

COB-2021-0334

INTERNAL COMBUSTION RECIPROCATING ENGINES PERFORMANCE AND EMISSIONS SIMULATION IN PYTHON

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Abstract.

This work aims to describe the method and results obtained of a reciprocating combustion engines simulation script developed in python language. The program uses graphic interface and has a didact purpose of illustrate the thermodynamic and combustion processes which occurs in a reciprocating engine allowing better understanding of its operation and design. Three cycles are available to assessment: Otto, Diesel and Dual. Type of fuel and air-to-fuel ratio can also be selected. Starting from the type of the operating cycle and the geometric, combustion parameters and the crankshaft rotation the program can simulate the engine performance and predicts the exhaust gases emissions if the combustion is considered complete. The output performance parameter are the state thermodynamic parameters, the indicated and brake power, torque, efficiencies, specific fuel consumption and exhaust gases emissions. Several simulations were carried out to compare the results with the actual engines data. The simulations presented results with values near to the of-the-shelf data found in research validating the program method for internal combustion reciprocating engines analysis.

Keywords: Reciprocating engines, Simulation, Python, Thermodynamics, Combustion

1. INTRODUCTION

In the teaching of thermal machines, the study of internal combustion reciprocating engines is of paramount significance. Based in the classic thermodynamic literature the air standard Otto and Diesel cycles are assessed to determine the performance parameters of the engine. As the real engines uses a combustion reaction as heat source the cycle cannot be closed, once the combustion products do not can be fired again. Thus, this cycle is called mechanical and can be assessed from the geometric parameters of the engine. The use of computational codes area always welcome to help the calculation of the performance parameters and to show graphically how the cycle operates. Spreadsheets were used by Rivas et al. (2006), Cruz-Peragón et al. (2012) and Matlab® by Thompson and Yoon (2020). Python is an open-source code which is fully available for the students use. It allows to develop analytical scripts to simulate the engine operation. So, this work shows a friendly program developed by the authors to analytically simulate internal reciprocating engines for didactical purposes from the geometric parameters of the engine. It is showing the theoretical background and two examples validating the software calculation.

2. THE SOFTWARE

The FATROMEIO (2020) software was developed using the Python Programming Language. The Tkinter library was used to provide a friendly and intuitive graphical interface. The program aims to provide a tool for didact purposes which can help both students and instructors to understand the actual operating cycle in reciprocating internal combustion engines using a free code language. Starting from the type of the operating cycle and the geometric, combustion parameters and the crankshaft rotation the program can analytically simulate the engine performance and predicts the exhaust gases emissions if the combustion is considered complete. The output performance parameter are the state thermodynamic parameters, the indicated and brake power, torque, efficiencies, specific fuel consumption and exhaust gases emissions. Developed in Portuguese, the input/output page is show in Figure 1. The initial data is input in the (I), (II) and (III) windows. The thermodynamic cycle, fuel and combustion parameters are input in the window (I), geometric parameters are input in window (II) and the fluid thermodynamic coefficients in the window (III). Once the input data was loaded the analytical simulation is performed by pushing the “calcular” button in the window (IV). Output results

are show in the window (V). Pressure x volume, mechanical efficiency, torque x rpm and effective brake power x rpm curves can by generated by selecting the proper buttons in window (VI).

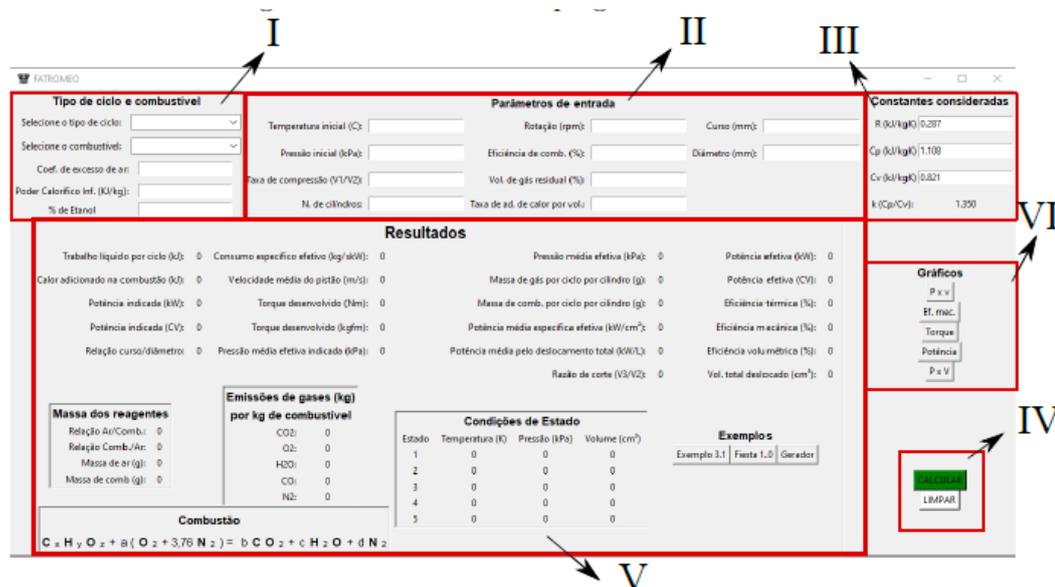


Figure 1. FATROMEIO input/output screen

3. THEORETICAL BACKGROUND

Theoretical background of both Otto and Diesel standard-air cycles can be found in the classical thermodynamic literature as Moran (2018), Çengel (2013), Borgnakke and Sonntag (2013) However, a more realistic approach is found in the specific literature for reciprocating internal combustion engines. The spine reference used for the script development was Pulkrabek (2004). Although both Heywood (2018) and Ferguson and Kirkpatrick (2015) were used as support. For combustion analysis reference Turns (2014) was used. So, the theoretical background described in this section is based in the above references

3.1 Basic cycle

Both Otto and Diesel air-standard cycles operates in four basic processes: iso-entropic compression of the air, heat transfer to the compressed air, iso-entropic expansion of the air and heat rejection to the environment. Compression, expansion and heat rejection are the same for both cycles. The main difference between them is in the heat transfer from the environment to the engine. It happens at constant volume for the Otto cycle and at constant pressure in the Diesel cycle. In the real cycle, were the thermodynamic processes turns into strokes, the heat amount input to the engine is replaced by the heat released in a combustion process and the heat rejection occurs via exhaustion of the burned gases. Besides the previous described difference at the combustion stroke another paramount characteristic takes place at the admission/compression stroke. While the Otto engine receives an air/fuel mixture inflow, at the diesel engine receives solely the atmospheric air. These peculiarities will be discussed as the theoretical model will be displayed. The Otto engine is known as spark ignition (SI) engine and the Diesel engine is called compression (CI) ignition engine.

3.2 Engine geometrical parameters

The main geometrical parameters for the reciprocating internal combustion engines are defined in Figure 2. They are the cylinder bore (B) and the stroke length of the piston (S). The top dead center (TDC) is the higher position of the piston, hence is the point where the cylinder presents the lowest volume. At this position the volume in the cylinder head is called clearance volume (V_c).The bottom dead center (BDC) is the position where the piston is further away from the engine head, so it's the position of larger volume of the cylinder.

The unitary displacement of a cylinder, or displacement volume (V_{du}) is the volume displaced by the piston when it travels from the BDC to TDC. To determine the total displacement of the engine V_{dt} shall be multiplied times the number of the engine cylinders (z). The displacement depends on the cylinder bore and piston stroke as show in Eq (1). The compression ratio of the engine (r_c) is defined as the ratio between the total of one cylinder (V_i) volume and the unitary

displacement volume of one cylinder. The total volume is the sum of the displacement and clearance volumes. For simulation both B , S and r_c shall be input. Also, the crankshaft rotation in rpm.

$$V_d = V_{du} \cdot z = (\pi/4) \cdot B^2 \cdot S \cdot z \tag{1}$$

$$r_c = V_t/V_c = (V_{du} + V_c)/V_c \tag{2}$$

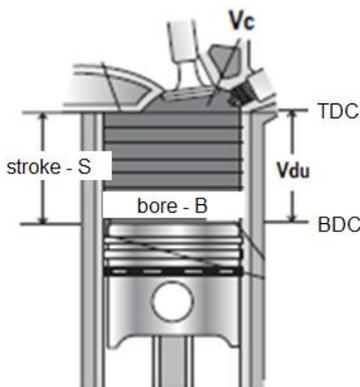


Figure 2. Geometrical parameters

3.3 Performance Parameters

Despite the differences at the combustion stroke, both SI and CI engines thermodynamic analysis can be performed by following the next steps.

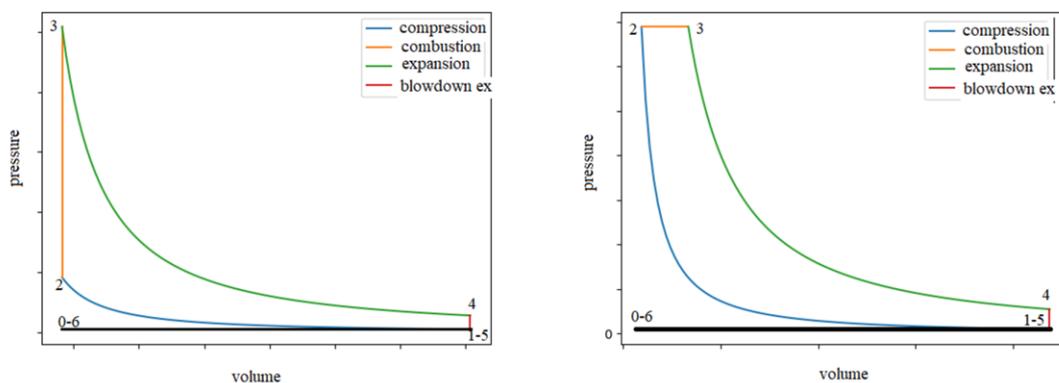


Figure 3. Otto cycle and Diesel Cycle

As show in Figure 3 the intake stroke occurs from point (6) to point (1). The piston moves downward from the TDC to the BDC. At this stroke the intake valve (IV) is fully open allowing the intake fluid (air/fuel mixture or atmospheric air) to enter the cylinder. The exhaust valve (EV) remains closed. Neglecting the pressure losses that occurs in the intake systems (filters, valves, intake ducts...) the pressure which the intake fluid enters the cylinder (P_1), for naturally aspirated engines, can be assumed as the surround pressure (P_0). For overcharged engines this pressure shall be given by the boost device. The intake temperature (T_1) also can be assumed as the surround temperature (T_0). Then, the intake work ($W_{6,1}$) is defined by Eq. (6) The mass of the fluid (m_m)inside the cylinder is then estimated by the equation of state for ideal gases (Eq. (7)).

$$P_1 = P_6 = P_0 \tag{3}$$

$$V_1 = V_t = V_{du} + V_c \tag{4}$$

$$T_1 = T_0 \tag{5}$$

$$w_{6-1} = P_0 \cdot (V_1 - V_6) \quad (6)$$

$$m_m = (P_1 V_1) / (R \cdot T_1) \quad (7)$$

The second stroke occurs when the piston travels from BDC to TDC with all valves closed. This stroke compresses the air-fuel mixture (SI) or only air (CI) increasing both the pressure and temperature. At this stroke there are work consumption. The thermodynamic state 2 and the compression work are defined from Eq. 8 to Eq. 11.

$$T_2 = T_1 \cdot (r_c)^{k-1} \quad (8)$$

$$P_2 = P_1 \cdot (r_c)^k \quad (9)$$

$$V_2 = V_c \quad (10)$$

$$w_{12} = c_v \cdot (T_1 - T_2) \quad (11)$$

Spark ignition engines combustion happens near stoichiometry. Compression ignition engines can occur at the stoichiometry or in very poor air-fuel ratio conditions. So, at this point there is a need to know the actual air-fuel mixture to determine the mass of fuel (m_f) and the mass of air (m_a) contained in the cylinder. Combustion of air-fuel mixture in SI engines happens at nearly constant volume when the piston is near TDC. At this point the clearance volume is assumed to be the combustion chamber of the engine. Combustion changes the composition of the gas mixture and increases the temperature and pressure to their peak values. So, the thermodynamic state 3 and the heat input (Q_{2-3}) can be computed from Eq. 12 to Eq. 14.

$$V_3 = V_c \quad (12)$$

$$Q_{2-3} = Q_{in} = m_f \cdot Q_{HV} \cdot \eta_{comb} = m_m \cdot c_v \cdot (T_3 - T_2) \quad (13)$$

$$P_3 = P_2 \cdot (T_3 / T_2) \quad (14)$$

The heat released by the combustion reaction is the result of the multiplication of the fuel amount (m_f), the lower heating value of the fuel (Q_{HV}) and the combustion efficiency (η_{comb}).

In the CI engines combustion happens when the piston leaves TDC and travels some length of the stroke while the fuel is injected into the cylinder at constant pressure. As there is volume variation some work is produced at this stroke. Is important to note that for CI engines, in the combustion stroke the pressure constant specific heat (c_p) is used in instead of volume constant specific heat (c_v) which us used in SI engines. A new parameter is introduced at this point: the cutoff ratio (β). The cutoff ratio is defined as the change in volume that occurs during combustion (Eq. (19)).

$$P_3 = P_2 \quad (15)$$

$$Q_{2-3} = Q_{in} = m_f \cdot Q_{HV} \cdot \eta_{comb} = m_m \cdot c_p \cdot (T_3 - T_2) \quad (16)$$

$$V_3 = (m_f + m_a) \cdot R \cdot T_3 / P_3 \quad (17)$$

$$w_{2-3} = P_2 \cdot (V_3 / (m_f + m_f) - V_2 / m_a) \quad (18)$$

$$\beta = V_3 / V_2 \quad (19)$$

With all valves close, the high pressure created by the combustion process pushes the piston away to the BDC. In SI engines this travel begins at TDC and for CI engines the expansion stroke continues from the point where the combustion ends. The expansion stroke, or power stroke, produces the work output of the engine cycle. As the piston travels to the BDC the volume increases leading to a pressure and temperature to drop. The thermodynamic state at the end of power stroke is defined through Eq. 20 to Eq. 23.

$$V_4 = V_t \quad (20)$$

$$P_4 = P_3 \cdot (1/r_c)^k \quad (21)$$

$$T_4 = T_3 \cdot (1/r_c)^{k-1} \quad (22)$$

$$w_{3-4} = c_v \cdot (T_3 - T_4) \quad (23)$$

At the end of the power stroke the pressure and temperature inside the cylinder are still high relative to surround. Then, the exhaust blowdown takes place when the EV is open near the BDC. The exhaust blowdown is the abrupt discharge of the combustion gases to the surroundings due the pressure differential between the cylinder and the environs. This exhaust gases still carries a large amount of enthalpy, leading to lowering the thermal efficiency. This stroke is assumed as constant volume heat rejection trough the control volume.

$$V_5 = V_1 \quad (24)$$

$$P_5 = P_0 \quad (25)$$

$$T_5 = T_0 \quad (26)$$

And finally, the piston goes from BDC to TDC (EV is still fully open) pushing the remaining exhaust gases out of the cylinder to the exhaust system at about atmospheric pressure leaving only that trapped in the clearance volume when the piston reaches TDC.

The indicated power is the total power developed within the cylinder, in one cycle, during the expansion stroke as the gas pressure pushes the piston downward. The indicated power is computed by the thermodynamic cycle of the engine considering only the losses due the heat transfer trough the control volume.

Once all thermodynamic states were defined the net indicated work ($W_{i,l}$), Eq. 27 for SI engines and Eq. 28 for CI engines, can be computed as the difference between the work produced in the power stroke and that spent in the compression stroke and then the indicated power (\dot{W}_i) is defined as function of the crankshaft revolutions (N) and the number of revolutions per power strokes (n). For engines that works at four stroke cycles $n = 2$ and for two stroke engines $n=1$). It is of paramount importance to remember that these parameters are calculated for only one cylinder, for the entire engine these values shall be multiplied by the number of cylinders.

$$W_{i,l} = w_{34} - w_{12} \quad (27)$$

$$W_{i,l} = m_g \cdot (w_{23} + w_{34}) - m_a \cdot w_{12} \quad (28)$$

$$\dot{W}_i = W_{i,l} \cdot (N/n) \quad (29)$$

The thermal efficiency is related to the compression ratio for SI engines. However, for CI engines the cutoff ratio shall be considered. Thus, for both SI and CI engines the thermal efficiencies are stated respectively in Eq. 30 and Eq. 31.

$$\eta_{t,SI} = 1 - (1/r_c)^{k-1} \quad (30)$$

$$\eta_{t,CI} = 1 - (1/r_c)^{k-1} \cdot [\beta^k - 1/k \cdot (\beta - 1)] \quad (31)$$

Finally, the brake power (\dot{W}_b) is defined. The brake power is the power which is effectively delivered by the engine. It considers the mechanical losses that happens in the engine as it operates. Brake power and indicated power are related via the mechanical efficiency (η_m) as show in Eq. 32. Mechanical efficiency depends on the design of the engine, so for didactical purposes the Eq. 33, which is an approach of a graphical curve show in Pulkrabek (2004), can be used. The average piston speed (\bar{U}_p) is function of the piston stroke and the crankshaft revolutions as in Eq. 34. And then the brake specific fuel consumption (*bsfc*), which is defined as the ration between the fuel mass flow rate and the brake power can be computed in Eq. 35. The torque (τ) an engine delivers through its crankshaft is always measured with a dynamometer. However, torque is related to the angular speed of the crankshaft and once the brake power is known it can be computed via Eq. (36). While torque is an important measure of the capacity of the engine to produce work, it depends on engine size. The brake mean effective pressure (*bmep*) is a better than torque parameter for comparing engines because it is independent of the size of the engine and its related to the brake power (for one cylinder) in Eq. (37).

$$\eta_m = \dot{W}_b / \dot{W}_i \quad (32)$$

$$\eta_m = -0,061 \cdot \bar{U}_p^2 - 1,441 \bar{U}_p + 92,62 \quad (33)$$

$$\bar{U}_p = 2 \cdot S \cdot N \quad (34)$$

$$bsfc = \dot{m}_f / \dot{W}_b \quad (35)$$

$$\tau = \dot{W}_b / 2 \cdot \pi \cdot N \quad (36)$$

$$bmep = \dot{W}_b \cdot n / V_{du} \cdot N \quad (37)$$

More are into the cylinder means more fuel can be added and more energy can be converted in work. Then, one of the most important parameters that shows how much power and performance can be obtained from an engine is the volumetric efficiency (η_v) which is the ratio between the actual air mass that enters the cylinder and the ideal amount of air which should be ingested(Eq. (38)). The ideal mass of air that would enter in the cylinder is the volumetric capacity (the volume displaced by the piston traveling in the cylinder) and the specific mass of the intaking air (ρ_a). For naturally aspirated engines the volumetric efficiency is lower than one due the losses in the intake system. As pressure increase leads to grater specific mass to rise, in overcharged engines the intake airflow is greater than the ideal one. The specific mass of the air is computed by using by the equation of state for ideal gases for the surrounding air temperature and pressure. The greater volumetric efficiency means larger mass air flow rate leading to better engine performance.

$$\eta_v = m_a / \rho_a \cdot V_{du} \quad (38)$$

3.4 Combustion and Fuels

For the simulation was assumed that the combustion reaction is complete, thus the combustion products are carbon dioxide and water. It is possible to input the air excess coefficient leading to oxygen and nitrogen presence in the flue gases. The fuels which can be set to the Otto cycle are gasoline and ethanol. It is also allowed to input a mixture of them.

For the compression ignition engine, the diesel fuel is set as default. The emission index (EI) is defined by Turns (2014) as the ration between the mass compound flow rate and the mass fuel flow rate. It is the amount of the specimen emission generated by one mass unity of fuel and it can be defined using the balance of the combustion reaction for an oxygenated fuel with some excess of air (α) (Eq. (39) to Eq.(44)) to first define the coefficients of the combustion products.

$C_c H_h O_o + \alpha. a. (O_2 + 3.76N_2) \rightarrow x. CO_2 + yH_2O + z_n N_2 + z_o O_2$	(39)
$a = (c + h/4 - z/2)$	(40)
$x = c$	(41)
$y = h/2$	(42)
$z_n = 3.76. \alpha. a$	(43)
$z_o = (\alpha - 1). a$	(44)

And the emission indexes are computed using the sequence from Eq. (45) to Eq. (48)

$EI_{CO_2} = (x. 44)/m_f$	(45)
$EI_{H_2O} = (y. 18)/m_f$	(46)
$EI_{N_2} = (z_n. 28)/m_f$	(47)
$EI_{O_2} = (z_o. 32)/m_f$	(48)

The fuels are gasoline (C_8H_{18}), diesel ($C_{10}H_{22}$) and ethanol (C_2H_5OH). It is also allowed to define any percentage of gas/ethanol blends and the composition of the mixture is given via a proportion weighted balance between them. The combustion reaction is assumed as complete and the products are carbon dioxide and water. The presence of nitrogen occurs once the reaction is processed with atmospheric air. The presence of oxygen happens due the excess of air in dome circumstances.

4. RESULTS AND DISCUSSION

To validate the script two simulations were performed. One of followed the example 3.1 described in Pulkrabek (2004) where the cycle of a SI engine was carried out. In the second example, looking for to validate the CI engine simulation, manufacturer data of a Cummins KTA50-G9 was used.

In the example, literature asks for a thermodynamic assessment of a 2.5 l spark ignition automobile engine operating in WOT (Wide Open Throttle), which means that there are no pressure losses through the intake system, at 3000 rpm. The engine has a compression ratio of 8.6:1. The fuel is gasoline assumed as iso-octane ($Q_{HV} = 44\ 300$ kJ/kg) reacting at stoichiometric ai-fuel ratio. The bore of cylinder is 91.91 mm, and the stroke of the piston is 94.42 mm. Mechanical efficiency is given as 86.00%. There are no emissions data available. The comparison between the simulation performed by the program and the example is show in Table 1. It can be noticed that the major discrepancies in results are due the difference of the mechanical efficiency. In fact, the mechanical efficiency is given in the example problem (86%) but its computed in the program (71%) leading to these divergencies. Then all the parameters that depends on the mechanical efficiency have show pretty much the same values of differences. Once it is clearly explained, these discrepancies do not invalidate the program results. There are no emissions data available to compare. However, the emissions indexes are shown in Table 2. The pressure x volume, brake power to rpm and torque to rpm curves are shown in Figure 4.

Table 1. Comparison for SI engine

Parameter	FATROMEIO	Pulkrabek	Difference %
\dot{W}_i [kW]	103.65	103	0.63
\dot{W}_b [kW]	73.71	88.6	-20.20
τ [N.m]	234.64	282	-20.18
bmep [kPa]	1179	1418	-20.24
η_t [%]	52.87	52.90	-0.06
η_m [%]	71.12	86.00	-20.92
η_p [%]	90.26	90.20	0.07
$bsfc$ [kg/kW.s]	$3.37.10^{-7}$	$5.00.10^{-7}$	-48.15

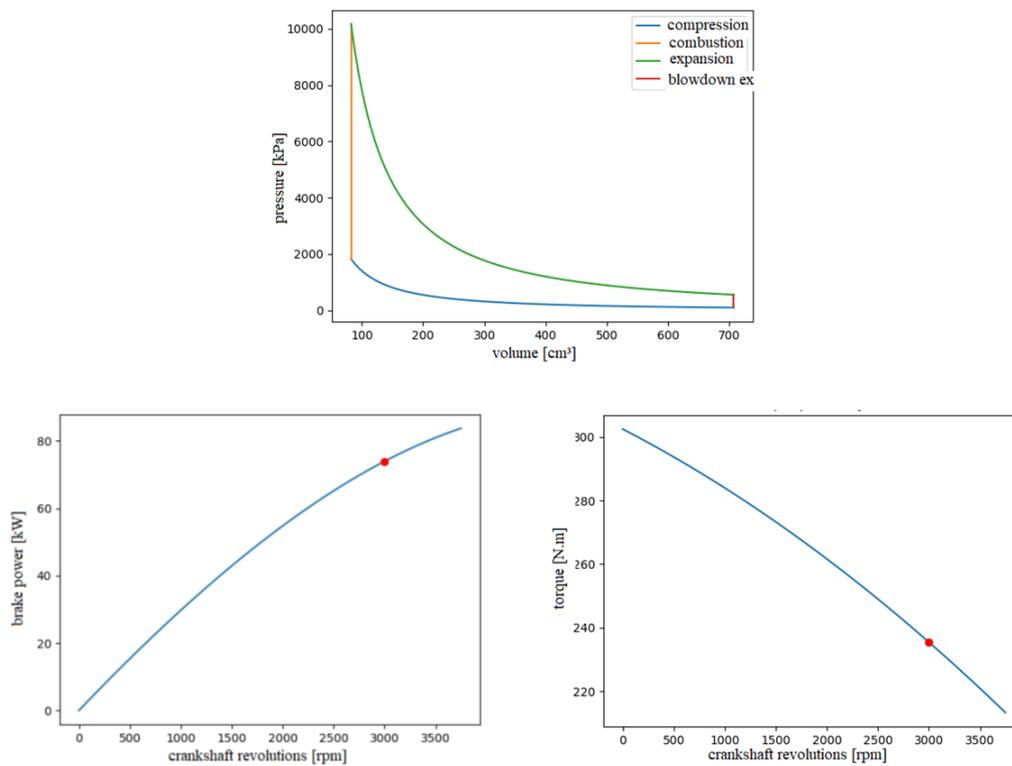


Figure 4. Pressure x volume; brake power x rpm; torque x rpm

Table 2. SI engine emission indexes

Parameter	EI [g/kg _f]
CO ₂	3.09
O ₂	0
H ₂ O	1.42
N ₂	11.54

For the validation of the CI engine the datasheet of a V16 Cummins KTA 50-G9 (Cummins, 2001) stationary engine was used. The engine is turbocharged and intercooled, so a pressure of 300 KPa and 25 °C were assumed. Also, the engine operates with air to fuel ratio of 25, 2:1 (excess air coefficient of 1.7). It is a square engine as both cylinder bore, and piston stroke length presents the value of 159 mm. The compression ratio is 13.9:1. The computed results show that for the brake power, torque and *bmep* are very near those for the actual engine, all of them are below 3%. Again, the great discrepancy occurs in the mechanical efficiency (-22%). The mechanical efficiency is an unique characteristic of an engine, and it must be taken in consideration when this parameter is explained in the class. There are no emissions data available to compare. However, the emissions indexes are shown in Table 4. The pressure x volume, brake power to rpm and torque to rpm curves are shown in Figure 5.

Table 3. Comparison for CI engine

Parameter	FATROMEIO	KTA 50-G9	Difference %
\dot{W}_i [kW]	2313	-	-
\dot{W}_b [kW]	1637	1656	-1.15
T [N.m]	8689	8785	-1.05
<i>bmep</i> [kPa]	2161	2221	-2.70
η_t [%]	49.30	-	-
η_m [%]	70.79	90,79	-22.03
η_v [%]	295	-	-
<i>bsfc</i> [kg/kW.s]	0.230	0.201	14.43

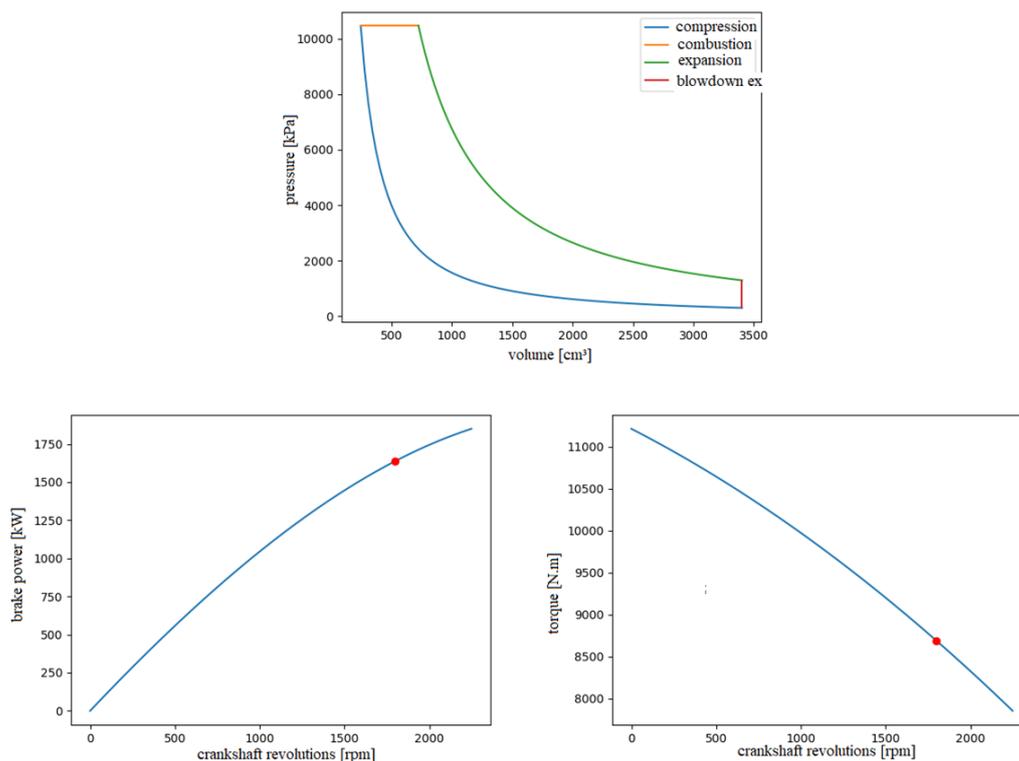


Figure 5. Pressure x volume; brake power x rpm; torque x rpm

Table 4. CI engine emission indexes

Parameter	EI [g/kg _f]
CO ₂	3.10
O ₂	2.45
H ₂ O	1.39
N ₂	19.54

In both simulations it is noticed that the greater discrepancies occur due the mechanical efficiency incertitude. In fact, Eq. 33 represents an approach from a graphical slope show in Pulkrabek (2004). The mechanical efficiency depends on the engine design and the amount of parasite load assembled in the engine. However, its behavior as function of the average piston speed can be demonstrated in the simulations. In despite of these results which depends on the mechanical efficiency, the script shows to be useful for the teaching of the reciprocating engines thermodynamic cycles.

5. CONCLUSION

The program was developed in open-source code and can be used for didactical purposes. Unless the value of the mechanical efficiency and the results that depends on this parameter, both Otto and Diesel mechanical cycles were validated and the differences in the performance parameters which appears between the example engines can be neglected. Despite of the mechanical efficiency accuracy, the behavior of the engine can be show, for teaching objectives, by varying the input conditions and beholding the output parameters. Thus, it can be concluded that:

1. The program computation method was validated for both Otto and Diesel cycles.
2. The program interface is friendly and intuitive.
3. The program is feasible for didactical purposes in teaching of thermodynamic cycles for reciprocating internal combustion engines.
4. The mechanical efficiency is the parameter which presents the greater discrepancy in results.

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