Turbulent Premixed Flames - BML and FGM Models

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BML - cont.

- The reactant mass fraction Y_F is non-dimensionalized, Y, using the initial reactant mass fraction in fresh gases Y_F^1

$$Y = \frac{Y_F}{Y_F^1} \tag{1}$$

so that Y varies from 1 in the fresh gases to 0 in the burnt gases.

- The reduced temperatura Θ is defined as

$$\Theta = \frac{c_p(T - T_1)}{QY_F^1} \tag{2}$$

and

$$Y + \Theta = 1.0 \tag{3}$$

Θ can also be viewed as a *Progress Variable*

Transport Equations in the BML Model

- Continuity Equation

$$\frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\right) = 0 \tag{4}$$

- Momentum Equation

$$\frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_i\widetilde{u}_j\right) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\frac{\partial \widetilde{u}_k}{\partial x_k}\right) - \overline{\rho u_i'' u_j''}\right] + \overline{\rho} g_i \tag{5}$$

- Progress Variable

$$\frac{\partial \overline{\rho}\widetilde{\Theta}\widetilde{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_k \frac{\partial \widetilde{\Theta}}{\partial x_j}\right) + \overline{\dot{\omega}}_\Theta, \tag{6}$$

where $\dot{\omega}_\Theta = \frac{\dot{\omega}_F}{Y_F^1}$

- 1-Step single irreversible reaction

$$\dot{\omega}_F = B\rho Y_F \exp\left(T_a/T\right) \tag{7}$$

BML - The ”no-Model” or Arrhenius Approach

1. The simplest approach is to neglect the effects of turbulence on turbulent combustion and to retain only the first term in the Taylor series:

$$\overline{\dot{\omega}}_\Theta = \dot{\omega}(\widetilde{\Theta}) = B\overline{\rho}\,\widetilde{Y_F}\exp\left(T_a/\widetilde{T}\right) = B\overline{\rho}(1-\widetilde{\Theta})\exp\left(\frac{T_a}{T_1+(T_2-T_1)\widetilde{\Theta}}\right) \tag{8}$$

2. This model is relevant only when chemical time e scales are larger than turbulent time scales ($\tau_{chem} >> \tau_{mixing}$, low Damkoehler number limit), corresponding to the “well stirred reactor” regime, where reactants mix rapidly and burn slowly.
3. This approach may be useful for simple analysis and is encountered for some specific applications such as supersonic combustion and chemical reactions in atmospheric boundary layers. In most situations, this model is completely inadequate.

BML - The Eddy Break Up (EBU) Approach

1. Range of application $Re >> 1$ and $Da >> 1$ - (opposite to the Arrhenius Model);
2. The chemistry does not play any explicit role while turbulent motions control the reaction rate:

$$\overline{\dot{\omega}}_{\Theta} = C_{EBU}\overline{\rho}\frac{\sqrt{\widetilde{\Theta''^2}}}{\tau_{EBU}} \tag{9}$$

where

$$\tau_{EBU} = \frac{k}{\varepsilon} \tag{10}$$

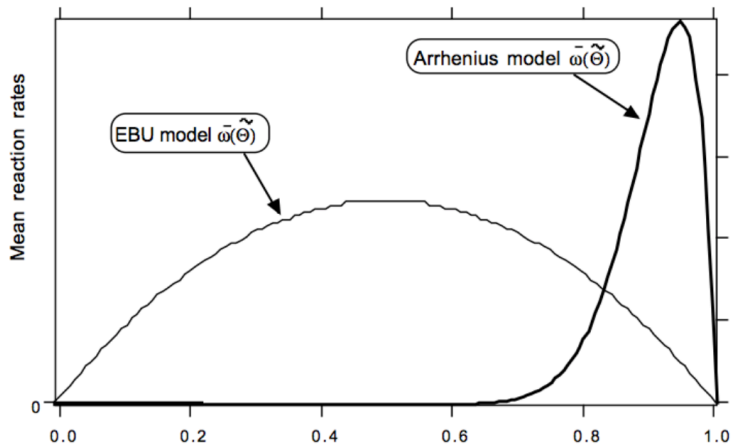
$$\overline{\rho}\widetilde{\Theta''^2} = \overline{\rho\left(\Theta - \widetilde{\Theta}\right)^2} = \overline{\rho}\left(\widetilde{\Theta^2} - \widetilde{\Theta}^2\right) = \overline{\rho}\widetilde{\Theta}\left(1 - \widetilde{\Theta}\right) \tag{11}$$

so that:

$$\overline{\dot{\omega}}_{\Theta} = C_{EBU}\overline{\rho}\frac{\varepsilon}{k}\widetilde{\Theta}\left(1 - \widetilde{\Theta}\right) \tag{12}$$

BML - The Eddy Break Up (EBU) Approach

1. - Obvious limitation: it does not include any effects of chemical kinetics.
2. - Comparison of the reaction rates predicted by the EBU and by the Arrhenius models:
3. - EBU gives a reaction rate for all values of Θ and not only at close to burned state;



The Bray Moss Libby (BML) model

1. Starting from the eq.(6), a transport equation for the quantity $\Theta(1-\Theta) = \Theta - \Theta^2$ can be derived:

$$\frac{\partial \rho \Theta(1-\Theta) u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_k \frac{\partial \Theta(1-\Theta)}{\partial x_j}\right) + 2\rho D_k \frac{\partial \Theta}{\partial x_j}\frac{\partial \Theta}{\partial x_j} - 2\Theta\dot{\omega}_\Theta + \dot{\omega}_\Theta, \tag{13}$$

2. Under the BML model assumptions, the reduced temperature Θ is equal to zero or to unity. So $\Theta(1-\Theta) = 0$ and the eq.(13) reduces to

$$2\rho D_k \frac{\partial \Theta}{\partial x_j}\frac{\partial \Theta}{\partial x_j} = 2\Theta\dot{\omega}_\Theta - \dot{\omega}_\Theta, \tag{14}$$

The Bray Moss Libby (BML) model

1. after averaging:

$$\overline{\dot{\omega}}_\Theta = \frac{1}{2\Theta_m - 1}\left(2\rho D_k \overline{\frac{\partial\Theta}{\partial x_j}\frac{\partial\Theta}{\partial x_j}}\right) = \frac{\overline{\rho}\widetilde{\chi}_\Theta}{2\Theta_m - 1} \tag{15}$$

where

$$\Theta_m = \frac{\overline{\Theta\dot{\omega}_\Theta}}{\overline{\dot{\omega}_\Theta}} = \frac{\int_0^1 \Theta\dot{\omega}_\Theta P(\Theta)d\Theta}{\int_0^1 \dot{\omega}_\Theta P(\Theta)d\Theta} \tag{16}$$

2. The scalar dissipation of the Reduced Temperature - $\overline{\rho\chi_\Theta} = \overline{\rho}\widetilde{\chi}_\Theta$, can be modelled as:

$$\overline{\rho\chi_\Theta} = \overline{\rho}\frac{\widetilde{\Theta''^2}}{\tau_{mixing}} = \overline{\rho}\frac{\widetilde{\Theta''^2}}{\frac{k}{\varepsilon}} \tag{17}$$

The Bray Moss Libby (BML) model

1. assuming an intermittency between fresh and burnt gases results $\Theta^2 = \Theta$ and then:

$$\overline{\dot{\omega}}_\Theta = \frac{1}{2\Theta_m - 1}\overline{\rho}\frac{\varepsilon}{k}\widetilde{\Theta}\left(1 - \widetilde{\Theta}\right) \tag{18}$$

2. It's easy to see that the BML Model incorporates both chemistry features through Θ_m and the turbulent mixing through τ_{mixing}

Favre decomposition

Carring out the Favre-decomposition for the mass fraction of specie k and modeling the unkown terms, one has

$$\frac{\partial \bar{\rho} \widetilde{Y_k}}{\partial t} + \frac{\partial \bar{\rho} \widetilde{Y_k} \widetilde{u_j}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_k \frac{\partial \widetilde{Y_k}}{\partial x_j} \right) + \widetilde{\dot{\omega}_k}, \tag{19}$$

and for the mixture fraction

$$\frac{\partial \bar{\rho} \widetilde{f}}{\partial t} + \frac{\partial \bar{\rho} \widetilde{f} \widetilde{u_j}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_t \frac{\partial \widetilde{f}}{\partial x_j} \right); \tag{20}$$

Favre decomposition

A transport equation for the Favre averaged variance of the mixture fraction can be obtained as

$$\frac{\partial \overline{\rho}\widetilde{f''^2}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i\widetilde{f''^2}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_t \frac{\partial \widetilde{f''^2}}{\partial x_j}\right) = C_{g,1}\overline{\rho} D_{Eff}\left|\frac{\partial \widetilde{f}}{\partial x_i}\right|^2 C_{g,2}\overline{\rho}\frac{\varepsilon}{k}\widetilde{f''^2} \tag{21}$$

where D_{Eff} is the effective coeficient of difusivity, including the turbulence effect. $C_{g,1} = 2.8$ e $C_{g,2} = 2$.
The Favre averaged absolute enthalpy equation reads

$$\frac{\partial \overline{\rho}\widetilde{h}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{h}\widetilde{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_t}\frac{\partial \widetilde{h}}{\partial x_j}\right), \tag{22}$$

Presume Probability Density Function

- If the Probability Density Function (PDF) were known, the mean value of $q(\psi)$ could be obtained as:

$$\bar{q} = \int_{-\infty}^{\infty} q(\psi) P(\psi) d\psi, \tag{23}$$

  where $P(\psi)$ is the PDF of the variable ψ.
- We don't know all statistical moments of a fluctuating signal;
- Based on previous knowledge of the Probability Density Function (PDF) on a reactive system, a presumed (ad hoc) PDF is proposed;

Presume Probability Density Function

Presumed $\beta - PDF$

Usually in combustion simulation, the Favre decompsiton is preferred, instead of the Reynolds decomposition. In this case, the Favre averaged value of the physical quantities can be evaluated with

$$\tilde{q} = \int_{-\infty}^{\infty} q(\psi)\, \tilde{P}(\psi)\, d\psi, \tag{24}$$

where $\tilde{P}(\psi)$ is related to the time PDF of the property ψ with

$$\tilde{P}(\psi) = \frac{\rho(\psi)}{\bar{\rho}} P(\psi). \tag{25}$$

Presume Probability Density Function

The Presumed $\beta - PDF$ can be obtained by

$$\tilde{P}(\psi) = \frac{f^{\alpha-1}(1-f)^{\beta-1}}{\int_0^1 f^{\alpha-1}(1-f)^{\beta-1}}, \; ou \; \frac{f^{\alpha-1}(1-f)^{\beta-1}\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\beta)} \tag{26}$$

$\Gamma(\psi)$ is the gamma function and

$$\alpha = \tilde{f}\left[\frac{\tilde{f}\left(1-\tilde{f}\right)}{\widetilde{f''2}}\right], \tag{27}$$

$$\beta = \frac{\left(1-\tilde{f}\right)}{\tilde{f}}\alpha. \tag{28}$$

one has to calculate the average and variance values of the mixture fraction.

Favre decomposition

A fluctuating quantity can be decomposed using Favre approach as:

$$\psi = \widetilde{\psi} + \psi'' = \frac{\overline{\rho\psi}}{\bar{\rho}} + \psi'', \tag{29}$$

$$\widetilde{\psi} = \frac{\overline{\rho\psi}}{\bar{\rho}}. \tag{30}$$

Flamelet Generated Manifolds Model

- In turbulent flames, the phenomenon of local extinction of the flame is often observed, which may be caused by very intense turbulence, for example.
- Only with the mixture fraction it is not possible to describe flames with local extinction. For this reason, a second variable is introduced, the reaction progress variable.
- The reaction progress variable is set to take the value of zero in the unburned mixture and the unit value in the completely burned mixture. It is not a passive scalar, as its value is changed by the combustion progress.

Flamelet Generated Manifolds Model

- The effect of turbulence on the averaged value of the source term can be modeled in several ways. One is to assume a probability density function, for example the beta function, and use the average values and variances of the mixture fraction and the reaction progress variable to calculate the mean value from the value of the laminar case without the effects of turbulence.

Flamelet Generated Manifolds Model

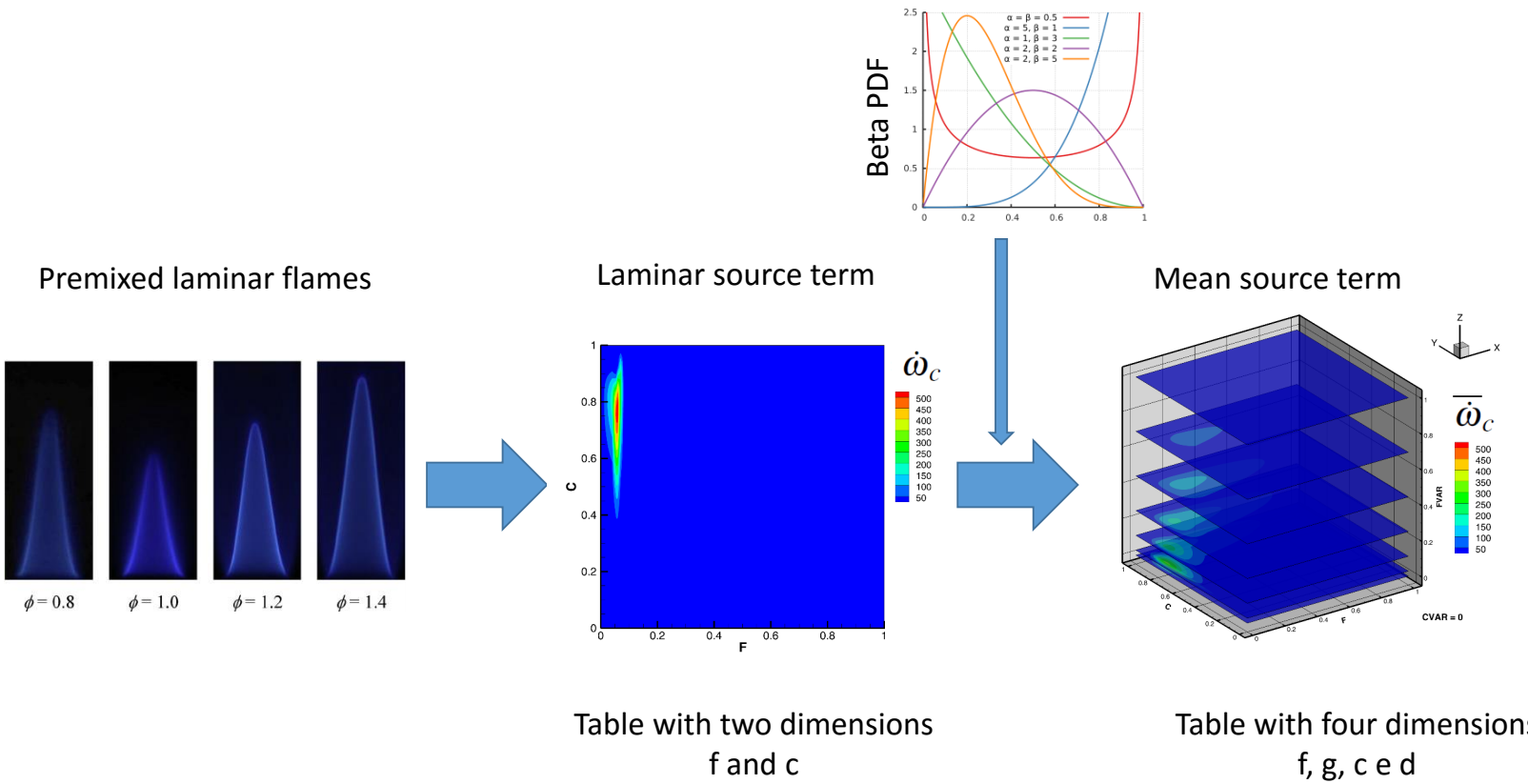
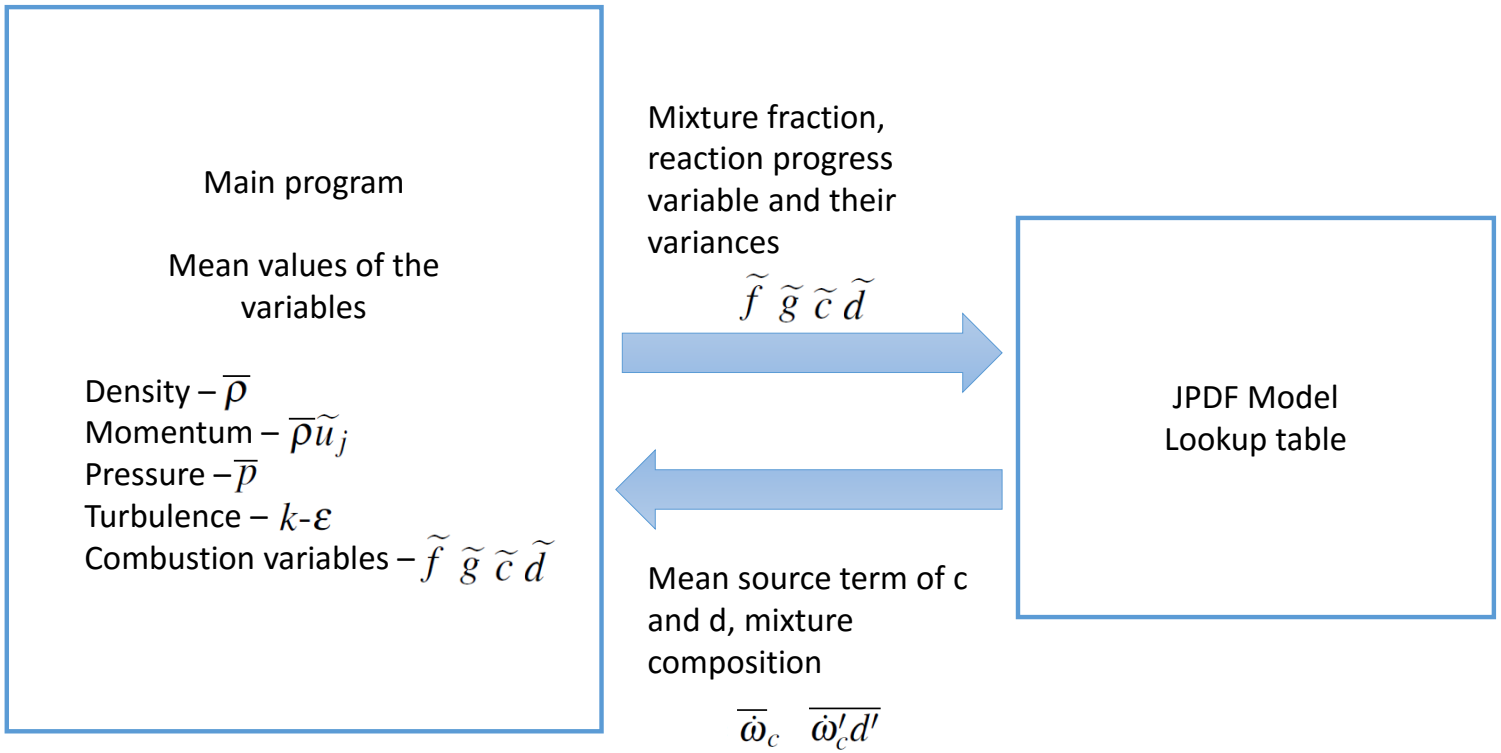


Figure:

Flamelet Generated Manifolds Model



Many contributors to the topic

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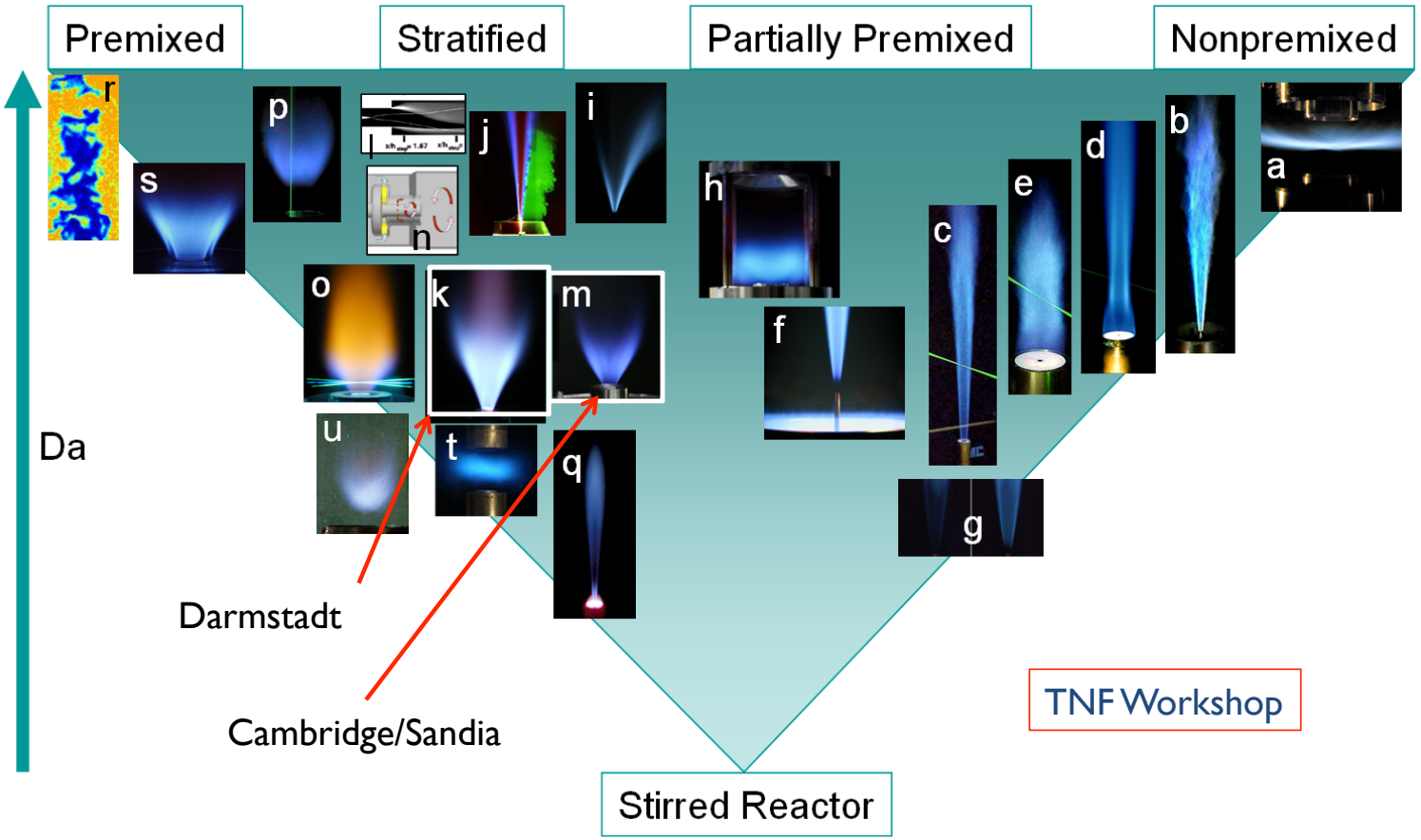


Nonpremixed flame - D

- Application - Nonpremixed flame - D; Sandia National Laboratories and Technische Universitäet Darmstadt

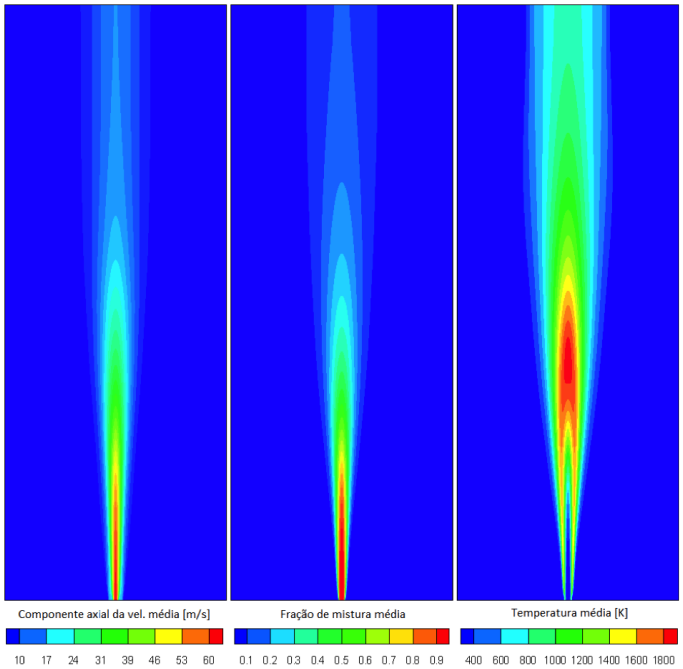


Figure: Campos de temperatura, fração de mistura e componente axial de velocidade da ”Simulação II”.

Nonpremixed flame - D

- Velocity boundary conditions

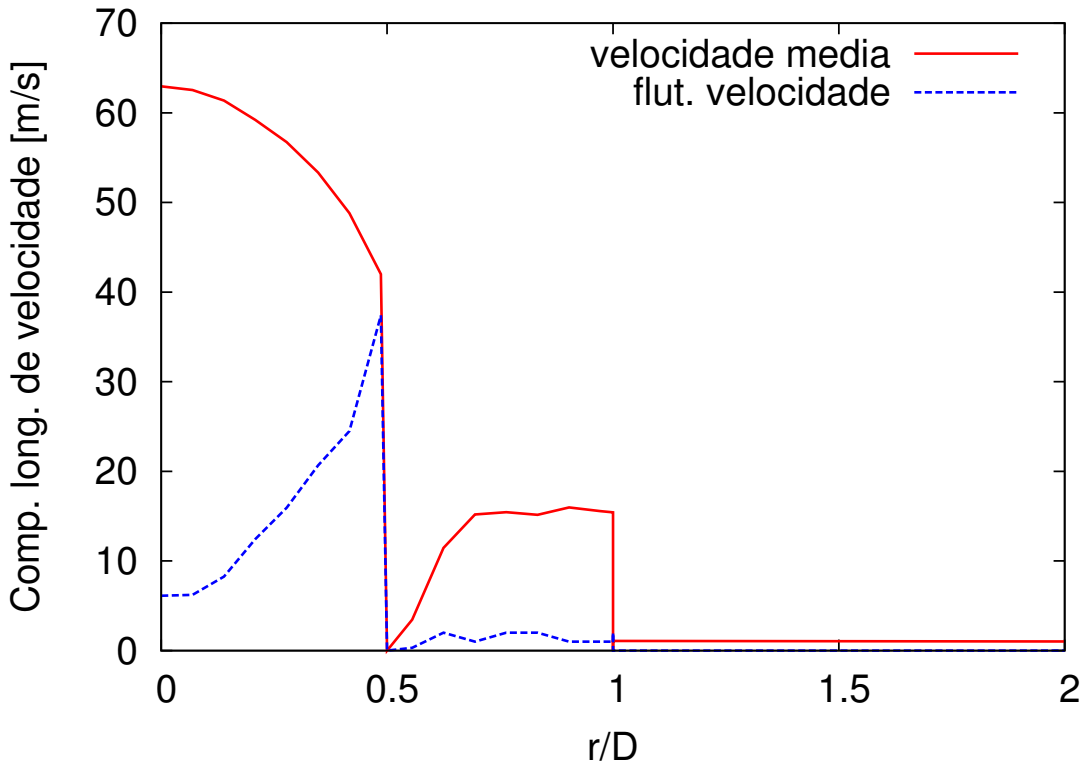
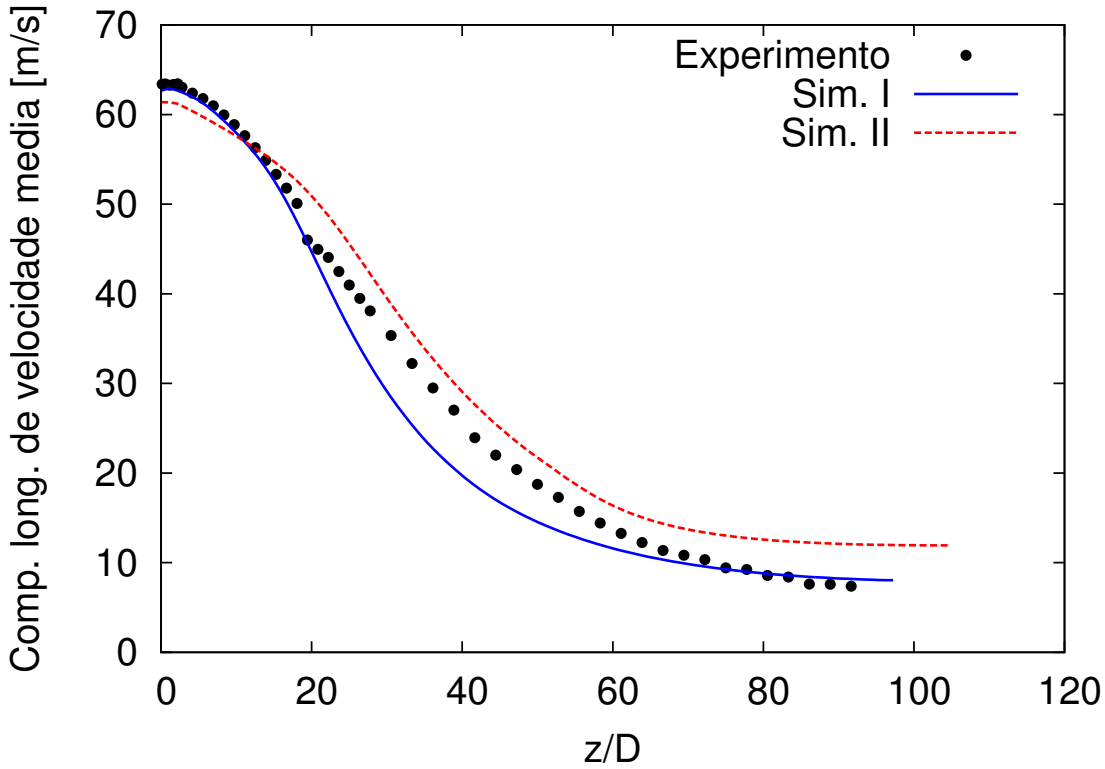


Figure: Perfil Mean value and fluctuaions of the axial velocity - data

Results Nonpremixed flame - D

- Results with $k - \varepsilon$ RANS equations + Flame sheet Model

- Axial velocity at the center line



Results Nonpremixed flame - D

- Mixture fraction at the center line

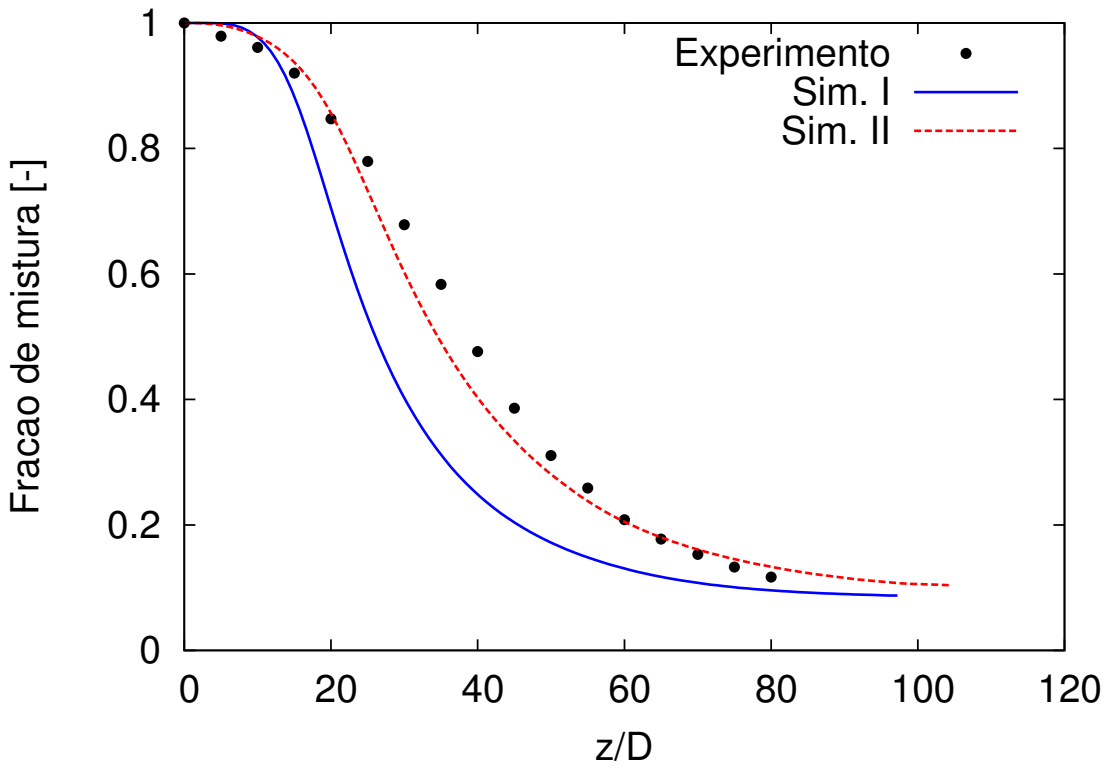


Figure: Comparação entre os resultados das simulações corrigidas e os

Results Nonpremixed flame - D

- Temperature at the center line

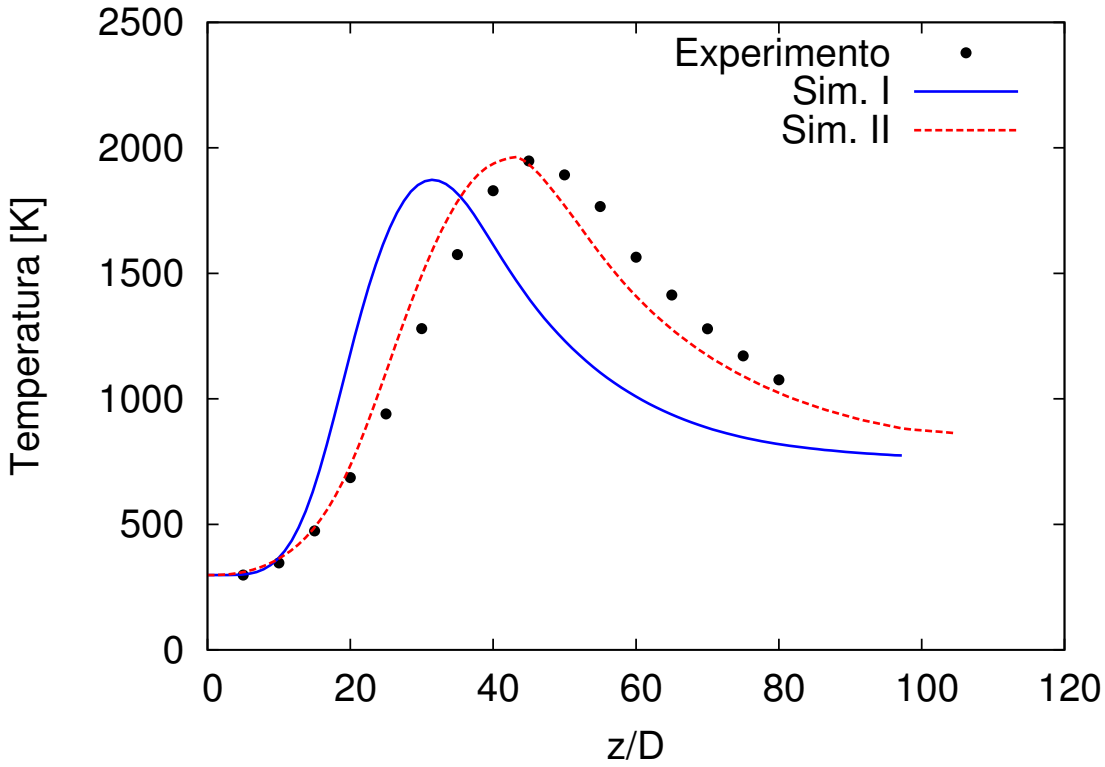


Figure: Perfis de temperatura média ao longo da linha de centro da chama.

Results Nonpremixed flame - D

- Results with $k - \varepsilon$ RANS equations + Chemical Equilibrium and Flamlet Models

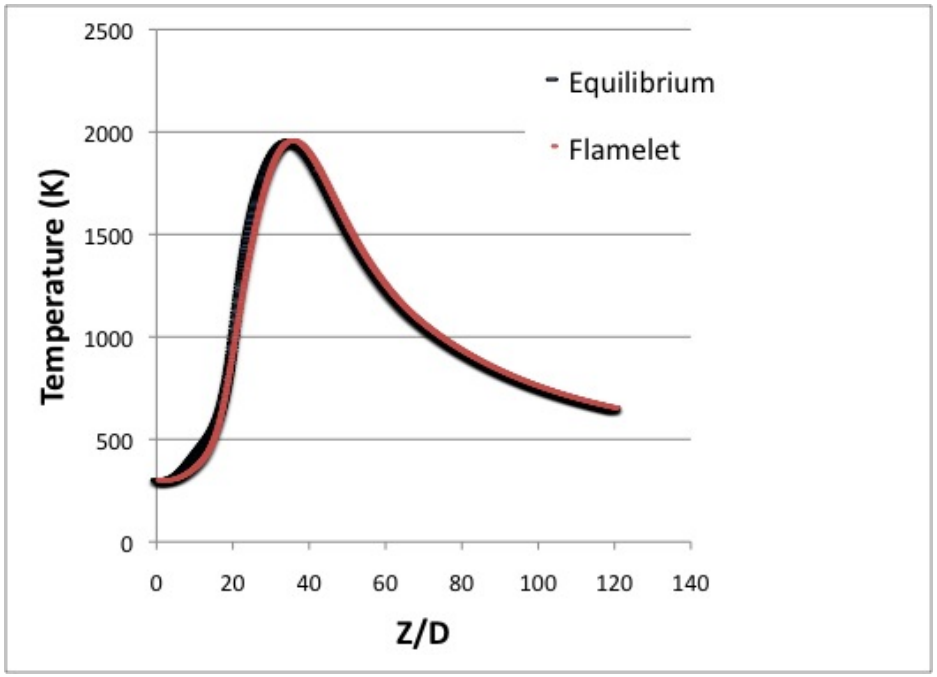


Figure: Flame D - Temperature at centreline - Equilibrium X Flamelet

Results Nonpremixed flame - D

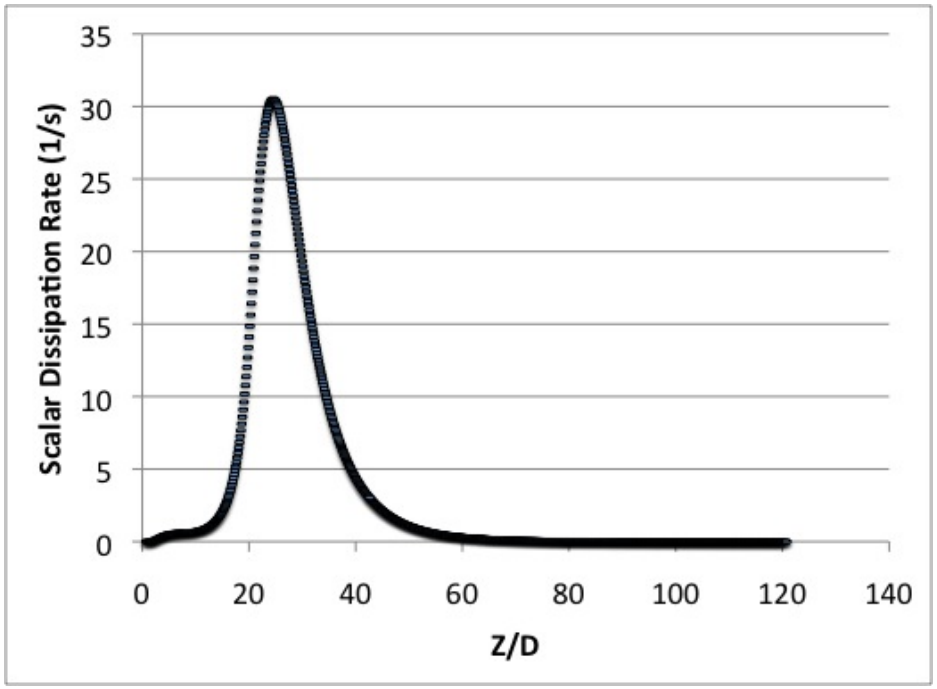


Figure: Averaged Scalar Dissipation Rate at the centreline

Results Nonpremixed flame - D LES - FGM

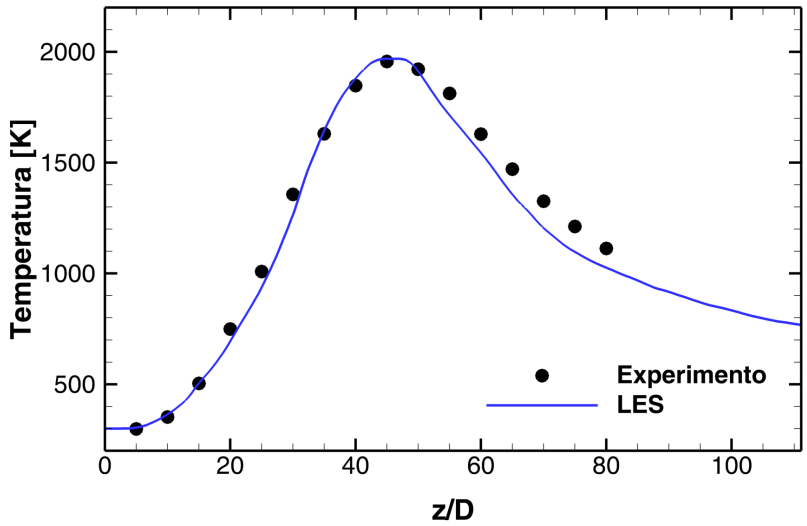


Figure: Flame D - Temperature at centreline LES-FGM

Summary

- Equilibrium, Da $\rightarrow \infty$, no time dimension
- Flamelet, Da ?, takes into account time in some extend
- FGM no Da dependency, explicit turbulence chemistry interaction
- LES with better flow prediction

Thank you!

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