Laminar Combustion Models

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Introduction

- Chemical reactions of the combustion process are tightly coupled to the other physical processes in a reactive flow.
- As a direct result of these reactions are the temperature increase and change in the chemical composition of the flow mixture.
- Inclusion of source terms in the energy conservation equations and chemical species;
- Changes in the thermodynamic and transport properties of the gas mixture.

Damköhler Number

A basic classification of the laminar combustion models can be done based on the adimensional Damköhler Number:

$$Da = \frac{\tau_{flow}}{\tau_{chem}}, \tag{1}$$

where (τ_{chem}) is the characteristic time for the chemical reactions and (τ_{flow}) is the characteristic time of the advection and diffusion transport processes in the flow.

The flame sheet and chemical equilibrium combustion models adopt the fundamental hypothesis that the characteristic time for the chemical reactions (τ_{chem}) is infinitely smaller than the characteristic time of the advection and diffusion transport processes in the flow (τ_{flow}).

This means, these two models are valid in combustion processes where $Da \rightarrow \infty$.

On the other hand, if transient processes are important, e.g. ignition, extintion and pollutant formation, this approximation does not hold.

Mixture Fraction

The definition of the mixing fraction was originally made for flames described by a single irreversible global reaction.

$$1\,kg\ of\ fuel + s\ kg\ of\ oxidizer \rightarrow (1+s)\,kg\ of\ products. \tag{2}$$

For stoichiometric conditions, the rate of comsumption of fuel,($\dot{\omega}_f$), and oxidizer, ($\dot{\omega}_{ox}$), are related by

$$\dot{\omega}_f = \frac{1}{s}\dot{\omega}_{ox}. \tag{3}$$

Mixture Fraction

The Transport Equation of the specie k

$$\rho \frac{\partial Y_k}{\partial t} + \rho u_i \frac{\partial Y_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Y_k}{\partial x_i}\right) = \dot{\omega}_k \tag{4}$$

can be used for the fuel(f) and oxidizer(ox) as

$$\frac{\partial \rho Y_f}{\partial t} + \frac{\partial \rho Y_f u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_f \frac{\partial Y_f}{\partial x_j}\right) + \dot{\omega}_f, \tag{5}$$

$$\frac{\partial \rho Y_{ox}}{\partial t} + \frac{\partial \rho Y_{ox} u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_{ox} \frac{\partial Y_{ox}}{\partial x_j}\right) + \dot{\omega}_{ox}. \tag{6}$$

The conservative variable φ is defined as

$$\varphi = sY_f - Y_{ox}, \tag{7}$$

Mixture Fraction

using equal diffusion coeficientes ($\rho D_f = \rho D_{ox} = \rho D = \Gamma_\varphi$) and subtracting the Eq. 6 from the Eq. 5 one has,

$$\frac{\partial \rho\varphi}{\partial t} + \frac{\partial \rho\varphi u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma_\varphi \frac{\partial \varphi}{\partial x_j}\right). \tag{8}$$

The mixture fraction is the result of the normalization

$$f = \frac{\varphi - \varphi_0}{\varphi_1 - \varphi_0} = \frac{(sY_f - Y_{ox}) - (sY_f - Y_{ox})_0}{(sY_f - Y_{ox})_1 - (sY_f - Y_{ox})_0}, \tag{9}$$

the subscripts $(.)_1$ and $(.)_0$ refer to a point at the flow where the fuel mass fraction and oxidizer mass fraction are respectively maxims.

Mixture Fraction

Applying the normalization into the Eq. 8, the transport equation for the mixture fraction is obtained:

$$\frac{\partial \rho f}{\partial t} + \frac{\partial \rho f u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma_f \frac{\partial f}{\partial x_j}\right). \tag{10}$$

Flame Sheet Model ou Burke Schumann Model

It is a model for Difusion Flames (Nonpremixed flames)

- There is a single global irreversible reaction
- The reaction is infinitely fast, i.e.,$Da \rightarrow \infty$
- The reaction takes place where fuel and oxidizer are mixed at stoichiometric proportion
- There is no coexistence of fuel and oxidizer (mixed is burned!)

Flame Sheet Model ou Burke Schumann Model

Let's use, for illustration purpose, the global irreversible reaction for the oxidation of ethanol:

$$C_2H_5OH + 3,00\left(O_2 + 3,76N_2\right) \rightarrow 2,00CO_2 + 3,00H_2O + 11,28N_2. \tag{11}$$

The mass stoichiometric rate oxidizer/fuel, s, can be evaluated as

$$s = \frac{n_{O_2}\, Mw_{O_2}}{n_{C_2H_5OH}\, Mw_{C_2H_5OH}} = \frac{3,00 \times 32,00}{1,00 \times 46,00} = 2,09, \tag{12}$$

Flame Sheet Model ou Burke Schumann Model

- If the $f > f_{st}$ the mixture is composed fuel and inerts;
- If the $f < f_{st}$ the mixture is composed oxidizer and inerts;

According with this, Equation 9 reads:

$$f = \frac{(sY_f - Y_{ox}) - (-Y_{ox,0})}{(sY_{f,1}) - (-Y_{ox,0})} = \frac{sY_f - Y_{ox} + Y_{ox,0}}{sY_{f,1} + Y_{ox,0}}. \tag{13}$$

The stoichiometric mixture fraction, f_{st}, is then

$$f_{st} = \frac{Y_{ox,0}}{sY_{f,1} + Y_{ox,0}}. \tag{14}$$

Flame Sheet Model ou Burke Schumann Model

For the lean side $f < f_{st}$

$$f = \frac{-Y_{ox} + Y_{ox,0}}{sY_{f,1} + Y_{ox,0}}, \tag{15}$$

and for the rich side $f > f_{st}$

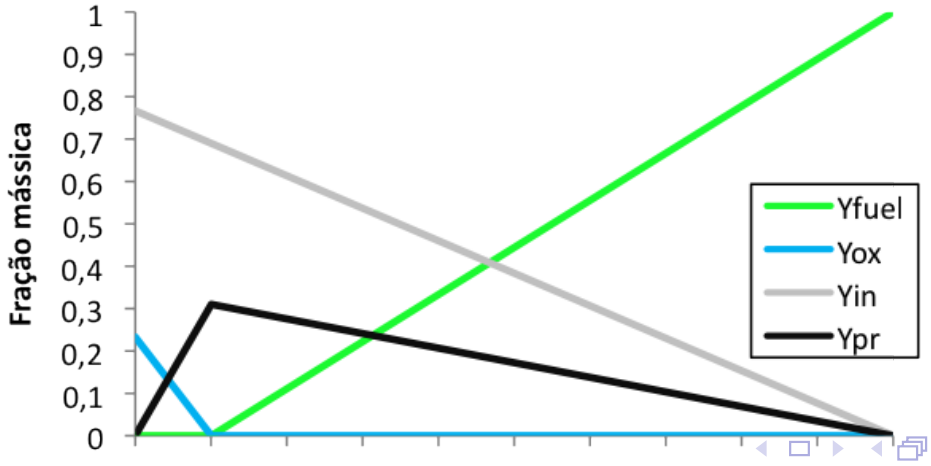
$$f = \frac{sY_f + Y_{ox,0}}{sY_{f,1} + Y_{ox,0}}. \tag{16}$$

Flame Sheet Model ou Burke Schumann Model

For a pure ethanol $(Y_{f_1} = 1,0)$ difusion flame in ar $(Y_{ox_0} = 0,233)$, one can evaluate the stoichiometric mixture fraction (14)as:

$$f_{st} = \frac{0,233}{2,09 * 0,233 + 0,233} = 0,323. \tag{17}$$

The mass fraction of fuel, oxidizer and products as fraction of the mixture fraction can be evaluated according to Eqs.15 and 16:



Flame Sheet Model ou Burke Schumann Model

The temperature and absolute enthalpy are related in the form:

$$T = \frac{h - \Sigma_k \left[Y_k \left(h_k^0 - c_{p,k} T_0 \right) \right]}{\Sigma_k Y_k c_{p,k}}, \tag{18}$$

Normalizing the absolute enthalpy with the maximum and minimum value in Eq. **??**, one has

$$h^* = \frac{h - h_{ox,0}}{h_{f,1} - h_{ox,0}}. \tag{19}$$

The transport equation for the normalized absolute enthalpy has the same structure as the Mixture Fraction Transport Equation,, so that

$$f = h^* = \frac{h - h_{ox,0}}{h_{f,1} - h_{ox,0}}. \tag{20}$$

Flame Sheet Model ou Burke Schumann Model

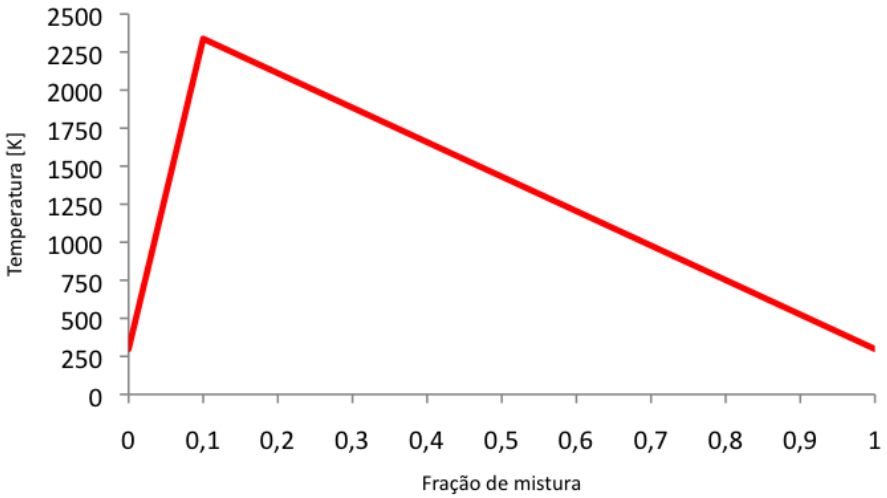


Figura: Temperatura da mistura em função da fração de mistura.

Flame Sheet Model ou Burke Schumann Model

The density of the mixture as a function of the mixture temperature by

$$\rho = \frac{p}{R_u T \sum_k \frac{Y_k}{Mw_k}}. \tag{21}$$

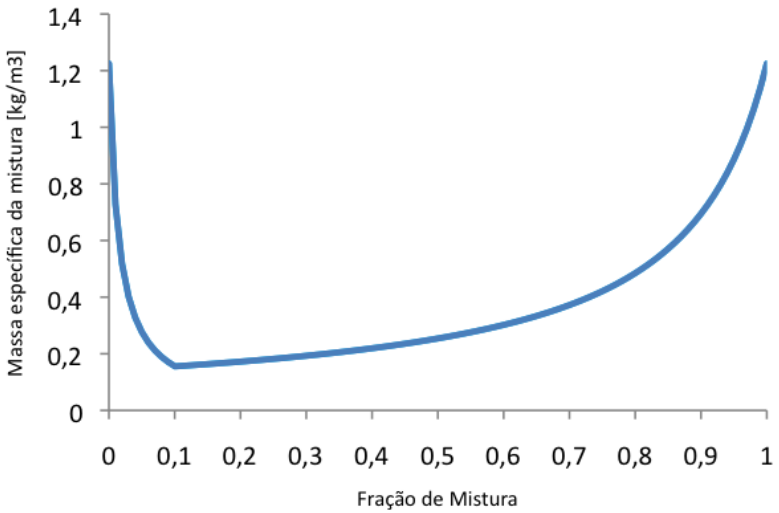


Figura: Density of the mixture as a function of the mixture fraction

Chemical Equilibrium Model - Free Gibbs Energy

- Model based on the 2nd Law of the Thermodynamic
- As the Flame Sheet Model, this model implies infinitely fast reaction, i.e.,$Da \rightarrow \infty$, (Mixed is burned!)
- It allows the coexistence of fuel and oxidizer

The 2nd Law of Thermodynamic says that for a thermodynamically isolated system the equilibrium state is that of the maximum entropia. For systems under constant pressure, is more convenient to use the Free Gibbs Energy, as follows:

$$G = H - TS. \tag{22}$$

The steady state that the reactive mixture will reach spontaneously in a system of constant mass, pressure and temperature must meet

$$(dG)_{P,T,m} \leq 0, \tag{23}$$

Chemical Equilibrium Model - Free Gibbs Energy

The Free Gibbs Energy for the gases mixture reads

$$G_{mist} = \sum N_i \bar{g}_{i,T} = \sum N_i \left[\bar{g}^o_{i,T} + R_u T ln \left(\frac{P_i}{P^o} \right) \right], \tag{24}$$

where N_i is the number of mols of the specie i in the mixture.

Chemical Equilibrium Model - Free Gibbs Energy

For a generic global reaction,

$$aA + bB + ... \Leftrightarrow +eE + fF + ..., \tag{25}$$

the mol changes is proportional to the stoichiometric coeficient:

$$\begin{aligned} dN_A &= -ka \\ dN_B &= -kb \\ &\vdots \quad \vdots \\ dN_E &= +ke \\ dN_F &= +kf. \end{aligned} \tag{26}$$

Chemical Equilibrium Model - Free Gibbs Energy

Doing the minization of the Free Gibbs Energy of the mixture (Eq. 24) one has:

$$-\underbrace{\left(e\bar{g}^o_{E,T} + f\bar{g}^o_{F,T} + \ldots - a\bar{g}^o_{A,T} - b\bar{g}^o_{B,T} - \ldots\right)}_{A} = \underbrace{R_u T ln \frac{\left(P_E/P^o\right)^e \left(P_F/P^o\right)^f .etc}{\left(P_A/P^o\right)^a \left(P_B/P^o\right)^b .etc}}_{B} \quad (27)$$

Chemical Equilibrium Model - Free Gibbs Energy

The term A is the variation of the Standard Gibbs Energy between reactants and products (ΔG_T^o):

$$\Delta G_T^o \equiv \left(e\bar{g}_{E,T}^o + f\bar{g}_{F,T}^o + \ldots - a\bar{g}_{A,T}^o - b\bar{g}_{B,T}^o - \ldots\right) \tag{28}$$

for $T = T_{ref}$

$$\Delta G_T^o = \left(e\bar{g}_{f,E}^o + f\bar{g}_{f,F}^o + \ldots - a\bar{g}_{f,A}^o - b\bar{g}_{f,B}^o - \ldots\right)_{T_{ref}=T} \tag{29}$$

Chemical Equilibrium Model - Free Gibbs Energy

The term B is defined as the Equilibrium Constant (Kp)

$$Kp \equiv \frac{\left(P_E/P^o\right)^e.\left(P_F/P^o\right)^f.etc.}{\left(P_A/P^o\right)^a.\left(P_B/P^o\right)^b.etc.} \tag{30}$$

So, for given pressure P and temperature T, the chemical equilibirum state is defined by:

$$\Delta G_T^o = -R_u T ln\left(Kp\right) \tag{31}$$

Chemical Equilibrium Model - Free Gibbs Energy

Para sistemas complexos com mais de uma reação global, pode-se escrever a Equação(31) para cada uma das reações. O lado esquerdo desta equação é somente função de propriedades termodinâmicas da mistura e dos coeficientes estequiométricos da reação global. Estes valores são facilmente encontrados na literatura de termodinâmica.

Chemical Equilibrium Model

Para exemplificar a aplicação do modelo de equilíbrio químico, considere a combustão de metano (CH_4) em ar, na proporção estequiométrica, pressão termodinâmica constante e sistema adiabático:

$$CH_4 + 2(O_2 + 3,76\ N_2) \Leftrightarrow b\ CO_2 + c\ CO + d\ H_2O + e\ H_2 + 2 * 3,76\ N_2. \tag{32}$$

Chemical Equilibrium Model

Deseja-se saber as pressões parciais da mistura, calculada com os coeficientes b, c, d e e e sua temperatura no equilíbrio químico. Assim o problema tem 5 incógnitas. O sistema de equações a ser resolvido é composto por:

- 1ª lei da termodinâmica para a mistura
  Aplica-se a 1ª lei da termodinâmica para um sistema adiabático e a pressão constante, na forma

$$H_{reagentes} = H_{produtos}, \tag{33}$$

  ou seja, a entalpia absoluta dos reagentes $H_{reagentes}$ é igual à entalpia absoluta dos produtos $H_{produtos}$.

Chemical Equilibrium Model

- Balanço atômico para os elementos C, H e O.
  É claro que se não fosse permitida a dissociação de CO_2, como no modelo de folha de chama, os coeficientes $b = 1$ e $d = 2$ seriam determinados diretamente do balanço atômico para os elementos C e H e o sistema estaria determinado.
  Considerando-se a dissociação, o balanço atômico para os elementos C, H e O fornece-se três equações para o sistema:

$$1 = b + c, \tag{34}$$

$$4 = 2d + 2e \tag{35}$$

e

$$4 = 2b + c + d \tag{36}$$

Chemical Equilibrium Model

- 2ª lei da termodinâmica, ou equilíbrio químico, na forma da Equação (31)
  A última equação vem da aplicação do equilíbrio químico à reação de dissociação de CO_2, conhecida como reação de deslocamento gás-água:

$$CO + H_2O \Leftrightarrow CO_2 + H_2. \tag{37}$$

Chemical Equilibrium Model

A equação do equilíbrio químico, Equação (31), para esta reação é:

$$Kp \equiv \frac{(P_{CO_2}/P^o).(P_{H_2}/P^o)}{(P_{CO}/P^o).(P_{H_2O}/P^o)} = \frac{(b/N_T).(e/N_T)}{(c/N_T).(d/N_T)} = \frac{be}{cd}, \tag{38}$$

em que N_T é o número total de mols da mistura. Kp, como já dito, é obtido de tabelas termodinâmicas em função da temperatura da mistura.

Chemical Equilibrium Model

Assim, resolve-se o sistema interativamente e são obtidas as pressões parciais das espécies e a temperatura.
É bastante comum utilizar-se a grandeza fração de mistura em conjunto com o modelo de equilíbrio químico. A fração de mistura é uma grandeza conservativa e portanto pode ser associada aos elementos químicos presentes na mistura. Assim pode-se relacionar a massa dos elementos C, H e O diretamente ao valor da fração de mistura. Com esta formulação pode-se obter a estrutura da chama laminar em função da fração de mistura como mostrado na figura a seguir.

Chemical Equilibrium Model

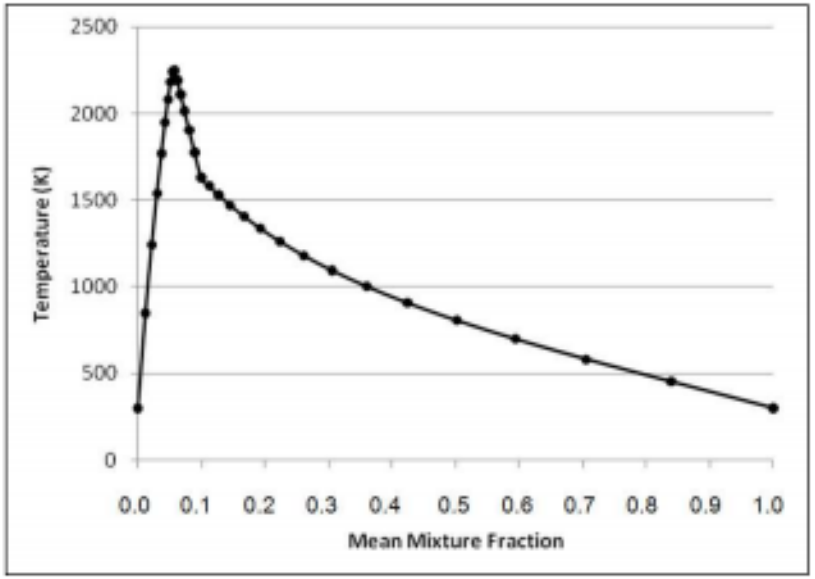


Figura: Evolução da temperatura com a fração de mistura usando o modelo de equilíbrio químico.

Flamelet Model

- Flamelet Model takes into account the time dimension
- It does not implies $Da \rightarrow \infty$
- For high Da, the rections take place on a thin layer attached to the $f = f_{st}$ surface. High gradients of mixture fraction in this region

Flamelet Model

A solução da equação de transporte da fração de mistura, com as devidas condições de contorno, possibilita a determinação do lugar geométrico dos pontos de fração de mistura estequiométrica, ou seja,

$$f(x_i, t) = f_{st} \tag{39}$$

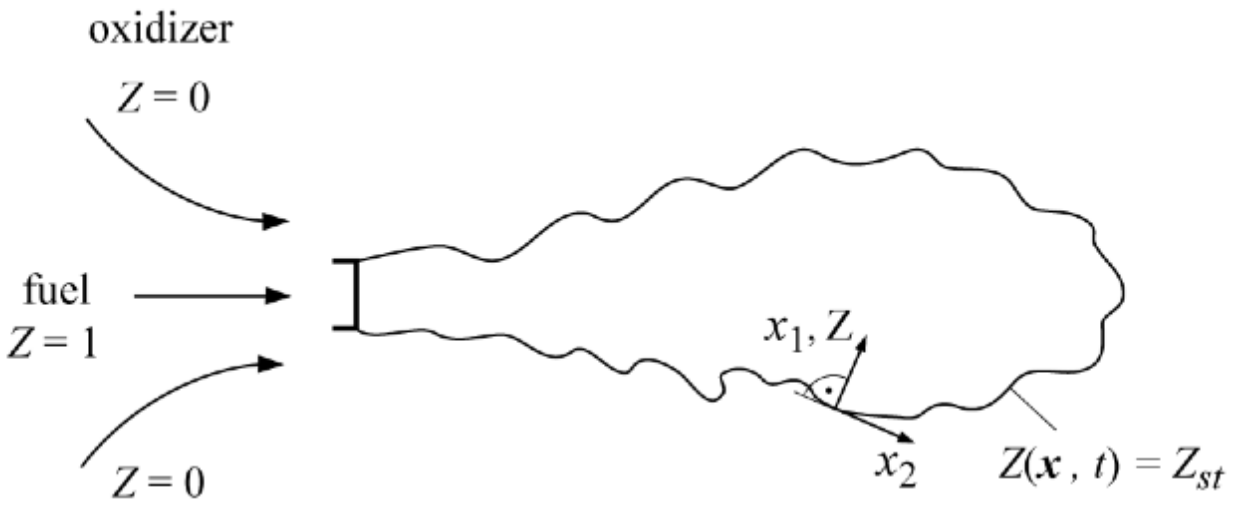


Figura: Flamelet - surface of stoichiometric mixture fraction (From ITV- Prof.

Flamelet

No modelo de Elemento de Chama Laminar faz-se a hipótese que as reações ocorrem numa fina camada na vizinhança da superficie definida pela Equação 39 e assim define-se um sistema de coordenadas ortogonais local $\zeta_1, \zeta_2, \zeta_3, t$ solidário com esta superficie de fração de mistura estequiométrica. Neste sistema de coordenadas local, a direção ζ_1 é normal à superficie $f = f_{st}$ e as direções ζ_2, ζ_3 são tangentes à mesma superfície. Para introduzir a fração de mistura no sistema de coordenadas, transforma-se a direção ζ_1 em f e o sistema de coordenadas torna-se $f, \zeta_2, \zeta_3, \tau$.

Flamelet

As regras da transformação do sistema de coordenadas ortogonais local são:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial f}{\partial t}\frac{\partial}{\partial f} \tag{41}$$

$$\frac{\partial}{\partial x_1} = \frac{\partial f}{\partial \zeta_1}\frac{\partial}{\partial f} \tag{42}$$

$$\frac{\partial}{\partial x_i} = \frac{\partial}{\partial \zeta_i} + \frac{\partial f}{\partial \zeta_i}\frac{\partial}{\partial f} \tag{43}$$

com $i = 2, 3$.

Flamelet

As regras de transformação são aplicadas à equação da temperatura (Equação 40). Adicionalmente, faz-se a aproximação de que a velocidade na direção ζ_1 é desprezível em relação às outras. Admite-se também que $\rho D \neq \rho(f)D(f)$. Chega-se, então à equação da temperatura

$$\rho\left(\frac{\partial T}{\partial \tau} + u_2\frac{\partial T}{\partial x_2} + u_2\frac{\partial T}{\partial x_2}\right) = \tag{44}$$

$$\rho D\left[\left(\sum_{i=1}^{3}\left(\frac{\partial f}{\partial \zeta_i}\right)^2\right)\frac{\partial^2 T}{\partial f^2} + 2\frac{\partial f}{\partial \zeta_2}\frac{\partial^2 T}{\partial f \partial \zeta_2} + 2\frac{\partial f}{\partial \zeta_3}\frac{\partial^2 T}{\partial f \partial \zeta_3} + \sum_{i=2}^{3}\frac{\partial^2 T}{\partial \zeta_k^2}\right] \tag{45}$$

$$-\frac{\partial(\rho D)}{\partial \zeta_2}\frac{\partial T}{\partial \zeta_2} - \frac{\partial(\rho D)}{\partial \zeta_3}\frac{\partial T}{\partial \zeta_3} - \frac{1}{c}\sum^{N} h_{f,i}^{o}\dot{\omega}_i + \frac{1}{c}\frac{\partial p}{\partial t}, \tag{46}$$

Flamelet

Fazendo-se a análise da ordem de grandeza das derivadas parciais, com a hipótese de que a espessura da camada de reação é pequena, conclui-se que o gradiente de temperatura normal à superfície de fração de mistura estequiometrica (Equação 39) é dominante. Assim,

$$\frac{\partial^2}{\partial f^2} >> \frac{\partial^2}{\partial \zeta_i^2} \tag{47}$$

com $i = 2, 3$. Com estas simplificações de ordem de grandeza, e negligenciando-se a variação temporal da pressão, reescreve-se a Equação 46 na forma

$$\left(\frac{\partial T}{\partial \tau} - \frac{\chi}{2} \frac{\partial^2 T}{\partial f^2} \right) = -\frac{1}{\rho c_p} \sum_{i=1}^{N} h_{f,i}^o \dot{\omega}_i \tag{48}$$

Flamelet

na qual χ é a Taxa de Dissipação Escalar

$$\chi \equiv 2D \sum_{i=1}^{3} \left(\frac{\partial f}{\partial \zeta_i} \right)^2 = 2D \left[\left(\frac{\partial f}{\partial \zeta_1} \right)^2 + \left(\frac{\partial f}{\partial \zeta_2} \right)^2 + \left(\frac{\partial f}{\partial \zeta_3} \right)^2 \right] \quad (49)$$

Flamelet

A dimensão da Taxa de Dissipação Escalar χ é s^{-1}. Assim, χ_{st} evidencia o tempo característico do processo de transporte difusivo na direção normal à superfície de fração de mistura estequiométrica. Este tempo concorre com o tempo característico das reações químicas do processo de combustão (lado direito da Equação (48)). Verifica-se, então, que no modelo de Elemento de Chama Laminar, o Número de Damköhler não é intrinsecamente infinito, como no caso dos modelo de folha de chama e equilíbrio químico.

Flamelet

Um caso limite interessante do modelo de Elemento de Chama Laminar é quando $\chi \rightarrow 0$, ou seja, o tempo característico para difusão da energia na chama é infinitamente maior que o tempo característico das reações químicas. Isto significa, veja a Equação 49, que os gradientes de temperatura tendem a zero e consequentemente a taxa de transferência de calor também. Assim, toda a energia das ligações químicas rompidas no processo de combustão é convertido em temperatura da mistura:

$$\left(\frac{\partial T}{\partial \tau}\right) = -\frac{1}{\rho c_p} \sum_{i=1}^{N} h_{f,i}^{o} \dot{\omega}_i. \tag{50}$$

Flamelet

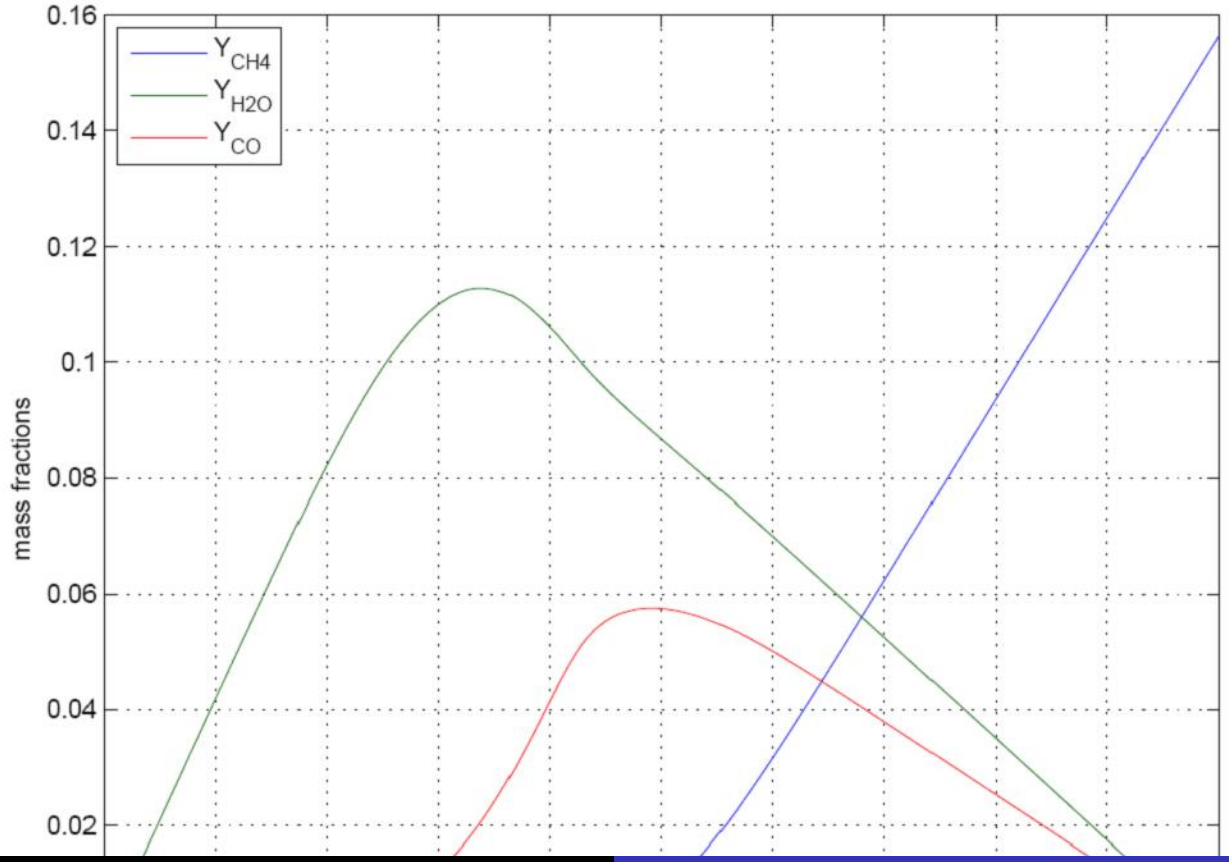
Da mesma forma como feito para a equação da energia e da temperatura, faz-se a transformação de coordenadas para a equação de transporte das espécies químicas (Equação 4) e tem-se

$$\left(\frac{\partial Y_k}{\partial \tau} - \frac{\chi}{2}\frac{\partial^2 Y_k}{\partial f^2}\right) = \frac{\dot{\omega}_k}{\rho} \tag{51}$$

Para o cálculo de uma chama com o modelo de elementos de chama laminar, deve-se usar as Equações (48) e (51), um modelo de cinética química adequado para o cálculo do termo de fonte $\dot{\omega}_k$ e um valor arbitrário de χ representativo.

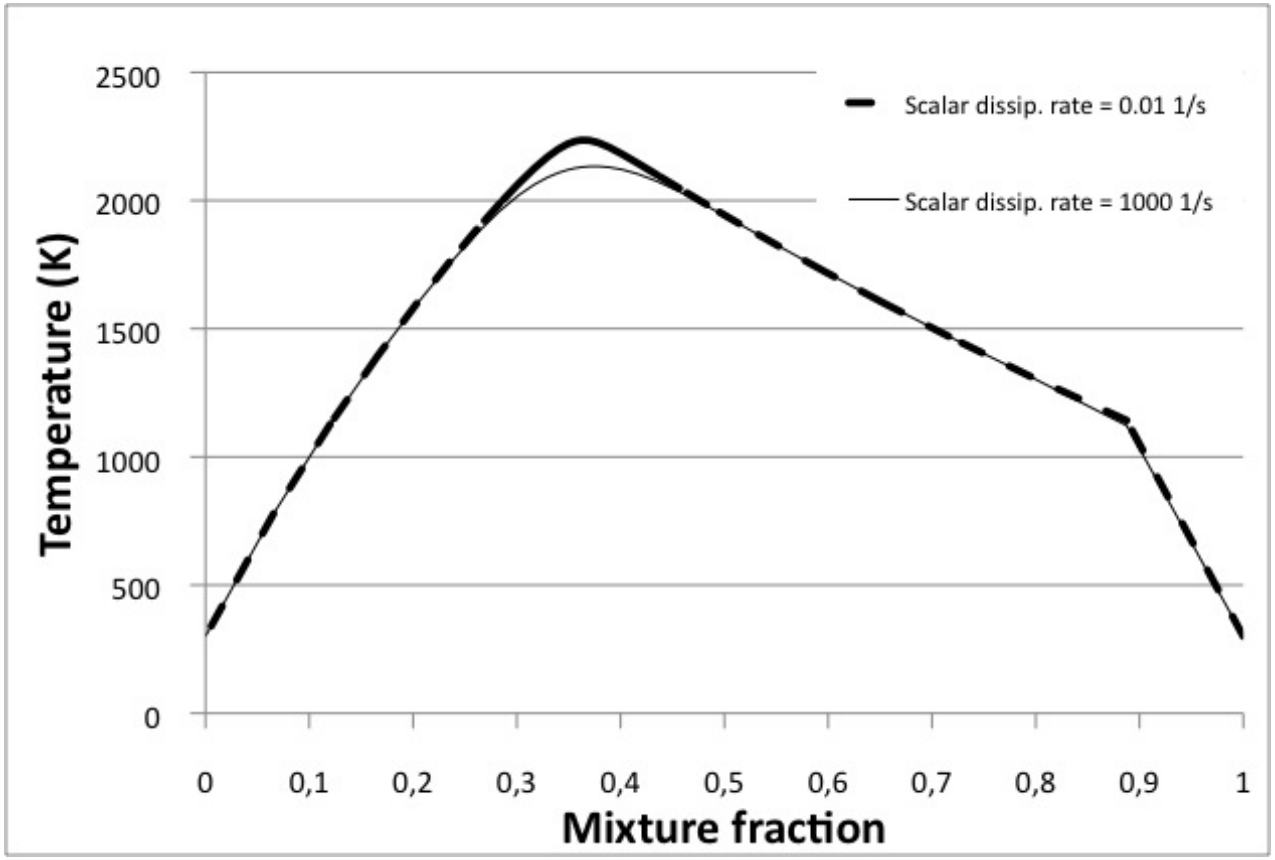
Flamelet - Results

A Figura 6 mostra a estrutura de uma chama laminar de ar com metano calculada desta forma.



Flamelet - Results

Influence of the scalar dissipation rate on the temperature



Laminar flame X Turbulent flame

- Laminar flame X Turbulent flame
- constant signal with respect to time X fluctuating
- comparison with experimental data (e.g. thermocouple measurements) and flamelet table
- influence of the fluctuating signal (e.g. temperature) on the non-linear chemical reactions equations (or radiation also)

Presume Probability Density Function

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

$$\bar{q} = \int_{-\infty}^{\infty} q(\psi)\, P(\psi)\, d\psi, \tag{52}$$

  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

$$\tilde{q} = \int_{-\infty}^{\infty} q(\psi)\,\tilde{P}(\psi)\,d\psi, \tag{53}$$

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

$$\tilde{P}(\psi) = \frac{\rho(\psi)}{\bar{\rho}} P(\psi). \tag{54}$$

Presume Probability Density Function

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

$$\tilde{P}(\psi) = \frac{f^{\alpha-1}(1-f)^{\beta-1}}{\int_0^1 f^{\alpha-1}(1-f)^{\beta-1}}, \; ou \; \frac{f^{\alpha-1}(1-f)^{\beta-1}\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\beta)} \tag{55}$$

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

$$\alpha = \tilde{f}\left[\frac{\tilde{f}\left(1-\tilde{f}\right)}{\widetilde{f''2}}\right], \tag{56}$$

$$\beta = \frac{\left(1-\tilde{f}\right)}{\tilde{f}}\alpha. \tag{57}$$

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:

$$\psi = \widetilde{\psi} + \psi'' = \frac{\overline{\rho\psi}}{\bar{\rho}} + \psi'', \tag{58}$$

$$\widetilde{\psi} = \frac{\overline{\rho\psi}}{\bar{\rho}}. \tag{59}$$

Favre decomposition

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

$$\frac{\partial \bar{\rho}\widetilde{Y_k}}{\partial t} + \frac{\partial \bar{\rho}\widetilde{Y_k}\widetilde{u_j}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_k \frac{\partial \widetilde{Y_k}}{\partial x_j}\right) + \widetilde{\dot{\omega}_k}, \tag{60}$$

and for the mixture fraction

$$\frac{\partial \bar{\rho}\widetilde{f}}{\partial t} + \frac{\partial \bar{\rho}\widetilde{f}\widetilde{u_j}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_t \frac{\partial \widetilde{f}}{\partial x_j}\right); \tag{61}$$

Favre decomposition

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

$$\frac{\partial \overline{\rho}\widetilde{f''^2}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u_i}\widetilde{f''^2}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_t \frac{\partial \widetilde{f''^2}}{\partial x_j}\right) = C_{g,1}\overline{\rho} D_{Eff}\left|\frac{\partial \widetilde{f}}{\partial x_i}\right|^2 C_{g,2}\overline{\rho}\frac{\varepsilon}{k}\widetilde{f''^2} \tag{62}$$

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

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t} + \frac{\partial \bar{\rho}\tilde{h}\widetilde{u_j}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_t}\frac{\partial \tilde{h}}{\partial x_j}\right), \tag{63}$$

Nonpremixed flame - D

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

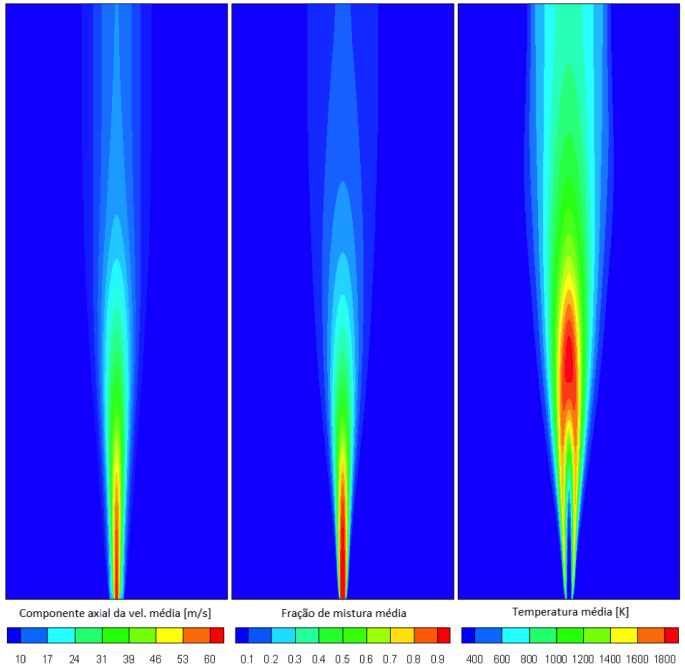
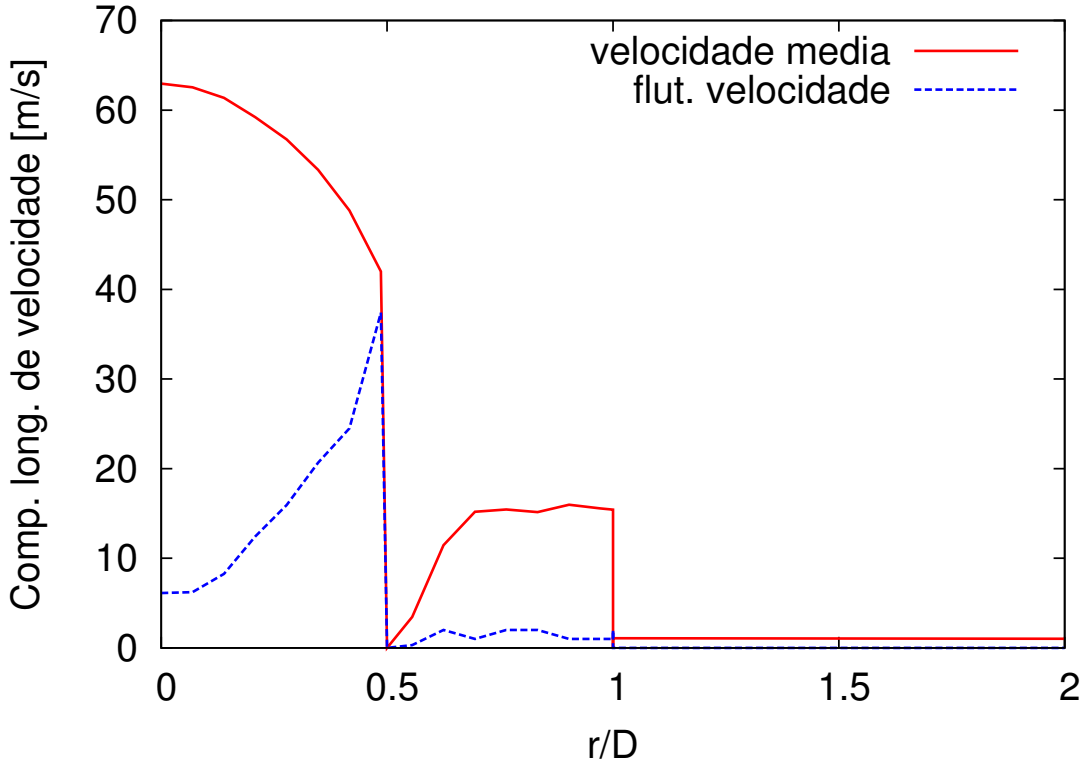


Figura: Campos de temperatura, fração de mistura e componente axial de velocidade da ”Simulação II”.

Nonpremixed flame - D

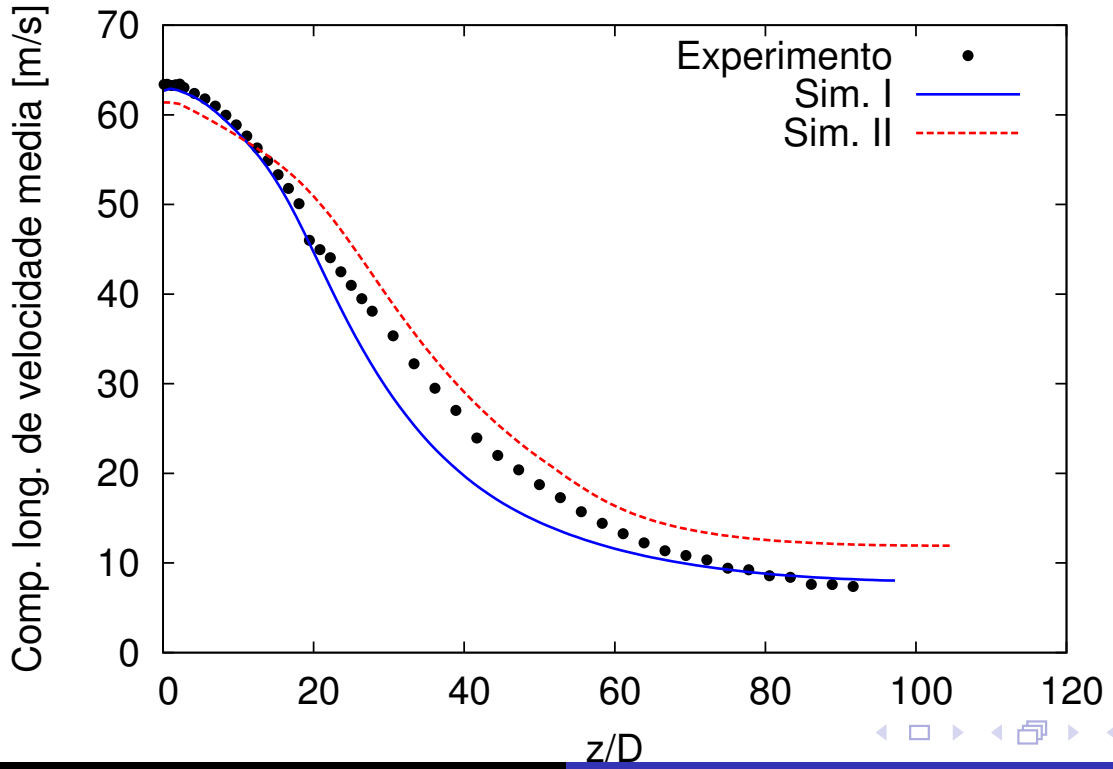
- Velocity boundary conditions



Results Nonpremixed flame - D

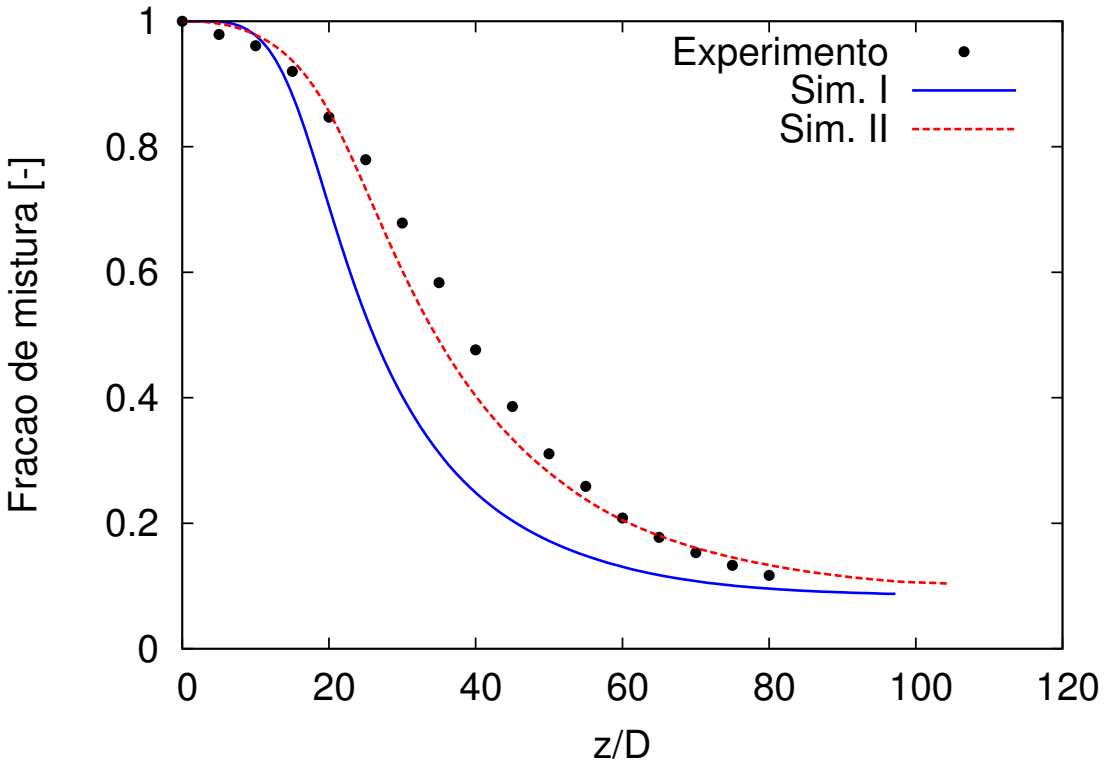
- Results with $k - \varepsilon$ RANS equations + Flame sheet Model

- Axial velocity at the center line



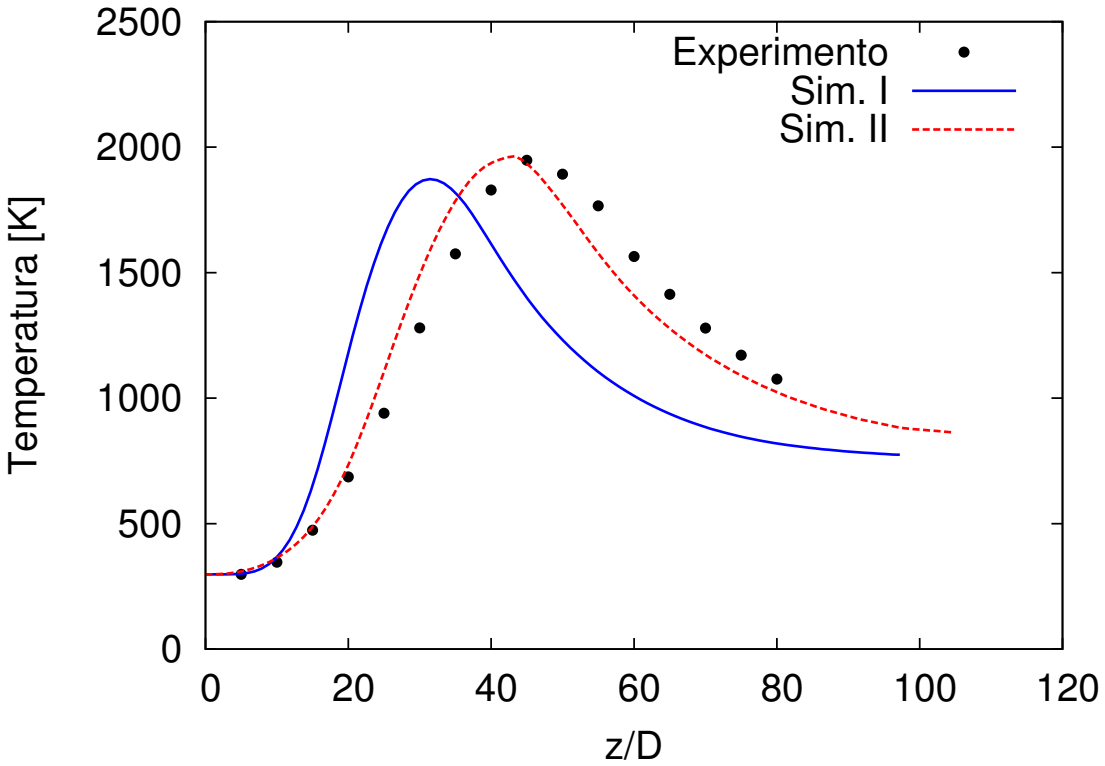
Results Nonpremixed flame - D

- Mixture fraction at the center line



Results Nonpremixed flame - D

- Temperature at the center line



Results Nonpremixed flame - D

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

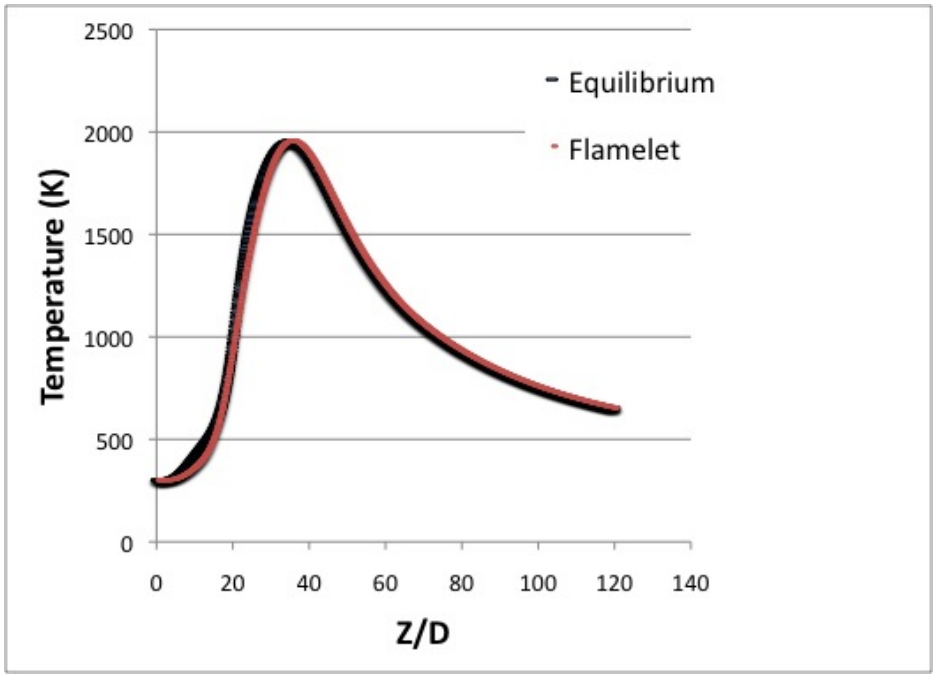


Figura: Flame D - Temperature at centreline - Equilibrium X Flamelet

Results Nonpremixed flame - D

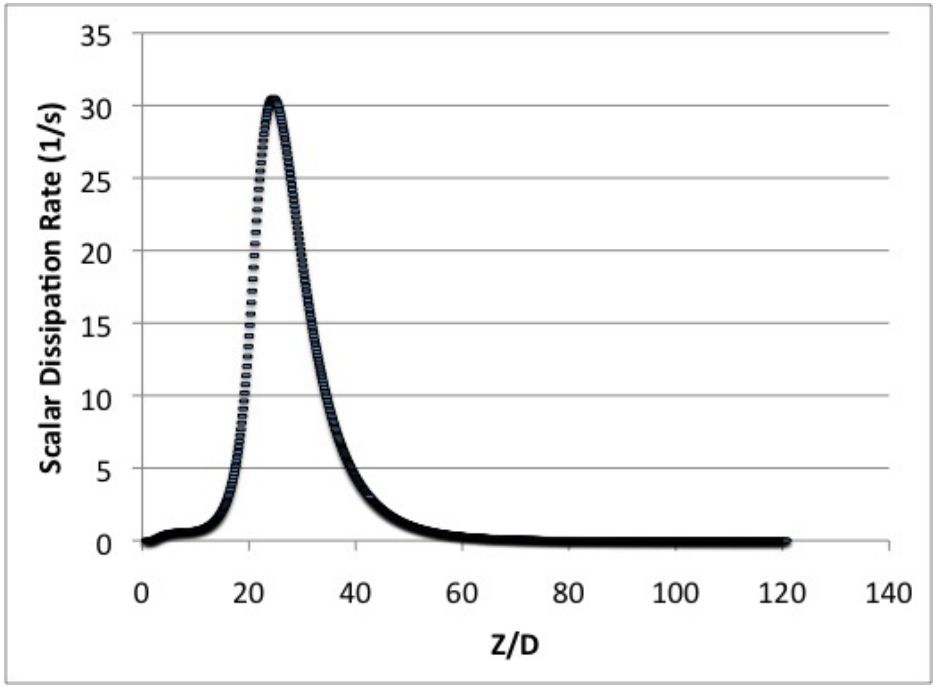


Figura: Averaged Scalar Dissipation Rate at the centreline

Results Nonpremixed flame - D LES - FGM

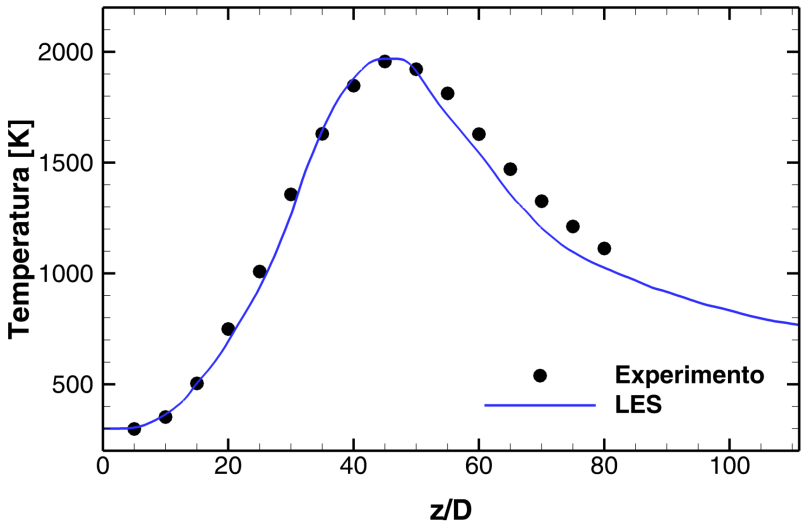


Figura: Flame D - Temperature at centreline LES-FGM

Summary

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