

MODELING AND NUMERICAL SIMULATION OF GREENHOUSE GAS EMISSIONS FROM A STATIONARY DIESEL ENGINE OPERATING WITH ETHANOL

André Bergel, 55(12)91499644, andrebergel84@yahoo.com.br¹

Sarah de Resende Viana, 55(12)78123617, srviana1@yahoo.com.br¹

¹ITA, Pç. Mal. Eduardo Gomes, 50 – Vila das Acácias – CEP 12228-900 – São José dos Campos – SP – Brasil.

Prof^a. Dr^a. Cristiane Aparecida Martins, 55(12)39475826, cmartins@ita.br¹

¹ITA, Pç. Mal. Eduardo Gomes, 50 – Vila das Acácias – CEP 12228-900 – São José dos Campos – SP – Brasil.

Prof. Dr. Francisco José de Souza, 55(34)32394040, R:615, fjsouza@mecanica.ufu.br²

²UFU, Av. João Naves de Ávila, 2121 – Campus Sta. Mônica – CEP 38408-100 – Uberlândia – MG – Brasil.

Abstract: *The present work aims at modeling and simulating a stationary, compression ignition motor, operating with ethanol at different levels of EGR. The objective is to quantify the influence of these parameters in the atmospheric pollutant emissions (CO, NO_x and Particulate Matter). Specifications of a diesel engine were used, with compression ratio 19:1, operating with ethanol with a percentile of EGR of 0, 10, 20 and 30%. In the simulation, the combustion model, ECFM-3Z, and the turbulence model k- ϵ -f were used, besides conditions for the temperatures of the combustion chamber, piston, cylinder head and glow plug. The spray characterization was done through the calculation of the injected fuel mass and parameters like spray angle, droplet size, number of holes, position of the injector and others. For the reduction of the simulation time, the crank angle range of is only 130[CAD], beginning at 30°BTDC and concluding at 100°ATDC. The assessment of the influence of the different EGR concentrations felt for the analysis of pollutant contained in the end of simulation. A very small delay in the ignition of the fuel injected and the emission of a minor amount of nitrogen oxides were observed in all cases as the EGR level used was increased.*

1. INTRODUCTION

The worldwide concerns with the reduction of greenhouse emissions in the atmosphere, jointly with the growing demand for renewable and economic fuels, are issues that are being hotly debated today. In view of the higher volumetric efficiency of compression ignition engine (CIE), Diesel cycle, comparing to spark ignition engine (SIE), Otto cycle, there is an untapped potential for these engines application with alternative fuels, like ethanol. The Diesel generator is a considerable source of pollutant emissions because of the gases released, namely Nitrogen Oxides (NO_x), Sulfur Trioxide (SO_x), Carbon Dioxide (CO₂), Carbon Monoxide (CO) and Particulate Matter (PM). With the ethanol application, the energy balance and emissions are very positive when compared to diesel oil. However, some engine modifications must be realized (e.g. spark plug application). It is worth remembering that the determining factor in Brazil petroleum imports is exactly the Diesel oil.

2. OBJECTIVES:

The purpose of this work is the simulation of a compression ignition engine operating with ethanol fuel, instead of Diesel, in order to analyze the exhaust gases concentration (Nitrogen Oxide (NO_x), Carbon Dioxide (CO₂), Carbon Monoxide (CO), Particulate Matter (PM) and Unburned Hydrocarbon (HC)) to assist the new engine designs that comply the limits required by the *U.S. Environmental Protection Agency* (EPA), which will be used in Brazil stationary engines regulation, from 2012 on and to analyze the NO_x emissions reduction potential, by varying the amount of exhaust gas recycled used (0,10,20 e 30%). An alternative to accomplish the study of emissions is the use of numerical methods to simulate the combustion process and the movement of the mixture inside the chamber. The software used was AVL Fire 2009, in which the chamber geometry, the fuel physical-chemical properties and the necessary boundary conditions are introduced.

3. THEORETICAL REVIEW

3.1. Ethanol

Ethanol is the most common alcohol, being found in alcoholic beverages and easily produced from sugar cane, maize and some fruits, by fermentation of carbohydrates. Its chemical structure is CH₃CH₂OH and is less toxic than methanol, having an average lethal dose (LD₅₀) of 7060mg/kg for a mouse oral consumption. The use of ethanol as a fuel was initially studied in 1897. Henry Ford designed his T1908 model to run on ethanol, but rising taxes limited its use. The ethanol was considered as a fuel again during the two world wars, but has not started a program for use during the oil crisis in the 70's. In 1973, the *Organization of the Petroleum Exporting Countries* (OPEC) quadrupled the crude petroleum purchase price, stimulating research, development and promotion of ethanol as an alternative fuel for internal

combustion engines. In view of recent Kyoto Conference, in which the U.S. pledged to reduce, by 2012, the emissions of greenhouse gases to the values found in 1990, gasoline and ethanol blends, such as E10 to E85, are an excellent way to reduce emissions of such gases. The Argonne National Laboratory showed that the greenhouse gases emission is 2.4 to 2.9% lower using E10 compared to gasoline. (Minteer, 2006)

3.2. Exhaust gas

In the second half of the twentieth century, the NO and NO₂, compounds named NO_x, emission became worrisome as they represented a major contributor to air pollution. In addition, the nitrogen oxides participate in a chain reaction that removes ozone from the stratosphere with consequent incidence raise of ultraviolet radiation on Earth's surface. Therefore, the minimization of NO_x production has become a very important issue with regard to the combustion theory (Warnatz, 2006). According to Turns, the main mechanisms of nitrogen compounds formation are: Thermal NO - Zeldovich and Prompt NO - Fenimore. (Turns, 2000)

3.2.1. NO Formation - Thermal NO (Zeldovich)

Obtained from the reaction of nitrogen from atmospheric air with oxygen dissociated by the high temperatures resulting from the combustion process. Its formation rate becomes significant at temperatures around 1850 K. The reaction scheme proposed for the thermal NO formation is based on the Zeldovich mechanism, which is described by the following reactions:



Where:

$$K_1 = 1,8 \times 10^{14} * e^{\left(\frac{-318 [kJ.mol^{-1}]}{RT}\right)} \left[\frac{cm^3}{mol.s}\right] \quad (4)$$

$$K_2 = 6,4 \times 10^9 * T * e^{\left(\frac{-26 kJ.mol^{-1}}{RT}\right)} \left[\frac{cm^3}{mol.s}\right] \quad (5)$$

$$K_3 = 3,8 \times 10^{13} \left[\frac{cm^3}{mol.s}\right] \quad (6)$$

Thus, Eq. (1) is the limiting factor in the thermal NO formation, because it has a high activation energy due to the triple bond in the N₂, occurring only at high temperatures.

According to Heywood, the estimate of thermal NO formation for certain operating conditions can be given by:

$$\frac{d[NO]}{dt} = \frac{6 \times 10^6}{T^{\frac{1}{2}}} e^{\frac{(-69090)}{T}} [O_2]_e^{1/2} [N_2]_e \quad (7)$$

where $K_1 = 7,6 \times 10^{13} * e^{\frac{-38000}{T}}$, with T ranging from 2000 to 5000 K. The great dependence of the NO formation rate $\left(\frac{d[NO]}{dt}\right)$ with temperature in the exponential term is evident. High temperatures and oxygen concentrations result in high rates of NO formation.

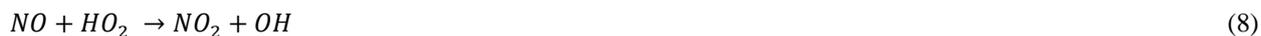
3.2.2. NO Formation - Prompt NO (Fenimore)

The Prompt or Fenimore mechanism was postulated by C. P. Fenimore (1979), who measured the NO concentration under a laminar flame coming from the burning of a hydrocarbon. The additional mechanism that produces NO immediately ahead of the flame is more complex than the thermal. It happens because prompt NO results from the CH radical, which was previously considered a negligible transient species generated through a complex scheme reactions in the Zeldovich mechanism. The CH, formed as an intermediate product in the flame front, reacts with nitrogen from the air, forming Hydrocyanic acid (HCN), which later forms NO.

3.2.3. NO formation in diesel engines

In engines, combustion occurs at high pressures, being the flame reaction zone extremely thin ($\cong 0.1$ mm) and the residence time in the zone very small. Moreover, the pressure inside the cylinder increases during the most combustion processes, so that the burned gases produced in the early combustion process are compressed at higher temperatures than those attained immediately after combustion. Thus, the NO formation in the gases produced after the flame should always dominate any NO formed in the flame front.

In Diesel engines, the NO₂ formation may be about 10-30% of total nitrogen oxides emitted. The next mechanism suggests that the NO formed in the flame zone is rapidly converted to NO₂ from reactions (Heywood, 1988):



Subsequently, the conversion of NO₂ to NO occurs via:



This mechanism occurs unless the NO₂ formed in the flame is dissipated by mixing in a cooler fluid. Since the critical formation of NO (15° after the TDC) occurs when the temperature of the exhaust gases is the highest, for example, between the start of combustion and shortly after cylinder pressure peak. After the pressure peak, the temperature of the burned gases decreases as the gases expand within the cylinder. The decrease in temperature due to expansion and to the high temperature gas mixture with air or with cooler burned gases, freezes the thermal NO. This second effect shows that the cooling occurs more rapidly in compression-ignition engines than in spark-ignition engines, and there is less decomposition of NO.

3.2.4. Particulate Matter

Particulate matter, also known as soot, consists mostly of carbon-based particles formed during incomplete combustion of hydrocarbons. The factors of the formation process are the unburned fuel availability, the oxygen shortage and high temperatures.

In solid state, these particles have very high emissivity compared to systems that do not contain them, so the flames in that way increase substantially the heat transfer by radiation.

The carbon deposited on the particulate matter consists of spherical particles with diameters ranging from 100-2000 Å, with most between 100 and 500 Å. It is known that the level of the particulate matter formation is directly related to the type of flame in the combustion process. Moreover, the fuel chemical structure has great influence on the formation of the same, with the descending order of formation obeying the following sequence: Aromatic > acetylenes > olefins > paraffins > alcohols (diffusive). (Glassman, 1987)

In Diesel engines, due to the peculiarities of the operating principle, the auto ignition is responsible for the combustion of an internal mixture with air in excess. Thus, due to different equivalence ratios contained in the spray, there are fuel rich regions, where high emissions of particulate matter are expected. (Smith, 2007)

3.2.5. Particulate Matter in Diesel engines

In "Diesel" engines with direct injection, the highest concentration of particles is found in the central region of the spray where the local equivalence ratios are very rich. Its concentration decays rapidly after the combustion initiation.

In practice, the soot formation rate tends to be governed by the physical characteristics of the atomization process as well as the dynamics of air-fuel mixture than by chemical kinetics (Lefebvre, 1999).

Soot particles are formed, primarily, of carbon contained in the Diesel. Thus, the formation process begins with fuel molecules with 12 to 22 carbon atoms and the ratio H/C \cong 2. The soot consists of particles compound with a diameter containing about hundreds of nanometers and is formed by spheres with 20-30 nm in diameter each. (Heywood, 1988).

3.2.6. Carbon Monoxide

The carbon monoxide emitted by internal combustion engines are controlled primarily by the equivalence ratio, (Heywood, 1988).

The Carbon oxidation, in hydrocarbons, occurs basically in two steps: the first, in which the carbon-based compounds are partially oxidized generating CO and, in a final step of this oxidation to CO₂. This second step is strongly dependent on the presence of hydrogen in the mixture. The local flame stoichiometry, residence time, rate of mixing between fuel and air and the extinction of combustion products from the cooling of them, are probable causes for the discrepancy between the emission values provided in chemical equilibrium and those measured. (Lacava et al, 2009)

3.2.7. CO formation in Diesel engines

In the CO formation mechanism in Diesel engines, it is assumed that the formation rate is proportional to the amount of unburned hydrocarbon and the temperature level, both controllers of decomposition and oxidation fuel.

$$\frac{dCO_{fo}}{dt} = A_{fo} \cdot m_{fu} \cdot P^{0.5} \cdot e^{\left(\frac{12000}{T}\right)} \quad (10)$$

Where T and P corresponding to the temperature and pressure, respectively, from each combustion zone in the region of the jet or the averages temperature and pressure of the air-fuel gas mixture, m_{fu} is the unburned fuel mass and A_{fo} is an empirical constant.

3.2.8. Unburned Hydrocarbon

Unburned hydrocarbons are gases and steams resulting from the incomplete burning of fuel due to lean or rich regions created inside the combustion chamber. In lean regions, the fuel injector characteristics and the air-fuel mixture patterns are important parameters to be considered, since the flame does not propagate through regions with low equivalence ratios. Thus, partial oxidation products are formed, among them, aldehydes and carbon monoxide. In rich regions, the unburned species formation occurs in the absence of a mechanism to mix enough to consume all oxygen available, or because of insufficient time for complete oxidation of fuel. (Turns, 2000)

3.2.9. Unburned Hydrocarbon in Diesel engines

Once the injection fuel is initiated into the cylinder, the equivalence ratio distribution is developed through the spray of fuel. The amount of poor mixture that has a lower lean limit to combustion ($\Phi \cong 0.3$) increases, rapidly, with time.

In the flow with swirl, the ignition occurs slightly in lean regions to the spray cone where the fuel is kept longer in the combustion limits. However, the fuel near the boundary has been mixed beyond the lean limit and there was no auto ignition or sustained a rapid reaction front. This mixture can only be oxidized by oxidation thermal reactions relatively slow, which cause incomplete oxidation. In this region, unburned fuel, decomposition products thereof and products of partial oxidation (aldehydes and other oxygenated compounds) must exist. Some of these are issued without being burned. The unburned hydrocarbons magnitude in this region depends on the fuel amount injected during the ignition delay, on the rate of mixing with air in that period and the extent of the conditions leading to auto ignition. (Heywood, 1988)

4. DEVELOPMENT

For this study, a six cylinder compression ignition engine was used, whose technical specifications are described in Table (1). The injection was modeled using typical values on references, for the amount and spray parameters. A glow plug was used to assist in the combustion process, ensuring the start of burning process in the simulation.

Table 1. Engine specifications used for numerical simulation.

Technical Specifications	
Bore × stroke, mm	128 × 160
Chamber displacement, liters	2.0
Compression Ratio	19:1
Speed, rpm	1800
Intake Pressure, Pa	1,5 × 10 ⁵

4.1. Geometry

The combustion chamber was designed to match the usual characteristics of diesel cycle combustion chambers. The piston bowl is axisymmetric, and there is a rebound representing the glow plug, which in the simulation was kept at a fixed temperature, 1173 K.

Figure (1) shows a solid representing the fluid inside the combustion chamber. The glow plug detail can be noticed. For the purpose of investigation, the injector was characterized by spray parameters which were kept constant in all cases, such as: injector position, injection crank angle, spray angle, fuel quantity injected, particle number, etc. The injector is not physically represented in simulation, but the fuel spray is simulated using the parameters mentioned in the previous sections.

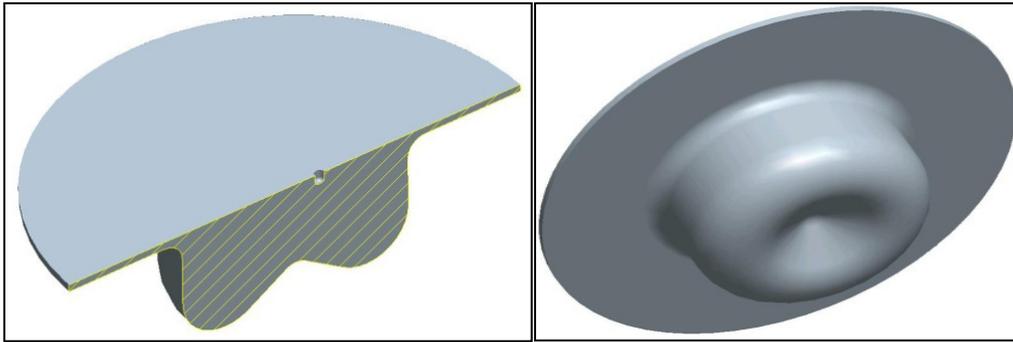


Figure 1. Details of the domain used in numerical simulation.

For the mesh generation, the piston must be positioned at top dead center (TDC), corresponding to 720 CAD (degrees of crankshaft - *Crank Angle Degrees*). This is used as a reference point for the meshes creation in various crankshaft angular positions, avoiding the use of negative values of the crankshaft position to reference injection parameters. By using the commercial computational code AVL Fire 2009, the surface and volumetric meshes for the numerical simulation were generated, as can be seen in Figs. (2) and (3).

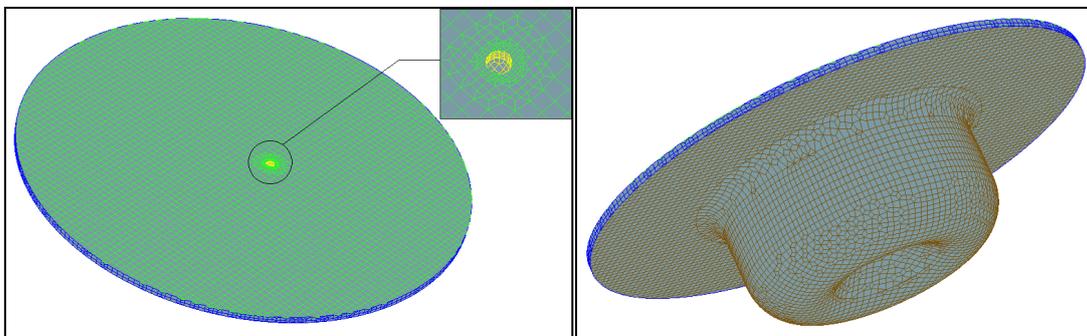


Figure 2. Mesh surface used in the simulation, showing the glow plug detail.

The meshes used have different refinement levels, ranging from about 80,000, at 690 CAD to 346,000, PMS and 820 CAD. Close to PMS there is an increase in the number of elements, although the computational domain is smaller. In the strategy solution of FIRE, multiple meshes are created. Each one is valid only for a certain range, in the case for 5 CAD. To perform the calculations at intermediate points, the commercial computational code interpolates values using the mesh created at the extremes of the range.

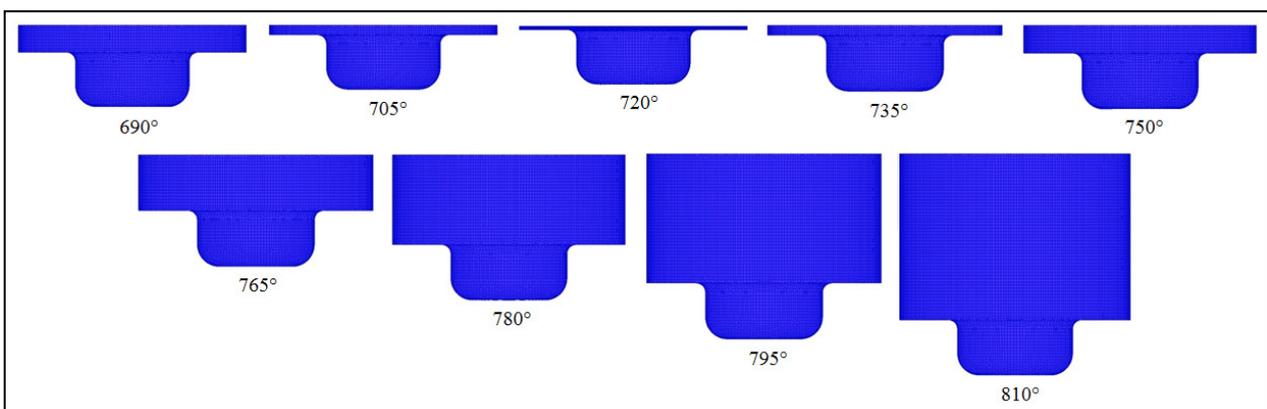


Figure 3. Evolution of volumetric mesh in the numerical simulation.

4.2. Boundaries and Initial Conditions

After the volumetric meshes creation, the boundary and initial conditions must be defined for the cases. The window of simulation was set at 130 CAD and different durations of time steps were used in this range, aiming the CPU time

reduction. It began with 0.2 crank-angle degrees, and, from the injection start (713 CAD) until 770 CAD it was reduced to 0.05. After 770 CAD, the time step value was set to baseline values.

The ECFM-3Z combustion model and the $k - \zeta - f$ turbulence model were used. The parameters of anhydrous ethanol fuel and injection parameters were defined. The latter has a single hole of 0.8 mm diameter, forming a spray angle of 150°. The distribution of particles size is uniform, with a diameter of 0.1 mm, injected at a constant rate over 10 CAD (713-723 DAC). Injector was positioned in the center of the cylinder head, just below the surface. The injected fuel mass was sufficient to obtain an equivalence ratio of 0.75 in the case without EGR and, for other cases, the injected fuel mass has not changed, resulting in a higher value for this rate, as can be seen in Table (2). The temperature of the ethanol injected was 500 K.

Table 2. Equivalence ratio obtained for the cases.

Case	Equivalence Ratio
No EGR	0,75
10% EGR	0,83
20% EGR	0,94
30% EGR	1,07

For momentum and continuity equations coupling, the algorithm SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) was used. Convergence at each time step was declared when the normalized residuals for the momentum and pressure equations dropped to 1.e-3 for residues of the momentum and pressure equations. These criteria were met in all time steps. The boundary conditions used in simulations are gathered in Table (3).

Table 3. Boundary conditions used in the simulations.

Surfaces:	Flow condition:	Temperature, K:
Piston	Non-slip	575
Cylinder wall	Non-slip	500
Cylinder Head	Non-slip	550
Glow Plug	Non-slip	1173

4.3. Equations solution

The computational code solves equations sets shown previously, calculating fluid flow, injection spray, combustion of the mixture and pollutants formation in parallel. The computational effort is considerable, requiring a large processing capacity and memory of the computers used in simulations. The computers specifications used in the simulations are as follows:

- Intel Core 2 Duo 2 GHz, model T7250;
- 04 GB of RAM;
- 800 MHz FSB
- 200 Gb HDD, 5400 RPM.

The average processing time of simulations was eight days each, approximately, with a total of 1534 time steps, and about 40 iterations per time step. The first time step, exceptionally, required about 120 iterations to achieve the convergence criteria.

5. RESULTS

5.1. Spray

Due to the high temperature of the injected fuel and air into the combustion chamber, there is a rapid fuel evaporation and low particles penetration in the chamber (about 1 cm) as can be seen in Fig. (4). This small penetration contributes to a very low value for ignition delay, indicating that oxygen reacts with the fuel immediately after the injection start and always close to injector and glow plug. This is due to the chamber conditions, because even the fuel having low cetane number, their reaction showed an almost zero delay.

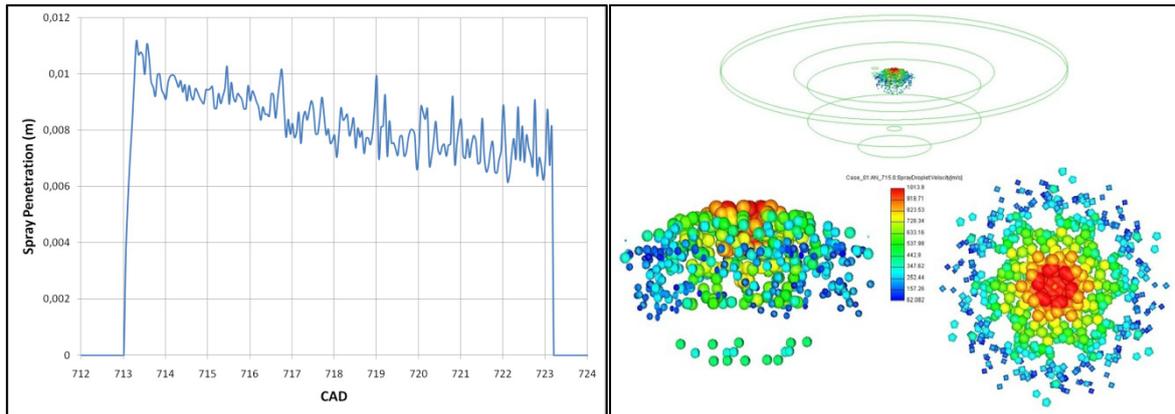


Figure 4. (A) Spray Penetration, (b) spray position and (c) velocities and droplet size distribution.

5.2. Temperature, Rate of Heat Release and Reaction Rate

Due to the different values for the equivalence ratio in the simulated cases, temperature has not changed as much as expected, as can be seen in Fig. (5). The instabilities presented in this graph, and others that will be shown later, arise from the results interpolation when changing of volumetric mesh used, a problem that repeats every 5 CAD, which was the chosen interval for mesh change.

As expected, the rate of heat release during premixed flame is greater than that in the diffusive phase, starting shortly after the injection, as shown in Fig. (5), which shows the rate of heat release in the case without EGR. For the remaining cases, there are no significant variations in the rate of heat release, with only a minor difference between premixed and diffusion flame phases.

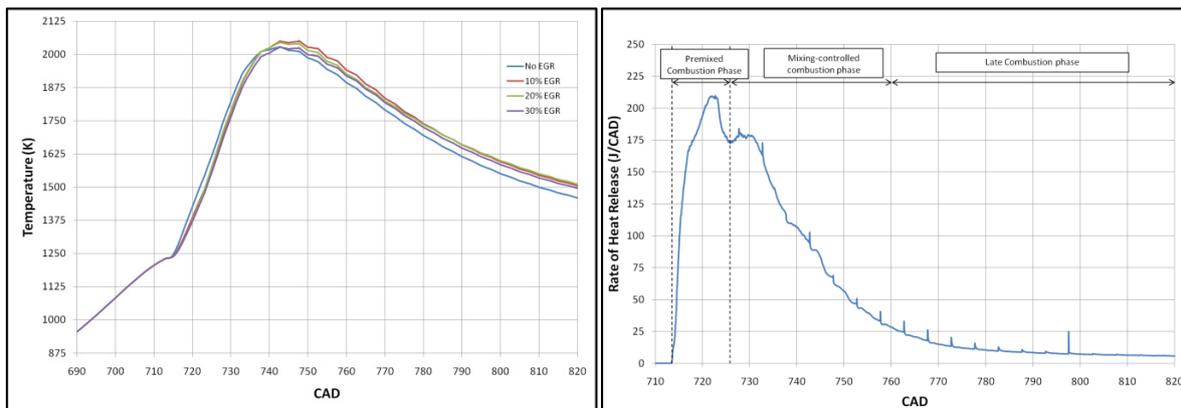


Figure 5. (a) Mean gas temperature inside the chamber and (b) rate of heat release.

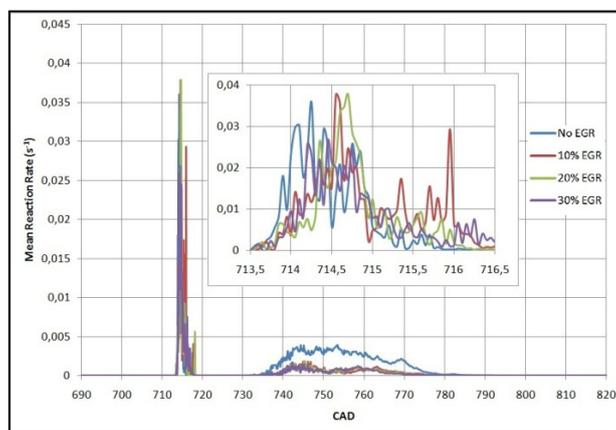


Figure 6. Mean reaction rates.

The highest reaction rates, for all cases, are found shortly after TDC, soon after the injection starts. This is because of the fuel being injected into the combustion chamber when temperature and pressure values were very high, therefore very close to self-ignition conditions. The temperature of the injected fuel also contributes to small delay found in all cases, with the combustion starting immediately after the injection start. In Fig. (6) may be noted that the highest values for reaction rates occur in the range from 713 CAD to 716 CAD.

5.3. Mass fraction of species

The mass fractions evolutions for the C_2H_5OH , O_2 , CO_2 , H_2O and CO species, for cases without EGR and with 30%, are shown in Fig. (7). Note that the variation was small, comparing the two extremes.

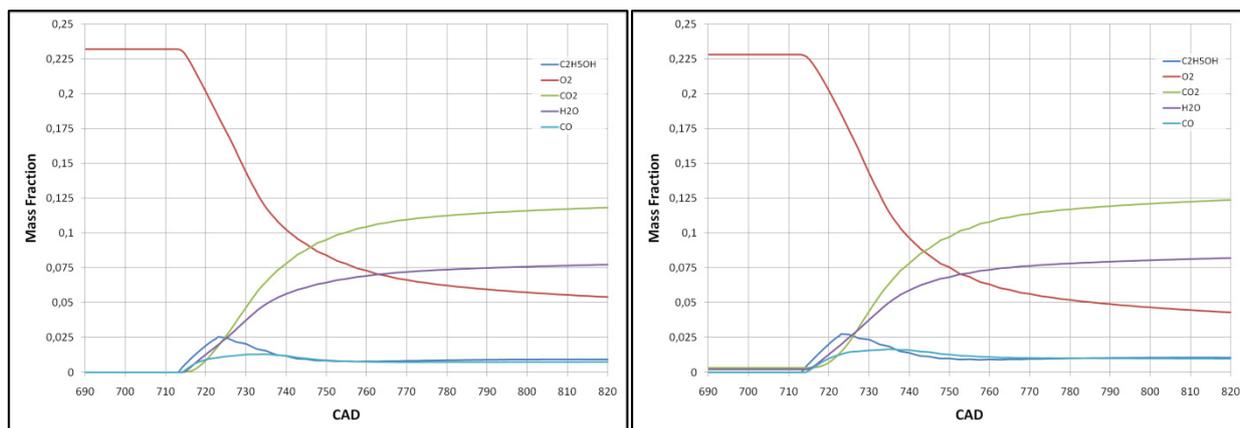


Figure 7. Mass fractions evolution for each species for cases (a) without EGR and (b) with 30% EGR.

5.4. Particulate Matter, CO and CO_2

For the cases of 0, 10 and 20% EGR, there is a tendency to increase the CO mass fraction due to the increase of equivalence ratio, while for the same interval, the value of Particulate Matter mass fraction decreased, probably due to the operating conditions imposed, favoring the oxidation, complete and partial, of available fuel. This can be seen in Figs. (8) and (9).

For the 30% EGR case, the value of CO mass fraction decreases, because the available carbon form particulate material, explaining the increase of this mass fraction due to reduction of initial concentrations of oxygen (initial mixture with $\phi > 1$).

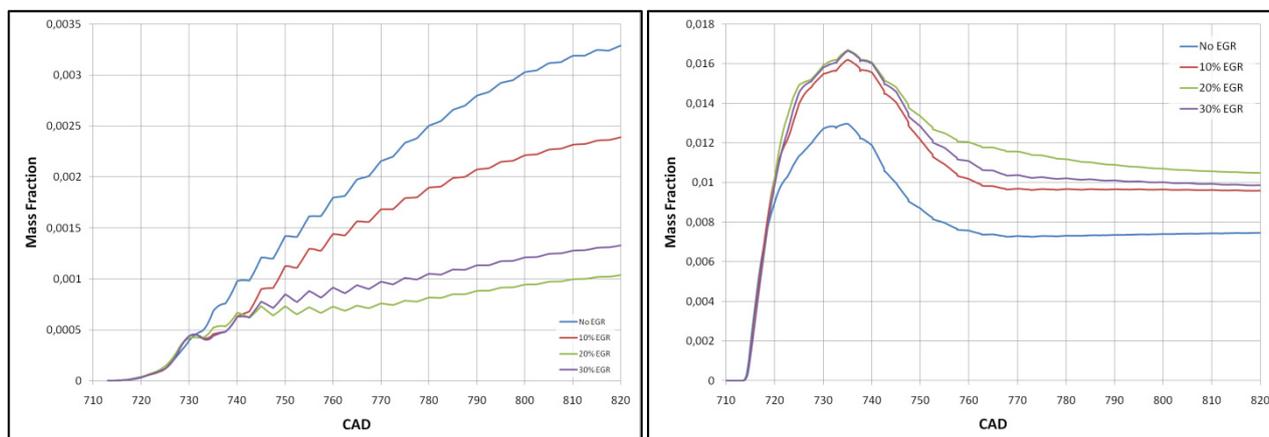


Figure 8. Mass fractions of (a) Particulate Matter and (b) CO.

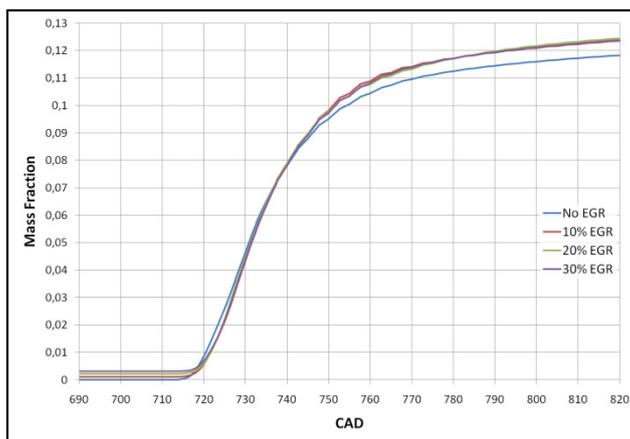


Figure 9. Mass fractions of CO₂.

5.5. Nitrogen Oxides

In accordance with the nitrogen oxides formation mechanisms described above, the highest formation rate occurs after peak pressure and very close to peak temperature (20° after the TDC), which can be seen in Fig. (10).

In Fig. (10) one can verify the reduction in NO_x mass fraction as the value of EGR is increased, obtaining a value up to 40% lower for the case with 30% EGR, in comparison with the case without EGR, shown in Tab. (4).

In the cases simulated, the NO_x formation reduction cannot be explained by Zeldovich mechanism because, as noted earlier, temperature remained the same for all cases. The explanation for the NO_x formation reduction is based on gradual reduction of oxygen available in each case, mainly due to increase in equivalence ratio value.

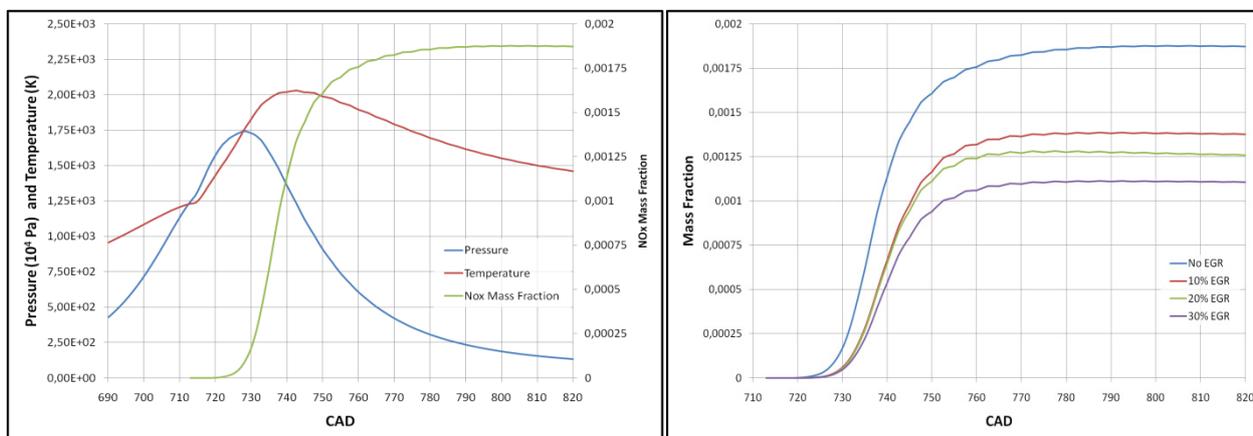


Figure 10. (a) Pressure, temperature and NO_x concentration evolution and (b) NO_x mass fractions Evolution.

Table 4. NO_x reduction for all cases.

Case	NO _x	Reduction, %
No EGR	0,001873	-
10% EGR	0,001376	26,6
20% EGR	0,001259	32,7
30% EGR	0,001106	40,9

6. CONCLUSIONS

The simulations require validation through experimental results, however, for this case, in which the results are based only on the engine operating terms variation, the numerical simulation represents well these trends caused by, for example, reducing NO_x emission by 40% using 30% EGR.

Therefore, for obtaining data representing real values of emissions in a diesel engine fueled with ethanol, it would be necessary to validate at least one of the simulated cases with experimental data.

Due to the imposition of initial conditions identical in all cases, some changes were necessary, such as maintaining a constant equivalence ratio, instead of keeping the injected fuel amount fixed. The initial conditions should also be altered, because the use of EGR would affect them, and this fact was not taken into account in the simulated cases

7. REFERENCES

- Glassman, I. "Combustion". 2. ed. New Jersey: Academic Press, 1986. 501p.
- Heywood, J. B. "Internal combustion engine Fundamentals". 1. ed. New York: McGraw-Hill, 1988. 930p.
- Lacava, P. T. et al. "Combustão em turbinas a gás". II Escola de Combustão, p.142-143, São José dos Campos, Junho 2009.
- Lefebvre, A. H. "Gas Turbine Combustion". 2.ed. Philadelphia: Taylor and Francis, 1999. 400p.
- Minteer, S. "Alcoholic Fuels". 1.ed. Boca Raton: CRC Press, 2006. 270p.
- SILVA, M. F. "Emissão de metais por veículos automotores e seus efeitos à saúde pública". 155f. Tese (Mestrado em Saúde Pública) – Universidade de São Paulo, São Paulo. 2007
- Turns, S. R. "An Introduction to combustion: concepts and applications". 2. ed. Pennsylvania: McGraw-Hill, 2000. 676p.
- Warnatz, J.; Maas, U.; Dibble, R. W. "Combustion: physical and chemical fundamentals, modeling and simulation, experiments, pollutant formation". 4.ed. Berlin: Springer, 2006. 378p.

8. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.