

SIMULATION OF COMBUSTION IN CYLINDRICAL CHAMBER

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Abstract. *The work presents the simulation of a combustion chamber using the Finite Volume based on Finite Elements using the software CFX 5.7. The numerical simulation of the process shows the importance of the combustion model when calculating the reaction rate in a combustion chamber. The work presents results using the “Eddy Dissipation Model” and “Finite Rate Chemistry Model”, being clear the sensibility of the model’s choice regarding the Damköler number. The case study treats a gas jet with expansion where there are regions with high and low flow timescales, showing a good opportunity to test a combined model. This model calculates reaction rates looking at different situations. When flow timescale is high comparing the reaction timescale, it uses the molecules collision, and when the flow timescale is low compared to reaction timescale, it uses the chemical kinetics of the reaction.*

Keywords: *Combustion, Thermal system, Natural gas, Cylindrical combustion chamber, Finite Volumes, CFX*

1. Introduction

The work shows the study of the combustion into a cylindrical chamber which is the most known geometry in use with furnaces for urban and industrial heating.

The calculus method presented in the paper for the combustion chamber is the Finite Volume method based in Finite Elements. It uses the commercial software CFX 5.7 for the simulation of the phenomena. This work intends to validate the model designed into the software comparing the case with experimental results and other simulation works, being capable to show the use of 3D non-structured grids to combustion phenomena and also parameters variation. The validation of the model and its physical interpretation for the reaction rate calculation are important for future works that intend to simulate complex conditions as turbines combustors, open combustors, pre-mixed and non pre-mixed flames, drying and incineration process burners.

There are mathematical models capable of simulate combustion processes of several fuels and several flow regimes. The calculation of the reaction rates of fuels and oxidizers is set by models based almost always in the Arrhenius law, being very complex to compute the coupled solution with the flow, species conservation, energy and reaction systems. Thanks to these reasons it’s adopted simplified mechanisms, with global reactions, to chemicals reactions rates (chemical species conservation). In Garretón and Simonin (1995) it was studied different models for the reaction rates, such as the coupling Eddy Breakup – Arrhenius model. The Eddy Breakup, that assume fast chemical reaction, considers that the time scale of chemical reaction rates due to mechanical mechanisms of the flow are faster compared to the time scale of mechanisms at the chemical species transport phenomena. The Arrhenius model determines the chemical reaction rates considering chocks at molecular scale. To the fast chemical reaction, the reactants collide, react and immediately form the products. In this situation the turbulent flows is the mainly driving force, and the mixing rate between the chemical species reactants at flow is proportional to the inverse of the relation between the turbulent kinetic energy and its dissipation, being a function of eddy dissipation scale (Kuo, 1996). For the coupling Eddy Breakup - Arrhenius model is used the smallest reaction rate calculated whit both models (CFX Inc., 2002). Nieckele et al. (2001) it was shown a good performance of this model, when make a comparison between your numerical results with the experimental data of Magel et al., (1996), for a cylindrical chamber burning natural gas and air for concentric jets.

da Silva et al. (2004) shows the performance, comparing with the same experimental case, of a numerical simulation using the called SCRS, which assumes fast chemical reaction and considers that the reactants and products do not exist together in the same control volume.

The major parameter for the choice of the model to be used in the reaction rate calculation is the Damköler number (Da); this number will tell the relation between the flow time scale and the chemical time scale. From this relation comes the decision looking if the flow is laminar, turbulent, with shear layers between fluid streams, with obstacles, vortex generators, etc, which model is a good option to use. For high Da is interesting to use models that take into account the flow mixing since the reaction time is small. For low Da , the models that determine the reactions rate is

hard dependent of chemical kinetic of the reactions. When calculating reactive mixing flows with high and low Damköler's zones is better to use mixed models.

2. Mathematical formulation

It's considered that the heat transfers has already happened reaching steady state. The heat transfer happens from the hot gases (products of the combustion processes) to the ambient; the objective of the work is to show the distribution of temperatures and concentrations. It's used the $k-\varepsilon$ model for modeling the turbulence through the turbulent viscosity μ_t , a property of the flow; But also it's tested the $k-\omega$ model. The radiative heat transfer is calculated through the DTRM - Discrete Transfer Radiation Model which solve for the intensity of radiation, I , along rays leaving from the boundaries. After integrate I over solid angle at discret points to find the incident radiation and the radiant heat flux and use homogeneity to extend the solution to the domain. Using the hypothesis of homogeneity to extend the solution to the whole dominium, it's considered gray gas with isotropic scattering of coefficient 0.5 (m^{-1}).

2.1. Phenomena equations

The equations to solve in the simulation of the combustion phenomena in steady state are mass conservation, momentum conservation, energy conservation and chemical species conservation, following:

2.1 Mass conservation

Adopting cylindrical coordinates and assuming axissymmetry, one obtains:

$$\frac{\partial}{\partial x}(\rho \bar{u}) + \frac{\partial}{\partial r}(\rho \bar{v}) + \frac{\rho \bar{v}}{r} = 0 \quad (1)$$

in which x and r are the axial and the radial coordinates, \bar{u} and \bar{v} are the average velocities in the respective directions, and ρ is the density. The bars over some terms indicate Reynolds Average.

2.2 Momentum equations in the axial (\bar{u}) and radial (\bar{v}) directions

$$\bar{u} \frac{\partial}{\partial x}(\rho \bar{u}) + \bar{v} \frac{\partial}{\partial r}(\rho \bar{u}) = -\frac{\partial p^*}{\partial x} + \bar{\nabla} \cdot [(\mu + \mu_t) \bar{\nabla} \bar{u}] + \frac{\partial}{\partial x} \left(\mu_t \frac{\partial \bar{u}}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu_t \frac{\partial \bar{v}}{\partial x} \right) \quad (2)$$

$$\bar{u} \frac{\partial}{\partial x}(\rho \bar{v}) + \bar{v} \frac{\partial}{\partial r}(\rho \bar{v}) = -\frac{\partial p^*}{\partial r} + \bar{\nabla} \cdot [(\mu + \mu_t) \bar{\nabla} \bar{v}] + \frac{\partial}{\partial x} \left(r \mu_t \frac{\partial \bar{u}}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu_t \frac{\partial \bar{v}}{\partial r} \right) - \frac{(\mu + \mu_t) \bar{v}}{r^2} \quad (3)$$

where μ is the dynamic viscosity, μ_t is turbulent viscosity, computed from the standard $k-\varepsilon$ model by $\mu_t = C_\mu \rho k^2 / \varepsilon$, $p^* = \bar{p} - (2/3)k$ represents the modified pressure, C_μ is an empirical turbulence model constant, \bar{p} is the average pressure, k and ε are the turbulent kinetic energy and its dissipation, respectively.

2.1.3. Energy conservation

For the energy transport due to the flow inside the chamber, neglecting the energy transport due to the diffusion of each species ($Le = 1$), one finds:

$$\bar{u} \frac{\partial}{\partial x}(\rho \bar{h}) + \bar{v} \frac{\partial}{\partial r}(\rho \bar{h}) = \bar{\nabla} \cdot \left[\left(\frac{\kappa}{c_p} + \frac{\mu_t}{Pr_t} \right) \bar{\nabla} \bar{h} \right] + \bar{S}_{rad} + \sum_{\alpha} \left[\frac{h_{\alpha}^0}{MM_{\alpha}} + \int_{\bar{T}_{ref,\alpha}}^{\bar{T}} c_{p,\alpha} dT \right] \bar{R}_{\alpha} \quad (4)$$

where \bar{h} is the average enthalpy of the mixture, c_p is the specific heat, defined as $c_p = \sum_{\alpha} \bar{f}_{\alpha} c_{p,\alpha}$, where $c_{p,\alpha}$ is the specific heat of the α -th chemical species, \bar{T} is the average temperature, κ is the thermal conductivity of the mixture, Pr_t is the turbulent Prandtl number, \bar{S}_{rad} is the source term due to the heat transfer by radiation, h_{α}^0 and $\bar{T}_{ref,\alpha}$ terms

are the enthalpy of formation and the reference temperature of the α -th chemical species. \overline{MM}_α is the molecular mass of the α -th chemical species.

2.1.4. Turbulence Models

Two equations turbulence models are largely used, they offer a commitment between numerical effort and computer accuracy. These models are much more sophisticated than the “zero-equation” model, in all models the velocity and the length scale are solved using separated transport equations, that’s why the two equations term. The models $k - \varepsilon$ and $k - \omega$ use the hypothesis of diffusion in the gradient to relate the Reynolds tensions to the average velocity and the turbulent viscosity. The turbulent viscosity is modeled with the product of the turbulent velocity and the length turbulent scale. In the two-equation models the turbulent velocity scale is estimated from the solution of these transport equations. The turbulent length is estimated of the two properties of the turbulent flow field, usually the turbulent kinetic energy and its dissipation. The dissipation rate is supplied by the solution of these transport equations. When observing trough time scales bigger than the real time scales of the turbulent fluctuations, it’s possible to say that the turbulent flow shows average characteristics, with an additional time variant component.

2.1.4.1. $k - \varepsilon$ model

Knetic energy conservation k and its dissipation ε are given by Eq. (5) and Eq. (6)

$$\bar{u} \frac{\partial}{\partial x} (\rho k) + \bar{v} \frac{\partial}{\partial r} (\rho k) = \bar{\nabla} \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \bar{\nabla} k \right] + P_k - \rho \varepsilon \quad (5)$$

$$\bar{u} \frac{\partial}{\partial x} (\rho \varepsilon) + \bar{v} \frac{\partial}{\partial r} (\rho \varepsilon) = \bar{\nabla} \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \bar{\nabla} \varepsilon \right] + C_{1,\varepsilon} \frac{\varepsilon}{k} P_k - C_{2,\varepsilon} \frac{\varepsilon^2}{k} \quad (6)$$

where $C_{1,\varepsilon}$ and $C_{2,\varepsilon}$ are constants defined experimentally and characteristics of the turbulence model, σ_k and σ_ε represent the respective Prandtl numbers of the kinetic energy and its dissipation, and P_k the production or dissipation of the kinetic turbulent energy, defined with Eq. (7).

$$P_k = \mu_t \left(2 \left(\frac{\partial \bar{u}}{\partial x} \right)^2 + \left(\frac{\partial \bar{u}}{\partial r} + \frac{\partial \bar{v}}{\partial x} \right)^2 + 2 \left(\frac{\partial \bar{v}}{\partial r} \right)^2 + 2 \left(\frac{\bar{v}}{r} \right)^2 \right) \quad (7)$$

2.1.4.2. $k - \omega$ model

One of the advantages of the formulation is the treatment near the wall for low Re numbers. The model does not involve complex functions of damping necessities into the $k - \varepsilon$ model. The model $k - \omega$ assume that the turbulent viscosity is related to the kinetic turbulent energy by Eq. (8).

$$\mu_t = \rho \frac{k}{\omega} \quad (8)$$

The model solve two transport equations, one for kinetic energy, k and one for the turbulent frequency, ω . The stress tensor is calculated by the concept of turbulent viscosity, Wilcox (2000). The kinetic energy conservation equation is given by Eq. (9)

$$\bar{u} \frac{\partial}{\partial x} (\rho k) + \bar{v} \frac{\partial}{\partial r} (\rho k) = \bar{\nabla} \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \bar{\nabla} k \right] + P_k - \beta' \rho k \omega \quad (9)$$

In addition to the independent variables, density, velocity vector, there are the quantities that come from the solution of the Navier-Stokes equations. P_k is the production of the turbulence rate, which is calculated for Eq. (7). The constants of the models are $\beta' = 0.09$, $\alpha = 5/9$, $\beta = 0.075$, $\sigma_k = 2$, $\sigma_\omega = 2$.

To avoid kinetic energy increase in the stagnation regions, a limiter (Eq. (10)) to the production term is introduced into the equations.

$$\tilde{P}_k = \min(P_k, c_{\text{lim}} \mathcal{E}) \quad (10)$$

with $c_{\text{lim}} \mathcal{E} = 10$.

2.1.5. Chemical species conservation

A conservation equation is required for all the components presents at the chemical reaction, except for the nitrogen. In this way, assuming a Lewis number of 1.0, one obtains the following conservation equation of the α -th chemical species, Eq.(11):

$$\bar{u} \frac{\partial}{\partial x} (\rho \bar{f}_\alpha) + \bar{v} \frac{\partial}{\partial r} (\rho \bar{f}_\alpha) = \bar{\nabla} \cdot \left[\left(\rho D + \frac{\mu_t}{Sc_i} \right) \bar{\nabla} \bar{f}_\alpha \right] + \bar{R}_\alpha \quad (11)$$

where D is the mass diffusivity, Sc_i is the Schmidt number, \bar{f}_α is the average mass fraction of the α -th chemical species of the mixture, and \bar{R}_α is the average volumetric rate of the formation or destruction of the α -th chemical species. This term is computed as the summation of all volumetric rates of formation or destruction in all chemical reactions k in which α is present, $\bar{R}_{\alpha,k}$. The source term is directly related to the reaction rate R_k , Eq. (12).

$$\bar{R}_\alpha = \overline{MM}_\alpha \sum_{k=1}^K (\eta_{\alpha,k}^{\leftarrow} - \eta_{\alpha,k}^{\rightarrow}) \bar{R}_{\alpha,k} \quad (12)$$

where $\eta_{\alpha,k}^{\leftarrow}$ and $\eta_{\alpha,k}^{\rightarrow}$ are the backward and the forward stoichiometric coefficient of the α -th chemical species that are present in the k -reactions.

2.1.6. Reaction rate models

The finite rate chemistry model is based on the Arrhenius law, where the average reaction rate is calculated by the Eq. (13)

$$\bar{R}_{\alpha,k} = \left(A_k \bar{T}^{\beta_k} e^{\left(\frac{-E_k}{RT} \right)} \prod_{\alpha=A,B,\dots}^{N_c} [\alpha]^{\gamma_{\alpha,k}^{\leftarrow}} - A_k \bar{T}^{\beta_k} e^{\left(\frac{-E_k}{RT} \right)} \prod_{\alpha=A,B,\dots}^{N_c} [\alpha]^{\gamma_{\alpha,k}^{\rightarrow}} \right) \quad (13)$$

where $\bar{R}_{\alpha,k}$ is the progress rate of the reaction k of the α -th chemical species, E_k is the activation energy, β is the dimensionless exponent of the temperature, and A_k is the pre-exponential factor that follow dimensions consistent with the unities of $R_{\alpha,k}$, $\gamma_{\alpha,k}$ is the exponent of the α -th chemical species into the reaction k and $[\alpha]$ is the molar concentration of the component α , where the subscript of $\gamma_{\alpha,k}$ identifies the direction of the reaction (\leftarrow) reactants-products and (\rightarrow) products-reactants.

The Eddy Breakup model is based in the concept that the chemical reaction is fast compared to the chemical kinetic. When the reactants mix in the molecular scale they immediately form products. In turbulent flows this characteristic time is determined by the properties of the turbulent structures (eddies). The mixing time between the components of the flow is proportional to the relation between kinetic energy k and the kinetic energy dissipation \mathcal{E} , Wilcox (2002). As a result the reaction rate is proportional to the inverse of this relation, Eq. (14) and Eq. (15).

$$\bar{R}_{\alpha,k} = A \frac{\mathcal{E}}{k} \min \left(\frac{[\alpha]}{\eta_{\alpha,k}^{\leftarrow}} \right) \quad (14)$$

$$\overline{R_{\alpha,k}} = AB \frac{\varepsilon}{k} \left(\frac{\sum_p [\alpha] \overline{MM_\alpha}}{\sum_p \eta_{\alpha,k} \overline{MM_\alpha}} \right) \quad (15)$$

Where in the equation, A and B are dimensionless empirical coefficients. In the Eddy-Breakup model (EBU) it's chosen the smallest reaction rate calculated. Equation (15) the limited rate of the products and it's not used in multiple steps reactions. It's widely employed in combustion simulation a model coupling the reaction rate calculation by the Arrhenius and the EBU model. However, in agreement with past works and validations, the simplified models achieved good representation of the physical phenomena. For modeling the chemical reaction in the present problem it's used the results of two reactions, Eq. (16) and Eq. (17).



The parameters used into the reactions are given by Tab. 1.

Table 1 – Adopted parameters for the reaction rate calculation.

Reaction	A_k	E_k	β_k	$\gamma_{CH_4,k}$	$\gamma_{O_2,k}$	$\gamma_{CO_2,k}$	$\gamma_{H_2O,k}^m$	$\gamma_{CO,k}$
1	$1.5 \left(\frac{1}{s} \right)$	$125400 \left(\frac{J}{mol} \right)$	0	-0.3	1.3	1	2	-
2	$10^{14.5} \left(\frac{1}{mol^{0.75} m^{4.5} s} \right)$	$167200 \left(\frac{J}{mol} \right)$	0	-	0.25	1	-	1

The dimensions of the pre-exponential factor should agree to get $\overline{R_{\alpha,k}}$ in $\left(\frac{mol}{s} \right)$ and the orders of the reaction γ give the result of the difference between A_k of the two reactions. For the value of the dimensionless empirical coefficients A and B of the EBU it is used the values 4 and 0.5, (Fluent Inc., 1997).

3. Problem presentation

3.1. Chamber geometry

Figure 1 shows the case studied is a cylindrical chamber with fuel injection, CH_4 (methane), and oxidizer, atmospheric air (22% O_2 , 78% N_2), in the form of coaxial jets in the center of one of the extremes of the chamber. The chamber dimensions agree with Garréton and Simonin (1995), da Silva et al. (2004), Magel et al. (1996) and Nieckele et al. (2001).

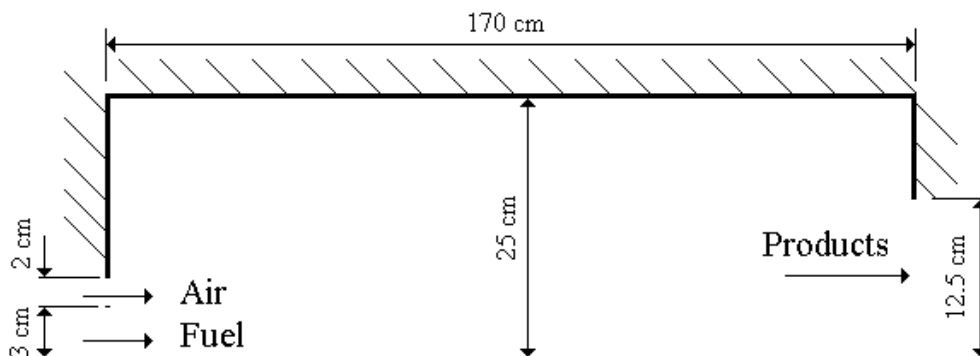


Figure 1. Combustion chamber geometry

The conditions for the oxidizer injection are 36.29 m/s, in the temperature of 323.15 K and the fuel with a velocity of 6.71 m/s with the temperature of 313.15 K. The turbulence intensity is given by the oxidizer with 6% value with turbulent length of 0.04 m, for the fuel the turbulent intensity is 1% and the turbulent length is 0.03 m. With these conditions and for atmospheric air with density 1.02 kg/m³ and methane 0.649 kg/m³, the chamber develops approximately 400 kW of power. The mass flows are 0.0125 kg/s and 0.186 kg/s for the air, in agreement with Garréton e Simonin (1995). The wall boundary condition is prescribed temperature, 393 K.

The study case is a god case because it's the geometry employed by almost all burners in the industry. It's also possible to obtain information for bigger systems as drying furnaces, rotatory dryers, incinerators, steam generators.

3.2 Domain discretisation

The domain is divided in tetrahedral volumes, in a 1 rad section, this is done for validation of the model with others works that use the same revolution, but with 2D approximations in structured grids. The grid in this paper is formed by 30 divisions in the radial direction, 60 in the axial direction and in the revolution it's developed a grid independence test to define the number to be used in the work. As a result of the grid independence test it was achieved the minimum element number of 53280, with 30 elements in the radial direction, 60 in the axial direction and 6 in the revolution. The grid with the same parameters, except to 4 elements in the revolution, a total of 35520, present good results only with very well defined initial value field. The refined mesh, 6 elements in the revolution does not show results that can justify the bigger computational effort, summing 80896 elements with a refinement near the wall of 25 mm of thickness and 4 elements in this layer.

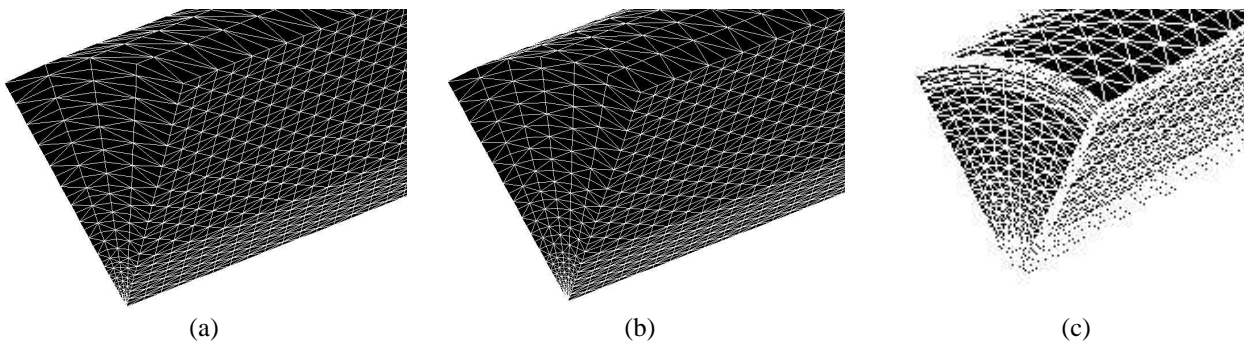


Figure 2. Meshes tested a) 4 elements in the revolution, b) 6 elements in the revolution and c) 6 elements plus refinement.

4. Results

To validate the results in the simulations with unstructured tetrahedral mesh, with the combustion models used and $k - \epsilon$ turbulence model; It's necessary to compare similar cases developed in the bibliography. The temperature field and temperature profiles in the chamber are used as parameter comparing with data from Nieckele et al. (2001), Garréton and Simonin (1995) e da Silva et al. (2004). The analysis of the data from Nieckele et al. (2001) shows a difference between the temperature fields in the chamber, Fig. 3.

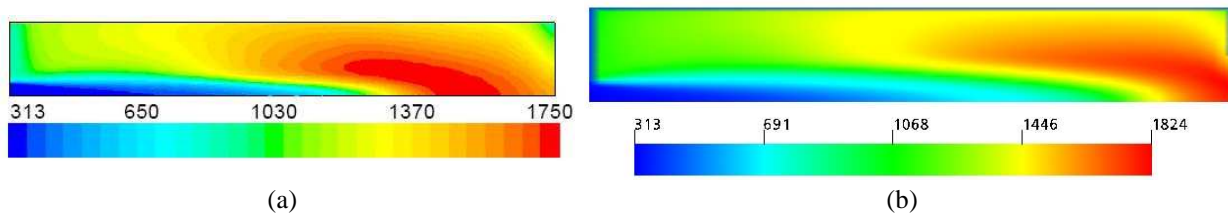


Figure 3. Temperature field a) Nieckele et al. (2001) and b) Present work.

Observing the two results it's possible to affirm that there's a small difference near the chamber wall and the temperatures are higher in the present work than Nieckele et al. (2001), showing higher values near the outlet.

It's also used to compare the experimental results of Garréton and Simonin (1995) and Magel et al. (1996), in the length 0.31 m and 0.91 m, for the temperature distribution along to the radial direction. Figure 4, shows results with wall boundary condition in the temperature of 393 K, according to the experiment of Garréton e Simonin (1995). Goods results are presented between the present work and the other results presents in this figure.

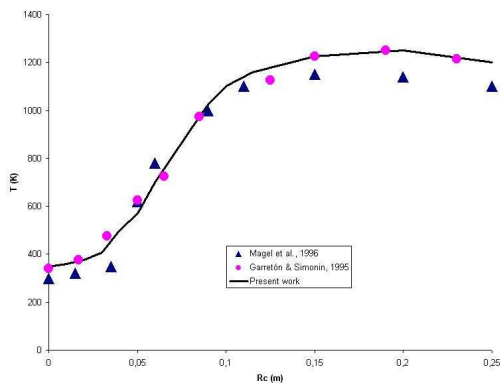


Figure 4. Temperature profile at the length 0.31 m.

Figure 5 shows temperature profile along the radius at 0.91 m from the entrance. One can observe that the gases temperature distribution presents a good agreement with the results obtained by Garréton and Simonin (1995), and by Magel et al. (1996).

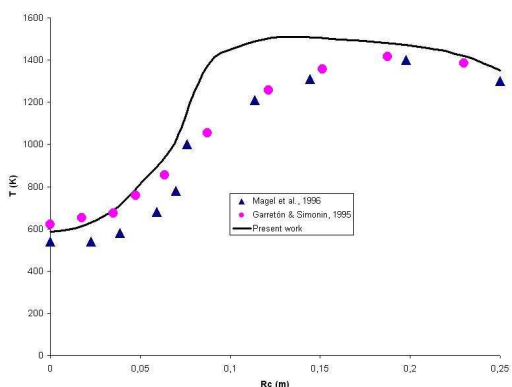


Figure 5 – Temperature profile for length 0.91 (m).

Two turbulence models are used, for a performance test when the chamber has an adiabatic wall. There is difference in the carbon monoxide concentration field between the simulations with using $k - \epsilon$ and $k - \omega$ turbulence model, Fig. 6. One can see that there are differences between the results of the Figs. 6-a and 6-b, this difference is due to the different way the models calculate the turbulent viscosity, which will influence directly the generation of turbulence in the flow. With higher turbulence, there will be higher reaction rate. However, the range of the value of monoxide of carbon presented is practically the same

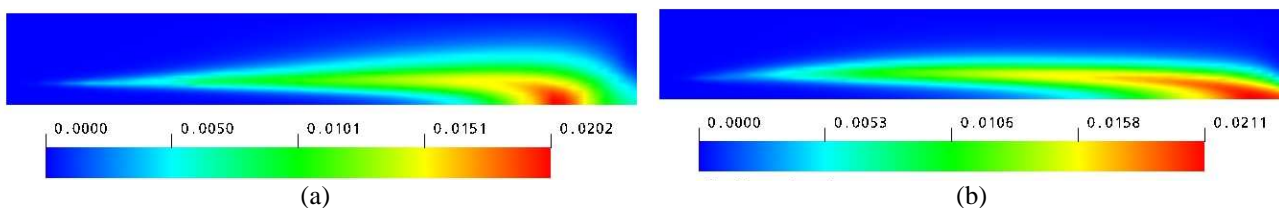


Figure 6 – CO mass fraction in the chamber: (a) $k - \epsilon$; (b) $k - \omega$.

Figure 7 shows temperature fields for the two models, first one using $k - \epsilon$ and the second one using $k - \omega$ turbulence model. The same characteristics are presented between the results. Here a little difference is too presented to the higher temperature arrived to the gases, for the same reason above mentioned.

For example of reaction rate model, it's presented the result of the same chamber when it's not well solved the flow region of low Da ($Da \ll 1$), Fig.8, in others words calculating the reaction rate mostly as a result of the components mixing, and not to the chemical kinetics. da Silva et al. (2004) do something similar to it using the SCRS model. The difference presented between the results, mainly close to the walls, occurs because in da Silva et al., (2004) was considered that the chamber had isolated walls.

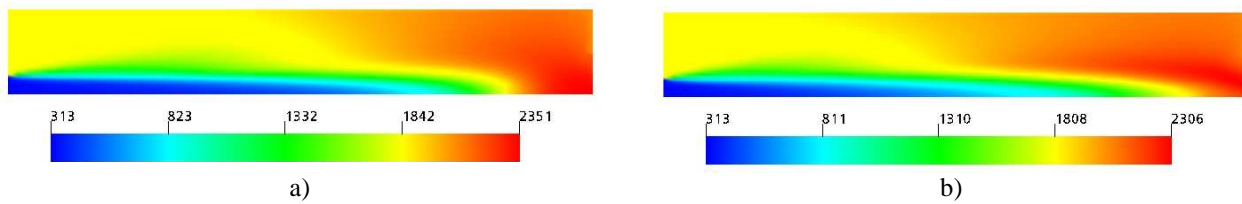


Figure 7 – Temperature (K) field in the chamber: (a) $k - \epsilon$; (b) $k - \omega$.

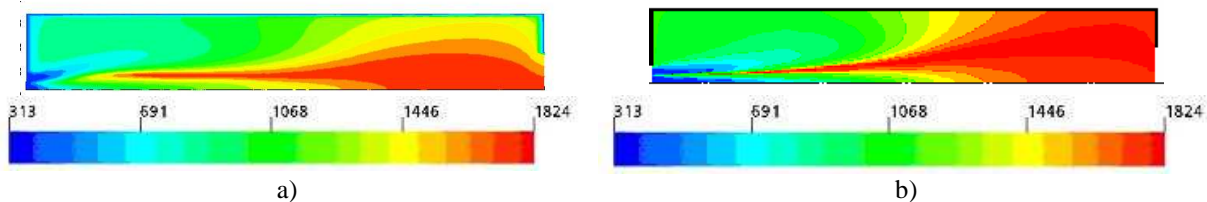


Figure 8. Temperature fields for: (a) EBU - present work; (b) SCRS - da Silva et al.(2004).

The important analysis is not the quantitative values but the reaction visualization only in the streams shear layer and the high temperature zone. In the central jet there's low mixing and also the temperature is smaller than the zone near the end of the chamber.

5. Conclusions

Even with small difference in the temperature field it's possible to observe that the reaction rate model is not well set to simulate the case, the main reason of it is that the reaction rate parameters were not changed as much as they could be thanks to numerical convergence problems. The model shows good performance in the beginning of the chamber, but at the end of the chamber, the model shows higher temperatures than the experimental case. A good step to continue the work is to show reaction parameters variation reaching numerical convergence and good physical results.

The two turbulence models used showed difference in the reaction products and temperature field for the adiabatic case, this difference is due to the different way the models calculate the turbulent viscosity, which will influence directly the generation of turbulence in the flow. With higher turbulence, there will be higher reaction rate.

A good reaction rate choice and parameters definition can avoid wrong reaction simulations as shown with the EBU and SCRS reaction rate models, which don't show good results for this chamber.

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7. Responsibility notice

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