PRELIMINARY DESIGN OF GAS TURBINE TUBULAR COMBUSTION CHAMBER USING POTENTIAL ALTERNATIVE FUELS FOR STATIONARY GAS TURBINES IN THE BRASILIAN CONTEXT

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Abstract. Moderate compression ratio and versatile combustion systems are requisites for the design of stationary gas turbines. In the present days, it is important to make allowance for the use of conventional and alternative fuels like petroleum distillates, gasified coal, natural gas or bio-syngas, bio-ethanol, bio-diesel. It is of great interest, therefore, to advance the knowledge of the implications of the use of such different fuels in the design of the combustor. This study is concerned with the preliminary design of gas turbine tubular combustion chamber and the numerical simulation of its performance using own computational program based in semi-empirical formulation. Ethanol and diesel were chosen as typical fuels. The characterization of conventional and alternative fuels for stationary gas turbines has been carried out in the Brazilian context. Inlet and outlet boundary conditions like air mass flow, fuel mass flow, pressure, temperature, and equivalence ratio were previously fixed having a specific gas turbine in mind. Direct fuel injection was adopted and diffusion flames used for both gaseous and liquid fuels. Calculations for the dimensions of the air admission holes have been performed and exhaust gas temperatures in the several zones of the combustion chamber have been determined. In this study has been analyzed the factors that influence the combustor performance, combustion efficiency, pressure loss, outlet temperature profile and the operation stability limits. Preliminary dimensions of the flex combustion chamber are shown and comments are made for the sake of choice of multi-fuel combustor.

Keywords: alternative fuels, fuel flexibility, numerical simulation, combustor design, gas turbine

1. INTRODUCTION

Gas turbines find enormous applications in aeronautical, automotive, naval, electric power generation and in oil industry. Pollutant emissions and the alternative fuels are being of much concern in the last years, so that high priority has been given to these subjects.

In the aeronautical industry, the reduction of the pollutant emissions is being deeply considered. Use of mixtures of aeronautical fuels and their possible substitutes, the bio and synthetic fuels is being, therefore, considered.

In the electric power industry the restrictions in the supply of natural gas and other low ashes content distilled fuels have driven the interest of researchers to identify other possible fuels, the alternative fuels (Dark *et al.*, 2001). Generally, all coal-derived fuels, heavy crude, tar, shale and biofuels are considered as alternative fuels.

In these applications, gas turbines are for large powers and their combustion systems are usually developed for a single specific fuel (natural gas or diesel). Conventional diffusion flame technology is used and high levels of NO_X and partially unburnt species are emitted.

Fossil fuels reserves are finite, non-renewable in nature and are increasingly difficult to be exploited. Moreover, problems in the international oil market are becoming increasingly common and their excessive utilization has caused serious environmental damages.

Given these facts, programs focused on the research of alternative energy sources have been strongly encouraged in the United States, Canada, European Union, Brazil and other countries. In recent years, aiming at making industrial processes environmentally friendlier, researches of potential fuels for use in gas turbines have been promoted. Among these are liquid and gaseous fuels from biomass, syngas from coal, biogas, refinery gas and other unconventional sources.

A major advantage of any thermal engine (in these specific case, gas turbines), using continuous processes of combustion, is its ability to successfully burn a wide variety of fuels, the "fuel flexible gas turbine combustor" (Barringer, 2001).

Much research is being carried out in this field, aiming at the design and development of gas turbine combustors to successfully burn low, medium and high calorific value liquid and gaseous fuels. This paper describes the development of a methodology focused on the design of stationary gas turbines combustion chambers with the ability to burn conventional and alternative fuels. This research studies the fuel combustion characteristics as function the major parameters used to calculate combustor performance: air mass flow, fuel mass flow, pressure, temperature, and equivalence ratio. In a later phase of the research, aerodynamics, temperature traverse quality and cooling will be considered.

Numerical models are used to calculate the combustion efficiency of these fuels in a specially designed combustor, as well as their influence on the pollutants emission under representative operating conditions, generating information that can be used during the design stage of the gas turbine, having control of pollutant emissions.

2. SIZING THE COMBUSTOR

Sizing of the combustion chamber was based on zero and one-dimensional approaches developed by Lefebvre, Melconian and Modak (1985), and Gordon and McBride's methodology for the thermokinetic equilibrium, flammability limit and near-global simplified kinetic mechanisms (1993). These approaches were used simultaneously into successive substitution using Newton-Raphson, LU factorization and Lagrange polynomials (Collins, 2003).

There is the necessity to analyze several aspects of combustion during the combustor design if fuel flexibility is sought. Stull and Prophet (1971) suggested and are considered in this work:

- Aerodynamic and chemical considerations to calculate the housing and liner cross-sectional areas, as well as determining the primary, secondary and dilution zone geometry;
- Calculation of the distribution for cooling air and air mass flow in the primary, secondary and dilution zone;
- Diffuser characteristics;
- Swirler characteristics;
- Calculation of flame temperature in the combustor zones;
- Calculation of the holes for air intake in the different zones of the combustor.

2.1. Aerodynamic considerations

Aerodynamic processes play vital part in the design and performance of gas turbine combustion systems. If the aerodynamic design is good and fuel injection system is matched appropriately then, it is ensured the operation of the combustor without major problems (Ramsden and Barbosa, 1994).

The process of mixing air with fuel is extremely important in the combustion and dilution zones. A good mixture in the primary zone is essential for high burn rate and minimization of NO_X and soot formation. Achieving appropriate temperature distribution in the combustor exhaust is dependent on the degree of mixing of dilution air and combustion products in the dilution zone. Satisfactory fuel-air mixture inside the liner and steady flow throughout the combustor are important features sought during the combustor design, to minimize the combustor length, parasitic losses and pressure loss (Darby, 2001).

Use is made of two dimensionless parameters related to pressure loss in the combustor during the design of the combustion chamber:

a) The ratio of total pressure loss in the combustor to the total pressure input ($\Delta P_{3-4}/P_3$).

b) The ratio of total pressure loss in the combustor to the reference dynamic pressure ($\Delta P_{3-4}/q_{ref}$).

Equation (1) shows how these parameters are related and how they are used to calculate the housing cross-sectional area of the combustor (Lefebvre, 1999).

$$A_{ref} = \left[\frac{R_a}{2} \left(\frac{\dot{m}_3 T_3^{0.5}}{P_3} \right)^2 \left(\frac{\Delta P_{3-4}}{q_{ref}} \right) \left(\frac{\Delta P_{3-4}}{P_3} \right)^{-1} \right]^{0.5} \tag{1}$$

where:

A_{ref}	- Cross-sectional area of the combustor housing, m^2;
$\left(\Delta P_{3-4} / P_3 \right)$	- Ratio of total pressure loss to input total pressure, dimensionless;
$\left(\Delta P_{3-4} / q_{ref} \right)$	- Ratio of total pressure loss to reference dynamic pressure, dimensionless;
$\dot{m}_3$	- Air mass flow at the combustor inlet, kg/s;
P_3	- Total pressure at the combustor inlet, Pa
R_a	- Air universal gas constant, Nm/kg·K;
T_3	- Total temperature at the combustor inlet, K.

2.2. Thermochemical considerations

The primary purpose of the combustion is to raise the air flow temperature through efficient fuel combustion. From the design point, one important requirement is how to relate to combustion efficiency to the operating parameters (pressure, temperature and air mass flow), together with the dimensions of the combustor (Zamuner et al., 2002). The methodology used in this research is based on the burning speed. For a given fuel-air ratio (F/A), the combustion

efficiency η_θ is correlated to the θ parameter, as shown in Eq. (2). When the value of θ is 73E+06 (SI units), the efficiency is highest, close to 100%.

The combustor housing cross-sectional area is calculated at that point. A correction factor, b in Equation (3), is used to correct the inlet temperature to the combustor. It is function of equivalence ratio in the primary zone.

$$\eta_\theta = f(\theta) = \theta = \left[\frac{P_3^{1.75} A_{ref} D_{ref}^{0.75} \exp\left(\frac{T_3}{b}\right)}{\dot{m}_3} \right] \tag{2}$$

$$b = 245[1.39 + \ln(\phi_{ZP})] \quad for \quad 0.6 < \phi_{ZP} \leq 1.0$$
$$or$$
$$b = 170[2.00 - \ln(\phi_{ZP})] \quad for \quad 1.0 < \phi_{ZP} \leq 1.5 \tag{3}$$
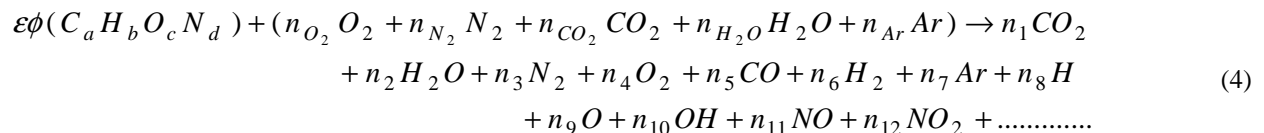
where:

b	- Temperature correction factor at combustor inlet, dimensionless;
D_{ref}	- Diameter of the housing cross-sectional area, m;
θ	- Correlation parameter of combustion efficiency, dimensionless;
ϕ_{ZP}	- Equivalence ratio at primary zone, dimensionless;
η_θ	- Combustion efficiency, dimensionless.

Equivalence ratios in the primary zone are guessed and, using a methodology based on thermokinetic equilibrium, the fuel flammability curve is built to delimit the gas turbine operational conditions.

The methodology used is the one developed by Gordon and McBride (1993), which had been used in gas turbine combustors by Lazaroiu (2007) for the free energy minimization. The chemical equilibrium condition was established using the Gibbs free energy minimization. Temperature and pressure were used as thermodynamic variables.

Fuel reaction with air is modeled by Eq. (4), which includes the equivalence ratio. For this study the most significant twelve combustion products were considered.

$$\varepsilon\phi(C_a H_b O_c N_d) + (n_{O_2} O_2 + n_{N_2} N_2 + n_{CO_2} CO_2 + n_{H_2O} H_2O + n_{Ar} Ar) \rightarrow n_1 CO_2$$
$$+ n_2 H_2O + n_3 N_2 + n_4 O_2 + n_5 CO + n_6 H_2 + n_7 Ar + n_8 H$$
$$+ n_9 O + n_{10} OH + n_{11} NO + n_{12} NO_2 + ... \tag{4}$$

where:

a	- Number of carbon atoms;
Ar	- Argon;
b	- Number of hydrogen atoms;
c	- Number of oxygen atoms;
d	- Number of nitrogen atoms;
n	- Number of moles for the reactants and products, mol;
ε	- Molar air-fuel ratio;
ϕ	- Equivalence ratio.

A set of 12 equations are, thus, needed to calculate the molar concentration of the twelve chemical species. Five equations are obtained from the chemical elements balance C/H/N/O/Ar between the reactants and products. The seven remaining equations are non-linear and they are obtained from chemical dissociation.

Equations (5) to (10) were obtained from the mass conservation of the main chemical elements (Ferguson, 1985):

$$(y_{CO_2} + y_{CO})N_t - \varepsilon\phi a - n_{CO_2} = 0 \tag{5}$$

$$(2y_{H_2O} + 2y_{H_2} + y_H + y_{OH})N_t - \varepsilon\phi b - 2n_{H_2O} = 0 \tag{6}$$

$$(2 y_{N_2} + y_{NO} + y_{NO_2}) N_t - \varepsilon \phi d - 2 n_{N_2} = 0 \tag{7}$$

$$(2 y_{CO_2} + y_{H_2O} + 2 y_{O_2} + y_{CO} + y_O + y_{OH} + y_{NO} + 2 y_{NO_2}) N_t$$
$$- \varepsilon \phi c - 2 n_{O_2} - 2 n_{CO_2} - n_{H_2O} = 0 \tag{8}$$

$$(y_{Ar}) N_t - n_{Ar} = 0 \tag{9}$$

$$N_t = \sum_{i=1}^{12} n_i \quad and \quad \sum_{i=1}^{12} y_i - 1 = 0 \tag{10}$$

where:

N_t - Total number of moles of the mixture, moles;

y - Mole fraction.

Using concepts of thermokinetic equilibrium for the final reactions, seven non-redundant equilibrium relationships were used to calculate the unknown mole fractions y_i and the number of total moles N_t. These expressions are part of the solution set involving the combustion products, as shown by Eq. (11, 12, 13, 14, 15, 16 and 17) (Ferguson, 1985).

$$\frac{1}{2} H_2 \Leftrightarrow H \quad and \quad K_1 = \frac{y_H P^{1/2}}{y_{H_2}^{1/2}} \tag{11}$$

$$\frac{1}{2} O_2 \Leftrightarrow O \quad and \quad K_2 = \frac{y_O P^{1/2}}{y_{O_2}^{1/2}} \tag{12}$$

$$\frac{1}{2} H_2 + \frac{1}{2} O_2 \Leftrightarrow OH \quad and \quad K_3 = \frac{y_{OH}}{y_{O_2}^{1/2} y_{H_2}^{1/2}} \tag{13}$$

$$\frac{1}{2} O_2 + \frac{1}{2} N_2 \Leftrightarrow NO \quad and \quad K_4 = \frac{y_{NO}}{y_{O_2}^{1/2} y_{N_2}^{1/2}} \tag{14}$$

$$H_2 + \frac{1}{2} O_2 \Leftrightarrow H_2O \quad and \quad K_5 = \frac{y_{H_2O}}{y_{O_2}^{1/2} y_{H_2} P^{1/2}} \tag{15}$$

$$CO + \frac{1}{2} O_2 \Leftrightarrow CO_2 \quad and \quad K_6 = \frac{y_{CO_2}}{y_{CO} y_{O_2}^{1/2} P^{1/2}} \tag{16}$$

$$NO + \frac{1}{2} O_2 \Leftrightarrow NO_2 \quad and \quad K_7 = \frac{y_{NO_2}}{y_{NO} y_{O_2}^{1/2} P^{1/2}} \tag{17}$$

where:

K - Equilibrium constant for constant pressure;

P - Total pressure at the combustor, atm.

The equilibrium constants of Eqn. (11) to (17) were taken from NIST-JANAF Thermochemical Tables as functions of temperature, calculated using Eq. (18).

$$\log K_i \big|_{reaction} = A_i \ln\left(\frac{T}{1,000}\right) + \frac{B_i}{T} + C_i + D_i T + E_i T^2 \tag{18}$$

where:

A, B, C, D, E	- Correlation coefficient of equilibrium curve at constant pressure;
i	- Index for each non-redundant equilibrium reaction;
T	- Total temperature at equilibrium state, K.

Equations 5 to 8 were linearized and a new set of equations (11 to 17) was obtained. Such equations are written in terms of y_{N2}, y_{O2}, y_{CO}, and y_{H2} respectively and are shown below (Ferguson, 1985):

$$f_i + \frac{\partial f_i}{\partial y_{CO_2}}\Delta y_{CO_2} + \frac{\partial f_i}{\partial y_{H_2O}}\Delta y_{H_2O} + \frac{\partial f_i}{\partial y_{O_2}}\Delta y_{O_2} + \frac{\partial f_i}{\partial y_{N_2}}\Delta y_{N_2} = 0 \quad for \quad i = 1,2,3,4 \tag{19}$$

where:

f	- Linear function based on y_{N2}, y_{O2}, y_{CO}, and y_{H2};
y_{CO}	- Mole fraction of carbon monoxide;
y_{H2}	- Mole fraction of carbon hydrogen;
y_{N2}	- Mole fraction of nitrogen;
y_{O2}	- Mole fraction of oxygen;
$\partial/\partial y_i$	- Partial derivative respect i mole fraction.

Equation (19) can be rewritten in terms of f_1, f_2, f_3 and f_4, as well as y_{N_2}, y_{O_2}, y_{CO} and y_{H_2} as follows.

$$\begin{bmatrix} f_1 + \dfrac{\partial f_1}{\partial y_{N_2}}\Delta y_{N_2} & \dfrac{\partial f_1}{\partial y_{O_2}}\Delta y_{O_2} & \dfrac{\partial f_1}{\partial y_{CO}}\Delta y_{CO} & \dfrac{\partial f_1}{\partial y_{H_2}}\Delta y_{H_2} & = & 0 \\[2mm] f_2 + \dfrac{\partial f_2}{\partial y_{N_2}}\Delta y_{N_2} & \dfrac{\partial f_2}{\partial y_{O_2}}\Delta y_{O_2} & \dfrac{\partial f_2}{\partial y_{CO}}\Delta y_{CO} & \dfrac{\partial f_2}{\partial y_{H_2}}\Delta y_{H_2} & = & 0 \\[2mm] f_3 + \dfrac{\partial f_3}{\partial y_{N_2}}\Delta y_{N_2} & \dfrac{\partial f_3}{\partial y_{O_2}}\Delta y_{O_2} & \dfrac{\partial f_3}{\partial y_{CO}}\Delta y_{CO} & \dfrac{\partial f_3}{\partial y_{H_2}}\Delta y_{H_2} & = & 0 \\[2mm] f_4 + \dfrac{\partial f_4}{\partial y_{N_2}}\Delta y_{N_2} & \dfrac{\partial f_4}{\partial y_{O_2}}\Delta y_{O_2} & \dfrac{\partial f_4}{\partial y_{CO}}\Delta y_{CO} & \dfrac{\partial f_4}{\partial y_{H_2}}\Delta y_{H_2} & = & 0 \end{bmatrix} \tag{20}$$

Equation (20) can be rewritten in matrix form, as indicated in Eq. (21) and (22). LU factorization and Newton-Raphson method were used for the solution of Eqn. (22).

$$\begin{bmatrix} \dfrac{\partial f_1}{\partial y_{N_2}} & \dfrac{\partial f_1}{\partial y_{O_2}} & \dfrac{\partial f_1}{\partial y_{CO}} & \dfrac{\partial f_1}{\partial y_{H_2}} \\[2mm] \dfrac{\partial f_2}{\partial y_{N_2}} & \dfrac{\partial f_2}{\partial y_{O_2}} & \dfrac{\partial f_2}{\partial y_{CO}} & \dfrac{\partial f_2}{\partial y_{H_2}} \\[2mm] \dfrac{\partial f_3}{\partial y_{N_2}} & \dfrac{\partial f_3}{\partial y_{O_2}} & \dfrac{\partial f_3}{\partial y_{CO}} & \dfrac{\partial f_3}{\partial y_{H_2}} \\[2mm] \dfrac{\partial f_4}{\partial y_{N_2}} & \dfrac{\partial f_4}{\partial y_{O_2}} & \dfrac{\partial f_4}{\partial y_{CO}} & \dfrac{\partial f_4}{\partial y_{H_2}} \end{bmatrix} \begin{bmatrix} \Delta y_{N_2} \\[2mm] \Delta y_{O_2} \\[2mm] \Delta y_{CO} \\[2mm] \Delta y_{H_2} \end{bmatrix} = \begin{bmatrix} -f_1 \\[2mm] -f_2 \\[2mm] -f_3 \\[2mm] -f_4 \end{bmatrix} \tag{21}$$

$$[A_{il}][\Delta y_j] = [-f_i] \quad for \quad i = 1,2,3,4 \quad and \quad j = 3,4,5,6 \quad and \quad l = 1,2,3,4 \tag{22}$$

where:

$[A_{il}]$	- Matrix of the $\partial f_i / \partial y_i$ partial derivatives;
$[-f_i]$	- Vector of linear functions based on y_{N2}, y_{O2}, y_{CO}, and y_{H2};
$[\Delta y_j]$	- Vector of the mole fractions variation based on N_2, O_2, CO, and H_2.

For several operating conditions, a set of solutions of Eq. (22) was obtained. Subsequently, based on energy conservation and adiabatic combustion, Eq. (23) was obtained. With equivalence ratio variation from lean to rich mixture, the flammability curve of each fuel was obtained. By inverse interpolation of Lagrange polynomials, for given temperature the equivalence ratio in the combustor primary zone was obtained.

$$\sum_r N_r \left({}^*h_{f,r} + {}^*\Delta h_{s,r} \right) - \sum_p N_p \left({}^*h_{f,p} + {}^*\Delta h_{s,p} \right) = 0 \tag{23}$$

where:

$*h_{f,p}$	- Enthalpy of formation for the products, kJ/kmol;
$*h_{f,r}$	- Enthalpy of formation for the reactants, kJ/kmol;
N_p	- Number of moles of the products, mol;
N_r	- Number of moles of the reactants, mol;
p	- Products;
r	- Reactants;
$*\Delta h_{s,p}$	- Sensible enthalpy of products, kJ/kmol;
$*\Delta h_{s,r}$	- Sensible enthalpy of reactants, kJ/kmol.

The equivalence ratio value in the combustor primary zone is used in Eq. (3) to calculate the correction factor of the inlet temperature in the combustion chamber and then this parameter is used in Eq. (2) to calculate the cross-sectional area of the combustor casing. In the sequence, Eq. (1) gives the cross-sectional area of the combustor liner.

2.3. Basic settings for the combustor

The largest values obtained for the cross-sectional areas, calculated from aerodynamic and thermochemical considerations, were chosen for the casing and combustor liner, what would be appropriate to accommodate the aerodynamics and chemistry at any operation regime. Other dimensions were, then, calculated using Eq. (24, 25, 26 and 27) (Sawyer, 1985).

$$L_{ZP} = 0.75 D_{ft} \tag{24}$$

$$L_{ZS} = 0.5 D_{ft} \tag{25}$$

$$L_{ZD} = \left(\frac{T_{max} - T_4}{T_4 - T_3} \right) D_{ft} \tag{26}$$

$$L_{T_{ZD}} = 0.5 L_{ZD} \tag{27}$$

where:

D_{ft}	- Diameter of the liner cross-sectional area, m;
L_{ZP}	- Length of combustor primary zone, m;
L_{ZS}	- Length of combustor secondary zone, m;
L_{ZD}	- Length of combustor dilution zone, m;
$L_{T_{ZD}}$	- Length of combustor transition dilution zone, m;
T_{max}	- Maximum combustor temperature, K;
T_3	- Temperature at the combustor inlet, K;
T_4	- Temperature at the combustor exit, K.

For the calculated equivalence ratio in the combustor primary zone, the air distribution at the other zones was obtained, using Eqn. (28, 29, 30 and 31) (Sawyer, 1985).

$$\% \, Air_{cooling} = 0.1T_3 - 30 \quad and \quad \dot{m}_{cooling} = (\% \, Air_{cooling})\dot{m}_3 \tag{28}$$

$$\dot{m}_{ZP} = \dot{m}_3 \left(\frac{\phi_{overall}}{\phi_{ZP}} \right) \tag{29}$$

$$\dot{m}_{ZS} = \dot{m}_3 \left(\frac{\phi_{overall_{max}}}{0.8} \right) - \dot{m}_{ZP} \tag{30}$$

$$\dot{m}_{ZD} = \dot{m}_3 - \dot{m}_{ZP} - \dot{m}_{ZS} - \dot{m}_{cooling} \tag{31}$$

where:

$\% \, Air_{cooling}$	- Percentage of cooling air, dimensionless;
$\dot{m}_{cooling}$	- Cooling air mass flow, kg/s;
$\dot{m}_{ZP}$	- Air mass flow at combustor primary zone, kg/s;
$\dot{m}_{ZS}$	- Air mass flow at combustor secondary zone, kg/s;
$\dot{m}_{ZD}$	- Air mass flow at combustor dilution zone, kg/s;
$\phi_{overall}$	- Overall equivalence ratio, dimensionless;
$\phi_{overall \, max}$	- Maximum overall equivalence ratio, dimensionless.

The diffuser, swirler and holes for air intake in the primary, secondary, dilution and cooling zones are, subsequently calculated.

3. ANALYSIS OF RESULTS

The tubular combustor performance parameters, for stationary gas turbine designed to burn diesel and ethanol, were calculated using the methodology detailed above. Special attention was given to flammability limits, overall equivalence ratio ($\phi_{overall}$), lean equivalence ratio (ϕ_{lean}), rich equivalence ratio (ϕ_{rich}), equivalence ratio in the combustor primary zone (ϕ_{ZP}), to name the most important for the study, having in mind the analysis of a newly designed combustor at all the operating conditions of the gas turbine in service. These results are summarized in Tab. 1, Fig. 1 and 2.

Table 1. Major characteristics of a stationary gas turbine combustor burning diesel and ethanol.

Parameters	Diesel fuel			Ethanol liquid fuel		
	Maximum Power	Base load	Idle	Maximum Power	Base load	Idle
Temperature at combustor inlet (K)	800	1,060	350	800	1,060	350
Temperature at combustor exit (K)	1,600	1,390	700	1,600	1,390	700
Overall equivalence ratio	0.35	0.29	0.13	0.35	0.286	0.128
Lean equivalence ratio	0.325	0.223	0.514	0.282	0.196	0.435
Rich equivalence ratio	2.8	2.74	2.215	2.8	2.8	2.8
$\phi_{overall}/\phi_{lean}$	1.07	0.65	0.24	1.232	0.74	0.294
$\phi_{overall}/\phi_{rich}$	0.124	0.052	0.058	0.124	0.0517	0.0457
ϕ_{ZP}	1.393	0.582	0.514	1.179	0.4925	0.435
Temperature correction factor (b)	283.61	208.03	177.47	312.05	167.05	136.49

Figures 1 and 2 show the equilibrium temperature changing with the equivalence ratio. The adiabatic flame temperature increases as equivalence ratio (ϕ) is increased until the equivalence ratio of approximately 1 to 1.1, decreasing subsequently.
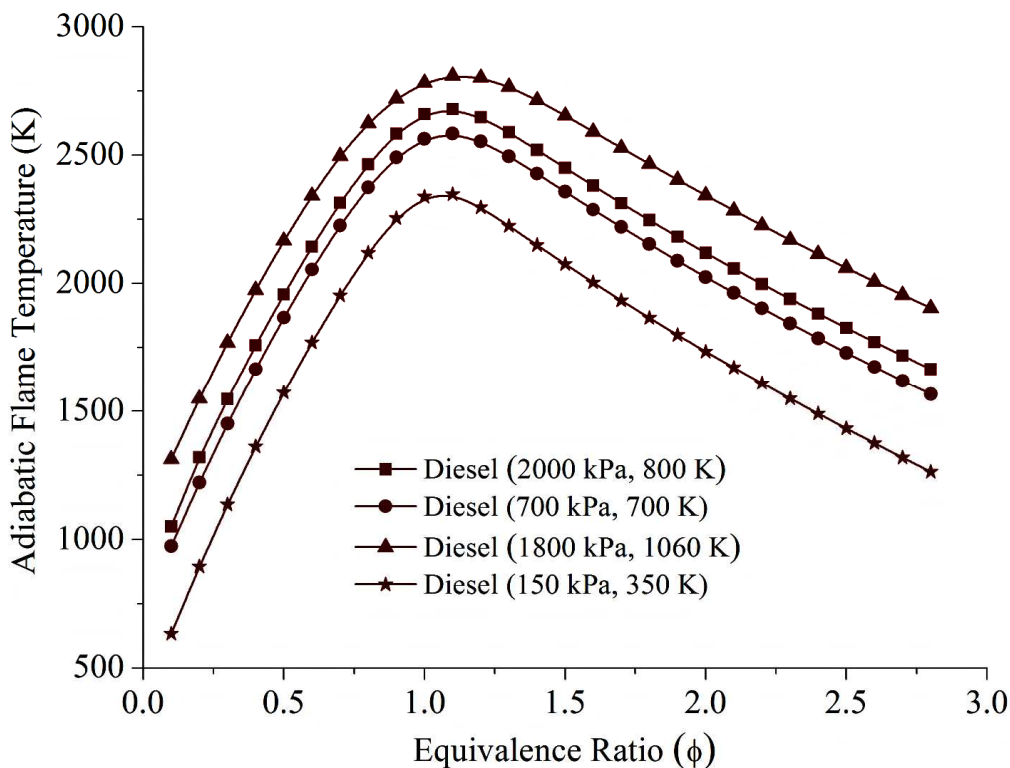
Figure 1. Equilibrium temperature as function of equivalence ratio for diesel fuel
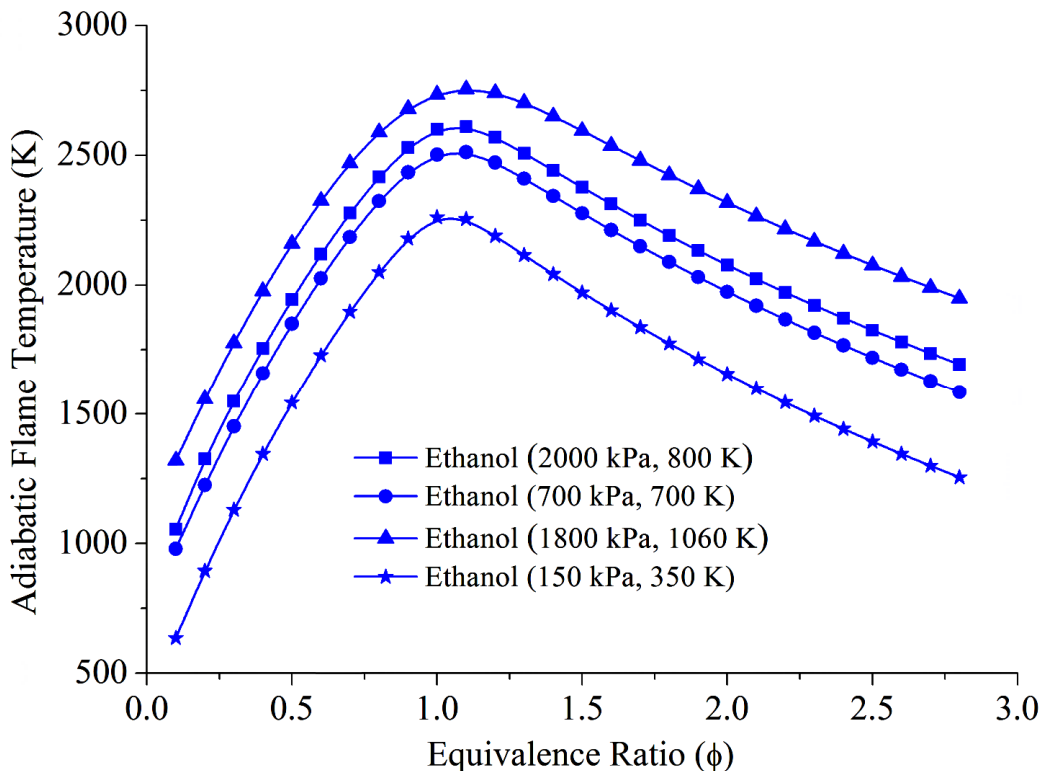
Figure 2. Equilibrium temperature as function of equivalence ratio for ethanol fuel

From Figures 1 and 2, the flammability zone narrows with decreasing combustor inlet temperature and pressure. Both temperature and pressure have significant influence on the combustion stability, as reflected by the stability curves. As can see in Fig. 1 and 2, when the operating temperature is 350 K and the pressure is 150 kPa, the stability zone is narrowest. The adiabatic flame temperature is smaller than the one obtained for the operating temperature of 800 K and pressure of 2,000 kPa.

Other important results that can be drawn from Fig. 1 and 2 are the lean and rich equivalence ratios. It can be observed that, for similar operating condition, the flammability curve of ethanol is narrower than the flammability curve of diesel fuel. It can also be seen that the equilibrium temperatures on the ethanol combustion stability curve is very close to the equilibrium temperature on the diesel flammability curve. This is of great importance because, for any gas turbine combustor, there is a limit in equivalence ratio, for both lean and rich mixtures, beyond which the flame will be unstable and flame out, would occur.

Table 2 shows the major geometrical characteristics calculated for a tubular combustion chamber, which fulfills both the aerodynamic and thermochemical requirements for a stationary gas turbine burning diesel or ethanol.

Table 2. Basic geometrical features of the stationary gas turbine combustor.

Features of Combustor	Diesel fuel	Ethanol liquid fuel
Combustors number	6	6
Housing combustor area (m^2)	0.088181	0.088181
Diameter of housing combustor area (m)	0.3351	0.3351
Liner combustor area (m^2)	0.061726	0.061726
Diameter of liner combustor area (m)	0.28031	0.28031
Cooling air (%)	51.4	51.4
Air in the combustor primary zone (%)	25.0	30.0
Air in the combustor secondary zone (%)	18.37	13.37
Air in the combustor dilution zone (%)	5.23	5.22
Air mass flow of cooling air (kg/s)	9.303	9.303
Air mass flow in combustor primary zone (kg/s)	4.525	5.430
Air mass flow in combustor secondary zone (kg/s)	3.326	2.421
Air mass flow in combustor dilution zone (kg/s)	0.946	0.946
Length of combustor primary zone (m)	0.2103	0.2103
Length of combustor secondary zone (m)	0.1402	0.1402
Length of combustor transition dilution zone (m)	0.1802	0.1802
Length of combustor dilution zone (m)	0.3603	0.3603
Total length of combustor (m)	0.7107	0.7107
Area at compressor exit (m^2)	0.096000	0.096000
Pressure loss in the diffuser (%)	1.0	1.0
Area at diffuser inlet (m^2)	0.016000	0.016000
Diameter at diffuser inlet (m)	0.1427	0.1427
Air velocity at diffuser inlet (m/s)	136.89	136.89
Air velocity at annular area (m/s)	72.44	70.37
Air at annular area (%)	87.5	85.0
Air mass flow at annular area (kg/s)	15.840	15.390
Expansion ratio coefficient (dimensionless)	1.89	1.95
Diffuser angle (º)	21.52	20.53
Snout angle (º)	30.92	29.23
Total length of diffuser (m)	0.2439	0.2569

From the results shown in Tab. 2, it can be seen how the geometric characteristics, calculated for a flex combustor burning diesel fuel, do not differ much from the calculated for the combustor burning ethanol. The major differences take place in the air distribution for the combustor primary and secondary zones, which would require a geometry optimization of the holes to obtain a stable combustion and high efficiency, allowing appropriate thermochemical development and reliable flame stability during the combustor operation.

Another important result is related to the quantification of the combustion products in the combustor primary zone, because the presence of high values of CO represents loss of combustion efficiency (Ferguson, 1985). This model is useful to calculate the variation of the main species: CO_2, H_2O, CO, H_2, O_2, N_2, Ar, OH, O, H, NO and NO_2. Figures 3 and 4 show these chemical species calculated as function of equivalence ratio (ϕ).
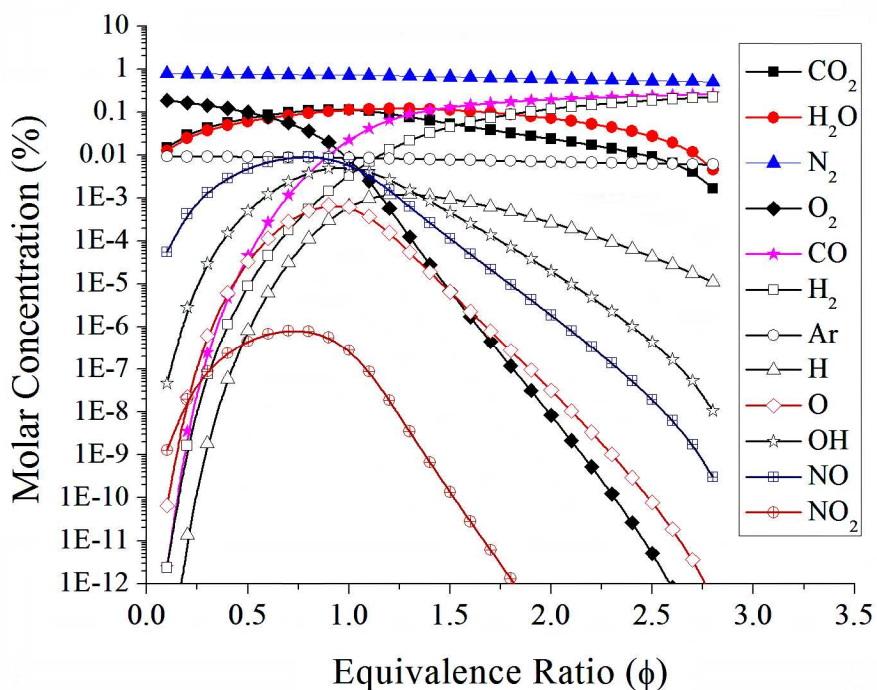

Figure 3. Combustion of diesel: molar concentration for products equilibrium composition.
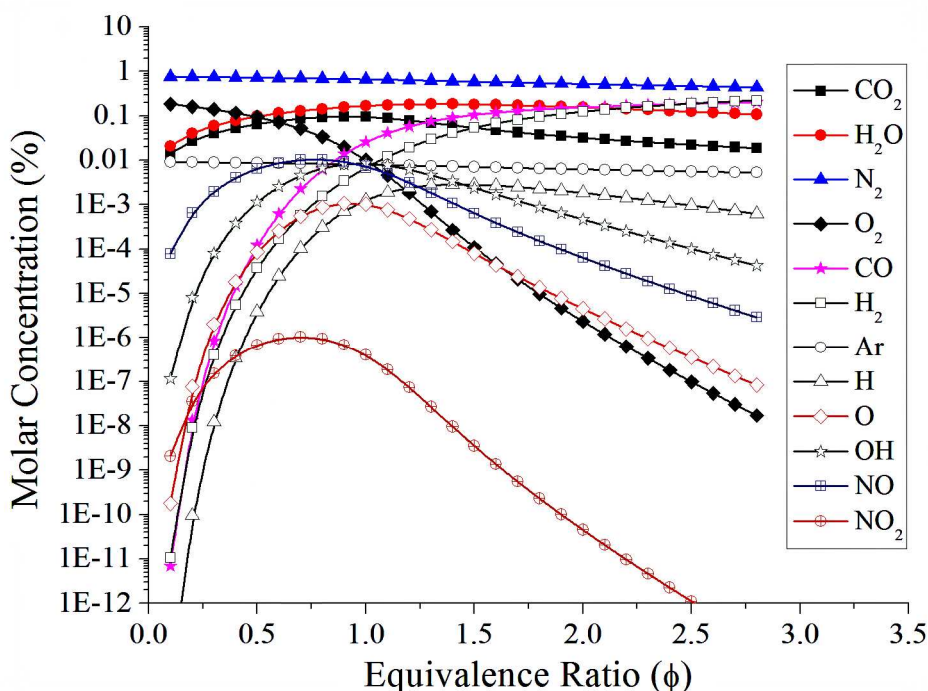

Figure 4. Combustion of ethanol: molar concentration for products equilibrium composition.

The results plotted on Fig. 3 and 4 are of much importance because of the qualitative changes of CO_2, CO, NO and NO_2 with the equivalence ratio. For CO emission, it can be observed that, when the equivalence ratio is increased from lean to rich, CO increases and the combustion of diesel is the largest emitter of this pollutant compared to the combustion of ethanol.

From the same Fig. 3 and 4, one can compare the water characteristic emission from hydroxide fuels (in this case, liquid ethanol) compared with diesel. The H_2O concentration from the combustion of diesel increases with the increase of equivalence ratio until a maximum is reached at the stoichiometric equivalence ratio, decreasing subsequently. Furthermore, the H_2O molar concentration from the combustion of ethanol increases with the increase of the equivalence ratio, reaching maximum at the stoichiometric ratio, slowly falling subsequently, maintaining a nearly constant trend.

4. CLOSURE

The aerodynamic and thermochemical models detailed above were implemented in a FORTRAN language code. Numerical simulations were carried out to validate the functionality and versatility of such models.

The non-linear system of equations was solved using successive substitution combined simultaneously with LU factorization and the Newton-Raphson method. The results, quickly obtained, were the concentration of chemical species at equilibrium in the combustion products and no problems were expedienced concerning singularities. These results were used to calculate the preliminary basic settings for the flex combustor burning diesel and liquid ethanol.

Description of the behavior of each chemical species concentration as function of equivalence ratio could be detailed for each type of fuel and combustor operating conditions. The computational tool turned to be particularly useful for determination and control of CO, CO_2, NO and NO_2 emissions during the combustion of diesel and ethanol in a flex stationary gas turbine.

5. ACKNOWLEDGEMENTS

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