Agronomy Research Biosystem Engineering Special Issue 1, 157-166, 2012

Simulation model of the combustion processes of a diesel engine

V. Mikita[1], J. Roots[2] and J. Olt[1]

[1]Institute of Technology, Estonian University of Life Sciences, Kreutzwaldi 56, EE51014, Tartu, Estonia; e-mail: villu.mikita@emu.ee,
[2]Institute of Economics and Social Sciences, Estonian University of Life Sciences, Kreutzwaldi 56, EE51014 Tartu, Estonia

Abstract. It is foreseen that in the near future in Estonia there will be growth in the consumption of alternative liquid fuels in internal combustion engines. The main share of it will be formed by the local raw material based diesel fuel and ethanol. In connection with this, the choice of fuels and the variety of their qualitative characteristics in filling stations will grow. This kind of situation will give rise to the necessity of creating new quality assessment methods which should be reliable, efficient and economical.

There may be several assessment methods for taking fuel samples. Drivers consider the fuel quality assessment express methods especially valuable. Working out a new method like that is at present also supported by the electronic control system of the engine and the use of digital diagnostic devices.

Creating and implementing the fuel quality assessment express method requires a considerable amount of effort. It includes the evaluation and prognosis of the fuels physical and chemical parameters, designing the simulation models of the engine combustion process pressure and temperature and carrying out the control testing.

Keywords: inside cycles of work processes of diesel engine, phases of the combustion process and their influence parameters, simulation model of computing the combustion process parameters, diesel engine test results.

Introduction

The simulation models of the internal combustion engine working process can be made on the basis of thermal, mathematical and physical parameters' changes. The present paper describes the engine working process simulation model that has been designed according to changes of physical parameters, such as the engine crankshaft angle of rotation; the amount of the injected fuel; cylinder pressure and temperature.

There are basically two stages in designing a simulation model. First a physical model is designed with sufficient accuracy, where certain parameters, e.g. the air-fuel mixture molecular heating value in the combustion process, have been substituted by constants. Next, stand tests are carried out with a selected internal combustion engine. The real values of the test object are determined according to the earlier prescribed conditions. Then the initially chosen constants are corrected and re-computations made. This way the reliability of the designed simulation model is achieved.

It is true that any simulation model includes uncertainty of measurement to some extent. It is even more so in the conditions of developing production technologies and more rigid environmental requirements. When describing the engine combustion process one has to take into account the obligation to direct part of the exhaust gases back to the working process. It is necessary to use extra catalytic converters for the after-treatment of the exhaust gases emitted to the environment. At the same time any additional device in the engine exhaust system is an obstacle for the exhaust gases and changes the conditions of the combustion process in the cylinder - that is, first of all, the parameters of pressure and temperature. A reliable simulation model has to include all the processes mentioned above.

The present paper investigates the changes of the engine input and output parameters values depending on the net calorific value. The methods of calculating the combustion process final pressure and temperature are analyzed and the physical calculation algorithm of the simulation model of compression and power processes parameters is presented. The paper includes comparison diagrams drawn on the basis of the stand tests and computing of the simulation model. The classification of the phases of the combustion process accompanied by the relevant terminology and preference list of the phases influence parameters is given. Possession of the piston engine combustion process simulation model enables to develop a new type of testing environment in future at the Estonian University of Life Sciences which will comply with the labour health regulations and help to save valuable testing resources. In the presence of a reliable working simulation model, the role of stand tests will be reduced. Future studies of the engine combustion process will be carried out on computers. A simulation model of a contemporary internal combustion engine has to enable to determine by computational methods the amount of work done by the fuels used in the combustion process. At the same time the parameters of pressure and temperature arising in the engine and the amount and components of exhaust gases being emitted should be indicated.

At present the authors of the article continue the relevant development activities with the purpose of making the fuels quality assessment express method easy and economical for the customer.

Materials and methods

When preparing a simulation model of the processes evolving over time, an important means is to divide time into parts, which is called time slicing. The values of the examined parameters’ variables are changed within the limits of a single time slice and while calculating a specific variable, the other variables remain constant. For calculating the combustion process simulation model, the time slice is the span during which the engine’s crankshaft changes its position by one degree. For the purpose of this article the following definition is used for characterizing the work of a four-stroke internal combustion piston engine: the cycle of the engine consists of induction, compression, combustion, expansion, and exhaust processes. For the calculations the technical specifications of the engine D–120 are used, which are shown in Table 1. The preparation of the combustion process simulation model is based on the patterns of the compression process pressure, combustion process pressure, and the pattern of the changes in temperature. When preparing a model of the abovementioned processes’ pressures and the changes in temperature, it is presumed that (Merker et al., 2004):

a) the cylinder is closed and does not depend on the changes in the conditions of the outside environment;
b) the working medium used for the combustion process consists of air and diesel fuel;
c) no molecular change of the working medium occurs in the combustion process;
d) the crank angle degree (α_{cr}) is measured with respect to the piston's top dead center (TDC), where $\alpha_{cr} = 0$;
e) the values of the crank angle degree position before and after TDC are respectively negative and positive.

Table 1. Diesel engine D–120 technical specifications

Number of cylinders	2
Cylinder diameter	105 mm
Piston stroke	120 mm
Volume	2.08 liters
Pump fuel delivery	59 ± 2 mm^3 stroke^{-1}
Power	18.4 kW
Maximum torque	99.5 Nm
Pressure ratio	16.0
Nominal rotational speed	1,800 rpm
Maximum torque achieved between	1,260 – 1,400 rpm
Maximum rotational speed	1,950 rpm
Minimal rotational speed	1,260 – 1,400 rpm
Specific fuel consumption	245 g (kWh)$^{-1}$
Fuel consumption nominal	6.37 kg h^{-1}
Fuel consumption on maximum idle	1.9 kg h^{-1}
Cooling system	air-cooled

The simulation model consists of three calculation algorithms: 1) modeling of the compression process pressure and working medium temperature dependent on compression; 2) modeling of the fuel-air mixture combustion process pressure and temperature; 3) modeling of the cooling system's influence on the changes in expansion process pressure and in temperature.

Modeling of the compression process pressure and working medium temperature dependent on compression

During the abovementioned process the parameters for piston movement are the stroke and crank angle degree. We will go through the following calculation algorithm to prepare a simulation model:

We determine the piston's distance from TDC (m) using the following formula:

$$h = \tfrac{S}{2}(1 - \cos\alpha), \qquad (1)$$

where S is piston stroke (m).

We will find out the cylinder total volume (m^3) in the given piston position:

$$V_a = V_c + h \cdot A, \qquad (2)$$

where V_c is the combustion chamber capacity (m^3) and A represents piston area (m^2).

We calculate how much the cylinder total volume changes (m^3):

$$\Delta V_{a.i} = V_{a.i} - V_{a.i-1}, \tag{3}$$

where $V_{a.i}$ represents the cylinder total volume in a given time slice (m^3) and $V_{a.i-1}$ stands for the cylinder total volume in the previous time slice (m^3).

After the intake valve closes as the piston moves towards TDC, the air in the cylinder will become pressurized. The cylinder volume will decrease during this process and the pressure and the temperature will increase.

We will use the Clapeyron formula (Taylor C.F. V1 and V2, 1998) to determine the relation of the changes in capacity, pressure and temperature:

$$p \cdot V = R \cdot T, \tag{4}$$

where p is gas pressure in the cylinder (MPa), V is total cylinder volume (m^3), T is the temperature of gas in the cylinder (K) and R is the universal gas constant.

We will calculate the increase in pressure which occurs during working medium pressurization at the given total volume of $V_{a.i}$ (2), presuming that the temperature does not change:

$$p_{c.1.i} = \frac{R \cdot T_{c.0}}{V_{a.i}}, \tag{5}$$

where $p_{c.1.i}$, $T_{c.0}$, $V_{a.i.}$ are respectively the compression process pressure (MPa), the temperature (K) and the total volume (m^3) of the cylinder in the given time slice.

We will find out the change in the compression process pressure (MPa) due to volume decrease:

$$\Delta p_{c.1.i} = p_{c.1.i} - p_{c.1.i-1}, \tag{6}$$

where $p_{c.1.i}$ is the compression process pressure in the given time slice (MPa) and $p_{c.1.i-1}$ is the compression process pressure of the previous time slice (MPa).

The main formula of one time slice (4) therefore looks like this:

$$(V_a + \Delta V_a) \cdot (p_c + \Delta p_c) = R(T_c + \Delta T_c), \tag{7}$$

where V_a , p_c , T_c are respectively the initial values of the total volume, pressure, and temperature in a specific time slice and ΔV_a , Δp_c , ΔT_c are the respective parameter changes which have occurred in the given time slice.

In case of modeling, the change in the total volume V_a is primary, which is determined by the piston movement position in the cylinder. The value of the latter cannot be changed during the given time slice.

Next we presume that in every elementary time slice the cylinder total volume is constant ($\Delta V_a = 0$). Therefore formula (7) will look like this:

$$V_a(p_c + \Delta p_c) = R(T_c + \Delta T_c), \tag{8}$$

After simplifying, we get:

$$V_a \cdot p_c + V_a \cdot \Delta p_c = R \cdot T_c + R \cdot \Delta T_c \, , \tag{9}$$

Considering that $V_a \cdot p_c = R \cdot T_c$ and that the elements with the same name can (9) be joined, we get:

$$V_a \cdot \Delta p_c = R \cdot \Delta T_c \, , \tag{10}$$

Using formula (10) we can find the value of temperature ΔT_c, as the remaining values are known:

$$\Delta T_{c.1.i} = \frac{\Delta p_c \cdot V_{a.i}}{R} \, , \tag{11}$$

The temperature (K) of the gases which are in the cylinder at the beginning of the next time slice can be found:

$$T_{c.1.i} = T_{c.1.i-1} + \Delta T_{c.1.i} \, , \tag{12}$$

where $T_{c.1.i\text{-}1}$ is the temperature in the cylinder during the compression process of the previous time slice (K) and $\Delta T_{c.1.i}$ represents increase in temperature (K) which occurs in this time slice.

As an increase in temperature by $\Delta T_{c.1.i}$ will cause an increase in pressure during the compression process, an increase in pressure $\Delta p_{c.2.i}$ (MPa) due to the rise in temperature will be calculated considering relations (10) and (11) as follows:

$$\Delta p_{c.2.i} = \frac{R \cdot \Delta T_{c.1.i}}{V_{a.i}} \, , \tag{13}$$

Next we will calculate the total value of the compression process pressure in the cylinder (MPa) at the end of the given time slice. This consists of a rise in pressure in the given time slice, to which the compression process pressure at the beginning of the given time slice will be added:

$$p_{c.i} = p_{c.i-1} + \Delta p_{c.1.i} + \Delta p_{c.2.i} \, , \tag{14}$$

where $p_{c.i\text{-}1}$, $\Delta p_{c.1.i}$ and $\Delta p_{c.2.i}$ are respectively the pressures of the compression process from the previous time slice (MPa), this time slice (MPa) and a rise in pressure in this time slice (MPa), which is caused by a rise in temperature.

The abovementioned operations are repeated when determining a new time slice. The stroke will next increase by Δh, which will cause a decrease in cylinder total volume by ΔV_a. A decrease in the cylinder total volume will apply pressure to the working medium, which in turn causes a rise in pressure $\Delta p_{c.1}$ (5 and 6). The latter will cause a rise in temperature (11). A rise in temperature will in turn cause an increase in pressure $\Delta p_{c.2}$ (12). The final pressure of the compression process will be calculated with formula (13).

The abovementioned method is used to calculate cylinder pressure value during the compression process and the expansion process. After TDC begins the expansion process, the volume gets bigger, the pressure and temperature will decrease. The only difference is that the changes in the pressure and temperature become negative.

Modeling of the fuel-air mixture combustion process pressure and temperature

The basis for the modeling of a piston engine's compression, combustion, and expansion process' pressure and temperature is the main equation (4) of the state of gas in its different variations. The differences can be caused by the various ways fuel-air mixture is formed or combustion takes place. This article is about a diesel engine in which fuel is injected straight into the cylinder. After that the fuel-air mixture will vaporize, ignite and burn, thereby releasing heat. The latter will in turn cause an increase in the temperature and pressure of the gases inside the cylinder.

The modeling of pressure and temperature changes caused by the combustion of fuel-air mixture takes place in the following stages:

Firstly, the amount of fuel which will be added in one cycle is distributed, dependent on the crank angle degree (the piston's position in the cylinder), in parts to single time slices. The amount of fuel (mm^3) which is added in a specific time slice can be calculated as follows:

$$\Theta_{f.i} = \Theta_f \cdot O_i , \tag{15}$$

where Θ_f is the amount of fuel injected into a cylinder during one cycle ($mm^3 cycle^{-1}$) and O_i is the proportion of fuel injected in time slice i.

The parameters Θ_f and O_i can be changed through various versions of modeling.

Secondly, we will model an increase in the temperature of the working medium which has been caused by the combustion of fuel-air mixture and which consists of several stages. The purpose of the division into stages is to give a better picture of how the model works. The modeling of fuel-air mixture combustion takes place with some delay as it takes a certain amount of time before the fuel will vaporize, burn and release heat so the temperature of gas in the cylinder can rise. With various versions of modeling the delay can be changed. The calculation for the rise in pressure and temperature has been presented below, which has been caused by the combustion of fuel-air mixture.

We will find the effective heat (MJ) of the fuel-air mixture injected in a given time slice:

$$q_{k.i} = Q_b \cdot \Theta_{f.i} \cdot \xi_u , \tag{16}$$

where Q_b is diesel fuel's specific heat of combustion ($MJ\ kg^{-1}$), $\Theta_{f.i}$ is the amount of fuel which is added in the time slice, and ξ_u is the actual efficiency.

We will determine the rise in temperature (K) of the gases, which has been caused by the released heat:

$$\Delta T_{2.i} = q_{k.i} \cdot W_a , \tag{17}$$

where W_a is an empirical multiplier, which characterizes the interdependence between the added heat amount and the rise in the temperature of gases inside the cylinder.

Next an equation (4) is used to find an increase in the pressure of the cylinder, which has been caused by a rise in temperature – presuming that the volume remains constant:

$$\Delta p_{z.3.i} = \frac{R \cdot \Delta T_{z.2.i}}{V_{a.i}} \tag{18}$$

Considering that the temperature and pressure of the gases inside the cylinder – and therefore also the total pressure (MPa) and temperature (K) – will change, the following relations can be seen:

$$T_{z.i} = T_{z.i-1} + \Delta T_{z.1.i} + \Delta T_{z.2.i}, \tag{19}$$

where $T_{z.i-1}$, $\Delta T_{z.1.i}$ and $\Delta T_{z.2.i}$ are respectively previous time slice's working medium's total temperature (K), the change in the temperature of the working medium caused by compression (K), and the change in the temperature of the working medium caused by fuel-air mixture combustion (K);

$$p_{z.i} = p_{z.i-1} + \Delta p_{z.1.i} + \Delta p_{z.2.i} + \Delta p_{z.3.i}, \tag{20}$$

where $p_{z.i-1}$, $\Delta p_{z.1.i}$, $\Delta p_{z.2.i}$ and $\Delta p_{z.3.i}$ are respectively previous time slice's working medium's total pressure (MPa), rise in the pressure of the working medium caused by compression (MPa), rise in the pressure of the working medium caused by temperature from compression (MPa), and rise in the pressure of the working medium caused by temperature from fuel-air mixture combustion (MPa).

The aforementioned formulas (19 and 20) are used to determine the changes in the cylinder pressure and the temperature of gases dependent on the added fuel. The presented model presumes that the working medium of the compression stroke is air and that in the combustion process vaporized diesel fuel will be added. In the current stage of the simulation model the molecular change of the working medium has not been considered. The latter characterizes the amount of exhaust gases, crankcase gases, and gases redirected to the current combustion cycle from the previous work process in an actual working medium. Therefore the values of the actual combustion mix gas constant R are different (Lide, 2010). At the moment $R = R_z$

Modeling of cooling system's influence on changes in the expansion process pressure and temperature

Besides the influence the change in the amount of heat caused by working medium compression and combustion of diesel fuel has on the change in the pressure and temperature of the cylinder, the environment of the working medium inside the cylinder also depends on the efficiency of the cooling system. In the expansion process, where the fuel-air mixture combustion takes place in the conditions of an increasing total volume, the cylinder's temperature and pressure decrease quickly. Besides the abovementioned, the working medium's parameters are also altered by the heat transferred from the cooling system. As a result of the latter, the pressure and temperature of the gases inside the cylinder will drop. Therefore it is necessary to consider the influence of the cooling system when modeling the pressure and temperature for the combustion process and the expansion process.

For this model the cylinder's pressure and temperature of the gases are most important. When calculating the cooling process, the temperature decrease in the gases and the pressure drop of the cylinder are primary.

It is important to determine during modeling the decrease in the temperature of the gases (K) in the cylinder for every time slice – for that purpose the following formula can be used:

$$\Delta T_{z.3.i} = T_{z.i} \cdot \zeta_a , \tag{21}$$

where ζ_a is a multiplier, which characterizes the temperature decrease in the gases inside the cylinder caused by the cooling system.

The temperature decrease in turn will cause the cylinder's pressure (MPa) to drop:

$$\Delta p_{z.4.i} = \frac{R_z \cdot \Delta T_{z.3.i}}{V_{a.i}} , \tag{22}$$

where R_z is the gas constant (MJ(kmol·K)$^{-1}$ of the working medium (Bosch, 2011).

Considering that the temperature and the pressure of the gases change inside the cylinder, the total temperature (K) and pressure (MPa) in time slice *i* can be expressed as follows:

$$T_{z.i} = T_{z.i-1} + \Delta T_{z.1.i} + \Delta T_{z.2.i} + \Delta T_{z.3.i} , \tag{23}$$

where $T_{z.i-1}$, $\Delta T_{z.1.i}$, $\Delta T_{z.2.i}$ and $\Delta T_{z.3.i}$ are respectively previous time slice's working medium's total temperature (K), change in the temperature of the working medium caused by the decrease in compression (K), change in the temperature of the working medium caused by a drop in the intensity of fuel-air mixture combustion (K), and temperature decrease caused by the cooling system (K);

$$p_{z.i} = p_{z.i-1} + \Delta p_{z.1.i} + \Delta p_{z.2.i} + \Delta p_{z.3.i} + \Delta p_{z.4.i} , \tag{24}$$

where $p_{z.i-1}$, $\Delta p_{z.1.i}$, $\Delta p_{z.2.i}$, $\Delta p_{z.3.i}$ and $\Delta p_{z.4.i}$ are respectively previous time slice's working medium's total pressure (MPa), decrease in the pressure of the working medium caused by the decrease in compression (MPa), decrease in the pressure of the working medium caused by a decrease in temperature due to a decrease in compression (MPa), decrease in the pressure of the working medium caused by a decrease in temperature due to a drop in the intensity of fuel-air mixture combustion (MPa), and the pressure decrease caused by the cooling system (MPa).

By using formulas (23) and (24), it is possible to model sufficiently accurately the internal pressure of the cylinder and the temperature of gases, depending on the work of the cooling system.

Results and discussion

Using the simulation model presented in this article the characteristics of the diesel engine's parameters of compression, combustion, and expansion processes have been developed. For the calculations the technical specifications of the D−120 test engine were used. Fig. 1 shows the D−120 diesel engine's combustion process characteristics from calculations and from test results. The imaginary zero point of the combustion process axis x (Heisler, 2001) in the figure is the TDC of the previous cycle.

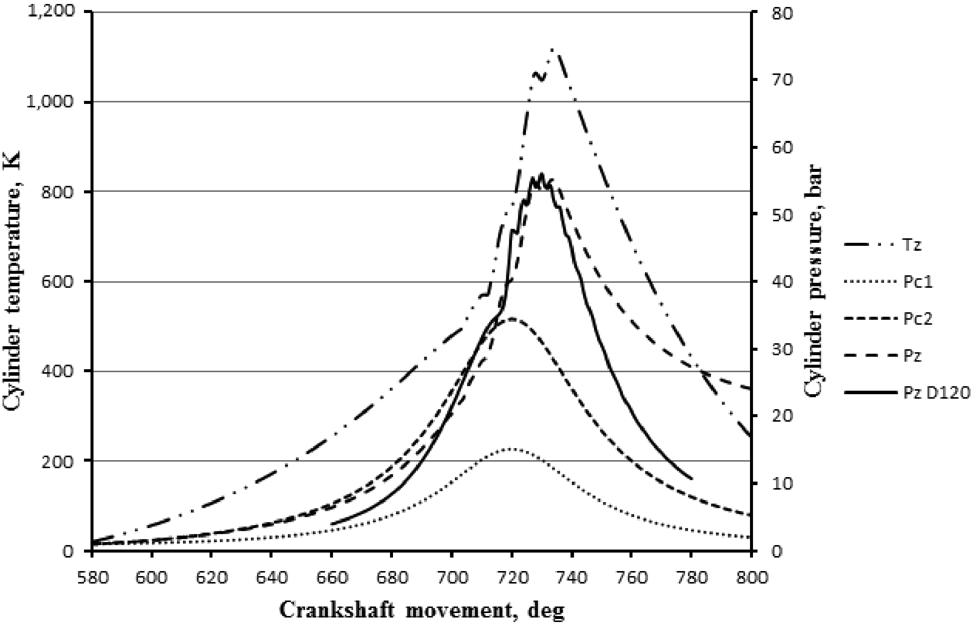

Fig. 1. The D−120 diesel engine's pressure and temperature parameters: Broken line – calculated value; continuous line – measured value; T_z – temperature of gases inside the cylinder; P_{c1} – cylinder pressure respective to the engine's pressure ratio; P_{c2} – engine compression; P_z – pressure of gases inside the cylinder obtained from the simulation model; P_{zD120} – pressure of gases inside the cylinder measured during tests.

The results of the research:

1. The difference between the theoretical and the actual characteristics depends on the physico-chemical properties of the studied fuel and the engine's workload and speed modes.
2. The combustion process pressure (P_z) calculated with the simulation model does not differ much from the pressure measured with bench testing (P_{zD120}) during the induction phase, but differs to a great extent during the afterburning phase.
3. During the induction phase the calculated cylinder pressure is greater than the actual pressure because the model does not consider the exhaust gases of the previous work process when preparing a working medium.
4. During the afterburning phase the calculated and the actual cylinder pressure is different because in a real combustion process the working medium's composition is altered and the authors do not yet have the experience for calculating it.

Conclusions

1. The computing algorithm presented in the article proves that the authors' methodology for preparing the simulation model is correct in principle.
2. This research is the first stage for developing the simulation model.
3. When improving the model's computing algorithm, the following has to be considered:
    a) influence of the engine's workload and speed mode;
    b) molecular change of the working medium inside the cylinder.
4. The authors of this paper have concluded that this research will hold great theoretical and practical value in the future and therefore will continue their work on the subject.
5. The simulation models of the internal combustion engine working process can be made on the basis of thermal, mathematical and physical parameters' changes.
6. In future, it is necessary to calculate extra catalytic converters for the after-treatment of the exhaust gases emitted to the environment.

References

Merker, G., Schwarz, Ch., Stiesch, G., Otto, F. 2004 Verbrennungsmotoren. Simulation der Verbrennung und Schadstoffbildung, Auflage 2. Wiesbaden, pp. 412.

Taylor, C. F. 1998. The internal-combustion engine in theory and practice: **1**, Thermodynamics, fluid flow, performance, pp. 574 and **2**: Combustion, Fuels, Materials, Design pp. 783, The Massachusetts Institute of Technology. 9-th printing. England.

David, R. Lide. 2010. CRC Handbook of Chemistry and Physics. Taylor & Francis Group. **90**-th edition, pp. 2475.

Robert Bosch GmbH. 2011. Bosch Automotive Handbook, 8 th edition, pp. 1460.

Heisler, H. 2001. Advanced engine technology. Butterworth-Heimann, Oxford, pp.794.