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3D ANALYSIS OF TURBULENT NON-PREMIXED COMBUSTION OF NATURAL GAS IN A HORIZONTAL CYLINDRICAL CHAMBER

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Abstract. *This work presents a tridimensional numerical simulation of the non-premixed combustion of natural gas in atmospheric air inside an axisymmetric cylindrical chamber, aimed at verifying the effect of buoyancy on the fluid flow, temperature and chemical species concentration fields. The simulation is based on the solution of mass, energy, momentum and chemical species conservation equations. Thermal radiation exchanges in the combustion chamber are computed through the Discrete Transfer Radiation Model (DTRM), and the gas absorption coefficient dependence on the wavelength is predicted by weighted sum of gray gases models. The turbulence is modeled by the standard* $k-\varepsilon$ *model, and the chemical reactions by a two-step reaction mechanism along with the combined Eddy-Break-Up - Arrhenius model. The finite volume method is employed to treat the differential equations by using the commercial software Ansys CFX in the simulations. The solution of the governing equations allows the determination of the region where combustion occurs, chemical species profiles, velocity fields and heat transfer rate by convection and radiation. For the considered system, results indicate that buoyancy has a small influence on the combustion processes and provided a minor deviation in relation to the case when the geometry was treated as axisymmetric for solution to this problem, as reported by Magel et al. (1996), Nieckele et al. (2001) and Silva et al. (2007). Also, the results obtained with these 3D simulations were closer to the experimental data (Garréton and Simonin (1994)) than the classical 2D model.*

Keywords*: Turbulent diffusion flames, Buoyancy, Eddy-Break-Up – Arrhenius model, Radiation heat transfer, WSGG model.*

1. INTRODUCTION

An efficient operation of combustion chambers depends on the knowledge of the oxidation reactions and heat transfer between the combustion products and the chamber walls, which requires a detailed analysis of the governing mechanisms, such as chemical kinetics, fluid flow and heat transfer. On the other hand, its modeling is a difficult task due to the highly complex interdependence between the involved phenomena. In addition, the radiative heat transfer, together with the complex dependence of the absorption coefficient with the wavenumber and both temperature and concentrations fields, makes the solution of the Radiative Transfer Equation (RTE) computationally expensive or even impossible without a model to solve the spectral problem. In the last years, many researchers have been developed and applied different models to predict the combustion process in combustion chambers, but only a few are able to account the process in its entirety. A review of the most commonly combustion modeling, used mainly in commercial software, was presented in Eaton et al. (1999). The models are generally based on the fundamental conservation equations of mass, energy, chemical species and momentum, while the problem closure is achieved by turbulence models such as the $k-\varepsilon$ (Launder and Spalding, 1972; Launder and Sharma, 1974), combustion models like Arrhenius (Kuo, 1996; Fluent, 1997), Magnussen - EBU - "Eddy-Break-Up" (Magnussen and Hjertager, 1976), and radiative transfer models based on the radiative transfer equation (Özisik, 1985; Carvalho et al., 1991). Appling this kind of modeling in methane diffusion flames, many authors can be cited: Magel et al. (1996), Nieckele et al. (2001), Miroslav et al. (2001), Zhou et al. (2002), Zhou et al. (2003), Guo et al. (2003), Yang and Blasiak (2004), Borjini et al (2007), Silva et al. (2007) and Centeno et al. (2013). Similarly, but taking into account another emphases, some investigations are focused on modeling of detailed chemical kinetics using mixing reactors, without great efforts in solving the fluid flow and heat transfer. A good example of work in this category is the investigation of Fairweather and Woolley (2004), who employed the first-order conditional moment closure (CMC) model to simulate the oxidation of methane in turbulent, non-premixed flames, using the finite volumes discretization scheme, while the chemical reactions were tackled with two chemical kinetics schemes from the CHEMKIN library: the GRI-Mech 2.11 with 279 reactions and 49 species; and the GRI-Mech 3.0 with 325 reactions and 53 species.

Looking to heat transfer by radiation, much effort has also been devoted. By the way, as a simplification, the Radiative Transfer Equation (RTE) is frequently solved with the gray gas (GG) model, where the dependence of the absorption coefficient over the wavenumber is neglected. In order to provide better results, global and spectral models

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are commonly used. Among the global models, the weighted-sum-of-gray-gases (WSGG), developed by Hottel and Sarofim (1967) is a method that is still widely used nowadays, especially in global simulation of combustion processes in which the RTE is solved together with fluid flow, chemical kinetics and energy equation. In the WSGG model the entire spectrum is represented by a few bands having uniform absorption coefficients, where each band corresponding to a gray gas. The weighting coefficients account for the contribution of each gray gas, and correspond to the fractions of the blackbody energy in the spectrum region where the gray gases are located. In practice, those coefficients are obtained from fitting experimental data, such as those presented in Smith et al. (1982) and Smith et al. (1987). In a recent study, Demarco et al. (2011) assessed several radiative models (narrow band, wide band, gray and global) and stated that the non-gray formulation of the WSGG is also very efficient from a computational point of view and yields considerably improved predictions, but can lead to significant discrepancies in high soot loadings. Simplified radiative property models, such as the WSGG (Bressloff et al. (1996); Pierce and Moss (2007)) or gray models (Wang et al. (1999); Wen and Huang (2000)), are often used in computational fluid dynamics (CFD) to simulate combustion problems. The main reason is that implementing more sophisticated models may become extremely time consuming when fluid flow/combustion/radiative heat transfer are coupled. Several researchers have studied new WSGG correlations and coefficients for application in combustion systems, among which it is possible to mention Galarça et al. (2008), Krishnamoorthy (2010), Johansson et al. (2011) and, most recently Dorigon et al. (2013) and Kangwanpongpan et al. (2012). As application of this approach, Bidi et al. (2008) employed the DOM (Discrete Ordinate Method) to solve RTE equation and the WSGG model to compute non-gray radiation effect of combustion gases in a cylindrical chamber, with the purpose of studying the radiation effect in the flame structure. The results indicated that the radiation can affect the temperature field and the species concentrations, and the numerical results including radiation were closer to the experimental data than the case in which radiation was neglected. Predictions of the radiative heat source with different gas models was analyzed in Mossi et al. (2010), where the authors simulated a laminar methane-air diffusion flame solving conservation equations (mass, momentum, species, soot, energy) through a finite volume code. In this work, the RTE was solved with DOM, and the authors compared the radiative effects obtained by a simple gray-gas model and the SLW model. Guedri et al. (2011) investigated the thermal radiation transfer effects on a fire scenario using the narrow-band based WSGG model. In Yadav et al. (2013) the combustion processes of turbulent non-premixed pilot stabilized flames (Sandia Flame D and Delft Flame III) were studied including radiative heat transfer by means of the WSGG model. Crnomarkovic et al. (2013) compared the numerical results obtained when the GG and the WSGG models were applied to model the radiative properties of the gas phase inside a lignite fired furnace.

This work presents a 3D numerical analysis of turbulent, non-premixed combustion of methane in air in a horizontal cylindrical chamber. For validation of the proposed solution, the similar case described by Garréton and Simonin (1994) was studied. The main objective of this investigation is to verify the effect of buoyancy on the combustion process. The finite volume method and the commercial software Ansys CFX was used for the solution of the conservation equations of mass, momentum, energy and the main chemical species involved in the combustion process. The chemical kinetics were described by two global steps of chemical reactions. The combined Eddy-Break-Up – Arrhenius (E-A) model (Magnussen and Hjertager (1976); Turns (2000)) was employed to determine the global reaction rates of the chemical species. To tackle the turbulence effects, the governing equations were time-averaged and the standard $k-\varepsilon$ model was used for problem closure. Thermal radiation was computed by the Discrete Transfer Radiation model (DTRM) for a cylindrical chamber, together with the WSGG model to account the spectral dependence of the gas absorption coefficient, with coefficients of the non-gray gases (CO_2 and H_2O) taken from the well-known Taylor and Foster (1974).

2. MATHEMATICAL FORMULATION

The proposed task can be stated as follows: considering steady combustion of natural gas (composed of 90% of methane and 10% of nitrogen) in air inside a horizontal cylindrical chamber, compute the temperature, chemical species concentrations and the velocity fields, modeling the radiation from non-gray gases by means of the WSGG model of Taylor and Foster (1974) and employing a 3D geometric configuration in order to consider buoyancy effects on the flame behavior.

The set of equations solved by Ansys CFX are mass, momentum, energy and chemical species conservation equations, as well as the equation of state of ideal gas. An Eulerian description for the fluid phase was adopted. The standard *k-ε* turbulence model was applied to closing the problem due to the averaged Navier-Stokes equations process. The methane oxidation by atmospheric air was modeled by two global steps, WD2 by Ansys Inc. (2004), given by:

$$2CH_4^{(16)} + 0.22N_2^{(28)} + 3(O_2^{(32)} + 3.76N_2^{(28)}) \rightarrow 2CO^{(28)} + 4H_2O^{(18)} + 11.5N_2^{(28)} \quad (1)$$

$$2CO^{(28)} + 1(O_2^{(32)} + 3.76N_2^{(28)}) \rightarrow 2CO_2^{(44)} + 3.76N_2^{(28)} \quad (2)$$

where the carbon monoxide oxidation is modeled by the second reaction above.

Scalar transport equations are solved for velocity, pressure, temperature and chemical species. The bulk motion of the fluid is modeled using single velocity, pressure, temperature, chemical species and turbulence fields (Ansys Inc., 2004).

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2.1. Mass and species conservation

Each component has its own Reynolds-Averaged equation for mass conservation which, considering incompressible and stationary flow can be written in tensor notation as:

$$\frac{\partial\left(\tilde{\rho}_i \tilde{U}_j\right)}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\tilde{\rho}_i\left(\tilde{U}_{ij} - \tilde{U}_j\right) - \overline{\tilde{\rho}_i "U_j"}\right) + S_i \tag{3}$$

where $\tilde{U}_j = \sum\left(\tilde{\rho}_i \tilde{U}_{ij}\right)\Big/\overline{\rho}$. $\tilde{\rho}_i$ and $\overline{\rho}$ are the mass-average density of fluid component i in the mixture and average density, respectively, x is the spatial coordinate, $\tilde{U}$ is the vector of velocity and $\tilde{U}_{ij}$ is the mass-averaged velocity of fluid component i. The term $\tilde{\rho}_i\left(\tilde{U}_{ij} - \tilde{U}_j\right)$ represents the relative mass flow, and S_i is the source term for component i which includes the effects of chemical reactions. If all the equations represented by Eq. (3) are added over all components, and the source term is set to zero, the result is the standard continuity equation.

The relative mass flow term accounts for differential motion of the individual components. At this work, this term is modeled for the relative motion of the mixture components and the primary effect is that of concentration gradient. Therefore,

$$\tilde{\rho}_i\left(\tilde{U}_{ij} - \tilde{U}_j\right) = \frac{\overline{\rho} D_i}{\overline{\rho}} \frac{\partial \tilde{\rho}_i}{\partial x_i} \tag{4}$$

where D_i is the kinetic diffusivity. The mass fraction of component i is defined as $\tilde{Y}_i = \tilde{\rho}_i \big/ \overline{\rho}$. Substituting these expressions into Eq. (3) and modeling the turbulent scalar flows using the eddy dissipation assumption it follows that:

$$\frac{\partial}{\partial x_j}\left(\overline{\rho}\tilde{U}_j \tilde{Y}_i\right) = \frac{\partial}{\partial x_j}\left(\left(\overline{\rho} D_i + \frac{\mu_t}{Sc_t}\right)\frac{\partial \tilde{Y}_i}{\partial x_j}\right) + \overline{S}_i \tag{5}$$

where μ_t is the turbulent viscosity and Sc_t is the turbulent Schmidt number. Note that the sum of component mass fractions over all components is equal to one.

2.2. Momentum conservation

For the fluid flow the momentum conservation equation is given by:

$$\frac{\partial}{\partial x_j}\left(\overline{\rho}\tilde{U}_i \tilde{U}_j\right) = -\frac{\partial p^*}{\partial x_j}\delta_{ij} + \frac{\partial}{\partial x_j}\left(\mu_{eff}\frac{\partial \tilde{U}_i}{\partial x_j}\right) + \frac{\partial \tilde{U}}{\partial x_j \partial x_i} + \overline{S}_U \tag{6}$$

where $\mu_{eff} = \mu + \mu_t$ and μ is the mixture dynamic viscosity and μ_t is the turbulent viscosity, defined as $\mu_t = C_\mu \rho\, k^2/\varepsilon$. The term $p^* = \overline{p} - (2/3)k$ is the modified pressure, C_μ is an empirical constant of the turbulence model equal to 0.09, $\overline{p}$ is the time-averaged pressure of the gaseous mixture, and δ_{ij} is the Krönecker delta function. $\overline{S}_U$ is the source term, introduced to model the buoyancy and drag force due to the transportation particles, and other mathematical terms due to turbulence models. The Boussinesq model is used to represent the buoyancy force due to density variations. The standard $k-\varepsilon$ model is used to provide the turbulence on the flow (Menter, 1994).

2.3. Energy conservation

Considering the transport of energy due to the diffusion of each chemical species, the energy equation can be written as (here the Lewis number, *Le*, was set to one)

$$\frac{\partial}{\partial x_j}\left(\overline{\rho}\tilde{U}_j \tilde{h}\right) = \frac{\partial}{\partial x_j}\left(\left(\frac{\kappa}{c_p}\right)\frac{\partial \tilde{h}}{\partial x_j} + \sum_i^{Nc}\overline{\rho} D_i \tilde{h}_i \frac{\partial \tilde{Y}_i}{\partial x_j} + \frac{\mu_t}{\mathrm{Pr}_t}\frac{\partial \tilde{h}}{\partial x_j}\right) + \overline{S}_{rad} + \overline{S}_{rea} \tag{7}$$

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where $\tilde{h}$ and c_p are the average enthalpy and specific heat of the mixture. The latter is given by $c_p = \sum_\alpha \tilde{Y}_\alpha c_{p,\alpha}$, where $c_{p,\alpha}$ and $\tilde{Y}$ are the specific heat and the average mass fraction of the α-th chemical species, κ is the thermal conductivity of the mixture, Pr_t is the turbulent Prandtl number, and $\overline{S}_{rad}$ and $\overline{S}_{rea}$ represent the sources of thermal energy due to the radiative transfer and to the chemical reactions. The term $\overline{S}_{rea}$ can be written as:

$$\overline{S}_{rea} = \sum_\alpha \left[\frac{h_\alpha^0}{\overline{MM}_\alpha} + \int_{\tilde{T}_{ref,\alpha}}^{\tilde{T}} c_{p,\alpha} d\tilde{T} \right] \overline{R_\alpha} \tag{8}$$

where $\tilde{T}$ is the average temperature of the mixture, h_α^0 and $\tilde{T}_{ref,\alpha}$ are the formation enthalpy and the reference temperature of the α-th chemical species. To complete the model, the density of mixture can be obtained from the ideal gas state equation (Kuo, 1996; Turns, 2000), $\overline{\rho} = p\overline{MM}\left(\overline{\Re}\tilde{T}\right)^{-1}$, where p is the combustion chamber operational pressure, which is here set to 1 atm, and $\overline{MM}$ is the mixture molecular mass, and $\overline{\Re}$ is the universal constant of ideal gas. The aforementioned equations are valid only in the turbulent core, where $\mu_t >> \mu$. Close to the wall, the conventional logarithmic law of the wall is used (Nikuradse, 1933).

To consider thermal radiation exchanges inside the combustion chamber, the Discrete Transfer Radiation Model (DTRM) is employed (Carvalho et al., 1991), considering that the scattering is isotropic. The effect of the non-gray gaseous mixture was considered by original WSGG (weighted-sum-of-gray-gases) model developed by Hottel and Sarofim (1967), using the coefficients obtained by Taylor and Foster (1974). The WSGG model coefficients employed in this work were those for partial pressures of 0.1 atm, 0.2 atm and 0.7 atm for CO_2, H_2O and N_2, respectively, being those values commonly considered for methane-air combustion and while the N_2 is considered transparent to radiation, as usual in combustion of gas fuel (Taylor and Foster, 1974).

2.4. The E-A (Eddy-Break-Up – Arrhenius) chemical reactions model

The reduced chemical reactions model employed in this work assumes finite rate reactions and a steady state turbulent combustion process. In addition, it is considered that the combined premixed and non-premixed oxidation occurs in two global chemical reaction steps, and involving only six species: O_2, CH_4, N_2, H_2O, CO_2 and CO. A conservation equation is required for each species but nitrogen. Thus, one has the conservation equation for the α-th chemical species, given by Eq. (5), where the source term, S_i, considers the average volumetric rate of formation or destruction of the α-th chemical species at all chemical reactions. This term is computed from the summation of the volumetric rates of formation or destruction in all the k-th equations where the α-th species is present, $\overline{R_{\alpha,k}}$. Thus, $\overline{R_\alpha} = \sum_k \overline{R_{\alpha,k}}$. The rate of formation or destruction, $\overline{R_{\alpha,k}}$, was obtained from a combined Eddy Break-Up - Arrhenius model, the E-A (Eaton et al., 1999). Such relations are appropriate for a wide range of applications, for instance, laminar or turbulent chemical reactions with or without pre-mixing. The rate of formation or destruction of the chemical species is taken as the lowest one between the values obtained from each model. Silva et al. (2007) used this formulation to simulate the combustion process of methane and air in a cylindrical chamber obtaining good results.

3. PROBLEM STATEMENT

The physical system consists of the same natural gas combustion chamber that was analyzed in Magel et al. (1996), Nieckele et al. (2001) and Silva et al. (2007), which was a test case proposed in Garréton and Simonin (1994). The cylindrical chamber has a length and a diameter of 1.70 m and 0.50 m, respectively, as shown in Fig. 1. Natural gas is injected into the chamber by a duct aligned with the chamber centerline. The burner is capable of providing the necessary amount of air and natural gas as required by the process. In all cases a fuel excess of 5% was prescribed. For a fuel mass flow rate of 0.01453 kg/s at a temperature of 313.15 K, this requires an air mass flow rate of 0.1988 kg/s, at a temperature of 323.15 K. The fuel enters the chamber through a cylindrical duct having diameter of 0.06 m, while air enters the chamber through a centered annular duct having a spacing of 0.02 m. For such mass flow rates, the fuel and air velocities are 7.23 and 36.29 m/s, respectively. The Reynolds number at the entrance, approximately 18,000, points that the flow is turbulent. The inlet air is composed of oxygen (23% in mass fraction), nitrogen (76%) and water vapor (1%), while the fuel is composed of 90% of methane and 10% of nitrogen. The burner power is about 600 kW. The fan and the other external components are not included in the computational domain, although their effects are taken into account through the inlet flow conditions. Buoyancy effects were considered and the Boussinesq approximation was adopted.

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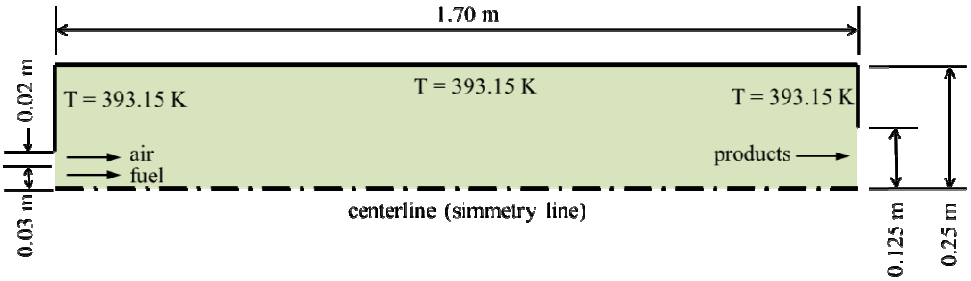


Figure 1. Combustion chamber geometry – Axisymmetric view.

The equations constants and the physical properties were taken from a number of different sources, and the constants of the Arrhenius equation for the methane combustion reactions are presented in Tab. 1.

Table 1. The constants of the Arrhenius equation WD2 (Ansys Inc., 2004).

Step (k)	E_k	A_k	β_k	γ_{CH_4}	γ_{O_2}	γ_{CO}	γ_{CO_2}	γ_{H_2O}
k =1 (CH_4)	30 [kcal/kmol]	$1.50x10^{7}[s^{-1}]$	0	-0.3	1.3	-	-	-
k =2 (CO)	40 [kcal/kmol]	$1.10x10[mol^{-0.75}cm^{2.25}s^{-1}]$	0	-	0.25	1	-	-

4. BOUNDARY CONDITIONS

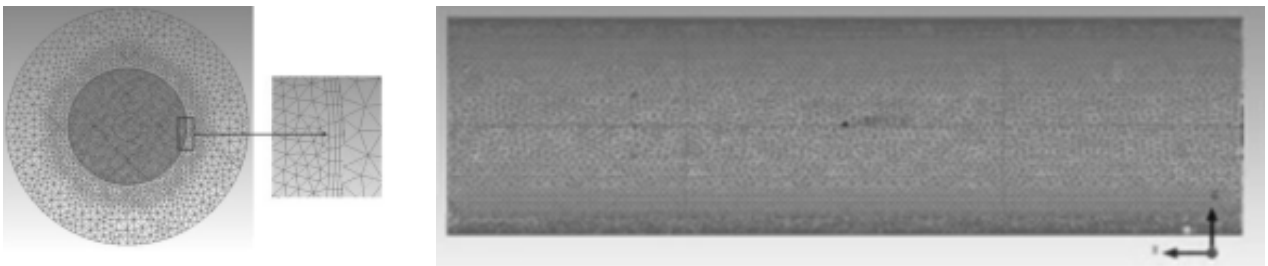
Keeping the same conditions as prescribed in Garréton and Simonin (1994) and Nieckele et al. (2001), the combustion chamber walls were kept at constant temperature of 393.15 K. In addition, impermeability and no-slip conditions were assumed on the wall. In the outlet duct null diffusive fluxes were assumed for all variables. The walls were assumed gray, diffusive emitters with an emissivity of 0.6. The inlet and the outlet reservoirs were modeled as black surfaces at the inlet and outlet temperatures. In the inlet, the velocity and concentration profiles were assumed uniform. The turbulence intensity was prescribed as 5% for the air and the fuel inlet flows, respectively.

5. NUMERICAL METHOD

The flow fields inside the boiler (velocity, temperature, concentrations, etc.) were numerically determined with the commercial software Ansys CFX 14.5, based on the finite volume method (Patankar, 1980). The "up-wind" for interpolation scheme was set. The velocity-pressure coupling was solved by the SIMPLE algorithm (Patankar, 1980). Since the conservation equations are non-linear, relaxation factors were used.

6. MESH SETTINGS AND CONVERGENCE CRITERIA

The domain under consideration comprises the cylindrical combustion chamber. The discretization was done using tetrahedral volumes. Prismatic volumes were used on the walls in order to capture the boundary layer behavior. The software Ansys © ICEM CFD was used to compute the geometry and the mesh. The mesh had approximately 2.15×10^{6} elements of unequal sizes, using mesh refinements in the reactive region near the burner. The convergence criterion adopted was the root mean square (RMS) of the residual values. RMS values lower than 1×10^{-6} were achieved at all equations. The CPU time for each simulation was approximately two days on desktop Intel ® Core 2 Quad 2.5 GHz with 8 Gb of RAM, with parallel processing. The Fig. 2 shows the frontal (a) and lateral (b) view of the mesh.



(a) (b)

Figure 2. (a) Frontal view of the mesh;(b) lateral view of the mesh.

7. MESH INDEPENDENCE TEST

A mesh independence test was performed considering tree different meshes in order to verify the accuracy of the results obtained with the computational mesh used. A finer mesh with 2,800,000 elements, another mesh with 2,150,000 (the adopted one) and a coarser mesh with only 510,000 elements were tested in order to verify the behavior of results regarding the size of the control volumes. Figure 3 shows the results obtained for the temperature profiles at

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the chamber centerline, where it can be observed that the two finer meshes present good agreement (nearly coincident) and, thereby, it can be concluded that the mesh of 2,150,000 elements used in the current simulation is sufficiently refined.

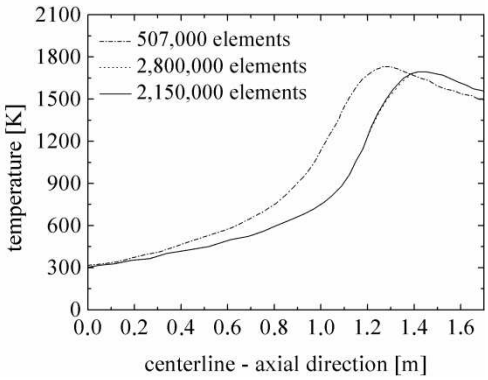

Figure 3. Temperature distribution in the line of symmetry of the chamber.

8. RESULTS ANALYSIS

Some works reported in the literature (Magel et al. 1996; Nieckele et al., 2001 and Silva et al., 2007) considered that the presently studied combustion chamber can be modeled in two-dimensional axisymmetric cylindrical coordinates, and also they considered that the buoyancy forces could be neglected based on the fact that the speed of the air and the fuel at the inlet are high, associated with the relatively short size of the flame, leading to a dominant effect of forced convection in relation to natural convection. The present study performs an analysis of three-dimensional methane-air combustion process considering that the chemical reactions occurs in two global steps, where the effect of buoyancy forces on the results is the main goal of this work. Then, in order to achieve the main goal previously mentioned, two scenarios are investigated here: (i) considering buoyancy into calculations, and (ii) neglecting buoyancy into calculations. Results for both scenarios are then recorded for velocity fields, profile of temperatures and chemical species concentration in regions of interest, with the purpose of comparing those results with experimental data from Garreton and Simonin (1994) and numerical results by Silva (2007).

Figures 4-a and 4-b depicts the temperature field at the plane of symmetry of the chamber for the scenarios without and with buoyancy, respectively. Similarly, Fig. 4-c and 4-d shows the velocity vectors distribution fields. Comparing results from scenarios without and with buoyancy shown in Fig. 4, it is observed that there is a small input offset of the jets downward relative to the line of symmetry of the flame due to the effect of buoyancy (Fig. 4-b and 4-d). Since the temperature increases in the lower portion of the chamber, the specific volume of gases are also increased, moving the gaseous mixture preferably to the top portion of the chamber, which increases the size of the recirculation above the inlet jets and increasing the pressure of this region, pushing the tip of the flame downwards, contrary to what would occur in a flame unconfined. However, generally it can be stated that the temperature distributions and the profile of the flame are not significantly influenced by the buoyancy. It is also observed that the velocity field for the flame without buoyancy (Fig. 4-c) shows similar magnitudes and forms if compared with the flame with buoyancy (Fig. 4-d).

By comparison between the velocity ranges (Figs. 4-c and 4-d), the highest speeds inside the chamber are approximately 35 m/s and the least are approximately 1 m/s. Thus, it can be seen that the highest velocities, due to the decrease in the specific mass of the gases as a result of the increase in temperature, are located closer to the center of the combustion chamber, and also closer to the outlet zone.

Figure 5 shows temperature profiles in the axial direction of the chamber and also for the radial position located at 1.312 m from the chamber inlet. In this region of the flame, which corresponds to the region close to the outlet duct of the chamber, it is observed differences between the results with and without buoyancy.

In Figs. 5-a and 5-b it appears that the presence of buoyancy actually generates no significant differences in the temperature profiles, both in the radial position (1.312 m from the entrance region) as in the chamber centerline. The results obtained in this study are also in good agreement with the experimental results by Garretón and Simonin (1994), as well as the Silva (2007). It is also verified that the effect of buoyancy, particularly in the end region of the flame, makes the computational results closer to the experimental data than the results previously reported in the literature considering the chamber as 2D axisymmetric cylindrical.

Figure 6 shows oxygen and carbon dioxide mass fraction profiles in the centerline of the chamber. It is noted that there is a deviation from the experimental data and results from the present investigation as well as Silva (2007) results for the oxygen mass fraction (Fig. 6-a) close to the inlet of the combustion chamber. The combustion model underestimates the chemical reactions rates and the oxygen consumption, which exhibits higher mass fractions. For the downstream region located at the after the middle of the chamber, results are in better agreement when compared to experimental data for all cases. Besides, it can be seen that the buoyancy effect was practically negligible and did not change the numerical results. In relation to carbon dioxide profile, there is a better agreement of the results of the

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present work with experimental data when compared to those reported in Silva (2007). Again, it was found that the buoyancy effect was negligible, without significant influence on the results.

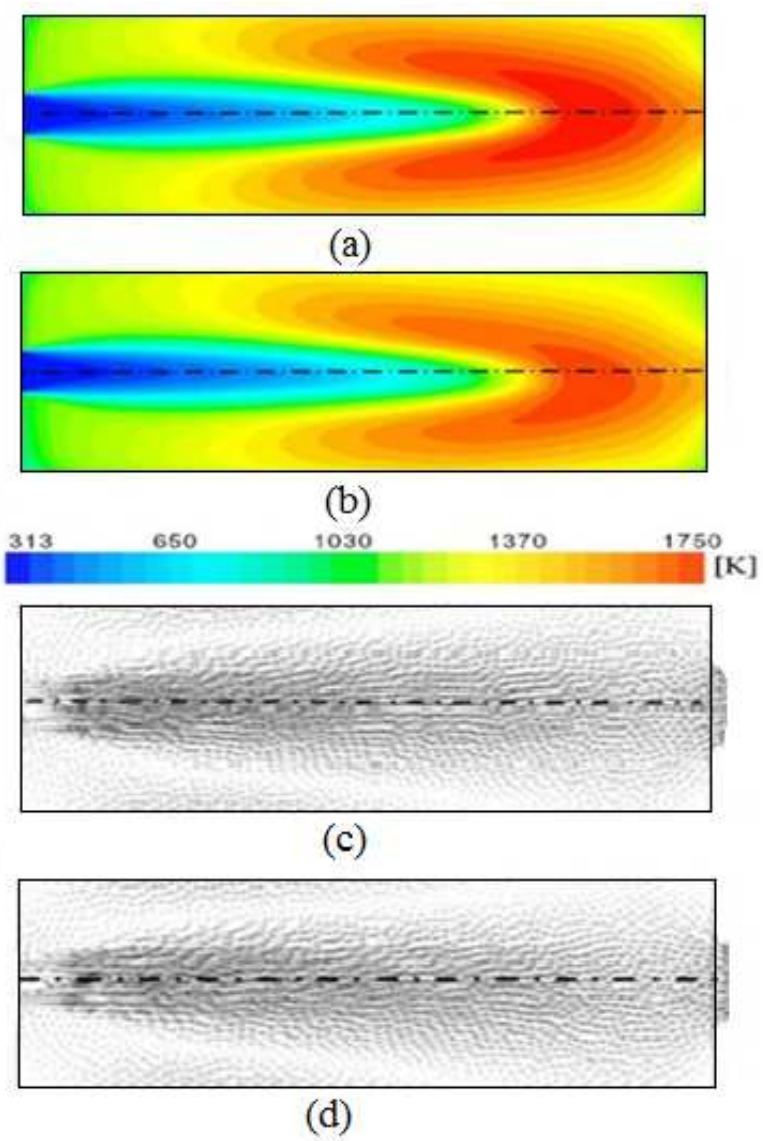
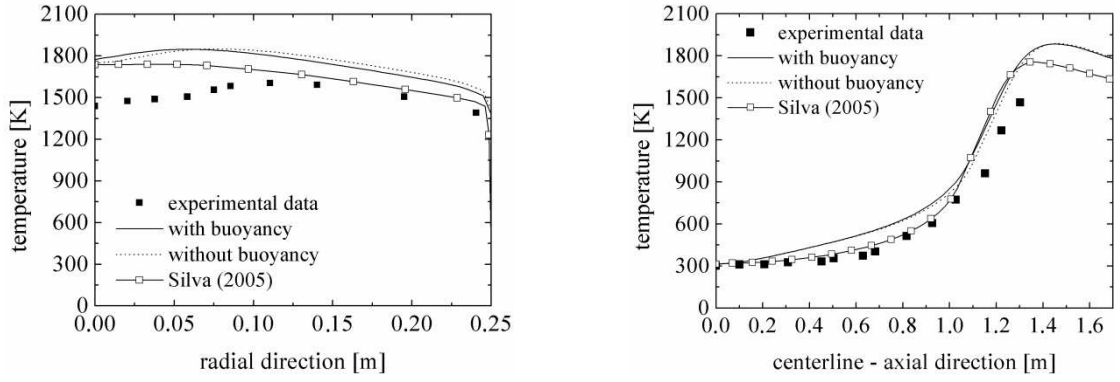


Figure 4. Temperature and velocity vectors distribution in the plane of symmetry of the chamber: (a) and (c) without buoyancy, (b) and (d) with buoyancy.



(a) (b)

Figure 5. Temperature profiles: (a) radial direction (1.312m), (b) axial symmetry of the chamber.

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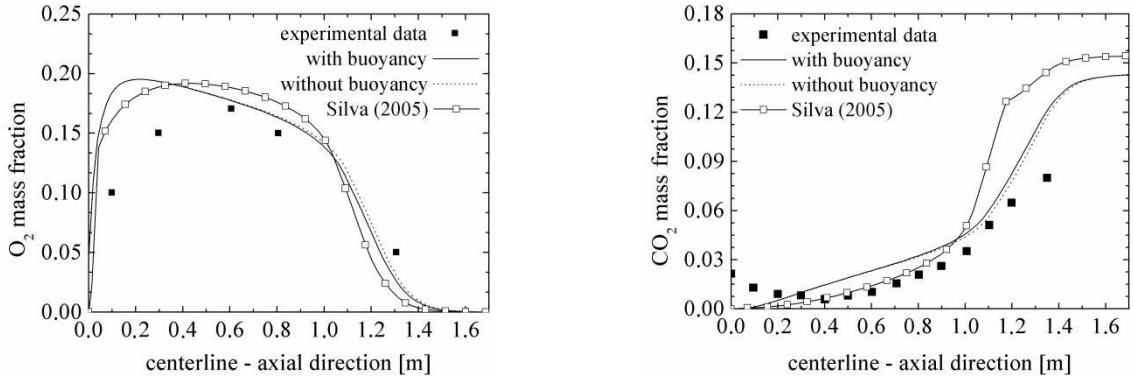

(a) (b)

Figure 6. Mass fraction profiles at the chamber centerline: (a) O_2; (b) CO_2.

At the beginning, making an evaluation of the conditions of inlet jets of methane and air, it was believed that the flame was predominantly diffusive, without pre-mixing of air and methane. However, after analysis of the computational results of the velocity field obtained with the three-dimensional study, it was found that the inlet region of the jets (region of the burner), due to the high velocity of the air jet against the fuel jet, leads to a vortex of high energy, which makes that the burning process passes to be partially-pre-mixed, as can be seen in Fig. 7-b, and, in detail, in Fig.7-c, fact which was not verified in results of Magel (1996), Nieckele et al. (2002) and Silva (2007) as a consequence of the model adopted by these studies, which was two-dimensional. This vortex generates better mixing between the fuel and oxidant, producing an additional element of premix in the process, which certainly affects the results. Note that the model adopted for chemical reactions is able to consider this premix effect (Eaton et al. 1999). It is noted that in Fig. 7-c the recirculation leads to a pre-mixing between fuel and air in the process, and also intensifies the turbulence in the region modifying the flame. If turbulence is larger, rates of chemical reactions are faster. Note also that the combustion model is sensitive to that, especially in the EddyBreak-Up model. Additionally, observe that the results of Silva (2007), Fig 7-a, this vortex was not present.

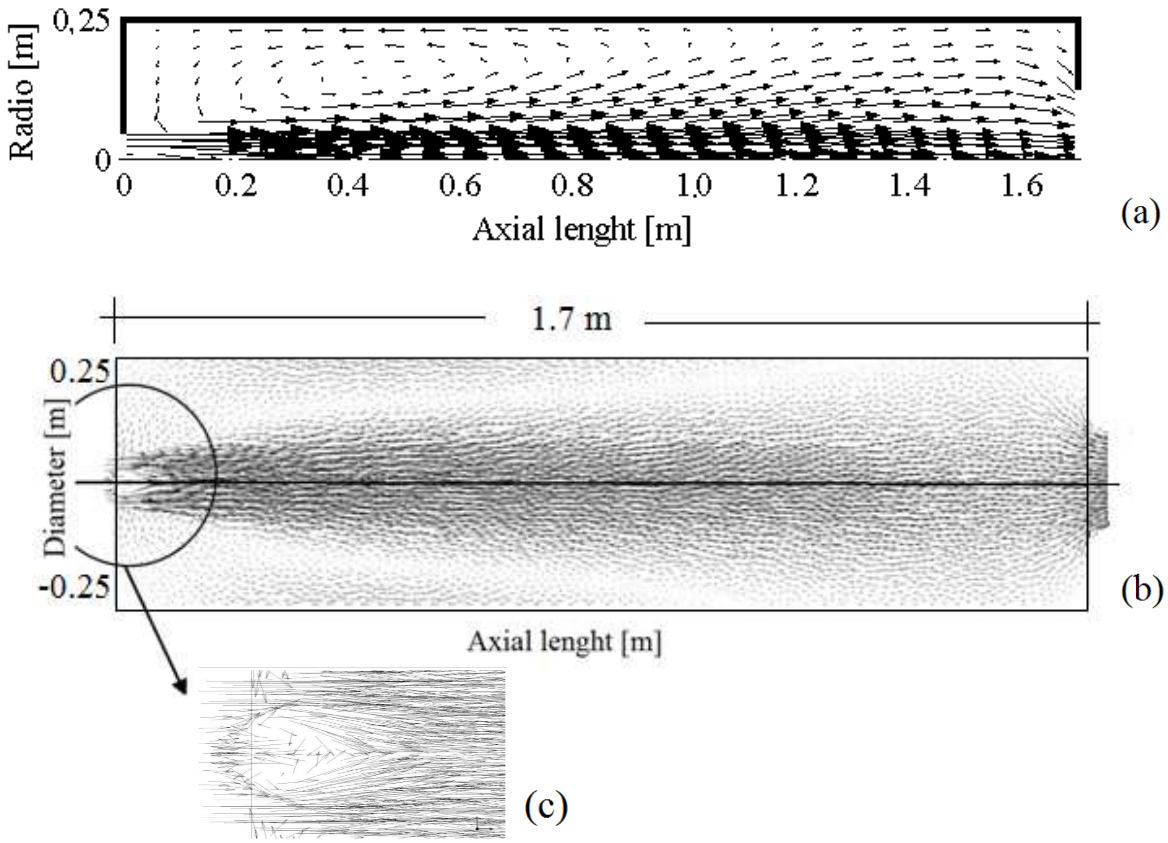

Figure 7 - Velocity field: (a) Silva (2007) no buoyancy – axisymmetric solution; (b) Present work - buoyancy tree-dimensional solution; (c) Present work – buoyancy - detail enlargement of the inlet region.

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9. CONCLUSIONS

Based on the study realized in this work, in the case analyzed, the main conclusion is that the buoyancy has a minor effect under the flame shape and it can be neglected without further consequences on the combustion process. On the other hand, the simplification of the problem to be considered two-dimensional adopted by Magel et al. (1996), Nieckele et al. (2001) and Silva et al. (2007) need a higher level of care, because the presence of recirculation in the inlet region of the jet changes the way it burns fuel, requiring further investigation.

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