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ENERGETIC AND EXERGETIC ANALYSIS SOFTWARE IN PYTHON: DEVELOPMENT, VALIDATION AND APPLICATION

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Abstract. *The research field in which Thermoelectric and Cogeneration Plants are analyzed works on the relationship between the various thermal machines used as primary drivers for thermoelectric generation and their relationship with the thermal energy supplied and/or used in order to identify, quantify and locate the irreversibilities inherent to these processes to the purpose of promoting increasing in overall efficiency. This paper aims to describe the development (including the theoretical thermodynamic background), validation, and the results of the application of an energetic and exergetic assessment software on a 12 kVA engine-driven generator. The program provides a graphic interface and was developed using SQLite in Python open-source language. The input parameters are the brake power, the fuel and air mass flow rates and the exhaust gases data which is obtained from a flue gas analyzer. The exhaust pipe gases data were collected on a molar dry basis and then converted to a molar wet basis and finally in mass fractions in order to compute the enthalpy and entropy contribution of each specimen. The thermomechanical and chemical exergy were then stated. Thus, both the first and second Law of Thermodynamics can be performed. The fuel composition and Lower Heating Value (LHV) were also set, after that, the chemical exergy of the fuel was computed. The energy and exergy of the entraining air were neglected due to their proximity to the dead state conditions. Output results are shown both numerically and in figures. The program was validated according to the existing literature, and the results obtained on the program were the same as the ones previously published. Ultimately the code was used on the laboratory test rig for the assessment of the results of an engine-driven generator set. The rig instrumentation was assembled by the following devices: the mass fuel flow rate was collected on a mass basis via an electronic scale and a stopwatch, while the air mass fuel flow rate was measured via a Pitot probe anemometer., The delivered electric power was measured by a wattmeter, and exhaust gas data were collected via a Greenline 8000 flue gas analyzer.*

Keywords: *Programming, Python, Energy, Exergy*

1. INTRODUCTION

Programming currently plays an important role in the modern world, whether on smartphones, computers or even through the internet. Programming has made possible many things that were previously considered unimaginable, such as data processing, software development, and solving complex mathematical problems.

Python is a programming language created in 1991 that, despite being quite recent in the current market, has been growing immensely, both by demand of young people with the intention of learning and of companies such as Spotify, Netflix, among others (Sanchez, 2021). Being an open-source language, its libraries and modules are reusable and are constantly updated by the community itself, the use of the libraries is free and most of them are already translated by other programmers, making it easier to learn (Revelo, 2021).

Considered a high-level language, Python 3 has a syntax geared to human understanding, i.e., it is more intuitive and friendly, which makes it perfect for novice programmers (Noleto, 2021).

For these reasons, Python 3 was chosen as the language used in the development of the program here presented, with the purpose of automating the calculations developed by the energetic and exergetic analysis method, based on the chemical balance of the real fuel combustion chemical equation, as well as on iterative calculations. It was necessary to implement a program for this method because, as said, it uses as a base iterative ways of checking enthalpy and entropy data for the exhaustion gases in tables that, if done manually are very time-consuming. There is also the future intention of the automatic integration of the gas analyzer with the program created, so that they communicate and generate the efficiencies in real-time of the engine's operation.

2. OBJECTIVE

The objective of the article is to describe the mathematical calculation of the developed energy and exergy method, and make it automatic by coding a new Program based on Python 3, validate both and then exemplify an application for the research in Universidade Federal da Grande Dourados.

3. METHODOLOGY

The developed program script aims to calculate the energetic and exergetic efficiency of combustion engines using the created method, which considers real and incomplete combustion. Eq. 1 shows the generic combustion reaction for hydrocarbons.

$$aC_xH_yO_z + b(O_2 + 3{,}76N_2) \rightarrow cO_2 + dCO + eCO_2 + fCH_4 + gNO + hNO_2 + iN_2 + jH_2O \quad (1)$$

3.1 Energetic analysis

Figure 1 shows the control volume of the system, which represents the mass flow and energy in balance, while the energy is defined in Eq. 2 by $\dot{Q}_c$, $\dot{Q}_{ex}$, $\dot{Q}_p$, characterizing the fuel, exhaust and loss energy respectively, $\dot{Q}_c$ and $\dot{Q}_{ex}$ are described in Eq. 3 and Eq. 4, and the mass flow is defined in Eq. 5 by $\dot{m}_c$, $\dot{m}_{ex}$ and $\dot{m}_a$, characterizing the fuel, exhaust and air mass flow. (Çengel at al., 2007)

Some considerations were applied to the control volume to make the calculations easier: the control volume is in a steady state, operating under permanent conditions, inertial and gravity effects are considered negligible, and the exhaust gas and inlet air are considered ideal gases. The temperature in the reference state is 25ºC (298,15 K) and the pressure is 1 atm, which is close to the temperature and pressure of air.

$$\dot{Q}_c = \dot{Q}_{ex} + \dot{Q}_p + \dot{W}el \quad (2)$$

$$\dot{Q}_c = \dot{m}_c + PCI_c \quad (3)$$

$$\dot{Q}_{ex} = \dot{m}_{ex} * h_{ex} \quad (4)$$

$$\dot{m}_{ex} = \dot{m}_c + \dot{m}_a \quad (5)$$

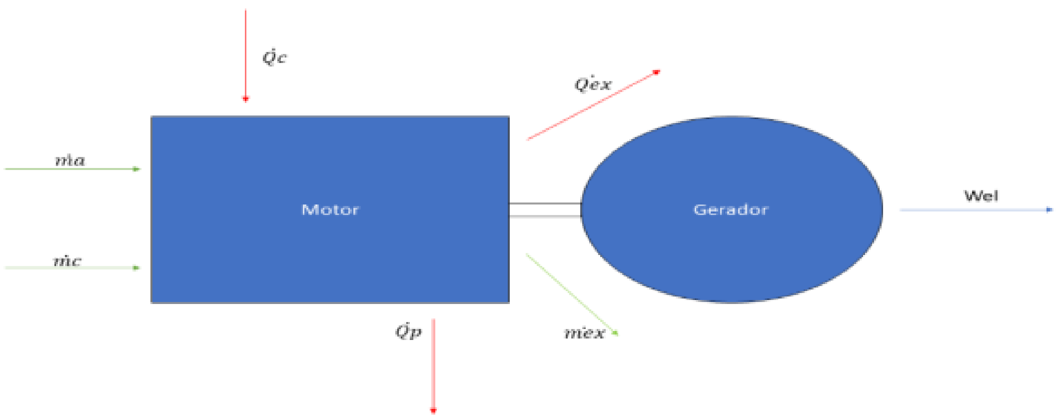

Figure 1. Mass and energy balance in control volume

For the calculation of the exhaust gas energy, the standard enthalpy $\bar{h}_i$, of the combustion products was used. Where Eq. (6), Eq. (7) and Eq. (8) were used for this purpose, where h_{ex} is the enthalpy of the exhaust gases, $\bar{h}_{ex}$ represents the specific enthalpy of the exhaust gases, and MW_{ex} characterizes the molar mass of the exhaust gases while X_i is the mole fraction of the exhaust gases. (Turns, 2013).

$$h_{ex} = \frac{\bar{h}_{ex}}{MW_{ex}} \tag{6}$$

$$\bar{h}_{ex} = \sum X_i * \bar{h}_i \tag{7}$$

$$\bar{h}_i = \bar{h}_f + \Delta\bar{h}_s \tag{8}$$

3.2 Exergetic analysis

To calculate the exergy it is necessary to take into account the specific entropy of the flue gases and the fuel used. The chemical exergy of the fuel is calculated using Eq. (9), where the terms are the mass fractions per carbon of the specific fuel elements. (Turns, 2013). The exergy of the exhaust gas was defined as the sum of its chemical and thermal exergy Eq. (10).

In Eq. (11), the thermal exergy of the exhaust gas is obtained, and, in Eq. (12), the chemical exergy of the exhaust gas is obtained (Canakci at al., 2006). For these equations, it is determined that a_i is the molar amount of the component, h_i the absolute enthalpy, s_i the absolute entropy, $\bar{R}$ symbolizes the universal gas constant and $\left(\frac{P}{Po}\right)$ the pressure ratio between the process pressure and that of the environment. It should be noted that, for very small pressures, the term $\left(\frac{P}{Po}\right)$ can be neglected and this has been taken into account.

$$\bar{e}_{ch}(C) = [1{,}0401 + 0{,}1728\mathrm{Hc} + 0{,}0432\mathrm{Oc} + 0{,}2169\mathrm{Sc} * (1 - 2{,}0628\mathrm{Hc})] * \mathrm{PCIc} \tag{9}$$

$$\bar{e} = \bar{e}_{th} + \bar{e}_{ch} \tag{10}$$

$$\bar{e}_{th}(Ex) = \sum_{i=1}^{j} a_i * \left\{h_i(T) - h_i(To) - To * \left[s_i(T) - s_i(To) - \bar{R} * \ln\left(\frac{P}{Po}\right)\right]\right\} \tag{11}$$

$$\bar{e}_{ch}(Ex) = \sum_{i=1}^{j} a_i * \bar{R} * To * \ln\left(\frac{y_i}{y_{(e)i}}\right) \tag{12}$$

3.3 Coeficients for the chemical equation

The Greenline 8000 flue gas analyzer delivers the combustion products data on a dry basis mole fractions, and must be converted to a wet basis so that both the specific enthalpy and the specific entropy of the combustion water are considered.

First, the transformation to mass fraction was performed with Eq. (13) and Eq. (14), where Y_i is the mass fraction, M_i is the molar mass of each component, and M_t is the molar mass of the mixture. Once the mass fractions were determined, the mass flow rates of the exhaust gas, the components were determined by Eq. (15) and the molar flow rate of the fuel n_{comb} was used to calculate a_i Eq (16). The coefficients of reactants *a* and *b* according to Eq. (1) were found by Eq. (17) and Eq. (18) where, M_{comb} is the molar mass with fuel, $\dot{m}_c$ is the mass flow rate of the fuel and M_{ar} consists of the molar mass of the air. The coefficient of water *j* was found by the chemical balance between the hydrogens of Eq. (1), to convert the coefficients of Eq. (1) from dry basis to wet basis; they were multiplied by the molar flow rate of the fuel and, finally, for wet basis mole fraction transformation they were divided individually by $\sum a_i * n_{comb}$

$$Y_i = \frac{X_i * M_i}{M_t} \quad (13)$$

$$M_t = \sum X_i * M_i \quad (14)$$

$$\dot{m}_i = Y_i * \dot{m}_{ex} \quad (15)$$

$$a_i = \frac{\dot{m}_i}{M_i * n_{comb}} \quad (16)$$

$$a = \frac{\dot{m}_c}{M_{comb}} \quad (17)$$

$$b = \frac{\dot{m}_{ex}}{M_{ar}} * a \quad (18)$$

3.4 Efficiency analysis

Once the flue gas energy and exergy are determined and the effective engine power is measured, the efficiencies are calculated. For the equations used, Eq. (19) is defined as energy efficiency, Eq. (20) as exergetic efficiency, Eq. (21) as exhaust gas energy and Eq. (22) as exhaust gas exergy.

$$\eta_{en} = \frac{P_{mot}}{\dot{Q}_c} \quad (19)$$

$$\eta_{ex} = \frac{P_{mot}}{\bar{e}_{ch}(C) * \dot{m}_{ex}} \quad (20)$$

$$En_{gas} = \frac{\dot{Q}_{ex}}{\dot{Q}_c} \quad (21)$$

$$Ex_{gas} = \frac{\bar{e}(Ex) * n_{comb}}{\dot{Q}_c} \quad (22)$$

4. THE PROGRAM

Combustion Viper is a program developed using Python 3 programming language, the methodology described above was transcribed into a script using Visual Studio Code, in which the input data were the initial variables of the methodology, these are:

Table 1. Input data.

Variables	**Acronyms**	**Unity**
Mass fuel flow	mc	g/s
Mass air flow	ma	g/s
Fuel PCI	pci	kJ/kg
Ambient temperature	tempa	K
Exaust gas temperature	tempg	K
Motor power	potm	W
Molar fraction O_2	io2	%
Molar fraction CO	ico	ppm
Molar fraction CO_2	ico2	%
Molar fraction CH_4	ich4	ppm

Molar fraction NO	ino	ppm
Molar fraction) NO_2	ino2	ppm

Some data used in the equations described are considered fixed and are found within the script itself, these are the molar masses and mass fractions. The units of the exhaust gases were selected as delivered by the gas analyzer, because it is with these units that the information of the exhaust gases is obtained and for a future automatic integration between the ICM and the program, the output data of the analyzer needs to be equal to the input data of the Greenline 8000.

4.1 Database - SQL

The specific enthalpies and exergies required in the methodology calculations were collected from tables in the reference books quoted, but, for the program the SQL (Structured Query Language) was used. Using SQL, a database was created to store information from all tables needed for the calculations in virtual tables, so that the script could access them and work with the same tables and data from the theoretical calculations (Çengel at al., 2007) (Turns, 2013).

SQL is a language used to execute commands in relational databases, i.e. tables, and Python 3 supports such tables. In order to avoid using external programs which would require the creation of an online database, *sqlite3* was used, a library available inside Python 3 that works with the SQL language in accordance with PEP 249 – Python Database API Specification v2.0. This PEP (Python Enhancement Proposals) was created in an attempt to establish a more coherent way of programming in Python and PEP 249 specifies a standard core set of interfaces to be used in the normalization between different packages available for database access, such as SQLite and MySQL, for example. To create the tables and check their data, two free external programs were used, DB Browser for SQLite and SQLiteStudio.

With these tools two databases were created, the first with the standard enthalpy tables of the exhaust gases used in the energy calculation and the second with the absolute enthalpy and entropy tables used in the exergetic calculation.

4.2 Graphics implementation

Having acquired the efficiency and heat loss values shown in Table 2, it was necessary to implement a pie chart to better represent their proportions. For this the *matplotlib* library was used along with *pyplot*.

4.3 Error treatment

Since the script used for the executable program is relatively simple and receives data input for mathematical calculations, it is possible that errors may occur in the process, causing the program to close. To avoid this, usage instructions have been placed in the program, indicating how to use it. There was also an implementation in the code to indicate which error was made, to do so the *PyQt5* online library was used and *QMessageBox* was imported.

4.4 Graphic design

A Python 3 script can be made executable through the *PyInstaller* library, but using only the latter, the code will just be opened and executed, without any kind of interface. For this reason, it was decided to implement a graphic design, i.e. an interface to the script, so that when executed it can be used in a more intuitive way.

One of the complications of making an interface is its programming language, which differs a lot from the standard Python 3, and for beginners and intermediate programmers it can be a big challenge. With this in mind, the PyQt5 library was used again, this library has a free program called QT Design that uses block programming to generate the interface script. The final design of the program can be seen in Fig. 2.

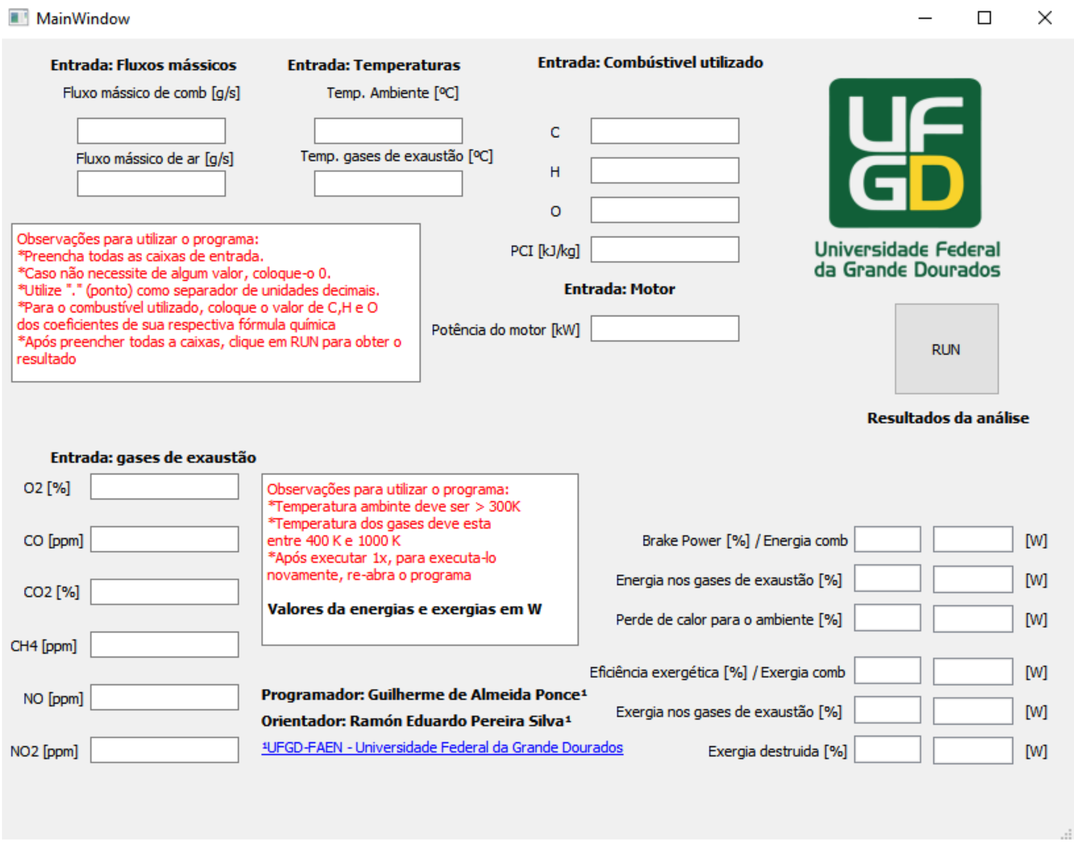

Figure 2. Combustion Viper graphic interface.

4.5 Turning into executable

As stated earlier, to make the code executable the PyInstaller library was used and installed on the machine. With the generated program, a folder was created with the same name as the old one, but with several internal files. The executable can be found on the "dist" folder and had the same name as the original script.

It is worth highlighting that if the programmer has used external files that communicate to the script such as photos, databases and even the GUI itself, they must be copied to the same folder where the executable is, so that the connection is maintained.

5. SIMULATION

For the validation of the Combustion Viper program a simulation was performed using energetic and exergetic analysis results published by Yoge Jeronimo (2007). The information used to run the program is: fuel mass flow, air mass flow, room and exhaust gas temperature, fuel data, engine data, and exhaust gas data. First, the simulation data and the results obtained with Combustion Viper are presented, followed by a comparative analysis of the result presented.

5.1 Validation

The simulations for program validation were performed using the data published by Yoge Jeronimo (2007) which are summarized in Table 2. The interface screen showing the results obtained is shown in Fig 3.

Table 2. Data for simulation

Variables	Value
Fuel	100% Diesel – C12H26
Mass fuel flow (g/s)	1.81
Mass air flow (g/s)	199.3
Fuel PCI (kJ/kg)	44,143.18
Ambient temperature (ºC)	32.4
Exaust gas temperature (ºC)	207.6

Variables	Value
Motor power (kW)	11.7
O_2 (%)	16
CO (ppm)	186
CO_2 (%)	2.4
CH_4 (ppm)	87
NO (ppm)	156
NO_2 (ppm)	2

Performing the simulation, the following results were obtained as shown in Fig. 3 and Table 3.

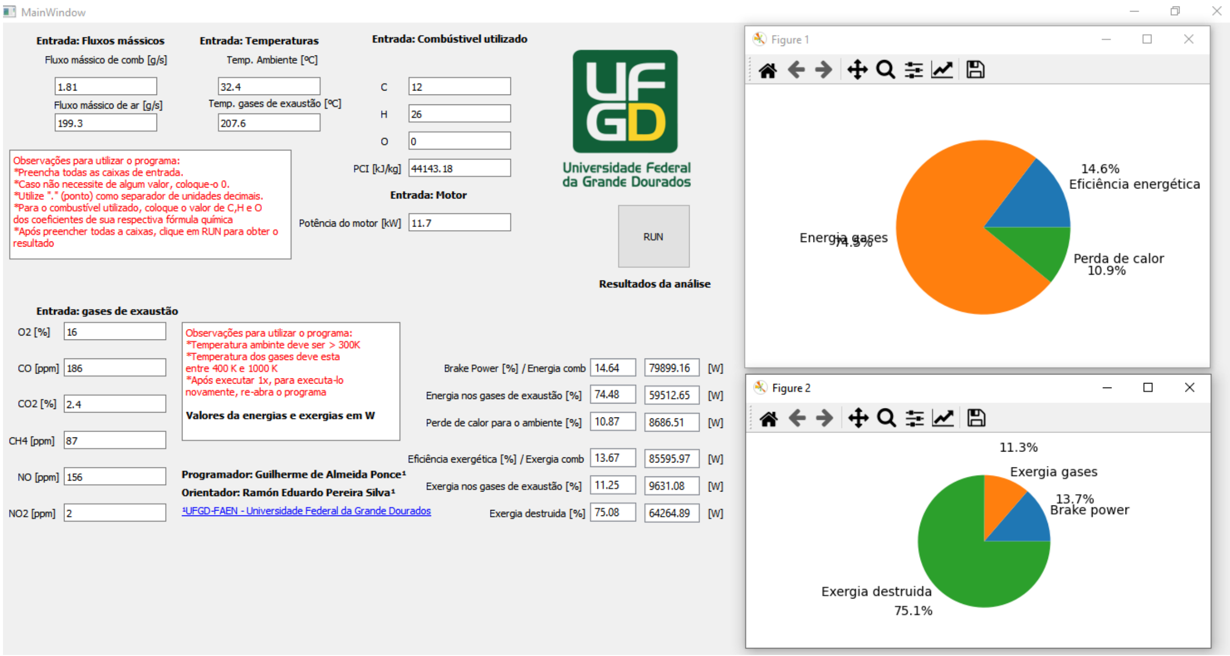

Figure 3. Combustion Viper results

Table 3. Results of the simulation.

Variables	[%]	[kW]
Brake Power	14.64	11.70
Exhaust gas energy – Wet Basis	74.48	59.51
Environment energy lost	10.87	08.69
Exergetic efficiency	13.67	85.50
Exhaust gas exergy	11.25	09.63
Environment and destroyed exergy	75.08	64.26
Exhaust gas energy – Dry Basis	---	28.15

The results of the energy and exergetic analysis of the base case for $C_{12}H_{26}$ diesel are found in Tab. 4 below.

Table 4. Base article results for the energy and exergy analisys. (Yoge, 2007)

Variables	[%]	[kW]
Brake Power	15.70	12.54
Exhaust gas energy	37.56	30.01
Environment energy lost	46.72	37.33
Exergetic efficiency	14.64	12.54
Exhaust gas exergy	8.71	07.47
Environment and destroyed exergy	76.49	65.64

Table 5. Comparation between simulation and article results.

Variables	Difference [%]
Exhaust gas energy – Dry Basis	06.19
Exhaust gas exergy	28.92

With the values observed in Tab. 3, Tab, 4 and Tab. 5 of energy for the exhaustion gases, the program obtained 59.51 kW and the article 30.01 kW, due to this big difference, the value for the energy of the exhaustion gases on a dry basis was also calculated, the result was 28.15kW, a difference of 6.19%. The Combustion Viper receives the exhaustion gases information on a dry basis and by chemical balance identifies the amount of water and transforms the molar fractions to a wet basis (Moran at al., 2014). The article doesn't do that, it calculates the energy and exergy of the exhaustion gases on a dry basis and analyzes the water separately. Thus, observing the water impact in the energetic calculation. Another topic of influence was the standard enthalpy calculation. In the base article, the sensitive enthalpy, a standard enthalpy component, is determined by linear and non-linear equations, the Combustion Viper gets the values of sensitive enthalpy from a table, and there is no intermediate calculation performed on the sensitive enthalpy part (Turns, 2013).

On the exergy calculations, the program value was 9.63kW and the one in the base article is 7.47 kW. The two results are close to each other, however, the difference between them may originate again from how the water was manipulated and its consideration. The Combustion Viper for the exergy calculations considers the exhaustion gases as ideal gases, this included the water present in the combustion products, in the base article the combustion products are also considered as ideal gases, however, as the water is treated and calculated separately from exhaustion gases, it's not informed if the consideration is also valid for it. Another point that influenced values was once again the conversion from dry base to wet base.

6. APPLICATION

With the program validated, an experiment was executed to measure the energy and exergy of a motogenerator system from the Faculdade de Engenharia (FAEN) laboratory of the Universidade Federal da Grande Dourados (UFGD). The workbench consisted of a 12kVA engine-driven generator set, the Greenline 8000 gas analyzer, an electronic scale and a stopwatch to collect the mass fuel flow data, a Pitot probe anemometer to measure the airflow rate and a wattmeter to measure the delivered electric power.

After assembling the workbench, the test was executed, and the needed data for the simulation in the Combustion Viper can be found in Tab.6 down below.

Table 6. Data for simulation

Variables	Value
Fuel	Diesel – $C_{14.09}H_{24.78}$
Mass fuel flow (g/s)	0.19
Mass air flow (g/s)	13.01
Fuel PCI (kJ/kg)	42,640
Ambient temperature (ºC)	31.90
Exaust gas temperature (ºC)	170.28
Motor power (kW)	1.17
O_2 (%)	19.93
CO (ppm)	84.07
CO_2 (%)	0.77
CH_4 (ppm)	16.38
NO (ppm)	67
NO_2 (ppm)	18

Performing the simulation, the following results were obtained as shown in Fig. 4 and Table 7.

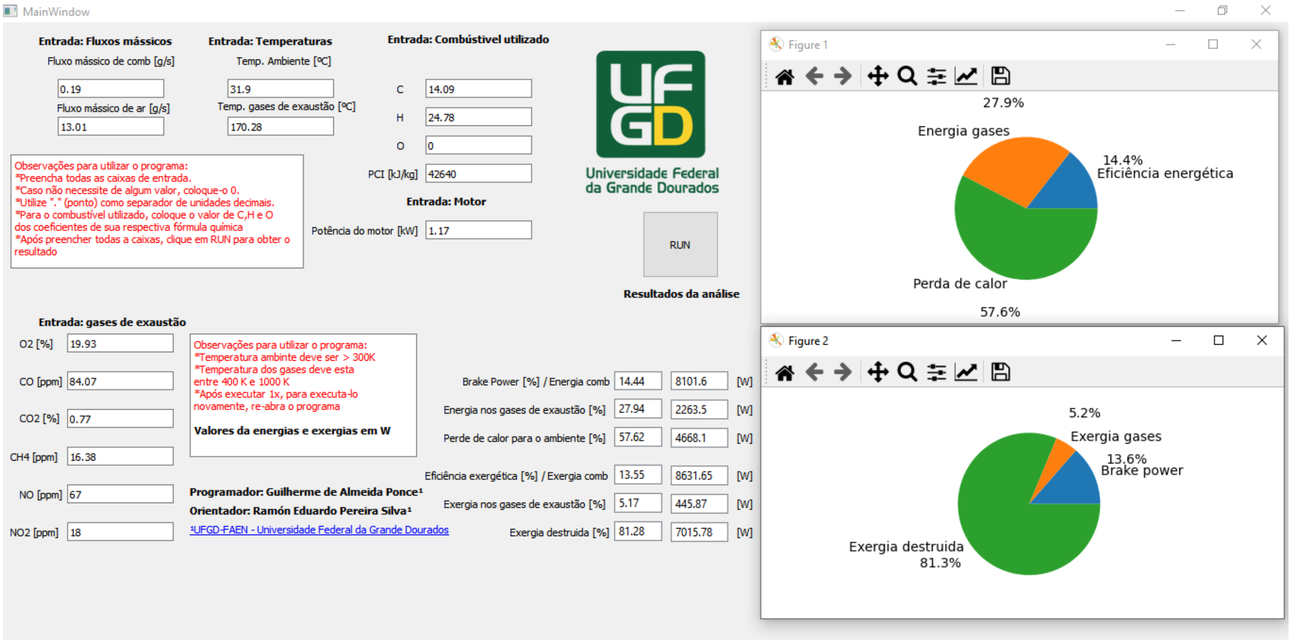

Figure 4. Combustion Viper results

The results of the energetic and exergetic analysis for $C_{14.09}H_{24.78}$ (Canakçi, 2006) diesel are found in Tab. 7 below.

Table 7. Results of the simulation.

Variables	[%]	[kW]
Brake Power	14.44	1.17
Exhaust gas energy – Wet Basis	27.94	2.26
Environment energy lost	57.62	4.67
Exergetic efficiency	13.55	1.17
Exhaust gas exergy	5.17	0.45
Environment and destroyed exergy	81.28	7.01

The simulation results for the test of the 12kVA motogenerator were very consistent since the bench is old and it has lost efficiency, this point is proved with the exhaustion gases low exergetic efficiency value.

7. CONCLUSION

According to the analysis in the previous section, it is concluded that: due to the small difference in dry bases between the program's results and the base article, the Combustion Viper was validated and it can be used to estimate the energy and exergy balance of thermal machines considering the real combustion. The application showed that the program can be used in real experiments to measure energy and exergy of internal combustion engines. A possible next step could be automatizing the process by the use of an Arduino system, so it can be possible to get the results in real-time.

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