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COB-2023-1060 STUDY OF BURN RATE MODELS IN A ZERO-DIMENSIONAL MODEL FOR SPARK IGNITION INTERNAL COMBUSTION ENGINES OPERATING ON BIOGAS, BIOMETHANE AND ETHANOL

Jullyane Raquel Almeida Nunes[1]
Ana Paula Mattos[2]

Federal University of Pará[1], Rua Augusto Corrêa 01, Guamá, 66075-110, Belém, Pará. jullyane.anunes@gmail.com[2]; anapmattos@ufpa.br[3];

Abstract. *The use of biofuels has increased throughout the country, demonstrating a remarkable transformation toward renewable energy sources. Factors that favor this increase are the territorial availability as it is an agricultural power and the suitable climatic conditions that contribute to the cultivation of raw materials for its production. This results in public policies in the social sector to encourage regional potentialities with the generation of jobs and income with sustainability. Therefore, Brazil has become an essential player in the development and growth of biofuels. On the other hand, the world continues to use fossil fuels heavily, despite growing concern about the effects of their use on global warming. In comparison, biofuels are a more ecological energy source since they release green* CO_2*. Therefore, they are suitable alternatives for replacing petroleum-derived fuels and natural gas in internal combustion engines (ICE). The transportation sector alone is responsible for 20% of the emissions of harmful gases to the environment, fostering the most incredible intensity of the greenhouse effect, without considering other gases released that are harmful to nature. The objective of this work is to study burn rate models for spark ignition (SI) for ICE, operating with biogas/biomethane e ethanol. The simple Wiebe and Double Wiebe in a two-zone zero-dimensional model will be used for a fraction of energy released. First, the experimental data used will be taken from the literature to analyze and make comparisons with the results obtained through numerical simulation. Additional studies on the double Wiebe are needed as there is a lack of data in the literature for all the parameters that the function requires. Parameters such as the onset and duration of combustion, shape coefficient, and combustion efficiency are essential. Biomethane is an alternative fuel to natural gas, and their potential for use in light vehicles needs further investigation to evaluate performance and emission notions. Consequently, making these fuels an innovation for the energy industry.*

Keywords: *MCI, Burn rate, Zero dimensional model, Wiebe, Double Wiebe.*

1. INTRODUCTION

Numerical modeling uses theoretical equations and laws, as well as empirical equations, to describe the parameters of interest. This results in the existence of various numerical models, depending on the assumptions and simplifications used in each one. Currently, with the advancement of technology, there has been an increase in the use of computational modeling. This advancement has contributed to progress in various fields of simulation, including helping to study the implementation of new technologies and biofuels to replace fossil fuels that are extremely harmful to the environment.

Known as a fossil fuel, oil is one of the main sources of energy used today and also generates several by-products widely used by society. Its exploitation began in the 19th century and its use expanded significantly with the emergence of gasoline and diesel engines. Oil is formed over time from the decomposition of organic matter, which undergoes various transformations until it becomes the dark, oily substance known as petroleum. It can be found in underground layers and in sedimentary basins, under specific pressure conditions. However, the exploitation of oil as an energy source generates several impacts on human health and the environment, including air and sea pollution and the increase in the greenhouse effect, contributing to global warming (SILVA, 2021). This occurs because the burning of this fuel releases gases such as methane (CH_4) and carbon dioxide (CO_2) which are greenhouse gases (GHG), carbon monoxide (CO) and sulfur dioxide (SO_2) which are polluting gases.

In the context of Brazil and the world's increasing search for alternative energy sources, aiming at an energy matrix less dependent on oil, renewable fuels, such as biofuels, emerge as solid options to achieve energy self-sufficiency without being linked to oil. Specifically for the transportation sector, which consumes about 50% of petroleum products, according to EPE (2021), biofuels represent a promising alternative.

According to the ANP (2019), around 45% of the energy and 18% of the fuels consumed in Brazil today come from renewable sources. In 2018, the country produced more than 33 billion liters of ethanol, used exclusively in flex fuel vehicles (hydrated) and in mixture with gasoline (anhydrous). In the same year, more than 5.3 billion liters of biodiesel were also produced (VIDAL, 2019).

Therefore, biofuels are a valuable alternative for use in internal combustion engines (ICE). Only the transportation sector in Brazil, according to information from EPE (2022), was responsible for 197.8 Mt of CO_2 as shown in figure 1, it is noted that from 2020 to the year in question, there was an increase of 12.4% in total CO_2 emissions. Becoming, then, one of the main gases causing the greenhouse effect, without considering the emission of other gases also harmful to the environment.

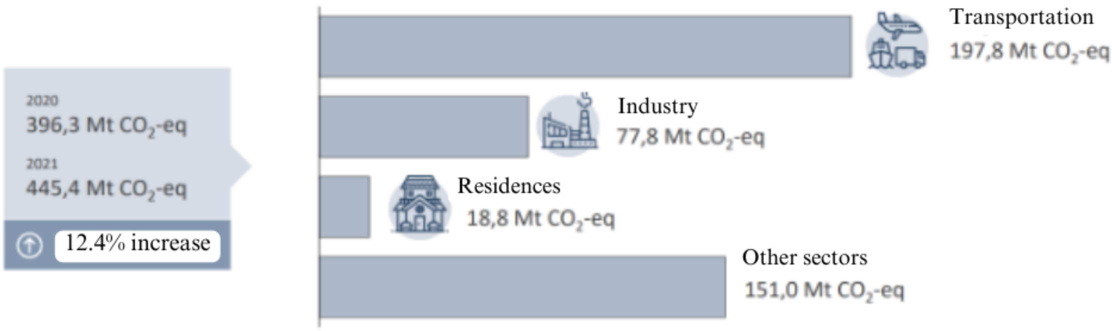

Figure 1 - Total emissions scenario of Brazil in 2021
Source: EPE, 2022.

In recent years, biomethane has been gaining ground in Brazil, especially with the bill PL 3865/2021, which proposes incentives to stimulate the production of biogas and biomethane. It is estimated that the country has the capacity to become the world's largest producer of biomethane, as shown in Figure 2a (number of biogas plants) and Figure 2b (biogas production in Brazil). It is worth noting that there are already 10 biomethane plants in operation, producing 522 thousand nm³/year of biogas and 435 thousand nm³/year of biomethane. Considering that 1 nm³ of biomethane is equivalent to 0.84 liters of diesel, the daily production would be equivalent to 378 thousand liters of diesel. Given this scenario, it is evident that biomethane has great potential to become a biofuel in engines to be a substitute for GNV (Vehicular natural gas).

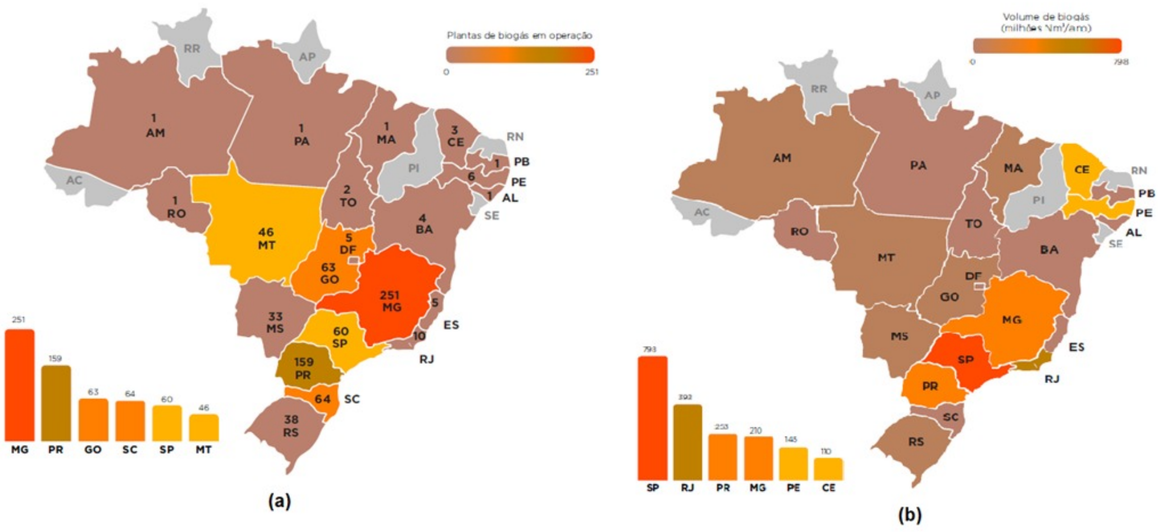

Figure 2 - Overview of plants (a) and production volume (b) of biogas and biomethane in Brazil in 2021.
Source: International Center for Renewable Energy, 2021.

In view of this, it is important to carry out studies of these alternative fuels in engines and also to analyze possible changes in order to have a long useful life, and the best possible performance reconciling the GHG and pollutant emission targets. With this in view, this article aims to study two combustion models widely used for conventional fuels, Single and Double Wiebe, and analyze which of these best represents the phenomenon for biogas and biomethane for ICE, port fuel ignition (PFI). The study carried out a comparison of the experimentally obtained performance parameters taken from the literature for biogas and ethanol. In addition to conducting a trend study for biomethane.

2. LITERATURE REVIEW

2.1 Theoretical background

In the combustion model in real Otto cycle engines, the combustion of the fuel occurs during the movement of the piston, changing the volume in the combustion chamber. The interval between the start and duration of combustion is extremely important for the best possible utilization of energy. Which depends on many factors such as engine type, operating condition, fuel type, factors that will require adjustments for best fit and functional use. This burning speed is a decisive factor for the elaboration of a model and for the description of the behavior of the combustion flame when consuming the reactants introduced into the chamber. This characteristic is closely related to thermal efficiency, which affects both the work done and the heat transfer to the cylinder walls (MELO, 2007).

Melo (2007), suggests that there are several methods to calculate the combustion rate or heat release rate: Heywood (1988), Caton (2000), Chan (2001), Alla (2002), Santos Junior (2004), among others. In the literature, these paths developed through equations with different particularities to predict the mass fraction of the fuel burned offer designers alternatives that better characterize the combustion behavior in a given fuel. The calculation of the mass fraction burned (MFB) is therefore one of the most relevant factors in the thermodynamic model of two-zone combustion. There are several ways to do this, the most used are: direct flame equations, single Wiebe function and double Wiebe (REZENDE, 2022).

The Wiebe function is widely used to model combustion in internal combustion engines and was developed in 1967 to describe the combustion mass ratio and the combustion profile (MELO, 2007). This function has a characteristic "S" shaped curve that increases from zero, indicating the beginning of combustion, and at the end of combustion (Xb=1). Due to its simplicity, this function is used instead of the turbulent flame front to predict the burning rate, whose calculation is complex and has a higher computational cost than the Wiebe function (YELIANA et al., 2011; MATTOS, 2018).

The Wiebe function as a function of the crank angle is given by equation 1.

$$x_b(\theta) = 1 - exp\left[- log(1 - \eta_c)\left(\frac{\theta-\theta_i}{\theta_b}\right)^{m+1}\right] \qquad [1]$$

Where $x_b(\theta)$ is the mass burned as a function of the crankshaft axis, m is the shape factor, which defines the shape of the heat release curve, $log(1 - \eta_c)$ is the efficiency parameter that will be admitted equal to "a", which will determine the fraction of fuel burned at the end of combustion, and η_c is the burning efficiency.

The simple Wiebe function is more applied to port fuel injection (PFI) engines of ICE, however, some authors use the double Wiebe function for ICE when there is indirect injection (MATTOS, 2018).

The dual function proposed by YELIANA et al. (2011) is presented in equation 2.

$$x_b = p\left(1 - exp\left[-\left(\frac{\theta-\theta_{b1}}{\alpha_1}\right)^{\beta_1}\right]\right) + (1 - p)(1 - exp)\left[-\left(\frac{\theta-\theta_{b2}}{\alpha_2}\right)^{\beta_2}\right] \qquad [2]$$

.

Where p is a weighting factor between the two combustion phases, $\beta_{1,2}$ are form factors $(m_{1,2}$ +1), $\alpha_{1,2}$ are combustion efficiency factors (Equation 3). b is combustion duration, i is combustion start, c combustion efficiency.

$$\alpha_{1,2} = \alpha^{\left(-\frac{1}{m_{1,2}}\right)}\theta_{b1,2} \qquad [3]$$

2.2 Biofuels

Ethanol is a chemical compound known as alcohol, with formula C_2H_5OH, obtained from sugar-rich vegetables such as sugarcane and corn. In Brazil, fuel ethanol, called E100, contains about 6.0 to 7.4% water in its composition. Ethanol production from sugarcane uses its own waste, such as bagasse, to generate energy during the process. This process involves fermenting the sugar present in molasses into alcohol and distilling it to separate the alcohol from the fermentation mash. However, the resulting residue, called vinasse, can cause ecological problems if not properly treated before disposal. Ethanol, despite having lower calorific value compared to gasoline and GNV, has a higher amount of energy available per mass of air due to its oxygen-rich composition (BERLINI, 2017).

Ethanol has advantages such as renewable fuel, high octane rating, lower pollutant emissions compared to gasoline and flexibility of use in engines without the need for adaptation. However, it has disadvantages such as low energy content, greater corrosiveness in certain materials and difficulty in cold starting due to its low vapor pressure and evaporation (BERLINI, 2017).

While biogas has been used as a fuel since the 1950, and in Brazil it seeks to replace gasoline with purified and compressed biogas in the automotive area. This biofuel has been gaining importance in both smaller and larger applications. There has been a significant increase in production and techniques to convert biogas into mechanical energy in modified internal combustion engines, as well as in the development of biogas-specific engines. However, the use of biogas in internal combustion engines requires treatment processes to make the fuel suitable for operation (GOMEZ, 2014).

Biomethane is obtained by enriching or upgrading biogas. This includes removing carbon dioxide (CO_2) and other elements that remain in the biogas and increasing the calorific value. It can be used as a substitute for GNV, after compression and subsequent storage, provided that the quality prerequisites of the corresponding regulatory body are met (adapted from PROBIOGÁS, 2015).

According to the following table 1, it is possible to visualize works that have been developed using numerical simulation in the cited biofuels.

Table 1 - Numerical models operating with ethanol or biogas/biomethane.

Author/ Year	Article	Methodology
Roberto Berlini Rodrigues da Costa (2017)	Experimental Study of Dual-Fuel Technology in Internal Combustion Engine Using Biogas, CNG and Ethanol.	Procedures include engine choice, preparation and testing. Includes design, manufacture of components, fuels and injection, instrumentation, calculation of uncertainties, assembly, testing and analysis. Three-stage testing: single-fuel, dual-fuel and iEGR.
Ana Paula Mattos (2018)	Performance Study of an Ethanol-Fueled Turbo Engine Employing EGR for NOx Emission Reduction and Denotation Contro	A two-zone phenomenological model, which was calibrated with experimental values for the aspirated engine and data for the engine with the turbocharger and EGR were stipulated from studies and typical values from the literature were used that fit with the conditions analyzed. The model can simulate different engine conditions, as well as geometry and valve train fuel.
Luan Murillo Duarte Rezende (2021)	Comparative Study of the Performance Parameters of a Spark Ignition Engine Using Phenomenological Model Operating with Biogas, Ethanol and Gasoline	Simulation with a phenomenological model of a spark ignition SCRE engine, fueled by biogas, ethanol and gasoline, analyzing some performance parameters obtained and applying comparison with the results obtained by a real SCRE engine.

3. Methodology

The phenomenological model developed by Mattos (2018) is applied to the Matlab® language used. The model was adapted by adding a biogas/biomethane model, in addition to the specifications of the engine under study.

The biogas/biomethane was modeled consisting of methane and CO_2, what differs the two biofuels is the amount of methane. The simulated biogas taken from Berlini (2017), has 64.5% methane, while biomethane according to ANP (2019) is formed by 90% methane. Thus, the cp of the biofuel is expressed by equation 4. It should be noted that the cp of CO2 is already part of the model library. The cp of methane is described by equations 5 and 6. The polynomial was divided in two according to temperature variations so that the values were close to those in the literature. They were developed using data from Barin and Platzki (1995).

$$cp_{fuel} = cp_{CH_4} * n_{CH_4} + cp_{CO_2} * \left(1 - n_{CH_4}\right) \quad [4]$$

$$cp_{CH_4} = 4x10^{-13}T^4 + 4x10^{-9}T^3 - 4x10^{-5}T^3 + 0.1006T + 0.9882 \quad [5]$$

$$cp_{CH_4} = 9x10^{-11}T^4 - 4x10^{-3}T^2 + 0.0003T^3 - 0.0687T + 36.74 \quad [6]$$

Where n_{CH_4} is the mole fraction of methane in the biogas, cp is in J/k.Mol and temperature is in K.

The parameters of peak pressure, thermal efficiency, volumetric efficiency and emissions are compared with the simulation results. The inserted engine parameters are from the work of Berlini (2017), which are presented in Table 2 and 3.

Berlini (2017), studied a spark ignition internal combustion engine with single-cylinder research with dual-fuel system, using some fuels, among them, ethanol, biogas and GNV. Mattos (2018), used the mathematical model as a basis for creating a numerical model that evaluates the performance parameters, such as combustion duration, ignition point, water content in ethanol and the amount of NOx and CO emission gases.

The model elaborated by Mattos (2018) had few changes, in order to make possible the comparison of the empirical experiment performed by Berlini (2017). Data from the physical engine were added to perform the comparison of the obtuse parameters in the work of Berlini (2017). In addition to the verification of the pressure versus volume, temperature versus crank angle diagrams, for knowledge and comparison between the fuels addressed by Berlini (2017).

3.1 Engine data

- **Engine geometry**

The engine used in the research is a SCRE (Single Cylinder Research Engine), spark ignition, four-stroke, aspirated engine equipped with a port fuel injection (PFI) system. The cylinder head has two intake and exhaust valves. It is naturally aspirated and the flow structure has a tumble coefficient to the lower swirl coefficient, which are coefficients related to the turbulence of the admitted mass flow (COSTA, 2017). Table 2 presents the engine geometry data.

Table 2 - Engine geometry data

Model	AVL 5495
Type	Monocilindrico
Diameter	82 mm
Course	86 mm
Connecting rod length	144 mm
Volumetric compression ratio	13;6;1
Displaced volume	454.16 cm^3
Number of valves	4

Source: Berlini, 2017.

- **Calibration variables**

In his work, Berlini (2017) presents in detail the calibration procedure used. Then, the values found in Table 3 proved to be of great influence on the results obtained for each fuel tested.

Table 3 - Calibration variables

Fuel	Speed (RPM)	Advanceof ignition	Temperature Cylinder wall	Intake pressure	Exhaust pressure	Intake temperature	Intake temperature
Ethanol	1800	-12.4°	850 K	0.96 bar	1.16 bar	306 K	865 K
Ethanol	3600	-14.5°	700 K	0.96 bar	0.88 bar	307.15 K	973.15 K
Biogás	1800	-24.0°	363 K	0.97 bar	0.11 bar	301 K	845 K
Biogás	3600	-31.1°	363 K	0.97 bar	0.68 bar	301 K	947.15 k

Source: Berlini, 2017.

3.2 Fuel modeling

It was considered that the biogas used comes from a pre-treatment, meeting some specific proportions of composition, with only methane (CH_4) and carbon dioxide (CO_2) present in its constitution, that is, no portions of other gases are present.

The best angle of combustion duration varies for each fuel and according to other parameters, such as speed and fuel-air ratio (MATTOS, 2018; PULKRABEK, 1997). For ethanol and biogas, Berlini (2017) provided the configurations that will be used in this work, obtained some data on the start and end angles of combustion, shown in Table 4, for biomethane the same values of biogas will be used to assess the trend of the results.

The specifications for the burning model of the fuels used are shown in Table 4. All the data of the engine parameters used, such as geometry, calibration and modeling parameters of the fuels are found in Berlini (2017).

Table 4 - Data obtained from the SCRE engine experiment.

Fuel	Speed (RPM)	MBF10-50 [°] (θ_{b1})	MBF10-90 [°] (θ_b)	MBF50-90 [°] (θ_{b2})	SOC [°] (θ_i)	Combustion efficiency [%] (η_c)
Ethanol	1800	10.2	19.6	10.3	-9.5	48.4
Ethanol	3600	11.7	23.5	10.5	-11.2	47.7
Biogas	1800	7.3	29.2	12.3	-17.8	60.4
Biogas	3600	7.0	33.6	13.4	-23.7	62.1

Source: Berlini, 2017.

4. Results

The simulation results are presented in tables 5 and 6. It can be observed that the single Wiebe function presents better results for ethanol, with smaller deviations from the experimental data. While Double Wiebe for Biogas. However, it is still necessary to refine the model to have even better results.

As the double Wiebe model has more parameters that depend on experimental data, which are not available in the literature in question, these values were stipulated based on other literature and conventional values, so the results obtained presented a higher percentage of error.

The 'Tb" in Tables 5 and 6, represents the peak temperature of the gases burned during combustion, and the IMEP is the average effective pressure. The temperature of the burned gases (tb) is important because it has a direct influence on NOx formation. In table 5 and 6 shows that the double Wiebe model better describes the phenomenon. It can be seen how the Wiebe function for biogas presents a very low temperature, lower than expected for 3600 rpm.

Table 5 - Biogas results for 1800 and 3600 rpm.

Fuel:	**Biogas**									
Parameters	**1800 RPM - Full Loud**			**Error [%]**		**3600 RPM - Full Loud**			**Error [%]**	
	Literature	**Simulation**		**W**	**WW**	**Literature**	**Simulation**		**W**	**WW**
		Wiebe (W)	**Double Wiebe (WW)**				**Wiebe (W)**	**Double Wiebe (WW)**		
Maximum temperature of the burned zone **(tb) [K]**	-	1618	1756	-	-	-	1618	1756	-	-
Maximum pressure [bar]	56.4	46.55	55.55	17.46	1.50	59.6	44.91	52.45	24.64	11.99
IMEP [bar]	7.65	9.86	5.7	-28.88	25.49	8.1	9.33	5.52	-15.18	31.85
Thermal efficiency [%]	50.1	36.12	34.23	27.90	31.67	49.4	37.92	34.8	23.23	29.55

Table 6 - Ethanol results for 1800 and 3600 rpm.

Fuel:	**Ethanol**									
Parameters	**1800 RPM - Full Loud**			**Error [%]**		**3600 RPM - Full Loud**			**Error [%]**	
	Literature	**Simulation**		**W**	**WW**	**Literature**	**Simulation**		**W**	**WW**
		Wiebe (W)	**Double Wiebe (WW)**				**Wiebe (W)**	**Double Wiebe (WW)**		
Maximum temperature of the burned zone (tb) [K]	-	2402	2523	-	-	-	2404	2523	-	-
Maximum pressure [bar]	57.4	58.74	78.79	-2.33	-37.26	57	58.48	67.89	-2.59	-19.10
IMEP [bar]	8.86	9.23	9.02	-4.17	-1.80	9.61	9.9	9.93	-3.01	-3.32
Thermal efficiency [%]	48.4	39.26	38.3	18.88	20.86	47.7	40	40.08	16.14	15.97

It is noted that the peak pressure of ethanol for the double Wiebe model is higher, overestimating the value (Figures 4 and 5). The value obtained using single Wiebe is more consistent with the experimental value, while for biogas the double Wiebe function better represents the phenomenon by obtaining values closer to the experimental ones. However, it is important to emphasize that engines operating with ethanol and biogas do not have such a high efficiency as presented in Berlini's experiments, and that the values found numerically correspond more to the typical values for ICE operating with such biofuels.

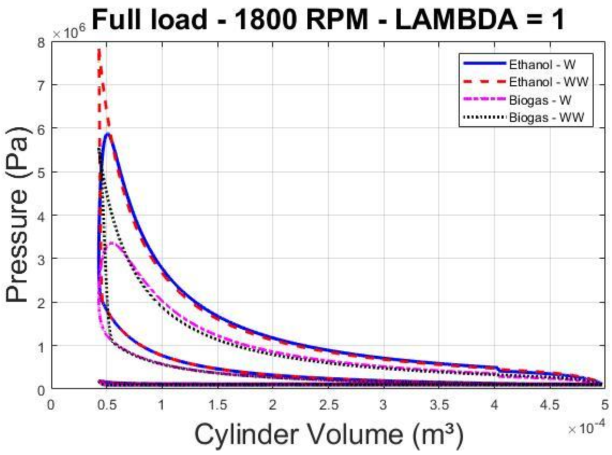

Figure 4 - Pressure by volume diagram for 1800 rpm.

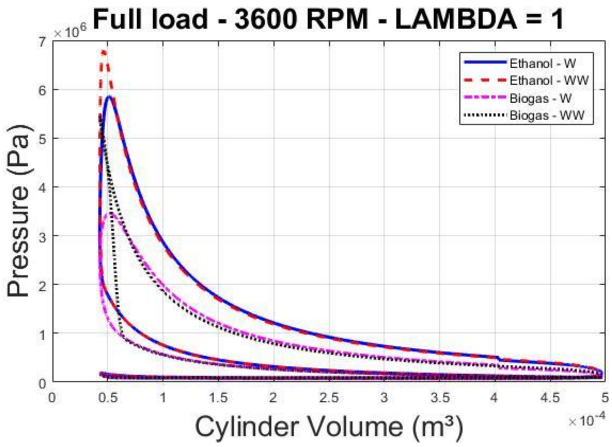

Figure 5 - Pressure by volume diagram for 3600 rpm.

The results for the biomethane simulation are represented in figure 6 and 7, with the pressure by volume graph. It can be seen that lower effective average peak pressures were found. This was shown to be due to the lack of parameters for the effective implementation of biomethane, in other words, experimental data is needed to find values closer to the real ones, and that the input parameters of biogas do not serve for biomethane, although they are biofuels with the same element base, but with different composition.

The biogas values cannot be used for biomethane, especially the data pertinent to the firing model. It was expected that biomethane would have higher pressures than biogas, and it has not occurred, proving that it is necessary to use values suitable for biofuel.

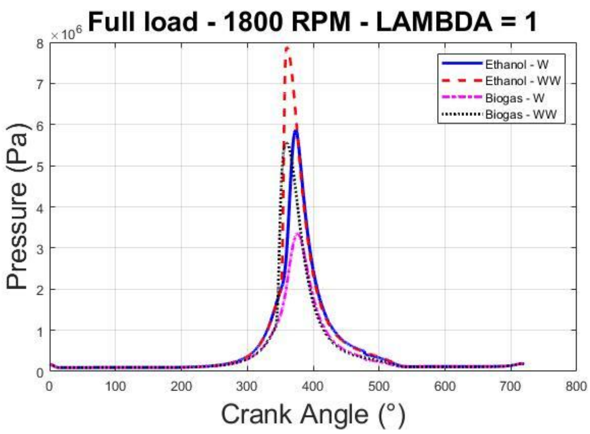

Figure 6 - Maximum pressure for 1800 rpm

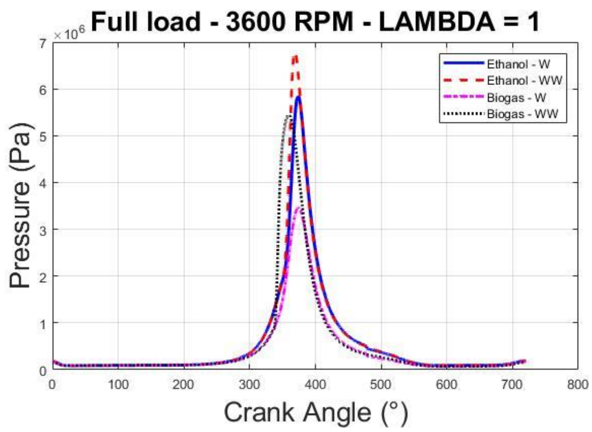

Figure 7 - Maximum pressure for 3600 rpm

In addition to the burn rate analysis, the impact of pollutant emissions with each fuel was evaluated. Figures 8 and 9 present the results of specific NOx emissions, and Figures 10 and 11 of CO for each load and rpm condition tested, using the Simple Wiebe function for burning rate calculation.

With regard to specific NOx emissions, ethanol showed higher levels of emissions in the 1800 rpm speed conditions, comparing it with biogas. However, biogas showed significant reduction of NOx emissions comparing it also with ethanol for 1800 rpm. For 3600 rpm, a trade-off occurred, where biogas showed more emissions than ethanol. In both simulations biomethane had lower emissions compared to ethanol and biogas, however as the input data was not validated a conclusive result cannot be reached.

NOx and CO emissions showed higher emissions for ethanol at 1800 rpm. However, for 3600 rpm speed, biogas showed higher NOx and CO rates. It was expected that ethanol would have higher temperatures of unburned gases, as it is one of the factors that influence NOx formation.

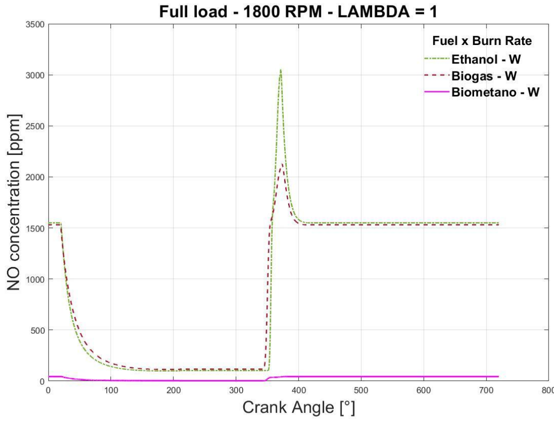

Figure 8 - NO emissions versus crank angle for 1800 rpm

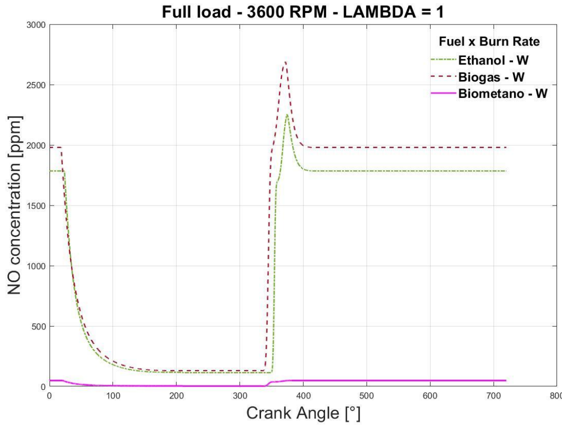

Figure 9 - NO emissions versus crank angle for 3600 rpm

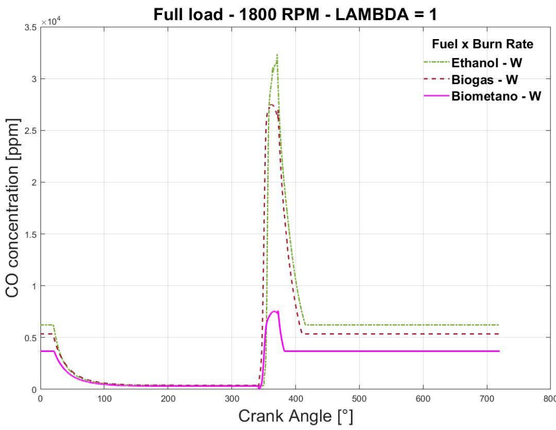

Figure 10 - CO emissions versus crank angle for 1800 rpm

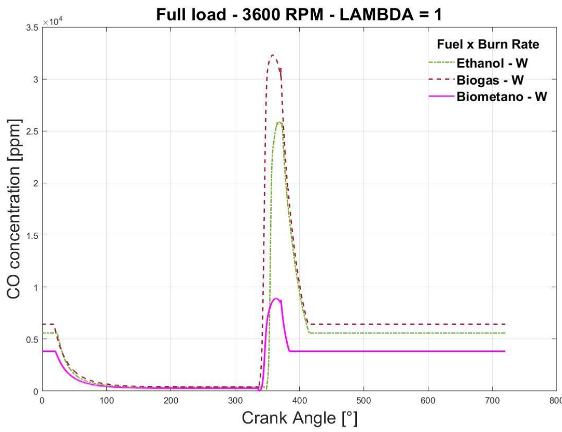

Figure 11 - CO emissions versus crank angle for 3600 rpm

5. Conclusions

The formation of pollutants such as CO and NOx has several reasons. In most vehicles, there is the lambda sensor, optimized to work with the stoichiometric mixture, where lower CO and NOx emissions are found simultaneously. This is because emissions are inversely proportional. Rich mixtures have high CO formations and low NOx formations, while poor mixtures have high NOx formations and low CO formations. This relationship occurs due to the availability of carbon for CO formation and the availability of oxygen at high temperatures for NOx formation. It is observed in the temperature graphs, in relation to the crank angle (Figure 6), that the temperatures of the burned zone (tb) are higher for ethanol compared to the other fuels. Therefore, it is noted that the NOx peaks are higher for ethanol, corroborating with the literature. Despite the expectation of higher NOx formation for ethanol at 3600 rpm, this did not occur. Therefore, it is necessary to study the mechanism of NOx formation for this specific case.

From the results obtained for the operating conditions with only one fuel it can be concluded that:

- Single Wiebe function gives better results for ethanol compared to literature. While Double Wiebe is better for biogas and biomethane.
- The double Wiebe implementation needs more input data to supply all the parameters that are requested in the function.
- Biomethane cannot be modeled using the biogas parameters, more studies need to be conducted for better modeling of the fuel.
- NOx and CO emissions showed lower values for biogas at 1800 rpm, while at 3600 rpm the opposite occurred.

6. Acknowledgements

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8. Responsibility notice

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