COBEM-2017-0212
EVALUATION OF EMISSIONS OF BURNING ALTERNATIVE LIQUID FUELS IN GAS TURBINE COMBUSTORS

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Abstract. Gas turbines are thermal machines with the great advantage of being capable of successfully burning a large variety of fuels in a continuous combustion process. Alternative liquid fuels are among possible fuels of interest, in addition to oil-derived fuels. Using a numerical methodology for sizing fuel flexible gas turbine combustor, this manuscript contributes at the analysis of the rate of emissions on those combustors and its objective is to evaluate the emissions of a gas turbine combustor operating with ethanol, methanol and kerosene. It was made by varying the input temperature, pressure and equivalence ratio, comparing the renewable fuels (ethanol, methanol) of the fossil fuel (kerosene). Stable equilibrium state were calculated to evaluate pollutants like NO_x, NO and CO. The chemical equilibrium was achieved when de individual species, in the burned products, react to produce and remove each species at equal rate. Results like air mass flow rate, fuel mass flow rate, pressure, combustion volume impacting on the production rate of combustion products (CO, CO_2, NO_X and OH) at the combustor exit. It can be concluded that the use of biofuels considerably improved the emission of polluting gases and maintains a very close range of operation with conventional fuel.

Keywords: gas turbine combustor, alternative liquid fuels, combustion, numerical simulation

1. INTRODUCTION

A gas turbine combustor is the device responsible of the incoming airflow increases temperature through the addition of fuel and its subsequent combustion. The combustor should perform several requirements, among which the capacity of easily starting the combustion and of operating steadily over a wide range of conditions. In all operating points the combustor should provide for complete fuel combustion, while minimizing the formation of undesirable emissions, such as NO_x. Much research is being carried out in this field, aiming at the design and development of gas turbine combustors to successfully burning several types of fuels (Odgers and Kretschmer, 1986).

Pollutant emissions from combustion processes have become of great public concern due to their impact on health and the environment. The past decade has witnessed rapid changes both in the regulations for controlling gas turbine emissions and in the technologies used to meet these regulations (Lefebvre and Ballal, 2003).

Using a numerical methodology for sizing fuel flexible gas turbine combustor, this manuscript contributes at the analysis of the rate of emissions on those combustors and its objective is to evaluate the emissions of a gas turbine combustor operating with different fuels.

The exhaust from an aircraft gas turbine is composed of CO, carbon dioxide (CO_2), water vapor (H_2O), unburned hydrocarbons (UHC), particulate matter (mainly carbon), NO_x, and excess atmospheric oxygen and nitrogen. Improvements in engine thermal efficiency not only reduce direct operating costs, but also reduce pollution (Lefebvre and Ballal, 2003).

Pressure, temperature and equivalence ratio of the mixture were set and the chemical reactions for a stable equilibrium state were calculated to evaluate those pollutants (Lois, *et. al.,* 2002).

2. PHYSICAL AND MATHEMATICAL MODELLING

2.1 Alcohol fuels characterization

The gas turbine combustion chamber corresponds to a continuous flow mechanism, which tends to develop a stable flame during its combustion. In theory, these machines can operate with a number of biofuels such as ethanol, methanol, biodiesel, gasified biomass, synthetic gas and hydrogen in addition to conventional natural gas. However, the replacement of the design fuel in gas turbine combustion chambers should be evaluate, since the fuel properties influence the overall efficiency, the pollutant emission rate and the combustion process (Dias, 2011).

The various types of liquid fuels that are available for gas turbines depend on various factors such as costs, availability, storage, handling, pollution and combustor type. In this study, for the numerical simulation, ethanol and methanol fuels were used. In Tab. 1 are shown some of their main characteristics (Lois, *et al*., 2002).

Table 1. Typical properties for ethanol and methanol fuels.

Property	Ethanol	Methanol	Unit
Formula	C_2H_5OH	CH_3OH	–
Enthalpy of vaporization	38.56	37.40	kJ/mol
Boiling point	351.2	337.7	K
Melting point	159	175.4	K
Flash point	286	285	K
Net Heating Value	27.2	22.7	MJ/kg
Critical temperature	514	513	K
Autoignition temperature	695	658	K
Critical pressure	6.3	8.07	MPa
Molecular weight	46.07	32.04	g/mol
Refractive index	1.36	1.33	–
Stoichiometric Air/Fuel	8.95	6.45	–
Specific gravity (15 ℃)	0.794	0.787	–
Energy density	21.6	15.6	MJ/l

In Brazil, the anhydrous alcohol (C_2H_5OH) is a natural candidate among biofuels. It contains 35% oxygen by weight, boils at a temperature of 78 ℃ and it has a high heat of vaporization due to its hydrogen bonding. These parameters are very important for fuel atomization and vaporization in the combustor. There are physical and chemical properties of ethanol that can be beneficially explored in gas turbine combustors, while other technical difficulties must be overcome (Hamelinck and Faaij, 2006).

Liquid methanol is an excellent motor fuel and fuel blending component. It can be produced from biomass and other energy sources. It is popular in the United States, with an annual output of about 1.2 billion gallons per year (U.S. Department of Energy, 2015).

2.2 Performance predictions

The mixing process and the fuel are extremely important in the combustion and dilution zones. In the primary zone a good mixing is essential to obtain a high burning rate and to minimize the formation of soot and NO_x. An important characteristic in the design of the combustor is to obtain a satisfactory air-fuel mixture inside the flame tube and a stable flow through of the entire combustor, it being necessary to achieve this in a minimum length, without pressure losses (Valverde-Salvador, 2004).

Two dimensionless parameters that relate the pressure loss in the combustor are important in the design of the combustor (Bohorquez and Barbosa, 2013). The first parameter is the reference area, A_{ref}, that is selected by considering the limitations of chemical or aerodynamic reactions as well as the maximum permissible pressure loss in the combustion chamber (Almeida, 2016). It is demonstrated at Eq. (1).

$$A_{ref} = \left[k \left(\frac{\dot{m}_3 \sqrt{T_3}}{P_3} \right)^2 \left(\frac{\Delta P_{3\_4} / q_{ref}}{\Delta P_{3\_4} / P_3} \right) \right]^{0,5} \tag{1}$$

Where *3* and *4* are the combustion chamber inlet and outlet stations, *A* is the cross-sectional area of the combustor shell, *k* is a constant which value is 143,5 (SI), $\dot{m}$ is the flow rate, *P* is the total pressure, *T* is the total temperature, *q* is the dynamic pressure and *ref* indicates reference.

The other dimensionless parameter is $\Delta P_{3-4}/q_{ref}$, shown in Eq. (2) , represents the resistance that the flow receives from the compressor output to the turbine inlet. It takes into account the sum of two portions of pressure loss: that of the diffuser and the flame tube (Almeida, 2016).

$$\frac{\Delta P_{3\_4}}{q_{ref}} = \frac{\Delta P_{diff}}{q_{ref}} + \frac{\Delta P_{ft}}{q_{ref}} \tag{2}$$

The subscripts *diff* indicates diffuser and *ft* flame tube.

2.3 Thermochemical parameters

Gas turbine combustors require a steady burning of fuel over a wide range of operating conditions with combustion efficiency levels approaching 100% (Bohorquez and Barbosa, 2013).

Using the burning speed methodology, for a given fuel / air ratio, the combustion efficiency, η_θ, is correlated with the θ parameter, presented in Eq. (3). Experimental data suggest that when θ value is 73E + 06 (SI), the designed combustors have a combustion efficiency close to 100% (Sawyer, 1985):

$$\eta_\theta = \theta = \frac{P_3^{1,75} A_{ref} D_{ref}^{0,75} e^{\left(\frac{T_3}{b} \right)}}{\dot{m}_3} \tag{3}$$

Where D_{ref} is the diameter of the cross-sectional area of the combustor housing, *b* is a temperature correction factor T_3, θ is the combustion efficiency correlation parameter and η_θ represents the combustion efficiency of the combustor.

The parameter *b* is a correction factor of the temperature of entry to the combustion chamber given by Eq. (4) and Eq. (5):

$$b = 245(1,39 + \ln \phi_{zp}) \quad 0,6 < \ln \phi_{zp} < 1,0 \tag{4}$$

$$b = 170(2,0 - \ln \phi_{zp}) \quad 1,0 < \ln \phi_{zp} < 1,4 \tag{5}$$

ϕ_{zp} is the equivalence ratio in the primary zone.

In order to obtain the appropriate value of the equivalence ratio in the primary zone, it is necessary to construct a flammability curve for the fuel to burn under the operating conditions of the gas turbine, using thermokinetic equilibrium concepts (Lefebvre, 1999).

The chemical equilibrium condition is established using Gibbs free energy minimization and the thermodynamic variables used are pressure and temperature (Bohorquez and Barbosa, 2013).

Considering for a fuel reacting and forming equilibrium combustion products, it is considered that *n* treats the chemical species and *k* the chemical elements. The law of conservation of chemical elements will provide *k* real equations to the concentrations of these *n* chemical species (McBride, et al., 1993).
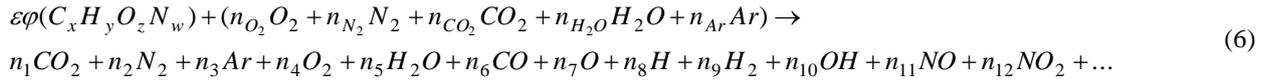
The fuel to be used may contain carbon, hydrogen, oxygen and nitrogen, with chemical formula $C_x H_y O_z N_w$. The air considered for combustion is composed of oxygen, nitrogen, argon, carbon dioxide and water vapor: $n_{O_2} O_2 + n_{N_2} N_2 + n_{Ar} Ar + n_{CO_2} CO_2 + n_{H_2O} H_2O$.
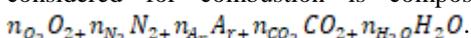
The combustion products contain 12 species, considered the most significant for the present study: $n_1 CO_2 + n_2 N_2 + n_3 Ar + n_4 O_2 + n_5 H_2O + n_6 CO + n_7 O + n_8 H + n_9 H_2 + n_{10} OH + n_{11} NO + n_{12} NO_2$.
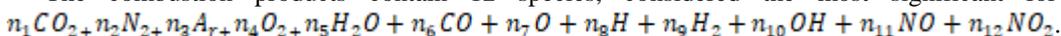
A generic equation of chemical reaction for these fuels, with an equivalence ratio ϕ, reacting with air, can be given by Eq. (6) (McBride, et al., 1993).

$$\varepsilon\varphi(C_xH_yO_zN_w)+(n_{O_2}O_2+n_{N_2}N_2+n_{CO_2}CO_2+n_{H_2O}H_2O+n_{Ar}Ar) \rightarrow$$
$$n_1CO_2+n_2N_2+n_3Ar+n_4O_2+n_5H_2O+n_6CO+n_7O+n_8H+n_9H_2+n_{10}OH+n_{11}NO+n_{12}NO_2+... \tag{6}$$

Considering the 12 chemical species n in the combustion products at a given temperature and pressure, it will be necessary 12 equations to obtain the molar concentration of these n chemical species. Five equations are obtained from the mass balance of the chemical elements C, H, N, O and Ar in the reagents and products. The remaining seven equations are relative to chemical dissociation, dependent on temperature (McBride, *et al.,* 1993). The resulting system of nonlinear equations can be obtained from the JANAF thermodynamic tables, using the Eq. (7):

$$\log K_p\Big)_{reação} = \sum_{produtos} n_e \log K_p - \sum_{reagentes} n_e \log K_p \tag{7}$$

Where K_p is a constant equilibrium when is constant pressure and n_e the molar coefficients in the equilibrium equation.

The equilibrium constants data shown in Eq. (7) can be polynomially adjusted to the temperature using a general functional relationship shown in Eq. (8):

$$\log K_p\Big)_{reação} = A_e \ln\left(\frac{T}{1000}\right)+\frac{B_e}{T}+C_e+D_eT+E_eT^2 \tag{8}$$

Equation (6) can be rearranged as a function of the equilibrium constants of Equation (7) and plotted against the molar fractions of N_2, O_2, CO e H_2 respectively. This set of equations is used to calculate the molar fraction of all chemical species in terms of y_{N2}, y_{O2}, y_{CO} and y_{H2}, using the system of equations indicated in Eq. (9):

$$\begin{bmatrix} \dfrac{\partial f_1}{\partial y_3}\Delta y_3 & \dfrac{\partial f_1}{\partial y_4}\Delta y_4 & \dfrac{\partial f_1}{\partial y_5}\Delta y_5 & \dfrac{\partial f_1}{\partial y_6}\Delta y_6 & = & -f_1 \\[2ex] \dfrac{\partial f_2}{\partial y_3}\Delta y_3 & \dfrac{\partial f_2}{\partial y_4}\Delta y_4 & \dfrac{\partial f_2}{\partial y_5}\Delta y_5 & \dfrac{\partial f_2}{\partial y_6}\Delta y_6 & = & -f_2 \\[2ex] \dfrac{\partial f_3}{\partial y_3}\Delta y_3 & \dfrac{\partial f_3}{\partial y_4}\Delta y_4 & \dfrac{\partial f_3}{\partial y_5}\Delta y_5 & \dfrac{\partial f_3}{\partial y_6}\Delta y_6 & = & -f_3 \\[2ex] \dfrac{\partial f_4}{\partial y_3}\Delta y_3 & \dfrac{\partial f_4}{\partial y_4}\Delta y_4 & \dfrac{\partial f_4}{\partial y_5}\Delta y_5 & \dfrac{\partial f_4}{\partial y_6}\Delta y_6 & = & -f_4 \end{bmatrix} \tag{9}$$

Where $\partial f_i/\partial y_i$ for $i=1,2,3,4$ and $j=3,4,5,6$ represents the partial derivatives of i equations with respect to j mole fractions, the Δy_j represent the vector of variations of the molar fractions based on N_2, O_2, CO e H_2. f_j represents the vector of linear functions based on the molar fractions y_j.

By means of computational methods such as LU Factoration simultaneously with the Newton-Raphson's method, it is possible to obtain the set of values of the molar fractions of the combustion products. Thus, it is possible to construct the flammability curve of each of the fuels used for every envelope of operations of the combustor, applying the matrix system under the conditions of energy conservation, with an adiabatic combustion hypothesis, shown at Eq. (10), varying the equivalence ratio from a poor mixture to a rich mixture.

$$\sum_r N_r(h_{f,r}^*+\Delta h_{s,r}^*)-\sum_p N_p(h_{f,p}^*+\Delta h_{s,p}^*)=0 \tag{10}$$

p represents the products, r the reactants, f formation, h specific sensitive enthalpy, Δh^* variation of specific enthalpy and N the total number of moles.

Each combustion stability curve represents the adiabatic flame temperature as a function of the equivalence ratio. Once the temperature is known, the inverse interpolation using the Lagrange polynomial gives the desired value of ϕ_{zp}.

The value of the equivalence ratio in the primary zone of the combustor ϕ_{zp} is used in Eq. (4) and Eq. (5) to calculate the correction factor of the input temperature of the combustion chamber and later this parameter is used in Eq. (3) to determine the cross-sectional area of the combustor carcass. Lastly, this value is applied at cross-sectional area of the liner for thermochemical considerations (Lefebvre, 1999).

2.4 Characteristics of a flex combustor

Several items must be specified for each operational envelope. These are air mass flow rate, fuel mass flow rate, combustor inlet parameters (temperature, pressure and velocity), exit temperature, pressure losses, combustion efficiency, maximum allowable wall temperature, combustor type, weight and physical space (O'Brien, 2002).

Stability loops are affected by air loading or fuel loading parameters (air mass flow rate, pressure, fuel mass flow rate, reaction order and volume of the combustor). It is assumed that the attainable stability limit is dependent upon reaction-rate control. The performance curves of gas turbine combustors had similar characteristics to those yielded by simple equations based on reaction rate theory (Odgers and Carrier, 1973).

3. EXPERIMENTAL PROCEDURE (OR COMPUTATIONAL PROCEDURE)

In order to evaluate the emissions from the combustion chamber of the gas turbine, it is required calculate the main characteristics, performance and reacting flow of a gas turbine combustor. A computational code, written in Matlab® and using the software Cantera, was developed for that purpose, enabling the gas turbine combustor burn fuels like ethanol (C_2H_5OH), methanol (CH_3OH) and kerosene ($C_{13}H_{26}$).

The use of successive substitutions, combined with LU-factorization and the Newton-Raphson procedure, as well as the application of other numerical methods allowed the rapid calculation of the adiabatic temperature as a function of the equivalence ratio and the concentration of chemical species in the combustion products avoiding the usual problems with singularities (Little *et al.*, 2004).

A main program calls several subroutines to perform specific sequential calculations. Some of these subroutines are described as follows:

a)   A subroutine to input fuel, air and operating conditions data. In this subroutine the equivalence ratio, air mole fraction and fuel mole fraction for each work condition are calculated;
b)   A subroutine to calculate the flammability curve for each fuel studied based on thermokinetic equilibrium and reaction mechanism;
c)   A subroutine to evaluate some performance characteristics of the calculated combustor;
d)   A subroutine to show the main results for the emissions rate.

The interaction among the computer codes for the calculation of the flammability curves, stability loops, design of a gas turbine combustion chamber, performance analysis and its emissions is schematically represented in Fig. 1.
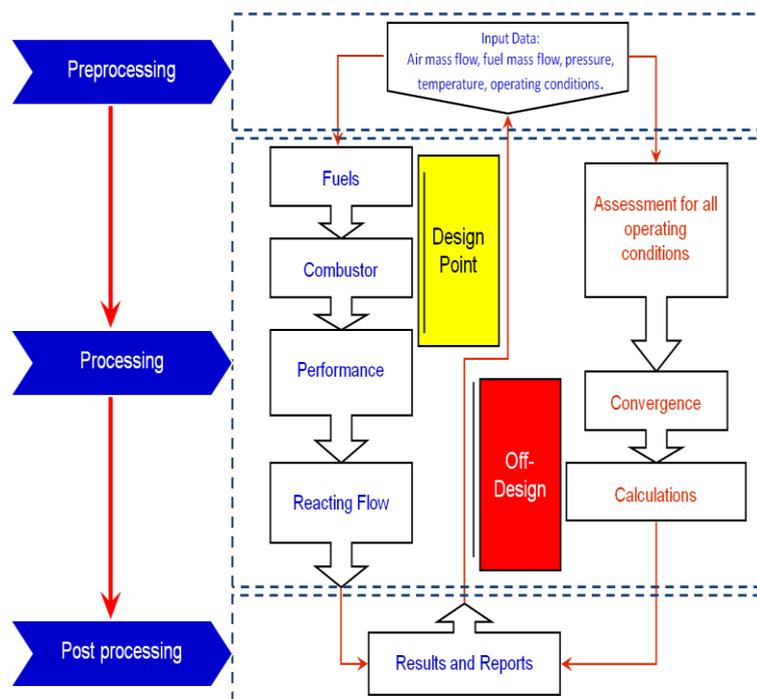

Figure 1 – Shematic diagram of the interactions among computer codes

4. RESULTS AND DISCUSSION

The combustor emission exhaust, for a gas turbine designed to burn ethanol, liquid methanol and kerosene, were calculated using the methodology detailed above using four conditions of temperature and pressure showed at Tab. 2.

Table 2 – Condition of input data

	Condition 1	*Condition 2*	*Condition 3*	*Condition 4*
Pressure [kPa]	501,56	186,29	627,00	182,39
Temperature [K]	491,43	419,23	523,92	357,88

It was possible to obtain the values of the molar fraction of the reactants involved in the combustion process in the test of the parameter of the combustor operating a turbine based on the condition of operation 1. These results are shown in Fig. 2, Fig. 3 and Fig. 4.
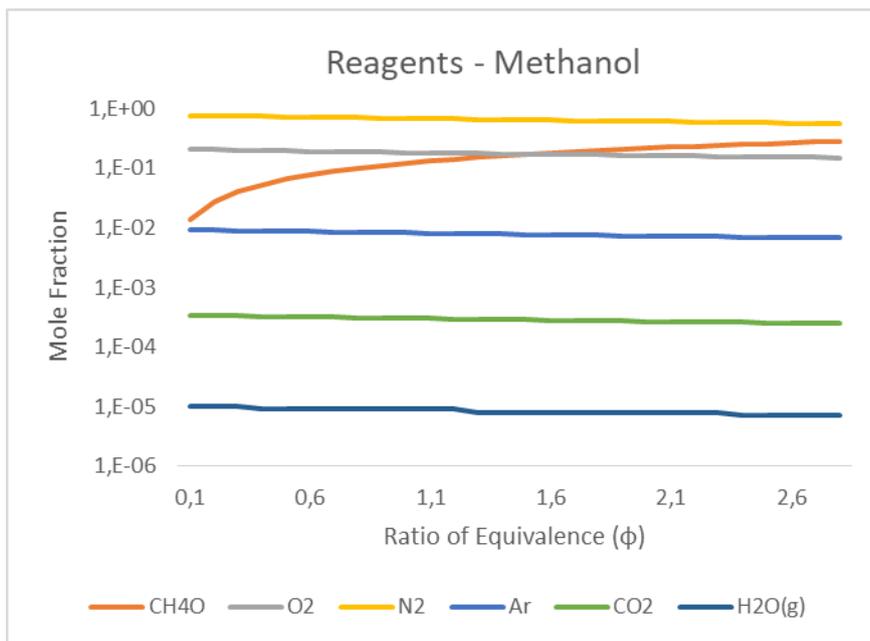

Figure 2: Reagents involved in the combustion of Methanol
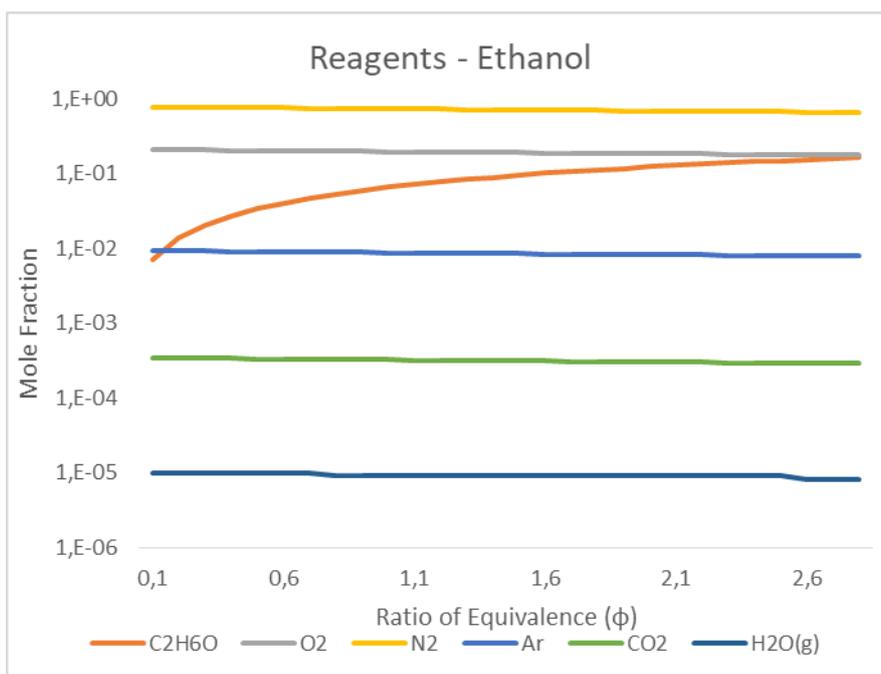
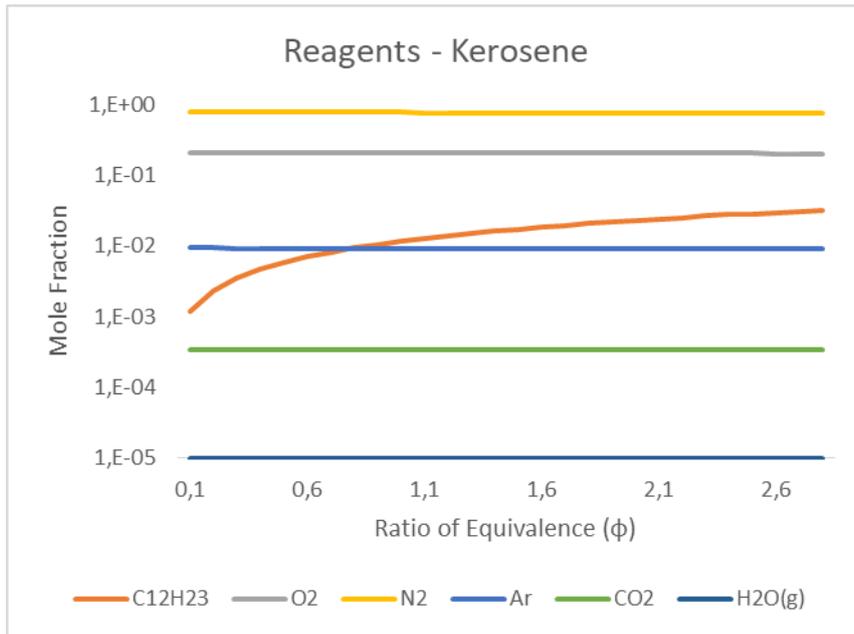Figure 3: Reagents involved in the combustion of Ethanol

Figure 4: Reagents involved in the combustion of Kerosene

The higher the equivalence ratio (the richer the mixture), higher is the fuel consumption, while the other reactants remain virtually unchanged, with a slight tendency towards lower consumption.

Figure 5, Fig. 6 and Fig. 7 show qualitative change in pollutant emissions as the equivalence ratio variation for condition 1 of operation. It is important to observe the trend of CO_2, CO, NO and NO_2 emissions because the quantities of these species are related to the inefficiency of the combustion chamber of the gas turbine and the environmental impact produced by it.
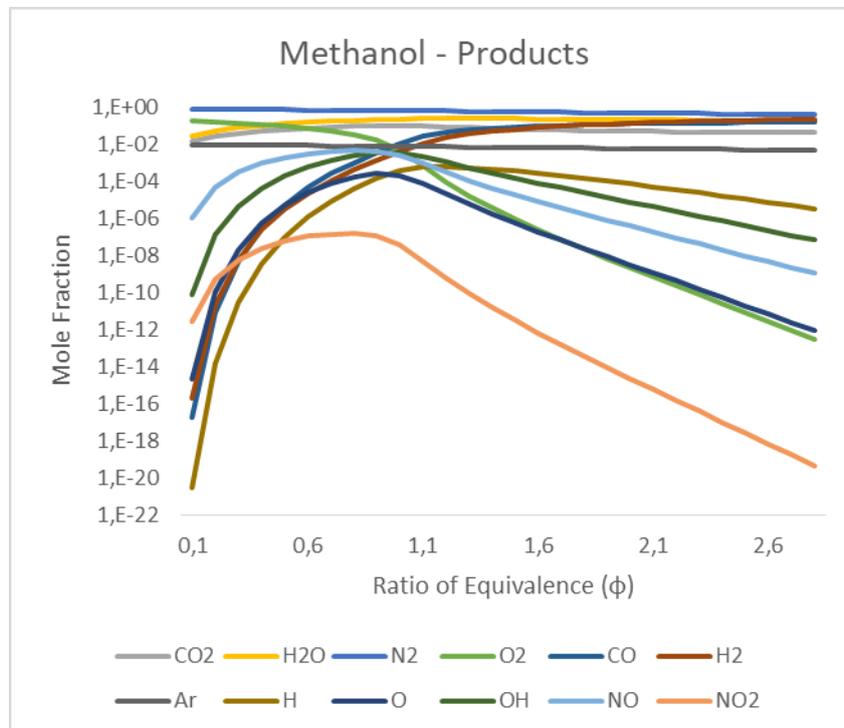

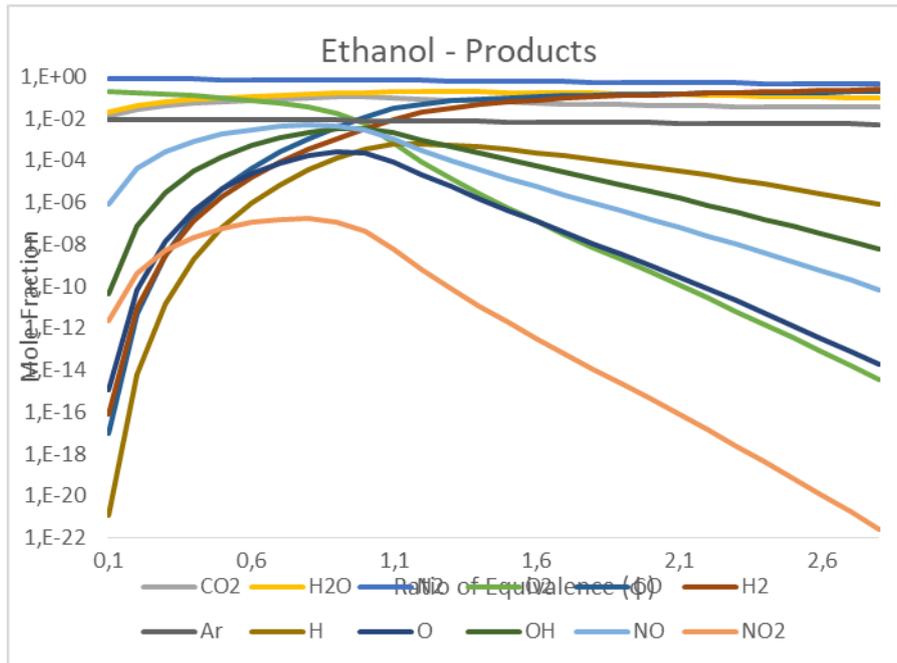Figure 5: Products involved in the Methanol reaction

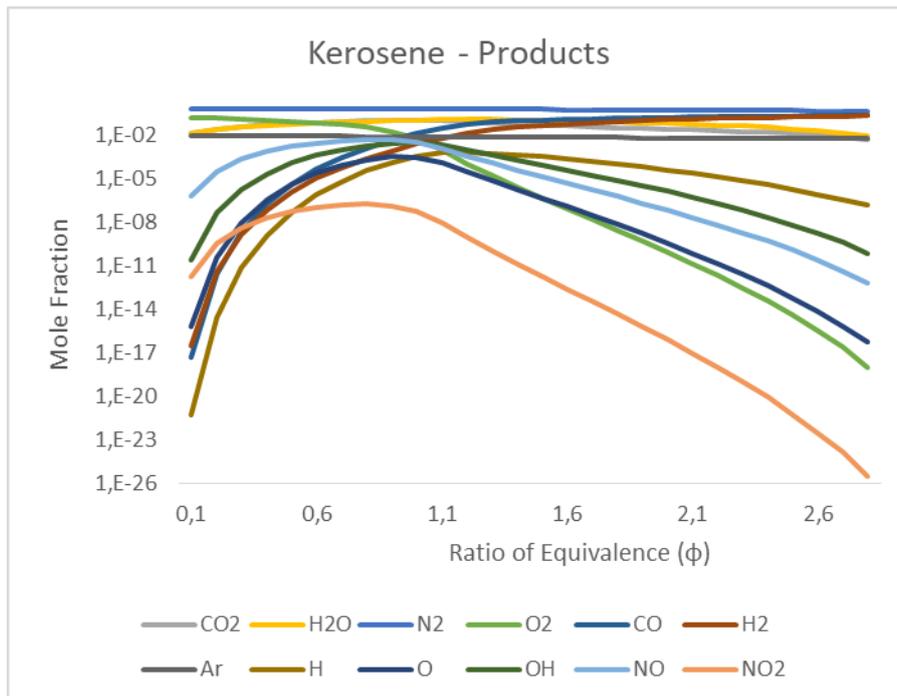Figure 6: Products involved in the Ethanol reaction

Figure 7: Products involved in the Kerosene reaction

It is possible to evaluate that higher the equivalence ratio, smaller the number of products generated in the reaction, since the combustion occurs in a more complete way.

For the emission of CO, it can be observed that when the equivalence ratio increases with a tendency to rich mixtures, there is an increase of the CO emissions and a decay of NOx, being that of kerosene is the largest emitter of this pollutant in comparison with the combustion of ethanol and methanol.

The concentration of H_2O increases with the increase of the equivalence ratio, until reaching a maximum value in the stoichiometric ratio, decreasing and maintaining an almost constant trend. In order to better visualize the emission of the NO and NOx gases, the following Fig. 8 and 9 were made, where their emissions are compared according to the fuel used:

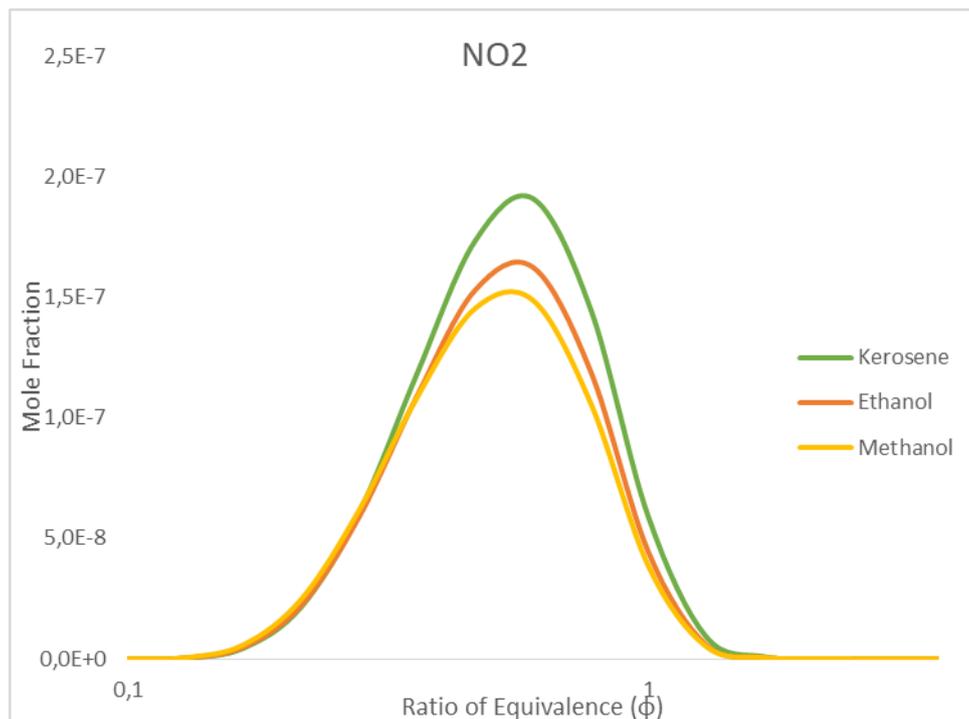Figure 8: Quantity of NO formed during fuel combustion

Figure 9: Quantity of NO2 formed during fuel combustion

In the results of the numerical simulation the reduction of the NO emission can be verified when comparing the biofuels burning in relation to the kerosene:
• Reduction of 36.59% of NO when the combustion chamber burns methanol in substitution of kerosene;
• Reduction of 12.03% NO when the combustion chamber burns ethanol instead of kerosene;

In the results of the numerical simulation the reduction of NO2 can be verified when comparing the burning of biofuels with kerosene:
• Reduction of 31.72% of NO2 when the combustion chamber burns methanol in substitution of kerosene;
• Reduction of 17.17% of NO2 when the combustion chamber burns ethanol instead of kerosene;

5. CONCLUSIONS

Using the computational methods highlighted, it was possible to perform the rapid calculation of the concentration of chemical species in equilibrium in the products of combustion avoiding the usual problems with singularities.

The computational code created is capable of using any type of fuel burned in gas turbines, requiring only the chemical composition of the fuel and its thermodynamic coefficients.

The behavior of each concentration of the chemical species studied was performed according to the equivalence ratio.

The results of the calculations can be used to control the emissions, with the proper dimensioning of the parts of the combustor that interfere in the studied parameters.

The results obtained of the emissions of the gas turbine combustor is quite important, since the Brazilian environmental legislation is very rigid with respect to the discharge of this pollutant through the operation of gas turbines. It can be concluded that the use of biofuels considerably improves the emission of polluting gases and maintains a very close range of operation with conventional fuels, its produces less nitrogen oxide, guaranteeing satisfactory results in the use of this fuel.

6. ACKNOWLEDGEMENTS

7. REFERENCES

Almeida, G.C., 2016. *Metodologia para avaliação do desempenho de câmars de combustão tubo-anulares de turbinas a gás flex com base no parâmetro do carregamento do combustor.* Monografia de Graduação, Universidade Federal de Juiz de Fora, Juiz de Fora.

Bohorquez, W.O.I., Barbosa, J.R., 2013. "Metodologia simplificada para a avaliação do uso de combustíveis alternativos no projeto de combustores em turbinas a gás flex usando equilíbrio termocinético e mecanismos quase-globais", R*evista Iberoamericana de Ingienieria Mecânica*, Vol. 17, Nº 1, pp. 121-140.

Dias, L.F.G., 2011. *Projeto preliminar e simulação computacional de câmara de combustão de turbina a gás considerando a queima de biocombustíveis*. Dissertação de Mestrado, Universidade de Itajubá, Itajubá.

Hamelinck, C. N., Faaij, A. P. C., 2006, "Outlook for advanced biofuels', Energy Policy, v. 34, n. 17, pp. 3268-3283.

Lefebvre, A.H., Ballal, D. R., 2003. *Gas Turbine Combustion: alternative fuels and emissions*, Taylor & Francis, Florida, Third edition.

Lefebvre, A.H., 1999. *Gas Turbine Combustion*, Taylor & Francis, New York, Second Edition.

Little, J.E., Nemets, S.A., Tornabene, R.T., 2004. "Fuel-Flexible Gas Turbine Combustor Flametube Facility", NASA Center for Aerospace Information, Hanover, 1-18.

Lois, E., Gupta, A., Keating, E., 2002. *Fuels*, John Wiley & Sons, New Jersey, Third edition.

McBride, B.J., Gordon, S., Reno, M.A., 1993. "Coeficientes for Calculating Thermodynamic and Transport Properties of Individual Species", NASA Technical Memorandum 4513, National Aeronautics and Space Administration, USA, 1-94.

O'Brien, W., 2002, "Performance prediction and simulation of gas turbine engine operation", NATO, Hull, pp. 1-356.

Odgers, J., Kretschmer, D., 1986. "Gas turbine fuels and their influence on combustion", *Energy and Engineering Science Series*, Vol. 65, pp. 1-185.

SAWYER, J.W., 1985. *Sawyer's Gas Turbine Engineering Handbook,* Turbomachinery International Publications, Connecticut, First edition.

U.S. DEPARTMENT OF ENERGY. "Biofuels for Sustainable". 7 Jun. 2016. http://www.nrel.gov/docs/fy00osti/25876.pdf

Valverde-Salvador, C.A.V., 2004. *Modelo matemático de câmaras de combustão bipropelentes*. Dissertação de Mestrado, Instituto Nacional de Pesquisas Espaciais, São José dos Campos.

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