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COMPUTATIONAL FLUID DYNAMIC APPLIED TO COMBUSTION CHAMBER FOR SMALL GAS TURBINES USING NATURAL GAS

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Abstract. This work focuses the development about a practical scheme using commercial softwares to study the flame behavior (combustion and flow) in annular combustion chambers for small gas turbines to attend its adaptability and economic feasible to use different fuels. For it, it is used the methane gas to represent the natural gas, whose chemical composition is done mainly by 88(%) in volume by methane. Among the softwares: Gatecycle® is applied to calculate the thermodynamic parameters of combustion chamber from thermal cycle for small gas turbine; GASEQ® to calculate the chemical reactions and concentration of reactants and products to esteemed the emissions; and CFX® is used to simulate the dynamic fluid for flow, combustion , heat transfer and emissions. The combustion in CFD is simulated by Eddy Dissipation Model with two steps of chemical reaction for the methane gas. The turbulence is simulated by RNG K-ε Model. The heat transfer by radiation is made by P1 Method and the NOx emission is calculated by Fenimore and Zeldovich Methods. The expected numeric results are the fields of velocity, pressure and temperature, to feature the load losses and the volume of flame. From this way, it intends to make available information about: the parameters that affect the position of flame; the maximum temperature of flame; the temperature of hot gas in exhaustion; the affects from nozzles; the affects of flame from methane gas in design; and the preliminary efficiency value for combustion chamber. Besides, it is presented a typical validation process for CFD in combustion chamber with tri-dimensional domain.

***Keywords**. CFD, Combustion Chamber, Small Gas Turbine, Natural Gas*

1. Introduction

The Small Gas Turbines are becoming a promise way for distributed power generation and combined heat and power applications. Its conception is from 40´s decade together others gas turbines for aeronautical and navy industry. Later, this system became alternative equipment to generate power and heat to attend the population located in isolated regions out to the interlinked electrical system, because of the Oil Crisis in 1973.

Part of its success is due to the advances in electronics, which allow unattended operation and interfacing with the commercial power grid. Electronic power switching technology eliminates the need for the generator used by gas turbine to be synchronized with the power grid.

These equipments can generate power until 350 (kW) and have the following advantages in relation to piston engine generators, Gurgel et al. (2002): (a) higher power density (with respect to footprint and weight); (b) low emissions; (c) few, or just one, moving parts; (d) its design uses foil bearings and air-cooling operate without oil, coolants or other hazardous materials; (e) its operation is simply; (f) its installation and maintenance are easy; and (g) its operation cost is low. However, piston engine generators are quicker to attend the changes in output power requirement.

Besides, the emission control of pollutant agents, such as NOx, CO and SOx, is adjusted by U.S. Environment Protection Agency (1993), where it is set that the maximum NOx emission for small gas turbines is 15 ppmv (15% Oxygen) for the flame temperature equal to 1900 [K], Lefebvre (1995).

Currently, the main manufactures of small gas turbines are: Turbo-Genset, Capstone Turbine Co., Solar Turbines, Allison Engine, Bowman Power, Turbec, Honeywell, lliott MagneTek Power Systen, General Electric, Turbomeca, ABB, Harvester Company and Rolls Royce Nimbus.

The small gas turbines are based on Ideal Brayton-Joule´s Cycles, which is a thermodynamic cycle where air is compressed isentropically in compressor, the combustion occurs at constant pressure in combustion chamber, and the expansion for hot gas over the turbine occurs isentropically until the back to the starting pressure, Lefebvre (1983).

Among the parts from small gas turbine, the combustion chamber is focused in earlier researches, mainly about the potential improvements in combustion efficiency, which has two basic factors that can limit its operation range: (a) friction losses; and (b) thermal limitations for blades in turbine.

The friction losses occur in bearings, in the blades and the metallic walls in compressor, turbine and nozzles in combustion chamber. Due to this friction, the small gas turbines need a compressor to supply more pressure. In case for annular chambers, the compressor is radial, while the compressor is axial for tubular chambers, Lefebvre (1983).

On the other hand, it is possible to compensate these losses using more fuel flow, although it can provoke higher temperatures than thermal limitations for blades in turbine, as well as the creep.

The main improvements that are done for small gas turbines are: (a) higher compression ratios; (b) higher temperature gradients in combustion chamber; (c) more efficient combustion; (d) better cooling of engine parts; and (e) reduced emissions. For it, two ways are applied: (a) the analysis of geometry; and (b) the development of fuels more reactive with low emissions.

The first way has been explored in relation to change of geometry, where can be sign the Dry Low NOx - DLN chambers, which are the cylindrical combustion chambers with big quantity of holes in Liners and dilution holes in downstream of combustion chamber, Allen (1998), Nickolaus et al. (2002) and Wakabayashi et al. (2002).

The second way has been studied in relation to the use of fuels without sulfur with high reactivity, like as, the natural gas, according to Lefevbre [16], Melick et al (1999), Vandebroek et al. (2003) and Williams (1985).

Allen (1998) explored the DLN chambers using other kind of fuel with liquid phase and generated by emulsion process. Vandebroek et al. (2003) explored the affects of chemical kinetic in combustion of methane with 4 steps to esteem the temperature for auto ignition. Lefevbre [15] and Melick et al. (1998) show other way to control the NOx emission based on the catalysts with NH_3, as well as its possible effects in environment.

In general, all of results can be obtained by experimental and numerical tests. While the first, it is necessary to raise enough money with expensive equipments and benches, the numerical tests have been a promise alternative with the advantage use of more quick computers with high capacity to save data, Kuo (1986) and Keating (1993).

In relation to numerical tests, different numerical methods have been tested to simulate the flame for combustion chambers. Among these methods, the Computational Fluid Dynamic (CFD) has more applications

The use of CFD for combustion chambers is not early and it has presented satisfactory results in some models, such as, tubular combustion chambers, Gosselin *et. al.* (2000), Lee *et. al.* (1990) and Nicklaus *et. al.* (2002), which executed the first simulations using CFD in cylindrical combustion chambers in bi-dimensional and three-dimensional geometry models. The turbulence models tested by them are K-ε, RNG K-ε and Reynolds Stresses Model (RSM), and the combustion models Fast Chemistry with PDF Model and Flamelet Laminar Model (FLM).

Besides, the works from Fuller and Smith (1994), Hamer and Roby (1997) introduced others combustion models, such as, Eddy Dissipation Model (EDM), with models of NOx emission of Fenimore and Zeldovich, in three-dimensional geometry models. In particular, Hamer and Roby (1997) archived satisfactory results with simulations until 4 steps for chemical reactions using methane gas.

Based on the satisfactory results for CFD from studies about tubular combustion chambers, new works has been developed too for the annular combustion chambers with the function to solve its particular problems, such as, low efficiency, high emission of pollution, and to check its economic feasibility.

Hence, considering the importance of CFD application in thermal-aerodynamics problems involving the combustion and its complex phenomena for annular combustion chambers, this work presents a methodology to guide researchers and engineers in the analysis of the flame behavior in annular combustion chamber for small gas turbines using natural gas by CFD. The tested geometric model uses an alternative fuel, the methane gas, once that its participation in chemical composition for natural gas is bigger than 88 (%) in volume. The adopted annular combustion chamber operates with conventional fuels, such as, diesel and kerosene oil, whose power can be until 50 (KW) at ISO conditions, according to the manufacturer of small gas turbine called Solar Turbines. The adopted chemical reactions use interactive steps based on the Minimization Principle of Free Gibbs Energy or Lewis – NASA Method, Svehla and McBride (1973).

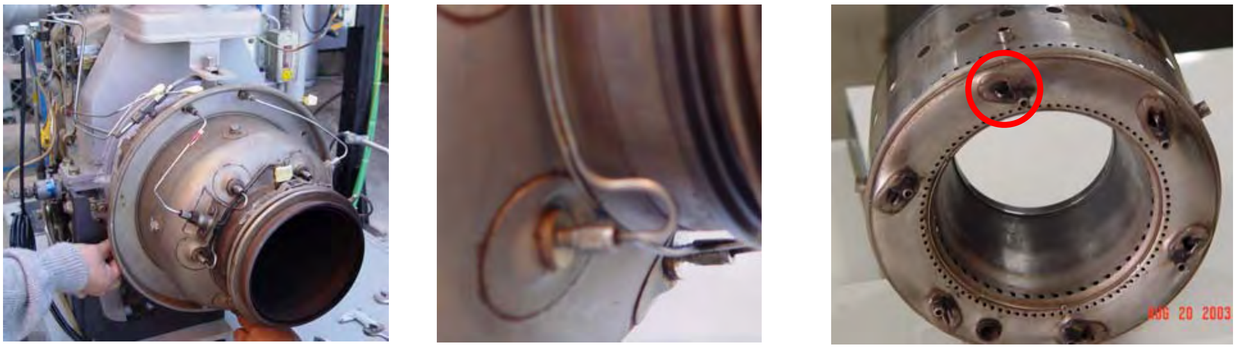
The knowledge about the flame behavior is achieved by the establishment of the fields of velocity, pressure and temperature, to describe the load losses and the volume of flame using the mathematical approximations, such as: of turbulent flow; of combustion; of heat transfer by radiation; and NOx and CO emissions.

2. The Combustion Chamber Tested

The tested combustion chamber is part of small gas turbine of kind Titan T-62T-32 Turbo shaft, 1-stage centrifugal compressor with annular profile, 1-stage turbine designed to work with diesel, kerosene and JP-4 oil according to the manufacturer Solar Turbines, whose main operation conditions are, Alencar et al (2005):

(a) Fuel pressure in inlet of nozzle: 275790 (Pa);
(b) Environment temperature and pressure in ISO condition: 25 (°C) and 1 (atm);
(c) Mass flow of fuel for 6 nozzles: 29 (kg/s);
(d) Fuel consumption 0.85 (kg / MWh);
(e) Pressure, temperature and mass flow of air in outlet from compressor, respectively: 206843 (Pa), 52 (°C) and 0.75 (kg/s);
(f) Maximal temperature of gas in outlet of combustion chamber: 637.9 (°C); and
(g) Maximal temperature of gas in exhaustion after turbine: 493.2 (°C).

In combustion chamber, the primary air is mixtured with fuel in nozzle with high pressure and velocity. Depend on its capillarity and viscosity, the fuel can be drafted by air, due to the decrease of relative pressure inside of nozzle, which is classified like as Venturi Nozzle. Figure 1 shows the equipment that is modeled.



(a) (b) (c)

Figure 1. (a) Small gas turbine; (b) External detail of nozzles; and (c) Combustion chamber with 6 nozzles (one of them is shown by red cycle), Alencar et al (2005)

Due to the inclination of the nozzles in relation to the axial axle of combustion chamber, it is generated a secondary flow with rotation. From this way, the time residence tends to be big in annular combustion chamber, which permits to improve the combustion efficiency.

This annular combustion chamber has 6 nozzles with inclination equal to 60 grades in relation to the axial axle of combustion chamber. This model has 86 primary holes and 46 secondary holes to the inlet of air that is used to the combustion and to the dilution and cooling of hot gas. The flow in nozzles obeys the basic principle of jets, like as it is shown in Fig. 2.

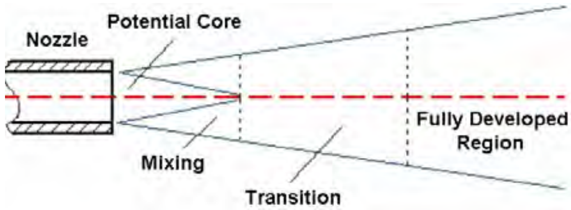


Figure 2 – Main regions of jets, Chigier (1983)

From Fig. 2, it is identified from jet: (a) Potential Core Region, where the air / fuel mixture have a jet that is not affected by environment; (b) Mixing Region, where the jet have load loss and air / fuel mixture presents a diffuse flow; (c) Transition Region, where the air / fuel mixture archives typical velocities for turbulence and it is affected by secondary flow in environment; (d) Fully Developed Region, where jet losses pressure and the flow is mixed with the secondary flow.

Considering the flow from lateral holes in Liner, a big recirculation is created near to the nozzles. From this, the flame can be anchored near to nozzles. Depend on the air / fuel reason, the flame can be classified as Diffusive Flame or Premixed flame. It is recommended to test different combustion models to identify the kind of flame, according to Louis et al. (2001).

The conventional fuels diesel and kerosene oil used by the small gas turbine have Lower Caloric Value equal to 10900 (Kcal/kg) and 10232 (Kcal/kg), respectively. The density for diesel and kerosene oil are 849.2 (kg/m^3) and 819.2 (kg/m^3), respectively. These fuels can have auto ignition in function of temperature, according to Fig.3, Lefebvre (1983).

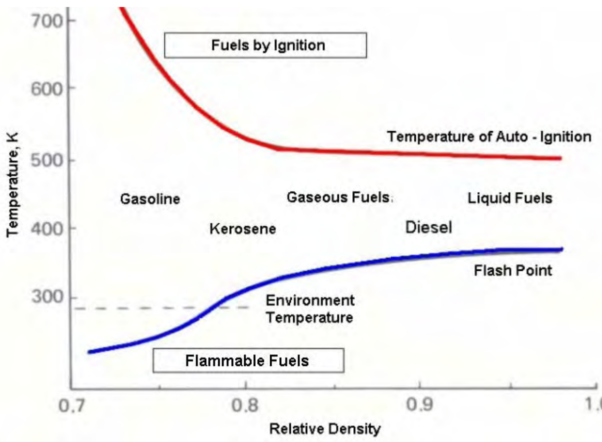


Figure 3 – Typical auto ignition for fuels in relation to relative density and the temperature, Lefebvre (1983)

From Fig. 3, it is possible to identify that in environment temperature, the auto ignition for fuels is not occurs. The temperature in that the fuels are flammables defines the Flash point. In this point, the fuel only can continue the combustion with the action of flash. This point is near to the environment temperature. From this, diesel can have auto ignition in temperature 500 (K), but it is flammable in temperature 350 (K), while the kerosene oil has auto ignition in temperature 630 (K), but it is flammable in environment temperature.

On the other hand, emission is the last step from combustion process and can be characterized by different types of substances, which cannot have more reactivity enough to interact with others, constituting the non-combustion species. Depending on the concentration of these species, the same can provoke damages to the environment. Table 1 shows the typical agents of pollution from emission at small gas turbines and its affects, using diesel and kerosene oil.

Table 1 – Typical emissions and its affects for environment and man, Lefebvre (1995)

Pollutant	**Effect**
Monoxide of Carbon – CO	Toxic.
Unburned Hydrocarbon - UHC	It contributes for the greenhouse effect in the urban region.
Particles of Carbon – C	It is visible and can provoke respiratory problems.
Oxides of Nitrogen - NOX	Toxic. It is precursory of chemical smoke and the ozone depletion in the atmosphere.
Oxides of Sulfur – SOX	Toxic and Corrosive.
Dioxides of Carbon – CO_2	It contributes the greenhouse effect in the atmosphere.

3. Thermodynamic Calculation

For the development of the thermodynamic calculations of the tested combustion chamber, it is used the program GateCycle® from GE Electronics, which permits to calculate the parameters from thermal cycle of small gas turbine considering the following conditions for Thermal System Laboratory at NEST: a) mechanic power 51.01 (+/-1) (kW); b) Heat Rate 37617.49 (kJ/kW); and c) Temperature of exhaustion 749 (K). The reference work fuel is natural gas in environment temperature 22 (°C) and pressure 693 (mmHg). Figure 4 presents the characteristics of each element that it composes the small gas turbine.

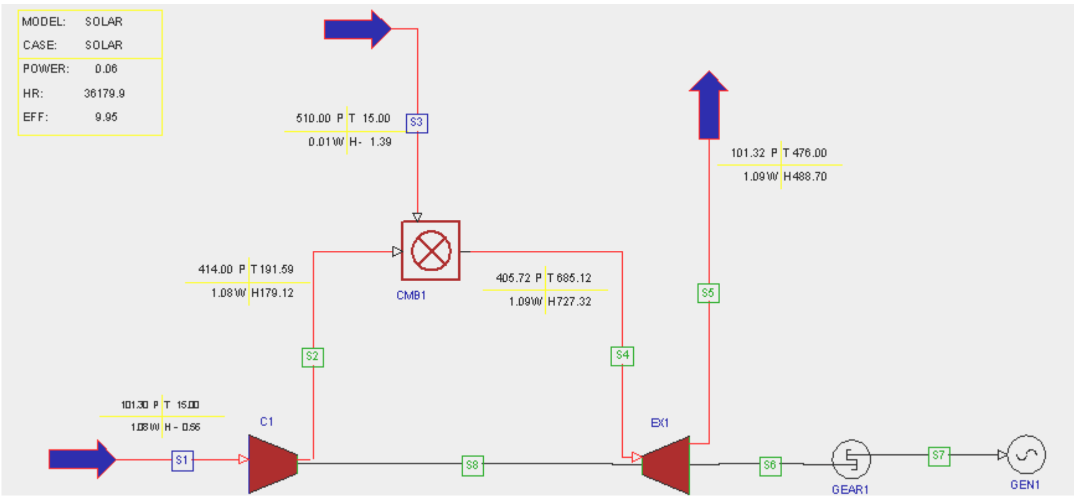


Figure 4 – Typical scheme from GateCycle® form small gas turbine tested

In Fig. 4, the temperature and the pressure are calculated for all point, based on thermal balance in an interactive way. Others parameters, such as: heat loss and pressure loss are obtained by references Borbely et al. (2001) and Lefebvre (1983).

Tab. 2 shows the final values calculated by GateCycle® for control points from **S1** to **S5** (see Fig. 4) in relation to Compressor, Combustion Chamber and Turbine.

Table 2 – Main values from GateCycle® for Small Gas Turbine

Generator Terminal Power	**Stream**	**Temperature (°C)**	**Pressure (kPa)**	**Flow (kg/s)**	**Enthalpy (kJ/kg)**
51.01 kW	S1	22	91.63	0.95609	6.54
	S2	199	368.14	0.95609	188.32
	S3	22	510.00	0.01144	14.29
	S4	685.08	360.78	0.96754	736.22
	S5	478.50	91.63	0.96754	497.52

In Tab. 2, the values calculated for control points from **S2** to **S4** can be used to define the Boundary Conditions for CFD.

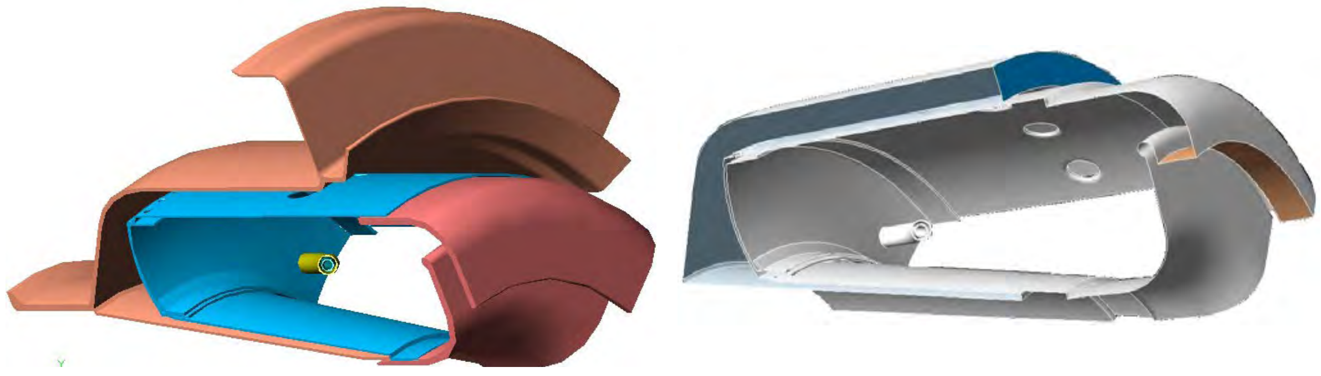
4. Methodology for Solution

The methodology consists to solver the physical problem relative to the behavior of flame in a model of annular combustion chamber for a small gas turbine, using CFD, which represents a part of science for Numerical Methods based on Eulerian Method known as Finite Volume Method to solve the Conservative Equations of Continuous, Momentum and Energy in differential way.

For this method, the physical domain is discretized by volume elements of type tetrahedrical or quadrilateral, whose geometries can be structured or not, i.e., the physical greatness is distributed in center of these elements, which permits to realize detailed analysis in geometrical model. The computational tool is the CFX® v 5.7 from ANSYS, which is used to define the three basic steps for the modeling: pre-processing, processing and post-processing.

In Pre-processing, the geometry model is generated from annular combustion chamber, which corresponds to 1 / 6 from original volume of chamber, because there are 6 nozzles and it is preserved the symmetry in relation to the axle of chamber. According to Gosselin *et al.* (2000), this modeling can get satisfactory results because of the symmetry, not considering the affects from heat transfer by convection.

Figure 5 shows the geometry generated by Mechanical Desktop ® v.6 for structural and CFD conceptions. Figure 6 presents details about this geometry for CFX ® v 5.7.



(a) (b)

Figure 5 – Geometric model tested: (a) Structural Conception; (b) CFD conception

Figure 6 – Geometry Details

The mesh generated is unstructured with 1915508 tetrahedral and prismatic elements and 4666141 nodes. Figure 7 shows a part of this mesh in a longitudinal surface that is paralleled to the axial axle of combustion chamber in a region near to the outlet of nozzle. Figure 8 presents the details of this mesh.

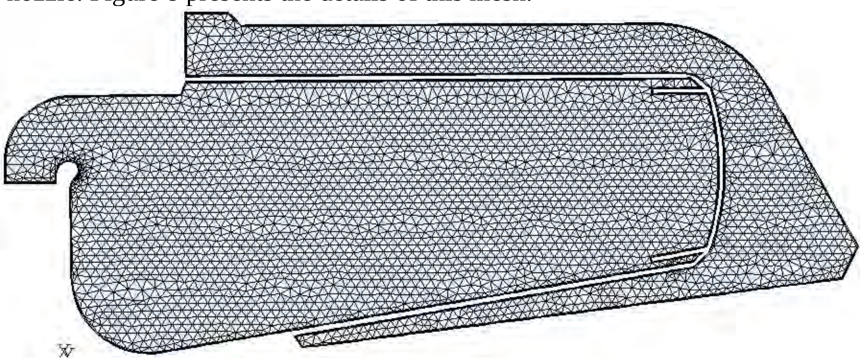


Figure 7 – Lateral view of mesh

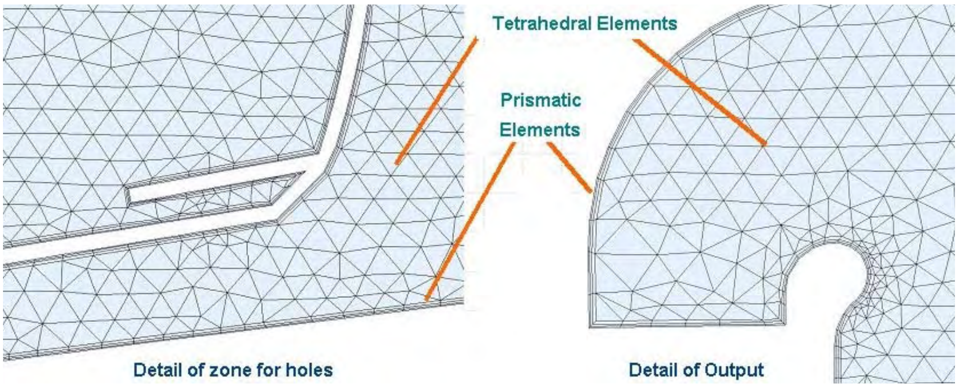


Figure 8 – Details of mesh: (a) in region near to the nozzle; and (b) in outlet of hot gas

The setting of this work fluid in CFD needs the knowledge about the thermal chemical balance, which is simulated by software GASEQ ® v 7.2, which applies the Minimization Principle of Free Gibbs Energy or Lewis – NASA Method, Svehla and McBride (1973).

This method is an interactive calculation that permits to simulate the thermal chemical process for some chemical reactions and by mass balance among reactants and products. It has a library has more than 120 chemical species. In general, this software permits to esteem the concentrations for products and, mainly, the emissions.

The adopted work fluid is the methane gas, because in chemical composition of natural gas, this specie corresponds to 88 (%) in volume and it is a reference fuel for every works in combustion. Table 3 shows the chemical composition for natural gas, according to Abreu and Martinez (1999). Table 4 presents the chemical composition for the combustion of methane gas by GASEQ ® v 7.2.

Table 3 – Chemical composition of alternative fuels for the model of small gas turbine

	Composition in volume (%)
Species	**Natural Gas**
N_2	1.2
CO_2	0.65
CO	0
CH_4	88.56
C_2H_6	9.17
C_3H_8	0.42
H_2S	0
H_2	0
H_2O	0
Low Caloric Value [kcal / kg]	11430

Table 4 – Composition of reactants and products in chemical reaction from GASEQ ® v 7.2 after 5 iterations.

Local	**Species**	**(Mol)**	**Mass (kg)**
Reactants	CH_4	0.105	1.68449
	O_2	0,21	6.71975
	N_2	0.76	22.1326
Products	CO_2	0.095	4.19314
	H_2O	0.204	3.6801
	N_2	0.788	22.1026
	O_2	0.005	0.15865
	CO	0.009	0.27232
	OH^-	0.003	0.05375
	H^+	0.0004	0.000418
	O^{-2}	0.0002	0.00361
	H_2	0.004	0.00794
	NO	0.002	0.06436

Some proprieties from natural gas are preserved, according to Abreu and Martinez (1999) and Lefebvre (1995):

a) it generates low emissions about CO_2 and NOx;

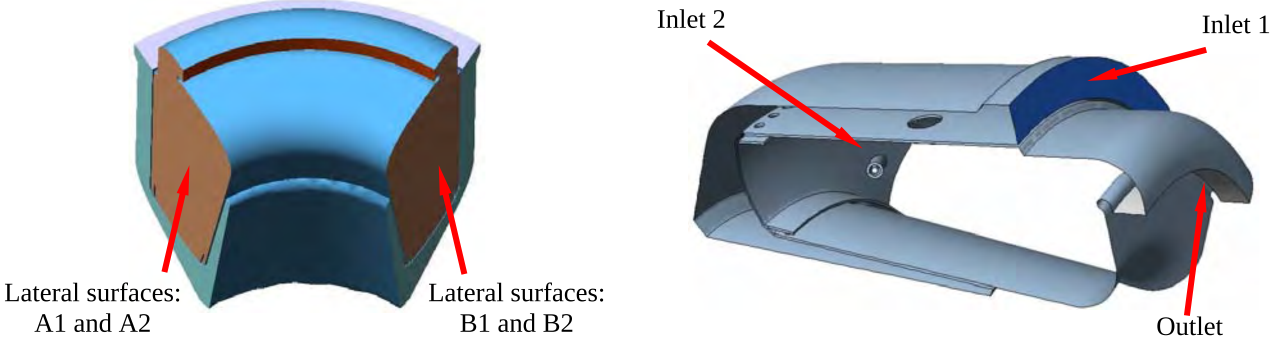
b) It has high combustion efficiency;

c) its combustion can be considered clean, because it does not have sulfur oxide emission, that combined with water molecules can form acid;

e) it has quick dispersion in air, due to its low molecular mass in relation to air; and

f) It presents agility in the transport and good level of safety.

Figure 9 shows the reference surfaces defined by boundary conditions for CFX ® v 5.7.



(a) (b)

Figure 9 – Surfaces defined by boundary conditions: (a) Frontal view; and (b) Lateral view.

Table 5 presents the values adopted for the boundary conditions for Fig. 9.

Table 5 – Boundary conditions used in CFD

Greatness	Local	Unit	Values
Mass flow of air	Inlet 1	(kg/s)	0.1593
Temperature of air		(K)	500
Mass flow of fuel	Inlet 2	(kg/s)	0.0341
Temperature of fuel		(K)	295
Relative pressure of hot gas	Outlet	(Pa)	0.0
Temperature of hot gas		(K)	918
Rotational symmetry in axle	Lateral surfaces A1 – pre-chamber	---	Periodic Interface
Rotational symmetry in axle	Lateral surfaces A2 - chamber	---	Periodic Interface
Rotational symmetry in axle	Lateral surfaces B1 – pre-chamber	---	Periodic Interface
Rotational symmetry in axle	Lateral surfacesB2 - chamber	---	Periodic Interface

In Processing, the domain for mixtures is controlled by the Conservative Equations of Continuous, Momentum (Navier Stokes) and Energy in differential way in relation to the time and the space, respectively:

$$\frac{\partial\left(\rho.\tilde{Y}_I\right)}{\partial t}+\frac{\partial\left(\rho.u_j.\tilde{Y}_I\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\Gamma ref.\frac{\partial \tilde{Y}_I}{\partial x_j}\right)+S_I \quad (1)$$

$$\frac{\partial(\rho.U)}{\partial t}+\nabla\bullet\left[\rho.U\otimes U-\mu.\left(\nabla U+\nabla U^T\right)\right]=-\frac{\partial p}{\partial x_j}+S_M \quad (2)$$

$$\frac{\partial(\rho.H)}{\partial t}-\frac{\partial P}{\partial t}+\frac{\partial\left(\rho.U_j.H\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\lambda.\frac{\partial T}{\partial x_j}+\sum_{N_i}^{Nj}\Gamma_i.h_i.\frac{\partial Yi}{\partial x_j}+\frac{\mu_t}{Pr_t}.\frac{\partial h}{\partial x_j}\right)+S_E \quad (3)$$

Where: **ρ** is the relative density of mixture, in (kg/m^3); **U** is the velocity, in (m/s); **T** is the temperature, in (K); **t** is the time, in (s); **p** is the relative pressure, in (Pa); **Γi** is the molecular diffusion coefficient of specie **i**; $\mathbf{S_{ct}}$ is the Schmidt's Number for high turbulence flows; **μ** is the average dynamic viscosity for fluid, in (m^2/s); $\mathbf{\mu_t}$ is the dynamic viscosity for turbulence in mixture, in (m^2/s); $\mathbf{S_I}$ is the source term due to the chemical reaction rate for specie **i**, which is given by $S_I = \omega_i / \rho$, function to reaction rate ω_i (**Kuramoto-Sivashinski' Equation**), Ariolli e Koch (2003), which is the key term to **Combustion Models**; $\mathbf{S_M}$ is the body force due to the gravity for each specie **i** in mixture, **i** and **j** is the Indicial Notation of Einstein, in relation to direction **x** and **y**, respectively, to discretization of space; **H** is the total enthalpy for mixture; **λ** is the Thermal Conductivity Coefficient of domain; **Γi** is the molecular diffusion coefficient; $\mathbf{S_E}$ is the molecular energy for species **i** in mixture; $\mathbf{P_{rt}}$ is the Prandtl's Number for turbulent flows; and $\rho.U\otimes U$ is the force due to Reynolds's Stress, in (N), which is the key term to **Turbulence Models**.

The equations (1),.(2) and (3) are obtained considering the following hypotheses: transient, compressible and turbulent flow; specific heat for species in mixture is constant; small convection effect; and uniform combustion.

Besides, the heat transfer for radiation can be analyzed by the Transportation Equation for Spectral Radiation (RTE), according to Beer *et al*. (1971) e Chung (2002):

$$\frac{d\,I_v\,(r,s)}{d\,s}=-\left(K_{av}+K_{sv}\right).\,I_v\,(r,s)+K_a\,.I_b\,(\nu,T)+\frac{k_{sv}}{4.\pi}.\int_{4.\pi} dI_v\,(r,s\acute{})\,.\,\Phi(s\bullet s\acute{})\,d\Omega+S \quad (4)$$

Where: **ν** is the emission frequency; **r** is the position vector; **s** is the direction vector; **s´** is the distance traveled by radiation; **Kav** is the absorption coefficient; **Ksv** is the reflexion coefficient; **Ib** is the intensity of emission in black body; **In** is the intensity of spectral radiation that depend on the position **r** and the direction **s**; **Ω** is the solid angle; **Φ** is function to phase of reflexion due to a immersed solid in domain; and **S** is the source term for the radiation (combustion).

From this way, the modeling of flow is done by application of different turbulence models to solve the term represented by Reynolds Stress Tensor, **Ui. Uj,** in Eq. (2).

Among the turbulence models applied by others authors, such as K-ε, RNG K-ε and Reynolds Stress Model (RSM), the RNG K-ε Model can be adopted because permits to describe flows in curved surfaces, where there is rotary flows, and have the capacity to capture the smallest vorticity generated by small holes in combustion chamber model. For this model, the Reynolds Stress Tensor **Ui. Uj** can be calculated by expression, Yadigaroglu (1998):

$$-\rho\,.\left(U_I\,.\,U_J\right)=2\,.\,\mu_t\,.\,S_{IJ}-\frac{2}{3}\,.\,\rho\,.\,k\,.\,\delta_{IJ} \tag{5}$$

Where $\boldsymbol{\delta_{IJ}}$ is the Dirac Function; and $\mathbf{S_{IJ}}$ is the Average Shear Tensor calculated by expression:

$$S_{IJ}=\frac{1}{2}\,.\left(\frac{\partial U_I}{\partial x_J}+\frac{\partial U_J}{\partial x_I}\right) \tag{6}$$

Where the turbulent viscosity $\boldsymbol{\mu_t}$ is given by:

$$\mu_t=C_\mu\,.\,\rho\,.\,\frac{k^2}{\varepsilon} \tag{7}$$

Where:

$$k=\frac{1}{2}\,.\left(U_I\,.\,U_J\right) \qquad \varepsilon=\nu\,.\left(\frac{\partial U_I}{\partial x_J}\,.\,\frac{\partial U_J}{\partial x_I}\right) \tag{8}$$

Thus, the main equations used to simulate the turbulence by RNG K-ε Model are:

$$\frac{\partial\left(\rho\,.\,U_J\,.\,k\right)}{\partial x_J}=\frac{\partial}{\partial x_J}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right).\,\frac{\partial k}{\partial x_J}\right]+2\,.\,\mu_t\,.\,S_{IJ}\,.\,S_{IJ}-\rho\,.\,\varepsilon \tag{9}$$

$$\frac{\partial\left(\rho\,.\,U_J\,.\,\varepsilon\right)}{\partial x_J}=\frac{\partial}{\partial x_J}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right).\,\frac{\partial \varepsilon}{\partial x_J}\right]+2\,.\,C_{\varepsilon 1}\,.\,\frac{\varepsilon}{k}\mu_t\,.\,S_{IJ}\,.\,S_{IJ}-C_{\varepsilon 2}\,.\,\rho\,.\,\frac{\varepsilon^2}{k} \tag{10}$$

Where there are five important constants, $\mathbf{C_\mu}$, $\mathbf{C_{\varepsilon 1}}$, $\mathbf{C_{\varepsilon 2}}$, $\boldsymbol{\sigma_k}$ e $\boldsymbol{\sigma_\varepsilon}$, whose typical values based on experimental tests for isotropic flows are presented by Tab. 6, where are shown others three auxiliary constants **η**, $\boldsymbol{\eta_0}$, and **β**:

Table 6 – Typical values for constants in turbulence model RNG K-ε

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	σ_k	σ_ε	η	η_0	β
0.076 to 0.094	$1.42-\dfrac{\eta\,.\left(1-\dfrac{\eta}{\eta_0}\right)}{1+\beta\,.\,\eta^3}$	1.51 to 1.85	0.6103 to 0.8256	0.6461 to 0.7897	$\left(\dfrac{k}{\varepsilon}\right).\left(2\,.\,S_{IJ}\,.\,S_{IJ}\right)^{1/2}$	3.94 to 4.82	0.012 to 0.017

Besides, among the combustion models such as, Eddy Dissipation Model (EDM), Finite Rate Chemistry (FRM), and Laminar Flamelet Model (LFM), the EDM Model or Eddy Break Up (EBU) can be adopted because it can describe combustion reactions with pre-mixture, where the effects of viscosity can be considered, between methane and air in nozzles, where the mechanism of reaction can be described by the following equations of combustion, Gurgel et al (2002):

Phase 1: the main reaction is given by expression:

$$CH_4+\left(O_2+3.76\,N_2\right)\rightarrow CO_2+2\,H_2O+3.76\,N_2 \tag{11}$$

Phase 2: the reaction is described using stoichiometric air in two steps:

$$CH_4+\left(O_2+3.76\,N_2\right)\rightarrow CO+2\,H_2O+3.76\,N_2+½\,O_2 \tag{12}$$

$$CO+½\,O_2\rightarrow CO_2 \tag{13}$$

According to Poinsot e Veynante (2005), the reaction rate can be affected by turbulence. From this way, the reaction rates for reactants and products are, respectively (kinetic chemical):

$$R_K = A \cdot \frac{\varepsilon}{k} \cdot \min\left(\frac{[I]}{\nu^{*}_{KI}}\right) \tag{14}$$

$$R_K = A \cdot B \cdot \frac{\varepsilon}{k} \cdot \left(\frac{\sum_P [I] \cdot W_I}{\sum_P \nu^{**}_{KI} \cdot W_I}\right) \tag{15}$$

Where **[I]** is the molar concentration of each species between the reagents; **A** is a proportionality constant, that depends on the physical properties of the reactants and if there is or not pre mixture and the conditions of reactions with or not free radicals; **P** tracks all the products generated in reaction **K**; $\mathbf{W_I}$ is the molecular weight of each component of the product; **B** is a numerical parameter that indicates if the simple reaction of or multiple stage. If **B** is negative, the formation of the products for determined reaction **K** is not performed; **ε** is the dissipation energy due the turbulence **k** is the turbulence in flow; and **ν** is the stoichiometric coefficient for reactants and products.

On the other hand, among the models for Heat Transfer by Radiation, such as, Rosseland (to opaque domains), P1, Monte Carlo, Discrete Transfer (the three to semi-transparency domains) and Spectral (to full transparency domains), Hottel and Sarofim (1967), the P1 Model can be adopted because permits to describe the radiation in domains with unitary emissive and unitary absorption in walls, which can be considered not catalytic (not affect the reactions).

The P1 Model or Radiation Differential Approximation, Raithby (1991), is a simplification of equation (4), considering that the radiation intensity is independent of direction and it is in an isotropic domain. In this model, the radiation heat flux in diffusion limit for domain is given by equation:

$$q_{r\nu} = -\frac{1}{3\cdot(K_{a\nu} - K_{s\nu}) - A \cdot K_{s\nu}} \cdot \nabla G_\nu \tag{16}$$

In equation (4), this term permits to get the following identity:

$$-\nabla \bullet \left[\frac{1}{3\cdot(K_{a\nu} - K_{s\nu}) - A.K_{s\nu}} \cdot \nabla G_\nu\right] = K_{a\nu} \cdot (E_{b\nu} - G_\nu) \tag{17}$$

Where **A** is the Linear Coefficient of Anisotropy.

From this, considering that the radiation emitted by walls in domain is independent of direction, the boundary condition can be calculated by equation:

$$n \cdot q_{r\nu} = -\frac{1}{3\cdot(K_{a\nu} - K_{s\nu}) - A.K_{s\nu}} \cdot \frac{\partial G_\nu}{\partial n^+} = \frac{\varepsilon_\nu}{2\cdot(2-\varepsilon_\nu)} \cdot [E_{b\nu} - G_\nu]_w \tag{18}$$

Where **n** is the normal vector in relation to the wall surface; $\mathbf{n}^+$ is the distance in the same direction of **n**; and **w** is the magnitude of $\mathbf{n}^+$ in the walls.

More details about the radiation model P1 are given by Raithby (1991).

On the other hand, the heat transfer mechanism in tested combustion chamber can be featured by the heating of domain and walls using radiation, while the cooling of walls and the dilution of heat gas is done by convection.

Thus, among the energy variation models used by CFD, such as, Isothermal Model; Thermal Energy Model; and Total Energy Model, it is adopted the Total Energy Model because the effects of the thermal energy and the kinetic energy are super posted in calculation of thermal balance by the first law of thermodynamic.

Besides, in general way, there are three different mechanisms for NOx emission. Table 7 shows these three mechanisms and its description, Lefebvre (1983).

Table 7 – Mechanisms for NOx generation, Lefebvre (1983)

Mechanism	Description
Thermal NOx	Zeldovich's Theory – It is produced NOx by the oxidation of atmospheric nitrogen in the gases after the flame.
Prompt NOx	Fenimore's Theory – it is generated NOx by the reactions of high speed in the front of the flame.
Fuel NOx	It is formed NOx by the oxidation of existing nitrogen in the fuel and can generates free radicals with low molecular weight, such as, NH_3, NH_2, NH, CN and others.

Among these models to simulate the NOx emission, the adopted models are Thermal Model of Zeldovich and Prompt Model of Fenimore, because of emission from methane combustion depends on oxidation of atmosphere nitrogen in front of flame and the high velocity reactions, respectively, given by the following basic reactions, Vandebroek *et al* (2003):

Thermal NOx:

$N_2 + O \leftrightarrow N + NO$

$N + O_2 \leftrightarrow NO + O$

$N + OH \leftrightarrow NO + H$

Prompt NOx:

$N_2 + CH \leftrightarrow HCN + N$

$N_2 + CH_2 \leftrightarrow HCN + NH$

5. Validation of CFD Calculation

In general, all CFD calculations shall be performed in comparison to the experimental results for simple geometries, in function to guarantee the right result with quality to represent the behavior of physical phenomena studied for more complex geometries.

A good example for it, which can be applied for combustion chambers, is the CFD validation for radiation calculation in a geometry proposed by Stuttaford (1997), which is used to validate the numerical method developed by Shah (1979).

This geometry domain consists of a little cylinder with length 5 (m) and diameter 2 (m). The walls have temperature of 227 (°C) and an emissivity of 0.8. The gas contains a hot region at a temperature of 1427 (°C) and has an absorption coefficient of 0.6 (m^{-1}). The external surface in cylinder is remain with temperature equal to 827 (°C) and has an absorption coefficient of 0.05 (m^{-1}), as it is shown by Fig. 10.

The calculation uses mesh with 89782 tetrahedral elements. The convergence condition has 50 iterations with goal error equal to 10^{-4} for heat transfer. Besides, the radiation model is Heat Transfer Discrete Model, where the radiation source can be discretized by 8, 64 and 128 rays with enough dimensions for that the average refraction is smaller than emission, because of work fluid is a hot gas without particles (photons). The adopted model to discrete the spectrum is Gray Model, because the spectrum is uniform. The Scattering Model is considered null, because that the term in transport equation for energy due the particles (photons) is not necessary and the domain is isotropic.

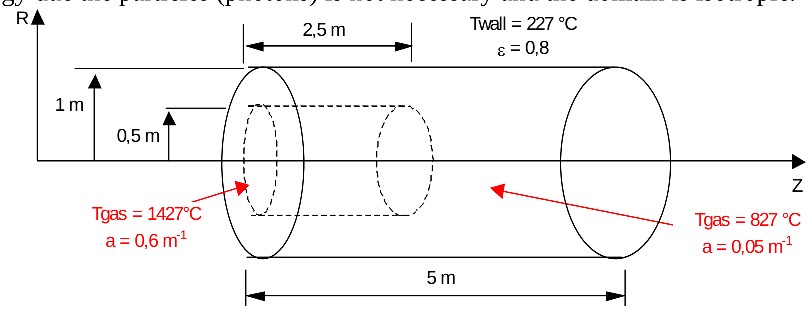


Figure 10 – Geometry Domain and boundary conditions for radiation calculation, Stuttaford (1997)

Table 8 presents the intensity of radiation in non-dimensional form obtained by experimental test and by CFD calculation, where **Io** is the maximum radiation intensity and equal to 80000 (W / m^2) and **L** is the length of cylinder and equal to 5 (m).

Table 8 – Results from Experimental Tests and CFD calculation

Distance Z / L	**0.0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**	**1.0**
Experimental Radiation Intensity I / Io	0.78	0.93	1.00	0.99	0.90	0.60	0.34	0.24	0.18	0.14	0.13
Numerical Radiation Intensity I / Io	0.74	0.90	0.98	0.97	0.86	0.56	0.31	0.21	0.15	0.11	0.09

From Tab. 8, it is possible to done a graphical comparison in relation to Non-dimensional Net Radiation Heat Flux for Axial Distance. In figure 8, this comparison is done, considering the maximum radiation intensity **Io** and the length of cylinder **L**.

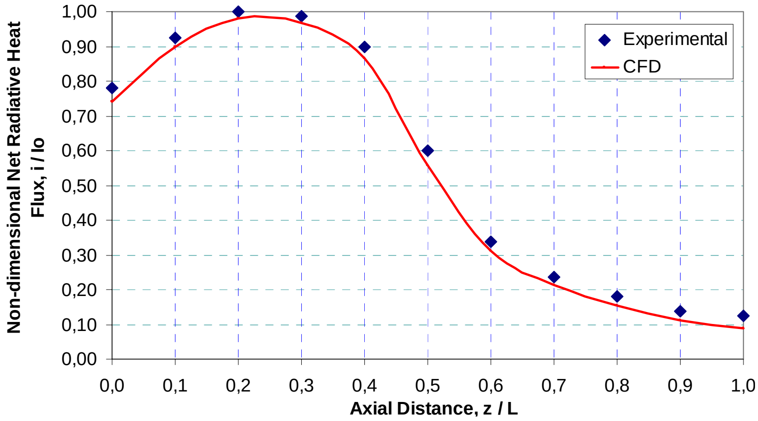


Figure 11 – Non-dimensional Radiation Heat Flux for Axial Distance

It is observed from Fig. 11 that the behavior of radiation intensity is due the characteristics of hot gas zone with temperature 1427 (°C) and the other hot gas zone with temperature 827 (°C).

The values of experimental and numerical tests are near and the CFD calculation permits to get satisfactory results in a simple geometry for radiation calculation. The maximum difference between the results is 4 (%) in non-dimensional axial distance equal to 0.5. From this, CFD can be used to study more complex geometries, where the heat transfer is done by radiation too, like as, in the combustion cases.

6. Analysis of Results

In general, the duration for the calculations is approximately equal to 14 hours using a computer DELL with double processor of 3.4 GHz and 1GByte of RAM, considering a goal error equal to 10^{-5} for mass flow, velocity, turbulence and turbulent dissipation energy in CFX ® v 5.7. Figure 12 presents the distributions of velocity and pressure.

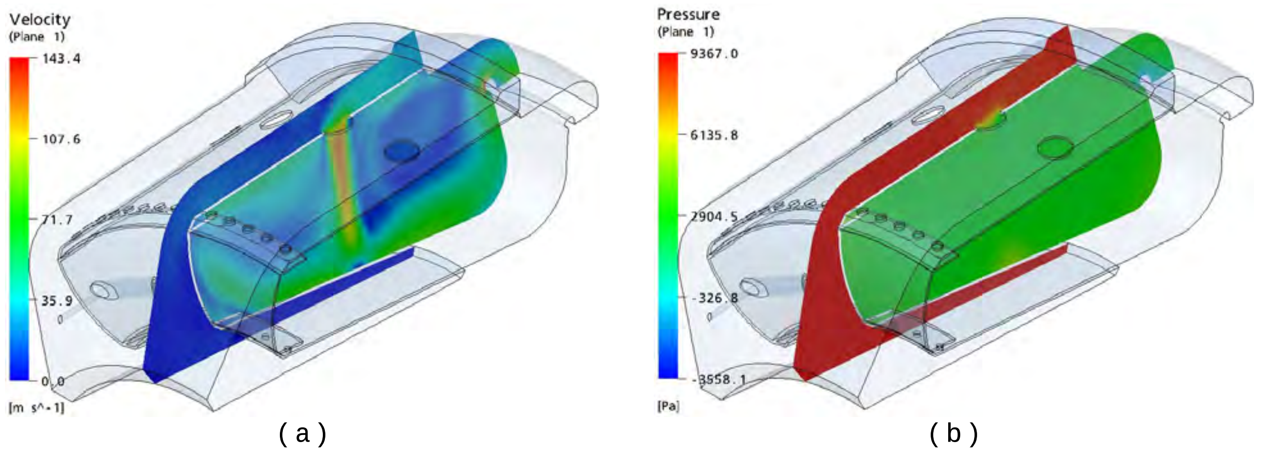


Figure 12 – (a) Velocity contour; (b) Pressure contour

Figure 13 shows the distribution of temperature and the format of flame from iso-surfaces of temperature, with gradients equal to 200 (°C), approximately, where is shown that the flame is formed from a specific distance in relation to the nozzle with low dispersion. It is a characteristic for this kind of annular combustion chamber.

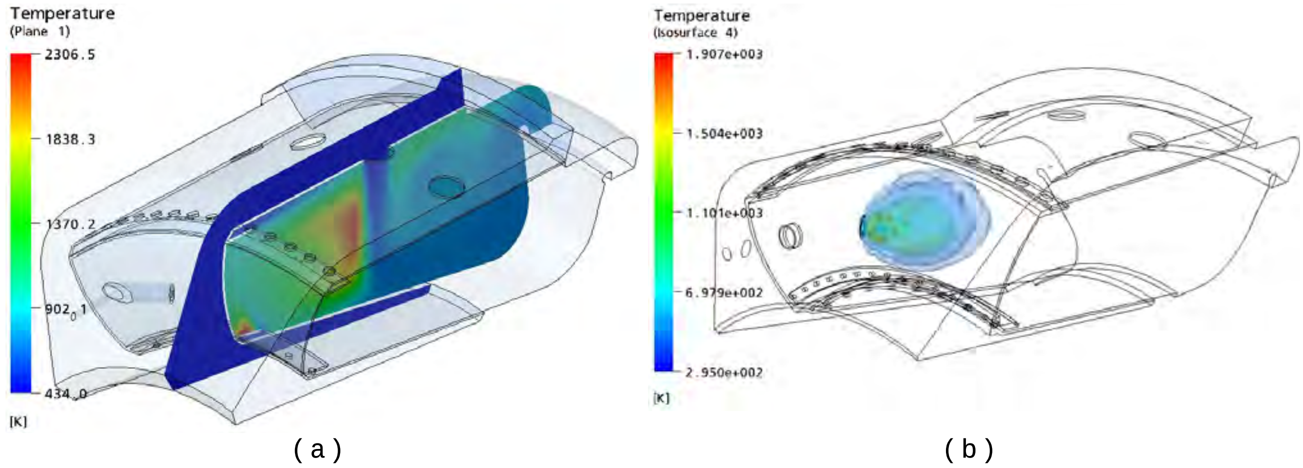


Figure 13 – (a) Temperature contour; (b) Iso-surfaces of temperature

The distribution of iso-surfaces of temperature shows that the flame has dispersion in annular combustion chamber, as well as, the temperature is affected by rotary flow. This flow changes the position where the flame has its maximum temperature after the ignition. Maybe, it is necessary to change the dimensions of lateral holes of dilution air in Liner.

Besides, in longitudinal surface that is shown in Fig. 12 and 13, it is possible to determine the variation for velocity, pressure and temperature along the local axle from nozzles, which is parallel to main axle of combustion chamber, according to Fig.14. Table 9 presents the values for these greatnesses for this local axle obtained after the convergence.

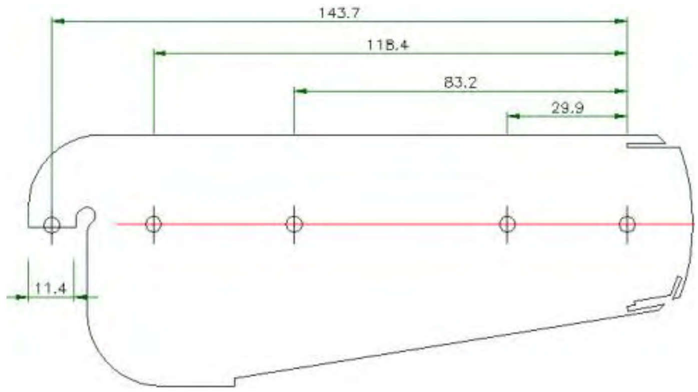


Figure 14 – Position of **Z** axle from nozzle

Table 9 – Values obtained after the convergence

Greatness	Symbol	Unit	Values				
Position in relation to nozzle	Z	(mm)	0	30	83	118	144
Average velocity of flow	V_{GAS}	(m/s)	52	45	32	27	62
Average pressure	P_{GAS}	(Pa)	2350	3200	3800	4100	0
Gas temperature	T_{GAS}	(°C)	907	2033	1012	810	630
Gas density	ρ_{GAS}	(kg/m^3)	0.35	0.18	0.36	0.42	0.52
Reynolds' number	RE_{GAS}	(--)	4.71E+07	4.07E+07	2.90E+07	2.44E+07	5.61E+07

Besides, others important parameters that can be determined are the maximum temperature of flame and the temperature of gas in exhaustion, whose values are 2033 (°C) and 630 (°C), respectively, which are coherent with data from manufacturer Solar Turbine, whose experimental values for temperature of gas in exhaustion is 637.9 (°C). Besides, this maximum temperature computed by Combustion Model EDM is near to the maximum temperature of flame esteemed by GASEQ ® V 7.2, approximately 2220 (°C) for methane gas.

From Tab. 9, it is possible to determine the characteristic curves of operation for the model, as it is shown from Fig. 15 to Fig. 17, whose reference is the Z-axle in longitudinal surface (see Fig. 14).

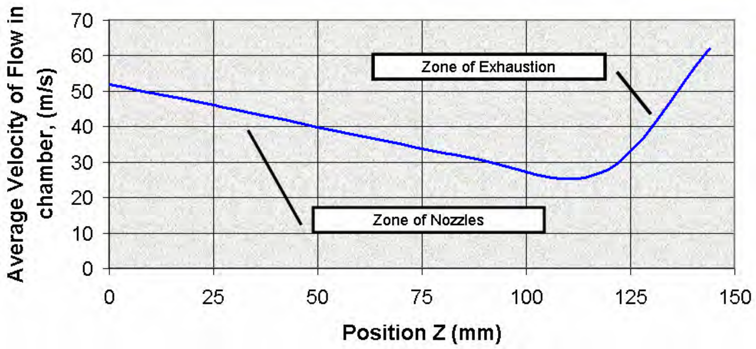


Figure 15 – Characteristic velocity curve

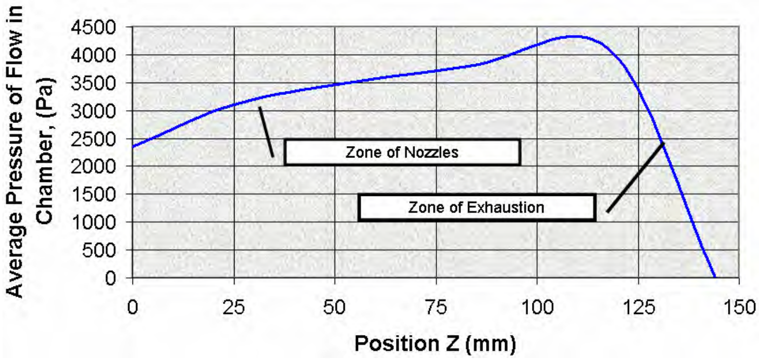


Figure 16 – Characteristic pressure curve

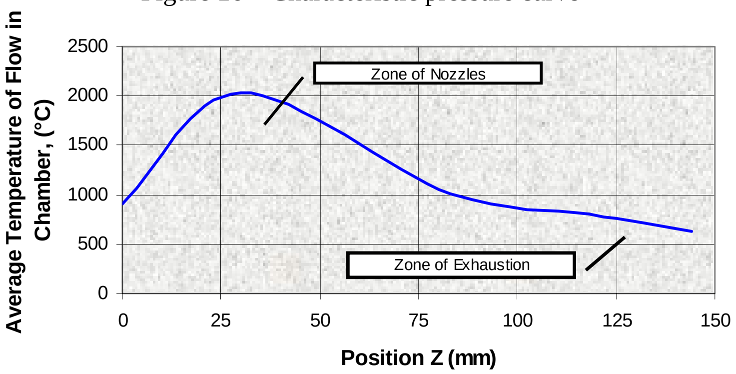


Figure 17 – Characteristic temperature curve

From Fig. 17, it is possible to identify the maximum temperature of flame is near to the nozzles, but its position is affected by the secondary flow, which can be represented by high flow of air from dilution holes in lateral surface (for distances between 60 and 90 (mm) from nozzles) and by the rotary flow due to the inclination of nozzles in relation to the main axle on combustion chamber, respectively, Figs 12(a) and 13(a). Because of it, it is possible to avoid the approximation of hot gases in relation to the metallic walls, too.

The velocity and pressure values obtained in Figs. 15 and 16, respectively, are affected by the turbulence zone near to the nozzles and exhaustion zones; see Fig. 13(a).

Other characteristic that can be identified is the rotary flow in zone of nozzles, which can benefit the combustion, because it contributes to increase the residence time.

Other important information is the efficiency of combustion chamber that can be estimated using the following equation, Odgers and Carrie (1973):

$$\eta_{CC} = 100 - \left(0.95 + \frac{37.5}{\%\ CO_2}\right).\frac{(T_{GAS} - T_o)}{100} \qquad (19)$$

Where **To** is the reference temperature in environment, in [°C].

In tested model, the reference temperature is 22 (°C). The percentage of CO_2 in outlet surface is, approximately, 17.5 (%) and the Temperature of gas or flame is 2033 (°C). So, the combustion efficiency is, approximately, 37.8 (%) for this combustion chamber in these operation condition.

According to manufacturer Solar Turbines, the combustion efficiency for this equipment is between 35 (%) and 40 (%) for the efficiency of cycle between 25 (%) and 30 (%) in relation to the power 50 (kW).

7. Conclusions

In this work, the important contribution is the development about a practical scheme using commercial softwares, like as Gatecycle®, GASEQ® and CFX ® to study the behavior of combustion and the flow in annular combustion chambers for small gas turbines to attend its adaptability and economic feasible to use different fuels.

Considering the methane gas to represent the natural gas, whose chemical composition is done mainly by 88(%) in volume of methane, as well as different models for flow, combustion, heat transfer and emission in CFD, whose boundary condition are set by parameters from thermal cycle of small gas turbine and chemical concentrations of reactants and products for combustion, the combustion chamber can be features by the following notes:

(a) From pressure, velocity and temperature distributions, the high flow of air from dilution holes in lateral surface in Liner affects the position where it is the maximum temperature of flame in relation to nozzles, whose value is 2033 (°C) for distances between 60 and 90 (mm) from nozzles;

(b) The inclination of nozzles can induce a rotary flow, which affects the position and stability of flame and the residence time for combustion;

(c) The methane gas signs that the flame can be dispersed, which obligates in new design of combustion chamber. This new design is to avoid the approximation of hot gases in relation to the metallic walls;

(d) The temperature of gas in exhaustion obtained by CFD is equal to 630 (°C), whose value is near to the temperature from manufacturer Solar Turbine, which is equal to 637.9 (°C); and

(e) The CFD simulation permits to esteem the combustion efficiency around 38 (%) for this tested model. This is a satisfactory precision, once that the manufacturer esteems this efficiency between 35 (%) and 40 (%) for power 50 (kW).

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