# ENC-2020-0464
# ANALYSIS OF THE INFLUENCE OF ETHANOL REFORMING GASES ON THE PERFORMANCE AND EMISSIONS OF A COMPRESSION COMBUSTION ENGINE

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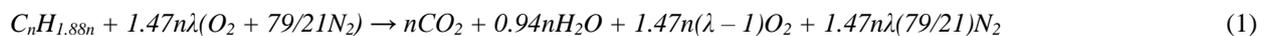*reydila.barbosa@sga.pucminas.br* *hanriot@pucminas.br* *cristianohbrito@gmail.com* *osmano.valente@gmail.com* *cristiana@pucminas.br*

***Abstract.*** *Currently, internal combustion engines power more than 99.9% of vehicles in circulation. When compared to SI engines, CI engines are more efficient, have better fuel economy, and lower $CO_2$ emissions. In contrast, they emit a greater quantity of nitrogen oxide ($NO_x$) and particulate matter (PM). One of the options to reduce emissions from CI engines is the addition of hydrogen ($H_2$) during the combustion process This study evaluated the effects of the application of gases obtained from the ethanol reforming on the performance and emissions of a diesel engine. Different proportions of ethanol/steam and reforming temperatures generated different percentages of $H_2$ and inert gases. For larger quantities of hydrogen added to the combustion chamber, there was an increase in the pressure and internal temperature of the cylinder. Regarding specific consumption, the addition of these gases caused an improvement of 17.22%. In terms of emissions, there was a decrease in the amount of $NO_x$. The addition of reformed gases increased the emissions of CO, particulate matter, and unburned hydrocarbons.*

***Keywords:*** *ethanol reforming, hydrogen, diesel engine, compression ignition engine.*

## 1. INTRODUCTION

Currently, internal combustion engines power more than 99.9% of vehicles in circulation (Kalghatgi, 2019). There are two types of internal combustion engines: spark-ignition (SI) engines, which operate on gasoline and ethanol, and compression ignition (CI) engines that use diesel as fuel (Heywood, 2018). When compared to SI engines, CI engines are more efficient, have better fuel economy, and lower $CO_2$ emissions. In contrast, they emit a greater quantity of nitrogen oxide ($NO_x$) and particulate matter (PM) (Karagöz et al., 2016a; Kumar et al., 2018; Tsolakis; Megaritis; Wyszynski, 2004; Tsolakis; Megaritis; Yap, 2008). The high efficiency, durability, reliability, and low operating cost of CI engines make them the best choice for heavy vehicles. According to Tsolakis and Megaritis (2005), the combustion reaction of a typical diesel engine is represented by eq. (1):

$$C_nH_{1.88n} + 1.47n\lambda(O_2 + 79/21N_2) \rightarrow nCO_2 + 0.94nH_2O + 1.47n(\lambda - 1)O_2 + 1.47n\lambda(79/21)N_2 \qquad (1)$$

One of the options to reduce emissions from CI engines is the addition of hydrogen ($H_2$) during the combustion process. Hydrogen is a clean-burning alternative fuel. The combustion of a lean mixture of $H_2$ and air as the final product is water and $NO_x$ (WANG et al., 2018). Other characteristics of $H_2$ include lower ignition energy and faster flame propagation speed. The high speed of propagation of the hydrogen flame increases the H/C ratio of the fuel and reduces the duration of combustion (Abu-Jrai; Tsolakis; Megaritis, 2007; Ghazal, 2013; Tsolakis; Megaritis, 2004). During the combustion process of diesel oil, recombination reactions occur, and the consequent emission of unburned HC. The higher speed of the $H_2$ combustion reduces these reactions and, as a consequence, increases the thermal efficiency of combustion (Morais, 2012). Due to its high ignition temperature (576 ºC), it is not possible to use $H_2$ directly in diesel engines (Bose; Maji, 2009; Karagöz et al., 2016a). For this reason, it is more common to add it as a complementary fuel (Karagöz et al., 2016b).

Hydrogen production methods include natural gas steam reforming, partial oxidation of heavy oils, coal gasification, and water electrolysis, among others. (Navarro Yerga et al., 2011) Most of the hydrogen produced nowadays is derived from natural gas and generates a high amount of $CO_2$, (Da Costa-Serra; Chica, 2018). The production of hydrogen from the steam reforming of ethanol is an alternative, since ethanol is non-toxic, with high hydrogen content and low

production cost (Wang; Lee; Lin, 2009). Another favorable condition for the use of reformed ethanol is that, in Brazil, there is an installed structure for its production and distribution, which makes it an alternative and renewable energy source present throughout the national territory (Evaristo, 2010). Moreover, steam reforming is the most efficient in terms of hydrogen productivity (Arslan Bozdag et al., 2019; Cheekatamarla; Lane, 2005; Cai et al., 2008). The stoichiometric reaction of ethanol steam reforming is given by eq. (2) (Basile et al., 2011; Casanovas et al., 2010; Lim; Gu; Oyama, 2012).

$$C_2H_5OH + 3H_2O \rightarrow 2CO_2 + 6H_2 \quad \Delta H_{298\ K} = 157.0\ kJ/mol \tag{2}$$
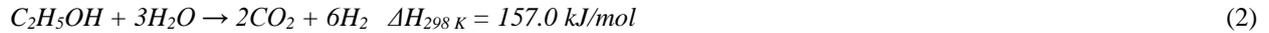
Another reaction that occurs in parallel with ethanol steam reforming is the water-gas shift reaction (eq. (3)), (Chen; Wang; Liu, 2019; Saidi; Jahangiri, 2018; Tosti et al., 2011). Methanation (eq. (4)) also takes place during ethanol reforming (Martin; Wörner, 2011; Specchia et al., 2006).

$$CO + H_2O \leftrightarrow H_2 + CO_2 \quad \Delta H_{298\ K} = -41.19\ kJ/mol \tag{3}$$

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O \quad \Delta H_{298\ K} = -165.4\ kJ/mol \tag{4}$$

Several noble metal-based catalysts, such as Pt, Pd, Rh, Au, Ir, and Ru, are suitable for ethanol steam reforming in different temperature ranges. Other metals (Ni, Co, Cu, and Ce), as well as bimetallic catalysts (NieRh, PteCo, Rh-Pt), have also presented high activity and selectivity to $H_2$ production (Chen; Wang; Liu, 2019; Hao; Guo; Han, 2019; Kourtelesis; Panagiotopoulou; Verykios, 2015; López; Divins; Llorca, 2012). In general, the choice of catalyst material aims to produce gas rich in hydrogen and to minimize the formation of products such as $CH_3CHO$, $C_2H_6$, $C_2H_4$, $CH_4$, and CO. The efficiency of the catalysis is also directly related, among other parameters, to the type of catalyst (Saidi; Jahangiri, 2018).

Brito (2019) numerically evaluated the influence of operational parameters in ethanol reforming by building a model in the ChemKin software, considering a Pt/Rh/Pd–5:1:1 catalyst, with 600 cells per square inch, a geometric surface area of 3,182 $m^2/m^3$ and the exhaust gas recirculation (EGR) with 5% and 10% as a heat source The temperature ranging from 523 K to 1023 K. The model of the simulation mechanisms considers 7 volumetric reactions and 33 surface reactions. For these conditions, the reforming products obtained were: CO, $H_2$, $H_2O$, $CH_4$ and $O_2$, as well as $CH_3CH_2OH$ and $CH_3CHO$ in smaller proportions.

Justino (2012) studied the effects of hydrogen and methane in a CI engine powered by diesel with 5% biodiesel in its composition. In his experimental analysis, he compared the combustion of an engine powered by diesel, diesel and $H_2$, and diesel and methane ($CH_4$). The addition of $CH_4$ reduced the specific consumption and decreased the temperature of the exhaust gases. $H_2$ showed similar results to those of methane.

Morais (2012) evaluated the behaviour of an engine powered by diesel and hydrogen. The lower calorific value was used as a substitution parameter. The percentages of $H_2$ used in the experiment were 5%, 10%, 15% and 20%. The results showed that the addition of hydrogen decreases the specific consumption.

Tsolakis et al. (2010) studied the effects of adding reformed exhaust gas (REGR) to a diesel engine. REGR containing $H_2$, CO, $CH_4$, and $CO_2$ was injected into the combustion chamber as a complementary fuel. The engine operated at low-load throughout the experiment, and different percentages of REGR were added. The use of REGR as a complementary fuel caused a decrease in $NO_x$ and soot emissions.

Kumar et al. (2017) studied the impact of reformed exhaust gases on a CI engine powered by diesel. A computational model was built on the ES-ICE software. They evaluated the behavior of pressure and temperature inside the cylinder, as well as soot and NOx emissions for different percentages of REGR. As a result, they found peak pressures up to 12.1% higher for simulations with 15% REGR. The piston work was also greater for 5% and 15% REGR. The addition of REGR caused a drop in soot emissions. There was a maximum decrease of 12.73% in the soot emission to 15% of REGR added to the combustion chamber.

## 2. METHODOLOGY

This work aims to make a numerical analysis of the influence of the mixture of EGR and ethanol reform gases on the performance and emissions of a diesel engine. The engine used in this study is a four-stroke diesel engine. It has four cylinders and operates at a speed of 1200 rpm. The positioning of the injection nozzle and some simplifications in the cylinder geometry allowed the use of only one-eighth of the combustion chamber during the simulation. Thus, the calculations started with the opening of the intake valve at -165 ° CA and ended with the closing of this exhaust valve at 125 ° CA.

In the simulation, using the ANSYS Forte software, a diesel mixture was considered and is composed of 87.4% nitrogen and 12.6% oxygen, totaling 100% of the gases present in the cylinder. With the addition of the reform gases, the amount of combustion chamber decreases. Table 1 shows the mass percentage of the reform gas, $N_2$ and $O_2$ used in

different simulations. The 5% EGR label indicates that, of a total of 100%, 5% of the combustion chamber gases are products of the ethanol reforming, while the other 95% are gases that precede air. One statement is valid for 10% EGR.

Table 1. Percentage of air and EGR added in the simulations

| % EGR | % $N_2$ | % $O_2$ | % of total air |
|---|---|---|---|
| 5 | 83.03 | 11.97 | 95 |
| 10 | 78.66 | 11.34 | 90 |

The data related to the reform gases were obtained by Brito (2019), using the ChemKin software, in his thesis on the study of the process of reforming the ethanol vapor to enrich the EGR in an internal combustion engine. The reactor used for the reforming was a Pt/Rh/Pd–5:1:1 reactor with six hundred cells per inch. Table 2 lists some reforming features that will be important in the course of this study, such as the percentage of EGR, the proportion of ethanol and water steam, and the temperature of the catalytic reaction.

Table 2. Reform gas characteristics

| Percentage of EGR | 5% and 10% |
|---|---|
| Ethanol/Steam ratio | 1/2, 1/3 and 1/5 |
| Catalytic reaction temperature | 523 K, 623 K and 723 K |

The simulation showed the products at the output of the reformer for each of these conditions, totaling eighteen simulated models. From these data, the amount of reforming gases present in the combustion chamber was calculated. Table 3 shows the chemical composition of the reforming gases added to the combustion chamber together with diesel oil.

Table 3. Chemical composition of reform gases

| Model | Model Characteristic | Mass Fraction of Species in the Combustion Chamber | | | | | |
|---|---|---|---|---|---|---|---|
| | | $CH_4$ | CO | $CO_2$ | $H_2$ | $H_2O$ | $O_2$ |
| M. 1 | 5%EGR-1/2 E/V-523K | 0.0165980 | 0.0082718 | 0.0017587 | 0.0000628 | 0.0231292 | 0.1198780 |
| M. 2 | 5%EGR-1/2 E/V-623K | 0.0140528 | 0.0072897 | 0.0009560 | 0.0006989 | 0.0262257 | 0.1204770 |
| M. 3 | 5%EGR-1/2 E/V-723K | 0.0119443 | 0.0091464 | 0.0010050 | 0.0040916 | 0.0231422 | 0.1203700 |
| M. 4 | 5%EGR-1/3 E/V-523K | 0.0135875 | 0.0064912 | 0.0018413 | 0.0000400 | 0.0267363 | 0.1210040 |
| M. 5 | 5%EGR-1/3 E/V-623K | 0.0120330 | 0.0060233 | 0.0010423 | 0.0007548 | 0.0299395 | 0.1199073 |
| M. 6 | 5%EGR-1/3 E/V-723K | 0.0102147 | 0.0082795 | 0.0011350 | 0.0041437 | 0.0255574 | 0.1203714 |
| M. 7 | 5%EGR-1/5 E/V-523K | 0.0105574 | 0.0043940 | 0.0016686 | 0.0000543 | 0.0325209 | 0.1205050 |
| M. 8 | 5%EGR-1/5 E/V-623K | 0.0123104 | 0.0062922 | 0.0009578 | 0.0007160 | 0.0288344 | 0.1205900 |
| M. 9 | 5%EGR-1/5 E/V-723K | 0.0060310 | 0.0057484 | 0.0014366 | 0.0042303 | 0.0317243 | 0.1205293 |
| M. 10 | 10%EGR-1/2 E/V-523K | 0.0306821 | 0.0130070 | 0.0041850 | 0.0000911 | 0.0503450 | 0.1150903 |
| M. 11 | 10%EGR-1/2 E/V-623K | 0.0285046 | 0.0128162 | 0.0026766 | 0.0014344 | 0.0521052 | 0.1158631 |
| M. 12 | 10%EGR-1/2 E/V-723K | 0.0242827 | 0.0170679 | 0.0041900 | 0.0084180 | 0.0455513 | 0.1138914 |
| M. 13 | 10%EGR-1/3 E/V-523K | 0.0284391 | 0.0107582 | 0.0035807 | 0.0000827 | 0.0546398 | 0.1158996 |
| M. 14 | 10%EGR-1/3 E/V-623K | 0.0255936 | 0.0106645 | 0.0033898 | 0.0015571 | 0.0577874 | 0.1144076 |
| M. 15 | 10%EGR-1/3 E/V-723K | 0.0208796 | 0.0146352 | 0.0047900 | 0.0086894 | 0.0506687 | 0.1137383 |
| M. 16 | 10%EGR-1/5 E/V-523K | 0.0249220 | 0.0066195 | 0.0030416 | 0.0001053 | 0.0641000 | 0.1146117 |
| M. 17 | 10%EGR-1/5 E/V-623K | 0.0195618 | 0.0066022 | 0.0044371 | 0.0017119 | 0.0664686 | 0.1146200 |
| M. 18 | 10%EGR-1/5 E/V-723K | 0.0139112 | 0.0103032 | 0.0058030 | 0.0089870 | 0.0596870 | 0.1147086 |

## 3. RESULTS

The results of a simulation are presented below, using ANSYS Forte, which shows the effects caused by the addition, in the combustion chamber, of the product of the ethanol and EGR reforming on the combustion parameters and derivatives of an ignition engine by compression.

## 3.1 Combustion chamber pressure

Figure 1 shows the pressure behavior in the combustion chamber after adding different reform gases to the fuel. The highest-pressure values occurred for Models 3, 6 and 9. For 5% EGR, there was a higher production of hydrogen in the reforming processes at 723 K, which accelerated the combustion reactions. The pressure increase in the combustion chamber for the Model 9 is 18.47%. The maximum pressure for this condition is 9.96 MPa. Model 3 shows an increase of 17.85% and a peak of 9.89 MPa. The maximum pressure for Model 9 is 9.66 MPa, which represents an increase of 15.88%.
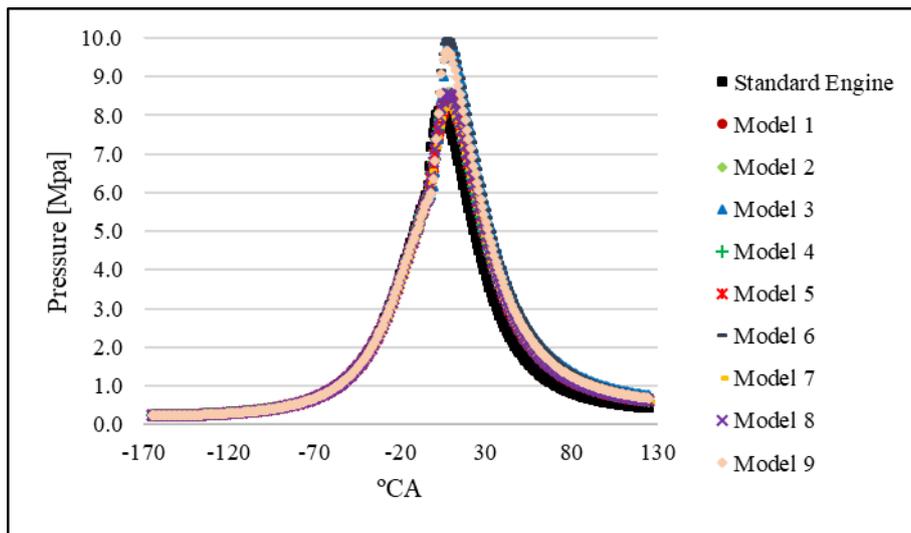


Figure 1. Pressure x Crank Angle for models with 5% of EGR

For 10% of the EGR, there is no increase in pressure in the combustion chamber. Compared to the pressure by the standard fuel, adding reform gas to the Model 12 fuel caused a 25.34% drop in the pressure of the cylinder. The pressure is 6.07 MPa for this model. For Model 15, the maximum pressure is 6.35 MPa, 21.80% less than that with standard fuel. At one point, the increase in the amount of reformed gas added began to cause both a decrease in peak pressure and a delay in the pressure phase. The addition of a larger amount of inert gases caused an increasing delay in the reaction of the fuel with the air, which reduced the conversion efficiency of the fuel reducing the pressure drop in the cylinder. The pressure for all reforming models is lower than that standard location.
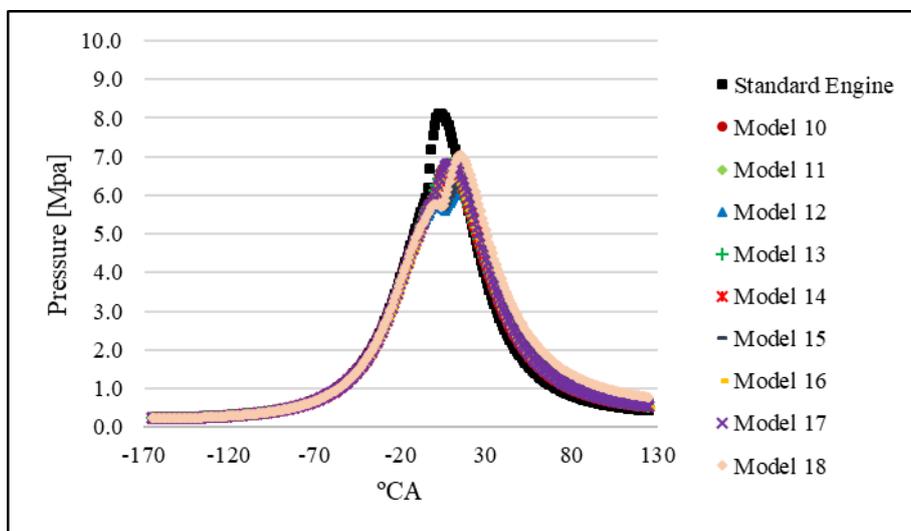


Figure 2. Pressure x Crank Angle for models with 10% of EGR

### 3.2 Combustion chamber temperature

Figure 3 shows the temperature behavior after adding different reform gases to the fuel. The biggest temperature rise occurred for Models 3, 6 and 9. Model 3 presented an increase of 26.04% in the temperature, with a peak of 1631.82 K. Model 6 showed a peak of 1617 K, an increase of 25.38% when compared to the standard model. There was an increase of 22.20% for Model 9, which presented a peak of 1551.38 K.
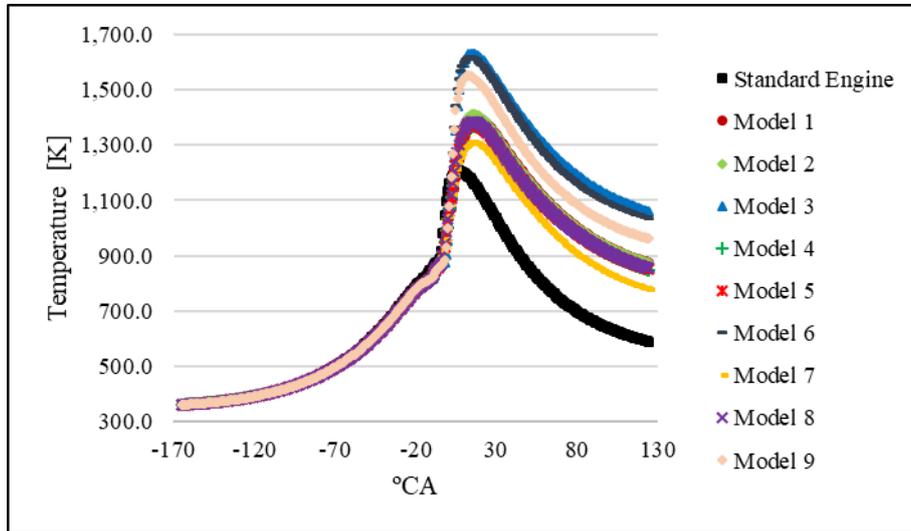


Figure 3. Temperature x Crank Angle for models with 5% of EGR

For combustion with 10% EGR, Model 18 showed a peak temperature of 1404.28 K, which represents an increase of 14.05% over the maximum standard fuel pressure. The other models did not gain significant temperature when compared to the standard model.
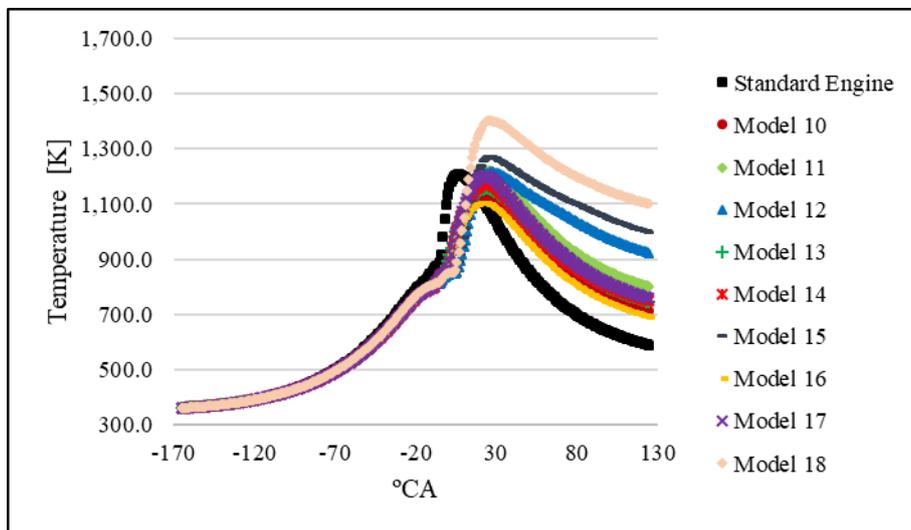


Figure 4. Temperature x Crank Angle for models with 10% of EGR

### 3.3 Heat release rate

Figure 5 shows the effect of adding reform gases on the heat release rate. The maximum rate of heat release, equal to 552.07 J/°CA, is observed in Model 9 (5% EGR), an increase of 37.91% when compared to the value produced by the standard fuel. Models 6 and 3 also show an increase in the heat release rate. For Model 6, this increase is 36.70% and the peak calorie release is 541.51 J/°CA. Model 3 shows a peak of 526.66 J/°CA, which represents an increase of 34.92%.
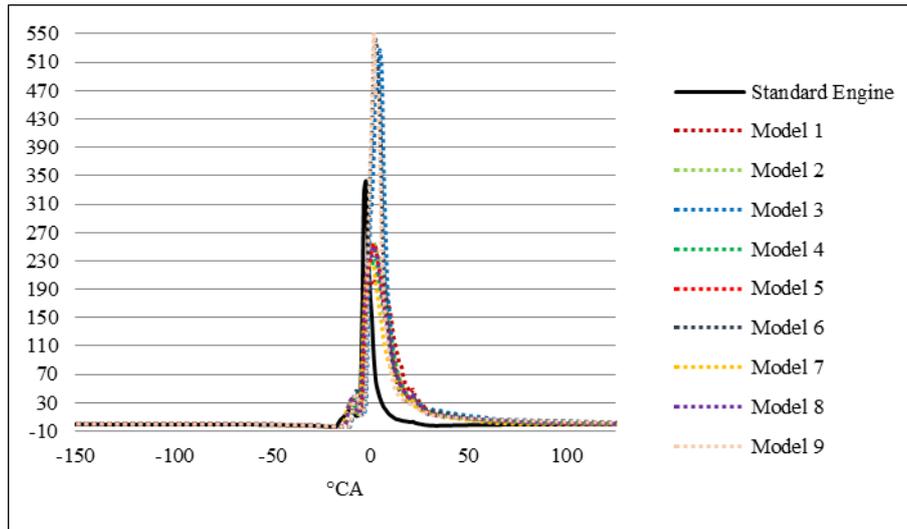
Figure 5. Heat release rate for 5% of EGR

Figure 6 shows the heat release rate for 10% EGR. In general, EGR works by slowing down combustion reactions, which justifies a lower peak in the heat release rate for 10% of the EGR added to the fuel, considering the same reforming temperature. For this same reason, when compared to standard fuel, other models tend to flatten and widen the curve that represents the heat released by combustion. The high temperature peak found for Model 18, due to the higher concentration of $H_2$, causes an increase in the heat release rate of this model.
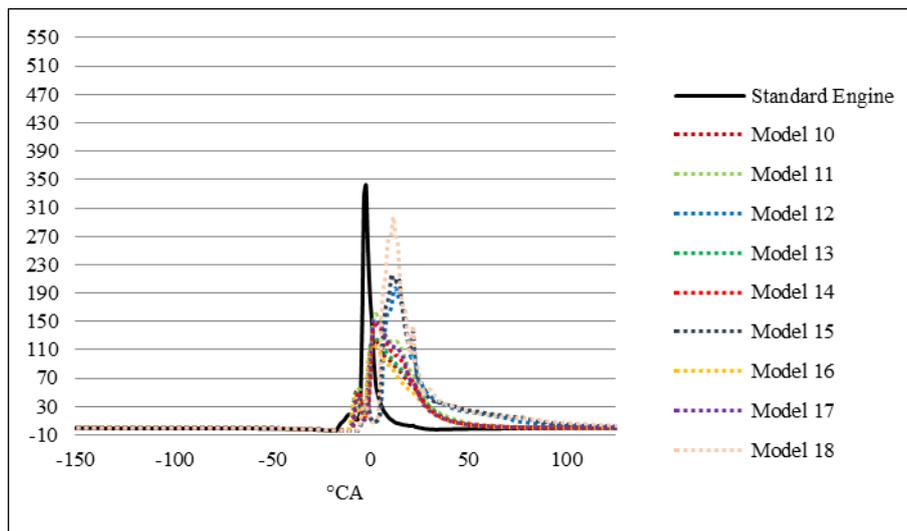


Figure 6. Heat release rate for 10% of EGR

## 3.4 Consumption and emissions

Figure 7 compares the specific consumption of all simulations. The minimum specific consumption, of 374.39 g/kWh, is found for Model 3 and represents a drop of 17.22% when compared to the standard engine. Model 16 obtained the maximum specific consumption, equivalent to 462.66 g/kWh, which corresponds to an increase of 2.25%. In Models 3, 6, and 9, where there was a higher production of $H_2$, the indicated specific consumption found its lowest values. On the other hand, where the action of inert gases was more intense (Models 10, 13, and 16), the specific consumption was higher.
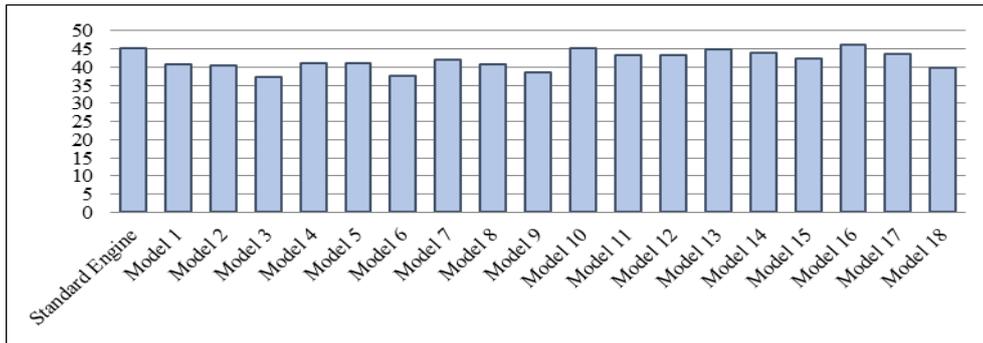
Figure 7 - Indicated specific consumption [g/kWh]

Figures 8 to 11 show the results of the characteristics simulation with the engine supplied with diesel and diesel over the products generated by the simulation model reform ethanol. Regarding the emission of carbon monoxide (Fig. 8), it is observed that the addition of the reformer gases present the highest values of that produced by the engine when fed with the standard fuel. Transfers increased by 94.68%, 94.58% and 94.04% for Models 12, 15 and 18. The maximum CO emission values were 558.22; 548.50 and 498.25 g/kg of fuel. The minimum gas emission, 112.06 g/kg of fuel, occurs for the Model 9. This result represents an increase of 73.51% in relation to the value produced by the standard fuel.
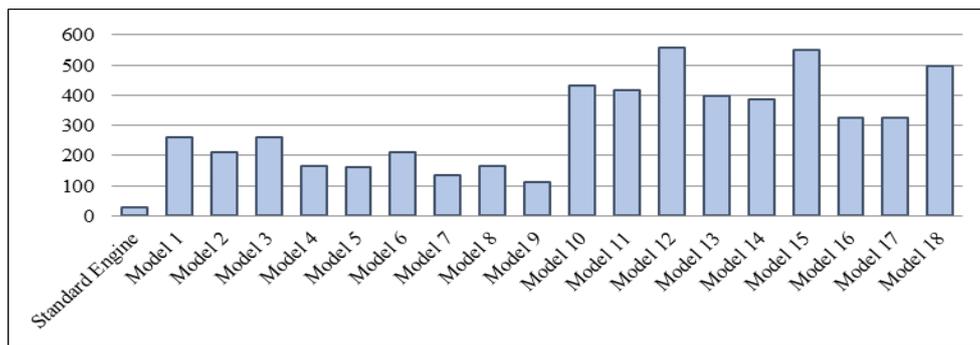


Figure 8. CO emission [g/kg$_{fuel}$]

There is also a decrease in the amount of $NO_x$ resulting from the simulation of the engine powered by diesel and diesel plus the products generated by the simulated models of ethanol reforming. (Fig. 11). The greatest reduction in the emission of this gas is equivalent to 85.06% and occurs in Model 1 (5% EGR). A greater amount of $H_2$ in the reformed gas tends to generate greater generations of $NO_x$.
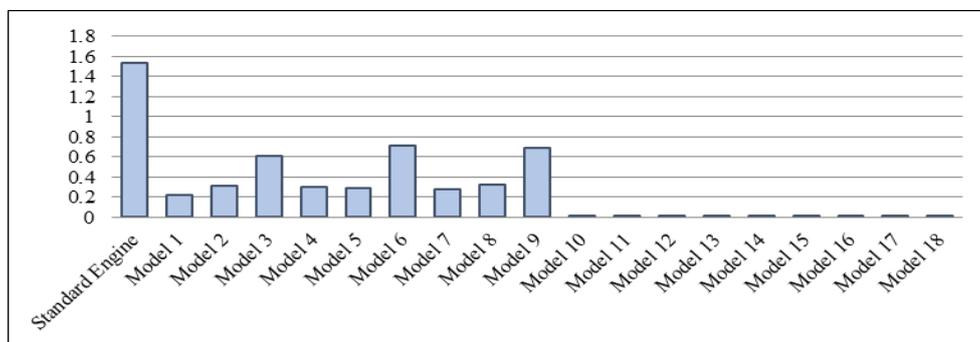


Figure 9. $NO_x$ emission [g/kg$_{fuel}$]

The soot emission increases with the addition of reformed gas to the fuel (Fig. 10). For Model 1, which has a higher soot emission, the value is 0.19 g/kg, which corresponds to an increase of 67.22% in relation to the value produced by the standard fuel. There is a reduction in soot emissions for models where 10% EGR has been added. Only Models 12, 15 and 18 emit less substances than standard fuel. Model 18 is the one with the greatest reduction in particulate material, 35.59%. For this model, the emission of particulate material corresponds to 0.038 g/kg of fuel.
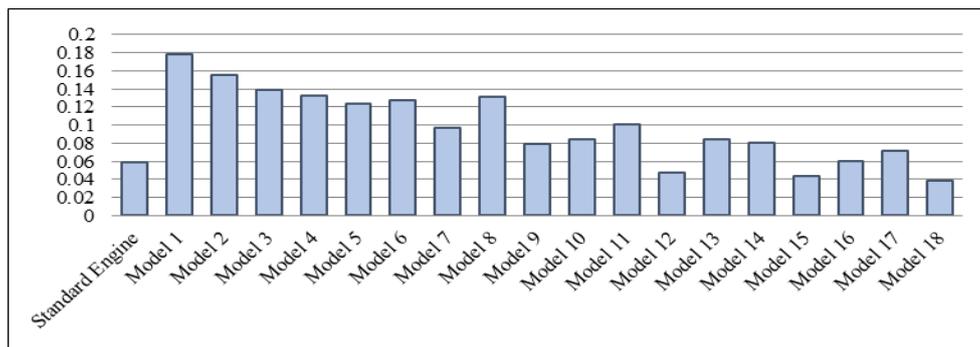
Figure 10. Soot emission [g/kg$_{fuel}$]

Figure 11 shows that the addition of reform gases causes an increase in the unburned or partially burned fuel emitted by the engine. This growth was higher for models in which 10% EGR was added. For Model 10, 596.8 grams of HC are emitted for each kilogram of fuel, which corresponds to an increase of 97.23%. Model 9 shows the lowest growth in the amount of HC emitted. In this model, there is an emission of 69.68 g/kg of fuel, which represents an increase of 76.34%.
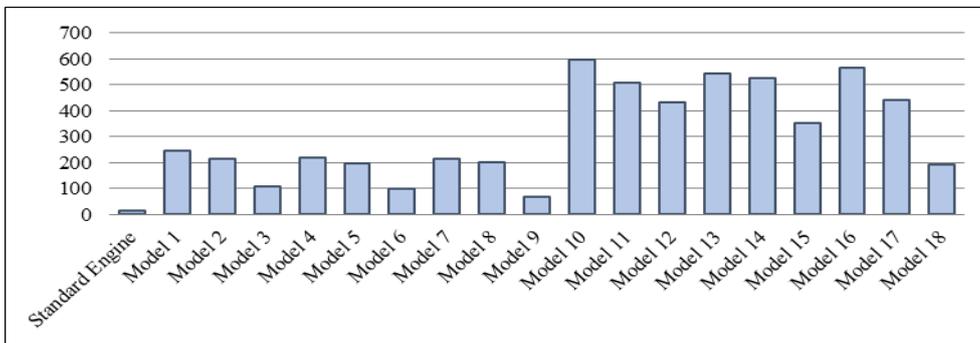


Figure 11. Unburned Hidrocarbons [g/kg$_{fuel}$]

## 4. CONCLUSION

The results show that the addition of the ethanol reform product and 5% EGR to the standard fuel produces in the combustion chamber:
1 - increased pressure for all simulation models, being more important for simulation Models 3, 6 and 9;
2 - temperature increase for all simulation models;
3 - increased heat release rate for simulation Models 3, 6 and 9.

With the product of 10% EGR ethanol reform for all models of simulation of combustion chamber performance results:
1 - less pressure;
2 - higher temperature;
3 - lower rate of heat release.

The consumption results and how to show:
1 - small reduction in specific consumption for all simulation models, except Models 10, 13 and 16;
2 - higher CO emission for all simulation models;
3 - reduction reduces NOx emission.
4 - higher soot emission for all simulation models;
5 - increased HC emission for all simulation models, with values obtained with 10% EGR being more evaluated.

## 5. ACKNOWLEDGEMENTS

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