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STUDY OF EMISSIONS IN COMBUSTION SIMULATION OF OXYGENATED FUEL MIXTURES

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Abstract. Renewable fuels are used in Internal Combustion Engines (ICE) as a way of solving economic and environmental issues. Biofuels, such as biodiesel and ethanol, pure or mixed with gasoline and diesel, have attracted several types of research since the burning of fossil fuels generates emissions of polluting gases, which have worrying consequences for the environment. The objective of this work is to simulate an internal combustion engine using mixtures of oxygenated fuels, diesel, biodiesel, and ethanol in the AVL Boost™ software, analyzing pollutant emissions of these blends. For this, a Fractal combustion model was developed based on data from the software, provided as an example, and from articles that model the use of internal combustion engines. Based on the AVL Boost™ fuel properties data and adding information of a generic biofuel, NOx, CO, and HC emission results were analyzed for different percentage amounts of fuels. For all simulations, the same physical configuration of the engine was maintained, changing only the amount of diesel, biodiesel, and ethanol in the fuel. Simulations were made for these three pure fuels; mixtures of diesel and ethanol (DE); diesel and biodiesel (DB) and finally, mixtures of the three fuels (DBE), considering D85B15 (15% biodiesel in diesel) were tested. The simulating results are in accordance with the literature, and it was observed that with increasing biodiesel concentration in the mixture, early ignition occurred, decreasing HC and CO levels, while NOx formation increased. However, adding ethanol to pure diesel or D85B15 blend increased ignition delay and reduced the emission of all pollutants.

Keywords: Engine simulation; Fuel mixture; Diesel; Biodiesel; Ethanol.

1. INTRODUCTION

The use of alternative fuels in Internal Combustion Engines (ICM) has attracted research, even though fossil fuels such as oil, natural gas and coal meet most industrial and commercial demands as an easy to transport solution and because they are relatively low cost, especially when compared to the high energy density they have. However, burning fossil fuels generates emissions of polluting gases, which have worrying consequences for the environment.

A possible solution that has already been studied is the use of adding biofuels to diesel, which at the same time verify a reduction in pollutant emission levels and an increase in efficiency, without increasing the complexity of current diesel engines. The evolution of this idea deals with the addition of two types of biofuels to diesel: ethanol and biodiesel. In this way, it is possible to carry out simulation analyzes that deal with the effects generated by the use of this fuel alternative in the engine, dealing especially with data that relate to efficiency, performance and emissions when blends of biodiesel, diesel and ethanol (BDE) are used, (CHEN et al., 2013; KNOTHE and RAZON, 2016; SÁNCHES et al., 2020).
BDE fuel has an energy value close to that of fossil fuels, and this is because biodiesel has excellent properties in terms of engine lubrication and, in addition, it can be considered as a fuel that affects the environment less harmfully (KHOOBBAKHT et al., 2018).

The study of fuel alternatives in engines based only on experimental data can limit the possibilities of observing the potential of fuel mixtures, and thus, it is necessary to intensify studies on internal combustion engines using software that can help in different types of analyses. This work can support a possible decision on which fuel would be the most suitable to be used with the greatest benefit, and if the BDE mixture is suitable for this purpose. But as Apollinario (2016) points out, there is no fuel that outperforms all others in all desirable parameters.

This work proposes the development of combustion simulation in a diesel cycle engine with the aid of the AVL Boost™ software that uses blends of diesel, biodiesel, and ethanol to analyze the effects of using this technique, presenting the potentials and possible problems in the use of this alternative.

Biodiesel is a renewable, biodegradable, non-toxic and environmentally friendly fuel. Safe to handle, store and transport. Biodiesel derived from vegetable oils and animal fats can be used in diesel engines with little or no modification (THAMILSELVAN, et al., 2017). Biodiesel and diesel blends have been successfully tested in compression-ignition

engines, but with results with some variations since biodiesel originates from many different types of biomasses. Properties such as viscosity, specific gravity and flash point vary between different types of biodiesels and therefore have different effects on emissions and efficiency when used as fuel for internal combustion engines (KNOTHE and RAZON, 2016). The most common attribute is that biodiesel consists of fatty acid methyl esters, which have a lower calorific value than regular diesel. This results in a higher specific fuel consumption compared to pure diesel (SHAMUN et. al, 2018).

Experiments with engines with fuel blends consisting of biofuel, diesel and ethanol yielded results with little variation. As might be expected, CO emissions generally decrease with a higher oxygen content in the fuel, while NOx emissions show an increase. A higher oxygen content in the fuel results in more complete combustion which increases the temperature during combustion (KHOOBBAKHT et al., 2018; SHAMUN et. al, 2018; HANSEN, 2005). The ethanol component increases the ignition delay and therefore a higher fraction of the fuel burns at the same time in pre-mixed mode, increasing the rate of heat release, also resulting in greater thermal NOx formation. In several studies, the amount of No emission is not deterministic and can vary in different experiments (HANSEN, 2005; SÁNCHES et al., 2020).

However, as highlighted by Khoobbakht et al. (2018), there are different results in some previous research, which can be attributed to the difference in the sources of biofuels, the percentages of ethanol and biodiesel and the types of engines.

Computational resources are increasingly used as an alternative to studies and internal combustion engines. Using some software, it is possible to mathematically predict what can happen in practice when a certain engine model is used under different conditions. In this way it is possible to draw conclusions about the effects of fuel mixtures on combustion, for example.

The use of fuel mixtures is also simulated and analyzed in different types of engines, such as the study by Matias (2014), which simulated the use of diesel, biodiesel and ethanol in constant rotation marine engines based on the Wiebe model in the AVL Boost software using also programming resources in Matlab software, which obtained satisfactory data via software when compared with the experimental data, as well as the work of Apollinario (2016), who also performed the computational simulation of a marine engine using diesel mixtures and biodiesel. Apollinario (2016) performed tests using combustion models in addition to the Wiebe also the Fractal, which presented satisfactory values in relation to the experimental results.

2. SIMULATION PROCEDURES

This work is based on the simulation of an internal combustion engine using the AVL Boost software to study the simulation of an internal combustion engine using a mixture of oxygenated fuels, diesel, biodiesel and ethanol. For that, a Fractal type model was developed based on the software's own data, provided as an example, and on articles that model the use of internal combustion engines. From software's own fuel properties data and adding information from a biofuel, it is possible to perform the analysis of NOx, CO, and HC emissions results for different percentage amounts of fuels. For all tests, the same physical engine configuration was maintained, changing only the amount of diesel, biodiesel and ethanol in the fuel. Simulations were performed for blends of diesel and ethanol (DE), diesel and biodiesel (DB), and finally blends of the three (DBE). In the mixture of the three fuels, ethanol was mixed with a composition of D85B15 (15% biodiesel in diesel in diesel).

AVL Boost is a one-dimensional simulator capable of calculating thermodynamic properties at each cycle or as a function of the crankshaft angle. Therefore, knowledge about the structure of the real engine to be simulated is necessary to deliver to the software information about characteristics that will influence the studied combustion.
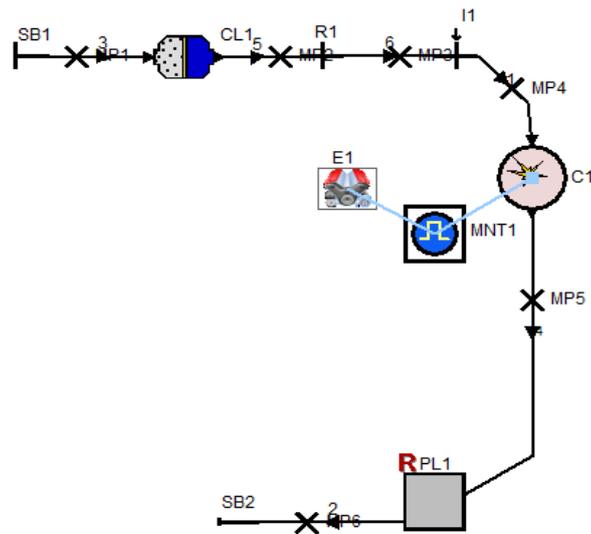
Figure 1. Representation scheme of the simulated model

Legend: air filter (CL1); carburetor (I1); butterfly valve (R1); exhaust (PL1 and ducts 2 and 4); and the cylinder (C1). The boundary conditions SB1 and SB2 were considered as input and output, respectively. For analysis of the tests, input conditions such as pressure at 1 bar and ambient temperature at 300K were considered, which were already standard conditions of the program.

For the analysis of combustion of diesel, biodiesel and ethanol mixtures, the fractal model was stipulated, which does not need the engine pressure curves, but the properties of the mixtures of the fuels used and their proportion ratios. The model created and simulated was based on the work of Appolinario (2016), Melo et al. (2014), making the characterization in a model provided by the software as an example.

The diesel and ethanol fuel characteristics given by the software and the physical characteristics of biodiesel were adapted in the simulation software based on the values provided in Table 1, from the work of Jamrozik, et al. (2017).

Table 1. Fuel Specifications

Fuel Properties	Unit	Diesel	Biodiesel	Ethanol
Molecular formula		$C_{13}H_{23}$	$CH_3(CH_2)nCOOCH_3$	C_2H_5OH
Cetane number	-	51	56	~11
Molecular weight	G	205.2	~300	46
Liquid density	kgm^{-3}	840	832.5	789
Lower heating value	$MJkg^{-1}$	42.5	37.8	26.8
Heat of evaporation	$kJkg^{-1}$	260	300	840
Auto-ignition temperature	K	503	534	698
Stoichiometric air-fuel-ratio	-	14.6	13.8	9.0
Viscosity at 25ºC	mPa·s	2.8	2-4.5	1.07
Carbon content	%	87	77.1	52.2
Hydrogen content	%	13	12.1	13.0
Oxygen content	%	0	10.8	34.8

(JAMROZIK, et al, 2017)

To study the effects of the quantities of different types of fuels in a mixture to be used in an internal combustion engine by compression, it was decided to carry out simulations with pure fuels and with 30 types of mixtures. For didactic purposes, we chose to use the nomenclature with the initial of the fuel followed by the percentage of it in the mixture, for example: D95E05, which means that in the mixture there is 95% diesel and 5% ethanol. In the case of simulations of diesel, biodiesel and ethanol mixtures, it was considered that a mixture of diesel and biodiesel, with 15% of this second fuel, that is, a D85B15 was considered as the basis for the addition of ethanol. Evidently, the calculations of the proportion of diesel and biodiesel in blends with different levels of ethanol were performed, keeping the final amount of fuel constant. The mixtures used for simulation are shown in Table 2.

Table 2. Fuel Mixtures

DIESEL-ETHANOL	DIESEL-BIODIESEL	DIESEL-BIODIESEL-ETHANOL
D95E05	D95B05	DB95E05
D85E15	D85B15	DB85E15
D75E25	D75B25	DB75E25
D65E35	D65B35	DB65E35
D55E45	D55B45	DB55E45
D45E55	D45B55	DB45E55
D35E65	D35B65	DB35E65
D25E75	D25B75	DB25E75
D15E85	D15B85	DB15E85
D05E95	D05B95	DB05E95

2.1 Fractal Model

The fractal combustion model is based on the physical flame propagation front model. For this it is necessary to know the combustion chamber geometry related to the piston position, the free flame surface geometries, and the burnt zone volume. Burnt zone volume growth is a function of burn threshold velocity and free flame geometry. The flame front is considered extremely thin.

According to the manufacturer AVL, the model then calculates the rate of heat released from the theory of fractal surface and turbulent flow, and in this case the experimental data of the engine pressure curves are not necessary for the simulation, but it is necessary to know the location of the spark plug, the composition of the gas to be flared and the turbulence of the fluid.

In this model it is considered that the combustion started smooth, but that during the progress of combustion its surface becomes wrinkled due to turbulence, to make an approximation of the burning model in cases of low-revving engine. Thus, the air mixture is basically divided into two zones: the burned and unburned zone, which are separated by the flame front (Figure 2).
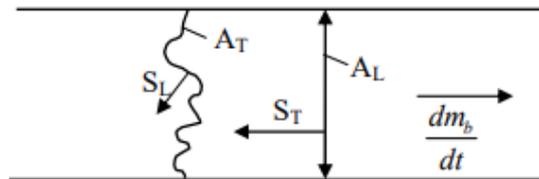

Figure 2. Representation of Fractal Model

Where: area A_T is the area of the flame front wrinkled by turbulence; A_L is considered an area of a theoretical flame front if there is no turbulence (laminar flow); S_L is the laminar velocity of the flame front; S_T is the turbulent velocity of the flame front; ρ_u is the specific mass of the mixture in the combustion chamber; and ρ_m is an average specific mass of the mixture. The mass burning rate (m_b) is characterized by Equation 1. AVL Boost is mainly based on the physical principles of combustion and thermodynamic properties presented in Heywood's book (1988), with species considered as ideal gases (RANZI, 2014).

$$\frac{dm_b}{dt} = \rho_u A_T S_L = \rho_m A_L S_t, \tag{1}$$

3. RESULTS

To analyze the results, the pressure curves inside the combustion chamber and the NOx, CO and HC emission curves were compared. The main objective was to analyze the changes in emissions when there are different amounts and fuels in the mixture directly injected into the engine. During the simulations, it was considered that homogeneous mixtures did not separate during the time of injection.

In the graphics, it is considered abscissa axis as the addition of ethanol in DE blends (Y), as addition of biodiesel in DB blends (X), and, as addition of ethanol in the DBE blends (Z).

3.1 Pressure curves inside the chamber

The pressure curve was analyzed because from its data the ignition moment can be inferred to compare the delay or advance of the ignition moment when the system receives a mixture with ethanol and diesel. The moment there is an inflection in the pressure rise curve, it is the moment of ignition. Therefore, it is possible to determine which mixture had delayed or advanced ignition, with the crank angle being the reference.

Another factor to be considered is the maximum internal pressure, as different amounts of ethanol and diesel interfere with this pressure value.

In the Figure 3 it is possible to observe the comparison of pressure curves as a quantity of pure diesel is mixed with an quantity of ethanol. It is observed that as the amount of ethanol increases proportionally in the mixture, the ignition delay becomes longer and longer, while the maximum internal pressure in the chamber is lower. This is due to the chemical properties of ethanol, which make it difficult for the mixture to self-ignite, delaying the ignition moment, and decreasing the internal pressure. Delays become more significant when there is an ethanol percentage of 55%.
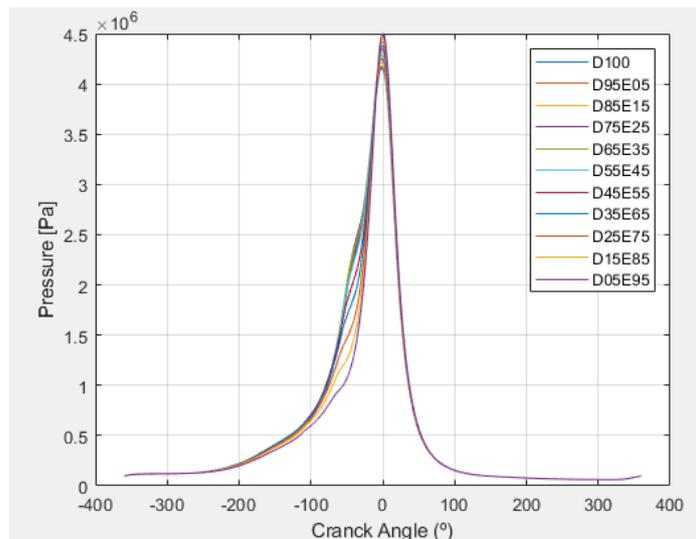

Figure 3. Pressure curves in Diesel and Ethanol mixtures

Unlike what happens with the addition of ethanol to diesel, as can be seen in Figure 4, when the percentage of biodiesel in the mixture increases, it is observed that there is an advance in ignition and an increase in the internal pressure in the chamber. This is clearly since biodiesel has chemical characteristics such as the cetane number that facilitates the self-ignition of the fuel, advancing the moment when the system ignites in relation to the angle. It should be noted that the advancing effect of biodiesel in the mixture is more discrete than the delaying effect of ethanol in the mixture.
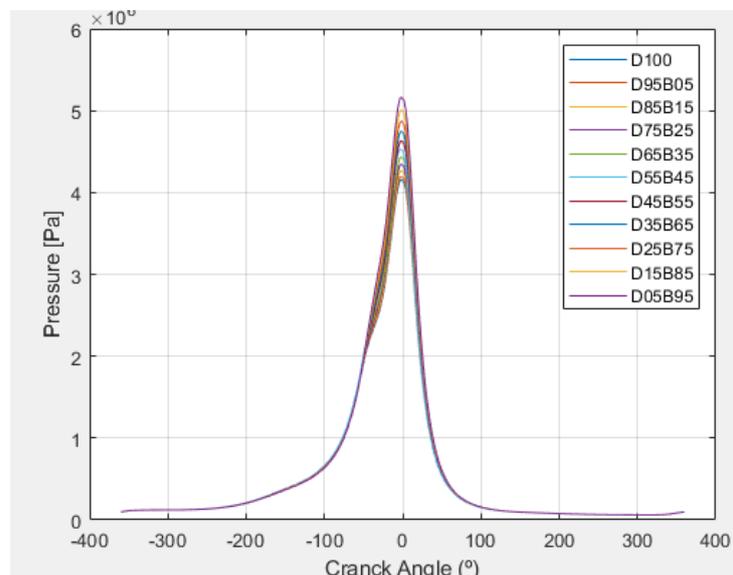

Figure 4. Pressure curves in Diesel and Biodiesel mixtures

In turn, diesel, and biodiesel blends – D85B15 – and ethanol behave similarly to diesel and ethanol blends, that is, there is a delay effect on ignition as there is an increase in ethanol in the final blend. In Figure 5, it is possible to observe that mixtures with about 45% of ethanol already present a significant ignition delay in relation to D85B15. In this way, as the amount of ethanol grows in the mixture, the effects of biodiesel are minimized.
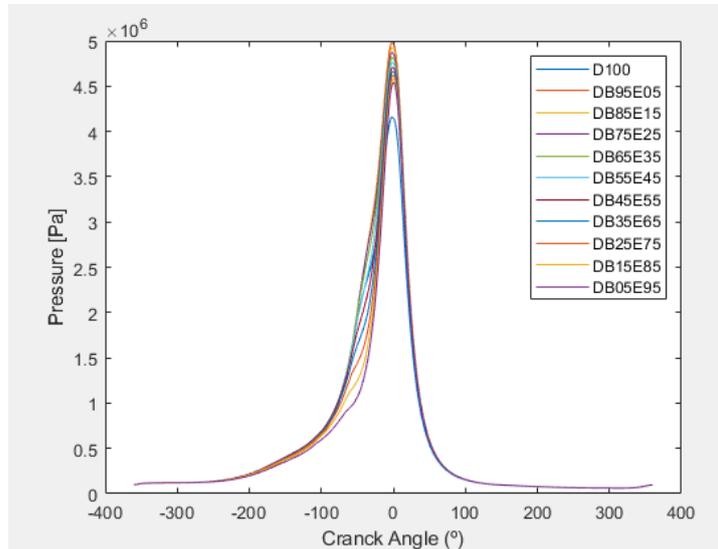

Figure 5. Pressure curves in Diesel-Biodiesel and Ethanol mixtures

3.2 NOX Emissions

Observing the plotted graphs shown in Figure 6A, for diesel and ethanol blends, 6B, for diesel and biodiesel blends and 6C for diesel-biodiesel and ethanol blends, it is understood that the behavior of NOx emissions decreases with the addition a lot of ethanol but increase as the amount of biodiesel is greater in percentage in the mixture. This fact corroborates different studies presented in this work, which show that NOx emission is a factor to be considered when it comes to choosing the use of biofuels.
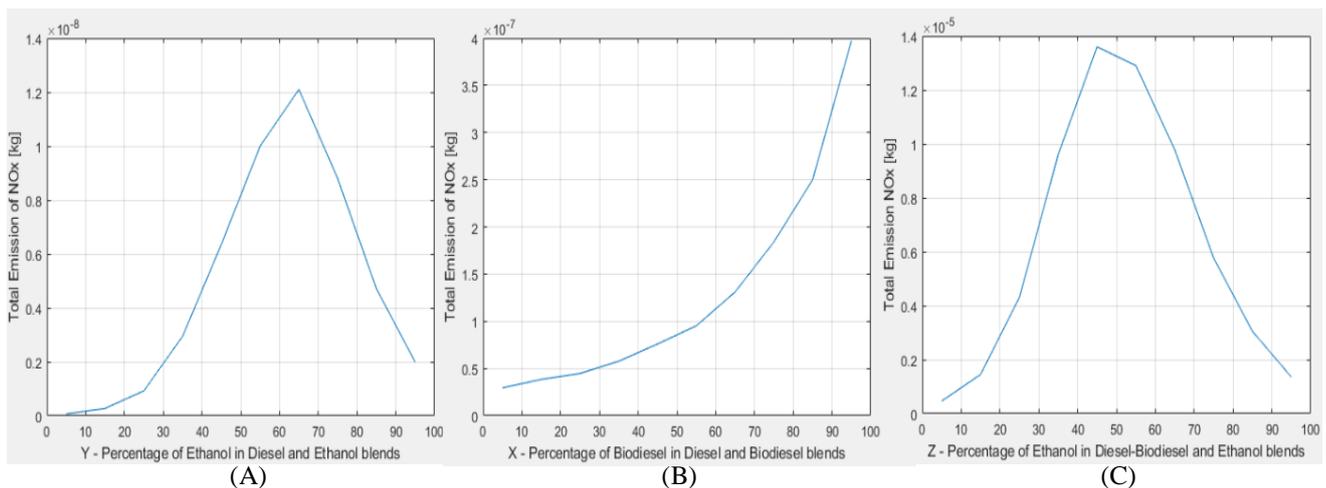

(A)   (B)   (C)

Figure 6A. NOX Emissions in Diesel and Ethanol blends
Figure 6B. NOX Emissions in Diesel and Biodiesel blends
Figure 6C. NOX Emissions in Diesel-Biodiesel and Ethanol blends

3.3. CO and HC Emissions

In all cases where a type of biofuel was added to the mixture, CO and HC emissions were reduced, that is, the more biodiesel or ethanol was added to the diesel mixture, lower amount of carbon monoxide and particulates, since combustion

tends to be more complete with a kind of help from the oxygen contained in oxygenated fuels. The total emissions throughout the cycle are shown in Figures 7A, 7B, 7C for CO emission analysis and 8A, 8B, 8C for HC emission analysis.

In the simulation, it is observed a disturbance in the calculation of CO emissions for some diesel and biodiesel blends, and for all diesel, biodiesel and ethanol blends. This may have happened due to the parameters stipulated for generic biodiesel, which may cause some inconsistency that conflicts with the chemical calculations of the fractal model. However, this does not affect the analysis at all, since the values stabilize after the transitory moment.
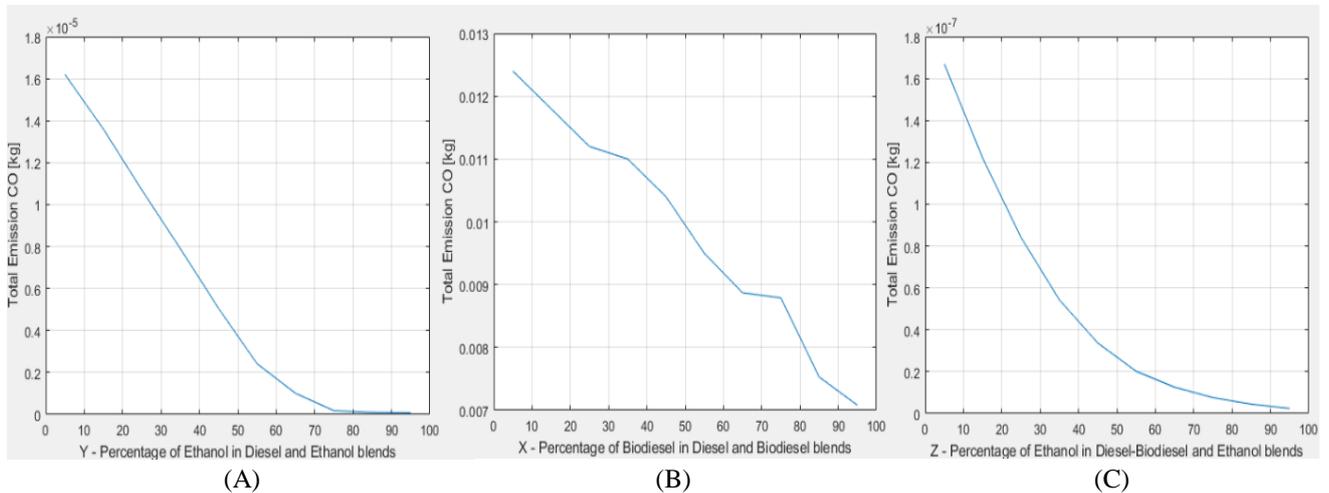
(A)	(B)	(C)

Figure 7A. CO Emissions in Diesel and Ethanol blends
Figure 7B. CO Emissions in Diesel and Biodiesel blends
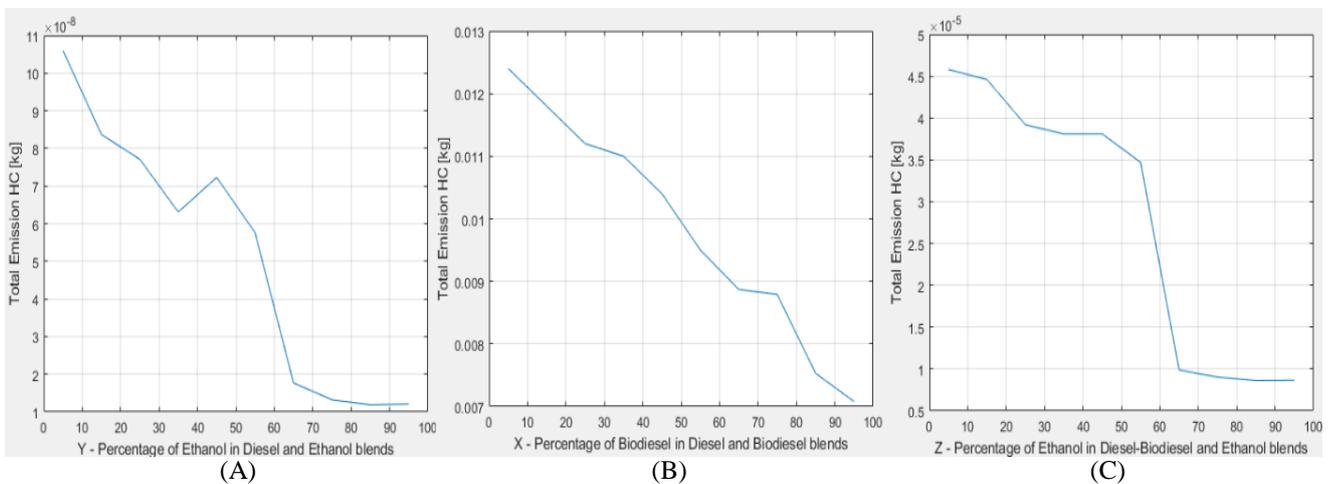Figure 7C. CO Emissions in Diesel-Biodiesel and Ethanol blends

(A)	(B)	(C)

Figure 8A. HC Emissions in Diesel and Ethanol blends
Figure 8B. HC Emissions in Diesel and Biodiesel blends
Figure 8C. HC Emissions in Diesel-Biodiesel and Ethanol blends

4. CONCLUSIONS

The mixture of biodiesel and ethanol in diesel modifies ignition and emission characteristics, considering that no changes were made to the physical characteristics of the simulated engine. From the analyzed graphs, it can be concluded that the obtained results are in agreement with the researched bibliography, as it was noticed that with the increase of biodiesel in the mixture, the ignition is anticipated and the HC and CO levels decrease, while the NOx increases. In the case of the percentage increase of ethanol to pure diesel, it delays the ignition moment, but reduces the emission of all pollutants when it is mixed in greater quantity. Something similar was observed when ethanol was added to the DB15 mixture, that is, there was a longer ignition delay as the proportion of ethanol was greater while CO, HC emissions were reduced.

As for the pressure levels in the chamber, it can be observed that the presence of ethanol decreases the pressure in the chamber, probably because it has a higher evaporation temperature, and the opposite happens with diesel, which increases the pressure in the chamber and has a higher temperature of smaller evaporation.

It should be remembered that for the use of oxygenated fuel mixtures, modifications must be made to the original diesel engine, aiming at a better use of fuels and the efficiency of the engine in general.

Another consideration that must be made is that, although the system simulates combustion with large proportions of ethanol, the self-ignition property of ethanol is very low, so it would not be possible to obtain all the results presented in an unmodified engine. Furthermore, the simulated results deal with the emissions resulting from a homogeneous mixture of fuels in different proportions, different values can be obtained in experimental tests.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE