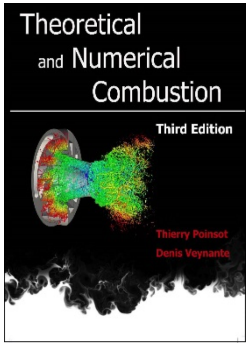
Iran First International Combustion School (ICS2019)
Tehran, 24-26 August 2019

Combustion modeling

6. Turbulent Combustion Modeling

Alberto Cuoci

References



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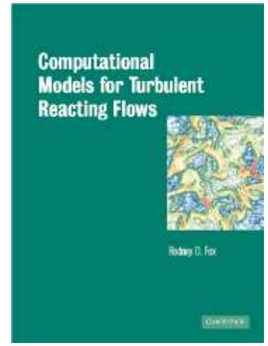

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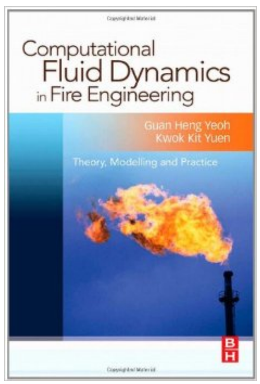

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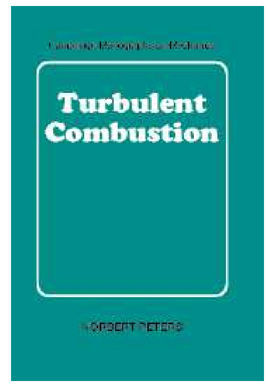

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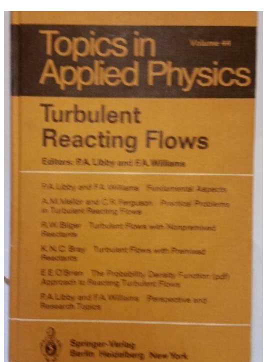

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Outline

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

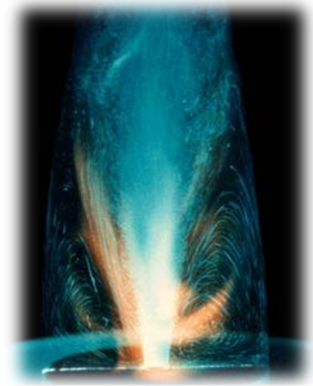
a) Eddy Dissipation models: ED, ED-FR, EDC
b) Steady Laminar Flamelet model
  i. Mixture fraction
  ii. Flamelet equations
  iii. Presumed PDF approach

3. Premixed combustion

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

Introduction



Numerical modeling of turbulent combustion

Complex numerical techniques

Computational resources

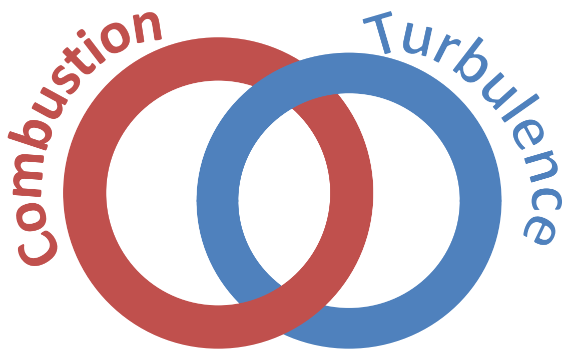
Large gradients of temperature and composition

Wide range of characteristic times (fludi dynamics and chemistry)

Detailed kinetic mechanisms

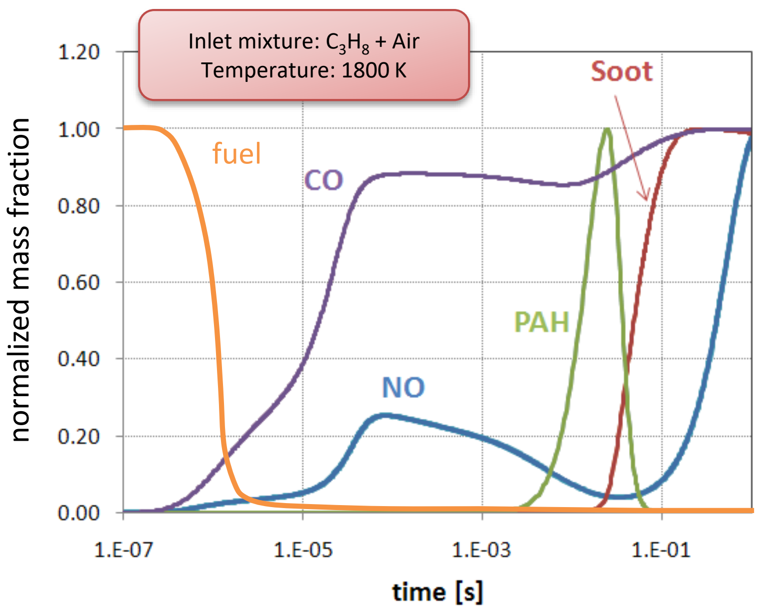
- hundreds of species
- thousands of reactions

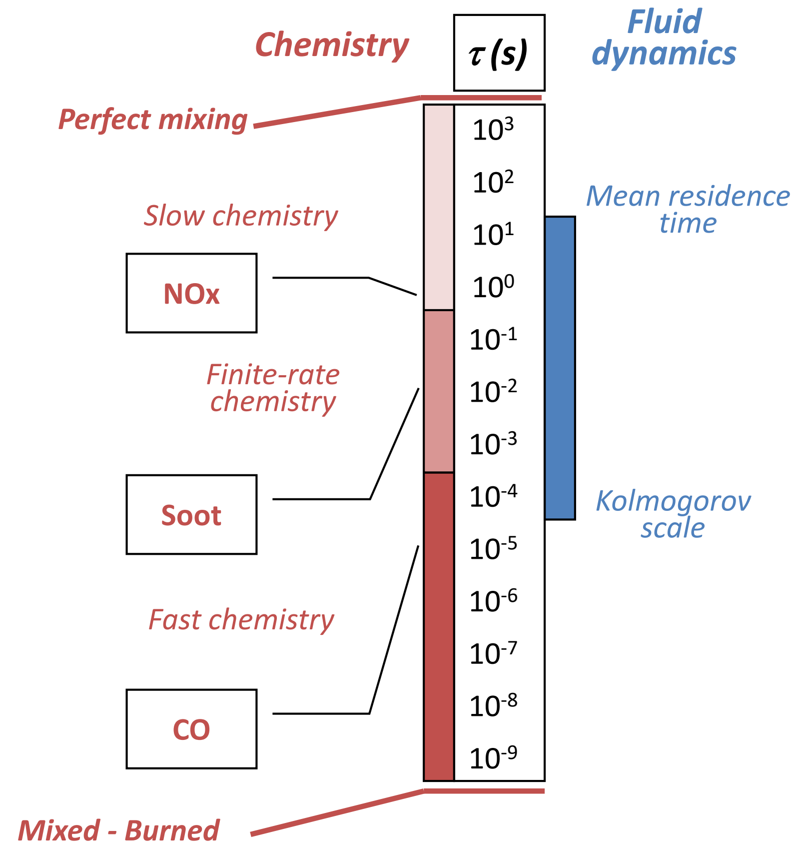
Turbulence-Chemistry Coupling



Combustion releases heat, strongly affecting the density of the mixture and therefore the fluid dynamics of the system

Turbulence can improve the mixing between fuel and oxidizer. However, if too large, extinction can occur





Adapted from **Fox R.O.**, *"Computational Models for Turbulent Reacting Flows"*, Cambridge, 2003

Characteristic times of chemistry

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

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

Reaction rates

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

Formation rates

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

Eigenvalues of Jacobian

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

Jacobian matrix (based on formation rates)

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

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

$$\boldsymbol{Da << 1}$$

Chemical reactions extremely slow. The system is under chemical control

Fluid dynamic regime

$$\boldsymbol{Da >> 1}$$

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

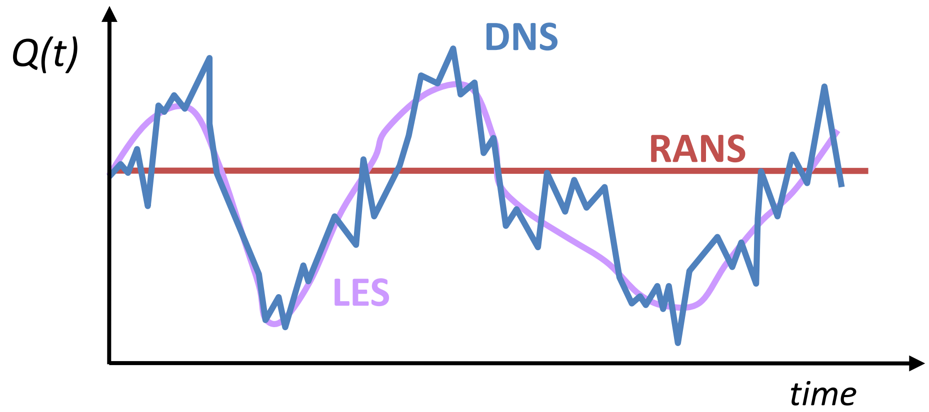
Peters N., *"Turbulent Combustion"*, Cambridge University Press, 2000

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

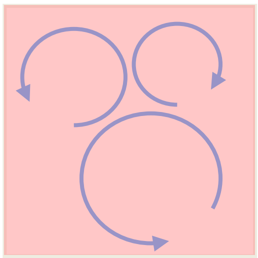
The conservation equations are filtered and only the largest vortices are described. Vortices smaller than a characteristic length are only modeled.

RANS

Reynolds-Averaged Navier-Stokes

Only the mean variables are described.

Formation rates have to be modeled



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

Effect of fluctuations of formation rates (I)

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

$$R = k(T)\prod_i c_i^{\alpha_i} \qquad\qquad k(T) = AT^n \exp\left(-\frac{E_a}{RT}\right)$$

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:

$$\overline{R}\left(\mathbf{c},T\right) = \overline{R}\left(\overline{\mathbf{c}}+\mathbf{c}',\overline{T}+T'\right) \neq R\left(\overline{\mathbf{c}},\overline{T}\right)$$

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

$$R\left(\mathbf{c},T\right) = R\left(\overline{\mathbf{c}}+\mathbf{c}',\overline{T}+T'\right) = R\left(\overline{\mathbf{c}},\overline{T}\right) + \sum_{i=1}^{NS}\left.\frac{\partial R}{\partial c_i}\right|_{\overline{c},\overline{T}} c_i' + \left.\frac{\partial R}{\partial T}\right|_{\overline{c},\overline{T}} T' + \frac{1}{2}\sum_{i=1}^{NS}\sum_{j=1}^{NS}\left.\frac{\partial^2 R}{\partial c_i \partial c_j}\right|_{\overline{c},\overline{T}} c_i' c_j' +$$

$$\frac{1}{2}\left.\frac{\partial^2 R}{\partial T^2}\right|_{\overline{c},\overline{T}} T'^2 + \frac{1}{2}\sum_{i=1}^{NS}\left.\frac{\partial^2 R}{\partial c_i \partial T}\right|_{\overline{c},\overline{T}} c_i' T' \qquad + \text{term of higher order}$$

Effect of fluctuations of formation rates (II)

If we apply the mean:

$$\overline{R}(\mathbf{c},T) \approx R(\overline{\mathbf{c}},\overline{T}) + \frac{1}{2}\sum_{i=1}^{NS}\sum_{j=1}^{NS}\frac{\partial^2 R}{\partial c_i \partial c_j}\bigg|_{\overline{c},\overline{T}}\overline{c_i' c_j'} + \frac{1}{2}\frac{\partial^2 R}{\partial T^2}\bigg|_{\overline{c},\overline{T}}\overline{T'^2} + \frac{1}{2}\sum_{i=1}^{NS}\frac{\partial^2 R}{\partial c_i \partial T}\bigg|_{\overline{c},\overline{T}}\overline{c_i' T'}$$

(I) (II) (III) (IV)

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

Terms (II), (III) and (IV) 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.

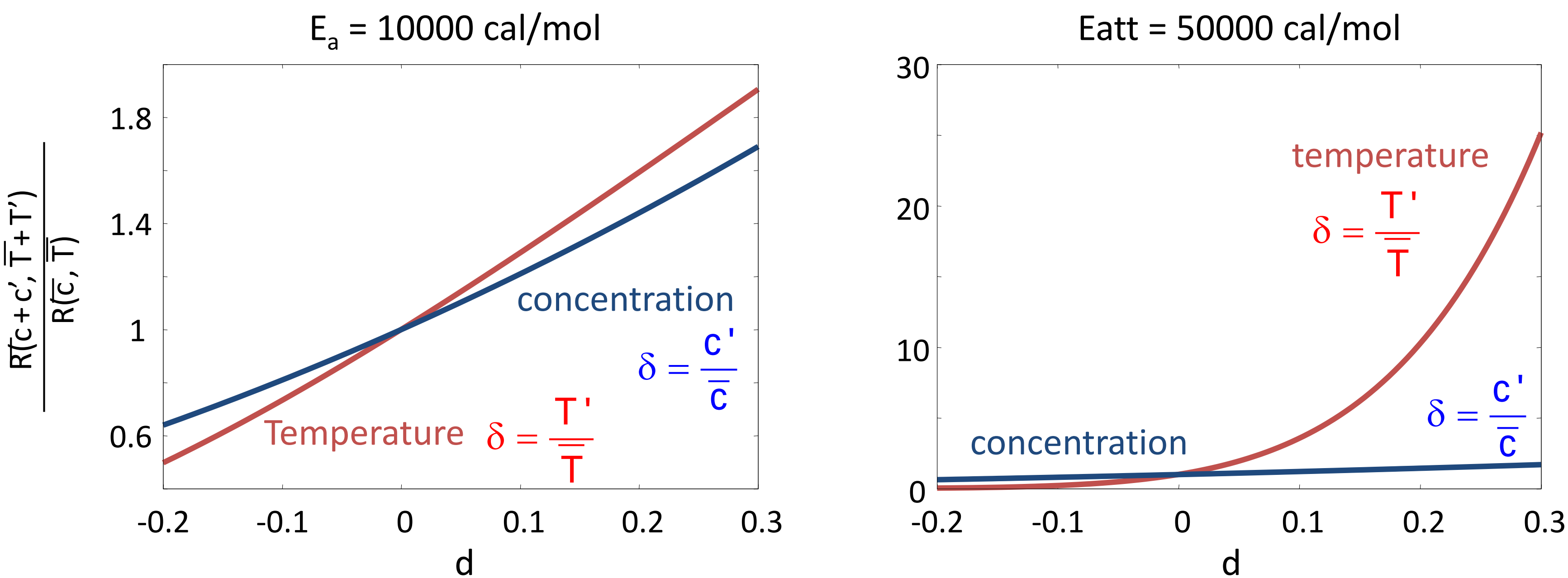
$$\overline{R}(\mathbf{c},T) = R(\overline{\mathbf{c}},\overline{T}) + C_C$$

Temperature and composition fluctuations

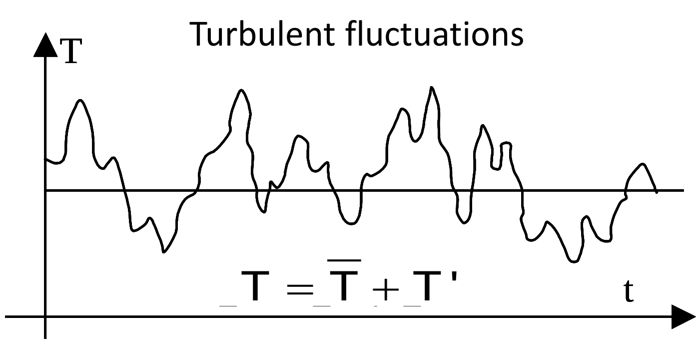
Temperature fluctuations have a strong impact especially onreactions with large activation energy (as an example formation of NOx)

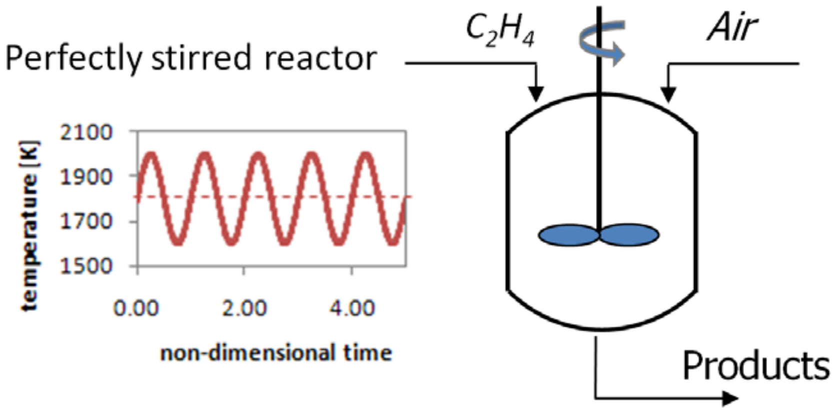
Example: second order reaction

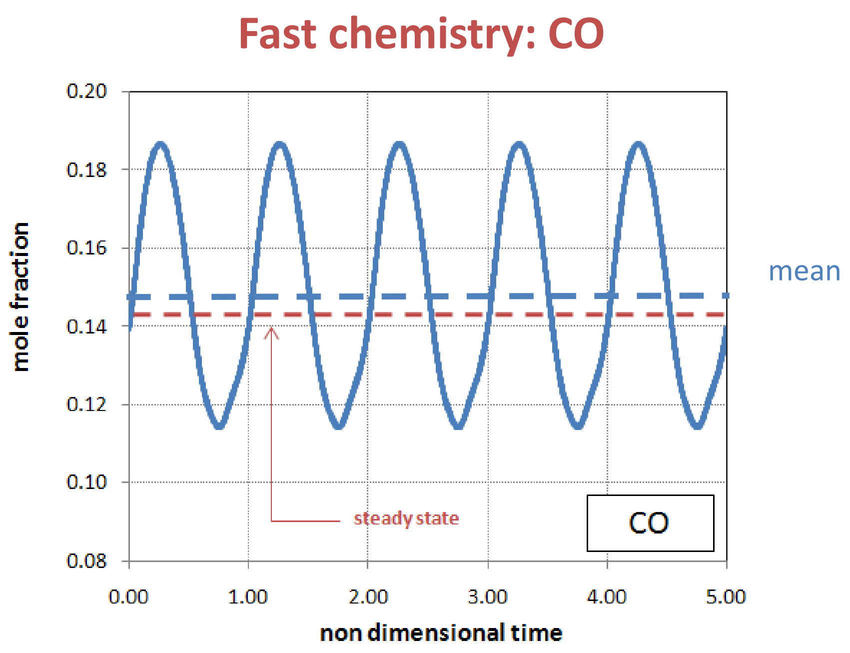
$$R = AT^n \exp\left(-\frac{E_a}{RT}\right)c^2$$

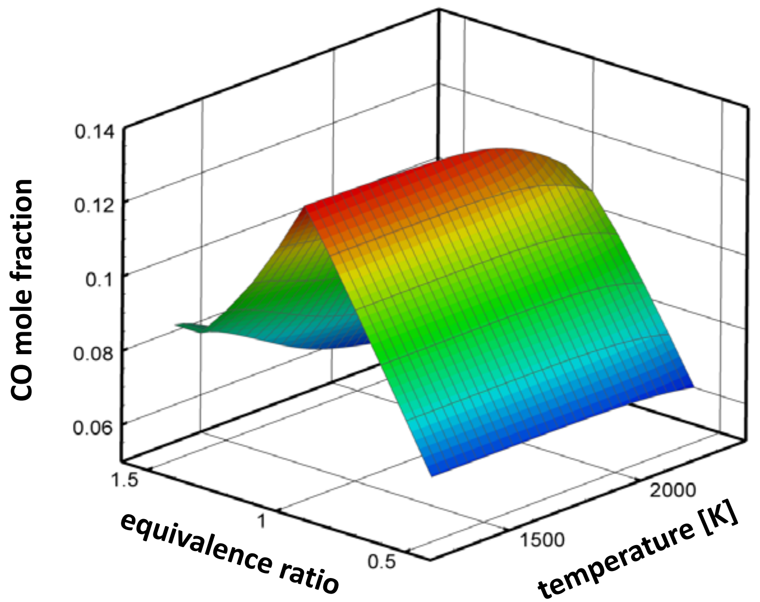


Effect of turbulent fluctuations (I)



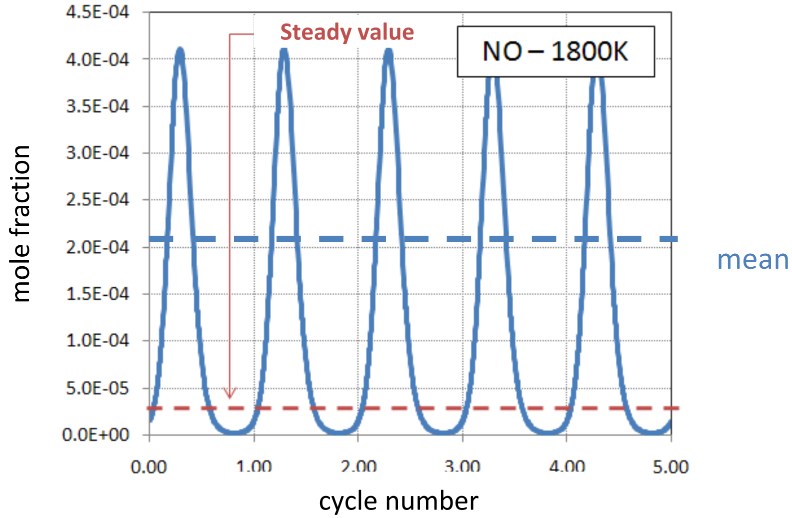


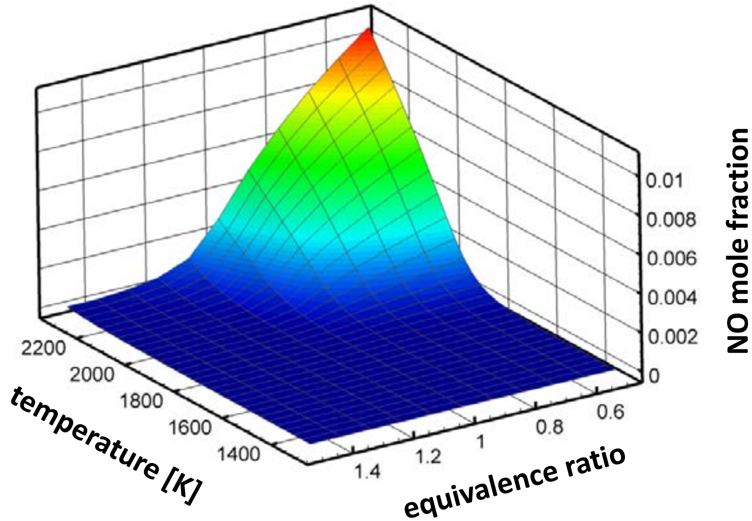




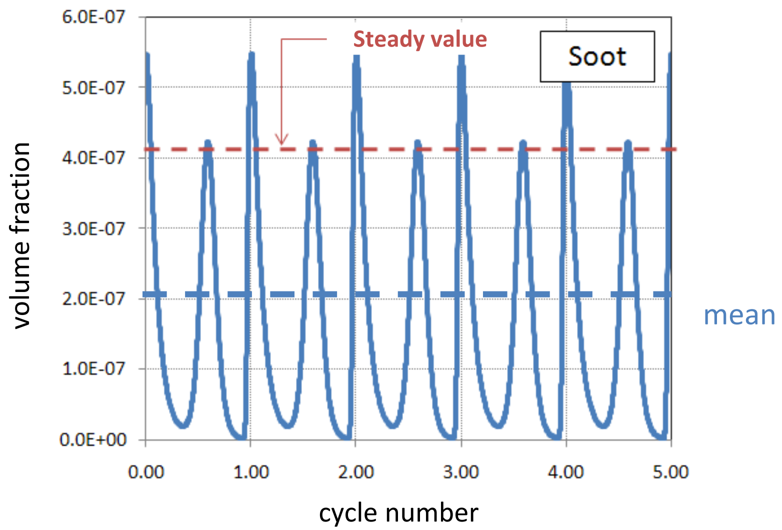
Effect of turbulent fluctuations (II)

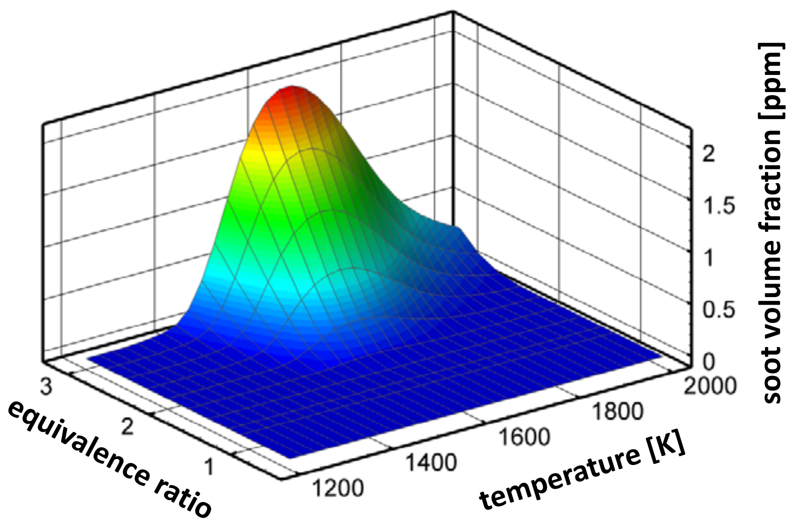
Slow chemistry: NOx





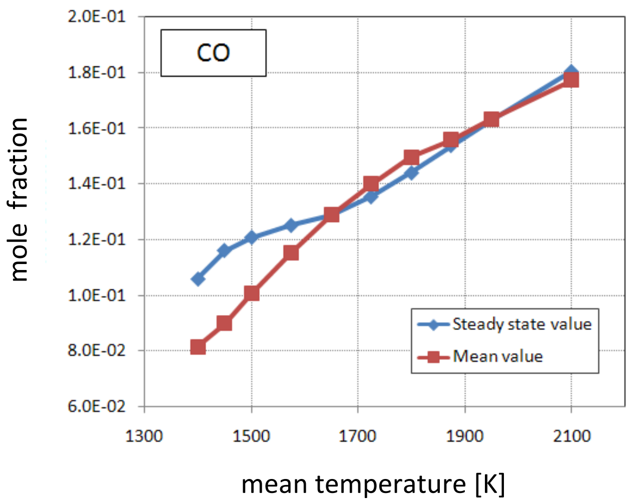
Finite-rate chemistry: Soot



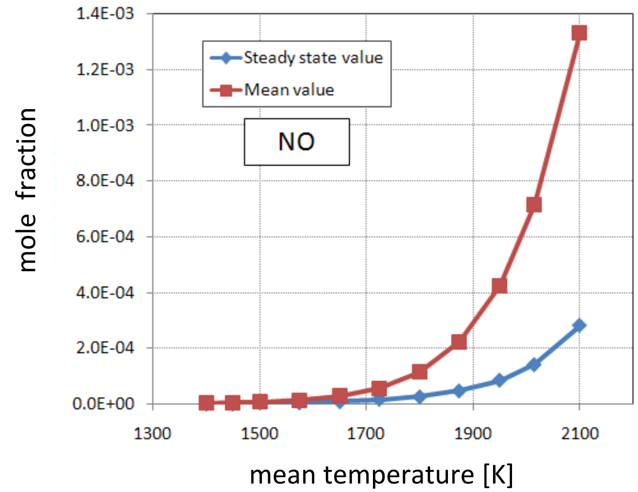


Effect of turbulent fluctuations (III)

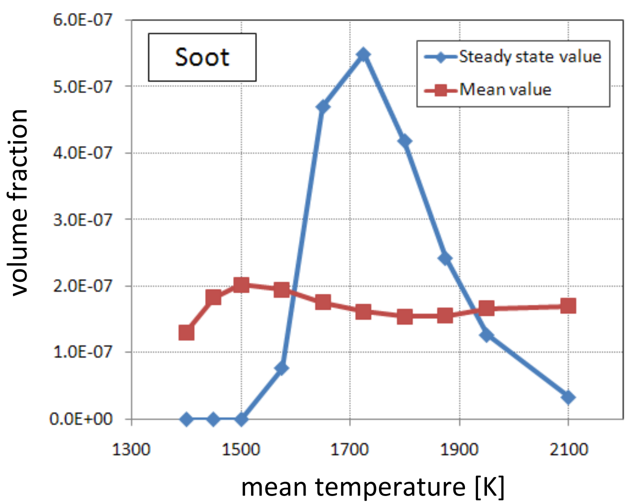
Fast chemistry: CO



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

Correction coefficient for reaction rates (I)

Rate constant is highly non linear function of temperature

$$k(T) = A \cdot T^{\beta} \cdot \exp\left(-\frac{E_{att}}{RT}\right)$$

Introduction of a proper probability distribution function p(T)

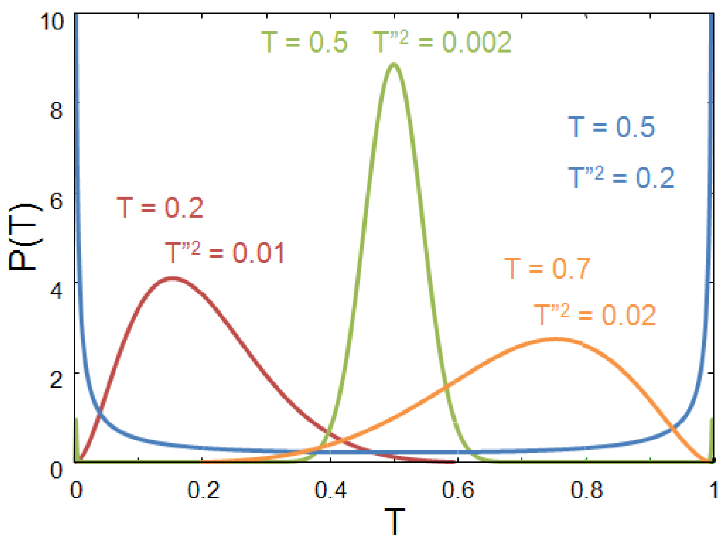
$$\tilde{k}(T) = \int_{T_{min}}^{T_{max}} k(T)p(T)dT = C_C\, k(\tilde{T})$$

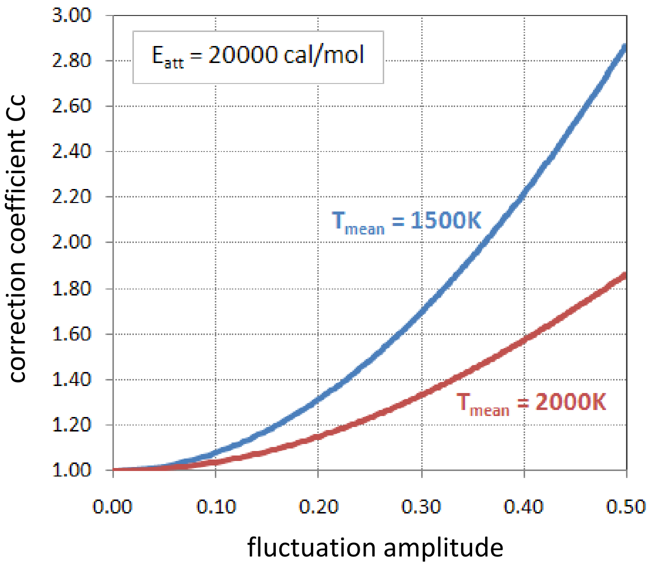
Correction coefficient

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

Requires the knowledge of the variance of temperature

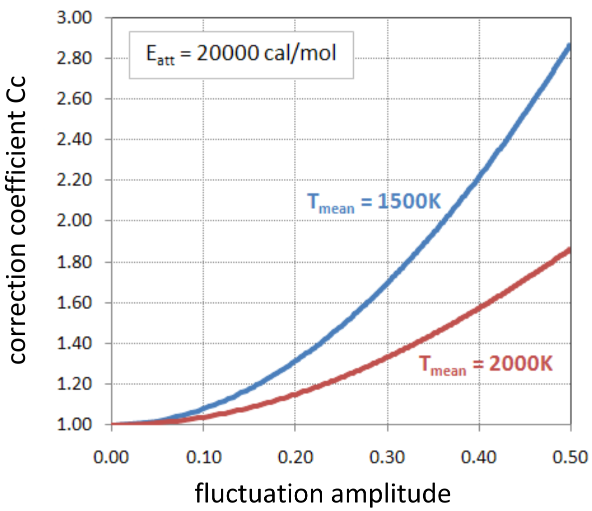
β-PDF

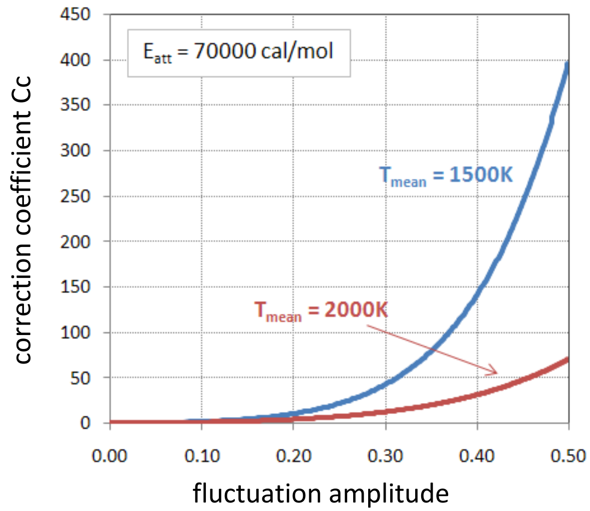




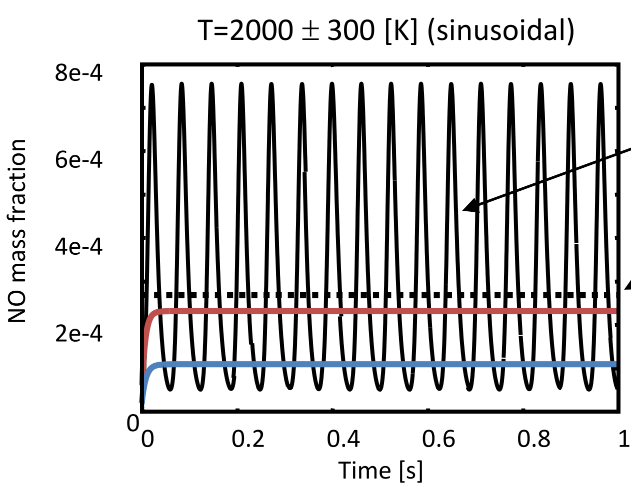
A. Cuoci, A. Frassoldati, G. Buzzi Ferraris, T. Faravelli, E. Ranzi, International Journal of Hydrogen Energy (32), p. 3486-3500 (2007)

Correction coefficient for reaction rates (II)





The correction Coefficient is significantly > 1 for high activation energies (Thermal NOx)



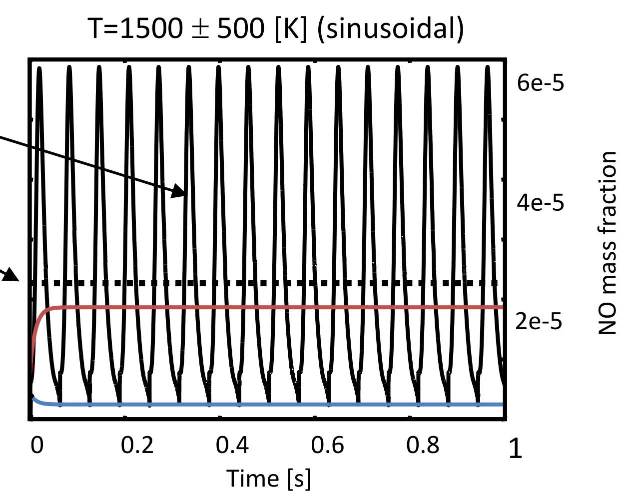
Φ=0.95 CH_4/Air

oscillating profile

mean value

Corrected: k=k(T)*Cc

Uncorrected: k=k(T)



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

Outline

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a) Eddy Dissipation models: ED, ED-FR, EDC
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   i. Mixture fraction
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Turbulent combustion models

	Reaction Rates Approach (RRA)	Primitive Variables Approach (PVA)
Infinitely Fast Chemistry	1. Eddy Dissipation 2. Eddy Dissipation – Finite Rate	1. Fast Chemistry – PDF mixture fraction
Finite Rate Chemistry	1. Eddy Dissipation Concept 2. Transported PDF Flamelet Model	1. Flamelet Approach

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 tabels

✓ 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

$\boldsymbol{Da \ll 1}$

Chemical reactions extremely slow. The system is under chemical control

Fluid dynamic regime

$\boldsymbol{Da \gg 1}$

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

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

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

Fluid dynamic control

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

Fuel reaction rate $\overline{r_f} = C_{ED}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Y}_f$

Oxidizer reaction rate $\overline{r_{ox}} = C_{ED}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Y}_{ox}$

Product reaction rate $\overline{r_p} = C_{ED}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Y}_p$

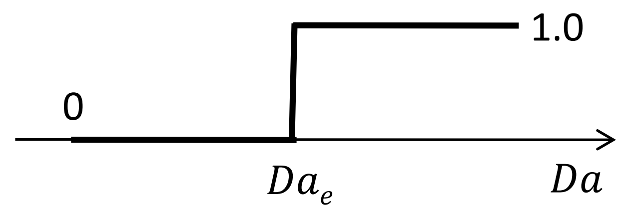
Reaction rate $\rightarrow$ $\bar{r} = min\left(\overline{r_f}, \frac{\overline{r_{ox}}}{r}, \frac{\overline{r_p}}{1+r}\right)$

Collision Mixing Model

$$min\left(\overline{r_f}, \frac{\overline{r_{ox}}}{r}, \frac{\overline{r_p}}{1+r}\right)\psi$$

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 $F + rO \rightarrow (1+r)P$

Fluid dynamic control

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

Fuel reaction rate $\overline{r_f} = C_{ED}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Y}_f$

Oxidizer reaction rate $\overline{r_{ox}} = C_{ED}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Y}_{ox}$

Product reaction rate $\overline{r_p} = C_{ED}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Y}_p$

Chemical control

Reaction rate expressed through the Arrhenius' Law

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

$$\overline{r_{chem}} = k_r \prod C_i^{\eta_i}$$

Reaction rate

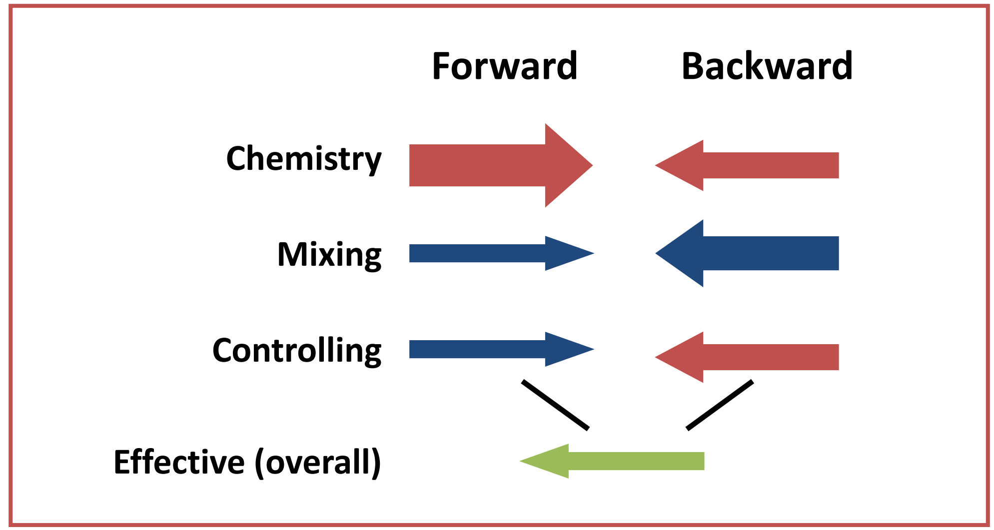
$$\bar{r} = min\left(\overline{r_f}, \frac{\overline{r_{ox}}}{r}, \frac{\overline{r_p}}{1+r}, \overline{r_{chem}}\right)$$

Thermodynamically consistent ED-FR model

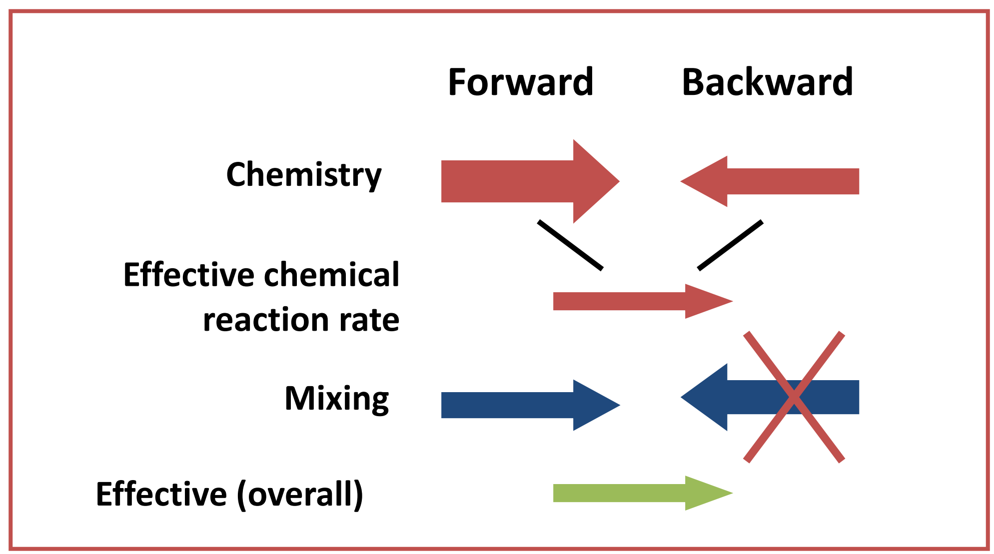
Reversible chemical reaction

$$A + B \rightleftharpoons C + D$$

Finite-Rate/Eddy-Dissipation



Consistent Finite-Rate/Eddy-Dissipation



Eddy Dissipation Concept (EDC)

Fine Structures

Hp: Isotropic turbulence

$$\gamma_\lambda = 2.13\left(\frac{\nu\varepsilon}{k^2}\right)^{1/4}$$

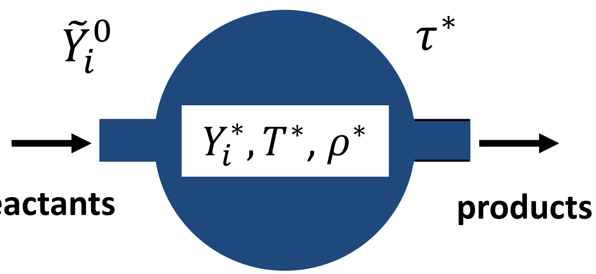
Volume fraction of *fine structures*

$$\tau^* = 0.4082\left(\frac{\nu}{\varepsilon}\right)^{1/2}$$

Mean residence time in the *fine structures*

Homogeneous, isobaric reactors

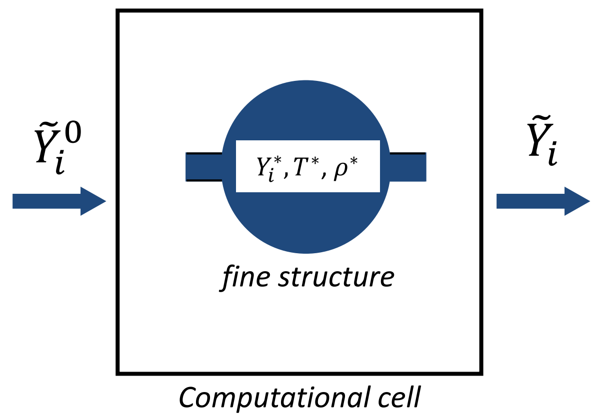
Steady-state perfectly stirred reactors



$$\Omega_i(T^*, \boldsymbol{Y}^*) = \frac{Y_i^* - \tilde{Y}_i^0}{\tau^*}$$

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



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

Outline

1. **Introduction to turbulent combustion modeling**
    a) Fluid dynamic and chemical time scales
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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 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 (CO_2, H_2O, 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 the 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

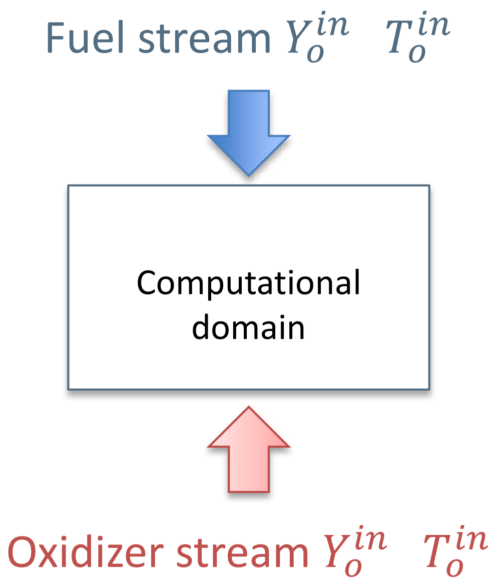
The mixture fraction (II)

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

Z_1	Z_2	Z_3
$Z_1 \stackrel{\text{def}}{=} rY_f - Y_o$	$Z_2 \stackrel{\text{def}}{=} \dfrac{C_P T}{\dot{q}} + Y_f$	$Z_3 \stackrel{\text{def}}{=} r\dfrac{C_P T}{\dot{q}} + Y_o$

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

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



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 ξ_j corresponding to the normalized Z_j variables previously defined

It is easy to demonstrate analytically that the new ξ_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 ξ_j are exactly the same, which means that actually they are the same variable, which is called the mixture fraction ξ :

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

$$\begin{cases} \xi(fuel\ stream) = 1 \\ \xi(ox\ stream) = 1 \end{cases}$$

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:

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

$$\Downarrow$$

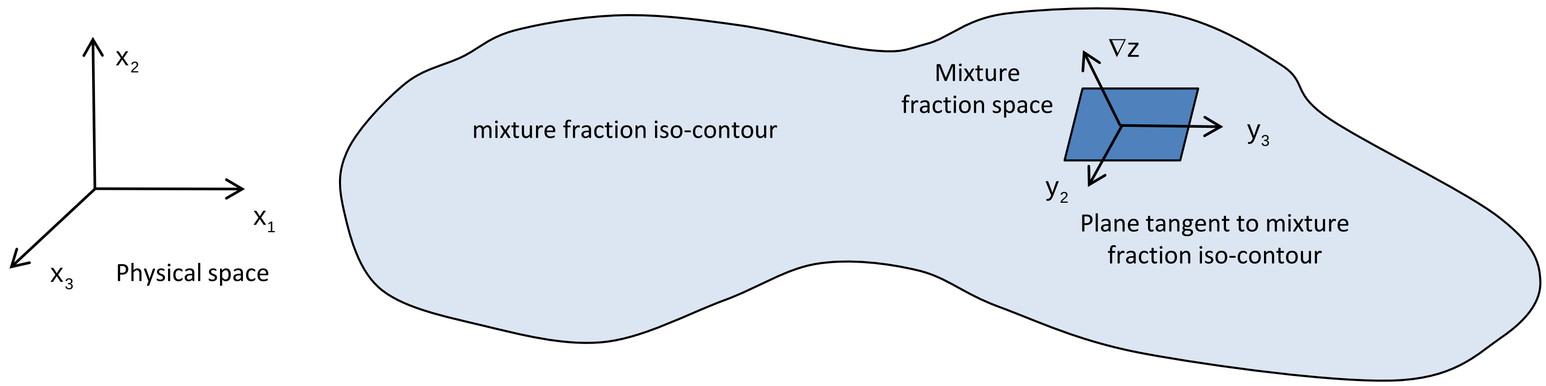
$$Z_j=Z_{j,o}^{in}+\left(Z_{j,f}^{in}-Z_{j,o}^{in}\right)\xi$$

$$\Downarrow$$

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

Flame structure in z-space (I)

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



1. Species equations are rewritten in the (ξ, y_2, y_3, t) space, where y_2 and y_3 are spatial variables in planes parallel to iso-ξ 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 ξ (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

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

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

The flamelet equations are typically rewritten introducing the scalar dissipation rate χ, defined as:

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

- 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 χ which controls mixing (because it controls the gradients of ξ).
- Once χ is specified, the flamelet equations can be entirely solved in the ξ 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 ξ-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 ξ 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 ξ and χ only. Flow information is entirely contained in the scalar dissipation rate χ whereas chemical effects are incorporated through the flame structure in ξ-space.

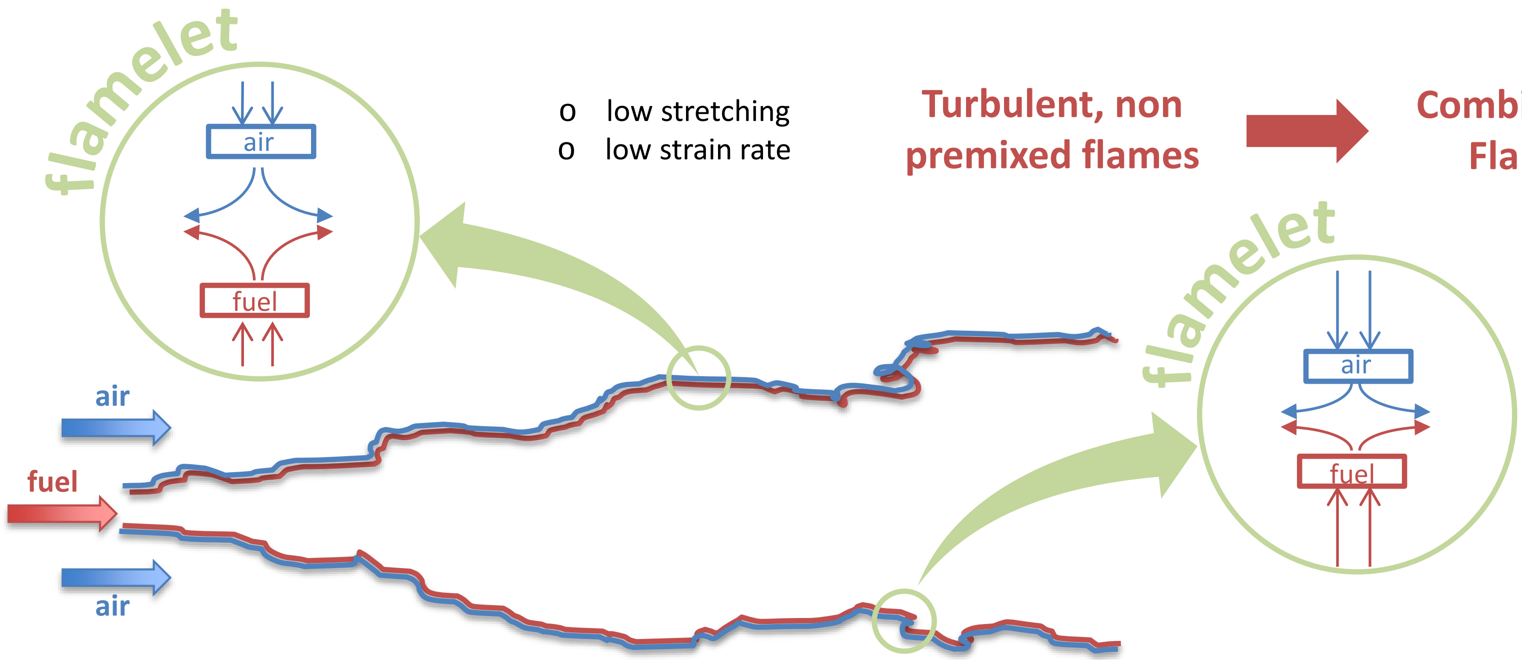
This important simplification is emphasized in the following slides.

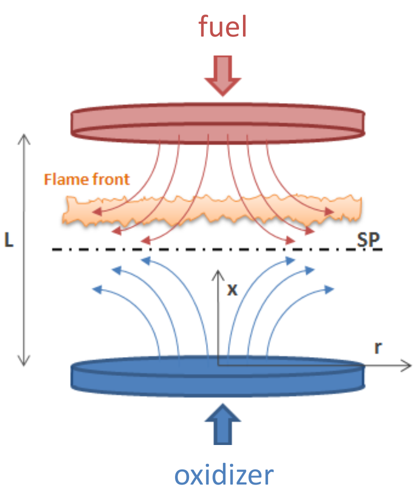
Physical interpretation

- low stretching
- low strain rate

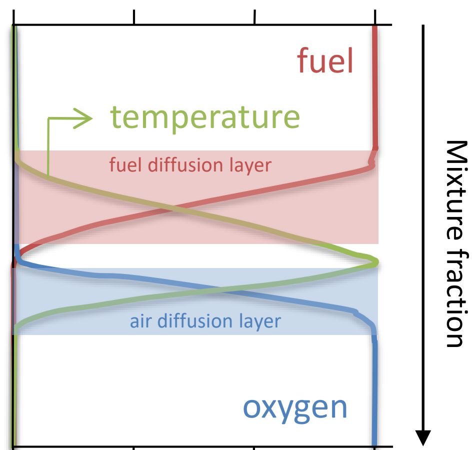
Turbulent, non premixed flames → **Combination of Flamelets**

- large stretching
- large strain rate





Laminar flamelet



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

Chemistry
Thermodynamics

Boundary conditions, Initial conditions, Geometry, Fluid dynamics

1. Flame structure

Composition and temperature as function of mixture fraction
$Y_k(\xi,\chi)$ *and* $T(\xi,\chi)$

scalar dissipation rate

2. Mixing

Mixture fraction in the physical space $\xi(x_i)$

Temperature and composition in physical space

$Y_k(x_i)$ *and* $T(x_i)$

The flame structure calculation can be performed through different approaches, with different degrees of accuracy:

- mixed-burned
- thermodynamic equilibrium
- laminar flamelets

scalar dissipation rate

The mixing effects on the flame structure are taken into account through the scalar dissipation rate

The mixture fraction in the physical space is calculated through the corresponding transport equation

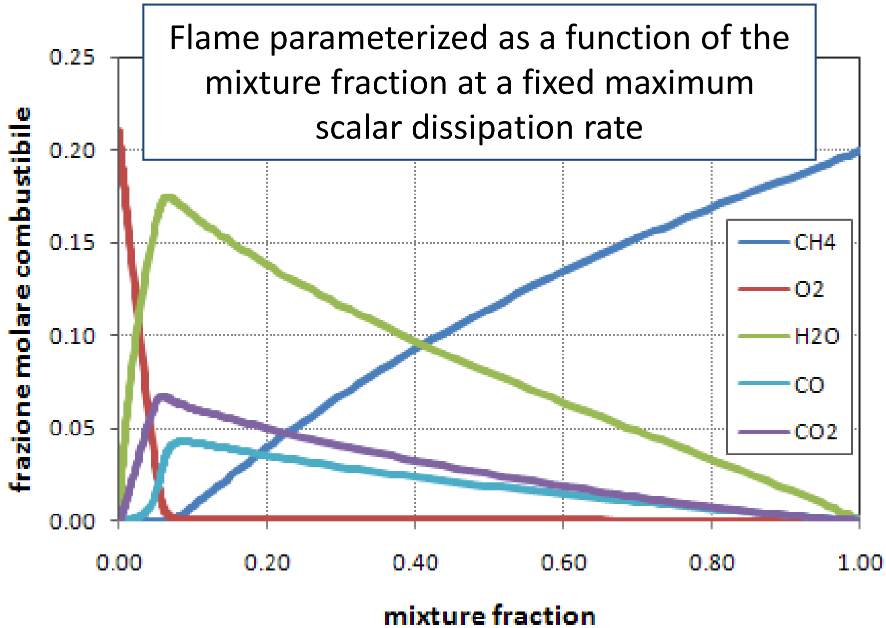
Flame structure (I)

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

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



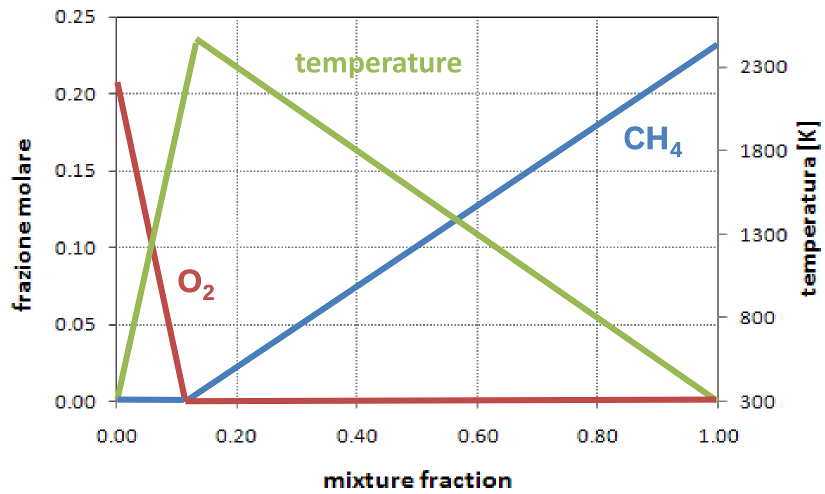
Pros

- 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)

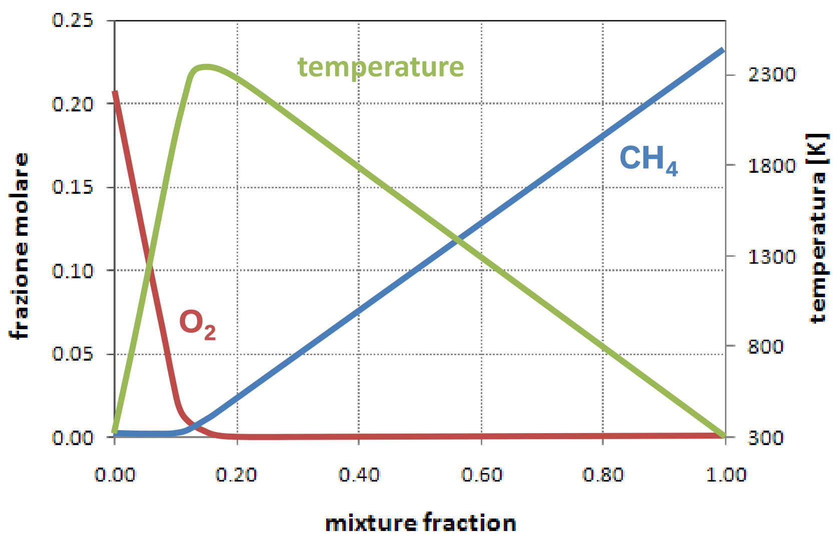


Approx. Solution: Mixed Is Burned

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

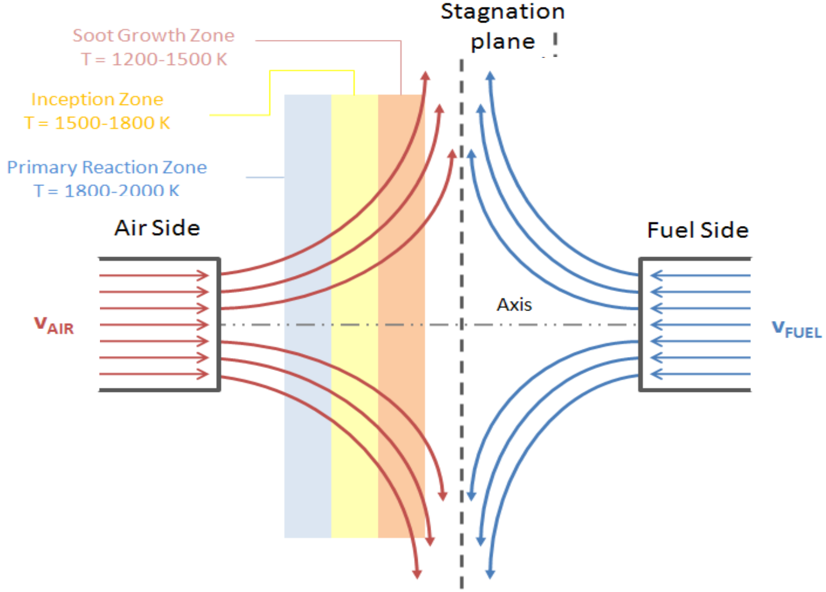


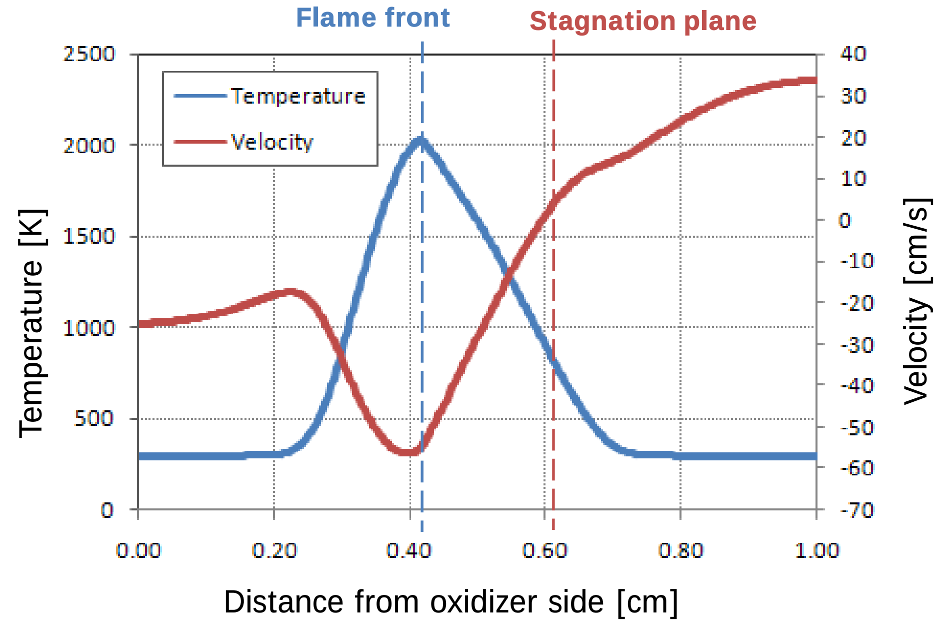
Approx. Solution: Equilibrium

Thisis the flamelet solution if the scalar dissipation rate approaches zero

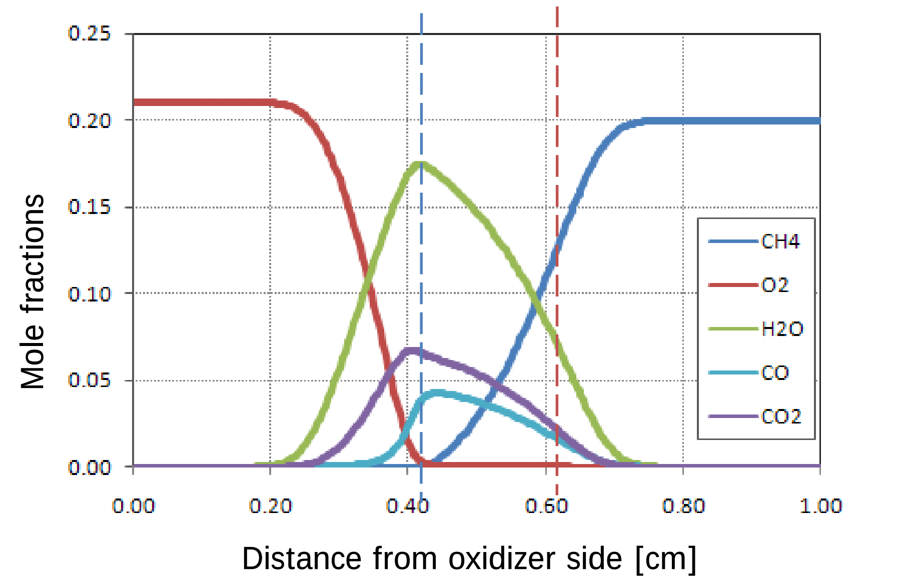
The solution does not depend on the scalar dissipation rate

Laminar counter-flow diffusion flames



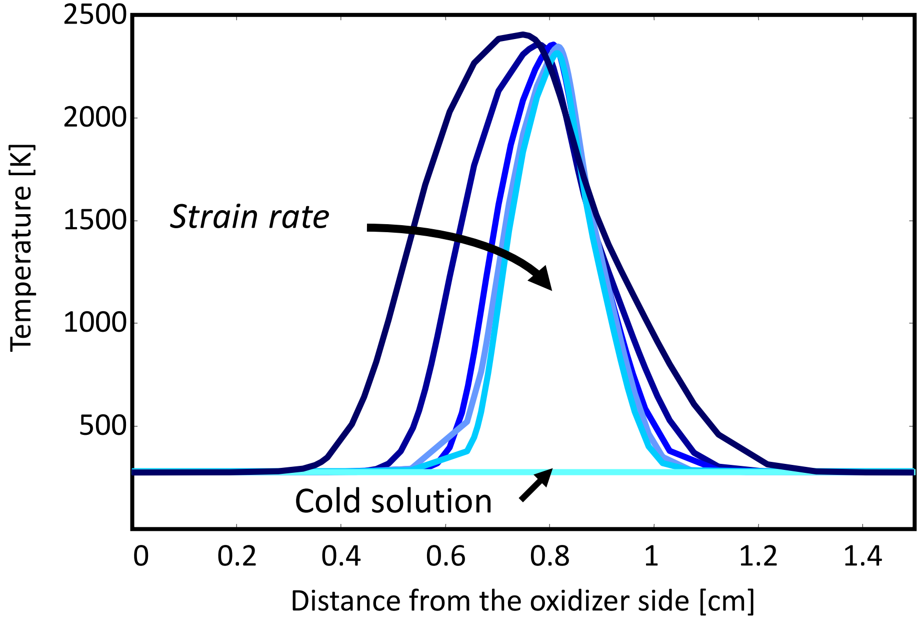


Usually, for conventional combustion in air, the flame front is on the oxidizer side



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

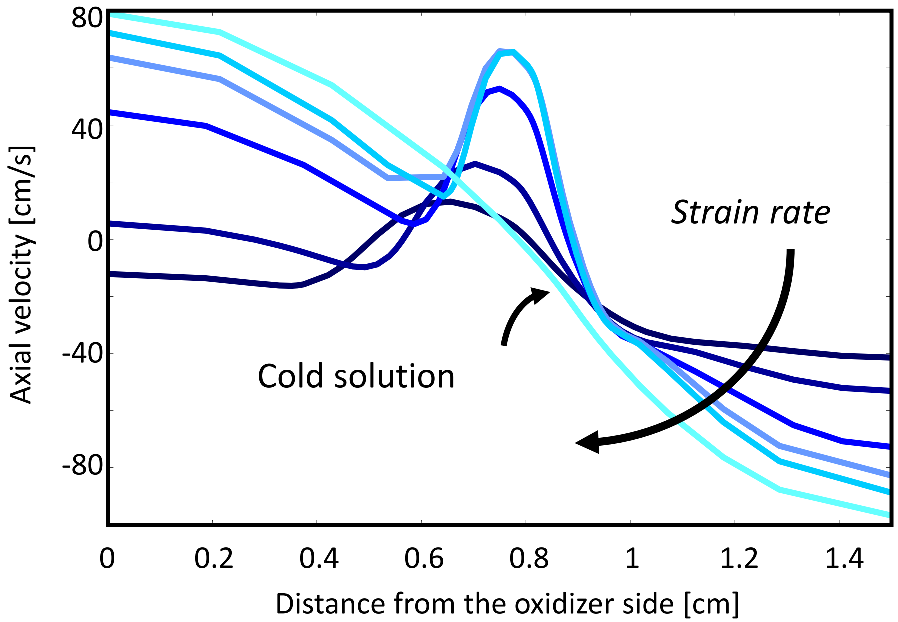
Strain rate



Strain rate is a measure of the residence time

$$K = \frac{2v_O}{L}\left(1 + \frac{v_C}{v_O}\left(\frac{\rho_C}{\rho_O}\right)^{0.5}\right)$$

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



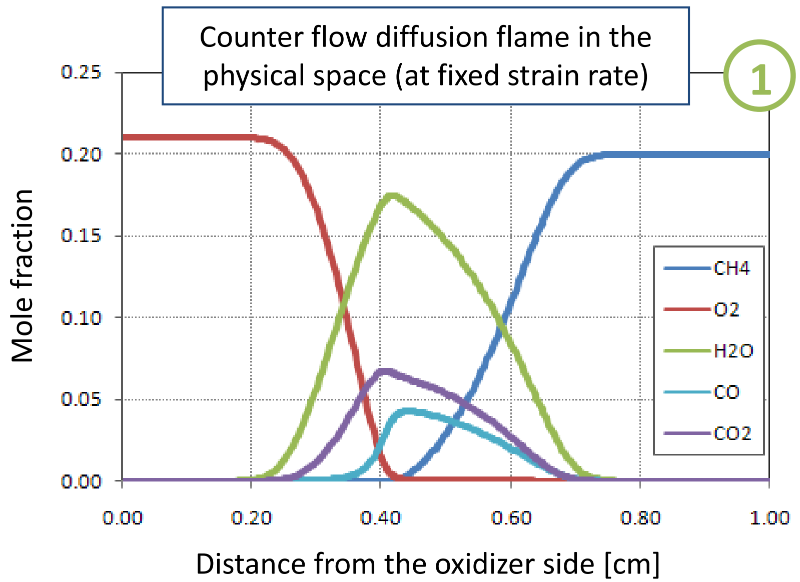
Solution: Counter-Flow Diffusion Flames

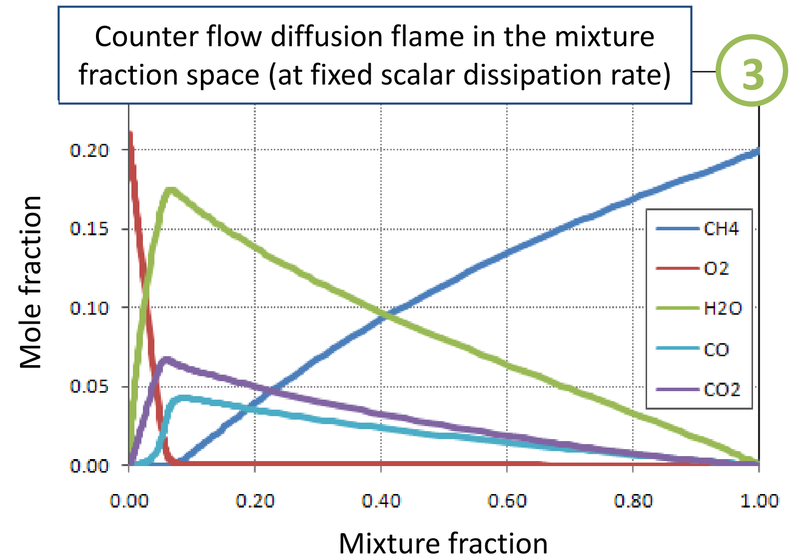
1. Counter-flow diffusion flame at fixed strain rate
2. **mixture fraction** is calculated in each point of the physical space
3. The solution is rewritten as a function of the **mixture fraction**

Usually the flame structures are parameterized as a function of the mixture fraction and the maximum scalar dissipation rate χ_0

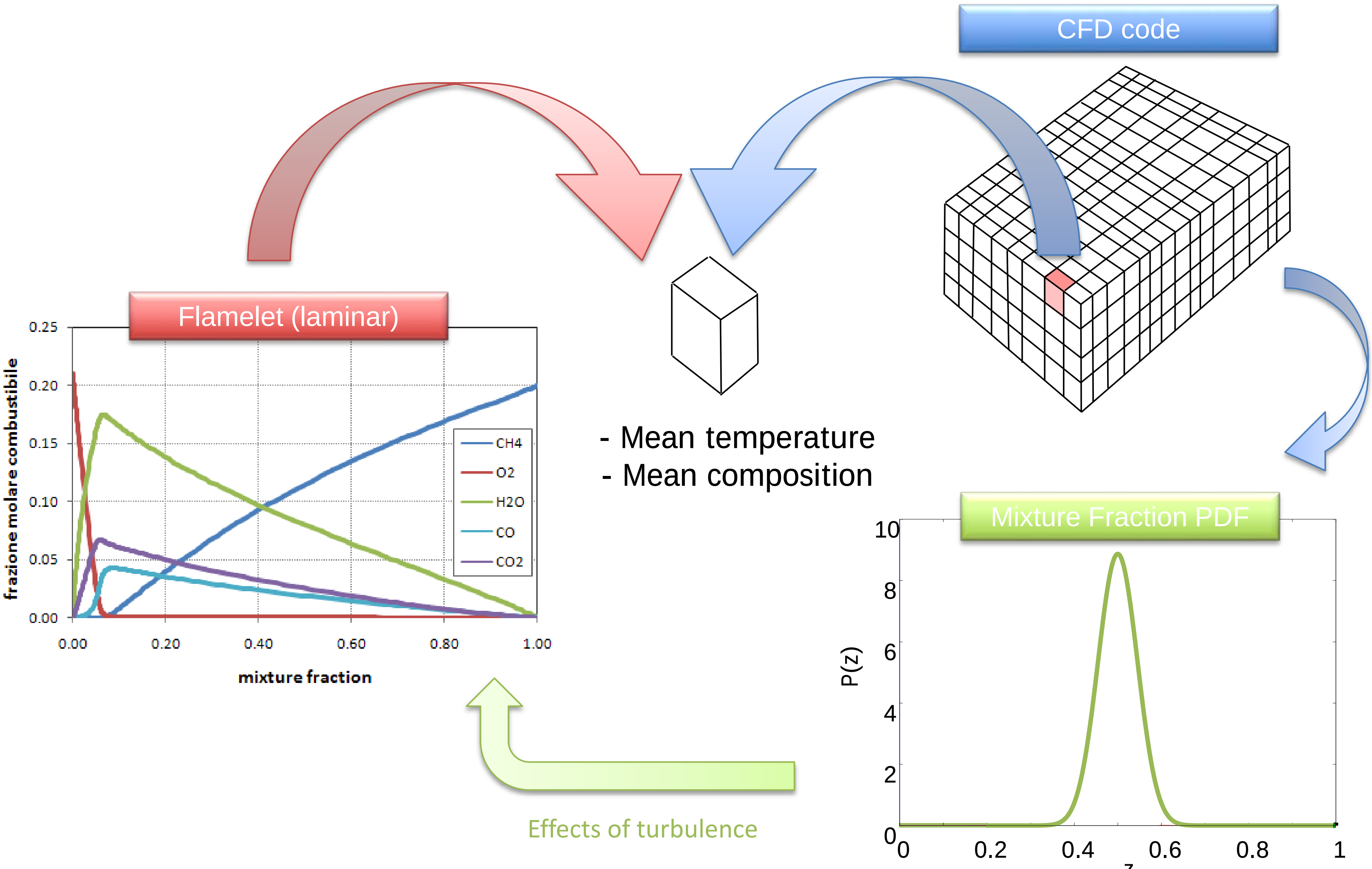
$$\chi_0 = \frac{a_S}{\pi}$$

scalar dissipation rate and strain rate

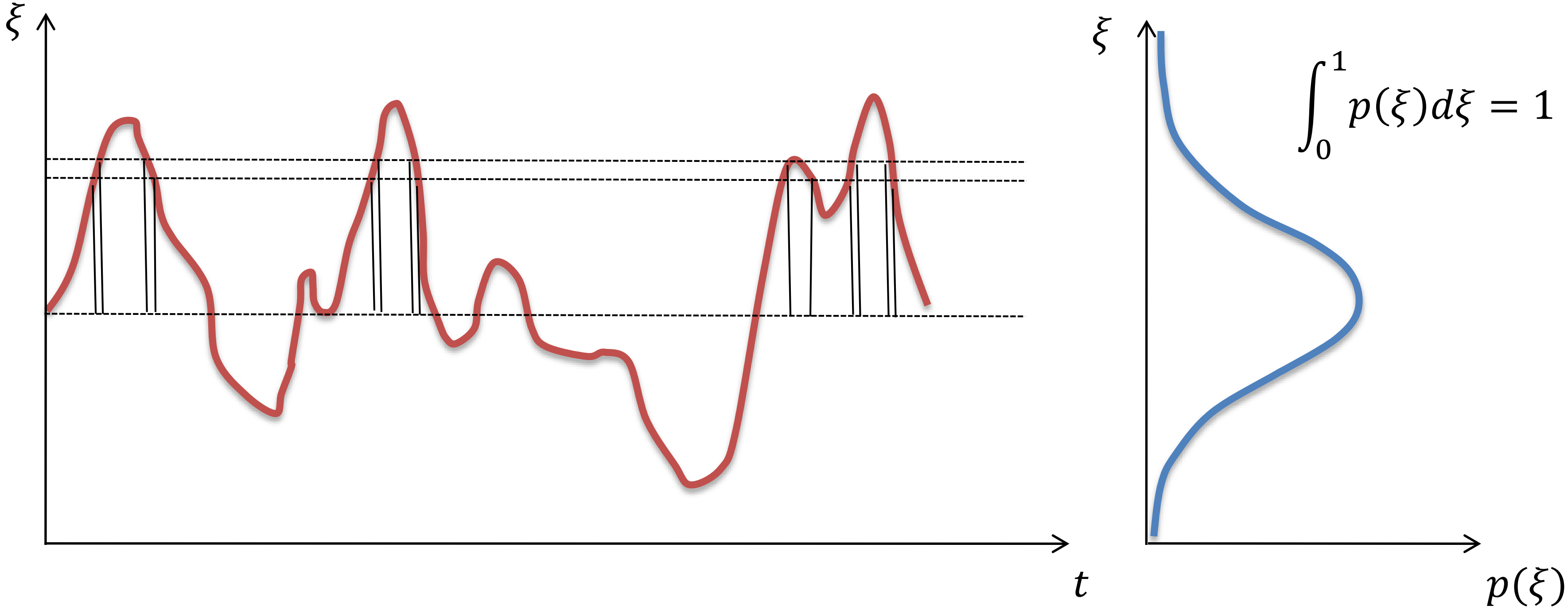




Coupling CFD - Flamelets



Probability Distribution Function (PDF)



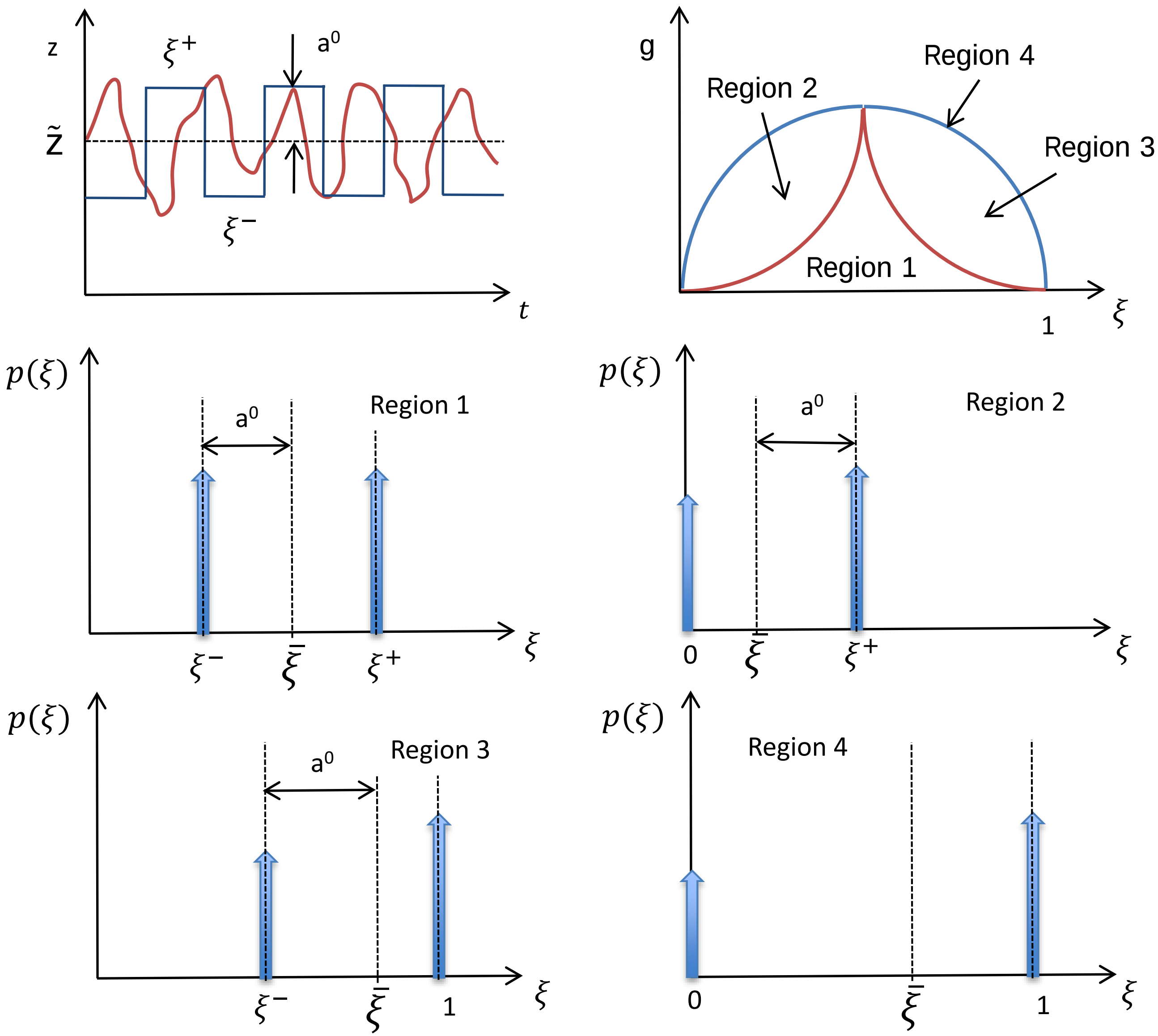
$$\bar{\xi} = \int_0^1 \xi p(\xi) d\xi$$

mean

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

variance

Double Delta Function (I)



Intermittent signal between ξ^- and ξ^+

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

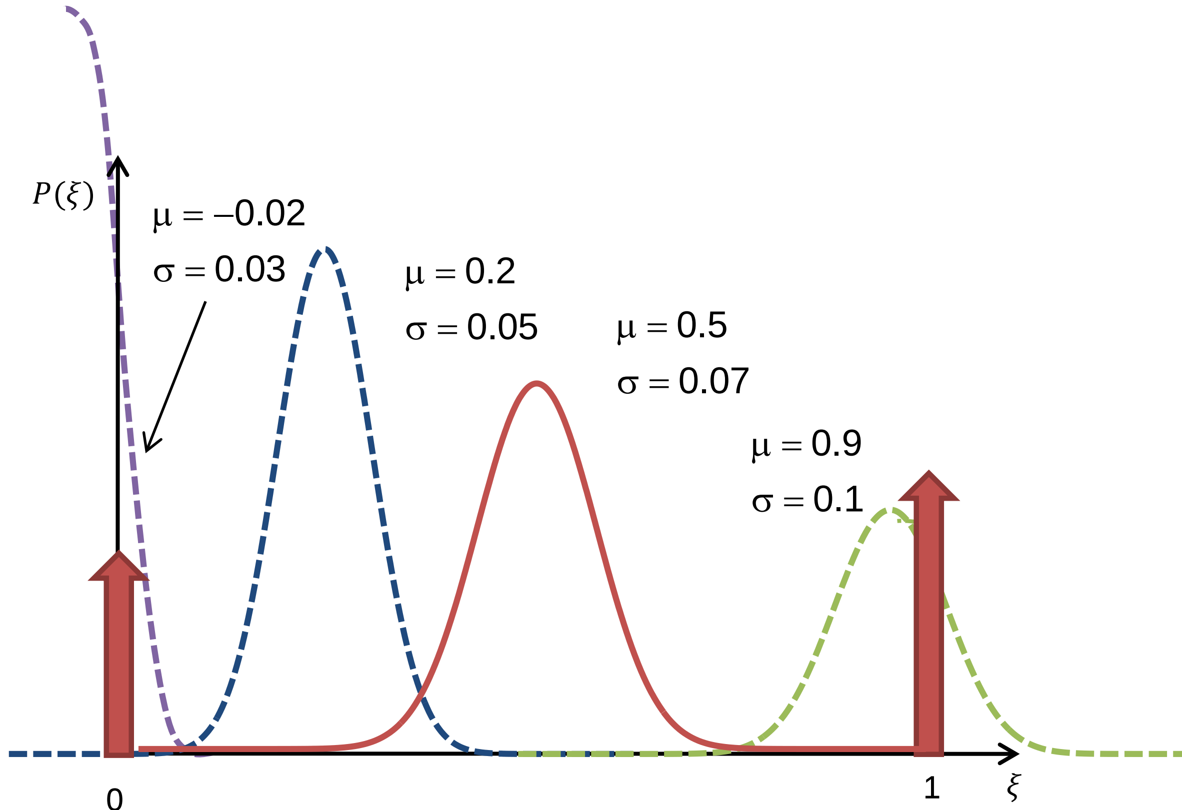
Double Delta Function (II)

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 funtions at z=0 (pure oxidizer) and z=1 (pure fuel)



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

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

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

β–PDF

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

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

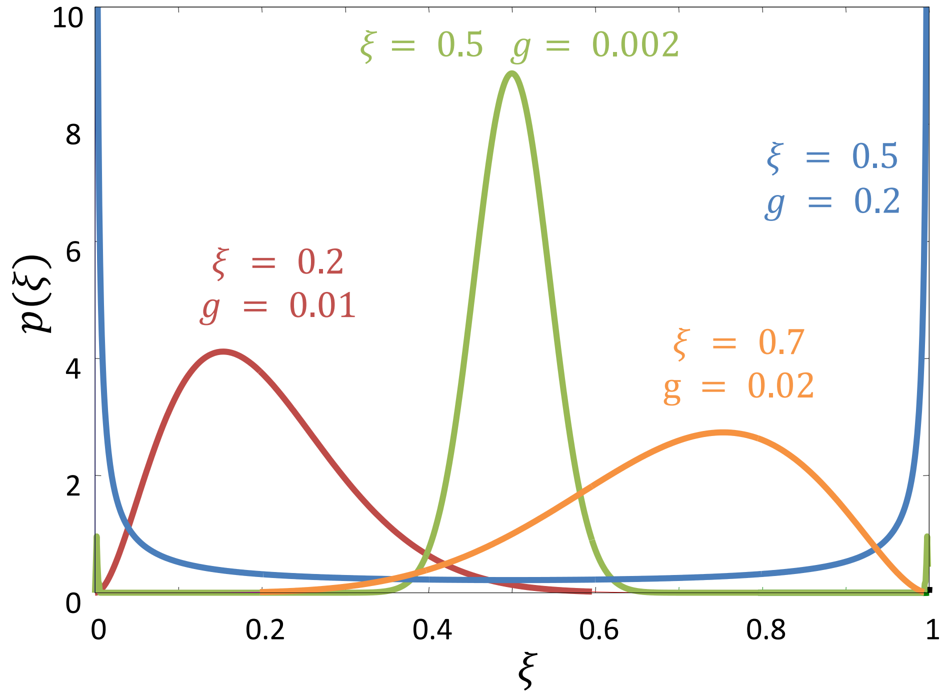
Where the **Γ** function is:

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

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 phisically 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

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

Variance of Mixture fraction

Mixture fraction (mean value)

Scalar Dissipation Rate

Infinitely Fast Chemistry

RANS Equations

$\rho = eos$

p

$\tilde{\boldsymbol{u}}$

$\tilde{\xi}$

$\widetilde{\xi''^2}$

Solution

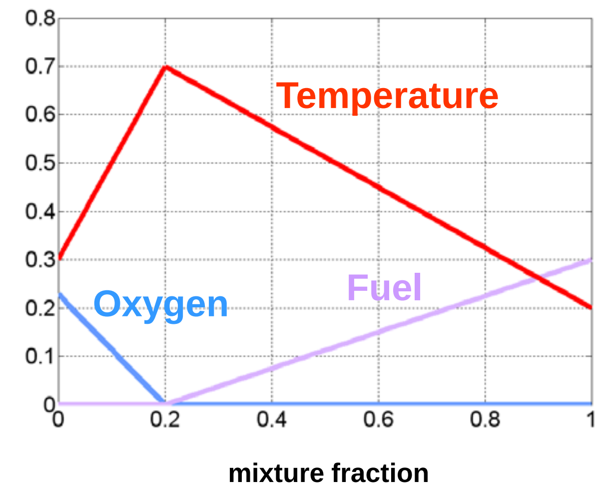
$\tilde{Y}_k \quad \tilde{T}$

Turbulence model

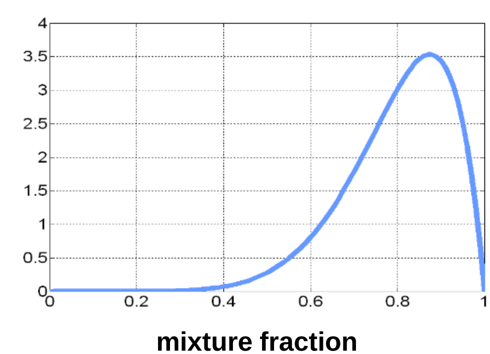
$\tilde{k} \quad \tilde{\varepsilon}$

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

Local flame structure



Mixture fraction PDF



Finite Rate Chemistry

RANS Equations

$\rho = eos$

p

$\tilde{\boldsymbol{u}}$

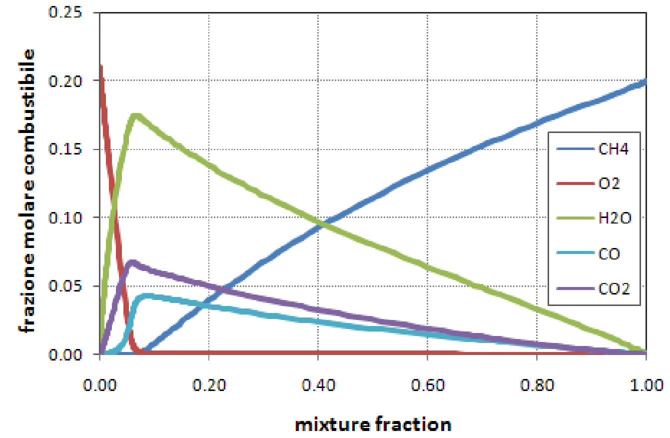
$\tilde{\xi}$

$\widetilde{\xi''^2}$

Solution

$\tilde{Y}_k \quad \tilde{T}$

Local flame structure



$$\bar{\rho}\tilde{\psi} = \int_0^1 \int_0^\infty \rho\psi(\xi)p(\xi)p(\chi)d\chi d\xi$$

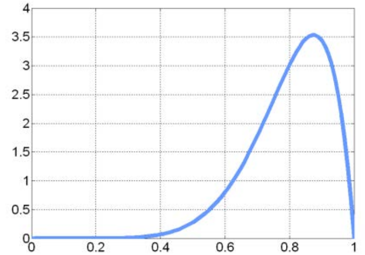
Turbulence model

$\tilde{k} \quad \tilde{\varepsilon}$

Scalar dissipation rate

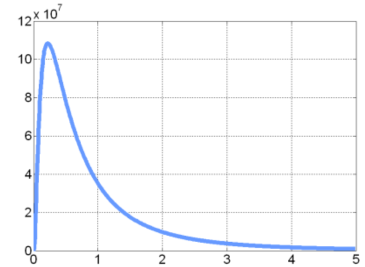
$$\chi_{st} = \chi_{st}\left(\tilde{k}, \tilde{\varepsilon}, \widetilde{\xi''^2}\right)$$

mixture fraction PDF



mixture fraction

scalar dissipation rate PDF



scalar dissipation rate

Reaction Rate - Flamelets

RANS Equations

$\rho = eos$

p

$\tilde{\boldsymbol{u}}$

$\tilde{Y}_k$

$\tilde{T}$

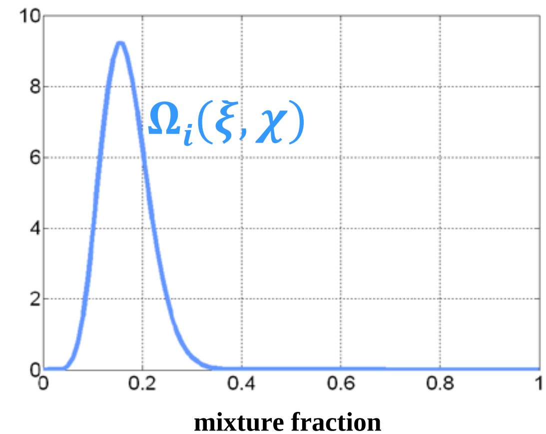
$\tilde{\xi}$

$\widetilde{\xi''^2}$

Formation rates

$\tilde{\Omega}_j$

Local flame structure

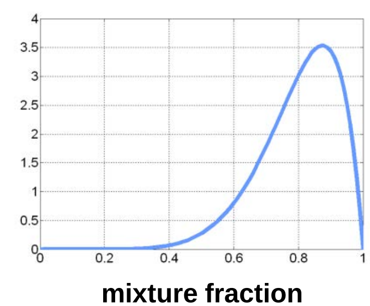


$$\tilde{\Omega}_j = \int_0^1 \int_0^\infty \dot{\Omega}_j(\xi) p(\xi) p(\chi) d\chi d\xi$$

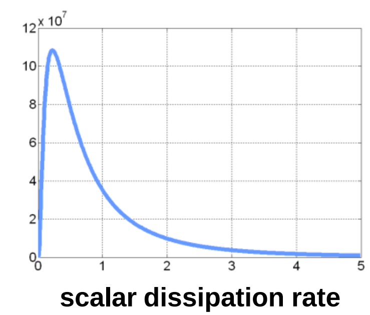
Turbulence model

$\tilde{k} \quad \tilde{\varepsilon}$

Mixture fraction PDF



Scalar dissipation rate PDF



Scalar dissipation rate

$$\chi_{st} = \chi_{st}\left(\tilde{k}, \tilde{\varepsilon}, \widetilde{\xi''^2}\right)$$

Outline

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 ($\boldsymbol{Re >> 1}$) and Damkohler ($\boldsymbol{Da >> 1}$) 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 τ_t and the normalized temperature (or product mass fraction) fluctuations θ and is expressed as:

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

C_{EBU} is a model constant of the order of unity. The turbulence time τ_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 θ is chosen as the normalized temperature, a first analysis assuming that the flame is infinitely thin leads to the simple result:

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

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:

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

- 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 θ is the fuel mass fraction. The fluctuations are estimated on the basis of a transport equation:

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

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

$$\bar{S}_{\widetilde{\theta''^2}} = \bar{P}_{\widetilde{\theta''^2}} + \bar{D}_{\widetilde{\theta''^2}} + \bar{K}_{\widetilde{\theta''^2}}$$

production dissipation interaction with chemistry

Mixing time

Da number

Chemical control

The **interaction with chemistry** term is very large

Fluid dynamic control

The **interaction with chemistry** term is negligible

Libby A.L., Williams F. A., *"Turbulent Reacting Flows"*, Academic Press, 1994

Outline

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

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:

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

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:

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

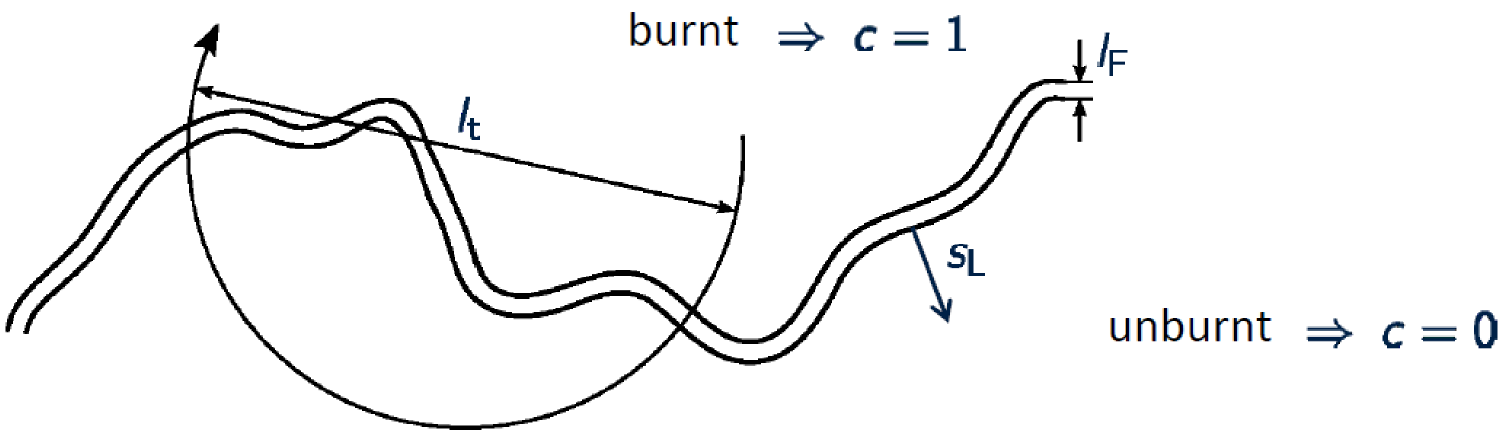
The terms on the right hand side are unclosed. Typically, the molecular transport is neglected. On the contrary, closure models for the turbulent transport and chemical source terms are required:

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

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:

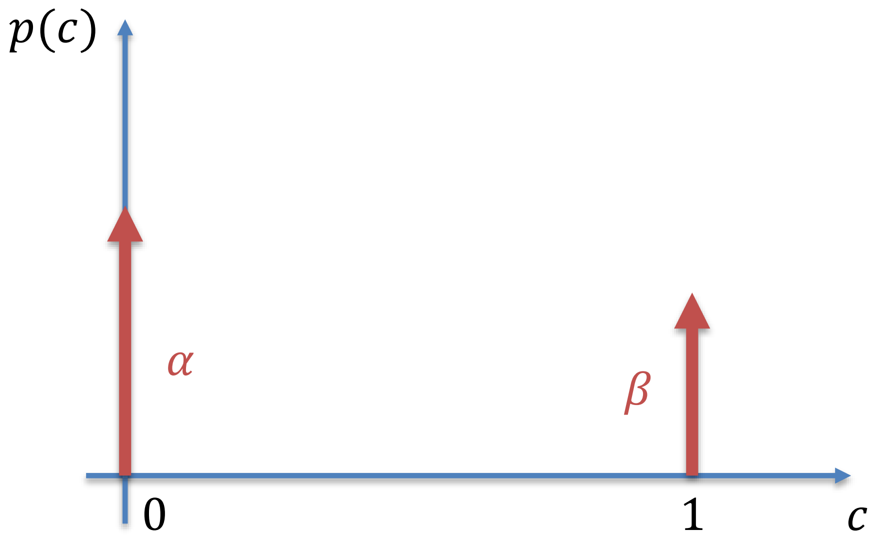
- the turbulent flame is made up of thin flamelets
- a probe inserted into the flame brush at a fixed location in space will detect reactants for some of the time and products for almost all the rest of the time
- since the flamelet interface is thin, the probe will detect reacting gases only for very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

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

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

Probability density function:

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



α and β are the probabilities to encounter the unburnt or the burnt mixture in the flow field

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

δ is the Dirac delta function

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

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

For a Favre average:

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

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

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

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

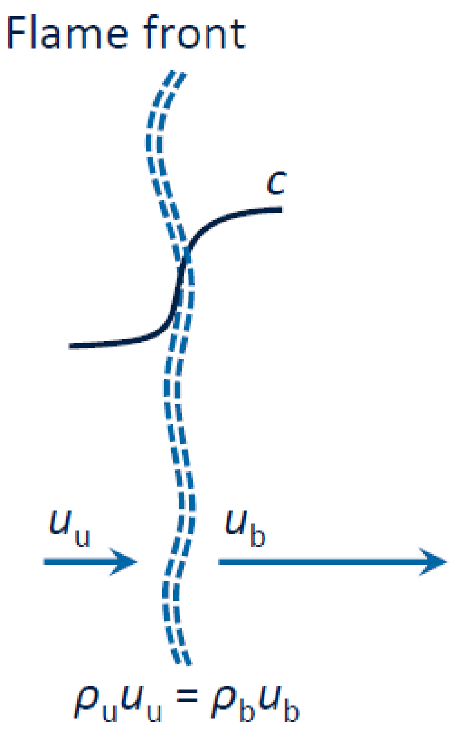
$$p_{\boldsymbol{u},c}(\boldsymbol{u},c) = \alpha\, \delta(c)\, \underbrace{p_{\boldsymbol{u}|c}(\boldsymbol{u}|c=0)}_{\text{conditional pdf}} + \beta\, \delta(c-1)\, p_{\boldsymbol{u}|c}(\boldsymbol{u}|c=1)$$

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

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

$$\bar{\rho}\widetilde{u_i''c''} = \int_0^1 \int_{u_{i,min}}^{u_{i,max}} \rho(u_i - \tilde{u}_i)(c - \tilde{c}) p_{\boldsymbol{u},c}(\boldsymbol{u},c) d\boldsymbol{u} dc = \cdots$$

$$\ldots = \bar{\rho}\tilde{c}(1-\tilde{c})(\bar{u}_b - \bar{u}_u)$$



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:

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

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

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

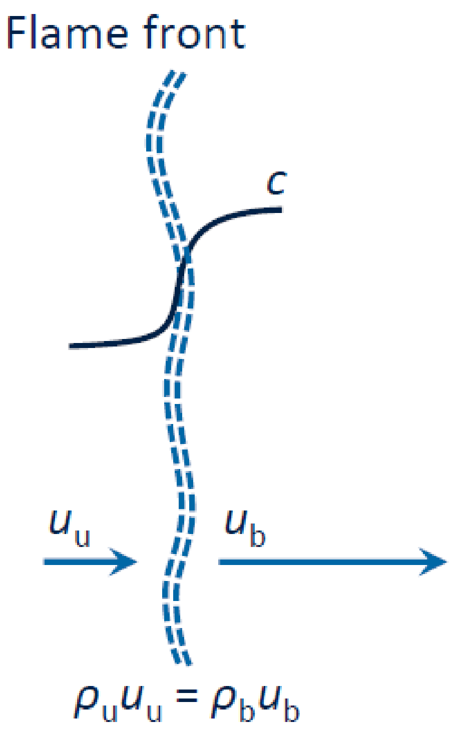
$$\frac{\partial \tilde{c}}{\partial x_i} \geq 0$$

Gradient transport model would be:

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

This is in conflict with the previous result:

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



Flame Surface Density model

- Closure by BML-model $p(c)$ leads to $\overline{S_c} = 0$

- Closure of the chemical source term, e.g. by **flame-surface-density-model**:

$$\overline{S_c} = \rho_u s_L^0 l_0 \, \Sigma$$

local mass conversion per area

flame-surface-density

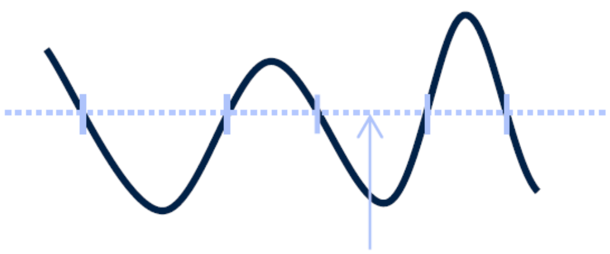
l_0: strain factor, i.e. a measure of local increase of burning velocity by strain

Σ: Flame-surface-density

- algebraic model:

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

- transport equation for Σ



L_y flame crossing length

Transport equation for Σ

Flame annihilation

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \tilde{u}_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\mathcal{D}_t \frac{\partial \Sigma}{\partial x_i}\right) + C_1 \frac{\varepsilon}{k}\Sigma - C_2 s_L \frac{\Sigma^2}{1-\tilde{c}}$$

production due to stretching of the flame

No chemical time scales

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

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c) **G-Equation**

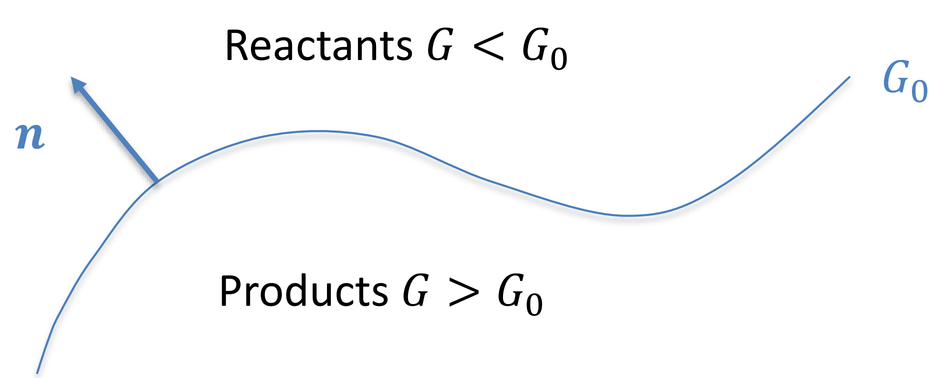
The G-Equation

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

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

And points into the reactants

The G-Equation

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

$$\frac{\partial \boldsymbol{x_F}}{\partial t} = \boldsymbol{u} + s_L \boldsymbol{n}$$

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

Then, using the expansion:

$$\frac{\partial G}{\partial t} + \nabla G \cdot \frac{\partial \boldsymbol{x_F}}{\partial t} = 0$$

We get the final G-equation:

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

Progress of flame front by burning velocity

Local change

convection

The G-Equation

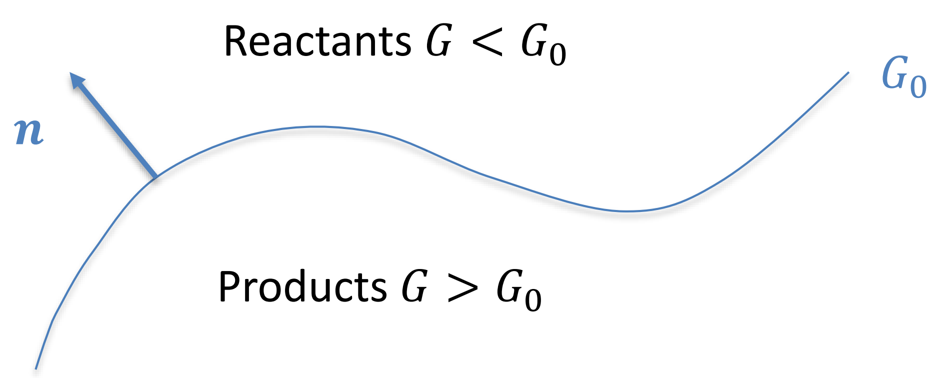
$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L |\nabla G|$$

- 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

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

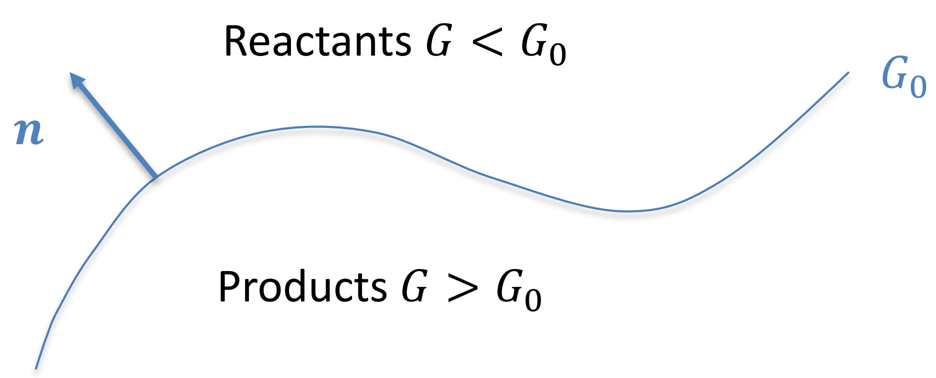
- This is a kinematic equation, i.e. the density does not appear in the equation
- Valid for flame position: $G = G_0$
  - For solving the field equation, G needs to be defined in the entire field
  - Different possibilities to define G, e.g. signed distance function:

$$|\nabla G| = 1$$



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

- 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



Laminar burning velocity: curvature

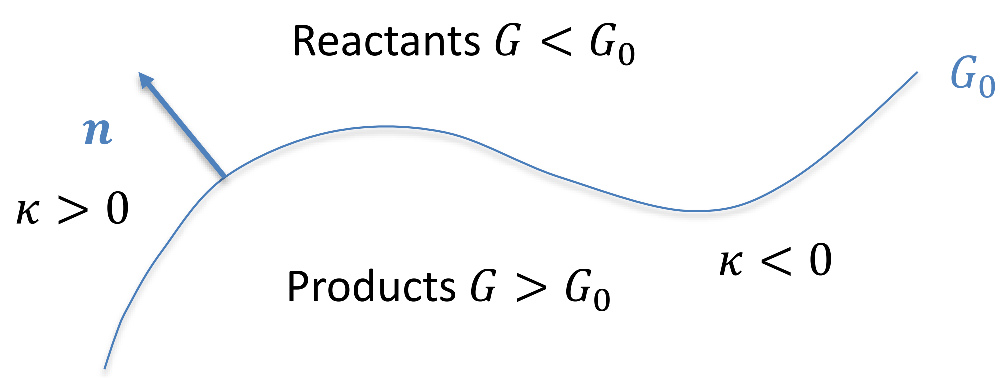
Curvature $\kappa = \frac{\partial n_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(-\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}\right)$

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

Influence of curvature $\boxed{s_L = s_L^0 - s_L^0 \mathcal{L}\kappa - \mathcal{L}S}$

$\mathcal{L}$ 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



Laminar burning velocity: Markstein length

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

$\mathcal{L}$ 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

Laminar burning velocity: curvature

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

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

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

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

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

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

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 $p(G; \boldsymbol{x}, t)$.

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

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

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

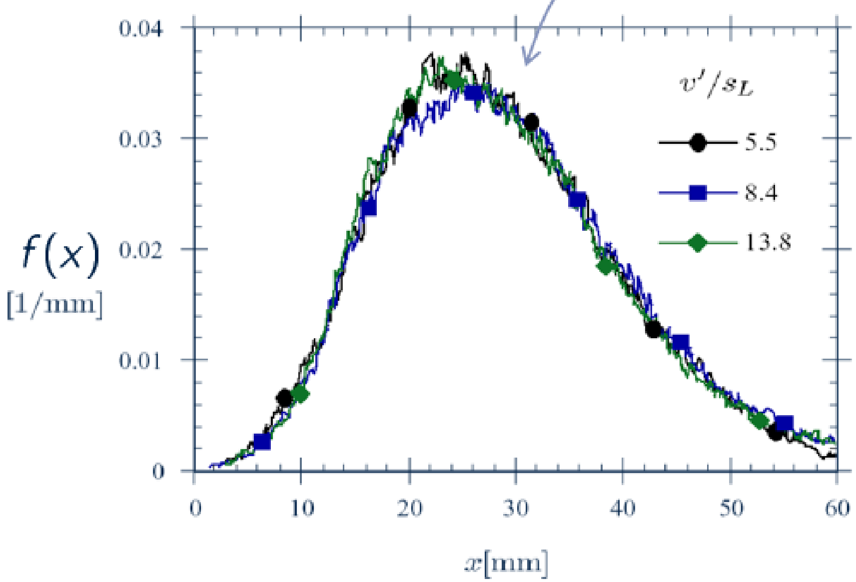
It would be straightforward to derive balance equations for these quantities, which could be modelled and solved.

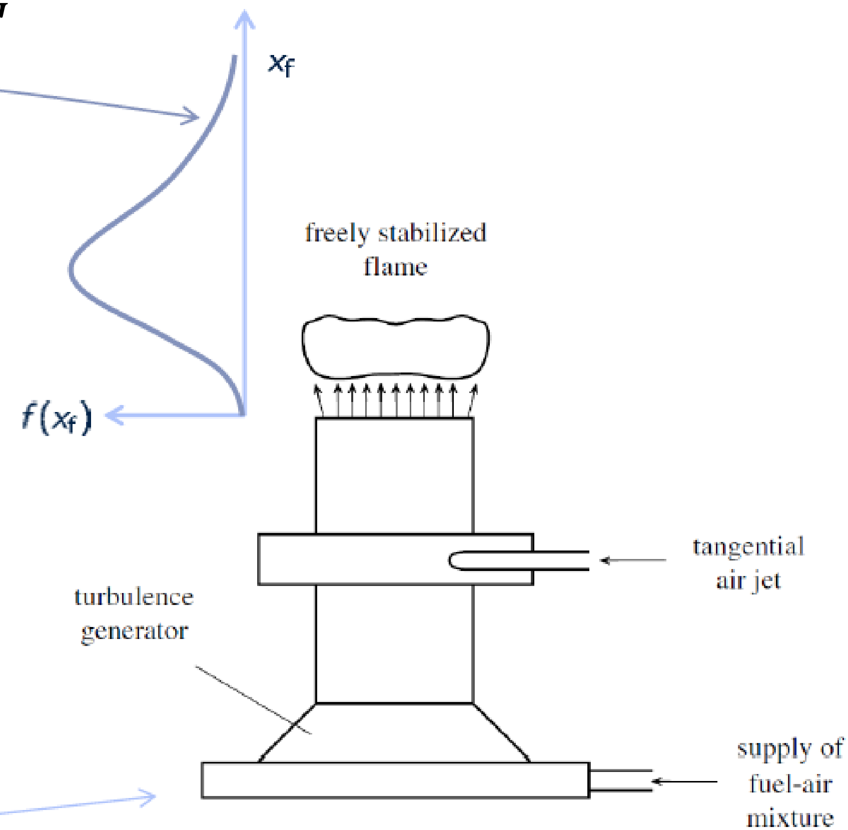
Instead it is more interesting to consider further the relationship between G and the distance field.

Statistical description of turbulent flame front (I)

Probability Density Function of finding $G = G_0$

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





Experimental determination
in weak swirl burner

Statistical description of turbulent flame front (II)

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

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

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:

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

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

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.:

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

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

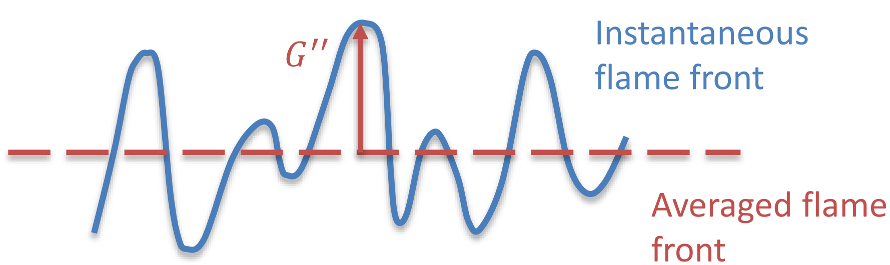
Favre Mean and Variance Equations

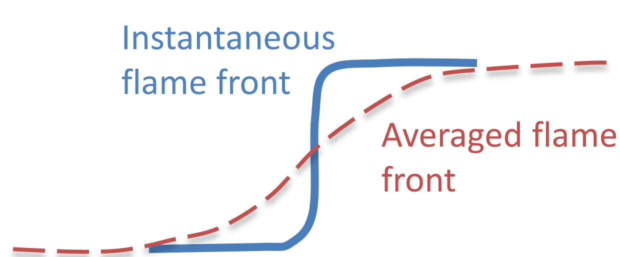
Using Favre averaging it is possible to derive equation for the Favre averaged mean and variance of G:

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

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

- $\sigma \stackrel{\text{def}}{=} |\nabla G|$ 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

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

Kinematic restoration

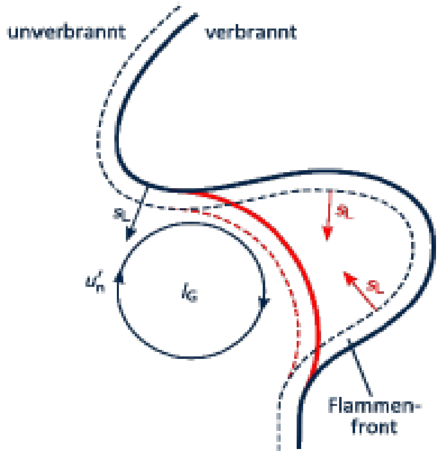
$$\widetilde{\omega} = -2(\rho s_L^0)\frac{\overline{G''\sigma}}{\bar{\rho}}$$

Scalar dissipation

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

They are typically modelled as:

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



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 2nd 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:

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

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

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

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

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

Turbulent burning velocity (II)

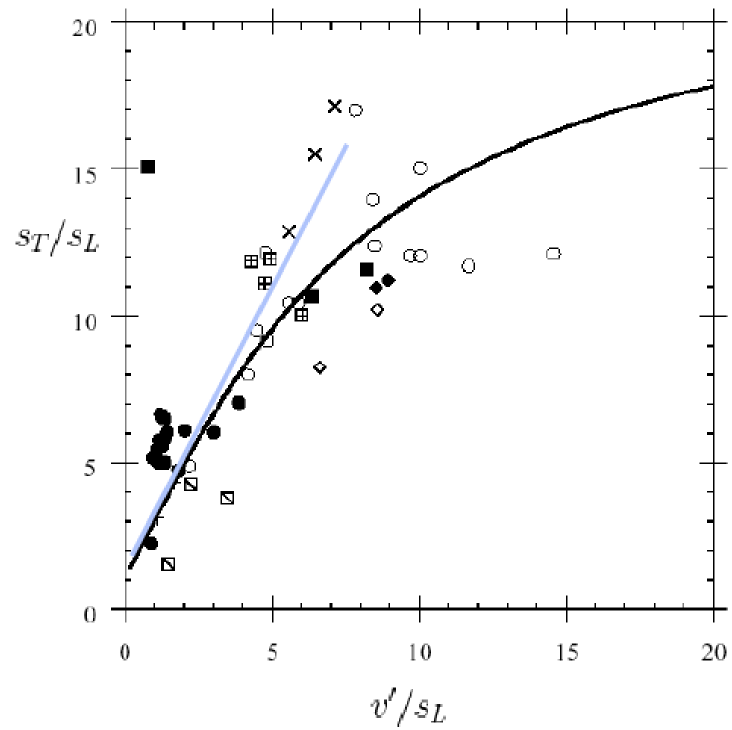
Introducing the turbulent burning velocity s_T^0:

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

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



Favre Mean and Variance Equations

Equation for the Favre mean

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

Equation for variance

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

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

Presumed PDF approach

Typically a Gaussian Distribution is assumed

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

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