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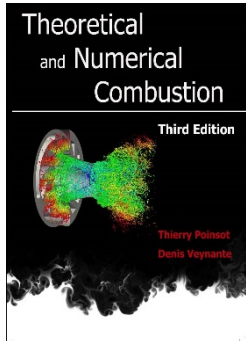
*Iran First International Combustion School (ICS2019)*  
*Tehran, 24-26 August 2019*

## **Combustion Modeling**

### **6. Turbulent Combustion Modeling**

**Alberto Cuoci**

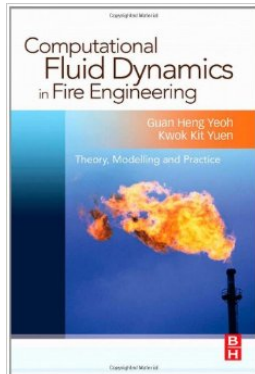
# References



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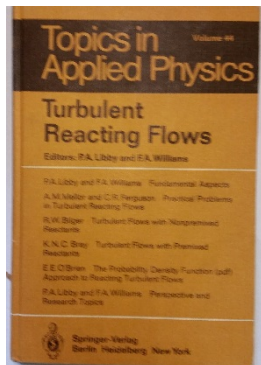
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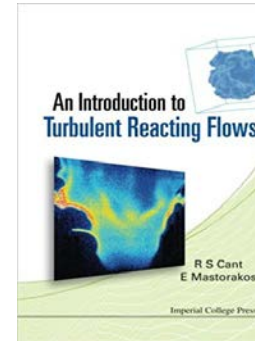
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Princeton Combustion Summer School 2018

<https://cefr.princeton.edu/combustion-summer-school/archived-programs/2018-session/lecture-notes>

## 1. Introduction to turbulent combustion modeling

- a) Averaged equations
- b) Effects of turbulent fluctuations on chemical reactions
- c) Need of turbulent combustion models

## 2. Non-premixed combustion

- a) Eddy Dissipation models: ED, ED-FR, EDC
- b) Steady Laminar Flamelet model
  - i. Mixture fraction
  - ii. Flamelet equations
  - iii. Presumed PDF approach

## 3. Premixed combustion

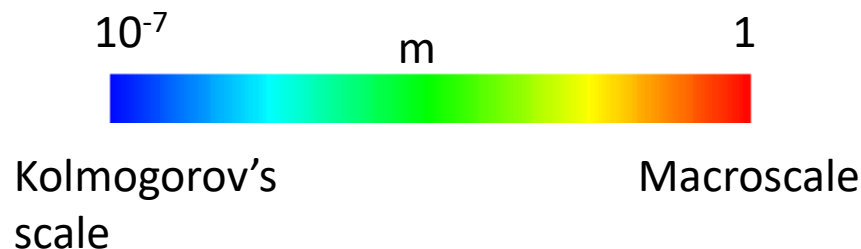
- a) Eddy Break-Up (EBU) model
- b) Bray-Libby-Moss (BLM) model
- c) G-Equation

# Solution of transport equations

The turbulent flows are described by the usual conservation equations of mass, species, momentum and energy

In principle, after assigning the proper boundary and initial conditions, we can solve the transport equations using the numerical techniques we discussed, in order to estimate the relevant variables in every point of the computational domain.

**Problem!** The number of grid points to describe the details of turbulent flows is huge, because of the wide range of scales (from the Kolmogorov's scale to the macroscale)



This direct approach (DNS or Direct Numerical Solution) is possible only for simple flows and for small Reynolds numbers:



**DNS:** Direct Numerical Simulation



# Example

Ratio between the Kolmogorov's and the integral scales:

$$\frac{\eta}{l_0} = Re_t^{-3/4}$$

Example

Turbulent jet

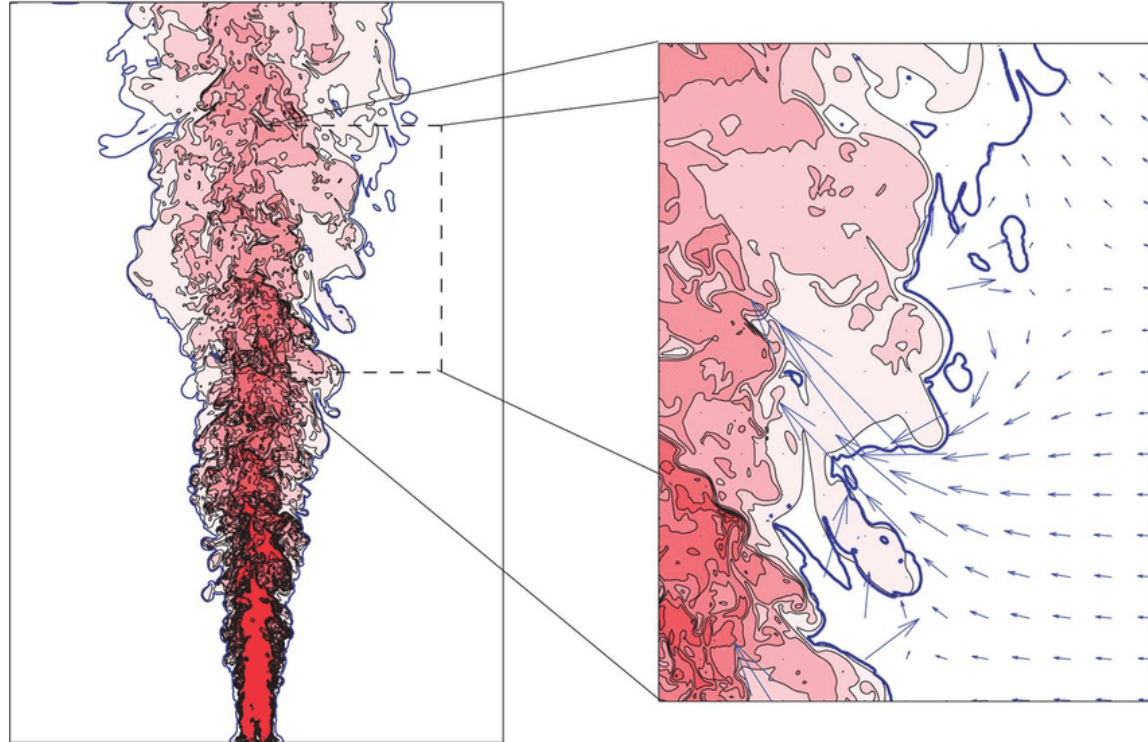
$$Re_{l_0} = 5,000$$

Number of points per direction

$$\frac{l_0}{\eta} = n \sim 600$$

Total number of mesh points:

$$n^3 \sim 0.21 \cdot 10^9$$



Craske, John. (2016). The properties of integral models for planar and axisymmetric unsteady jets. IMA Journal of Applied Mathematics. 82. hxxw043. 10.1093/imamat/hxxw043.

# Numerical modeling of turbulent flows

**Semi-empirical correlations:** this methodology is very simple and useful for some applications of interest for Chemical Engineering. However, this approach is not very general (it is valid only for the conditions for which the correlation was developed) and not always it is very useful for the understanding of the phenomenon under investigation

**Integral equations:** they can be derived from the integration of conservation equations along one or more than one coordinates; the resulting problem to be solved is describe by one or more differential equations

**Reynolds Averaged Navier-Stokes (RANS):** this methodology consists of a system of PDE (partial differential equations) which is derived from a proper averaging in time of conservation equations of relevant variables (momentum, pressure, energy and species). The RANS equations however need a proper closure, i.e. sub-models describing non-linear effects

**Large Eddy Simulation (LES):** in this approach a new set of partial differential equations is solved, in which the new variables are filtered in space (i.e. only the scales larger than a so called filter width are solved). Only LES approach requires a proper closure, i.e. submodels describing the effects of small scales (which are not resolved)

**Direct Numerical Simulation (DNS):** the transport equations of relevant species are solved directly

Computational cost



# Numerical modeling of turbulence (I)

## DNS

### Direct Numerical Simulation

The transport equations are resolved as they are, with any filtering or averaging

## LES

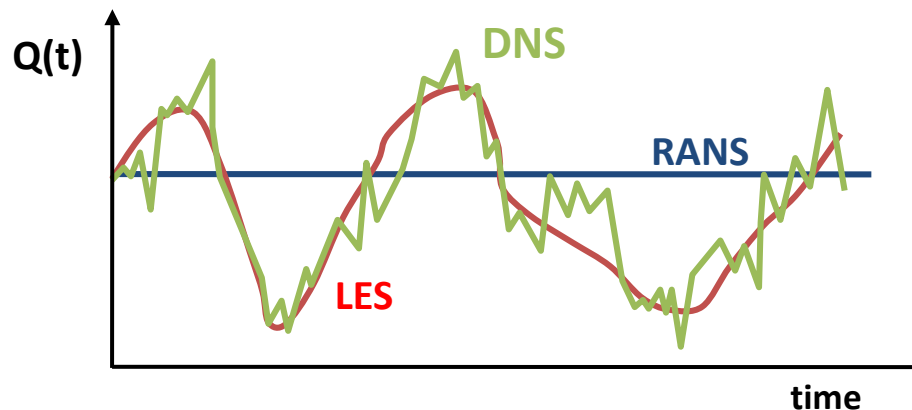
### Large Eddy Simulation

Only largest vortices are transported. Computational cells are too large to describe small vortices, which are modeled using proper sub-grid scale models

## RANS

### Reynolds-Averaged Navier-Stokes

Only the mean quantities are transported. The transport equations require closure models.

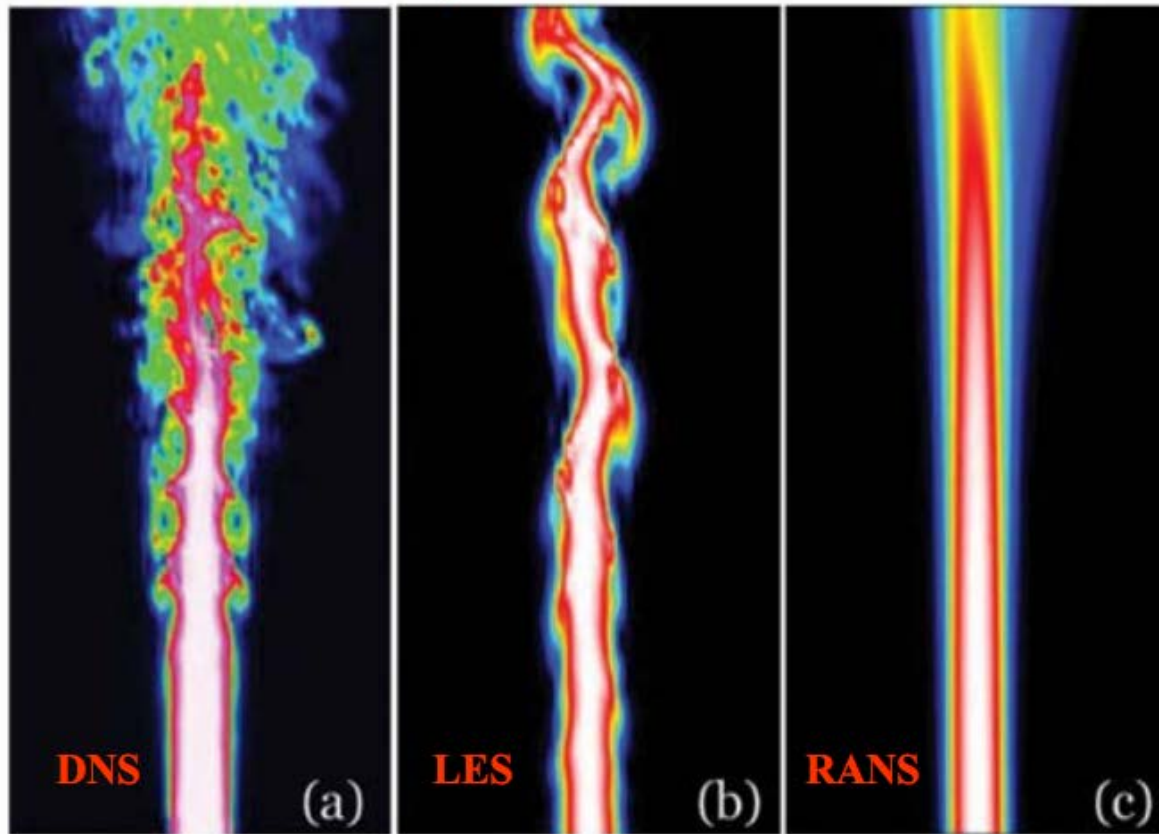


RANS

**Advantages:** computational cost very low

**Disadvantages:** inaccuracy of closure models

# Numerical modeling of turbulence (II)



Small vortices are not transported, but modelled

Only mean quantities are available in RANS



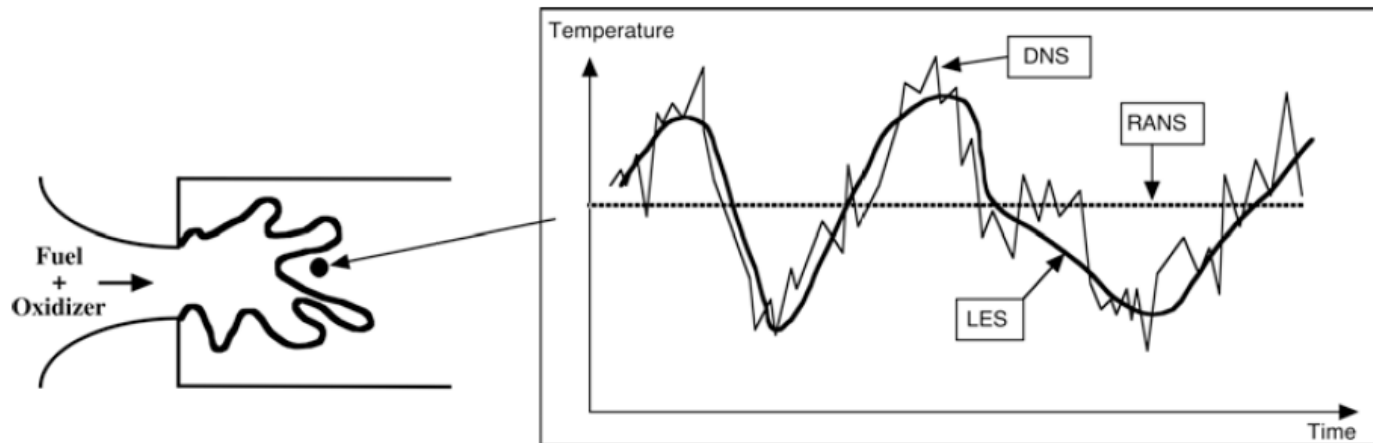
# Reynolds Averaged Navier-Stokes (RANS)

- Reynolds Averaged Navier-Stokes (or RANS) computations have **historically** been the first possible approach because the computation of the instantaneous flow field in a turbulent flame was impossible.
- Therefore, RANS techniques were developed to solve for the **mean values** of all quantities.
- The **balance equations for Reynolds or Favre averaged quantities** are obtained by averaging the instantaneous balance equations.
- The averaged equations require **closure rules**: a **turbulence model** to deal with the flow dynamics in combination with a **turbulent combustion model** to describe chemical species conversion and heat release.
- Solving these equations provide averaged quantities corresponding to **averages over time** for stationary mean flows or **averages over different realizations** (or cycles) for periodic flows like those found in piston engines (i.e. phase averaging).
- For a stabilized flame, the temperature predicted with RANS at a given point is a constant corresponding to the mean temperature at this point.

Poinsot T., Veynante D., *"Theoretical and Numerical Combustion"*, R.T. Edwards, 2<sup>nd</sup> Edition, 2005

# Large Eddy Simulation (LES)

- The turbulent large scales are explicitly calculated whereas the effects of smaller ones are modeled using subgrid closure rules.
- The balance equations for large eddy simulations are obtained by filtering the instantaneous balance equations.
- LES determines the instantaneous position of a “large scale” resolved flame front but a subgrid model is still required to take into account the effects of small turbulent scales on combustion.
- LES would capture the low-frequency variations of temperature.

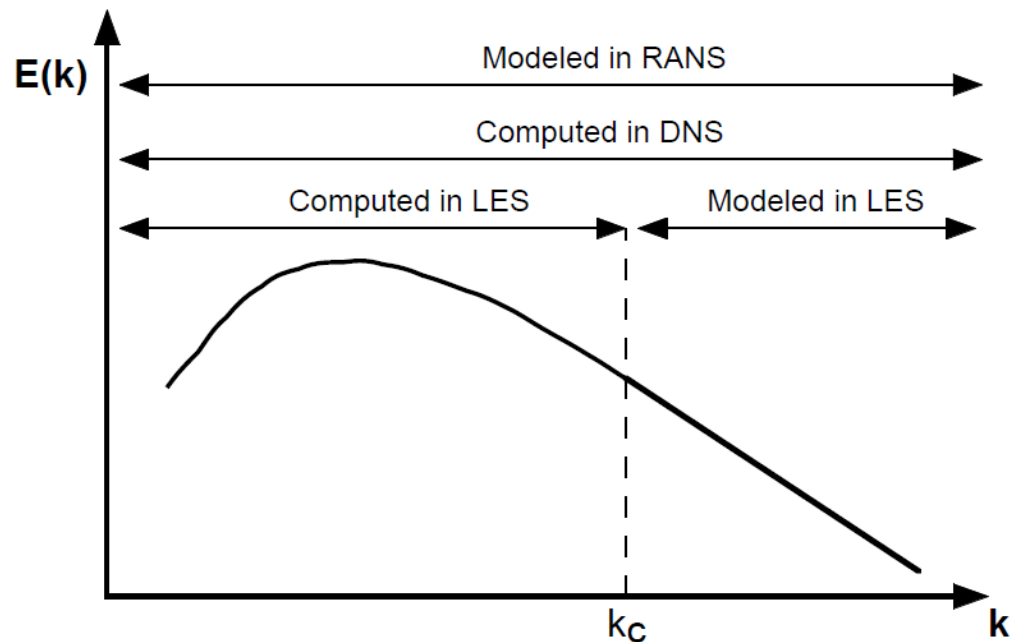


Poinsot T., Veynante D., “Theoretical and Numerical Combustion”, R.T. Edwards, 2<sup>nd</sup> Edition, 2005

# Comparison: DNS, LES, and RANS

- All spatial frequencies in the spectrum are resolved in direct numerical simulations
- Only the largest ones (up to a cut-off wave number  $\kappa_c$ ) are computed in LES (the effects of motions smaller than the cut-off length scale, having a wave number  $\kappa$  larger than  $\kappa_c$ , are modeled).
- In RANS, only mean flow fields are resolved: no turbulent motion is explicitly captured.

Turbulence energy spectrum plotted as a function of wave numbers. RANS, LES and DNS are summarized in terms of spatial frequency range.  $\kappa_c$  is the cut-off wave number used in LES (log-log diagram).



Poinsot T., Veynante D., "Theoretical and Numerical Combustion", R.T. Edwards, 2<sup>nd</sup> Edition, 2005

# Computational requirements

- In terms of computational requirements, CFD for non-reacting and reacting flows follow similar trends: DNS is the most demanding method and is limited to fairly low Reynolds numbers and simplified geometries.
- LES works with coarser grids (only larger scales have to be resolved) and may be used to deal with higher Reynolds numbers but require subgrid scale models. The computation quality and the results accuracy are directly linked to these physical subgrid models.
- In current engineering practice, RANS is extensively used because it is less demanding in terms of resources but its validity is limited by the closure models describing turbulence and combustion

Poinsot T., Veynante D., *"Theoretical and Numerical Combustion"*, R.T. Edwards, 2<sup>nd</sup> Edition, 2005

# Comparison: DNS, LES, and RANS

|      | Advantages  | Drawbacks  |
|------|---|--|
| RANS | <ul style="list-style-type: none"><li>- Coarse numerical mesh</li><li>- Geometrical simplifications (2D, symmetries, etc.)</li><li>- Limited computational cost</li></ul> | <ul style="list-style-type: none"><li>- Only mean flow fields</li><li>- Closure models required</li></ul>  |
| LES  | <ul style="list-style-type: none"><li>- Unsteady features</li><li>- Reduced modelling impact (if compared to RANS)</li></ul>  | <ul style="list-style-type: none"><li>- Subgrid models required</li><li>- 3D simulations</li><li>- Advanced/accurate numerical techniques</li><li>- Computational cost</li></ul> |
| DNS  | <ul style="list-style-type: none"><li>- No closure/subgrid models for turbulence and turbulence/combustion interactions</li><li>- Tool to study closure models</li></ul>  | <ul style="list-style-type: none"><li>- Prohibitive computational cost</li><li>- Limited to academic problems</li></ul>  |

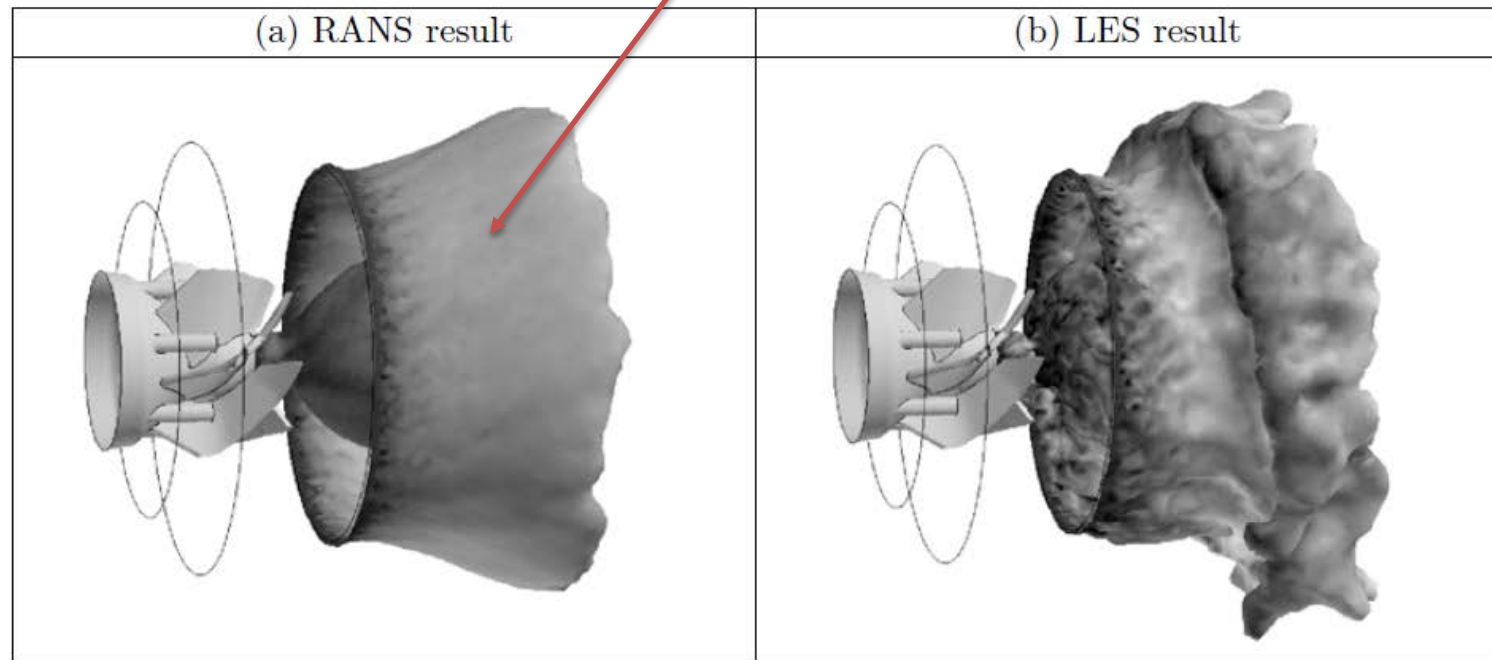
Poinsot T., Veynante D., *"Theoretical and Numerical Combustion"*, R.T. Edwards, 2<sup>nd</sup> Edition, 2005



# Computational advantages of RANS (I)

The advantage of RANS is its applicability to any configuration and operating conditions: a standard RANS mesh can contain  $10^5 - 10^6$  cells and the domain of calculation may be as large as needed.

On the iso-surface, the average temperature is 1100 K but RANS does not explicitly solve for possible turbulent fluctuations around this mean value.



Iso-surface of mean high temperature (1100 K) in a turbulent premixed flame stabilized by swirl. (Selle et al., 2004).

# Computational advantages of RANS (II)

The same example, simulated via a DNS, would be basically unfeasible. Indeed, while for the RANS simulation the cell size is  $\sim 1 - 5 \text{ mm}$ , for the DNS it would be  $\sim 10 - 50 \text{ }\mu\text{m}$ , i.e.  $\sim 100$  times smaller. Thus, the required computational mesh (in terms of number of cells) would be  $\sim 100^3 = 10^6$  times larger!

## Why do similar problems treated with DNS and RANS require so different grid sizes?

- DNS has to describe the smallest scales contained in the flow field and to resolve the inner instantaneous structure of the flame front. This last condition determines the grid size. For hydrocarbon/air flames at atmospheric pressure, fronts have a thickness of the order of  $0.1 \text{ mm}$  so that mesh sizes of the order of  $\mu\text{m}$  are required.
- In contrast, RANS considers an average flame front which extends over a broader region: only mean turbulence characteristics and average statistical position of the front are solved for. Typical mean flame brushes in burners, aircraft or piston engine have a thickness of 1 to 2 cm and may be easily resolved with a 2 mm mesh.
- Engineering codes using RANS techniques (the majority of current computational tools) never resolve the inner structure of the flame and provide average flow fields featuring scales which are much larger than the instantaneous flame thickness.

# Reynolds' and Favre's averaging

**Reynolds' Average:** mean and fluctuation, e.g. for the flow velocity  $u_i$ :

$$u_i = \bar{u}_i + u'_i$$

Mean of the fluctuation is zero (applies for all quantities):

$$\bar{u}'_i = 0$$

Mean of the squared fluctuation is not zero:

$$\sqrt{\overline{u'_i u'_i}} = \sqrt{\overline{u'^2_i}} = \sqrt{\overline{u'^2_1} + \overline{u'^2_2} + \overline{u'^2_3}} \neq 0$$

**Favre's Average** (density-weighted mean velocity):

$$\overline{\rho u_i} = \overline{\rho(\tilde{u}_i + u''_i)} = \bar{\rho}\tilde{u}_i + \overline{\rho u''_i} = \bar{\rho}\tilde{u}_i \quad \rightarrow \quad \tilde{u}_i = \frac{\overline{\rho u_i}}{\bar{\rho}}$$

# Passive-scalar transport equations (I)

Let us consider the transport equation for a passive scalar  $\phi$ , i.e. a scalar without any source term and without impact on the main fluid dynamic variables (velocity, pressure, and density). Let us also consider the general case of a compressible fluid:

$$\rho \frac{\partial \phi}{\partial t} + \rho u_i \frac{\partial \phi}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho \mathcal{D}_\phi \frac{\partial \phi}{\partial x_i} \right)$$

If we apply the Reynolds average to every term and we consider the definition of Favre average (i.e. density-weighted average), we get the following averaged equation:

$$\bar{\rho} \frac{\partial \tilde{\phi}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \tilde{\phi}}{\partial x_i} = \underbrace{\frac{\partial}{\partial x_i} \left( \overline{\rho \mathcal{D}_\phi \frac{\partial \phi}{\partial x_i}} \right)}_{\text{molecular transport}} - \underbrace{\frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' \phi''})}_{\text{turbulent transport}}$$

**Unclosed terms**

# Passive-scalar transport equations (II)

A typical simplification is to assume that the molecular transport is negligible with respect to the turbulent transport (this simplification implies the assumption of high Reynolds' number)

The turbulent transport term is usually modelled using the gradient transport model:

$$\widetilde{u_i''\phi''} = -\mathcal{D}_t \frac{\partial \tilde{\phi}}{\partial x_i}$$

$\mathcal{D}_t$  is the turbulent diffusivity, proportional to the turbulent viscosity:

$$\mathcal{D}_t = \frac{\nu_t}{Sc_t}$$

Thus, the transport equation for the mean passive scalar is:

$$\bar{\rho} \frac{\partial \tilde{\phi}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \tilde{\phi}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \mathcal{D}_t \frac{\partial \tilde{\phi}}{\partial x_i} \right)$$



# Passive-scalar transport equations (III)

It is possible to derive a transport equation for the variance of a passive scalar  $\phi$ . The demonstration is reported in many textbooks and in [Pitsch2018]:

$$\bar{\rho} \frac{\partial \widetilde{\phi''^2}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \widetilde{\phi''^2}}{\partial x_i} = - \frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' \phi''^2}) + 2\bar{\rho} (-\widetilde{u_i'' \phi''}) \frac{\partial \tilde{\phi}}{\partial x_i} - 2\bar{\rho} \mathcal{D}_\phi \left( \frac{\partial \phi''}{\partial x_i} \right)^2$$

dissipation

$$\widetilde{u_i'' \phi''^2} = -\mathcal{D}_t \frac{\partial \widetilde{\phi''^2}}{\partial x_i}$$

Turbulent transport

$$\widetilde{u_i'' \phi''} = -\mathcal{D}_t \frac{\partial \tilde{\phi}}{\partial x_i}$$

production

$$\bar{\rho} \frac{\partial \widetilde{\phi''^2}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \widetilde{\phi''^2}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \mathcal{D}_t \frac{\partial \widetilde{\phi''^2}}{\partial x_i} \right) + 2\bar{\rho} \mathcal{D}_t \left( \frac{\partial \tilde{\phi}}{\partial x_i} \right)^2 - \bar{\rho} \chi$$

Scalar dissipation  $\chi \stackrel{\text{def}}{=} 2\mathcal{D}_\phi \left( \frac{\partial \phi''}{\partial x_i} \right)^2$

# Scalar dissipation model

Integral time  $\tau_\phi$  (dimensional analysis,  $[\chi] = s^{-1}$ )

$$\tau_\phi \sim \frac{\widetilde{\phi''^2}}{\chi}$$

Typically proportional to  $\tau$

$$\tau = \frac{\tilde{k}}{\tilde{\varepsilon}} = C_\chi \tau_\phi \quad 1.5 \leq C_\chi \leq 3$$

This leads to

$$\chi = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{\phi''^2}$$

**Pitsch H.**

*“Combustion Theory and Applications in CFD”*  
Princeton Combustion Summer School 2018

# Passive-scalar transport equations: summary

Transport equation for mean passive scalar  $\phi$ :

$$\bar{\rho} \frac{\partial \tilde{\phi}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \tilde{\phi}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \mathcal{D}_t \frac{\partial \tilde{\phi}}{\partial x_i} \right)$$

Transport equation for mean variance of passive scalar  $\phi$ :

$$\bar{\rho} \frac{\partial \widetilde{\phi'^2}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \widetilde{\phi'^2}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \mathcal{D}_t \frac{\partial \widetilde{\phi'^2}}{\partial x_i} \right) + 2 \bar{\rho} \mathcal{D}_t \left( \frac{\partial \tilde{\phi}}{\partial x_i} \right)^2 - \bar{\rho} C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{\phi'^2}$$

# Reactive species transport equations (I)

Let us consider the transport equation for a reactive species whose mass fraction is  $Y_k$ :

$$\rho \frac{\partial Y_k}{\partial t} + \rho u_i \frac{\partial Y_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho \mathcal{D}_k \frac{\partial Y_k}{\partial x_i} \right) + \rho S_k$$

The “only” difference with the passive scalar case is the presence of the source term  $S_k$  due to the chemical reactions (actually we will see this is a huge difference). If we apply the averaging, we have:

$$\bar{\rho} \frac{\partial \bar{Y}_k}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \bar{Y}_k}{\partial x_i} = \underbrace{\frac{\partial}{\partial x_i} \left( \overline{\rho \mathcal{D}_k \frac{\partial Y_k}{\partial x_i}} \right)}_{\text{molecular transport}} - \underbrace{\frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' Y_k''})}_{\text{turbulent transport}} + \underbrace{\rho \tilde{S}_k}_{\text{source term}}$$

**Unclosed terms**

# Reactive species transport equations (II)

We can proceed similarly to what we already did for the passive scalar case. In particular, we can neglect the molecular transport contribution and we can use the gradient transport model for the turbulent transport term:

$$\bar{\rho} \frac{\partial \widetilde{Y}_k}{\partial t} + \bar{\rho} \widetilde{u}_i \frac{\partial \widetilde{Y}_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \mathcal{D}_t \frac{\partial \widetilde{Y}_k}{\partial x_i} \right) + \boxed{\rho \tilde{S}_k} \quad \begin{array}{l} \text{Unclosed} \\ \text{terms} \end{array}$$

source  
term

The source term is unclosed. Its modeling is quite complex, because it is a strongly non linear function of temperature and composition. Moreover, its expression is not general, but it depends on the kinetic mechanism describing the reactions in which the species is involved.



Modeling of turbulent combustion!

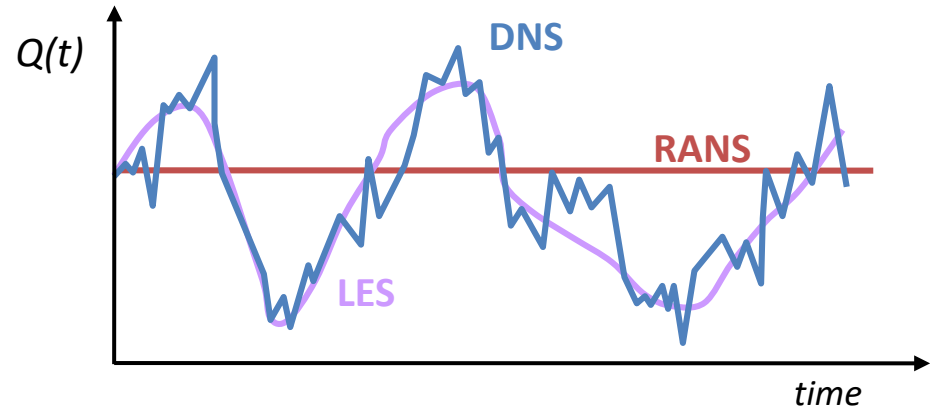


# Numerical modeling of turbulent reacting flows

## DNS

### Direct Numerical Simulation

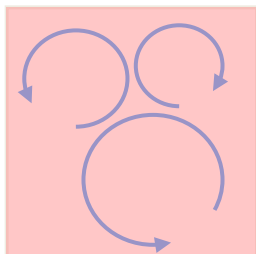
The equations of continuity, momentum, energy and species are solved directly without any manipulation. Extremely expensive from a computational point of view



## LES

### Large Eddy Simulation

The conservation equations are filtered and only the largest vortices are described. Vortices smaller than a characteristic length are only modeled.



## RANS

### Reynolds-Averaged Navier-Stokes

Only the mean variables are described.

*Formation rates have to be modeled*

$$\bar{\rho} \frac{\partial \bar{Y}_k}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \bar{Y}_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \overline{\rho D_k} \frac{\partial \bar{Y}_k}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left( \bar{\rho} \widetilde{u_i'' Y_k''} \right) + \bar{\rho} \tilde{\dot{\Omega}}_k$$

# Characteristic times of chemistry

How to estimate the chemical characteristic times in a system with  $NS$  species and  $NR$  chemical reactions?

$$r_j = k_j \prod_{i=1}^{NS} C_i^{\eta_i^j} \quad j = 1, \dots, NR$$

Reaction rates

$$\dot{\Omega}_i = \sum_{j=1}^{NR} \nu_i^j r_j \quad i = 1, \dots, NS$$

Formation rates

**Fox R.O.**,  
“*Computational Models  
for Turbulent Reacting  
Flows*”, Cambridge  
University Press, 2003

## Eigenvalues of Jacobian

$$J_{ij} = \frac{\partial \dot{\Omega}_i}{\partial C_j} \quad i, j = 1, \dots, NS$$

Jacobian matrix (based on formation rates)

$$\tau_i = \frac{1}{|\lambda_i|} \quad i = 1, \dots, NS$$

Chemical characteristic times

# Chemical vs Fluid dynamic control

Dimensionless parameter to characterize the combustion: **Damköhler Number**

$$Da = \frac{\tau_{flow}}{\tau_{chem}}$$

The fluid dynamic time depends on the features of the system. Each species has a proper characteristic time, depending on the formation rate

Two asymptotic behaviors can be observed:

Chemical regime

$$Da \ll 1$$

Chemical reactions extremely slow. The system is under chemical control

Fluid dynamic regime

$$Da \gg 1$$

Chemical reactions extremely fast. The system is under fluid dynamic control

Peters N., "Turbulent Combustion", Cambridge University Press, 2000

# Effect of fluctuations on formation rates (I)

The formation rate of each chemical species is a function highly non linear of temperature and composition (especially temperature)

$$r(\mathbf{C}, T) = k(T) \sum_i C_i^{\lambda_i} \quad k(T) = AT^n \exp\left(-\frac{E}{RT}\right)$$

Arrhenius' Law

This means that the mean formation rate is not equal to the reaction rate calculated at the mean values of temperature and composition:

$$\bar{r}(\mathbf{C}, T) = \bar{r}(\bar{\mathbf{C}} + \mathbf{C}', \bar{T} + T') \neq r(\bar{\mathbf{C}}, \bar{T})$$

This can be easily demonstrated if we perform a Taylor expansion around the mean values of temperature and composition:

$$\begin{aligned} r(\mathbf{C}, T) = r(\bar{\mathbf{C}} + \mathbf{C}', \bar{T} + T') &= r(\bar{\mathbf{C}}, \bar{T}) + \sum_{i=1}^{NS} \left. \frac{\partial r}{\partial C_i} \right|_{\bar{\mathbf{C}}, \bar{T}} C'_i + \left. \frac{\partial r}{\partial T} \right|_{\bar{\mathbf{C}}, \bar{T}} T' + \dots \\ &\dots + \frac{1}{2} \sum_{i=1}^{NS} \sum_{j=1}^{NS} \left. \frac{\partial^2 r}{\partial C_i \partial C_j} \right|_{\bar{\mathbf{C}}, \bar{T}} C'_i C'_j + \frac{1}{2} \left. \frac{\partial^2 r}{\partial T^2} \right|_{\bar{\mathbf{C}}, \bar{T}} T'^2 + \frac{1}{2} \sum_{i=1}^{NS} \left. \frac{\partial^2 r}{\partial C_i \partial T} \right|_{\bar{\mathbf{C}}, \bar{T}} C'_i T' + h.o. terms \end{aligned}$$

# Effect of fluctuations on formation rates (II)

If we apply the mean:

$$\bar{r}(\mathbf{C}, T) \approx r(\bar{\mathbf{C}}, \bar{T}) + \dots$$

$$\dots + \underbrace{\frac{1}{2} \sum_{i=1}^{NS} \sum_{j=1}^{NS} \left. \frac{\partial^2 r}{\partial C_i \partial C_j} \right|_{\bar{\mathbf{C}}, \bar{T}} \overline{C'_i C'_j} + \frac{1}{2} \left. \frac{\partial^2 r}{\partial T^2} \right|_{\bar{\mathbf{C}}, \bar{T}} \overline{T'^2} + \sum_{i=1}^{NS} \left. \frac{\partial^2 r}{\partial C_i \partial T} \right|_{\bar{\mathbf{C}}, \bar{T}} \overline{C'_i T'}}_{\text{These terms have to be modelled}}$$

These terms have to be modelled, i.e. they have to be expressed as function of mean variables only

They are directly associated to the non linearity of formation rates with respect to the temperature and composition.

They are strongly dependent on the fluctuations of temperature and composition and in most cases are not negligible.

$$\bar{r}(\mathbf{C}, T) \approx r(\bar{\mathbf{C}}, \bar{T}) + C_C$$

Is this term really relevant?

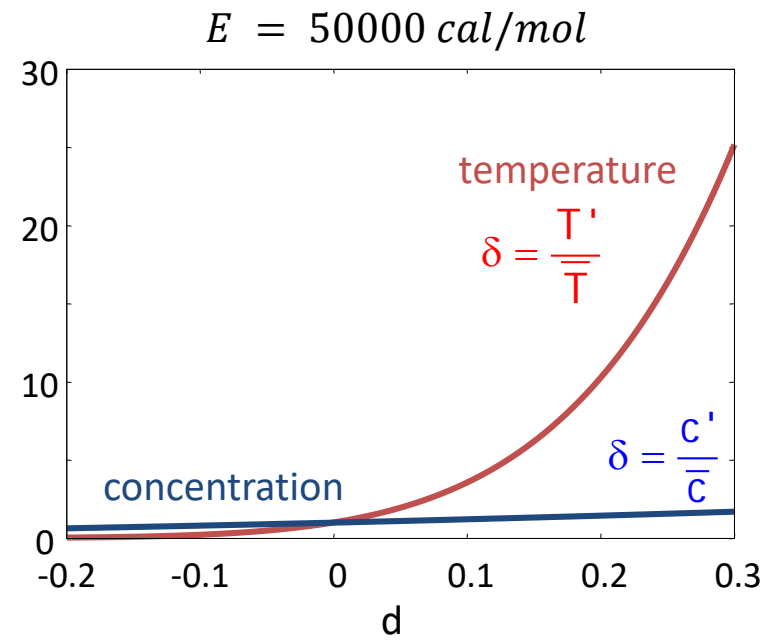
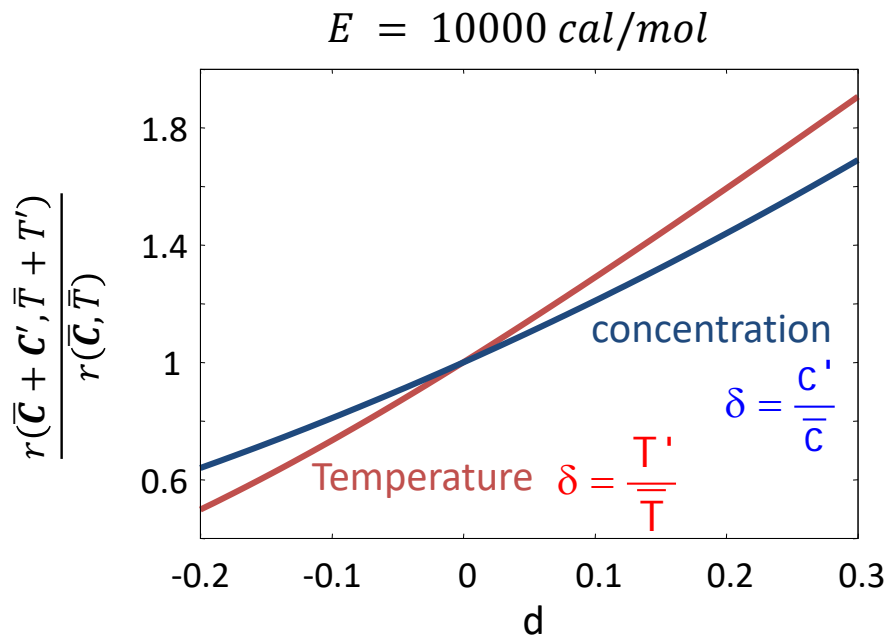


# Temperature and composition fluctuations

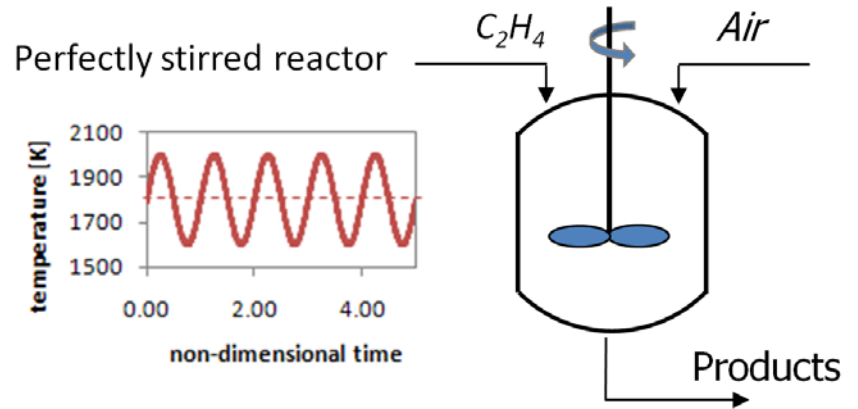
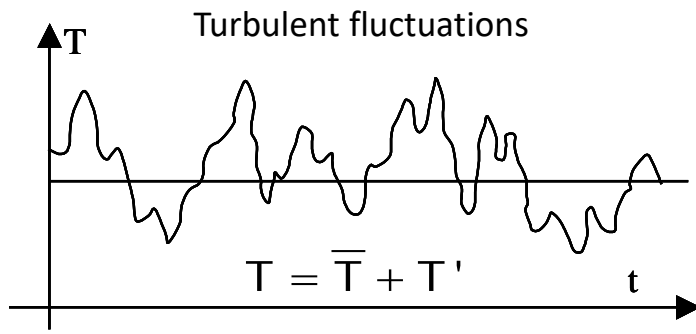
Temperature fluctuations have a strong impact especially on reactions with large activation energy  
(as an example formation of NO<sub>x</sub>)

Example: second order reaction

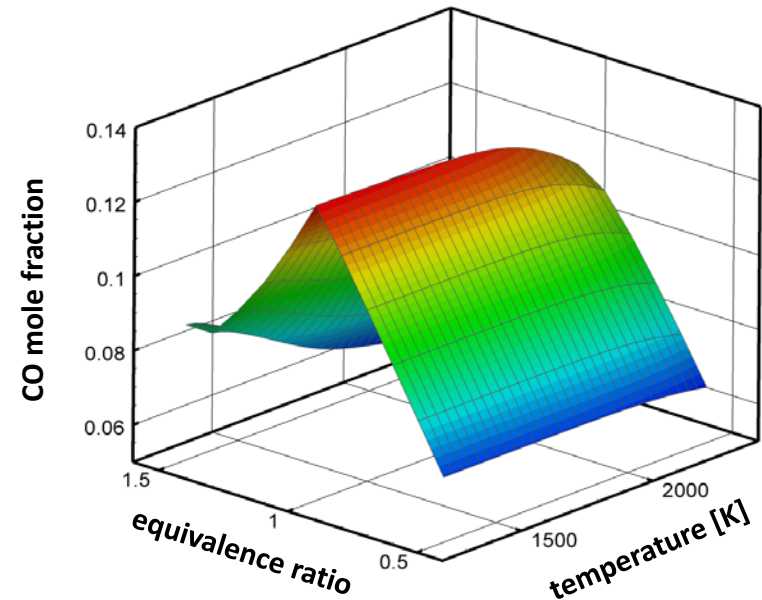
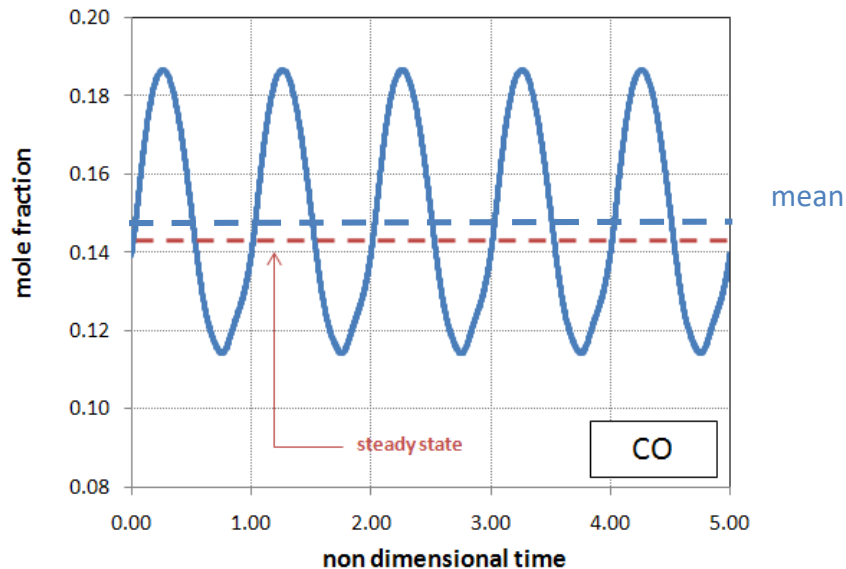
$$r(C, T) = A \exp\left(-\frac{E}{RT}\right) C^2$$



# Effect of turbulent fluctuations (I)

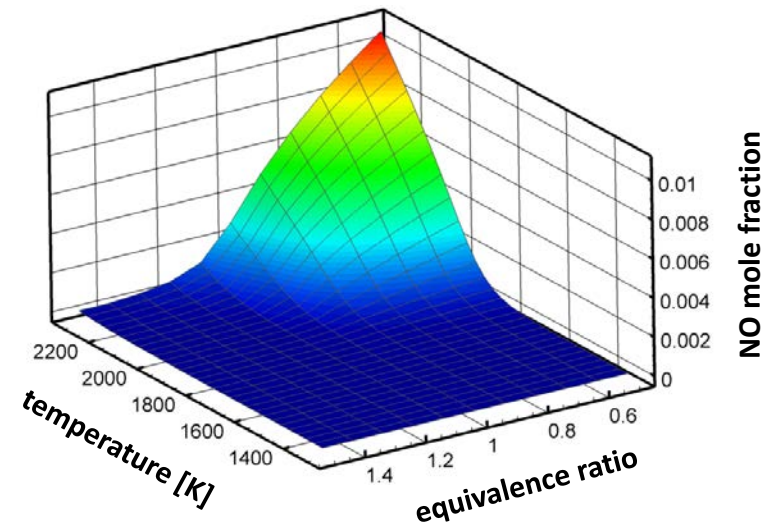
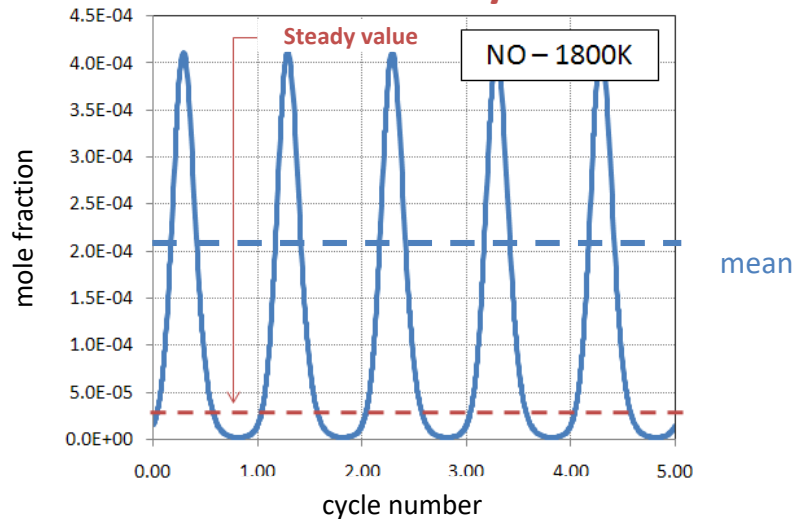


## Fast chemistry: CO

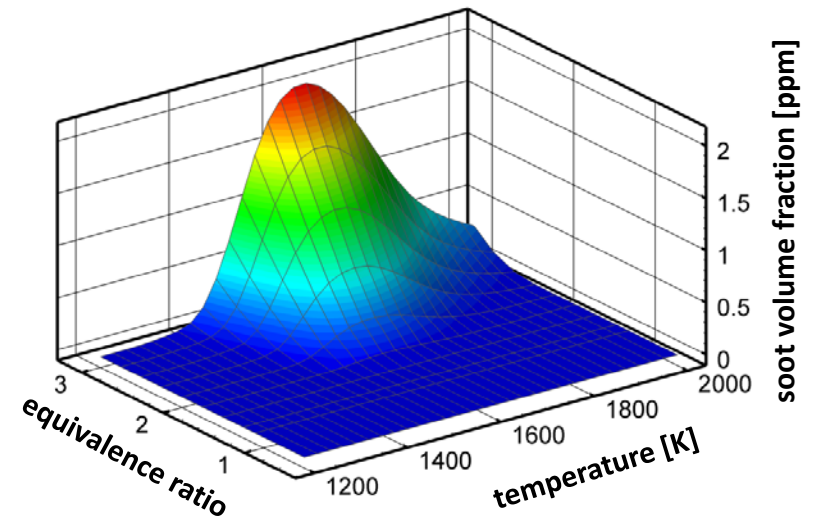
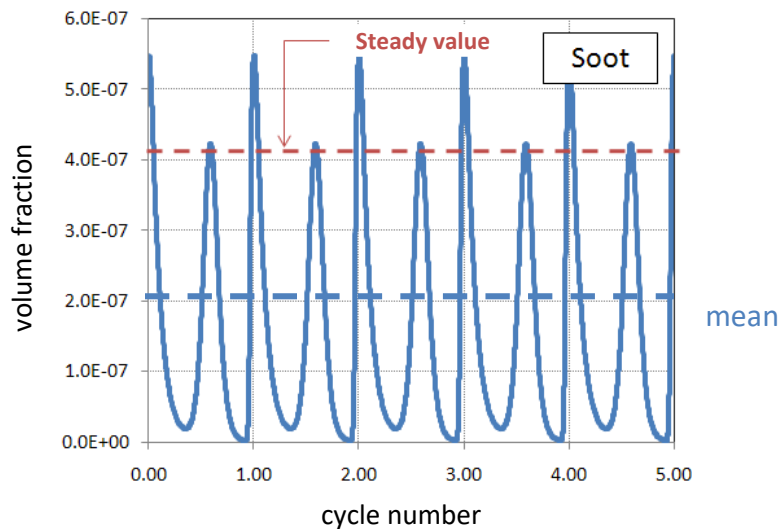


# Effect of turbulent fluctuations (II)

## Slow chemistry: NOx

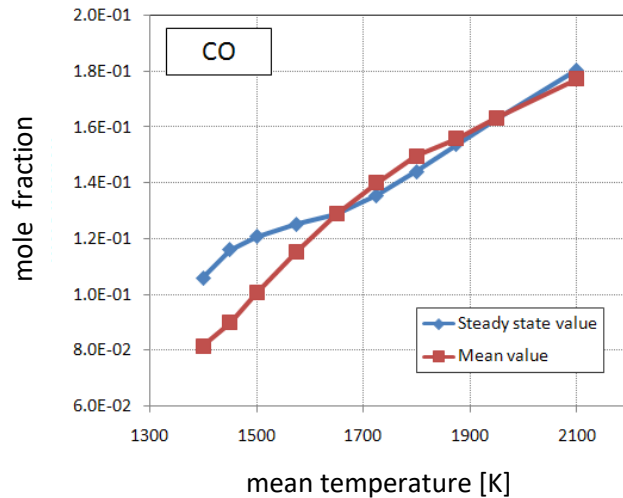


## Finite-rate chemistry: Soot

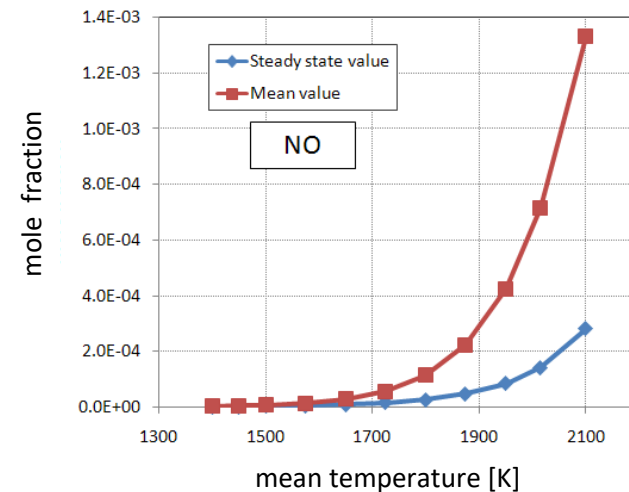


# Effect of turbulent fluctuations (III)

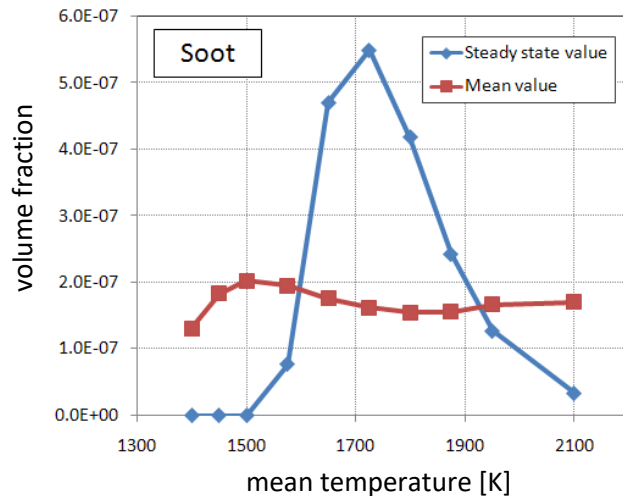
Fast chemistry: CO



Slow chemistry: NO



Finite-rate chemistry: Soot



The effect of fluctuation of temperature on soot production is quite complex to describe, since the dependence of soot on temperature is complex from a chemical point of view

# A first, unsuccessful attempt to close mean reaction

Let's go back to the expansion previously carried out:

$$\bar{r}(\mathbf{C}, T) \approx r(\bar{\mathbf{C}}, \bar{T}) + \frac{1}{2} \sum_{i=1}^{NS} \sum_{j=1}^{NS} \left. \frac{\partial^2 r}{\partial C_i \partial C_j} \right|_{\bar{\mathbf{C}}, \bar{T}} \overline{C'_i C'_j} + \frac{1}{2} \left. \frac{\partial^2 r}{\partial T^2} \right|_{\bar{\mathbf{C}}, \bar{T}} \overline{T'^2} + \sum_{i=1}^{NS} \left. \frac{\partial^2 r}{\partial C_i \partial T} \right|_{\bar{\mathbf{C}}, \bar{T}} \overline{C'_i T'}$$

- It is clear that this direct approach to evaluate mean reaction rates, based on series expansion, cannot be applied for practical simulations.
- In particular, new quantities such as  $\overline{C'_i C'_j}$ ,  $\overline{C'_i T'}$ , and  $\overline{T'^2}$  have to be closed, using algebraic expressions or transport equations. Transport equations are unfeasible in case of large kinetic mechanisms: as an example, for  $NS = 30$ , we should write  $30^2/2 = 450$  transport equations for the  $\overline{C'_i C'_j}$  terms.
- For these reasons, reaction rate closures in turbulent combustion are not based on the equation above, but are derived from physical analysis.

# Series expansion for 1-step, irreversible reaction

Nevertheless, the approach based on series expansion can be used in some practical simulations **where chemical times are not negligible compared to flow times**, for example in supersonic reacting flow or to describe chemical reactions in atmospheric boundary layer where the temperature  $T$  may be roughly assumed to be constant.

The approach is limited to the case of a single, irreversible reaction between fuel and oxidizer  $F + sO \rightarrow P$ .

The series expansion would give, arrested to second-order terms, gives:

$$\bar{r}(\mathbf{C}, T) \approx r(\bar{\mathbf{C}}, \bar{T}) + Q_{F,O} \overline{C'_F C'_O} + Q_F \overline{C'^2_F} + Q_O \overline{C'^2_O} + Q_T \overline{T'^2} + Q_{F,T} \overline{C'_F T'} + Q_{O,T} \overline{C'_O T'}$$

In the situations mentioned above, the most relevant expansion term is the first one (i.e.  $Q_{F,O} \overline{C'_F C'_O}$ ). All the remaining terms are neglected. Thus, the average reaction rate is written as:

$$\bar{r}(\mathbf{C}, T) \approx r(\bar{\mathbf{C}}, \bar{T}) + Q_{F,O} \overline{C'_F C'_O} = r(\bar{\mathbf{C}}, \bar{T})(1 + \alpha_S)$$

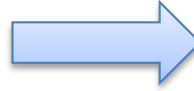
The segregation factor  $\alpha_S$  measures the mixing between fuel and oxidizer ( $\alpha_S = 0$  for perfectly mixed reactants and  $\alpha_S = -1$  for perfectly separated ones).

This factor is modeled or provided by a balance equation.

# Series expansion for kinetic post-processing (I)

Rate constant is highly **non linear** function of temperature

$$k(T) = AT^n \exp\left(-\frac{E}{RT}\right)$$

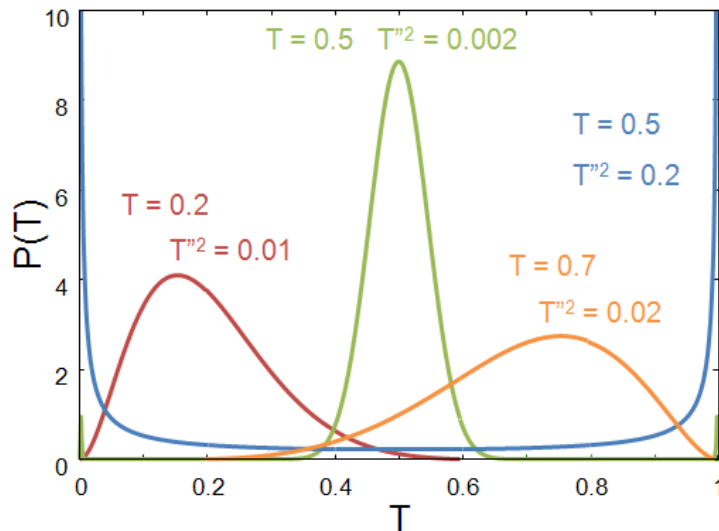


Introduction of a proper **probability distribution function**  $p(T)$

$$\bar{k} = \int_{T_{min}}^{T_{max}} k(T)p(T)dT = C_C k(\bar{T})$$

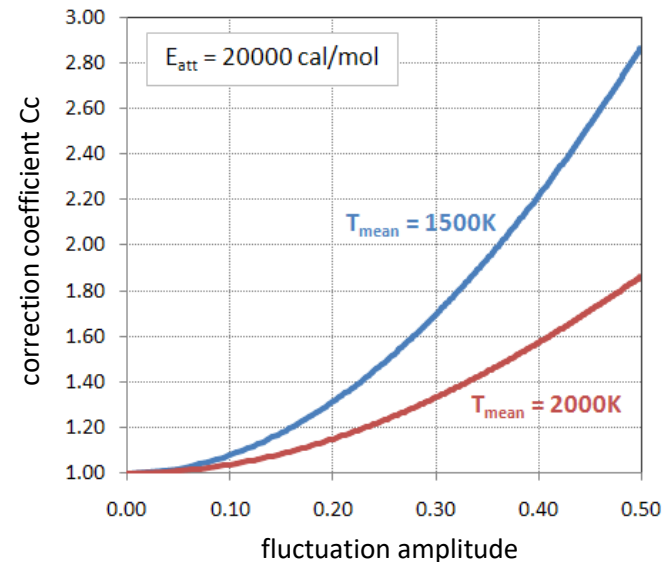
Requires the knowledge of the **variance of temperature**

$\beta$ -PDF



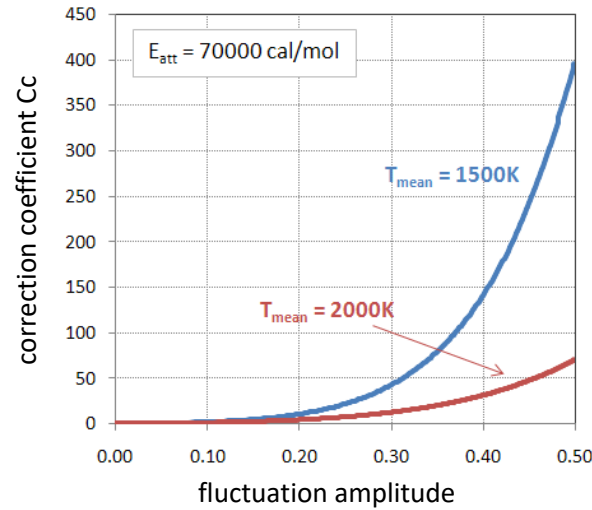
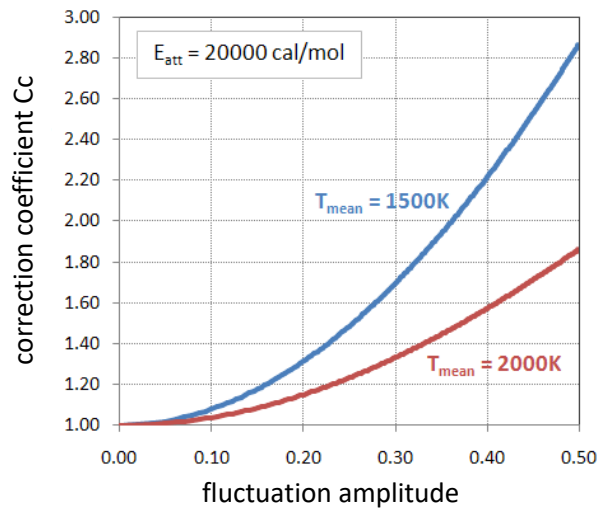
Correction coefficient

$$C_C = \frac{\int_{T_{min}}^{T_{max}} k(T)p(T)dT}{k(\bar{T})}$$

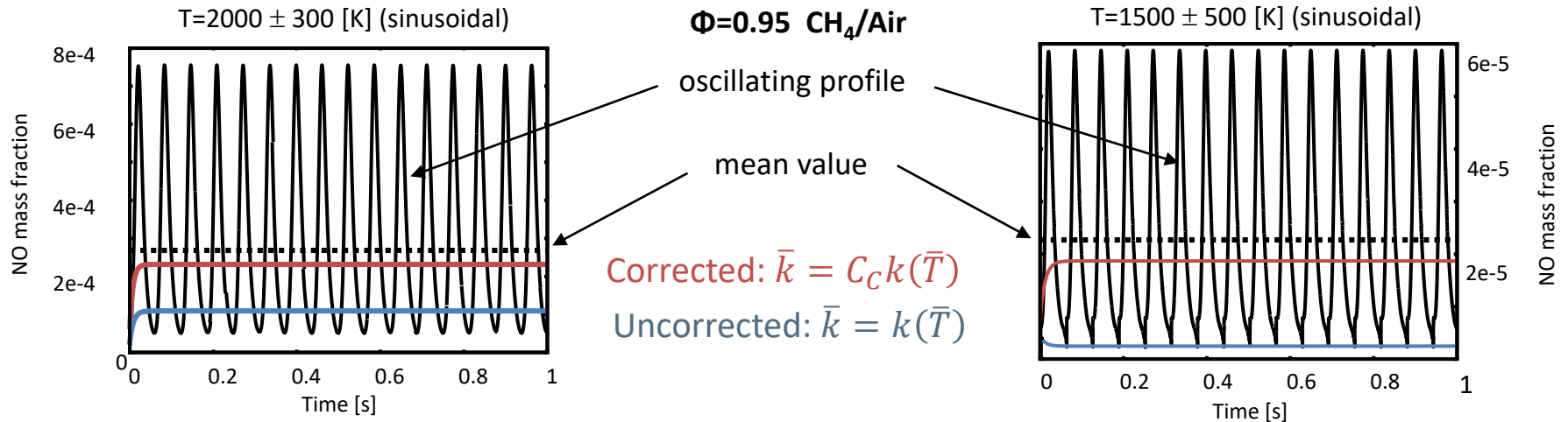


A. Cuoci, A. Frassoldati, G. Buzzi Ferraris, T. Faravelli, E. Ranzi,  
International Journal of Hydrogen Energy (32), p. 3486-3500 (2007)

# Series expansion for kinetic post-processing (II)



The correction Coefficient is significantly  $> 1$  for high activation energies  
(Thermal NO<sub>x</sub>)



The error ( $< 15\%$ ) is also due to the fluctuations of composition (neglected)



## 1. Introduction to turbulent combustion modeling

- a) Fluid dynamic and chemical time scales
- b) Effects of turbulent fluctuations on chemical reactions
- c) Need of turbulent combustion models

## 2. Non-premixed combustion

- a) **Eddy Dissipation models: ED, ED-FR, EDC**
- b) Steady Laminar Flamelet model
  - i. Mixture fraction
  - ii. Flamelet equations
  - iii. Presumed PDF approach

## 3. Premixed combustion

- a) Eddy Break-Up (EBU) model
- b) Bray-Libby-Moss (BLM) model
- c) G-Equation

# Turbulent combustion models

|  |  |   |
|--|--|---|
| <b>Infinitely Fast Chemistry</b><br><br><b>Finite Rate Chemistry</b> | <b>1. Eddy Dissipation</b><br><b>2. Eddy Dissipation – Finite Rate</b>         | <b>1. Fast Chemistry – PDF mixture fraction</b> |
|  | <b>1. Eddy Dissipation Concept</b><br><b>2. Transported PDF Flamelet Model</b> | <b>1. Flamelet Approach</b>                     |
|  | <b>Reaction Rates Approach (RRA)</b>   | <b>Primitive Variables Approach (PVA)</b>       |

## Reaction rates approach (RRA)

- ✓ only the formation rates of species are modeled
- ✓ the formation rate is usually calculated on-line
- ✓ high computational cost
- ✓ very accurate
- ✓ able to describe non-conventional cases

## Primitive variables approach (PVA)

- ✓ only a limited number of scalar variables, the primitive variables, must be solved
- ✓ no equations of conservation of species have to be solved
- ✓ the flame structure is solved before the fluid dynamic simulation and stored in so-called look-up tables
- ✓ low computational cost

# Eddy Dissipation (ED) model (I)

- Most fuels are fast burning, and the overall rate of reaction is controlled by turbulent mixing.
- In non-premixed flames, turbulence slowly convects/mixes fuel and oxidizer into the reaction zones where they burn quickly. In premixed flames, the turbulence slowly convects/mixes cold reactants and hot products into the reaction zones, where reaction occurs rapidly.
- In such cases, the combustion is said to be mixing-limited, and the complex, and often unknown, chemical kinetic rates can be safely neglected.

Chemical regime

$$Da \ll 1$$

Chemical reactions extremely slow. The system is under chemical control

Fluid dynamic regime

$$Da \gg 1$$

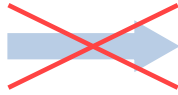
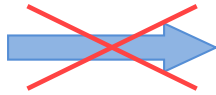

Chemical reactions extremely fast. The system is under fluid dynamic control


# Eddy Dissipation (ED) model (II)

One-step non reversible reaction  $F + rO \rightarrow (1 + r)P$

## Fluid dynamic control

The reaction rate is controlled by the mixing velocity of fuel and oxidizer vortices

|                        |  |  |
|------------------------|--|--|
| Fuel reaction rate     | $\bar{r}_f = C_{ED} \bar{\rho} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Y}_f$       |  |
| Oxidizer reaction rate | $\bar{r}_{ox} = C_{ED} \bar{\rho} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Y}_{ox}$ |  |
| Product reaction rate  | $\bar{r}_p = C_{ED} \bar{\rho} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Y}_p$       |  |

Reaction rate   $\bar{r} = \min \left( \bar{r}_f, \frac{\bar{r}_{ox}}{r}, \frac{\bar{r}_p}{1 + r} \right)$

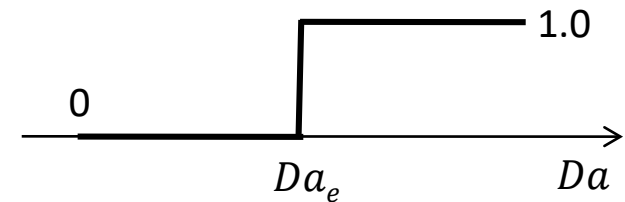
**Magnussen B.F., Hjertager B.,H.** "On mathematical modeling of turbulent combustion", 16th Symposium (International) on Combustion, 1976

## Collision Mixing Model

$$\min \left( \bar{r}_f, \frac{\bar{r}_{ox}}{r}, \frac{\bar{r}_p}{1 + r} \right) \psi$$

Chemical control

Fluid dynamic control

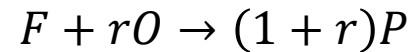


In order to take into account a possible chemical control

$$Da_e \sim 10^{-3}$$


# Eddy Dissipation – Finite Rate (ED-FR) Model

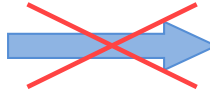
One-step non reversible reaction




## Fluid dynamic control

The reaction rate is controlled by the mixing velocity of fuel and oxidizer vortices

Fuel reaction rate  $\bar{r}_f = C_{ED} \bar{\rho} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Y}_f$  

Oxidizer reaction rate  $\bar{r}_{ox} = C_{ED} \bar{\rho} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Y}_{ox}$  

Product reaction rate  $\bar{r}_p = C_{ED} \bar{\rho} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Y}_p$  

## Chemical control

Reaction rate expressed through the Arrhenius' Law

$$k_r = A \tilde{T}^n \exp\left(-\frac{E}{R \tilde{T}}\right)$$

$$\bar{r}_{chem} = k_r \prod C_i^{\eta_i}$$



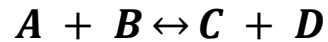
Reaction rate



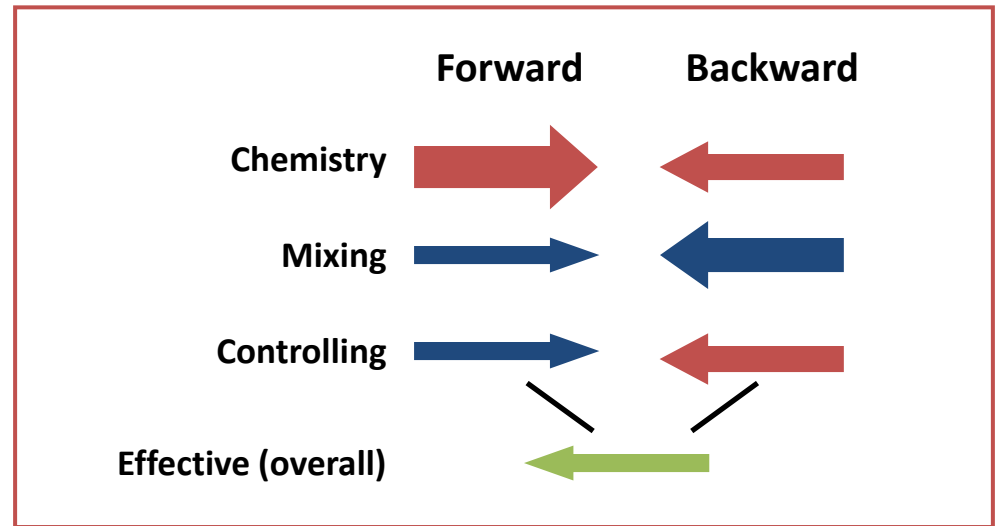
$$\bar{r} = \min\left(\bar{r}_f, \frac{\bar{r}_{ox}}{r}, \frac{\bar{r}_p}{1+r}, \bar{r}_{chem}\right)$$

# Thermodynamically consistent ED-FR model

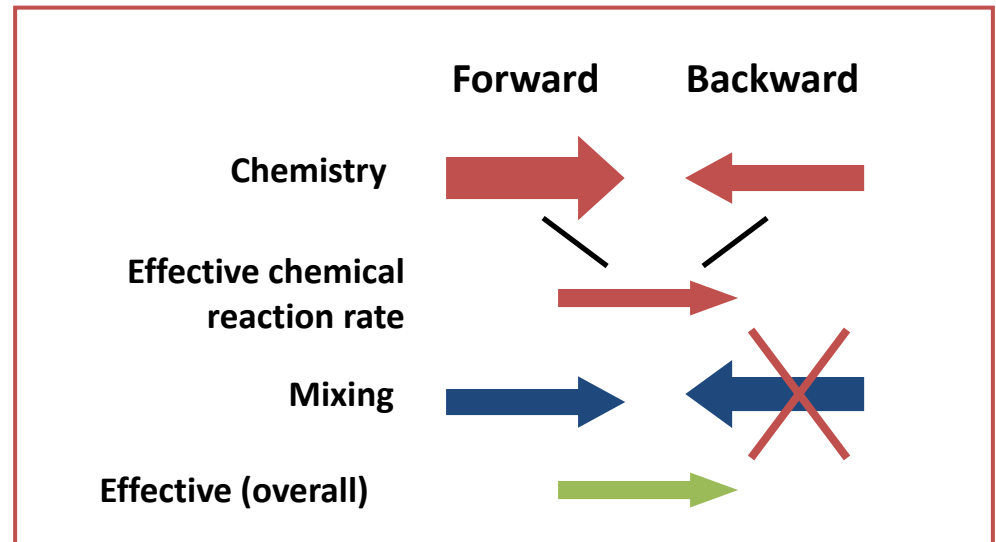
Reversible chemical reaction



Finite-Rate/Eddy-Dissipation



Consistent  
Finite-Rate/Eddy-Dissipation



# Eddy Dissipation Concept (EDC)

## Fine Structures

Hp: Isotropic turbulence

$$\gamma_\lambda = 2.13 \left( \frac{\nu \varepsilon}{k^2} \right)^{1/4} \quad \text{Volume fraction of fine structures}$$

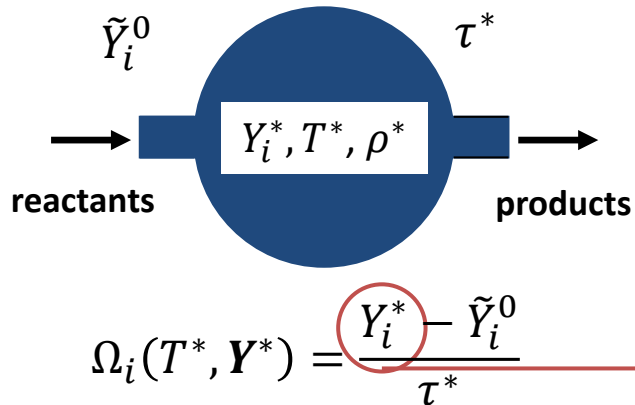
$$\tau^* = 0.4082 \left( \frac{\nu}{\varepsilon} \right)^{1/2} \quad \text{Mean residence time in the fine structures}$$



Homogeneous, isobaric reactors



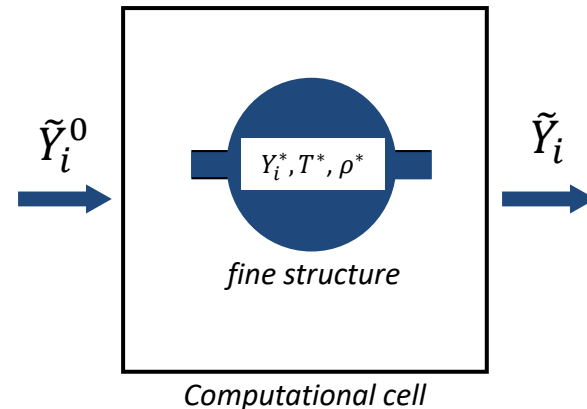
Steady-state perfectly stirred reactors



Gran I.R., Magnussen B.F. "A numerical study of a bluff-body stabilized diffusion flame", Combustion Science and Technology, 119 (1-6), 1996

RANS Variables

$$\bar{\rho} \quad \tilde{u} \quad \tilde{T} \quad \tilde{Y}_i \quad \tilde{k} \quad \tilde{\varepsilon}$$



$$\dot{\Omega}_i = \frac{\bar{\rho} \gamma_\lambda^3}{\tau^* (1 - \gamma_\lambda^3)} (Y_i^* - \tilde{Y}_i)$$

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- b) **Steady Laminar Flamelet model**
  - i. **Mixture fraction**
  - ii. **Flamelet equations**
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# The Steady State Flamelet (SSF) model

- Under certain assumptions, the thermochemistry can be reduced to a single parameter: **the mixture fraction**.
- The mixture fraction, denoted by  **$z$** , is the mass fraction that originated from the fuel stream. In other words, it is the local mass fraction of burnt and unburnt fuel stream elements (C, H, etc.) in all the species ( $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{O}_2$ , etc.).
- The approach is elegant because atomic elements are conserved in chemical reactions. In turn, the mixture fraction is a conserved scalar quantity, and therefore its governing transport equation **does not have a source term**.
- Combustion is simplified to a **mixing problem**, and the difficulties associated with closing non-linear mean reaction rates are avoided. Once mixed, the chemistry can be modeled as being in chemical equilibrium with the Equilibrium model, being near chemical equilibrium with the Steady Laminar Flamelet model.

# The mixture fraction (I)

One-step non reversible reaction  $F + rO \rightarrow (1 + r)P$

## Simplifying assumptions

- Unitary Lewis' numbers for all the species
- Constant specific heat (i.e. independent of temperature)

Conservation equation of species

$$\rho \frac{\partial Y_k}{\partial t} + \rho u_i \frac{\partial Y_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho \mathcal{D} \frac{\partial Y_k}{\partial x_i} \right) + \dot{\Omega}_k$$

Conservation equation of energy

$$\rho \frac{\partial T}{\partial t} + \rho u_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\lambda}{C_p} \frac{\partial T}{\partial x_i} \right) + \frac{\dot{q} \dot{\Omega}_f}{C_p}$$

**Poinsot T., Veynante D.**, *"Theoretical and Numerical Combustion"*, Edwards, 2001

**Peters N.**, *"Turbulent Combustion"*, Cambridge University Press, 2000

# The mixture fraction (II)

Let's define 3 dimensionless variables as proper linear combinations of mass fractions and T:

| $Z_1$   | $Z_2$  | $Z_3$  |
|---|--|--|
| $Z_1 \stackrel{\text{def}}{=} rY_f - Y_o$   | $Z_2 \stackrel{\text{def}}{=} \frac{C_P T}{\dot{q}} + Y_f$ | $Z_3 \stackrel{\text{def}}{=} r \frac{C_P T}{\dot{q}} + Y_o$ |
| $\rho \frac{\partial Z_j}{\partial t} + \rho u_i \frac{\partial Z_j}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho \mathcal{D} \frac{\partial Z_j}{\partial x_i} \right)$ |  |  |

| Passive scalar | Fuel side                                 | Oxidizer side                               |
|----------------|---|---|
| $Z_1$          | $rY_f^{in}$                               | $-Y_o^{in}$                                 |
| $Z_2$          | $\frac{C_P T_f^{in}}{\dot{q}} + Y_f^{in}$ | $\frac{C_P T_o^{in}}{\dot{q}}$              |
| $Z_3$          | $r \frac{C_P T_f^{in}}{\dot{q}}$          | $r \frac{C_P T_o^{in}}{\dot{q}} + Y_o^{in}$ |

Fuel stream  $Y_o^{in} \quad T_o^{in}$



Oxidizer stream  $Y_o^{in} \quad T_o^{in}$

# The mixture fraction (III)

$$\xi_j \stackrel{\text{def}}{=} \frac{Z_j - Z_{j,o}^{in}}{Z_{j,f}^{in} - Z_{j,o}^{in}}$$

Let us define new variables  $\xi_j$  corresponding to the normalized  $Z_j$  variables previously defined

It is easy to demonstrate analytically that the new  $\xi_j$  are governed by the same transport equation, without any source term (i.e. passive scalars)

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

The interesting point is to recognize that the boundary conditions for the three  $\xi_j$  are exactly the same, which means that actually they are the same variable, which is called the mixture fraction  $\xi$  :

$$\rho \frac{\partial \xi}{\partial t} + \rho u_i \frac{\partial \xi}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho \mathcal{D} \frac{\partial \xi}{\partial x_i} \right) \quad \begin{cases} \xi(\text{fuel stream}) = 1 \\ \xi(\text{ox stream}) = 1 \end{cases}$$

# The mixture fraction (IV)

It is clear that instead of solving the transport equations for all the species (F, O, and P) and for the temperature, we can solve only the mixture fraction transport equation and reconstruct from it every variable of interest:

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



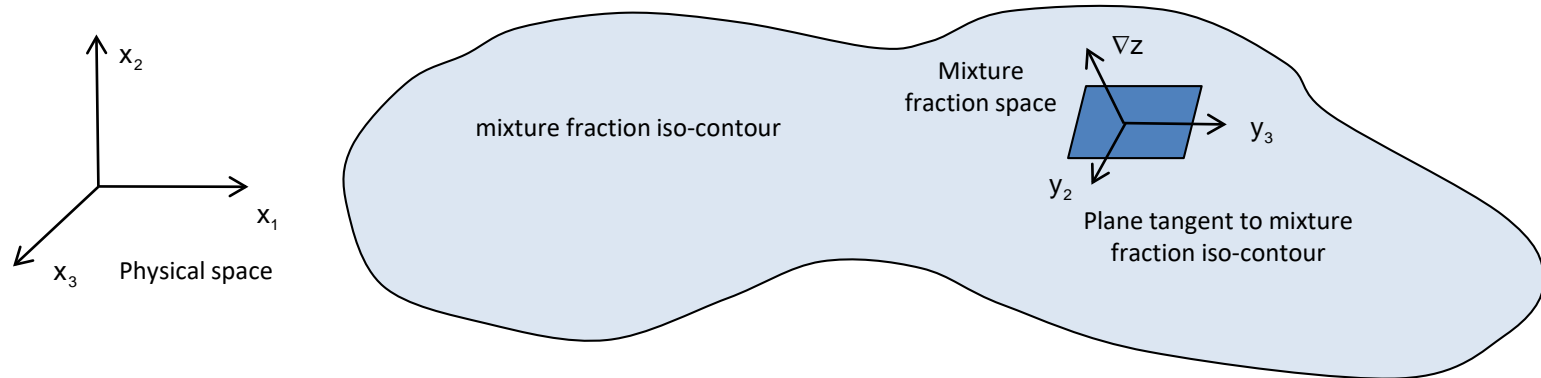
$$Z_j = Z_{j,o}^{in} + (Z_{j,f}^{in} - Z_{j,o}^{in})\xi$$



$$\begin{bmatrix} r & -1 & 0 \\ 1 & 0 & \frac{C_P}{\dot{q}} \\ 0 & 1 & r \frac{C_P}{\dot{q}} \end{bmatrix} \begin{bmatrix} Y_f \\ Y_o \\ T \end{bmatrix} = \begin{bmatrix} Z_1 \\ Z_2 \\ Z_3 \end{bmatrix}$$


# Flame structure in z-space (I)

Poinsot T., Veynante D., “Theoretical and Numerical Combustion”, Edwards, 2001

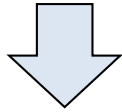


1. Species equations are rewritten in the  $(\xi, y_2, y_3, t)$  space, where  $y_2$  and  $y_3$  are spatial variables in planes parallel to iso- $\xi$  surfaces
2. In the resulting equations, the terms corresponding to gradients along the flame front (i.e. along  $y_2$  and  $y_3$ ) are neglected in comparison to the terms normal to the flame
3. This means that we are assuming that **the flame structure is locally 1D**, depending only on  $t$  and on  $\xi$  (i.e. the flame is thin compared to other flow scales)
4. Each element of the flame front can then be viewed as a small laminar flame called **flamelet**

# Flame structure in z-space (II)

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_k) = \frac{\partial}{\partial x_i} \left( \rho \mathcal{D} \frac{\partial Y_k}{\partial x_i} \right) + \dot{\Omega}_k$$


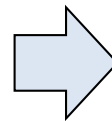
$$\rho \frac{\partial Y_k}{\partial t} + Y_k \left[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) \right] + \frac{\partial Y_k}{\partial \xi} \left[ \rho \frac{\partial \xi}{\partial t} + \rho u_i \frac{\partial \xi}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \rho \mathcal{D} \frac{\partial \xi}{\partial x_i} \right) \right] - \rho \mathcal{D} \left( \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i} \right) \frac{\partial^2 Y_k}{\partial \xi^2} = \dot{\Omega}_k$$



## Unsteady flamelet equations

$$\rho \frac{\partial Y_k}{\partial t} = \rho \mathcal{D} \left( \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i} \right) \frac{\partial^2 Y_k}{\partial \xi^2} + \dot{\Omega}_k$$

$$\rho \frac{\partial T}{\partial t} = \rho \mathcal{D} \left( \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i} \right) \frac{\partial^2 T}{\partial \xi^2} + \frac{\dot{Q}}{C_P}$$



## Flame structure

$$Y_k = Y_k(t, \xi)$$

$$T = T(t, \xi)$$

# The unsteady flamelet equation

$$\rho \frac{\partial Y_k}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 Y_k}{\partial \xi^2} + \dot{\Omega}_k$$

The flamelet equations are typically rewritten introducing the **scalar dissipation rate**  $\chi$ , defined as:

$$\rho \frac{\partial T}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 T}{\partial \xi^2} + \frac{\dot{Q}}{C_p}$$

$$\chi = 2\mathcal{D} \left( \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i} \right)$$

- The flamelet equations are key elements in many diffusion flame theories: in these equations, the only term depending on spatial variables  $x_i$  is the scalar dissipation rate  $\chi$  which controls mixing (because it controls the gradients of  $\xi$ ).
- Once  $\chi$  is specified, the flamelet equations can be entirely solved in the  $\xi$  space to provide the **flame structure**, i.e.  $Y_k = Y_k(t, \xi)$  and  $T = T(t, \xi)$
- Although this is not explicit in the present notation, the  $T$  and  $Y_k$  functions are **parametrized by the scalar dissipation rate**: different scalar dissipation levels lead to different flame structures.
- The scalar dissipation rate has the dimension of an inverse time (like strain). It measures the  $\xi$ -gradients and the molecular fluxes of species towards the flame.



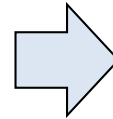
# Steady flamelet equations

The structure of the flamelet can be assumed to be steady, even though the flow itself (and especially the  $\xi$  field) depends on time.

## Unsteady flamelet equations

$$\frac{1}{2}\rho\chi\frac{\partial^2 Y_k}{\partial \xi^2} + \dot{\Omega}_k = 0$$

$$\frac{1}{2}\rho\chi\frac{\partial^2 T}{\partial \xi^2} + \frac{\dot{Q}}{C_p} = 0$$



## Flame structure

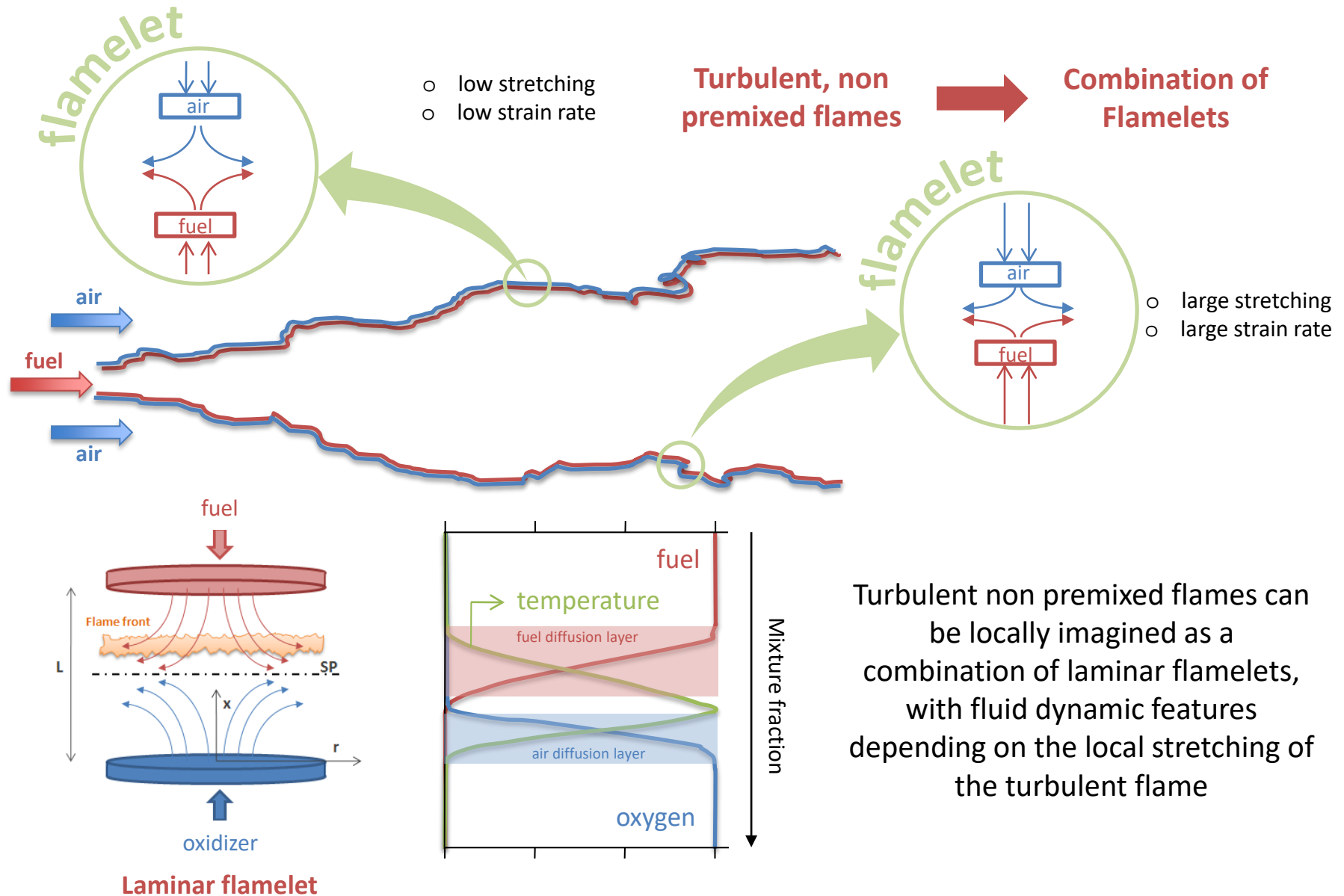
$$Y_k = Y_k(\xi, \chi)$$

$$T = T(\xi, \chi)$$

Reaction rates for species or temperature depend on  $\xi$  and  $\chi$  only. Flow information is entirely contained in the scalar dissipation rate  $\chi$  whereas chemical effects are incorporated through the flame structure in  $\xi$ -space.

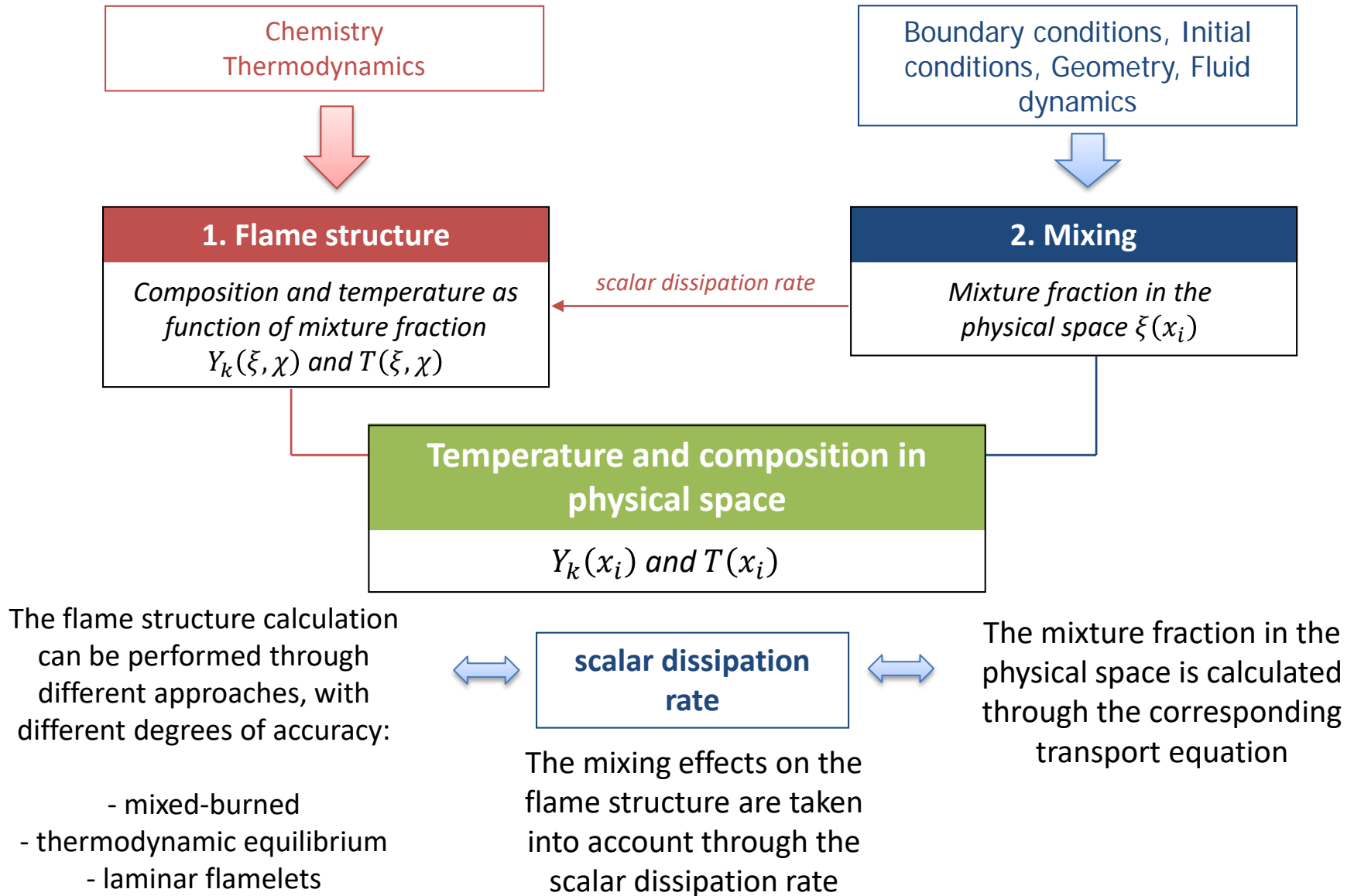
This important simplification is emphasized in the following slides.

# Physical interpretation



Turbulent non premixed flames can be locally imagined as a combination of laminar flamelets, with fluid dynamic features depending on the local stretching of the turbulent flame

# Flame Structure + Mixing



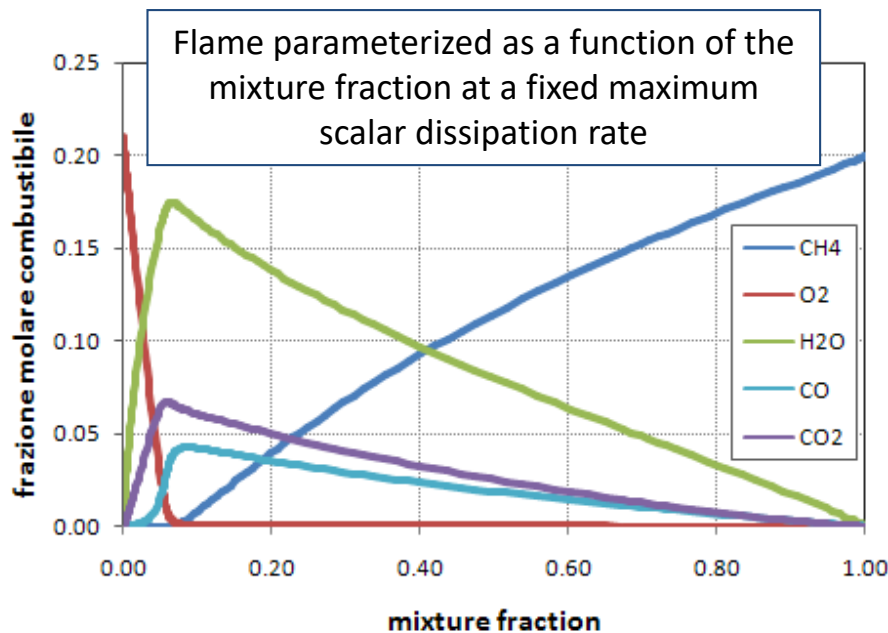
# Flame structure (I)

The steady state flamelet equations are solved directly in the mixture fraction space

$$\frac{1}{2}\rho\chi\frac{\partial^2 Y_k}{\partial \xi^2} + \dot{\Omega}_k = 0 \qquad \frac{1}{2}\rho\chi\frac{\partial^2 T}{\partial \xi^2} + \frac{\dot{Q}}{C_P} = 0$$

The scalar dissipation rate is usually written as a function of the mixture fraction

$$\chi = \chi_0 e^{-2\left(\text{erf}^{-1}(1-2\xi)\right)^2}$$



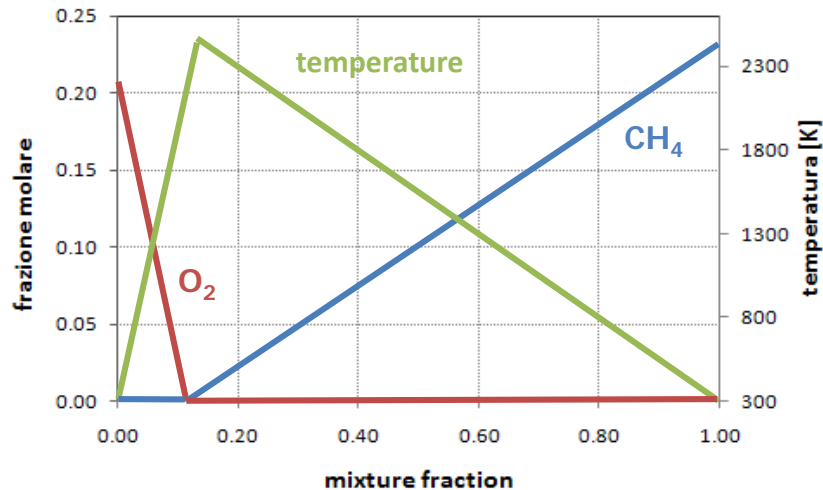
## Pros

- Low computational resources
- Satisfactory accuracy for fast species

## Cons

- Unitary Lewis' numbers for all the species (no differential diffusion)
- Not appropriate for slow species (as an example nitrogen oxides)

# Flame structure (II)

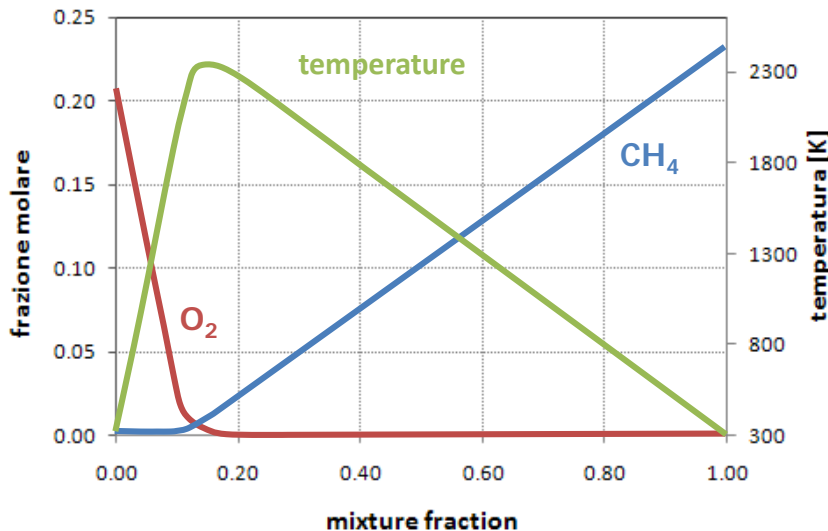


## Approx. Solution: Mixed Is Burned

If we assume an infinitely fast one-step chemical reaction, the flamelet equations have the Burke-Schumann analytical solution

The solution does not depend on the scalar dissipation rate

Fuel and oxygen cannot co-exist

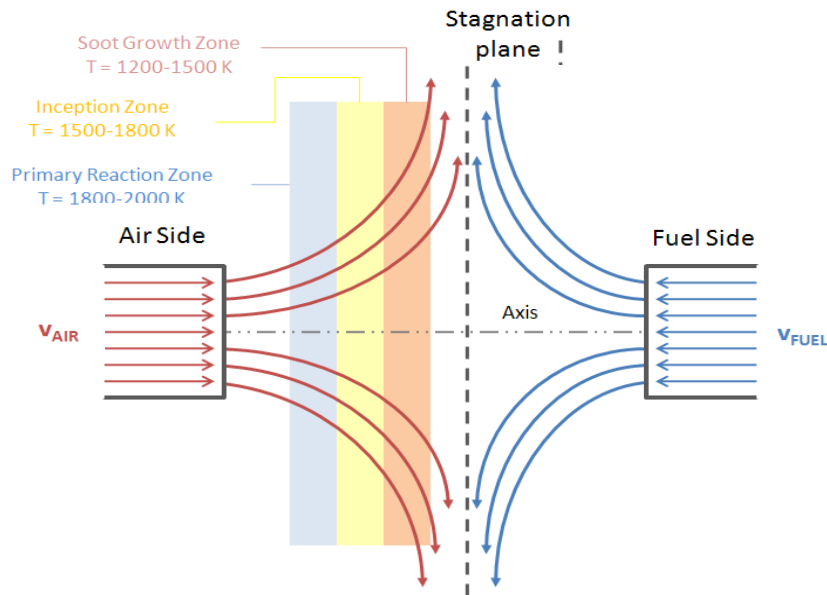


## Approx. Solution: Equilibrium

This is the flamelet solution if the scalar dissipation rate approaches zero

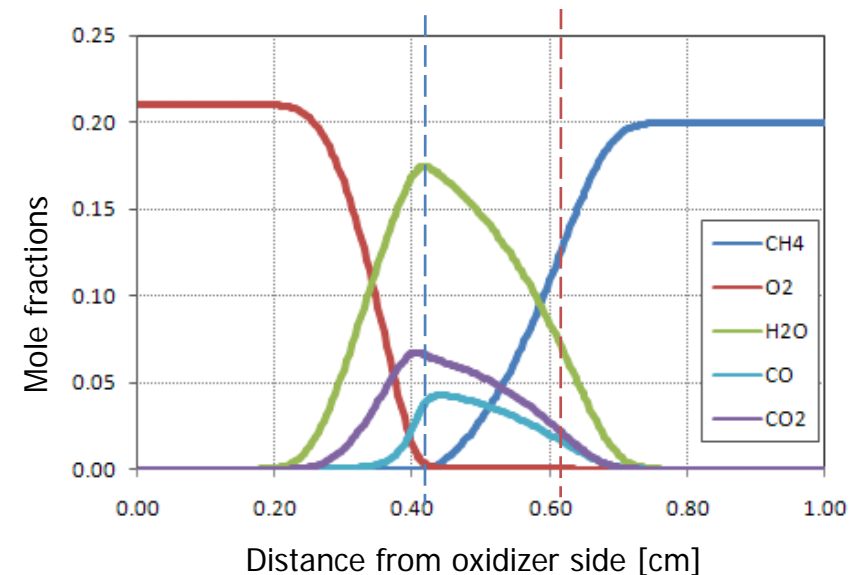
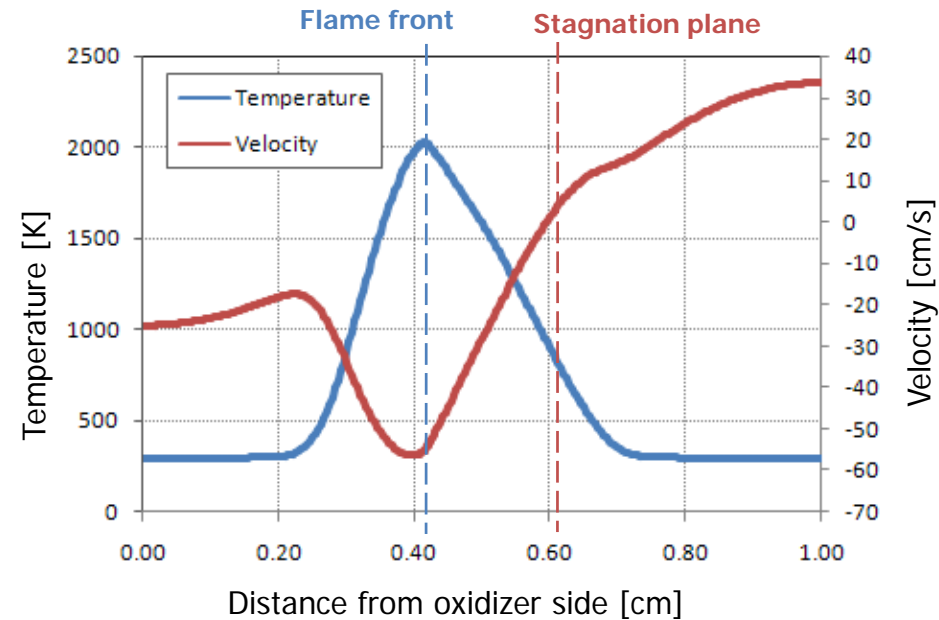
The solution does not depend on the scalar dissipation rate

# Laminar counter-flow diffusion flames

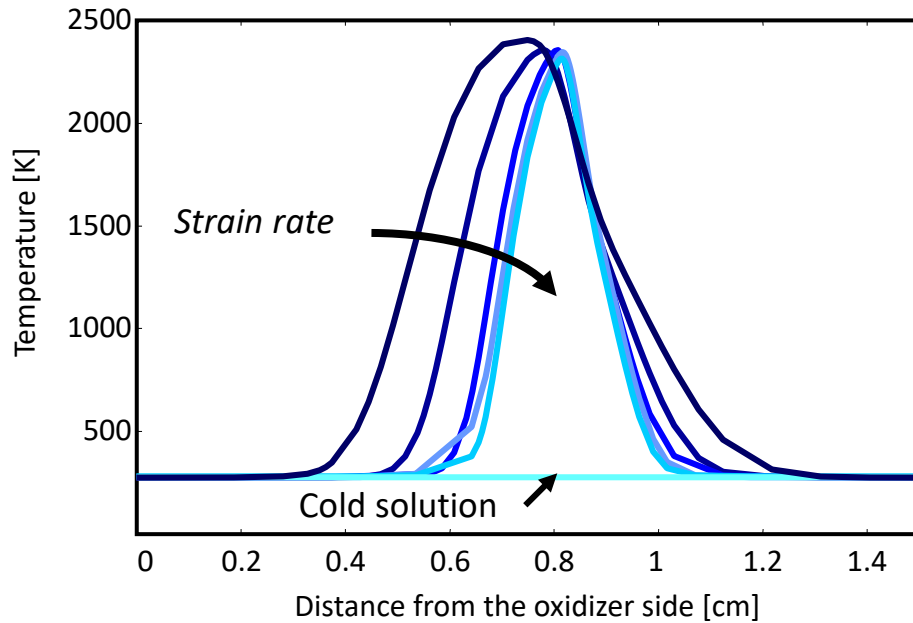


Usually, for conventional combustion in air, the flame front is on the oxidizer side

Peaks of temperature and main products can be usually find at the location of stoichiometric composition



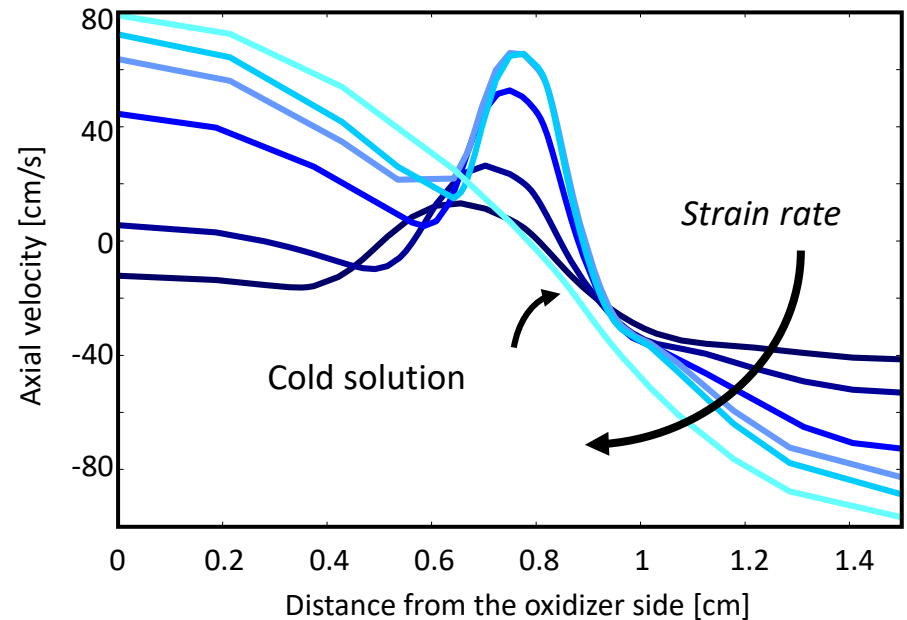
# Strain rate



If we increase the strain rate, the residence time decreases. If we exceed the maximum strain rate the flame extinguishes.

Strain rate is a measure of the residence time

$$K = \frac{2v_o}{L} \left( 1 + \frac{v_c}{v_o} \left( \frac{\rho_c}{\rho_o} \right)^{0.5} \right)$$



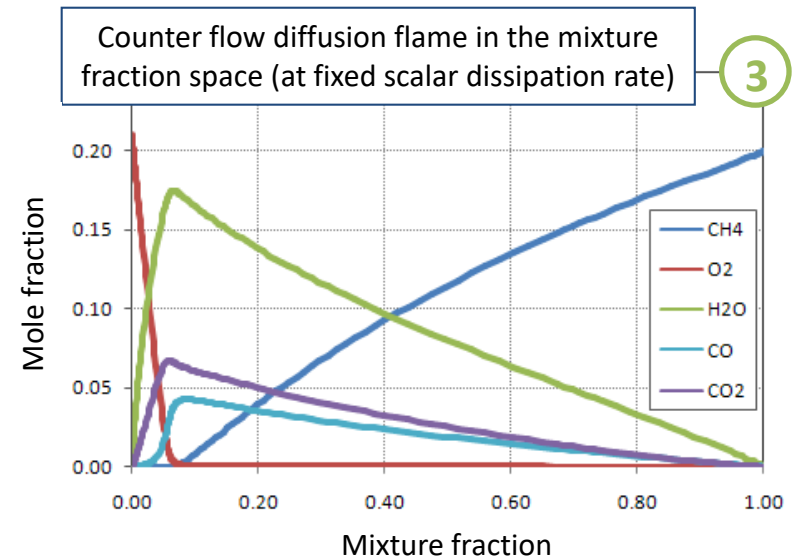
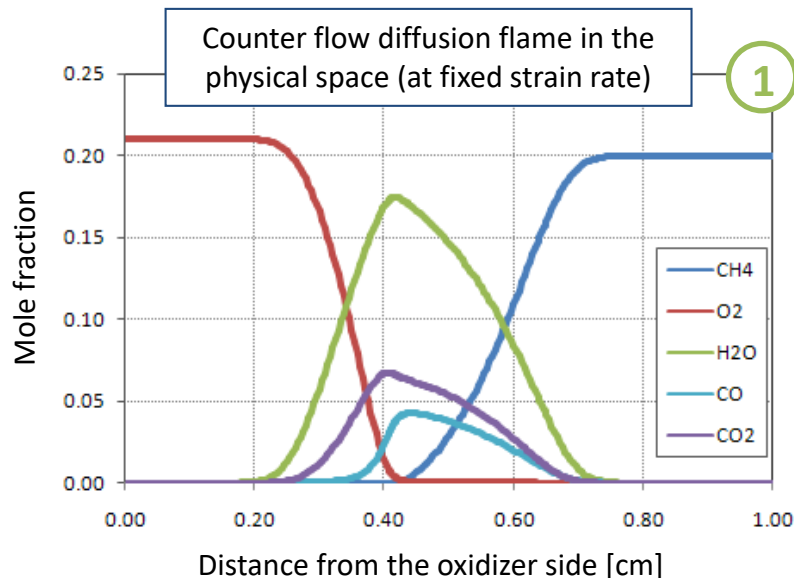
# Flame structure (I)

## Solution: Counter-Flow Diffusion Flames

1. Counter-flow diffusion flame at fixed strain rate
2. **mixture fraction** is calculated in each point of the physical space
3. The solution is rewritten as a function of the **mixture fraction**

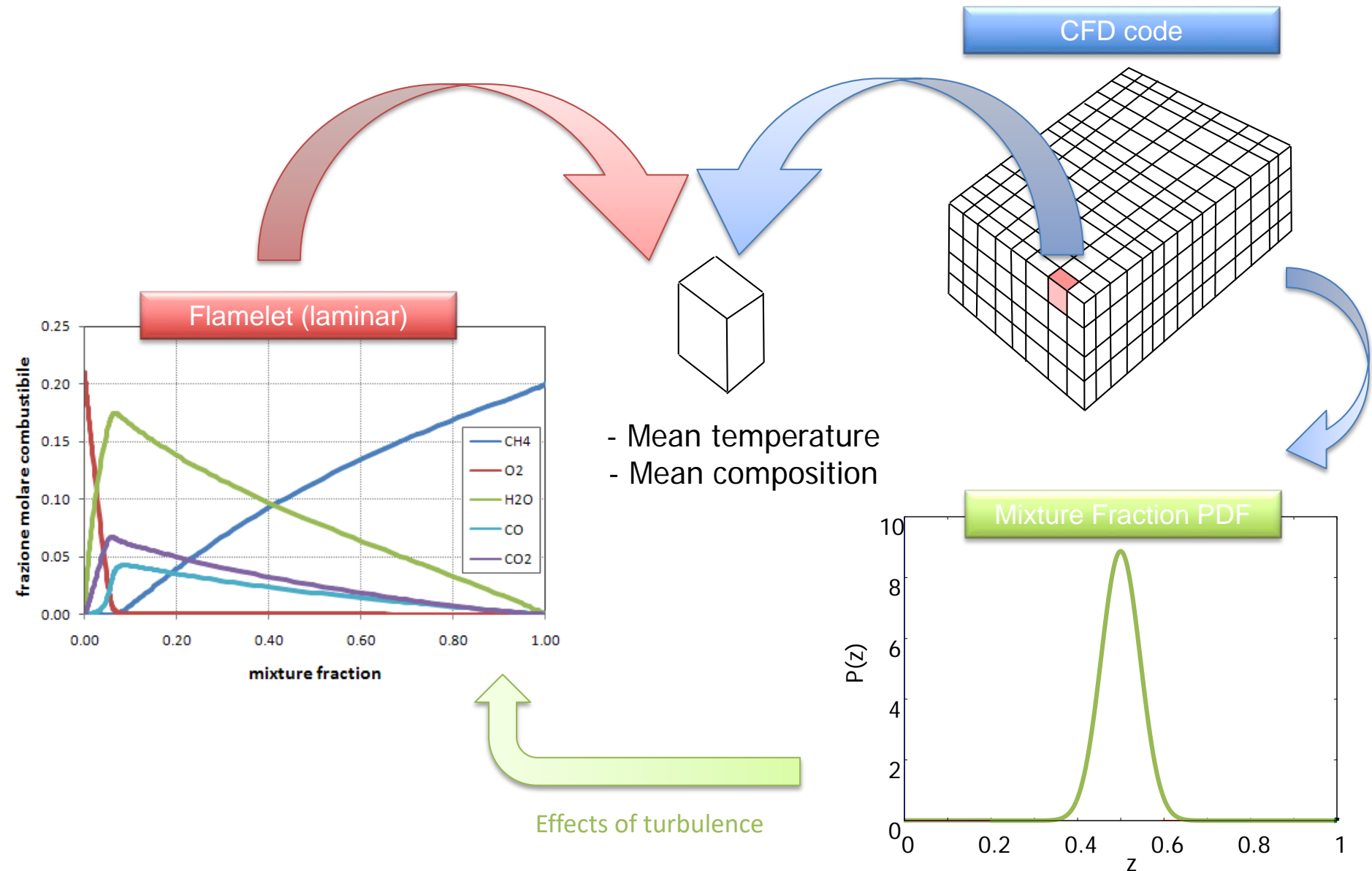
Usually the flame structures are parameterized as a function of the mixture fraction and the maximum scalar dissipation rate  $\chi_0$

$$\chi_0 = \frac{a_S}{\pi} \quad \text{scalar dissipation rate and strain rate}$$

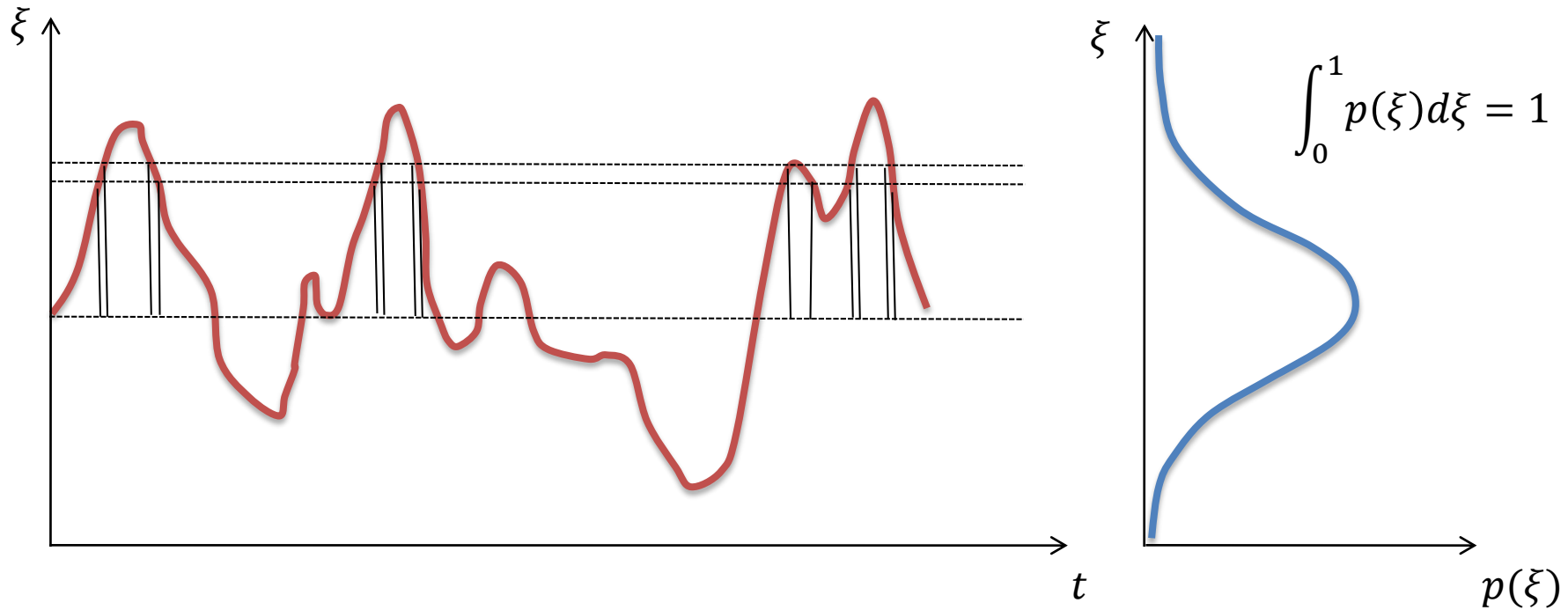




# Coupling CFD - Flamelets



# Probability Distribution Function (PDF)



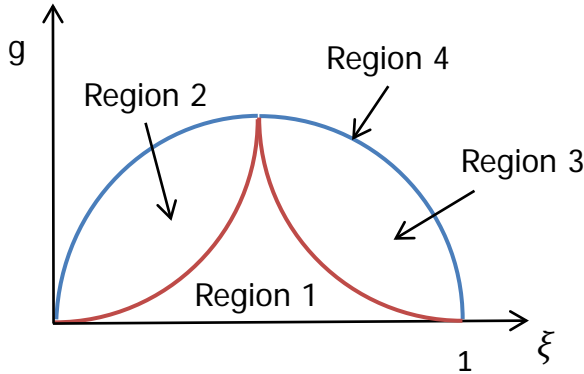
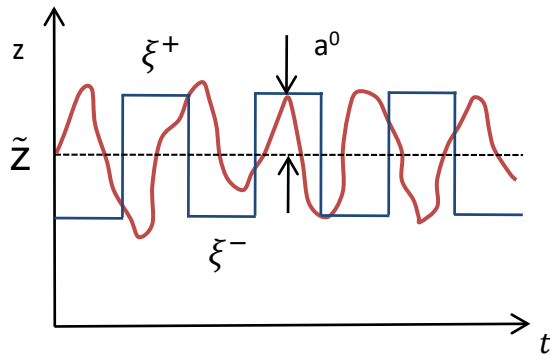
$$\bar{\xi} = \int_0^1 \xi p(\xi) d\xi$$

mean

$$g = \overline{\xi'^2} = \int_0^1 (\xi - \bar{\xi})^2 p(\xi) d\xi$$

variance

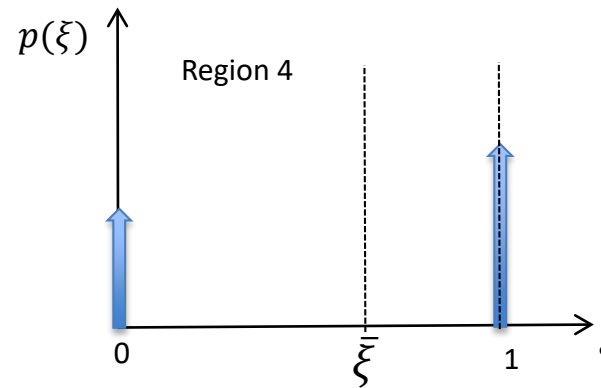
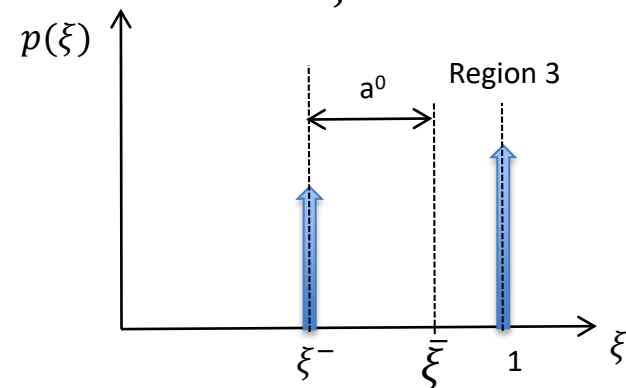
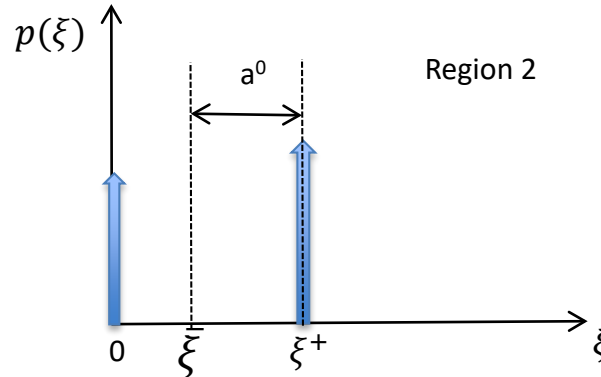
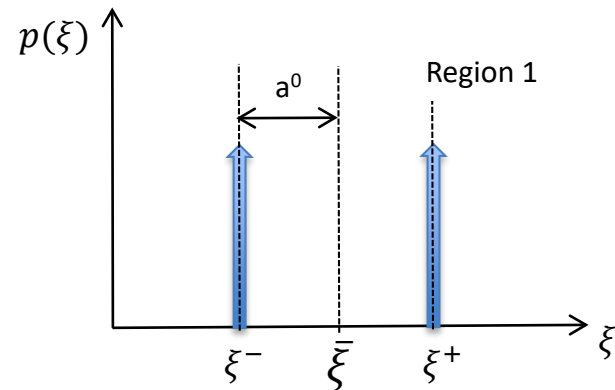
# Double Delta Function (I)



Intermittent signal  
between  $\xi^-$  and  $\xi^+$

Usually not  
accurate

Computational  
cost negligible



**Yeoh G.H., Yuen K.K.,**  
“Computational Fluid  
Dynamics in Fire Engineering  
Theory, Modelling and  
Practice”, Butterworth-  
Heinemann Ltd, 2009

# Double Delta Function (II)

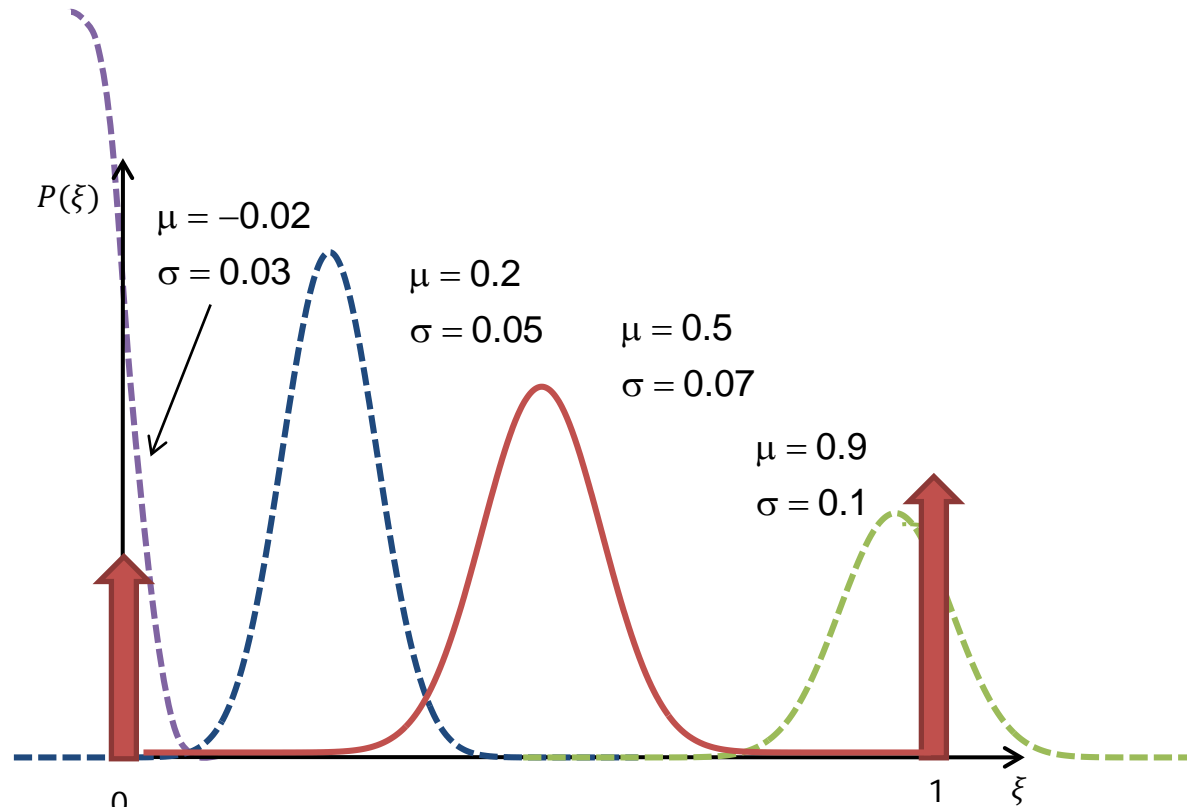
| Region 1   | Region 2   |
|--|--|
| $p(\xi) = \frac{1}{2} \delta(\xi^-) + \frac{1}{2} \delta(\xi^+)$ $\begin{cases} \xi^- = \bar{\xi} - \sqrt{g} \\ \xi^+ = \bar{\xi} + \sqrt{g} \end{cases}$  | $p(\xi) = \frac{1 - \bar{\xi}}{1 - \bar{\xi} + \frac{g}{1 - \bar{\xi}}} \delta(\xi^-) + \frac{g}{(1 - \bar{\xi})^2 + g} \delta(1)$ $\begin{cases} \xi^- = \bar{\xi} - \sqrt{g} \\ \xi^+ = 1 \end{cases}$ |
| Region 3   | Region 4   |
| $p(\xi) = \left( \frac{g}{g + \bar{\xi}^2} \right) \delta(0) + \left( \frac{\bar{\xi}}{\bar{\xi} + \frac{g}{\bar{\xi}}} \right) \delta(\xi^+)$ $\begin{cases} \xi^- = 0 \\ \xi^+ = \bar{\xi} + \sqrt{g} \end{cases}$ | $p(\xi) = (1 - \bar{\xi}) \delta(0) + \bar{\xi} \delta(1)$ $g = \bar{\xi}(1 - \bar{\xi})$  |

# Clipped Gaussian

The Gaussian probability distribution function cannot be directly applied because the mixture fraction is a scalar which is defined between 0 and 1



The solution is a **Clipped Gaussian**, i.e. a modified Gaussian distribution defined between 0 and 1 and coupled with two delta Dirac functions at  $z=0$  (pure oxidizer) and  $z=1$  (pure fuel)



$$p(\xi) = A_0 \delta(0) + \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\xi - \mu}{\sigma} \right)^2 \right] [H(\xi) - H(\xi - 1)] + A_1 \delta(1)$$

$$A_0 = \int_{-\infty}^0 \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\xi - \mu}{\sigma} \right)^2 \right] d\xi$$

$$A_1 = \int_1^{+\infty} \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\xi - \mu}{\sigma} \right)^2 \right] d\xi$$

The most appropriate probability distribution function is the **β-PDF**

$$p(\xi) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \xi^{a-1} (1-\xi)^{b-1}$$

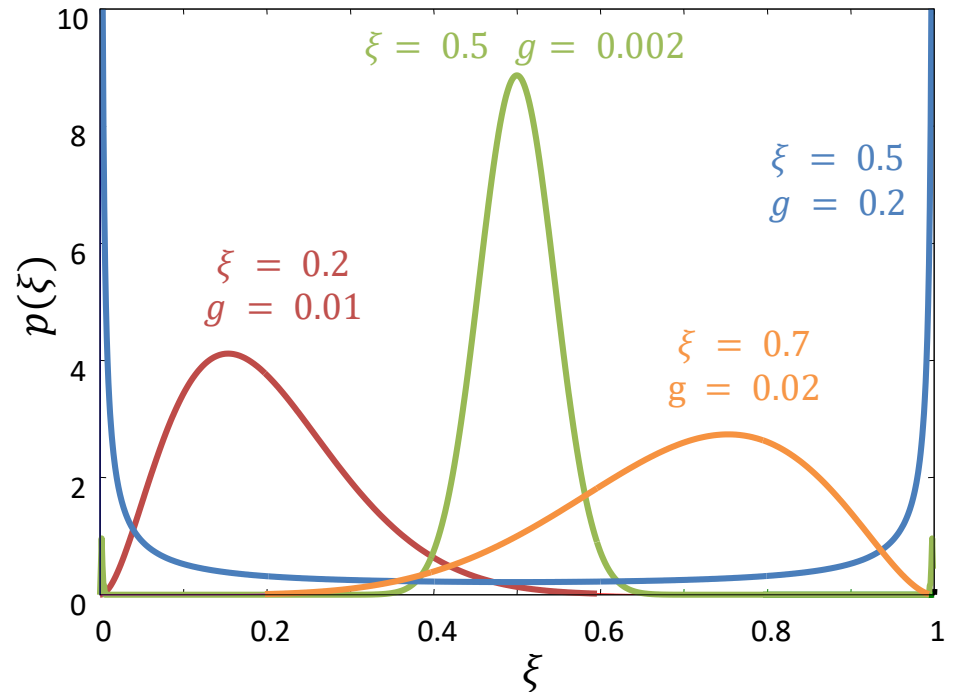
Where the  $\Gamma$  function is:

$$\Gamma(x) = \int_0^{\infty} e^{-t} t^{x-1} dt$$

The parameters **a** and **b** can be estimated from the mean value of mixture fraction and its variance

$$a = \tilde{\xi} \left[ \frac{\tilde{\xi}(1-\tilde{\xi})}{g} - 1 \right]$$

$$b = \frac{a}{\tilde{\xi}} - a$$



The b-PDF is physically appropriate to model the real probability distribution function of mixture fraction.

The behavior is similar to a double delta Dirac if the variance is extremely large.

On the contrary, the behavior is similar to a Gaussian PDF when the variance is small.

# Mixing

The mixture fraction field can be calculated through the solution of the corresponding transport equation in the physical space:

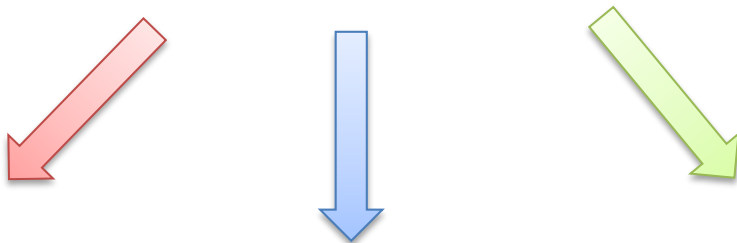
**Transport equation  
of mixture fraction**

$$\bar{\rho} \frac{\partial \tilde{\xi}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \tilde{\xi}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \mathcal{D}_t \frac{\partial \tilde{\xi}}{\partial x_i} \right)$$

The mixture fraction field is not enough to solve the turbulent flame problem. The fluctuations of mixture fraction must be also estimated:

**Transport equation  
of mixture fraction  
variance**

$$\bar{\rho} \frac{\partial \widetilde{\xi'^2}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \widetilde{\xi'^2}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \mathcal{D}_t \frac{\partial \widetilde{\xi'^2}}{\partial x_i} \right) + 2 \bar{\rho} \mathcal{D}_t \left( \frac{\partial \tilde{\xi}}{\partial x_i} \right)^2 - \bar{\rho} C_\chi \frac{\tilde{\epsilon}}{\tilde{k}} \widetilde{\xi'^2}$$

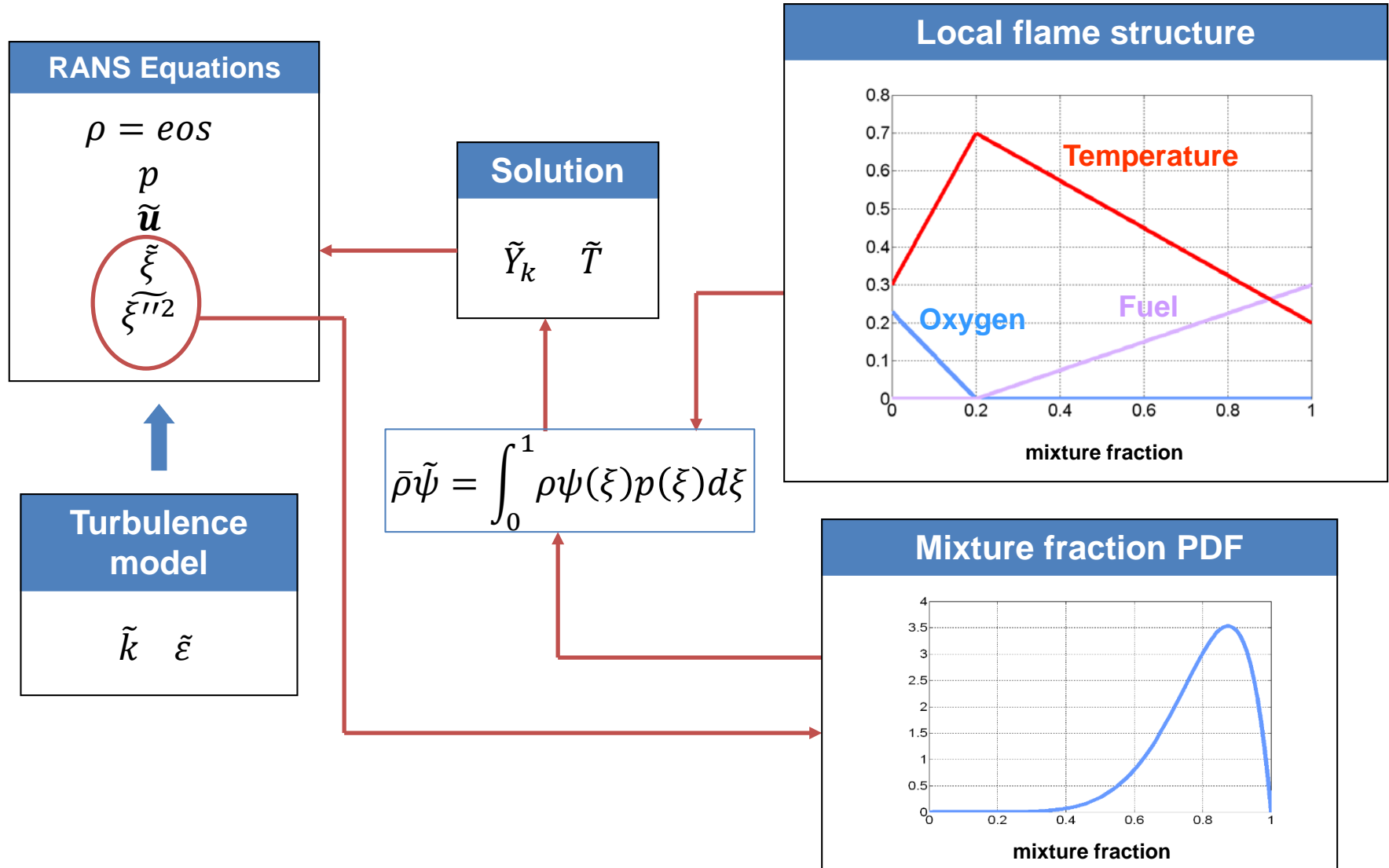


**Variance of  
Mixture  
fraction**

**Mixture fraction  
(mean value)**

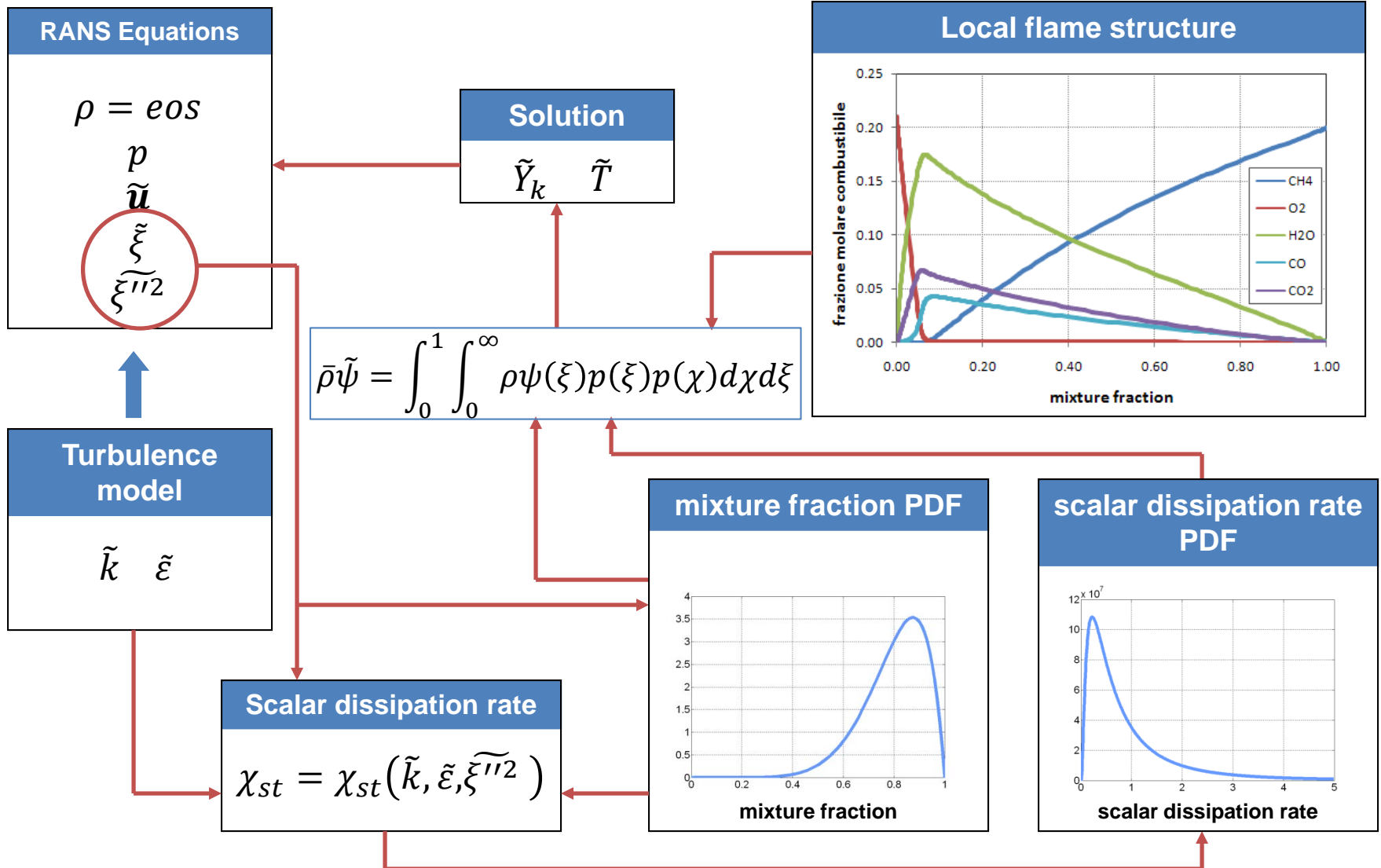
**Scalar  
Dissipation Rate**

# Infinitely Fast Chemistry

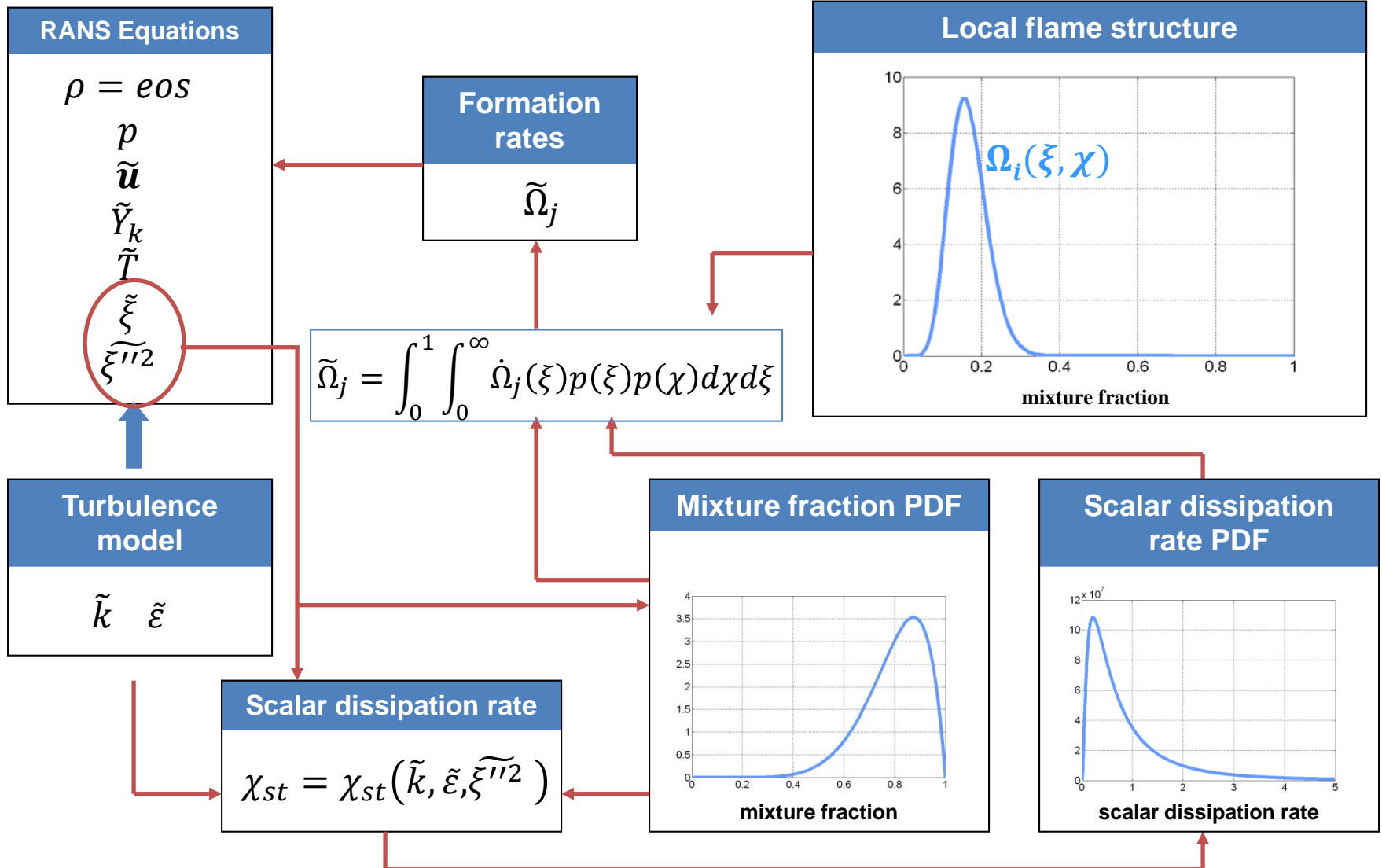




# Finite Rate Chemistry



# Reaction Rate - Flamelets



# Final remarks on flamelet model

- A **large variety of flamelet approaches** exist and have been successfully applied to various configurations.
- Flamelet models are particularly adapted to LES, which provides good prediction of the filtered and subgrid variables, as well as their time evolution, to be used in the flamelet library.
- One important feature of flamelet methods is that they give **access to the fully detailed chemical structure of the flame, including all minor species**.
- **Optimized and efficient tabulation techniques (e.g. ILDM, ISAT, FPI)** enable the use of flamelet libraries in complex flow simulations. This is of major importance to predict pollutant emissions and soot.
- Flamelet models are still being developed, in particular to account for heat losses or liquid fuel sprays or to predict diesel engine auto-ignition.
- Although a large majority of industrial systems are fed with separate fuel and oxidizer flows, the flame in the chamber is usually partially-premixed, with premixed and non-premixed flame elements. In this case **unified models adapted to both premixed and diffusion flames** must be developed. Flamelet methods are good candidates, as they are able to involve both the mixture fraction and the progress variable.

# Training Session 5 (optional)

## Numerical simulation of Sandia CO/H<sub>2</sub>/N<sub>2</sub> turbulent Jet Flames.

The test case is a CO/H<sub>2</sub>/N<sub>2</sub> non-premixed, unconfined, turbulent jet flame. The fuel is injected from a straight circular tubing with squared-off ends (inner diameter 4.58 mm, outer diameter 6.34 mm) at 76 m/s and the corresponding Reynolds number is 16700. The air coflows at 0.75 m/s. The syngas percent composition is 40/30/30 in volume. The fuel tubing length is sufficient to make the assumption of fully developed turbulent pipe flow appropriate. Detailed description of operating conditions and experimental data are available at <https://www.sandia.gov/TNF/DataArch/SANDchn.html>

The simulations are carried out using the flameletSMOKE code, freely available at the following GitHub address: <https://github.com/acuoci/flameletSMOKE>

Detailed instructions on how to compile and install flameletSMOKE are reported in the associated README file:

<https://github.com/acuoci/flameletSMOKE/blob/master/README.md>

Detailed instructions on how to setup and run the H<sub>2</sub>/N<sub>2</sub> flames are available here:

<https://github.com/acuoci/flameletSMOKE/tree/master/cases>

## 1. Introduction to turbulent combustion modeling

- a) Fluid dynamic and chemical time scales
- b) Effects of turbulent fluctuations on chemical reactions
- c) Need of turbulent combustion models

## 2. Non-premixed combustion

- a) Eddy Dissipation models: ED, ED-FR, EDC
- b) Steady Laminar Flamelet model
  - i. Mixture fraction
  - ii. Flamelet equations
  - iii. Presumed PDF approach

## 3. Premixed combustion

- a) Eddy Break-Up (EBU) model
- b) Bray-Libby-Moss (BLM) model
- c) G-Equation

# Eddy Break-Up Model (I)

- Proposed by Spalding, the Eddy Break Up (EBU) model is based on a phenomenological analysis of turbulent combustion assuming **high Reynolds ( $Re \gg 1$ ) and Damkohler ( $Da \gg 1$ ) numbers**.
- A simple idea is to consider that **chemistry does not play any explicit role** while turbulent motions control the reaction rate
- The reaction zone is viewed as a collection of fresh and burnt gaseous pockets transported by turbulent eddies
- The mean reaction rate is mainly controlled by a **characteristic turbulent mixing time  $\tau_t$**  and the normalized temperature (or product mass fraction) fluctuations  $\theta$  and is expressed as:

$$\bar{r} = C_{EBU} \bar{\rho} \frac{\sqrt{\overline{\theta'^2}}}{\tau_t}$$

$C_{EBU}$  is a model constant of the order of unity. The turbulence time  $\tau_t$  can be interpreted as the rate of turbulent mixing between reactants and products and is estimated as:

$$\tau_t = \tilde{k} / \tilde{\varepsilon}$$

# Eddy Break-Up Model (II)

The EBU Model requires the estimation of fluctuations  $\widetilde{\theta''^2}$ . In case  $\theta$  is chosen as the normalized temperature, a first analysis assuming that the flame is infinitely thin leads to the simple result:

$$\bar{\rho}\widetilde{\theta''^2} = \overline{\rho(\theta - \tilde{\theta})^2} = \bar{\rho}(\widetilde{\theta^2} - \tilde{\theta}^2) = \bar{\rho}\tilde{\theta}(1 - \tilde{\theta})$$

because the normalized temperature can only take two values,  $\theta = 0$  (in the fresh gases) or  $\theta = 1$  (in the fully burnt gases) so that  $\theta^2 = \theta$ . The final EBU model for the mean reaction rate is:

$$\bar{r} = C_{EBU}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{\theta}(1 - \tilde{\theta})$$

- This model is attractive because the reaction rate is written as a simple function of known mean quantities without additional transport equations.
- Despite its success, its basic form has an obvious limitation: it does not include any effects of chemical kinetics. However, the EBU model generally gives better results than the simple Arrhenius model.

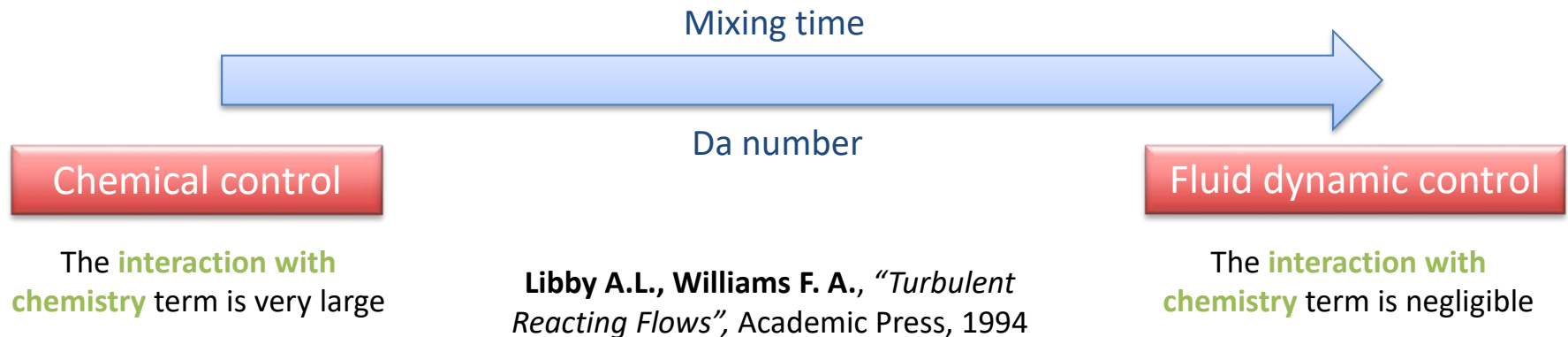
# Eddy Break-Up Model (III)

Some adjustments have been proposed to incorporate chemical features. Libby and Williams proposed a more advanced model in which  $\theta$  is the fuel mass fraction. The fluctuations are estimated on the basis of a transport equation:

$$\bar{\rho} \frac{\partial \overline{\theta''^2}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \overline{\theta''^2}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{\rho} \frac{\mathcal{D}_t}{Sc_t} \frac{\partial \overline{\theta''^2}}{\partial x_i} \right) + \bar{S}_{\overline{\theta''^2}}$$

The source term is given by the sum of three contributions:

$$\bar{S}_{\overline{\theta''^2}} = \underbrace{\bar{P}_{\overline{\theta''^2}}}_{\text{production}} + \underbrace{\bar{D}_{\overline{\theta''^2}}}_{\text{dissipation}} + \underbrace{\bar{K}_{\overline{\theta''^2}}}_{\text{interaction with chemistry}}$$





## 1. Introduction to turbulent combustion modeling

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## 3. Premixed combustion

- a) Eddy Break-Up (EBU) model
- b) Bray-Libby-Moss (BLM) model**
- c) G-Equation

# Bray-Libby-Moss (BLM) Model (I)

Flamelet concept for premixed turbulent combustion: **Bray-Moss-Libby-Model (BML)**

The formulation is based on a reaction **progress variable** equal to 0 in unburned reactants ( $u$ ), rising monotonically to a value of 1 in fully-burned products ( $b$ ).

The reaction progress variable can be related to a particular species mass fraction, for a specific product  $Y_p$  or for the fuel itself  $Y_f$ :

$$c = \frac{Y_p}{Y_{p,b}} \quad or \quad c = \frac{Y_f - Y_{f,u}}{Y_{f,b} - Y_{f,u}}$$

For adiabatic flames with Lewis number equal to 1 it is possible to adopt a definition directly based on the temperature:

$$c = \frac{T - T_u}{T_b - T_u}$$

# Bray-Libby-Moss (BLM) Model (II)

Favre averaged transport equation:

$$\bar{\rho} \frac{\partial c}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial c}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \overline{\rho \mathcal{D}_c} \frac{\partial c}{\partial x_i} \right) - \frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' c''}) + \bar{S}_c$$

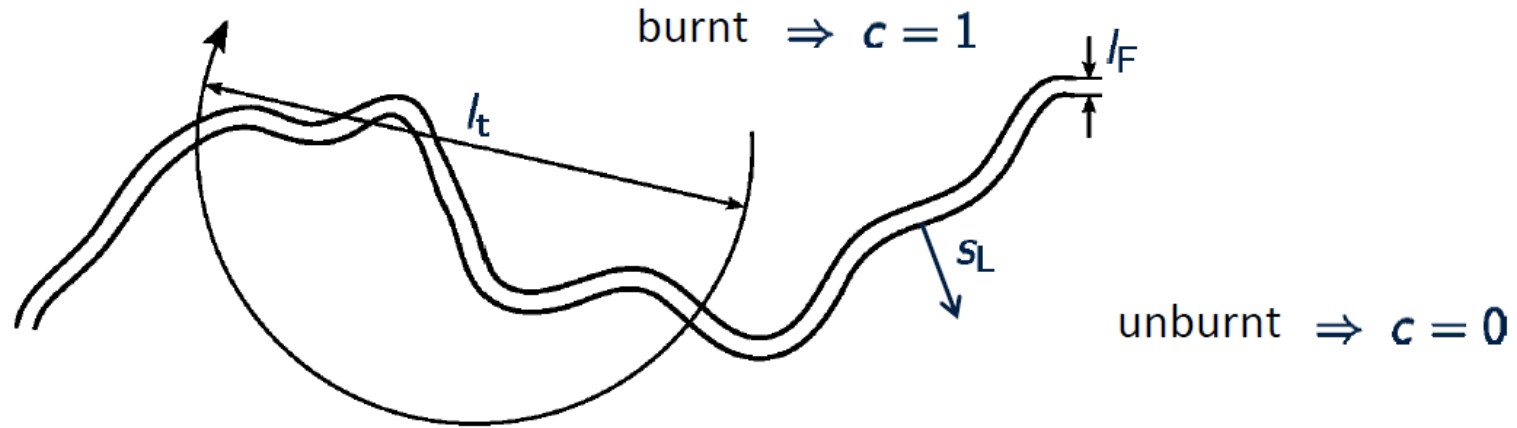
The terms on the right hand side are unclosed. Typically, the molecular transport is neglected. On the contrary, closure models for the turbulent transport and chemical source terms are required:

$$\bar{\rho} \frac{\partial c}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial c}{\partial x_i} = \underbrace{-\frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' c''})}_{\text{turbulent transport}} + \underbrace{\bar{S}_c}_{\text{source}}$$

**Unclosed terms**

# Bray-Libby-Moss (BLM) Model (III)

Assumption: (very) fast chemistry, flame size  $l_F \ll \eta \ll l_t$



Specification of a PDF (probability distribution function) for the progress variable:

- the turbulent flame is made up of thin flamelets
- a probe inserted into the flame brush at a fixed location in space will detect reactants for some of the time and products for almost all the rest of the time
- since the flamelet interface is thin, the probe will detect reacting gases only for very short intervals

Pitsch H., "Combustion Theory and Applications in CFD", Princeton Combustion Summer School 2018

# Bray-Libby-Moss (BLM) Model (IV)

Simplification: progress variable is expected solely to be  $c = 0$  (unburnt) or  $c = 1$  (burnt)

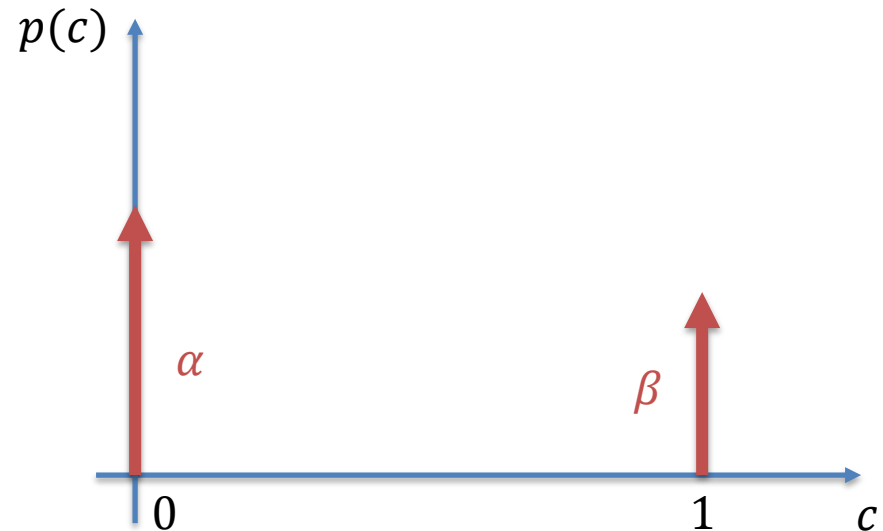
Probability density function:

$$p(c) = \alpha\delta(c) + \beta\delta(c - 1)$$

$\alpha$  and  $\beta$  are the probabilities to encounter the unburnt or the burnt mixture in the flow field

No intermediate states are allowed, which means that  $\alpha + \beta = 1$

$\delta$  is the Dirac delta function



$$\delta(c) = \begin{cases} \infty & \text{if } c = 0 \\ 0 & \text{elsewhere} \end{cases} \quad \int_{-\infty}^{+\infty} g(c)\delta(c - c_0) = g(c_0)$$

# Bray-Libby-Moss (BLM) Model (V)

For a Favre average:

$$\bar{\rho} \tilde{Q} = \int_0^1 \int_{-\infty}^{+\infty} \rho Q(\mathbf{u}, c) p_{\mathbf{u},c}(\mathbf{u}, c) d\mathbf{u} dc$$

Therefore, the unclosed correlation  $\widetilde{u_i'' c''}$  can be calculated on the basis of the joint pdf for  $\mathbf{u}$  and  $c$ :

$$p_{\mathbf{u},c}(\mathbf{u}, c) = p_c(c) p_{\mathbf{u}|c}(\mathbf{u}|c)$$

Introducing the BML approach for  $p_c(c)$  leads to:

$$p_{\mathbf{u},c}(\mathbf{u}, c) = \alpha \delta(c) \underbrace{p_{\mathbf{u}|c}(\mathbf{u}|c=0)}_{\text{conditional pdf}} + \beta \delta(c-1) p_{\mathbf{u}|c}(\mathbf{u}|c=1)$$

Pitsch H., "Combustion Theory and Applications in CFD", Princeton Combustion Summer School 2018

# Bray-Libby-Moss (BLM) Model (VI)

$$\bar{\rho}\tilde{Q} = \int_0^1 \int_{-\infty}^{+\infty} \rho Q(u, c) p_{\mathbf{u},c}(\mathbf{u}, c) d\mathbf{u} dc$$

$$\begin{aligned} \bar{\rho} \widetilde{u_i'' c''} &= \int_0^1 \int_{u_{i,min}}^{u_{i,max}} \rho (u_i - \tilde{u}_i) (c - \tilde{c}) p_{\mathbf{u},c}(\mathbf{u}, c) d\mathbf{u} dc = \dots \\ &\dots = \bar{\rho} \tilde{c} (1 - \tilde{c}) (\bar{u}_b - \bar{u}_u) \end{aligned}$$

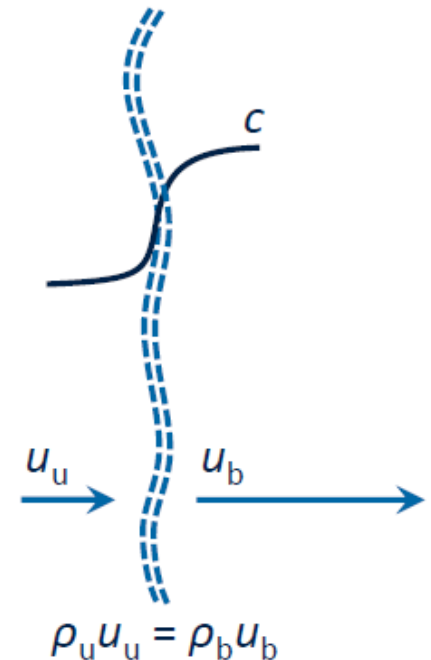
Since the density of products (i.e. burnt mixture) is much smaller than density of reactants, we have:

$$\bar{u}_b - \bar{u}_u > 0$$

Since the progress variable is by definition is  $0 \leq c \leq 1$ , at the end we have:

$$\widetilde{u_i'' c''} = \bar{\rho} \tilde{c} (1 - \tilde{c}) (\bar{u}_b - \bar{u}_u) \geq 0$$

Flame front



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# Bray-Libby-Moss (BLM) Model (VII)

Within the flame zone the progress variable, by definition, increases, i.e.:

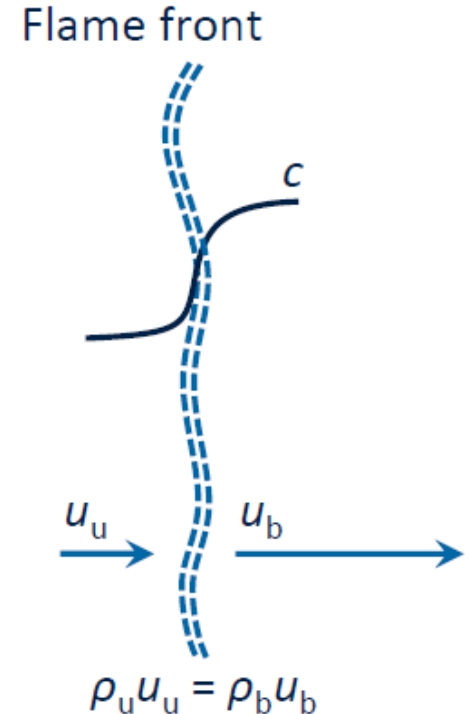
$$\frac{\partial \tilde{c}}{\partial x_i} \geq 0$$

Gradient transport model would be:

$$\widetilde{u_i'' c''} = -\mathcal{D}_t \frac{\partial \tilde{c}}{\partial x_i} \leq 0$$

This is in conflict with the previous result:

$$\widetilde{u_i'' c''} = \bar{\rho} \tilde{c} (1 - \tilde{c}) (\bar{u}_b - \bar{u}_u) \geq 0$$



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# Flame Surface Density model

- Closure by BML-model  $p(c)$  leads to  $\bar{S}_c = 0$
- Closure of the chemical source term, e.g. by **flame-surface-density-model**:

$$\bar{S}_c = \rho_u s_L^0 l_0 \Sigma$$

local mass conversion per area

flame-surface-density

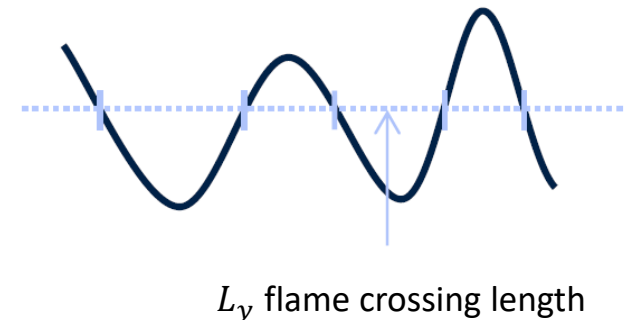
$l_0$ : strain factor, i.e. a measure of local increase of burning velocity by strain

$\Sigma$ : Flame-surface-density

- algebraic model:

$$\Sigma \sim \frac{\tilde{c}(1 - \tilde{c})}{L_y}$$

- transport equation for  $\Sigma$



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# Transport equation for $\Sigma$

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \tilde{u}_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mathcal{D}_t \frac{\partial \Sigma}{\partial x_i} \right) + \underbrace{C_1 \frac{\varepsilon}{k} \Sigma}_{\text{production due to stretching of the flame}} - \underbrace{C_2 s_L \frac{\Sigma^2}{1 - \tilde{c}}}_{\text{Flame annihilation}}$$

No chemical time scales

- Turbulent time ( $\tau = k/\varepsilon$ ) is the determining time scale
- Limit of **infinitely fast chemistry**
- By using transport equations  $\rightarrow$  model for chemical source term independent of  $s_L$

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## 1. Introduction to turbulent combustion modeling

- a) Fluid dynamic and chemical time scales
- b) Effects of turbulent fluctuations on chemical reactions
- c) Need of turbulent combustion models

## 2. Non-premixed combustion

- a) Eddy Dissipation models: ED, ED-FR, EDC
- b) Steady Laminar Flamelet model
  - i. Mixture fraction
  - ii. Flamelet equations
  - iii. Presumed PDF approach

## 3. Premixed combustion

- a) Eddy Break-Up (EBU) model
- b) Bray-Libby-Moss (BLM) model
- c) **G-Equation**

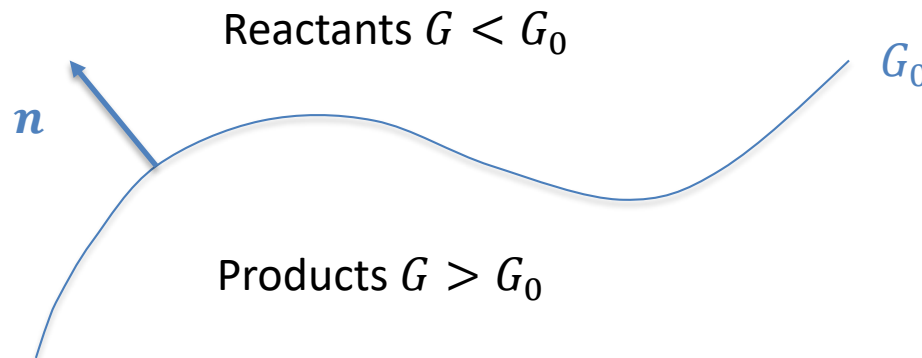
# The G-Equation

The G-Equation is widely used for turbulent combustion modeling and it has proved especially useful as a basis for sub-grid modelling for LES

There are strong similarities with the FSD approach, but there are significant differences too and the G-equation offers a greater degree of flexibility in modeling

The formulation makes use of a non-reacting variable denoted by  $G$

The flame surface is represented by a level set (i.e. iso-surface) of the scalar at  $G(x, t) = G_0$ , where  $G_0$  is an arbitrary fixed value (typically chosen as zero)



The flame normal vector is defined by

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|}$$

And points into the reactants

# The G-Equation

The propagation of the surface  $G = G_0$  is described by the kinematic equation:

$$\frac{\partial \mathbf{x}_F}{\partial t} = \mathbf{u} + s_L \mathbf{n}$$

where  $\mathbf{u}$  is the flow velocity at the surface  $G = G_0$  that is located instantaneously at  $\mathbf{x}_F$  and  $s_L$  is the displacement speed of the surface relative to the underlying fluid.

Then, using the expansion:

$$\frac{\partial G}{\partial t} + \nabla G \cdot \frac{\partial \mathbf{x}_F}{\partial t} = 0$$

We get the final G-equation:

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L |\nabla G|$$

Local change      convection      Progress of flame front by burning velocity

# The G-Equation

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L |\nabla G|$$

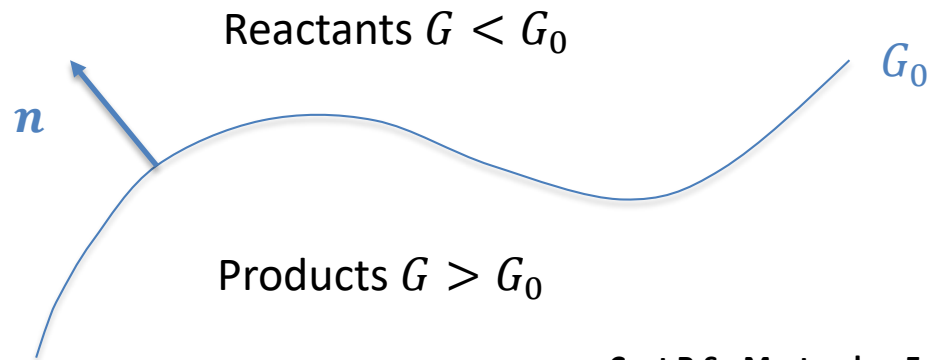
- The G-equation contains no diffusion and no reaction terms
- The quantity G is a field variable in three-dimensional space while the level set  $G=G_0$  defines a two-dimensional surface within that field
- The application to premixed flames depends only on the description of the propagation of the surface at  $G=G_0$ , and in principle the rest of the G field can remain arbitrary
- The G-Equation model can be applied for thin flames and well-defined burning velocities, i.e. in the regime of corrugated flamelets

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$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L |\nabla G|$$

- This is a kinematic equation, i.e. the density does not appear in the equation
- Valid for flame position:  $G = G_0$ 
  - For solving the field equation,  $G$  needs to be defined in the entire field
  - Different possibilities to define  $G$ , e.g. signed distance function:

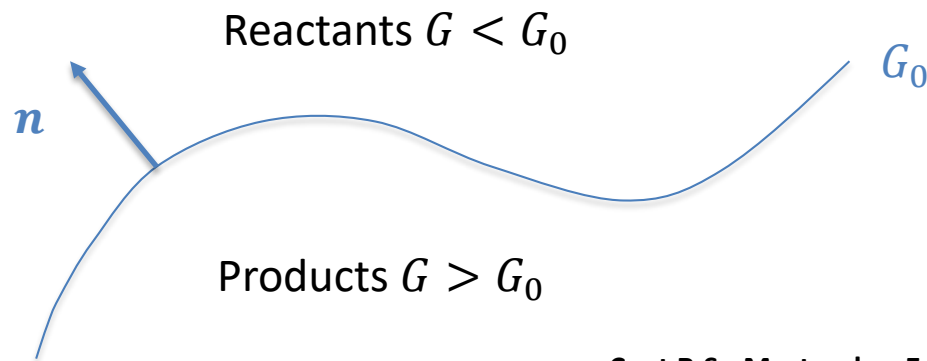
$$|\nabla G| = 1$$



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$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L |\nabla G|$$

- Influence of chemistry by  $s_L$
- $s_L$  is not necessarily constant, but it is influenced by
  - Strain  $S$
  - Curvature  $K$
  - Lewis number
- Modified laminar burning velocity



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# Laminar burning velocity: curvature

Curvature  $\kappa = \frac{\partial n_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( -\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|} \right)$

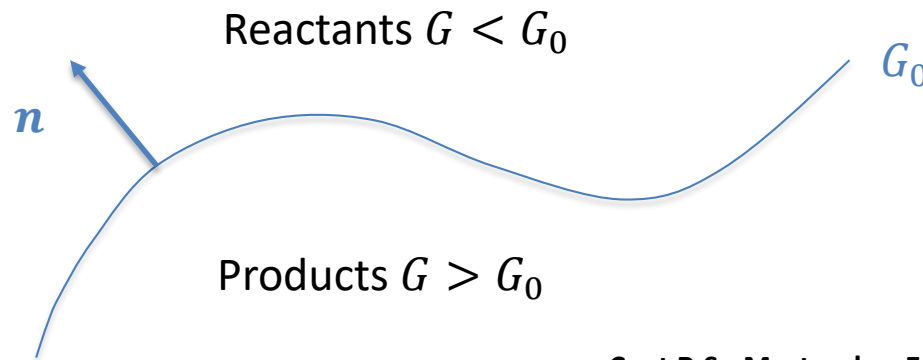
Is the curvature of the surface at  $G = G_0$  expressed simply as the divergence of the local normal vector

Influence of curvature

$$s_L = s_L^0 - s_L^0 \mathcal{L} \kappa - \mathcal{L} S$$

$\mathcal{L}$  is a Markstein length, expected to be  $\sim \delta_L$

This is a linear model for the dependence of the burning velocity on the curvature



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# Laminar burning velocity: Markstein length

$$s_L = s_L^0 - s_L^0 \mathcal{L} \kappa - \mathcal{L} S$$

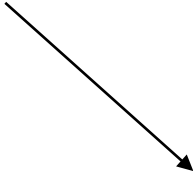
$\mathcal{L}$  is a Markstein length, expected to be of the same order of the laminar flame thickness, i.e.  $\mathcal{L} \sim \delta_L$

The Markstein length can be:

- Determined by experiments
- Determined by asymptotic analyses

$$\mathcal{L} = \mathcal{M} \delta_L$$

The larger the Markstein length, the greater the effect of curvature on localized burning velocity.



the Markstein number  $\mathcal{M}$  characterizes the effect of local heat release of a propagating flame on variations in the surface topology along the flame and the associated local flame front curvature

# Laminar burning velocity: curvature

Strain rate  $\mathcal{S} = -n_i \frac{\partial u_i}{\partial x_j} n_j$

$S$  is the strain rate in the plane of the surface. It is equal to the tangential strain rate provided that the velocity divergence is zero, i.e. in the absence of compressibility or heat release effects

Influence of strain rate

$$s_L = s_L^0 - s_L^0 \mathcal{L} \kappa - \mathcal{L} \mathcal{S}$$

$\mathcal{L}$  is a Markstein length, expected to be  $\sim \delta_L$

This is a linear model for the dependence of the burning velocity on the strain rate

Incorporating the expression above in the G-equation, we have the following modified G-equation:

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = (s_L^0 - s_L^0 \mathcal{L} \kappa - \mathcal{L} \mathcal{S}) |\nabla G|$$

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# Turbulent premixed flames with $G$

In a turbulent flow field it is helpful to assume that  $G$  is both well-defined and well-behaved outside the surface at  $G = G_0$ . Then it is possible to define the PDF of  $G$  denoted by  $p(G; \mathbf{x}, t)$ .

The mean and the variance of  $G$  are given by the integration over the pdf as:

$$\bar{G} = \int G p(G; \mathbf{x}, t) dG$$

$$\overline{G'^2} = \int (G - \bar{G})^2 p(G; \mathbf{x}, t) dG$$

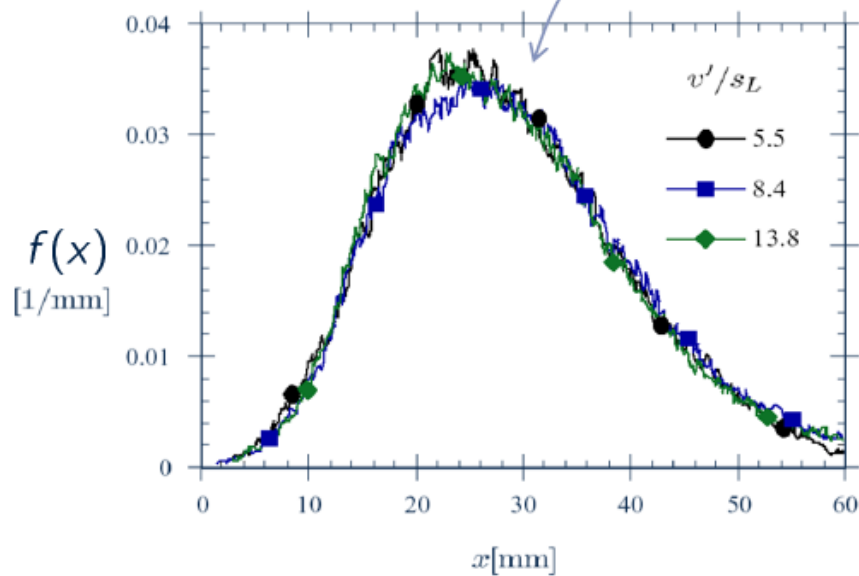
It would be straightforward to derive balance equations for these quantities, which could be modelled and solved.

Instead it is more interesting to consider further the relationship between  $G$  and the distance field.

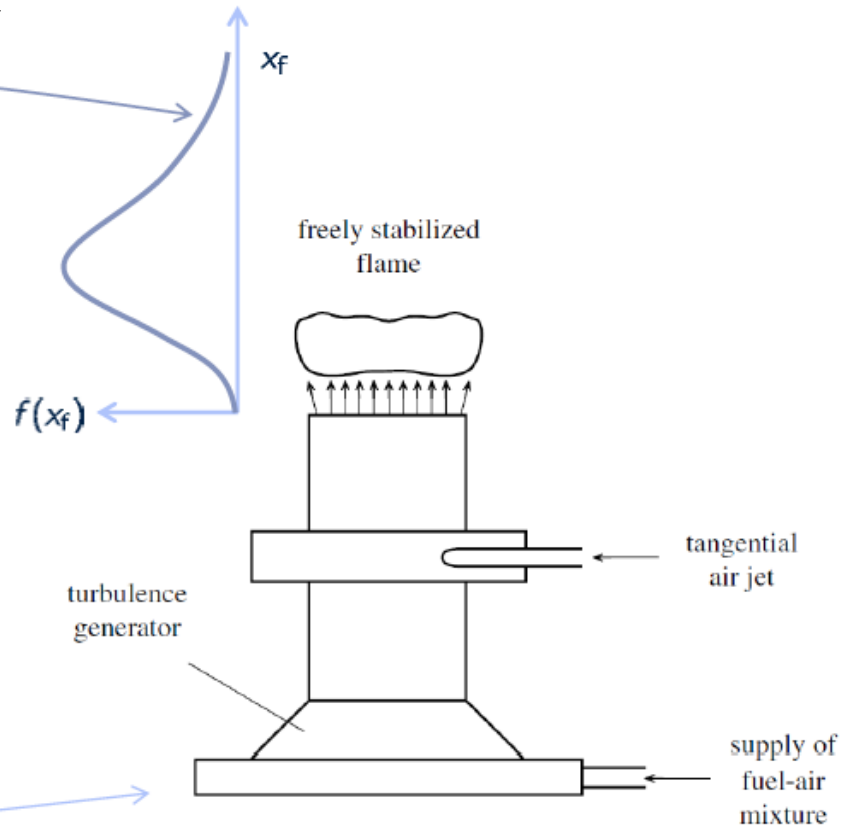
# Statistical description of turbulent flame front (I)

Probability Density Function of finding  $G = G_0$

$$p(G_0; \mathbf{x}, t) = \int \delta(G - G_0) p(G; \mathbf{x}, t) dG$$



Experimental determination  
in weak swirl burner



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# Statistical description of turbulent flame front (II)

The PDF of finding the surface  $G = G_0$  at an arbitrary spatial location  $\mathbf{x}$  at time  $t$  may be stated as:

$$p(G_0; \mathbf{x}, t) = \int \delta(G - G_0) p(G; \mathbf{x}, t) dG$$

It is clear that this PDF provides information about the statistical geometry or spatial distribution of the flame surface, similarly to that provided by the BML flame cross frequency and the FSD approach.

Let us now focus on the ideal case of a locally 1D statistically stationary turbulent flame (see previous slide). All the quantities can be considered as functions of a single spatial coordinate  $x$ .

Then, the mean and variance of the flame position  $x_F$  are given by:

$$x_F = \int x p(G_0; x, t) dx$$

$$\overline{(x - x_F)^2} = \int (x - x_F)^2 p(G_0; x, t) dx$$

# Statistical description of turbulent flame front (III)

The variance of the flame position can be also interpreted as the squared flame brush thickness, i.e.:

$$l_f = \sqrt{(x - x_F)^2}$$

It is helpful to relate the mean and variance of flame position more closely to the mean and variance of  $G$ :

$$\bar{G}(x) - G_0 = x - x_F$$

Which means that the mean flame position  $x = x_F$  is fixed at the location where  $\bar{G} = G_0$ .

Fluctuations of  $G$  about the mean are given by:

$$G' = G - \bar{G} = G - (G_0 + x - x_F)$$

Setting  $G = G_0$  at the surface provides:

$$G' = -(x - x_F)$$

# Statistical description of turbulent flame front (IV)

Thus, the scalar variable  $G$  can be interpreted as the scalar distance between the instantaneous and the mean flame positions, measured in the direction normal to the mean turbulent brush.

The analysis we carried out was limited to 1D cases. However, it can be extended to more general 2D and 3D cases. The mean flame location can be defined by  $G(x, t) = G_0$  and by the expression for the normal distance:

$$x = x_F + \frac{\bar{G} - G_0}{|\nabla G|}$$

Note that the re-initialization condition  $|\nabla G| = 1$  must be applied in order to guarantee the regularity of the  $G$  field away from the mean flame location.

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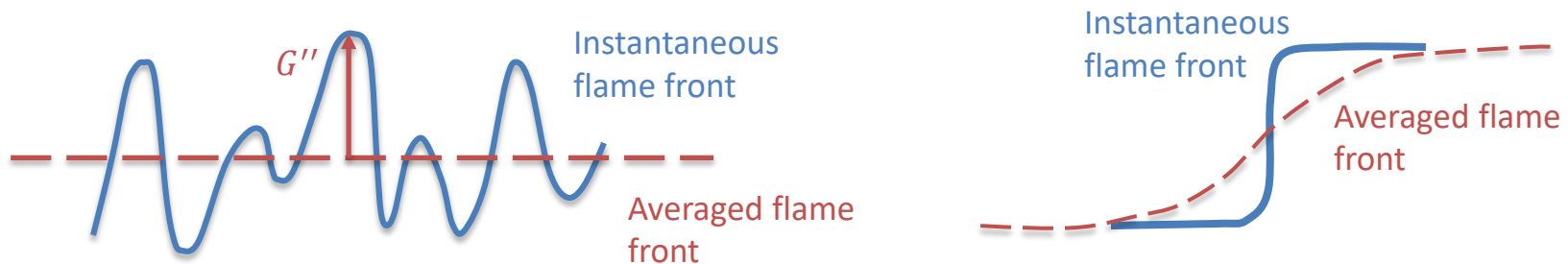
# Favre Mean and Variance Equations

Using Favre averaging it is possible to derive equation for the Favre averaged mean and variance of G:

$$\bar{\rho} \frac{\partial \tilde{G}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \tilde{G}}{\partial x_i} = \overline{(\rho s_L^0) \sigma} - \overline{(\rho \mathcal{D}) \kappa \sigma} - \frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' G''})$$

$$\bar{\rho} \frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \widetilde{G''^2}}{\partial x_i} + \frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' G''^2}) = -2 \bar{\rho} \widetilde{u_i'' G''} \frac{\partial \tilde{G}}{\partial x_i} - \bar{\rho} \tilde{\omega} - \bar{\rho} \tilde{\chi} - (\rho \mathcal{D}) \overline{\kappa \sigma}$$

- $\sigma \stackrel{\text{def}}{=} |\nabla G|$  can be interpreted as the area ratio of the flame  $A_T/A$
- As already mentioned, the variance describes the average size of the flame



# Sink terms in the variance equation

$$\bar{\rho} \frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \widetilde{G''^2}}{\partial x_i} + \frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' G''^2}) = -2 \bar{\rho} \widetilde{u_i'' G''} \frac{\partial \tilde{G}}{\partial x_i} - \bar{\rho} \tilde{\omega} - \bar{\rho} \tilde{\chi} - (\bar{\rho} \mathcal{D}) \bar{\kappa} \sigma$$

Kinematic restoration

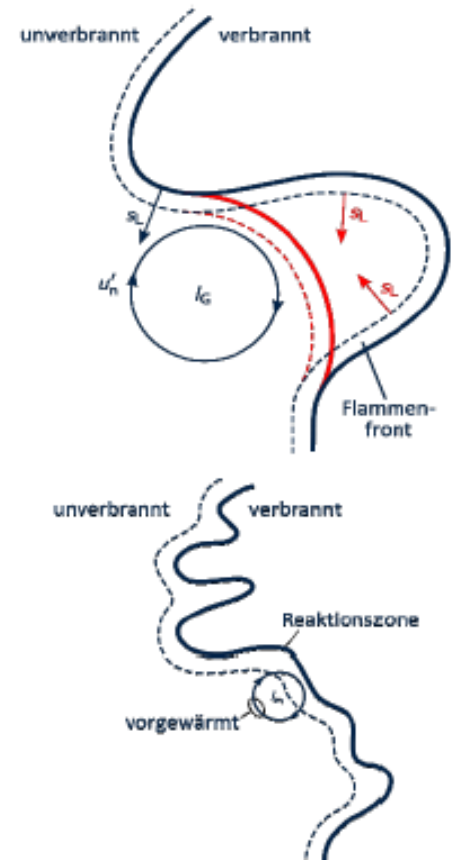
$$\tilde{\omega} = -2(\bar{\rho} s_L^0) \frac{\overline{G'' \sigma}}{\bar{\rho}}$$

Scalar dissipation

$$\tilde{\chi} = 2 \frac{\overline{\rho \mathcal{D}}}{\bar{\rho}} \left( \frac{\partial \widetilde{G''}}{\partial x_i} \right)^2$$

They are typically modelled as:

$$\tilde{\omega} + \tilde{\chi} = C_s \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{G''^2}$$



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# Turbulent burning velocity (I)

Turbulent transport is commonly treated using a gradient transport model:

$$\bar{\rho} \widetilde{u_i'' G''} = -\bar{\rho} \mathcal{D}_t \frac{\partial \tilde{G}}{\partial x_i}$$

However, this would introduce a 2<sup>nd</sup> order derivative of G, changing the mathematical character of the G equation. Instead, the modelled gradient diffusion term may be decomposed into normal and tangential components:

$$\nabla \cdot (\bar{\rho} \mathcal{D}_t \nabla \tilde{G}) = n \cdot \nabla (\bar{\rho} \mathcal{D}_t n \cdot \nabla \tilde{G}) - \bar{\rho} \mathcal{D}_t \tilde{\kappa} |\nabla \tilde{G}|$$

Thus, after neglecting the molecular diffusion contribution, the sum of RHS terms in the G equation can be rewritten as:

$$\overline{(\rho s_L^0) |\nabla G|} - \nabla \cdot (\bar{\rho} \widetilde{u'' G''}) = [\overline{(\rho s_L^0) |\nabla G|} + n \cdot \nabla (\bar{\rho} \mathcal{D}_t n \cdot \nabla \tilde{G})] - \bar{\rho} \mathcal{D}_t \tilde{\kappa} |\nabla \tilde{G}|$$

The term in the square brackets is written introducing the turbulent burning velocity:

$$(\rho s_T^0) |\nabla \tilde{G}| \stackrel{\text{def}}{=} \overline{(\rho s_L^0) |\nabla G|} + n \cdot \nabla (\bar{\rho} \mathcal{D}_t n \cdot \nabla \tilde{G})$$

# Turbulent burning velocity (II)

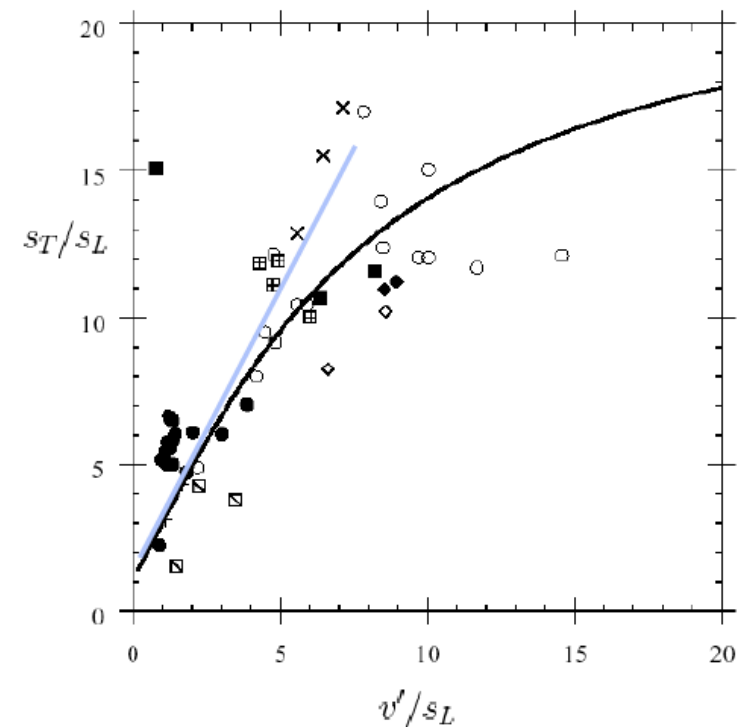
Introducing the turbulent burning velocity  $s_T^0$ :

$$(\rho s_T^0) |\nabla \tilde{G}| \stackrel{\text{def}}{=} \overline{(\rho s_L^0) |\nabla G|} + n \cdot \nabla (\bar{\rho} \mathcal{D}_t n \cdot \nabla \tilde{G})$$

Example: modeling of turbulent burning velocity by the Damkohler theory:

$$\frac{s_T^0}{s_L^0} = 1 - \alpha \frac{l_t}{l_F} + \sqrt{\left(\alpha \frac{l_t}{l_F}\right)^2 + 4\alpha \frac{u' l_t}{s_L l_F}}$$

It is interesting to note that the turbulent burning velocity appears as an input to the Favre averaged G-equation formulation and it is not part of the solution



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# Favre Mean and Variance Equations

Equation for the Favre mean

$$\bar{\rho} \frac{\partial \tilde{G}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \tilde{G}}{\partial x_i} = (\rho s_T^0) |\nabla \tilde{G}| - \bar{\rho} \mathcal{D}_t \tilde{\kappa} |\nabla \tilde{G}|$$

Equation for variance

$$\bar{\rho} \frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \widetilde{G''^2}}{\partial x_i} = \nabla_{||} \cdot (\bar{\rho} \mathcal{D}_t \nabla_{||} \widetilde{G''^2}) - 2 \bar{\rho} \mathcal{D}_t \left( \frac{\partial \tilde{G}}{\partial x_i} \right)^2 - \bar{\rho} C_s \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{G''^2}$$

Similar arguments  
have been applied to  
the closure of the  
turbulent transport  
term  $\frac{\partial}{\partial x_i} (\bar{\rho} \widetilde{u_i'' G''^2})$

# Presumed PDF approach

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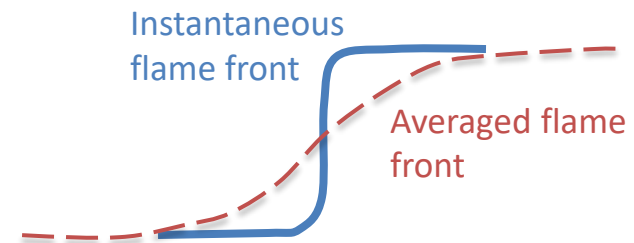
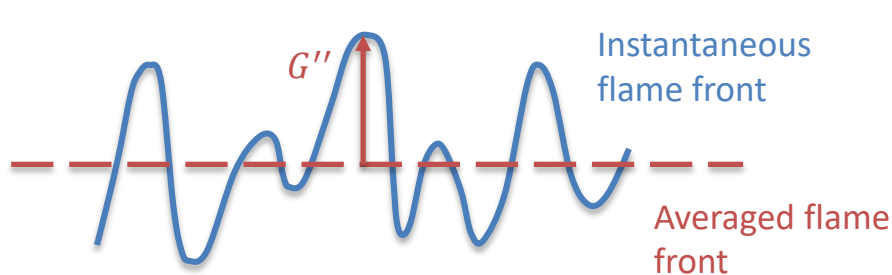
Typically a Gaussian Distribution is assumed

$$p(G; x, t) = \frac{1}{\sqrt{2\pi\widetilde{G''^2}|_0}} \exp\left(-\frac{(G - \tilde{G})^2}{2\widetilde{G''^2}|_0}\right)$$

Mean temperature (and other scalars)

$$\tilde{T}(x, t) = \int T(G) p(G; x, t) dG$$

$T(G)$  is taken from the laminar premixed flame without strain



# Other methods: tabulation of chemistry (I)

- In general, turbulent premixed flames well away from extinction can be modelled without explicit consideration of the chemical reaction rate. Chemical information is encapsulated in quantities such as the **laminar burning velocity** and its response to straining.
- The computational costs of detailed chemistry are high, and it is preferable to treat the chemistry separately from any turbulent flame calculation. This is true especially in LES where computational costs are already high due to the demand for fine spatial resolution and the need for unsteady solutions.
- **Chemistry can be precomputed and stored in tabulated form** using a number of different approaches. Perhaps the simplest is a **premixed flamelet library**, in which the laminar burning velocity can be stored as a function of mixture strength, pressure and reactant temperature.
- Other independent variables can be included, such as strain rate and mean curvature. In order to avoid the computational costs of searching in tables, it is possible to make use of correlations for laminar burning velocity which have been derived from either experimental or one-dimensional computations .

## Other methods: tabulation of chemistry (II)

An approach such as Flamelet Generated Manifolds (FGM) or Flamelet Prolongation of ILDM (FPI) allows for a reasonable level of chemical detail that is computationally inexpensive - at least within the turbulent flame calculation - and which is largely free from the restrictions of the original flamelet concept.

**Gicquel, O., Darabiha, N., Thevenin, D.,** Laminar premixed hydrogen/air counterflow flame simulations using flame prolongation of ILDM with preferential diffusion. *Proc. Combust. Inst.* 28, 1901–1908 (2000)

**van Oijen, J.A., de Goey, L.P.H.,** Modelling of premixed laminar flames using flamelet generated manifolds. *Combust. Sci. Technol.* 161, 113–138 (2000)



# Other methods: Transported PDF

- The transported pdf approach makes no assumptions about the structure of the flame and has proved successful in its application to turbulent non-premixed flames.
- There have been applications of PDF transport modelling to premixed flames in which convincing results have been obtained.
- The advantages of the approach lie in its potential for generality especially in cases where direct chemical effects may be important, but the computational cost is high and there are technical issues concerned with the modelling of mixing processes in the presence of the high scalar gradients typical of premixed flames.

**Pope, S.B.**, PDF methods for turbulent reacting flows. Prog. Energy Combust. Sci. 11, 119– 192 (1985)

**Pope, S.B., Cheng, W.K.**, The stochastic flamelet model of turbulent premixed combustion. Proc. Combust. Inst. 22, 781–815 (1989)

**Jones, W.P.**, The joint scalar probability density function. In: Launder, B.E., Sandham, N.D. (Eds.) Closure Strategies for Turbulent and Transitional Flows, Cambridge University Press, Cambridge, UK (2002)

**Lindstedt, R.P., Vaos, E.M.**, Transported PDF modelling of high-Reynolds number premixed turbulent flames. Combust. Flame 145, 495–511 (2006)

# Other methods: Conditional Moment Closure (CMC)

- Another approach that has proved successful in non-premixed combustion is the Conditional Moment Closure (CMC) approach, in which the fluctuations of all variables about the conditional mean mixture fraction are assumed to be small.
- In principle the CMC approach could be extended to treat premixed flames, possibly by using the reaction progress variable as a conditioning variable. The use of a marker field variable has been suggested, but it is questionable whether this would bring any advantage over the existing G-equation approach.
- One promising avenue is the Conditional Source Term Estimation (CSTE) approach, which is closely related to CMC and which may provide a more realistic way to model chemical effects in premixed flames.

**Bilger, R.W.**, Marker fields for turbulent premixed combustion. *Combust. Flame* 138, 188–194 (2004)

**Grout, R.W.**, An age extended progress variable for conditioning reaction rates. *Phys. Fluids* 19, 105107 (2007)

**Grout, R.W., Bushe W.K., Blair C.**, Predicting the ignition delay of turbulent methane jets using conditional source term estimation. *Combust. Theory Model.* 11, 1009–1028 (2007)