# **COURSE OVERVIEW**

#### DAY 2

#### **Combustion with Flame Propagation**

- a. One Dimensional Steady Flow formulation.
- b. Rayleigh and Rankine-Hugoniot equations.
- c. Detonation.
- d. Deflagration. Thermal theory. Flame Speed Dependencies.

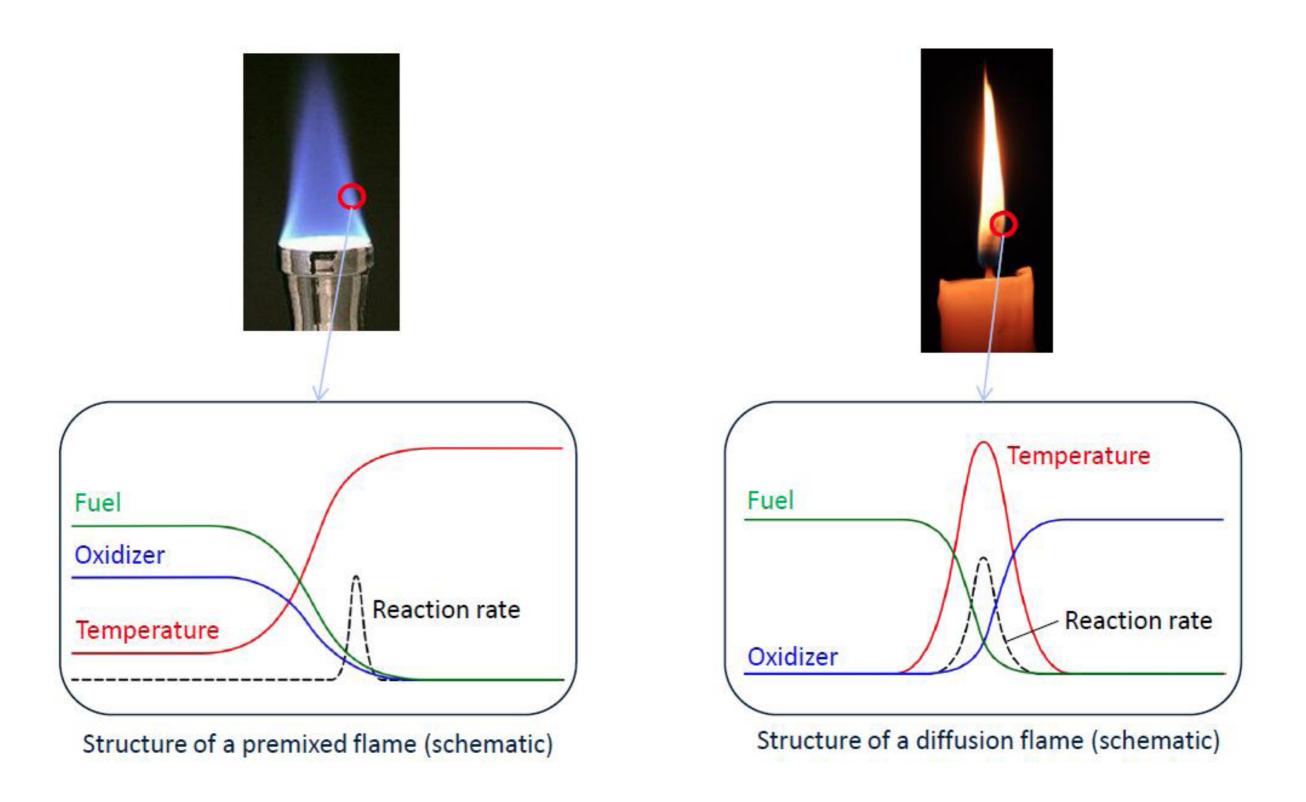
#### Laminar Diffusion Flames

- a. Flame Structure and Mixture Fraction.
- b. Infinitely fast chemistry. Flamelet concept.
- c. 1D Unsteady Diffusion flames. Unstrained.
- d. 1D Steady Diffusion flames. Strained.
- e. 1D Unsteady Diffusion flames. Strained.
- f. Diluted conditions. Diffusion Ignition processes.



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### **PREMIXED vs DIFFUSION flames**

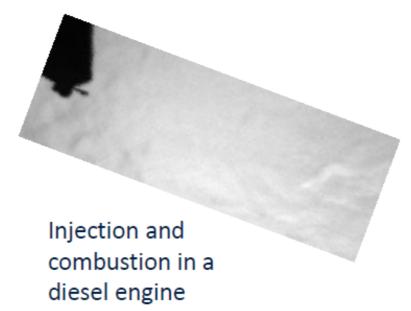




<u>DI</u> <u>C</u> <u>Ma</u> PI

## LAMINAR DIFFUSION flames

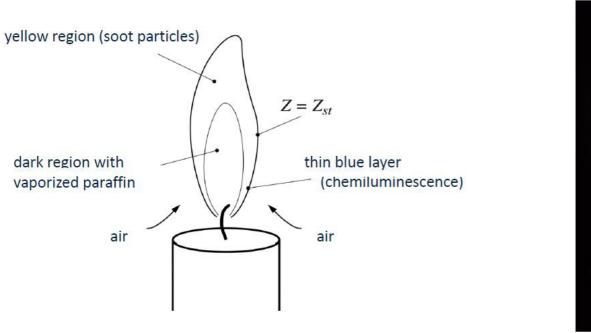
- Seperate feeding of fuel and oxidizer into the combustion chamber
  - Diesel engine
  - Jet engine
- In the combustion chamber:
  - Mixing
  - Subsequently combustion
- Mixing: Convection and diffusion
  - On a molecular level
     → (locally) stoichiometric mixture
- Simple example for a diffusion flame: Candle flame
  - Paraffin vaporizes at the wick
    - ightarrow diffuses into the surrounding air
- Simultaneously: Air flows towards the flame due to free convection and forms a mixture with the vaporized paraffin







### A very difficult flame: the candle flame



•The solid fuel is first heated by heat transfer induced by combustion. The liquid fuel reaches the flame by capillarity along the wick and is vaporized.

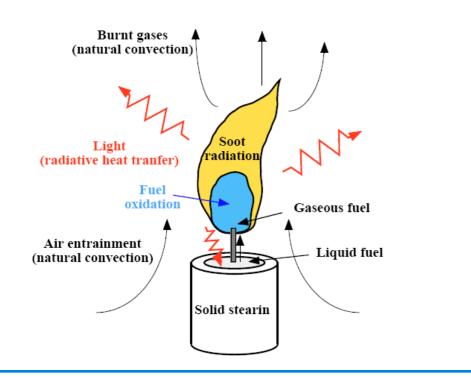
•Fuel oxidation occurs in thin blue layers (the color corresponds to the spontaneous emission of the CH radical)

•Unburnt carbon particles are formed because the fuel is in excess in the reaction zone. The this soot is the source of the yellow light emission.

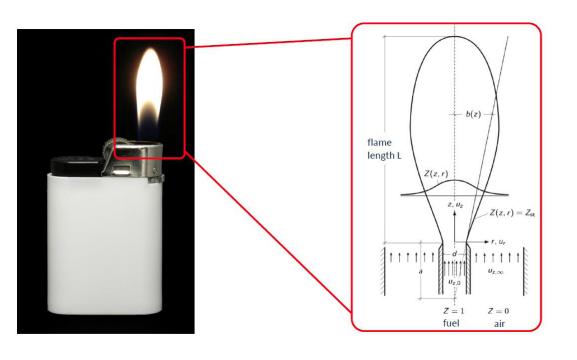
•Flow (entrainment of heavy cold fresh air and evacuation of hot light burnt gases) is induced by natural convection



• In a first approximation, combustion takes place at locations, where the concentrations of oxygen and fuel prevail in stoichiometric conditions.



# **Example : gas lighter**

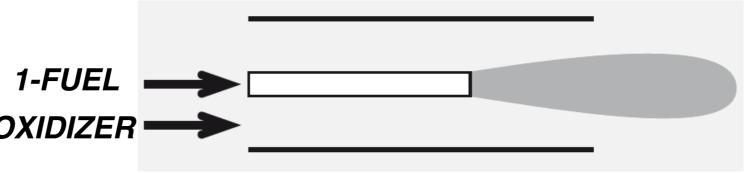


- Fuel enters into the combustion chamber as a round jet
- Forming mixture is ignited
- Example: Flame of a gas lighter
  - Only stable if dimensions are small
  - Dimensions too large: flickering due to influence of gravity
  - Increasing the jet momentum → Reduction of the relative importance of gravity (buoyancy) in favor of momentum forces
  - At high velocities, hydrodynamic instabilities gain increasing importance: laminar-turbulent transition



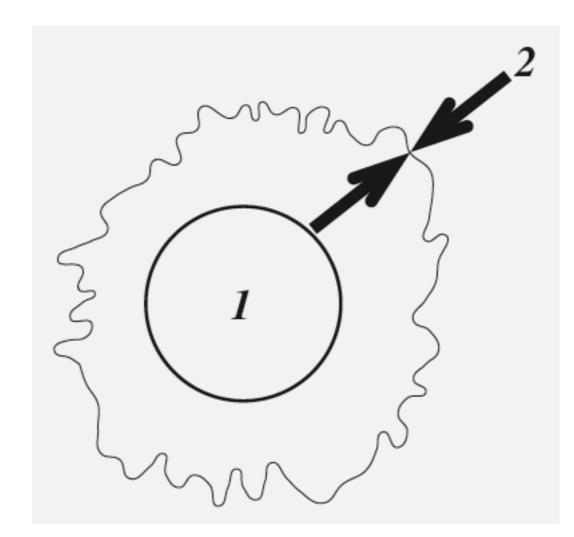
# LAMINAR DIFFUSION FLAME STRUCTURE

In diffusion flames the fuel and the oxidant flows are separated **1-FUEL** and mixed immediately before or **2-OXIDIZER** during the oxidation reaction.



There is a difference between flames in which the two streams are partially mixed before reacting and flames in which they mix while reacting.

Only the latter are real "diffusion flames" even if this diction is generally used also for the former when only a minority fraction of fuel is mixed before the oxidative phase.



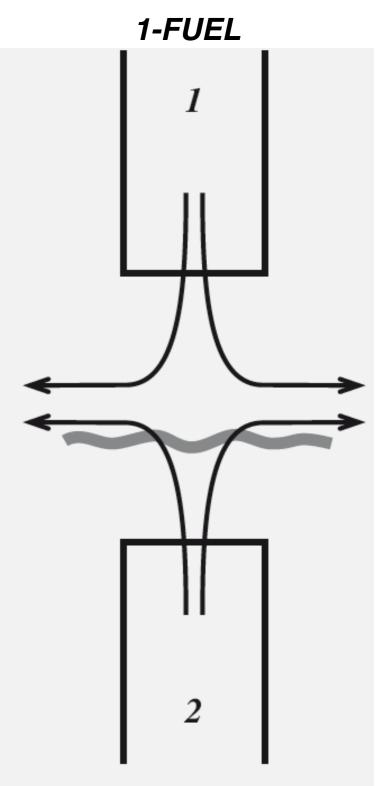
## LAMINAR DIFFUSION FLAME STRUCTURE

#### **MIXTURE FRACTION**

is a conserved scalar quantity

$$Z = \xi = \frac{\beta - \beta_2}{\beta_1 - \beta_2}$$

**Opposed Counterflow Diffusion Flames** 



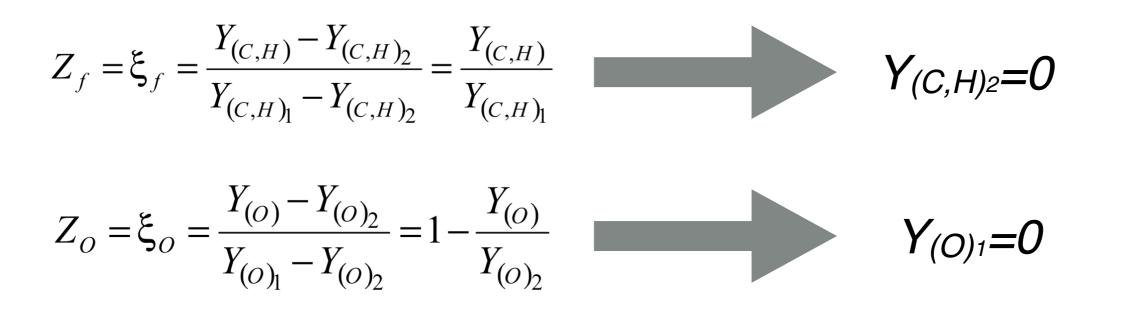
2-OXIDIZER



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### MIXTURE FRACTION CONSERVED VARIABLES

$$\begin{split} Y_{(C,H)} &= \sum a_{C,i} \ \frac{m_C}{m_i} \ Y_i \ + \sum a_{H,i} \ \frac{m_H}{m_i} \ Y_i \\ Y_{(O)} &= \sum a_{O,i} \ \frac{m_O}{m_i} \ Y_i \end{split}$$



 $Z_f = Z_o$  for equidiffusivity



### MIXTURE FRACTION CONSERVED VARIABLES

if diluent is present in the jet 1, the mass fraction of Diluent is:

if diluent is present in the jet 2, the mass fraction of Diluent is:

$$1 - Y_{(C,H)_1} = Y_{(C,H)_1} \frac{1 - Y_{(C,H)_1}}{Y_{(C,H)_1}}$$

$$\eta = \left(1 - Y_{(C,H)}\right) / Y_{(C,H)}$$

$$Y_{(O)} \frac{1 - Y_{(O)_2}}{Y_{(O)_2}}$$

sum of mass fraction equal to 1  $Y_{(C,H)} + Y_{(C,H)} \frac{1 - Y_{(C,H)_1}}{Y_{(C,H)_1}} + Y_{(O)} + Y_{(O)} \frac{1 - Y_{(O)_2}}{Y_{(O)_2}} = 1$ 



### MIXTURE FRACTION CONSERVED VARIABLES

$$Y_{(C,H)}\left(1 + \frac{1 - Y_{(C,H)_1}}{Y_{(C,H)_1}}\right) + Y_{(O)}\left(1 + \frac{1 - Y_{(O)_2}}{Y_{(O)_2}}\right) = 1$$

$$Y_{(C,H)}\left(1 + \frac{1}{Y_{(C,H)_1}} - 1\right) + Y_{(O)}\left(1 + \frac{1}{Y_{(O)_2}} - 1\right) = 1$$

$$\frac{Y_{(C,H)}}{Y_{(C,H)_1}} = 1 - \frac{Y_{(O)}}{Y_{(O)_2}}$$

and therefore is verified:

$$Z_f = Z_o$$

## STOICHIOMETRIC MIXTURE FRACTION

$$v_s = Y_{(O)_s} / Y_{(C,H)_s}$$
 STOICHIOMETRIC RATIO

$$Z_{st} = \xi_{st} = \left(1 + v_s \frac{Y_{(C,H)_1}}{Y_{(O)_2}}\right)^{-1}$$

### S T O I C H I O M E T R I C MIXTURE FRACTION

$$\begin{split} Z_{st} &= 1 - \frac{Y_{(O)_{st}}}{Y_{(O)_{2}}} \to Z_{st} = 1 - \frac{V_{s}}{Y_{(C,H)_{st}}} \\ Z_{st} &= \frac{Y_{(C,H)_{st}}}{Y_{(C,H)_{1}}} \to Y_{(C,H)_{st}} = Z_{st}Y_{(C,H)_{1}} \\ Z_{st} &= 1 - \frac{V_{s}}{Y_{(C,H)_{1}}} \frac{Y_{st}}{Y_{(O)_{2}}} \end{split}$$



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## STOICHIOMETRIC MIXTURE FRACTION

$$Z_{st} Y_{(O)_2} - Y_{(O)_2} + v_s Z_{st} Y_{(C,H)_1} = 0$$

$$Z_{st} \left( Y_{(O)_2} + v Y_{(C,H)_1} \right) = Y_{(O)_2}$$

$$Z_{st} \left( 1 + v \frac{Y_{(C,H)_1}}{Y_{(O)_2}} \right) = 1$$

$$Z_{st} = \xi_{st} = \left( 1 + v_s \frac{Y_{(C,H)_1}}{Y_{(O)_2}} \right)^{-1}$$

Relation with equivalence ratio

$$\phi = \frac{Z}{1-Z} \frac{(1-Z_{st})}{Z_{st}}$$

- Pure oxidizer  $(\phi = 0)$ : Z = 0

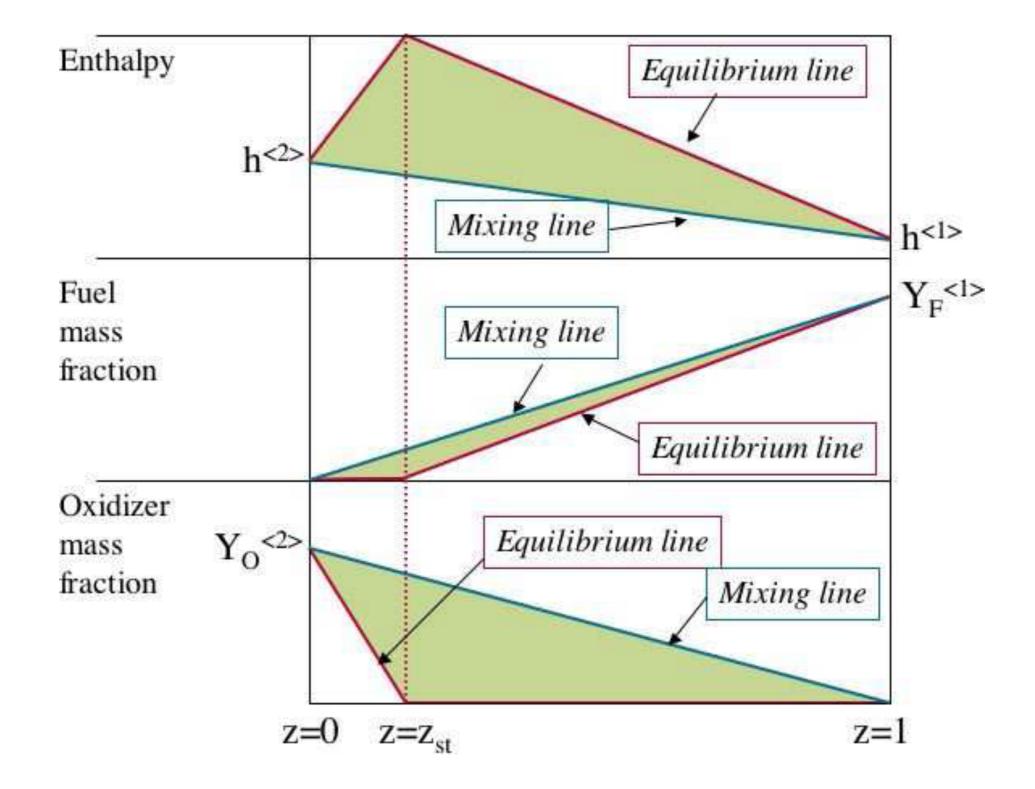
Pure fuel

(φ = ∞): Z = 1



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# MIXING AND EQUILIBRIUM







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### **INFINITELY FAST CHEMISTRY**

INFINITELY FAST CHEMISTRY ASSUMPTION:

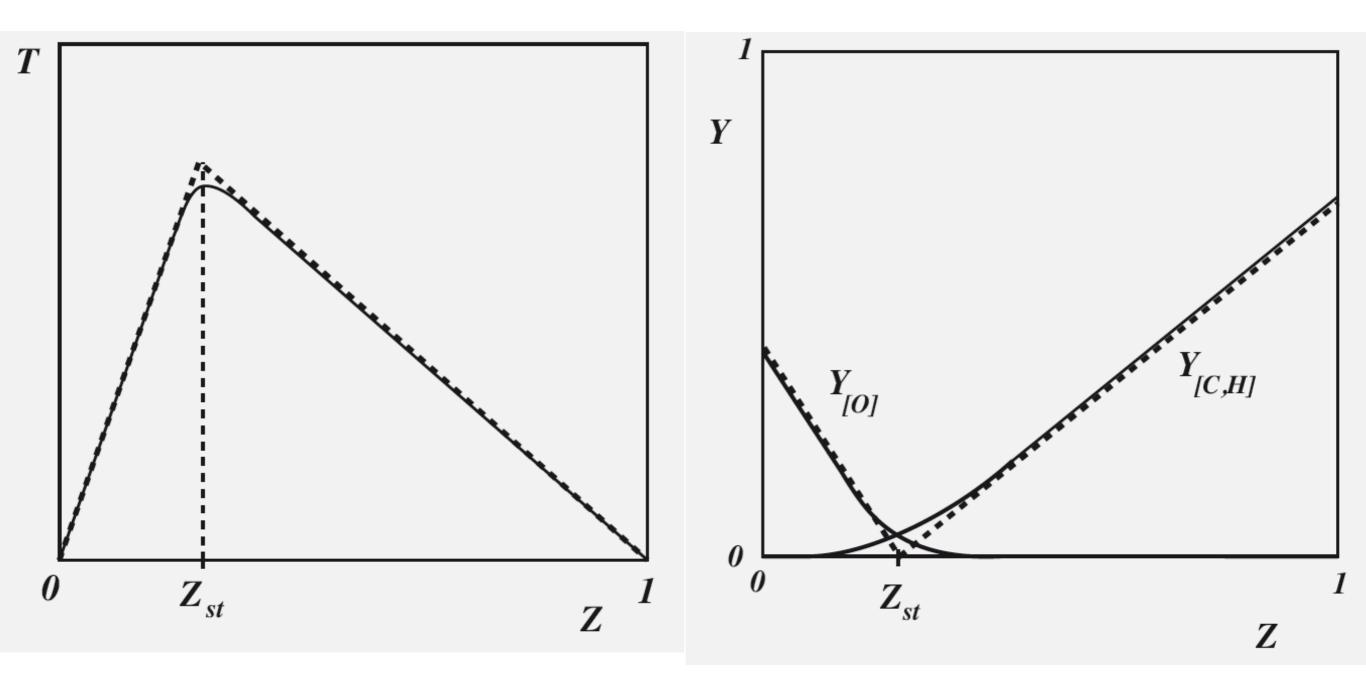
1) 
$$\dot{\rho}_i = \infty$$
  $Z = Z_{st}$   
 $\dot{\rho}_i = 0$   $AT$   $Z \neq Z_{st}$ 

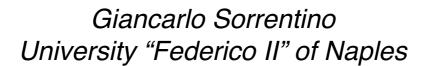
II)  
$$Y_{(C,H)} = 0 \qquad AT \qquad Z < Z_{st}$$
$$Y_{(O)} = 0 \qquad AT \qquad Z > Z_{st}$$



### INFINITELY FAST CHEMISTRY

INFINITELY FAST CHEMISTRY AND EQUILIBRIUM





#### - Assumption of fast chemical reactions

• If characteristic timescales of the flow and the reaction are of same order of magnitude: Chemical reaction processes have to be considered explicitly

•Flamelet formulation for non-premixed combustion

- Mixture fraction as independent coordinate

- Asymptotic approximation in the limit of sufficiently fast chemistry leads to onedimensional equations for reaction zone



• Assumptions: Equal diffusivities of chemical species and temperature

$$\operatorname{Le}_i = \lambda/(c_p \rho D_i) = 1, \quad i = 1, 2, \dots, k \qquad \Rightarrow \qquad D = \lambda/(\rho c_p)$$

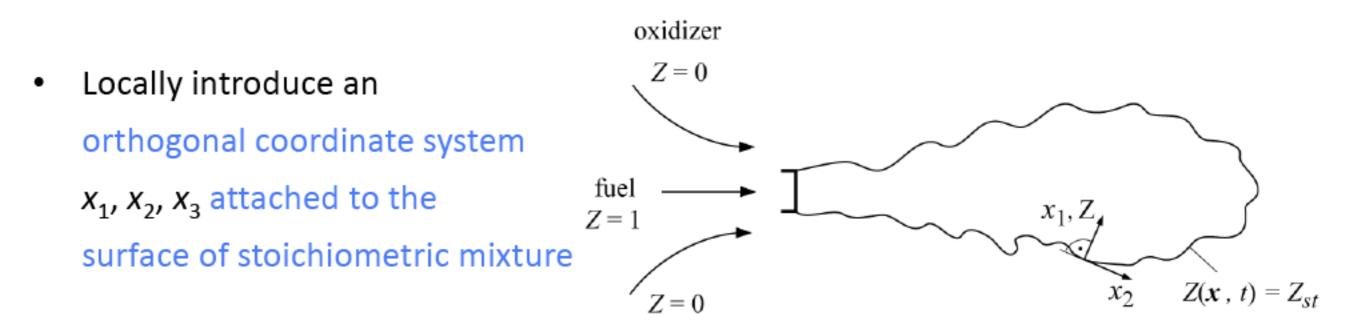
• The balance equation for mixture fraction, temperature and species read

$$\rho \frac{\partial Z}{\partial t} + \rho v_{\alpha} \frac{\partial Z}{\partial x_{\alpha}} - \frac{\partial}{\partial x_{\alpha}} \left( \rho D \frac{\partial Z}{\partial x_{\alpha}} \right) = 0 \quad \longleftarrow \quad \begin{array}{l} \text{No chemical source term!} \\ \rho \frac{\partial T}{\partial t} + \rho v_{\alpha} \frac{\partial T}{\partial x_{\alpha}} - \frac{\partial}{\partial x_{\alpha}} \left( \rho D \frac{\partial T}{\partial x_{\alpha}} \right) &= \sum_{i=1}^{k} \dot{m}_{i} \frac{h_{i}}{c_{p}} + \frac{\dot{q}_{R}}{c_{p}} + \frac{1}{c_{p}} \frac{\partial p}{\partial t} \\ \rho \frac{\partial Y_{i}}{\partial t} + \rho v_{\alpha} \frac{\partial Y_{i}}{\partial x_{\alpha}} - \frac{\partial}{\partial x_{\alpha}} \left( \rho D \frac{\partial Y_{i}}{\partial x_{\alpha}} \right) &= \dot{m}_{i} \quad i = 1, 2, \dots, k \end{array}$$

- Low Mach number limit
  - Zero spatial pressure gradients
  - Temporal pressure change is retained



- Surface of the stoichiometric mixture:  $Z(x_{\alpha}, t) = Z_{st}$
- If local mixture fraction gradient is sufficiently high:
  - → Combustion occurs in a thin layer in the vicinity of this surface



- $x_1$  points normal to the surface  $Z_{st}$ ,  $x_2$  and  $x_3$  lie within the surface
- Replace coordinate  $x_1$  by mixture fraction Z and  $x_2$ ,  $x_3$  and t by  $Z_2 = x_2$ ,  $Z_3 = x_3$  and t =  $\tau$



- Here temperature *T*, and similarly mass fractions *Y<sub>i</sub>*, will be expressed as function of mixture fraction *Z*
- By definition, the new coordinate Z is locally normal to the surface of stoichiometric mixture
- With the transformation rules:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t} \frac{\partial}{\partial Z}, \qquad \frac{\partial}{\partial x_1} = \frac{\partial Z}{\partial x_1} + \frac{\partial}{\partial Z}$$
$$\frac{\partial}{\partial x_{\alpha}} = \frac{\partial}{\partial Z_{\alpha}} + \frac{\partial Z}{\partial x_{\alpha}} \frac{\partial}{\partial Z} \quad (\alpha = 2, 3)$$

we obtain the temperature equation in the form

$$\rho \frac{\partial T}{\partial \tau} + \rho v_2 \frac{\partial T}{\partial Z_2} + \rho v_3 \frac{\partial T}{\partial Z_3} - \frac{\partial (\rho D)}{\partial x_2} \frac{\partial T}{\partial Z_2} - \frac{\partial (\rho D)}{\partial x_3} \frac{\partial T}{\partial Z_3} +$$

$$-\rho D\left(\left(\frac{\partial Z}{\partial x_{\alpha}}\right)^{2}\frac{\partial^{2}T}{\partial Z^{2}}+2\frac{\partial Z}{\partial x_{2}}\frac{\partial^{2}T}{\partial Z\partial Z_{2}}+2\frac{\partial Z}{\partial x_{3}}\frac{\partial^{2}T}{\partial Z\partial Z_{3}}+\frac{\partial^{2}T}{\partial Z_{2}^{2}}+\frac{\partial^{2}T}{\partial Z_{3}^{2}}\right)=\sum_{i=1}^{k}\dot{m}_{i}\frac{h_{i}}{c_{p}}+\frac{\dot{q}_{R}}{c_{p}}+\frac{1}{c_{p}}\frac{\partial p}{\partial t}$$

Transformation of equation for mass fractions is similar



 If flamelet is thin in the Z direction, an order-of-magnitude analysis similar to that for a boundary layer shows that

 $\left(\frac{\partial Z}{\partial x_{\alpha}}\right)^2 \frac{\partial^2 T}{\partial Z^2}$ 

is the dominating term of the spatial derivatives

• This term must balance the terms on the right-hand side

$$\rho \frac{\partial T}{\partial \tau} - \rho D \left(\frac{\partial Z}{\partial x_{\alpha}}\right)^2 \frac{\partial^2 T}{\partial Z^2} \approx \sum_{i=1}^k \dot{m}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

- All other terms containing spatial derivatives can be neglected to leading order
- This is equivalent to the assumption that the temperature derivatives normal to the flame surface are much larger than those in tangential direction





$$\rho \frac{\partial T}{\partial \tau} - \rho D \left( \frac{\partial Z}{\partial x_{\alpha}} \right)^2 \frac{\partial^2 T}{\partial Z^2} \approx \sum_{i=1}^k \dot{m}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

• Time derivative  $\partial T/\partial \tau$  important if very rapid changes occur, e.g. extinction

- Formally, this can be shown by introducing the stretched coordinate  $\xi$  and the fast time scale  $\sigma$ 

$$\xi = (Z - Z_{st})/\varepsilon, \quad \sigma = \tau/\varepsilon^2$$

•  $\epsilon$  is small parameter, the inverse of a large Damköhler number or large activation energy, for example, representing the width of the reaction zone



 If the time derivative term is retained, the flamelet structure is to leading order described by the one-dimensional time-dependent flamelet equations

$$\rho \frac{\partial T}{\partial t} - \rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \sum_{l=1}^r \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

$$\rho \frac{\partial Y_i}{\partial t} - \rho \frac{\chi_{st}}{Z} \frac{\partial Y_i}{\partial Z^2} = \dot{m}_i \quad i = 1, 2, \dots, k.$$

Here

$$\chi_{st} = 2D \left(\frac{\partial Z}{\partial x_{\alpha}}\right)_{st}^2$$

is the instantaneous scalar dissipation rate at stoichiometric conditions

- Dimension 1/s → Inverse of characteristic diffusion time
- Depends on t and Z and acts as a external parameter, representing the flow and the mixture field



• As a result of the transformation, the scalar dissipation rate

$$\chi_{st} = 2D \left(\frac{\partial Z}{\partial x_{\alpha}}\right)_{st}^2$$

implicitly incorporates the influence of convection and diffusion normal to the surface of the stoichiometric mixture

• In the limit  $\chi_{st} \rightarrow 0$ , equations for the homogeneous reactor are obtained



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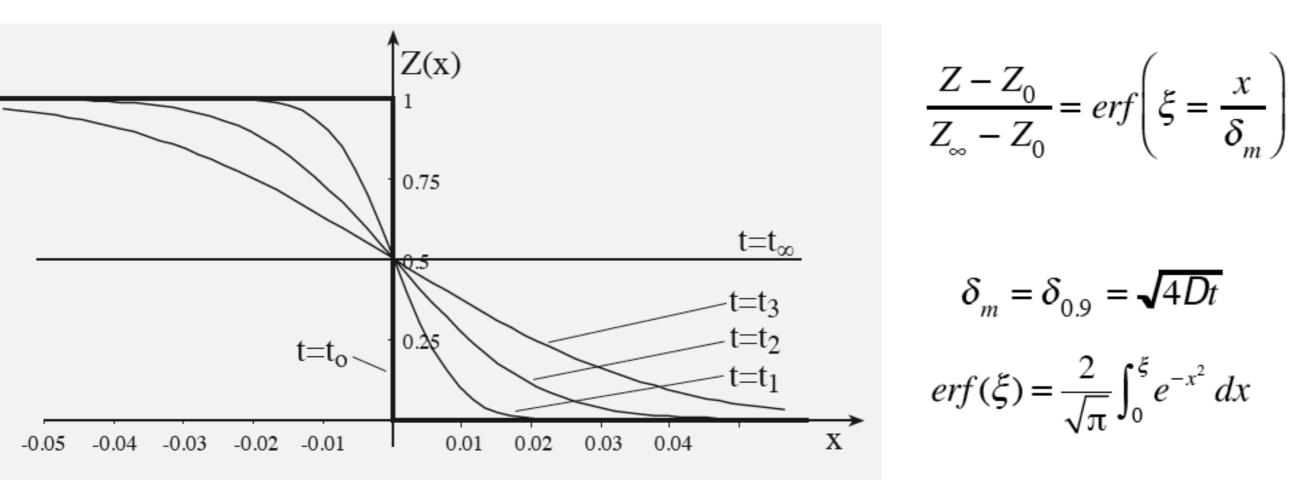


### 1D UNSTEADY DIFFUSION FLAMES/ UNSTRAINED

BOLTZMANN VARIABLE

 $\xi = x / \sqrt{4Dt}$ 

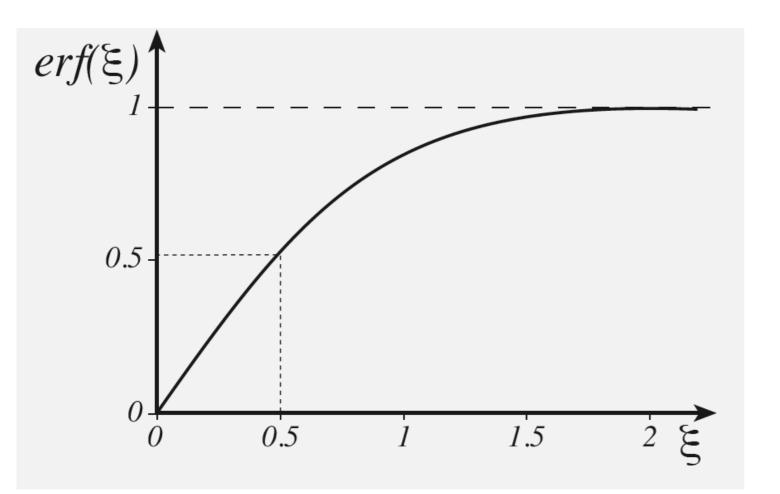
$$u\frac{dZ}{dx} - D\frac{d^2Z}{dx^2} = 0$$





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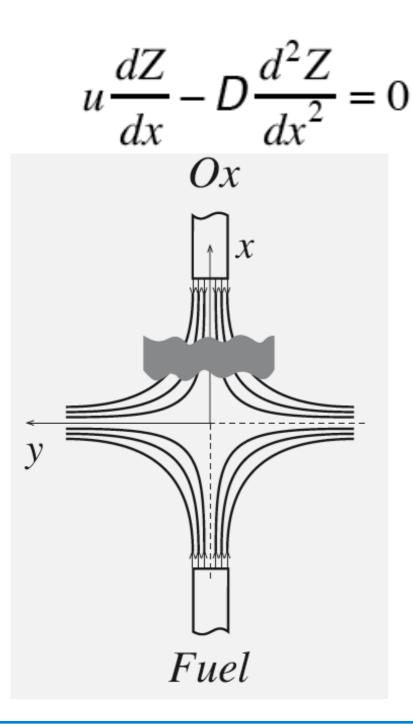
### 1D UNSTEADY DIFFUSION FLAMES/ UNSTRAINED



$$\xi = x / \sqrt{4Dt}$$

$$\delta_m = \delta_{0.9} = \sqrt{4Dt}$$
$$erf(\xi) = \frac{2}{\sqrt{\pi}} \int_0^{\xi} e^{-x^2} dx$$





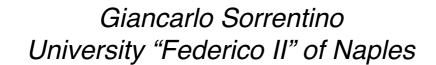
$$-\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} = a$$

$$\begin{cases} u = -ax \\ v = ay \end{cases}$$

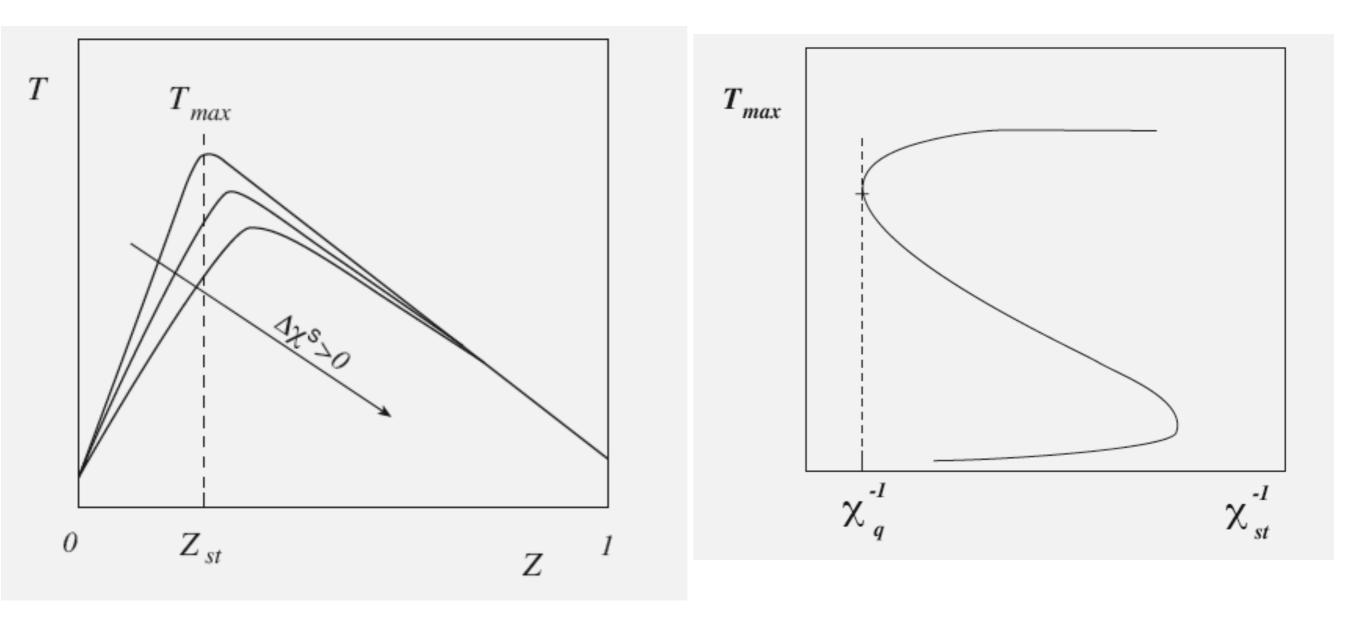
$$-ax\frac{dZ}{dx} - D\frac{d^2Z}{dx^2} = 0 \qquad \delta_m = (D/a)$$

$$x = 2\alpha \left(\frac{dZ}{dx}\right)^2$$

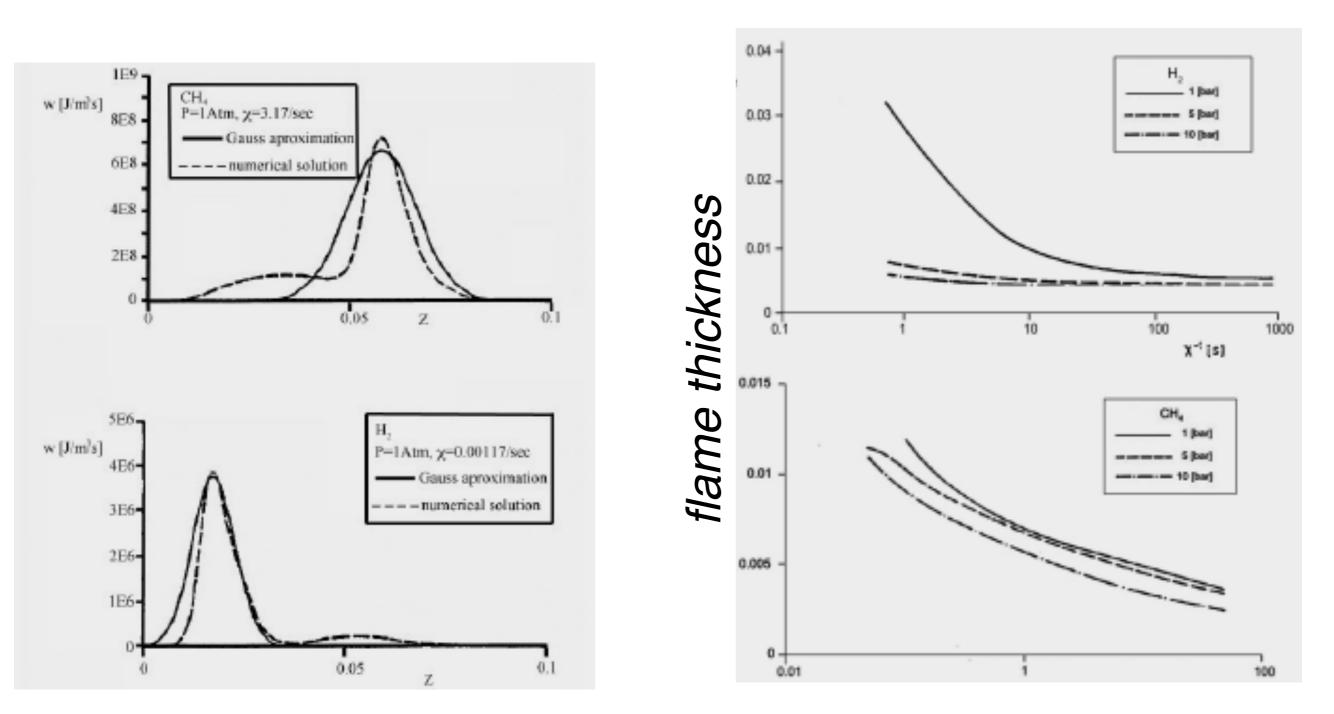
dx

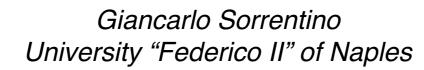




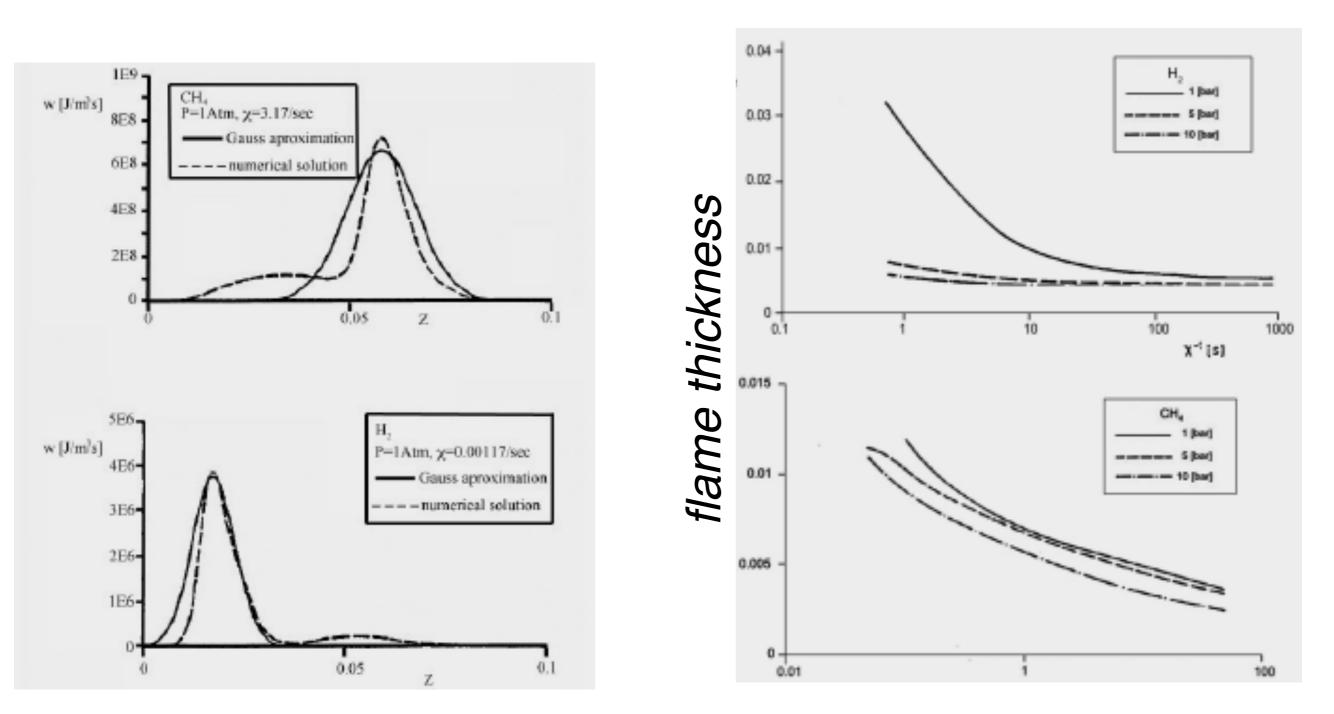


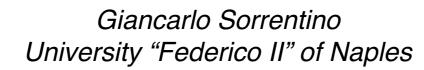






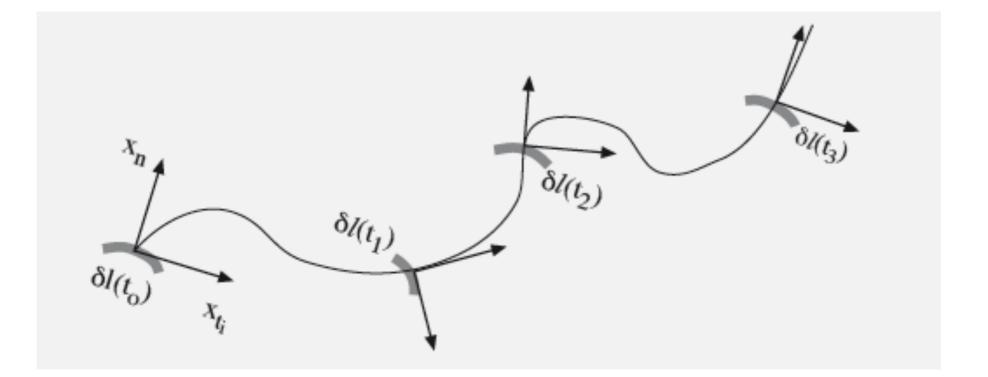


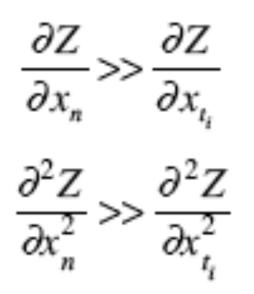






#### **1D STEADY DIFFUSION FLAMES/UNSTRAINED**



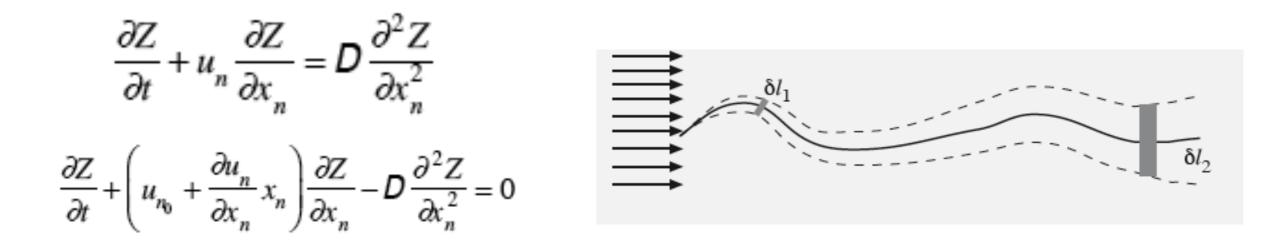


 $\frac{\partial Z}{\partial t} + u \frac{\partial Z}{\partial x} - D \frac{\partial^2 Z}{\partial x^2} = 0$ 

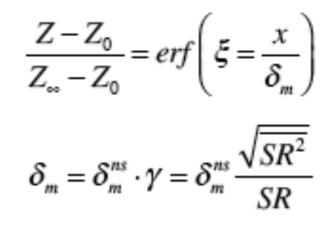




#### **1D STEADY DIFFUSION FLAMES/UNSTRAINED**



$$K = \underline{\nabla}_{t} \cdot \underline{\mathbf{v}}_{t}$$
$$\frac{\partial Z}{\partial t} - K \cdot x_{n} \frac{\partial Z}{\partial x_{n}} - D \frac{\partial^{2} Z}{\partial x_{n}^{2}} = 0$$



 $\gamma = \sqrt{SR^2}/SR$ 



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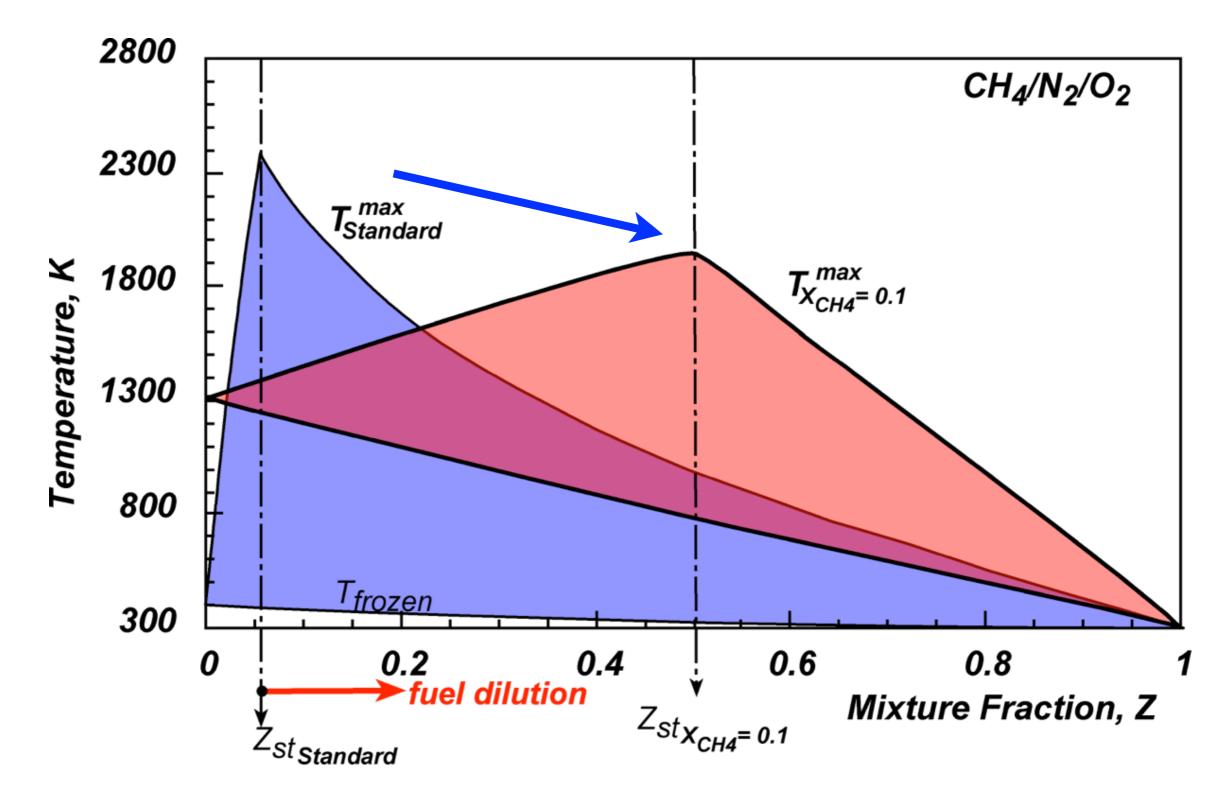
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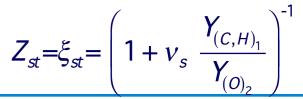
## **DILUTION EFFECTS**





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## **DILUTION EFFECTS** non premixed reactants oxidant standard hot and/or diluted hot and/or diluted diffusion flame fuel **Diluted Fuel** $\frac{\partial Y_i}{\partial t} - \chi \frac{\rho}{2} \nabla^2 Y_i = \dot{\rho}_i$ $Z = \frac{Y - Y_{(O)_1}}{Y_{(O)_2} - Y_{(O)_1}} = \frac{Y - Y_{(C,H)_1}}{Y_{(C,H)_2} - Y_{(C,H)_1}}$ $\frac{\partial h^s}{\partial t} - \chi \frac{\rho}{2} \underline{\nabla}^2 h^s = -\sum_i \dot{\rho}_i h_i^0$



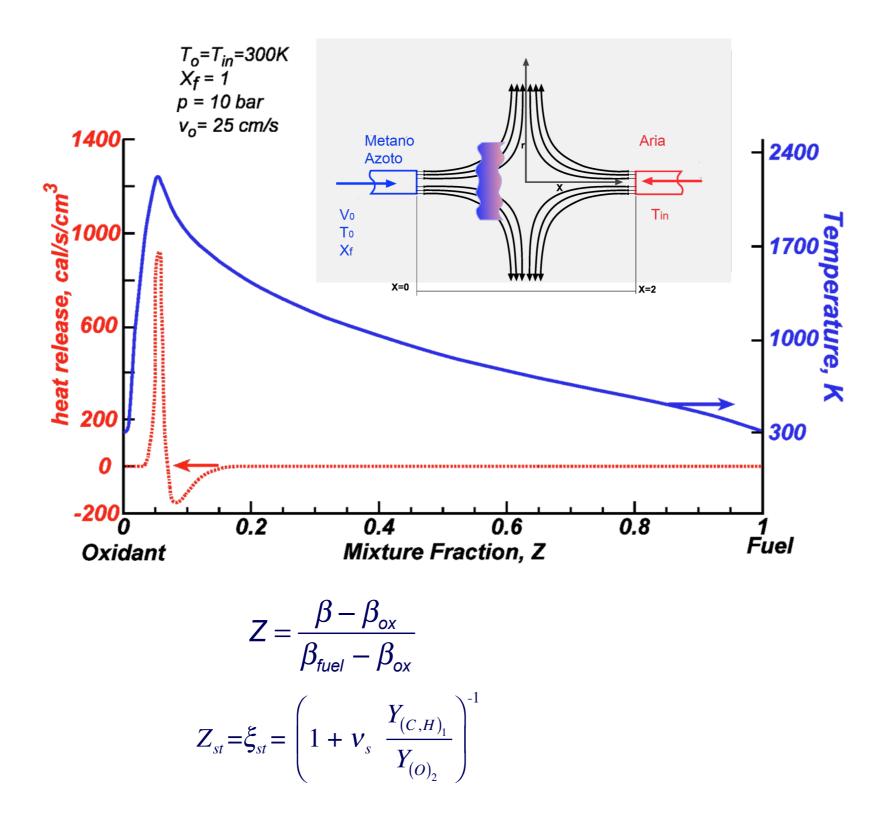


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Hot Oxidant

 $\chi = 2\alpha (\nabla Z)^2$ 

## **DILUTION EFFECTS**

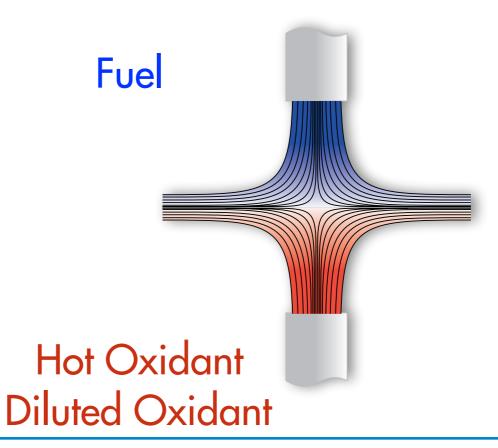




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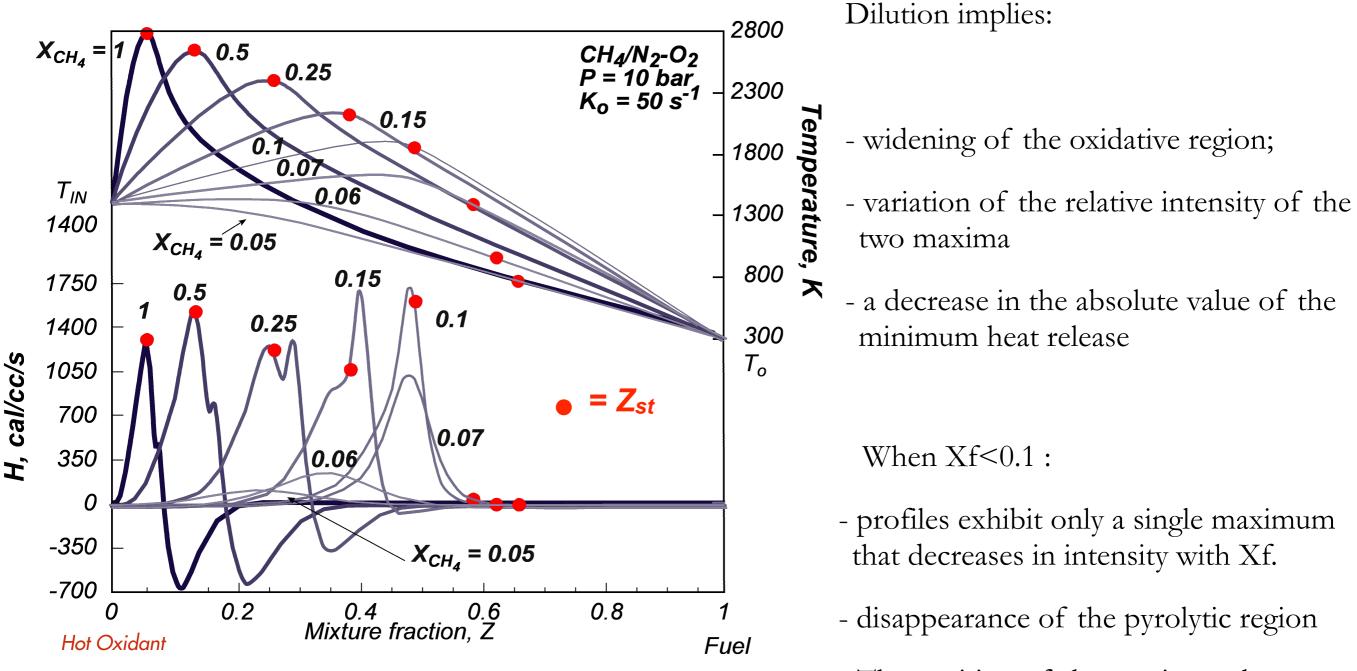
## **DILUTION EFFECTS**

	Oxidant	Fuel	
1	hot diluted		HODO
2	hot	diluted	HODF
3	diluted	hot	HFDO
4		hot diluted	HFDF



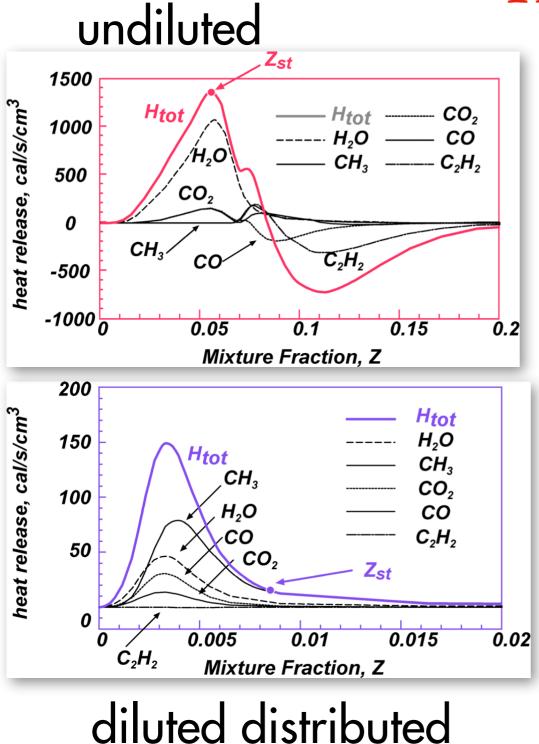
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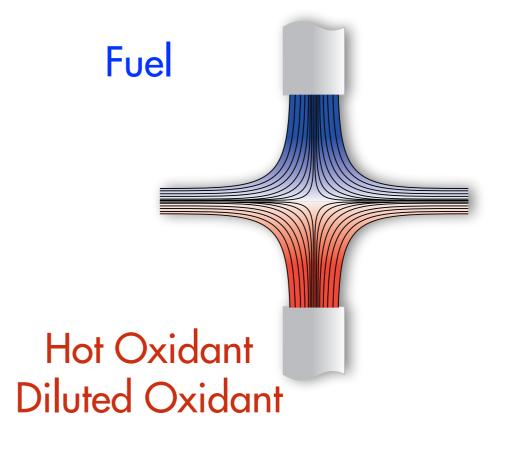


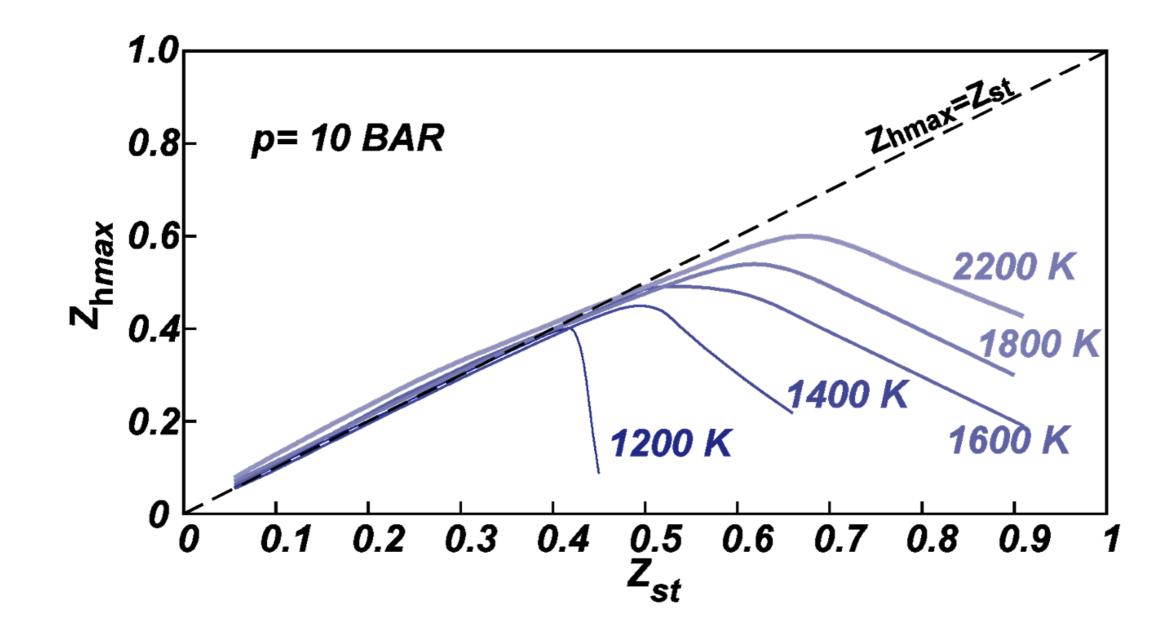


- The position of the maximum heat release is not related to Zst.

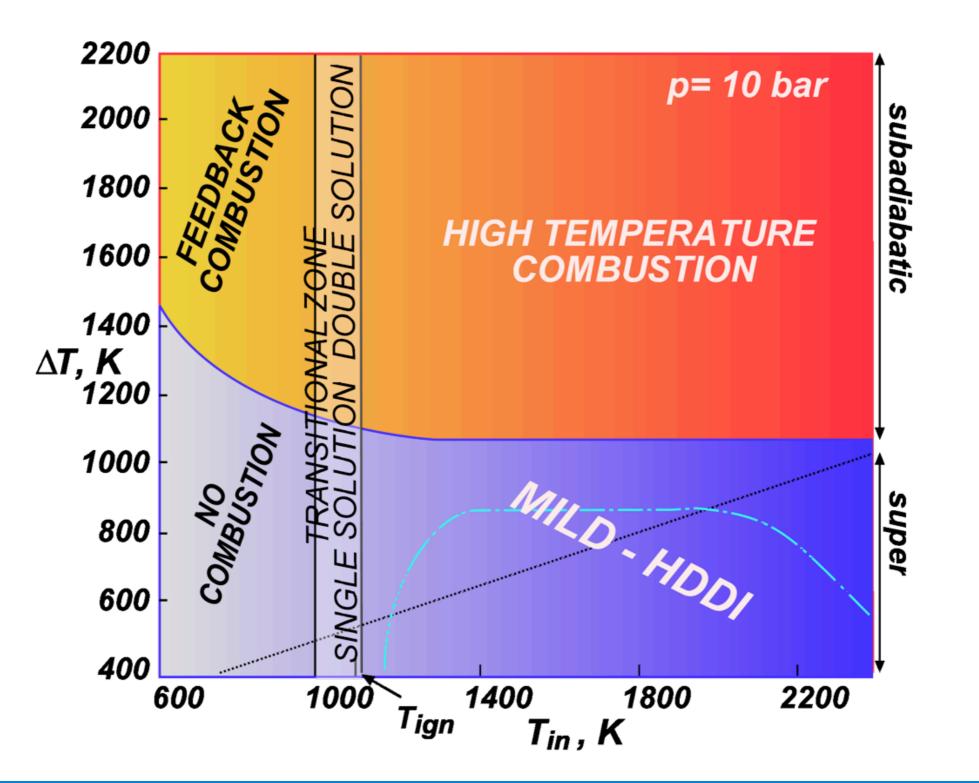


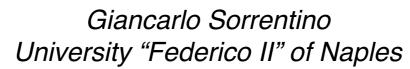














### DILUTION EFFECTS HDDI (HOT DILUTED DIFFUSION IGNITION)

•Pyrolytic region disappears (Flameless)

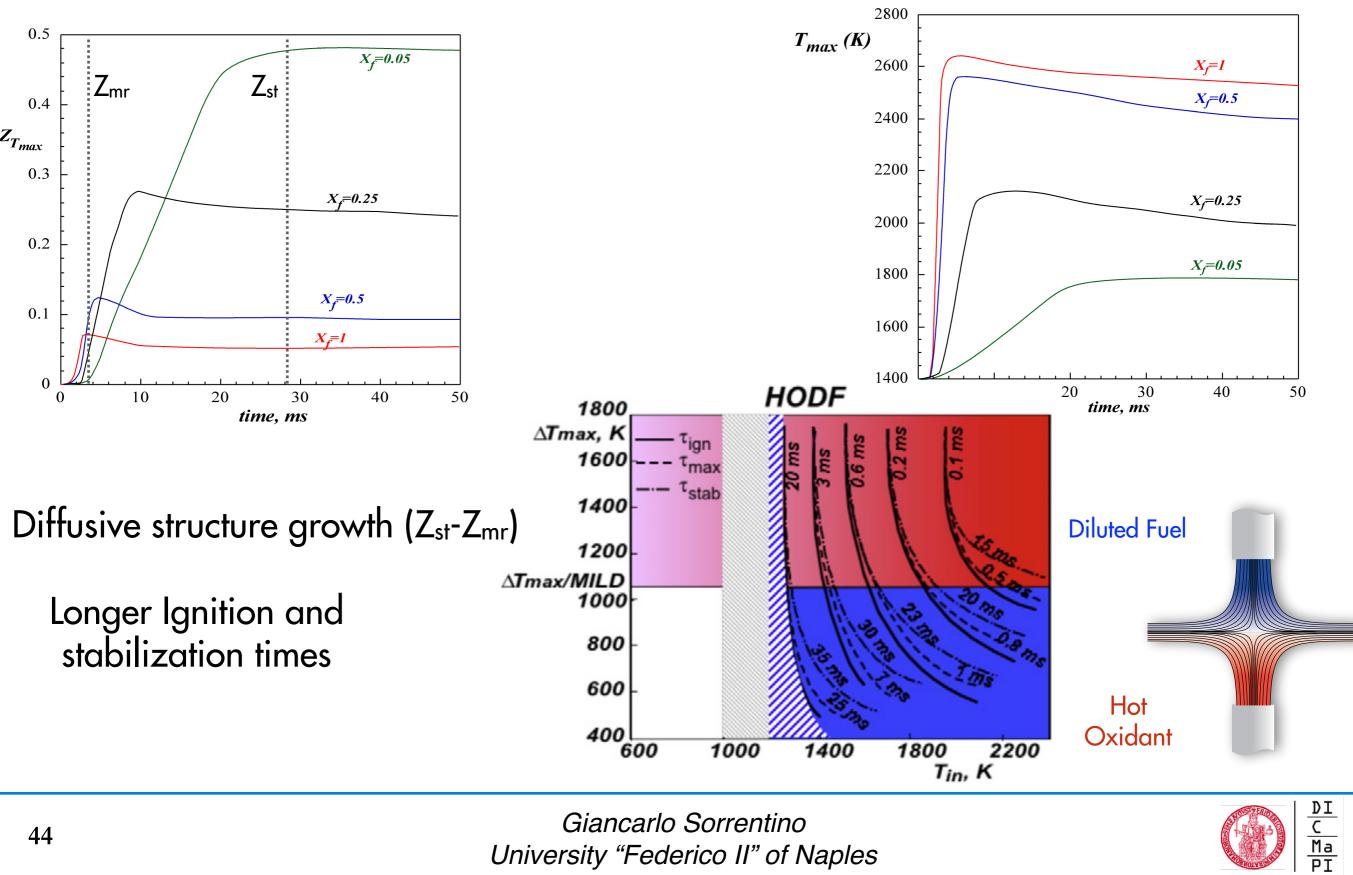
Reactive Region broadening (Distributed)

- heat release toward the hot side
- H no longer correlated with  $Z_{st}$

# **IGNIDIFFUSION PROCESS**

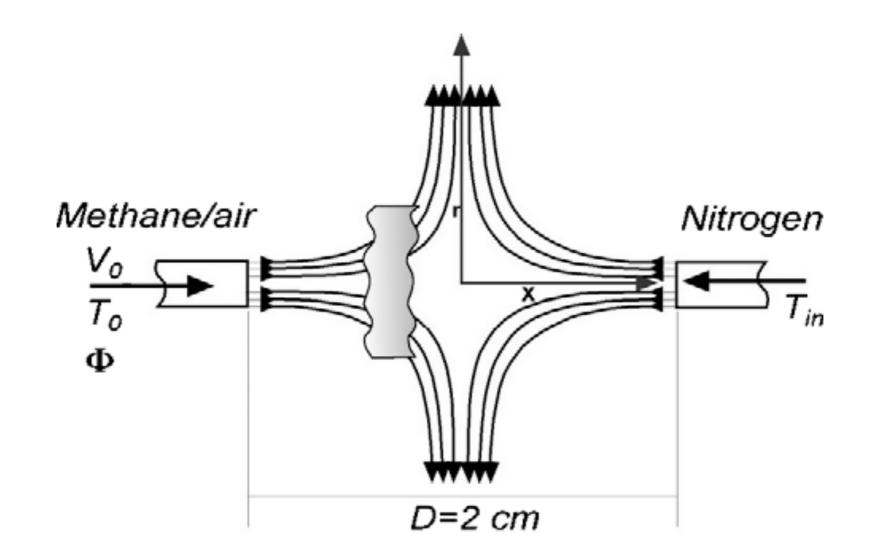


### **DILUTION EFFECTS UNSTEADY HDDI**



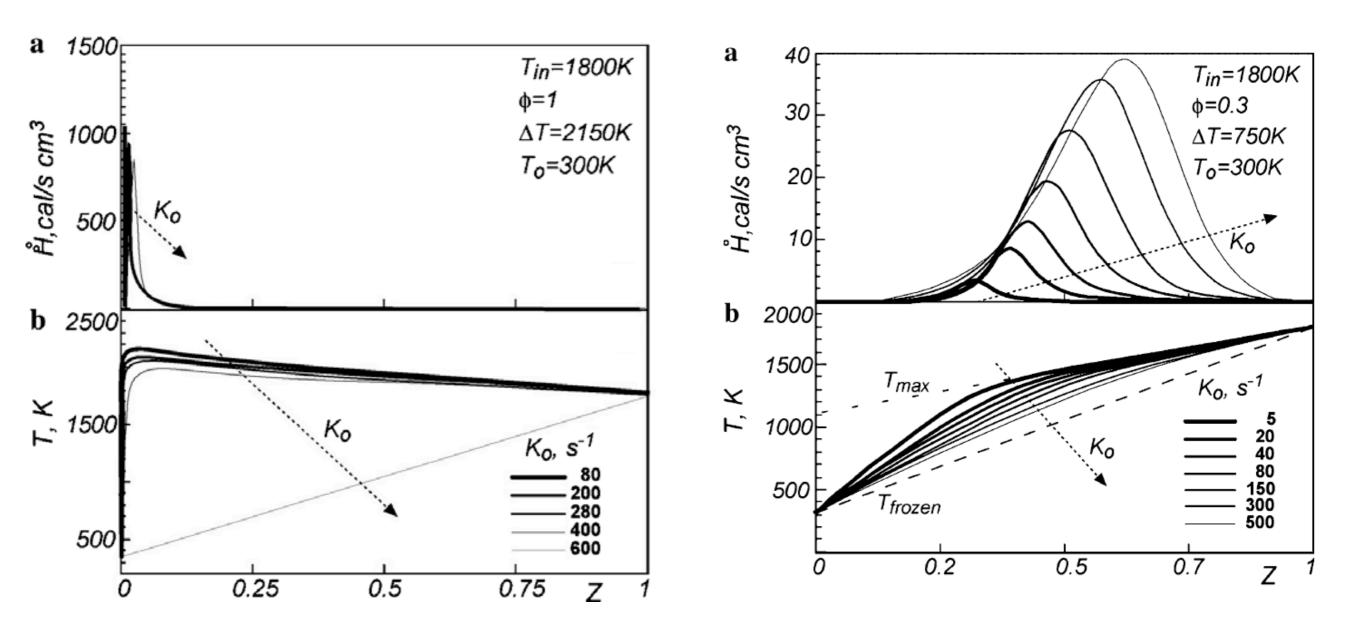
Giancarlo Sorrentino University "Federico II" of Naples

### DILUTION EFFECTS HOMOGENEOUS CHARGE DIFFUSION IGNITION (HCDI)



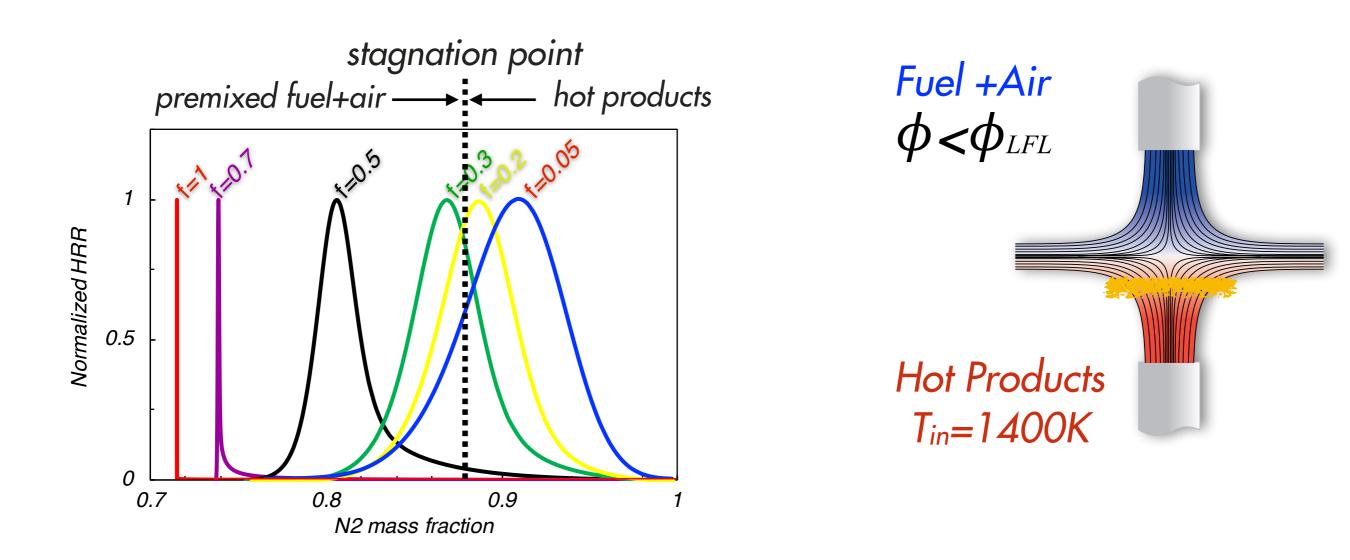


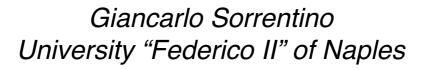
#### DILUTION EFFECTS HOMOGENEOUS CHARGE DIFFUSION IGNITION (HCDI)





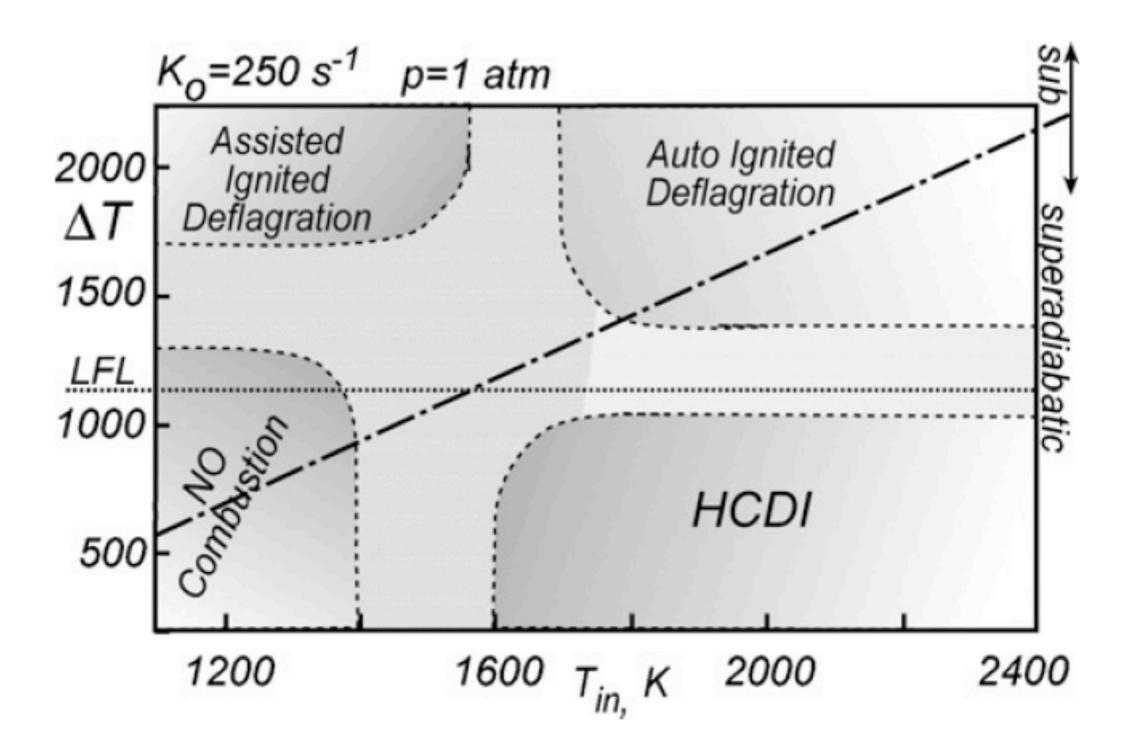
### DILUTION EFFECTS HOMOGENEOUS CHARGE DIFFUSION IGNITION (HCDI)





## **DILUTION EFFECTS**

**HOMOGENEOUS CHARGE DIFFUSION IGNITION (HCDI)** 





## IGNIDIFFUSION

#### HOT DILUTED DIFFUSION IGNITION

HOMOGENEOUS CHARGE DIFFUSION IGNITION

- Distribution of heat release rate is wider (with respect to the other reference elementary processes: deflagration, flame diffusion)
- The maximum heat release does not occur where could be expected (in terms of local chemical composition)
- Stabilization in mixing diffusion layer relies on autoignition



# **COURSE OVERVIEW**

#### DAY 2

#### **Combustion with Flame Propagation**

- a. One Dimensional Steady Flow formulation.
- b. Rayleigh and Rankine-Hugoniot equations.
- c. Detonation.
- d. Deflagration. Thermal theory. Flame Speed Dependencies.

#### Laminar Diffusion Flames

- a. Flame Structure and Mixture Fraction.
- b. Infinitely fast chemistry. Flamelet concept.
- c. 1D Unsteady Diffusion flames. Unstrained.
- d. 1D Steady Diffusion flames. Strained.
- e. 1D Unsteady Diffusion flames. Strained.
- f. Diluted conditions. Diffusion Ignition processes.