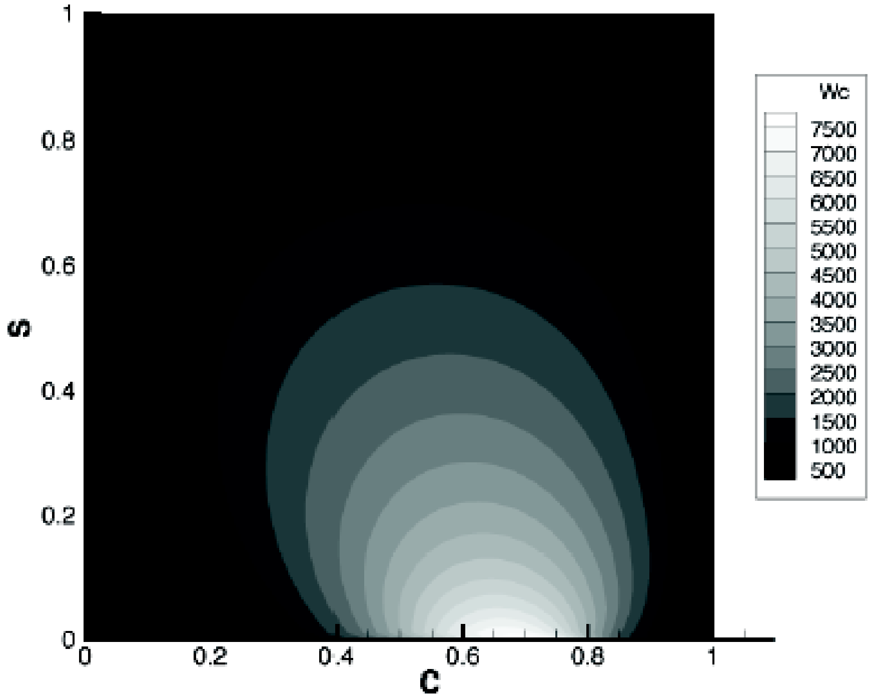
Scalar dissipation rate $+ \quad 2\overline{\rho}\left(D|\nabla \widetilde{c}|^2 + C_D \frac{\nu_t}{Sc_T}\frac{\widetilde{c}_v}{\Delta^2}\right)$

Chemical source $+ \quad \overline{\rho}\left(\widetilde{\dot{\omega}}_c - 2\widetilde{\dot{\omega}_c c}\right)$

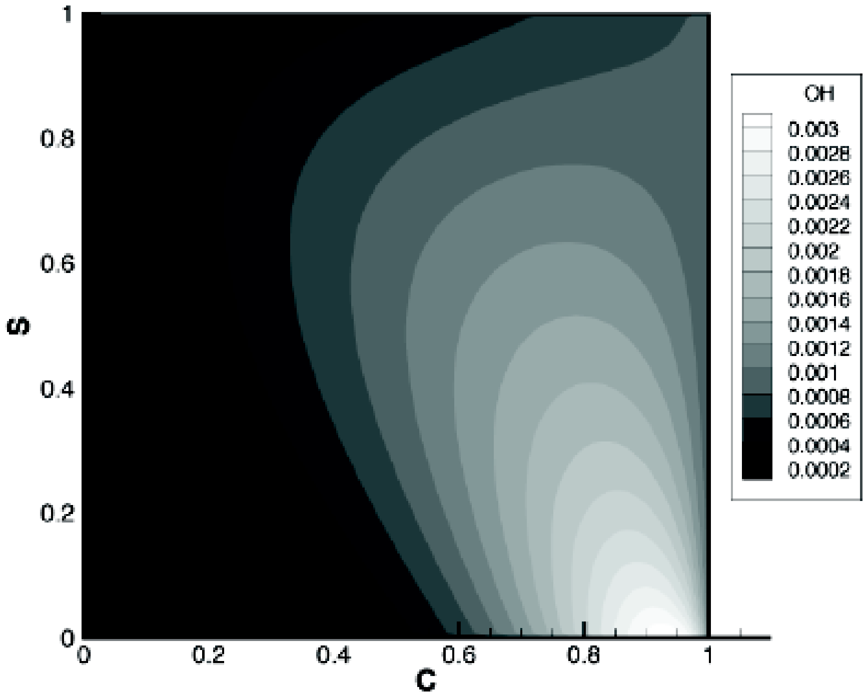
LES CHEMICAL TABLES
Averaging FGM or FPI

FPI (Flame Prolongation of ILDM): Gicquel et al Proc. Combust. Inst.Vol. 28, 1901-1908, 2000.
FGM (Flame Generated Manifod): Oijen et al Combust. Flame, 127(3):2124-2134, 2001.

$$\widetilde{\dot{\omega}}_c$$



$$\widetilde{Y}_{OH}$$



SGE:

- ✓ **Fully Compressible Flow.**

- ✓ **4th ordre in space, 2nd in time.**

  Skew symmetric like, Ducros et al, J. Comput. Phys., 161: 114-139, 2000.

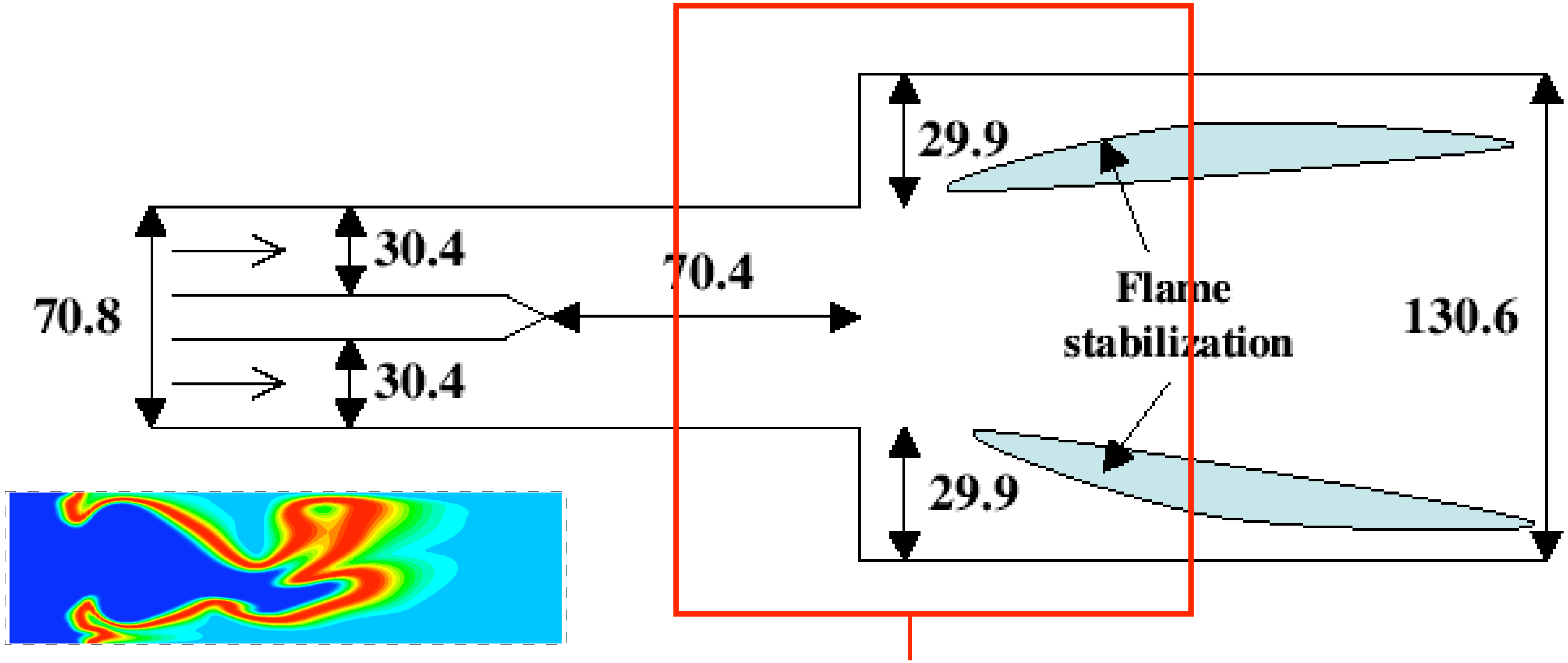
- ✓ **Dynamic Lagrangian Modeling.**

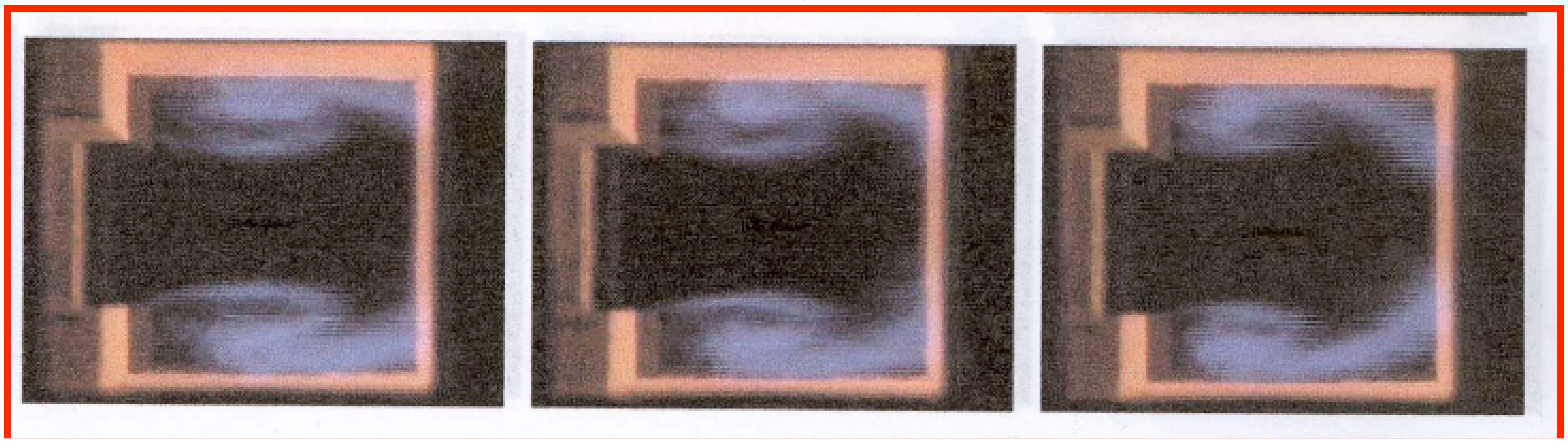
  Meneveau et al, JFM, 353-386, 1996.

- ✓ **Structure Function.**

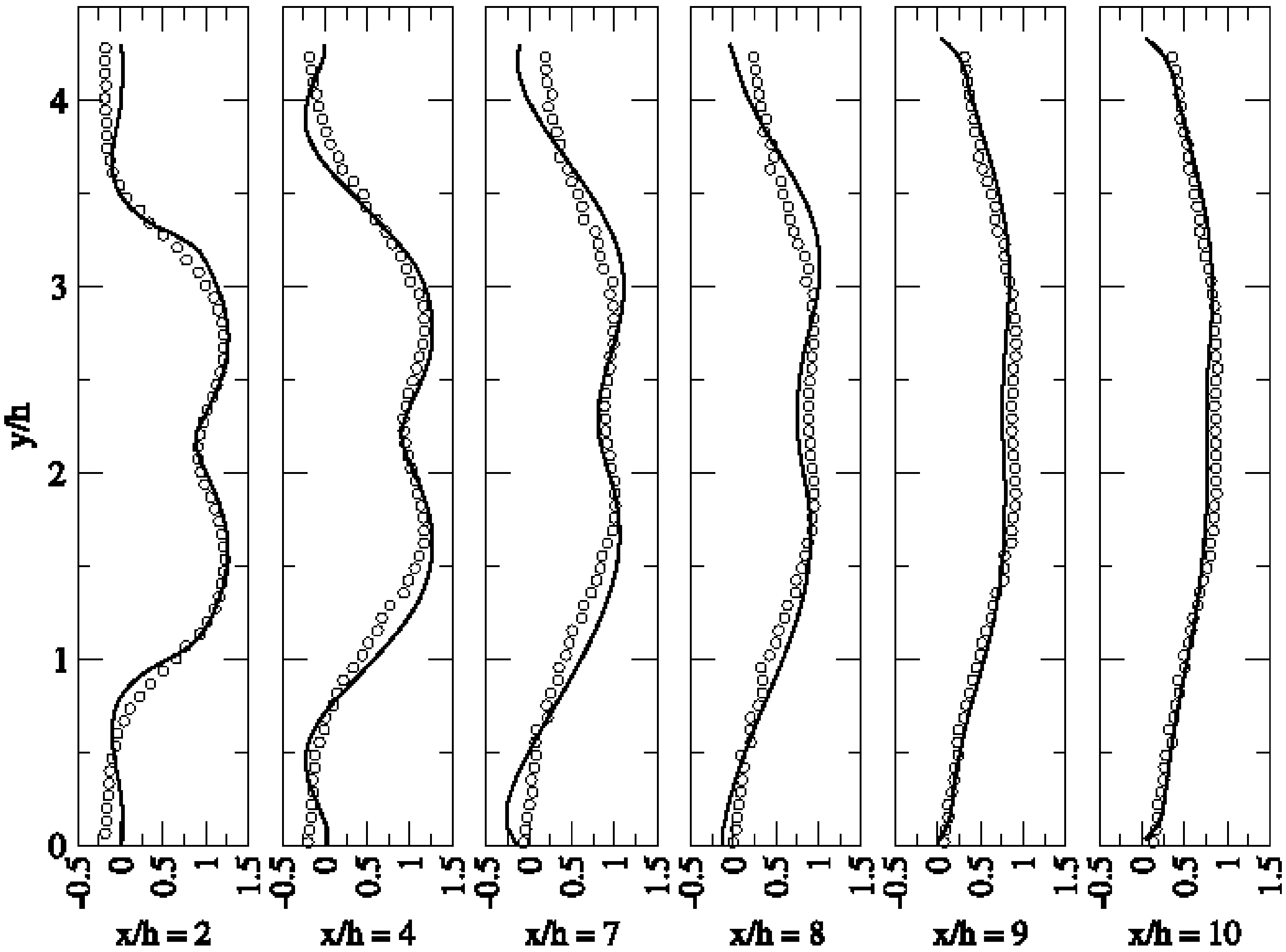
  M. Lesieur Team.

Test premixed SGS modeling on ORACLES (Nguyen and Bruel, AIAA-2003-0958.)

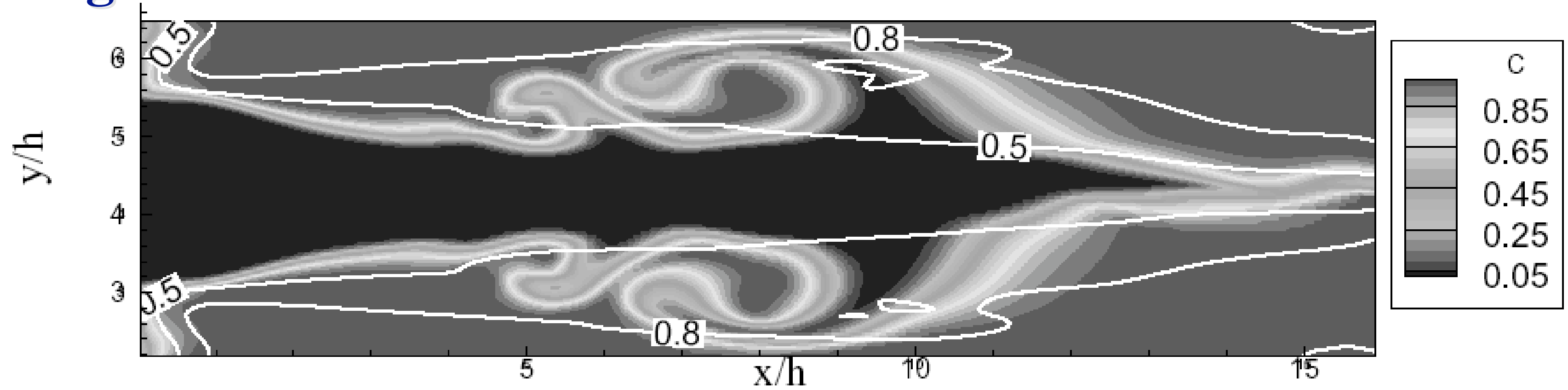




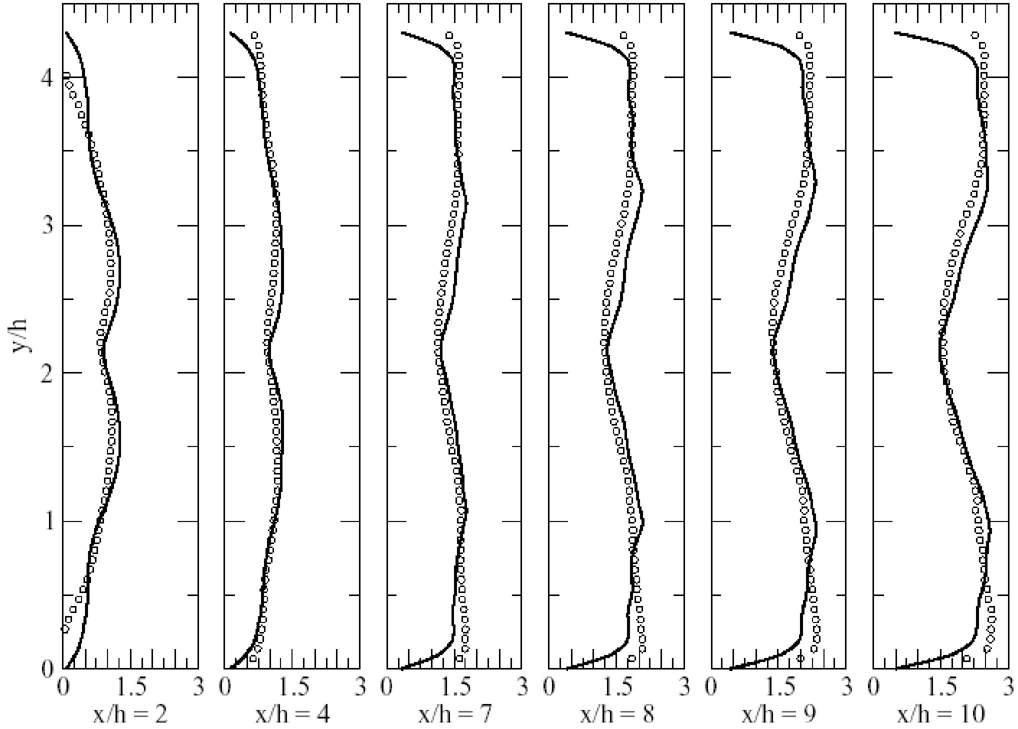
Time averaged streamwise velocity frozen flow mixing:



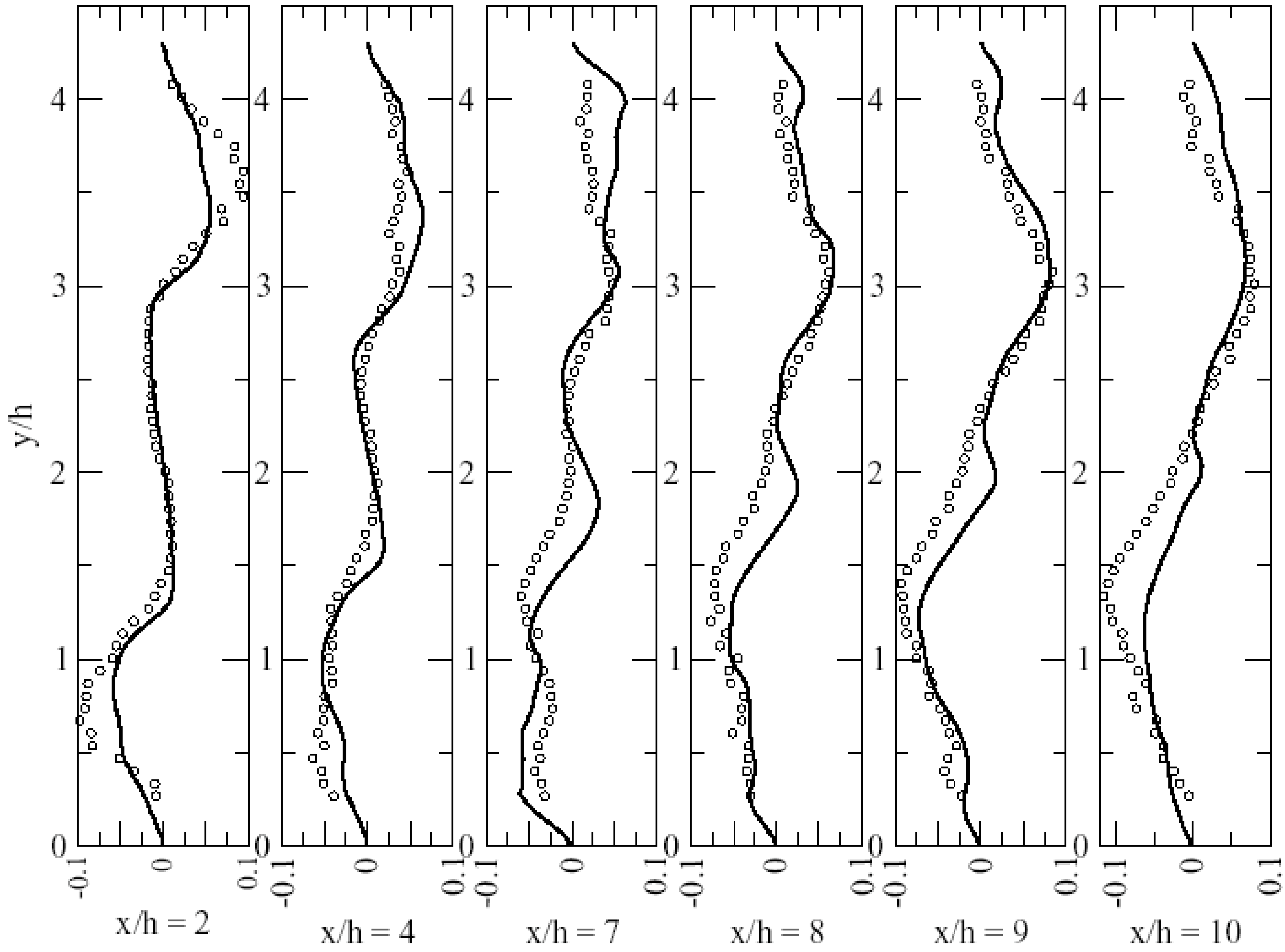
Progress variable:



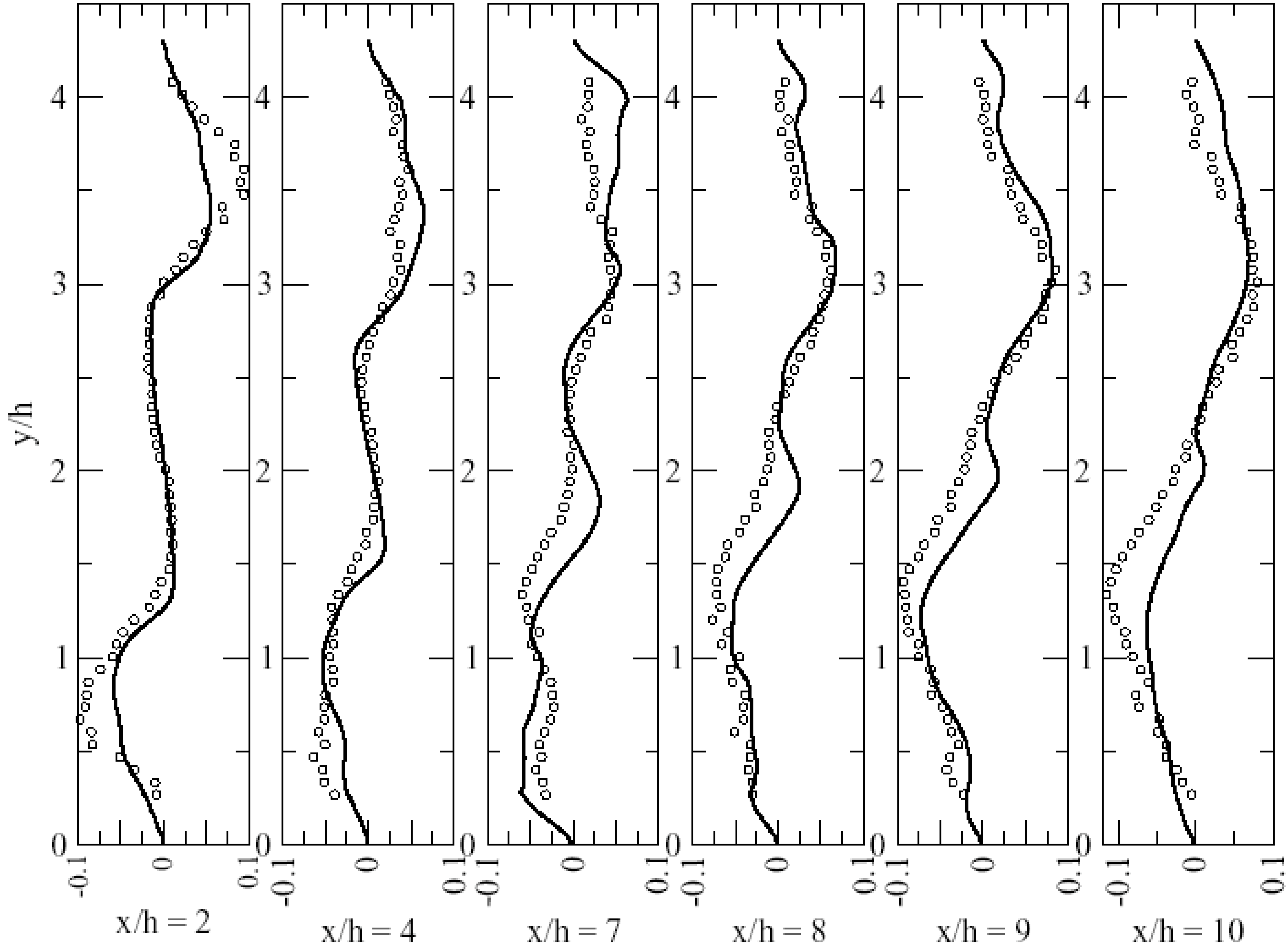
Time averaged streamwise velocity:



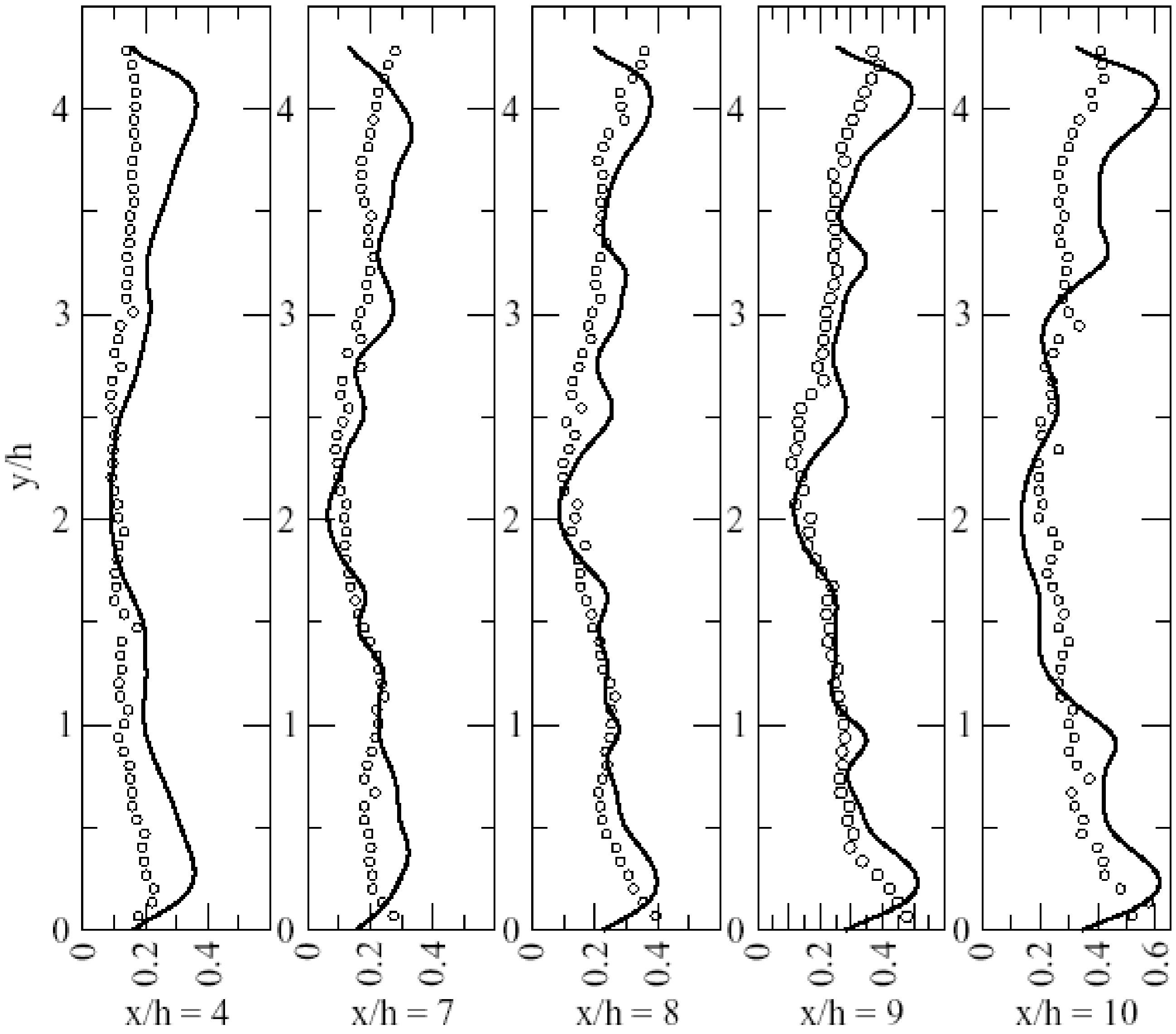
Time averaged spanwise velocity:



Time averaged spanwise velocity:



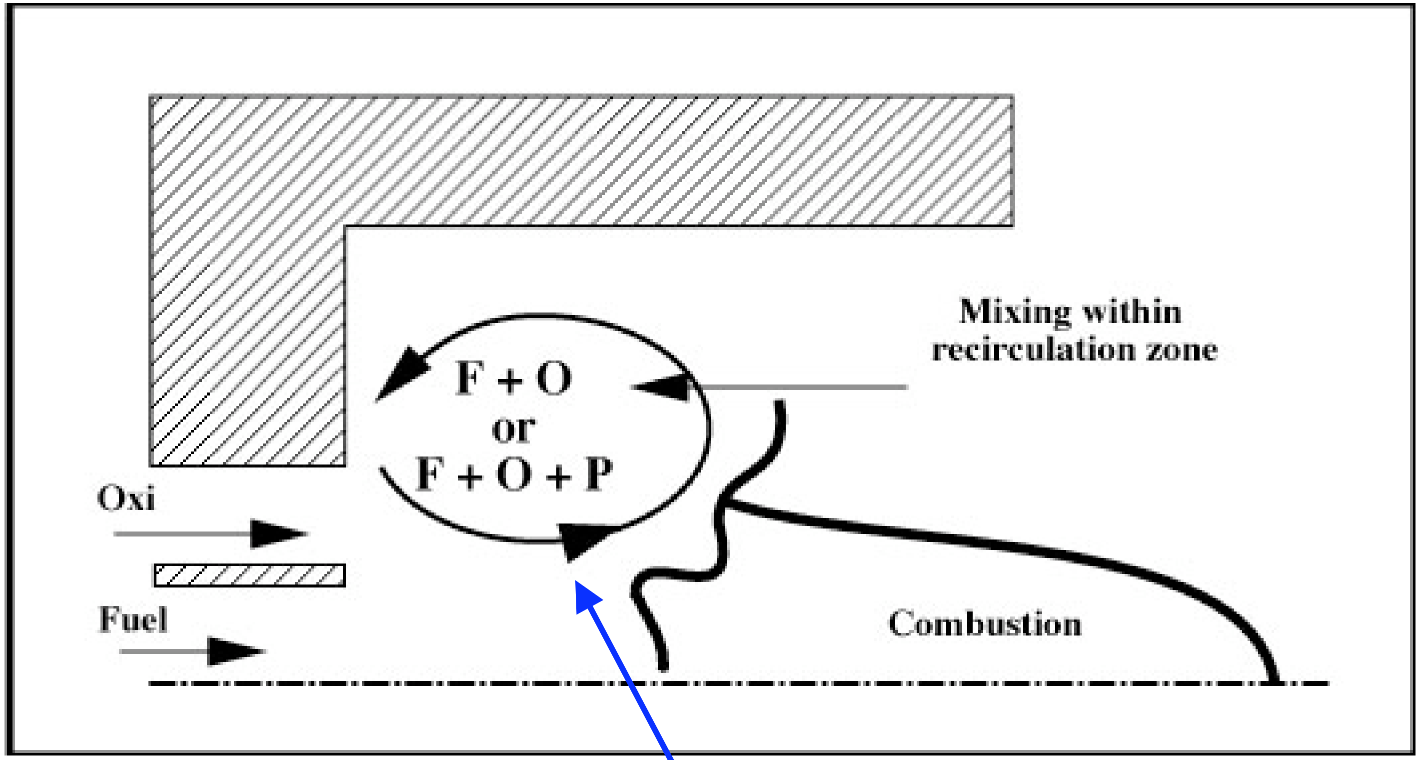
Time averaged RMS velocity:



OUTLINE

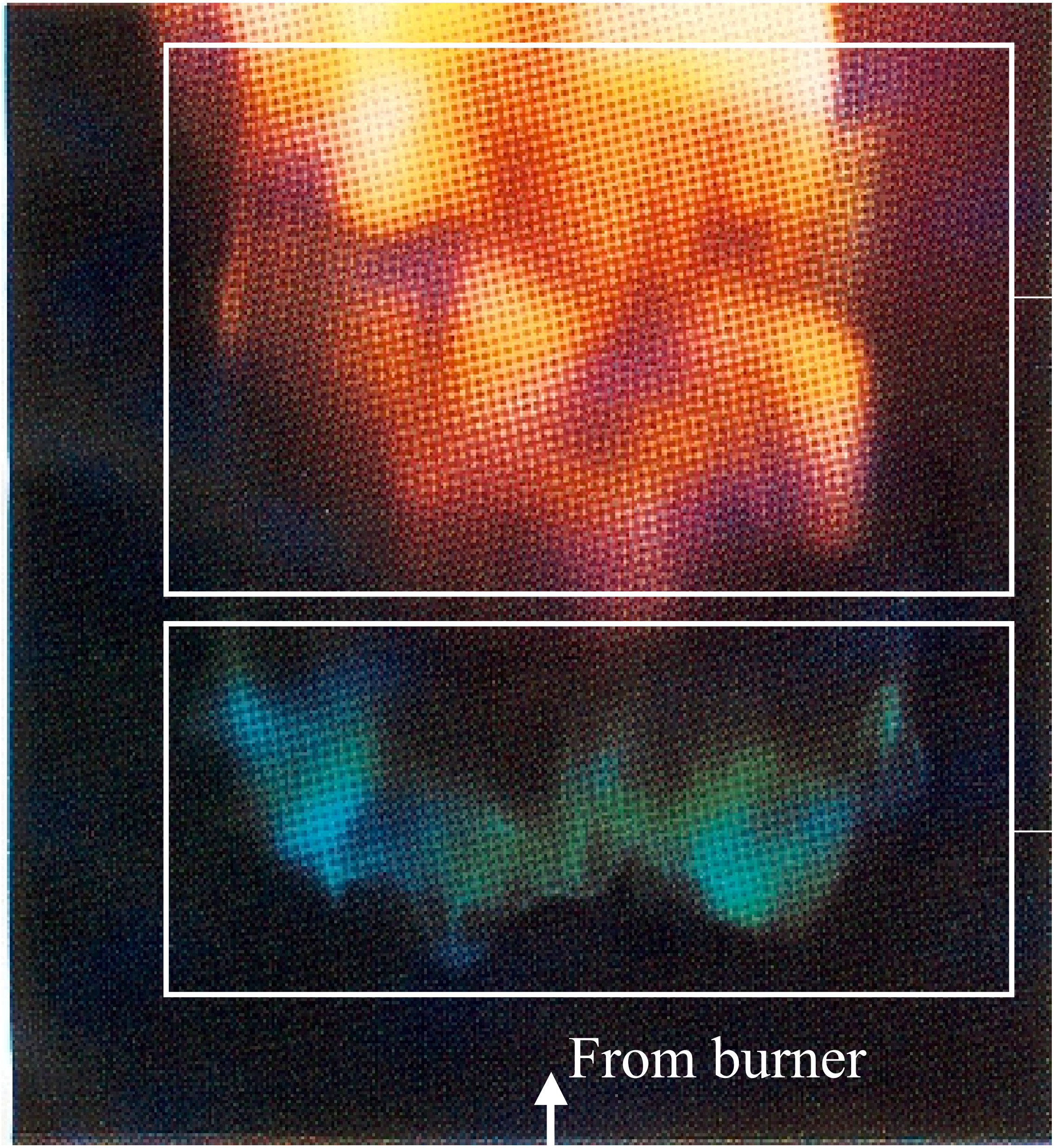
- ✓ DNS of turbulent combustion.
- ✓Overview of turbulent combustion modeling.
- ✓ One example of SGS modeling for LES of premixed turbulent combustion.
- ✓ **SGS modeling of partially premixed combustion.**

Industrial combustion



Nox emission control

Nonpremixed turbulent flame base:

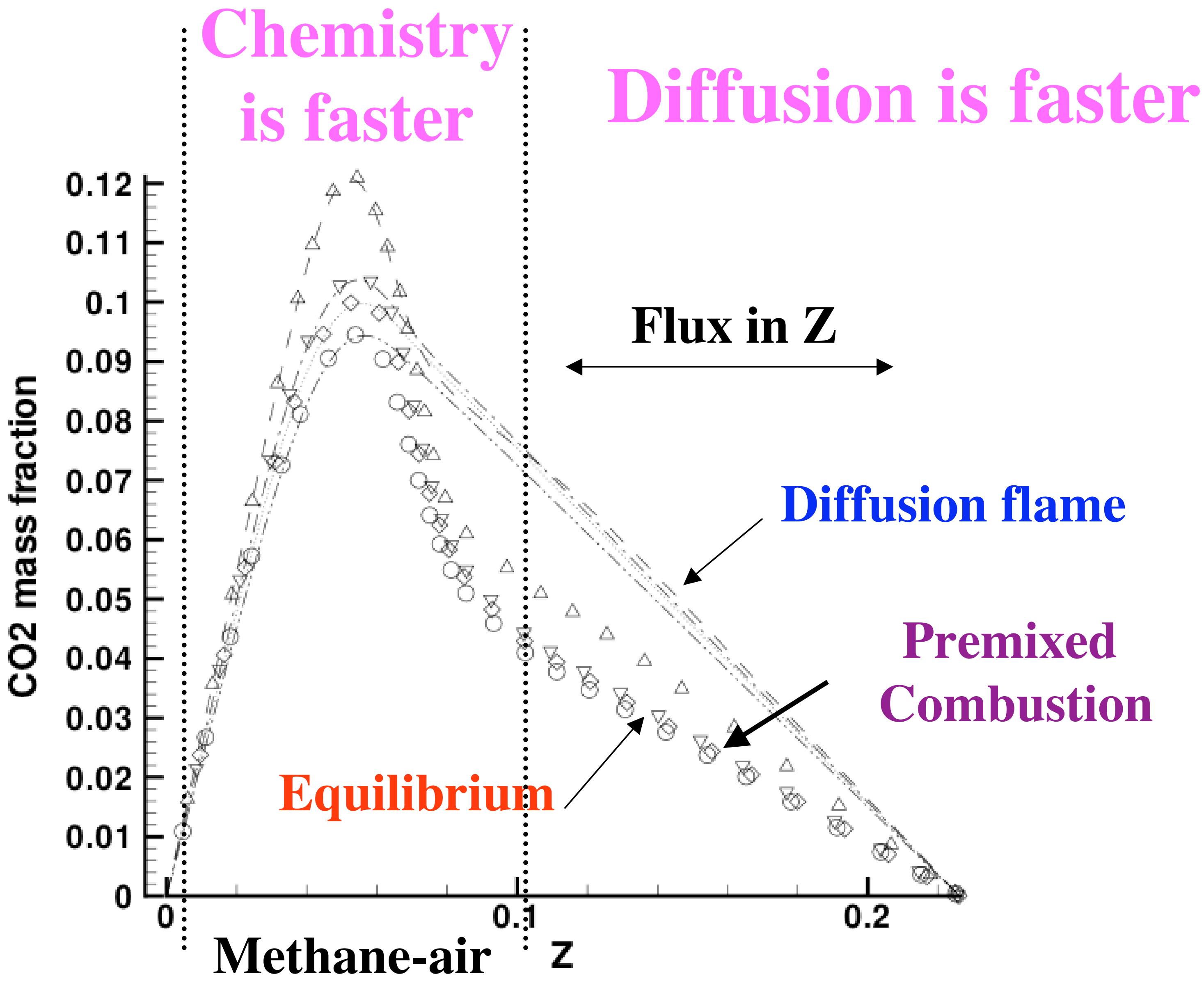


Muniz & Mungal, Combust. Flame 111(1/2), 1997

Zone 2: **Diffusion properties**
- **Mixing controlled**
- **Pollution**
- **Flame length**

Zone 1: **Premixed properties**
- **Thin reaction zones**
- **Interface fresh/burnt**
- **Propagation**
- **Stabilization**

Premixed/Diffusion combustion



Chemistry is faster

Diffusion is faster

Flux in Z

Diffusion flame

Premixed Combustion

Equilibrium

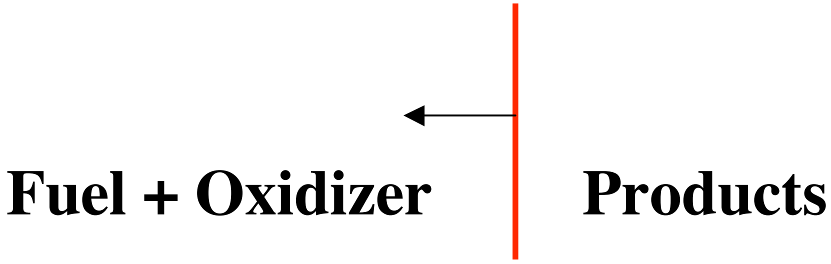
Methane-air

Fiorina et al. Combust. Flame, 140(3), 147-160, (2005)

Takeno’s flame index to determine combustion regime:

$$G_{FO} = \nabla Y_F \cdot \nabla Y_O$$

Premixed



Fuel + Oxidizer

Products

$$G_{FO} > 0$$

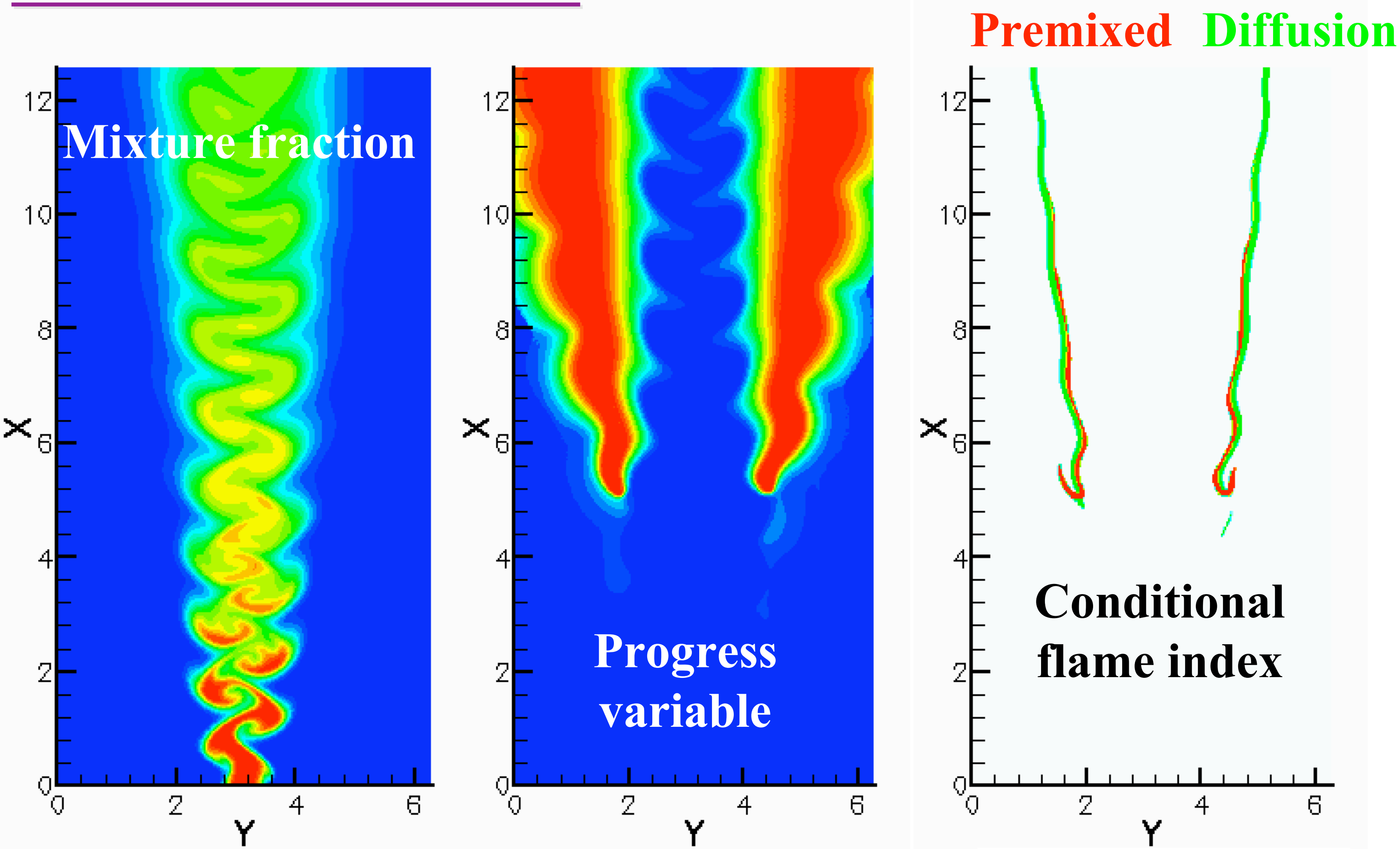
Diffusion

Fuel

Oxidizer

$$G_{FO} < 0$$

DNS of lifted flames:



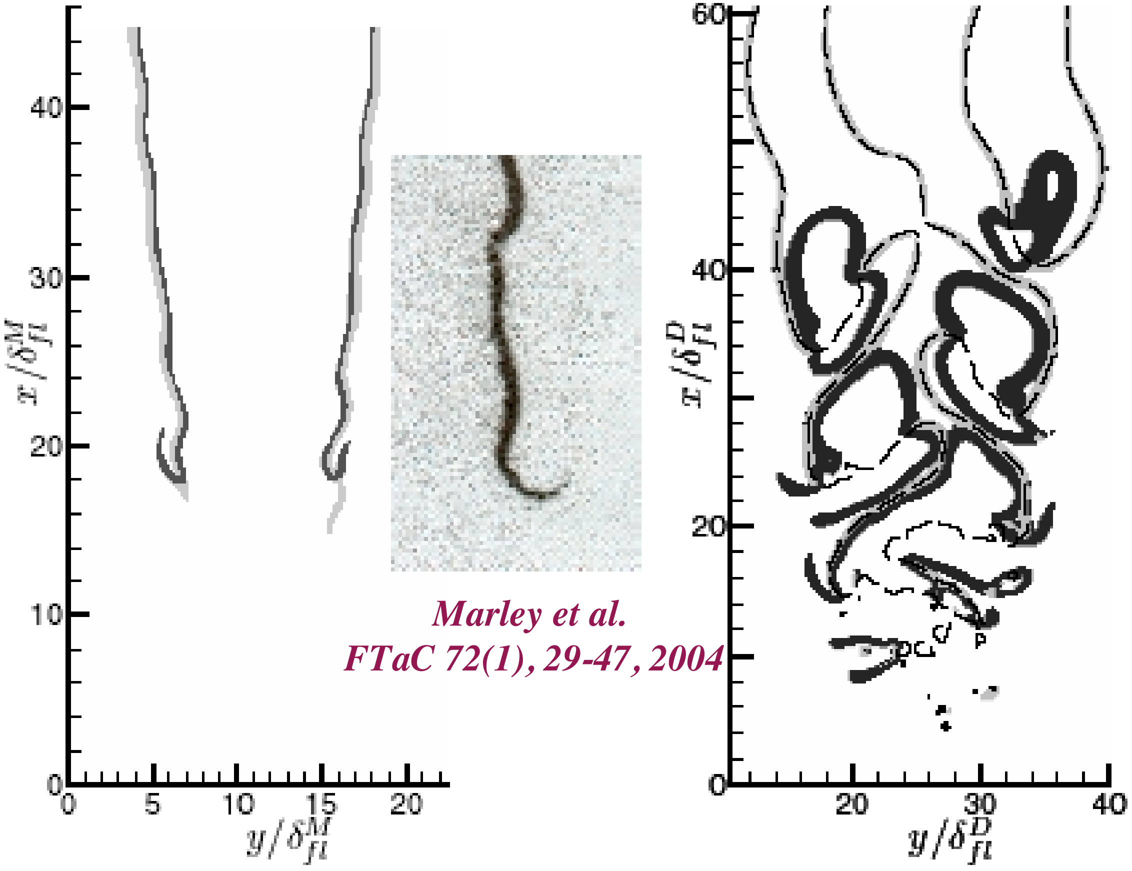
$$\xi_p = \frac{1}{2}\left(1 + \vec{n}_F \bullet \vec{n}_O\right)$$

Hot air 900K St = 0.4

Sixth order PADE, Third order time stepping, NSCBC Boundary conditions

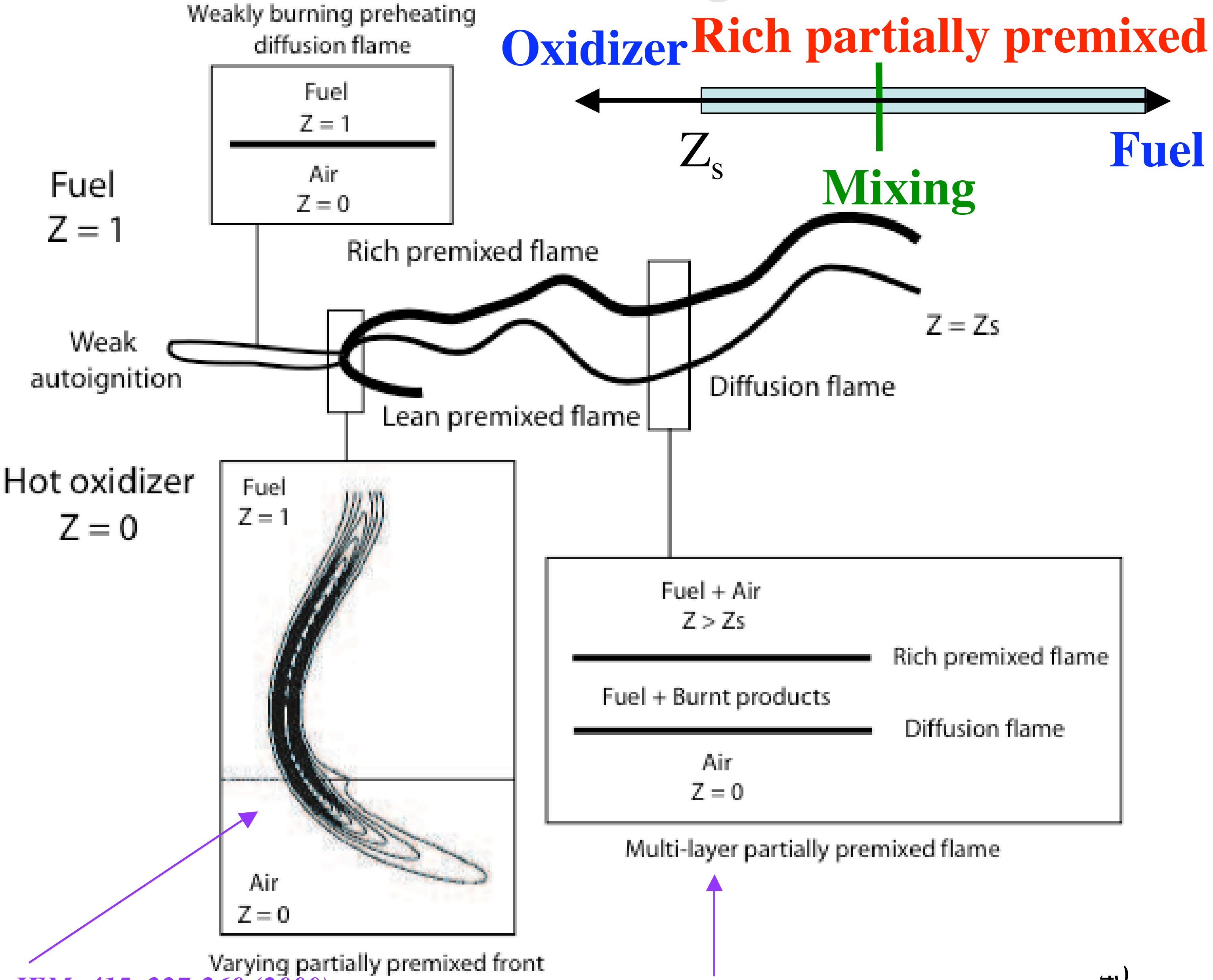
DNS of weakly turbulent flame bases:

Gaseous **Spray**



Marley et al.
FTaC 72(1), 29-47, 2004

Turbulent flame base structure (gaseous case):



Ghosal & Vervisch, JFM, 415, 227-260 (2000)

Li & Williams, Combust. Flame, 118(3):399-414, (1999)

Amplitude of the burning rate in premixed mode:

$$\xi_p = \frac{1}{2}\left(1 + \frac{\nabla Y_F}{\mid \nabla Y_F \mid} \cdot \frac{\nabla Y_O}{\mid \nabla Y_O \mid}\right)$$

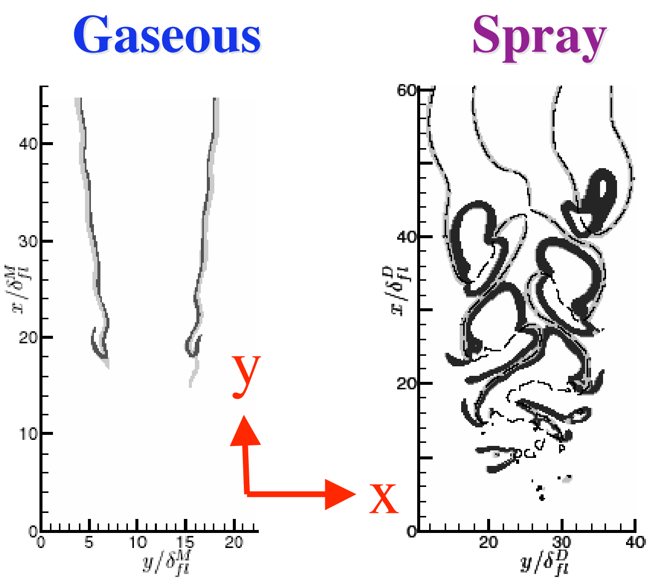
= 1 Premixed

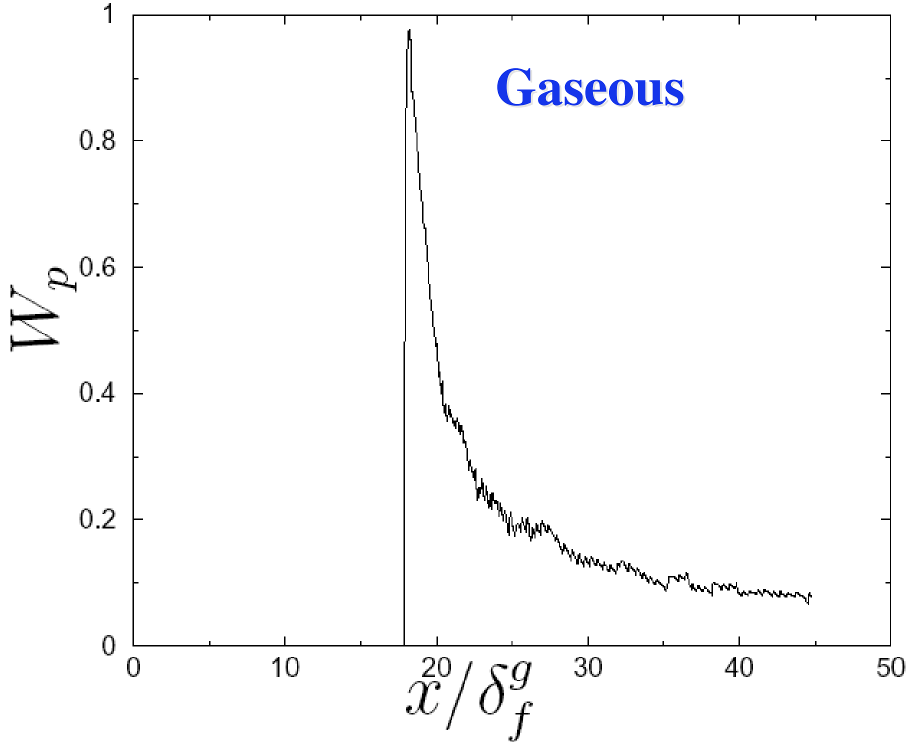
= 0 Diffusion

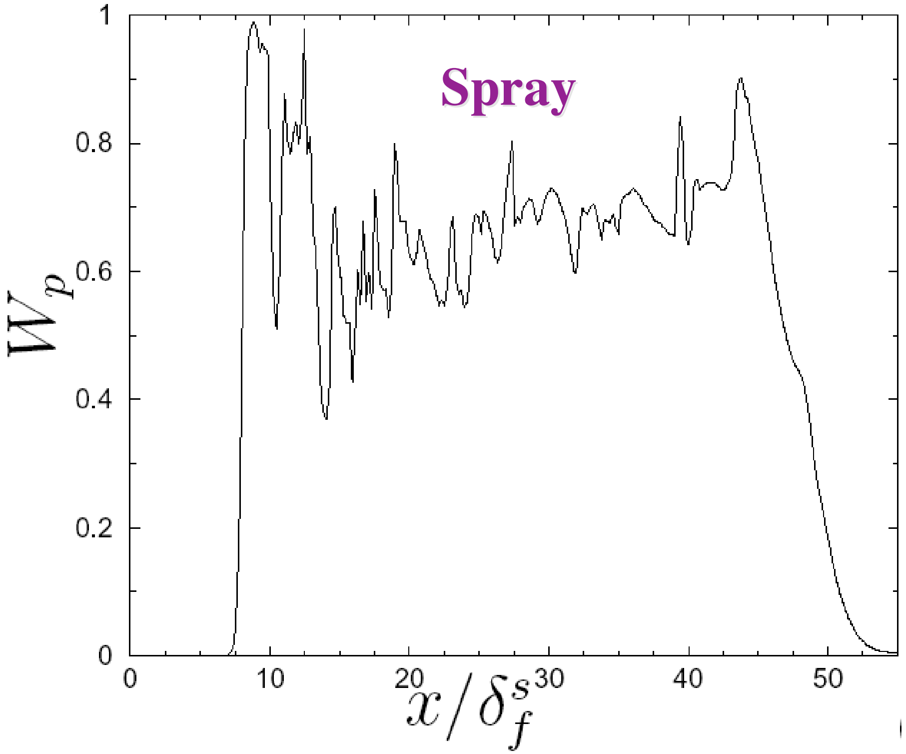
$$\boxed{W_p(x) = \frac{\int_y \xi_p \dot{\omega} dy}{\int_y \dot{\omega} dy}}$$

Fraction of premixed burning:

$$W_p(x) = \frac{\int_{L_y} \xi_p \dot{\omega}_F dy}{\int_{L_y} \dot{\omega}_F dy}$$





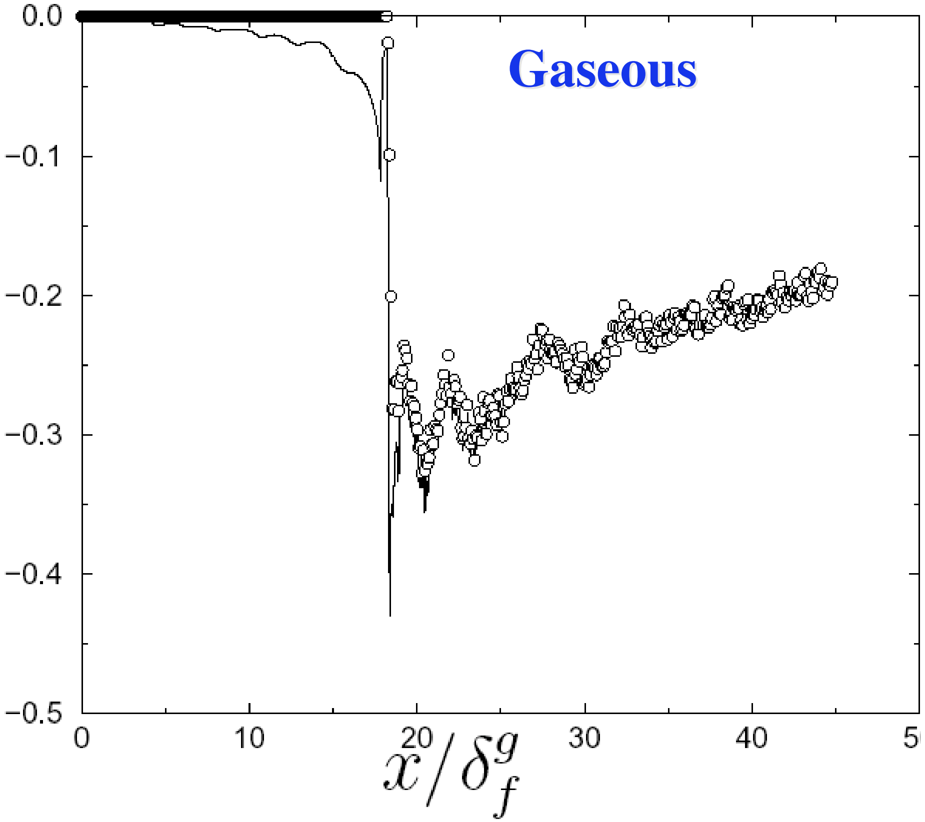


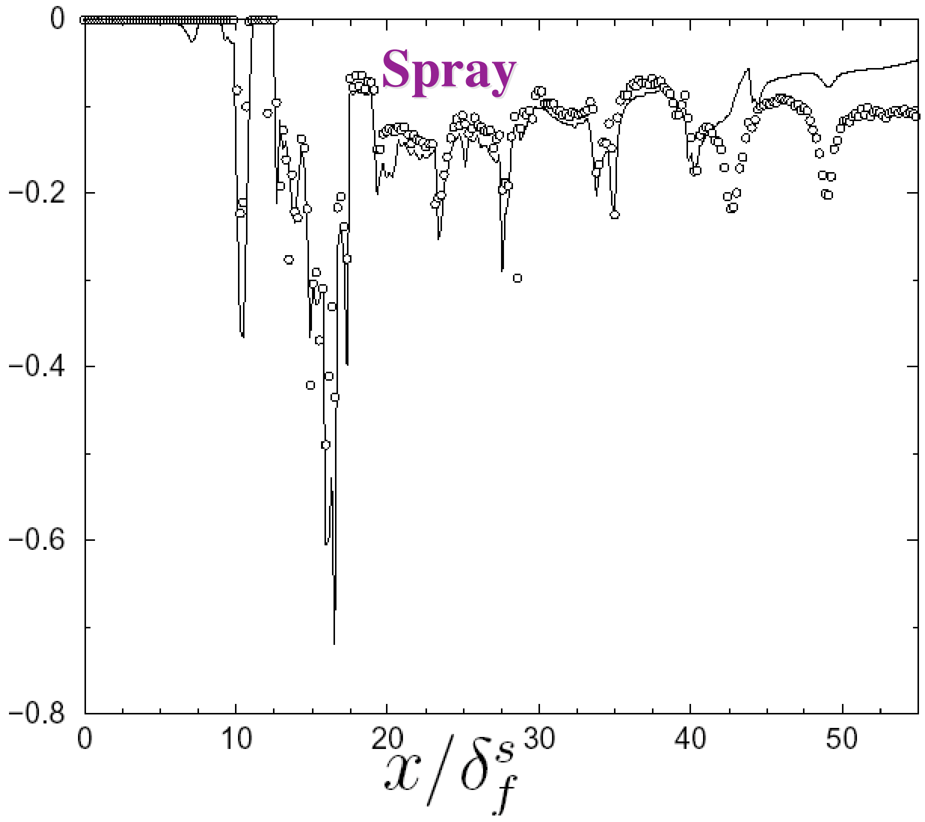
Diffusion flamelet, but only for the “diffusion-part”:

$$\chi_Z \frac{dY_F^d}{dZ^2} = -\dot{\omega}_F^d(Z, \chi_Z)$$

$$\mathcal{I}_d^{DNS} = \int_{L_y} (1-\xi_p)\dot{\omega}_F dy$$

$$\mathcal{I}_d^{Eq.38} = \int_{L_y} (1-\xi_p)\dot{\omega}_F^d(Z, \chi_Z) dy$$





Flame decomposition:

$$\overline{\dot{\omega}_F} = \overline{\xi_p \dot{\omega}_F^p} + \overline{(1 - \xi_p) \dot{\omega}_F^d}$$

Modeled decomposition:

$$\overline{\dot{\omega}_F} = \overline{\alpha}_p \overline{\dot{\omega}_F^p} + \overline{\alpha}_d \overline{\dot{\omega}_F^d}$$

Modeled coefficients:

$$\overline{\alpha}_p = \frac{\overline{\xi_p \dot{\omega}_F^p}}{\overline{\dot{\omega}_F^p}} \quad \overline{\alpha}_d = \frac{\overline{(1 - \xi_p) \dot{\omega}_F^d}}{\overline{\dot{\omega}_F^d}}$$

Modeled decomposition:

- *Domingo et al, “DNS analysis of partially premixed combustion in spray and gaseous turbulent-flame bases stabilized in hot air”, Combust. Flame, 103(3): 172-195, 2005.*

- *Reveillon & Vervisch, “Analysis of weakly turbulent diluted-spray flames and spray combustion regimes”, JFM, 537:317-347, 2005.*

$$\overline{\dot{\omega}_F} = \overline{\alpha_p}\overline{\dot{\omega}_F^p} + \overline{\alpha_d}\overline{\dot{\omega}_F^d}$$