The determination of the rate of heat release in the diesel cylinder taking into account the change in the composition of the working substance

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Abstract. The thermodynamic efficiency of the cycle of the internal combustion engine and its efficiency are related to the law of supply of heat to the working fluid. The characteristics of heat release allow us to evaluate and improve the combustion process from the point of view of the thermodynamic efficiency of the cycle, from thermodynamic positions. To optimize the combustion process in compression-ignition engines, including when working on unconventional fuels, it is necessary to develop an algorithm for determining the rate of heat release, taking into account the current composition of the working fluid, since when working on fuels with a changed chemical composition, the ratio of gases in the combustion products can significantly change. The type of heat dissipation characteristic is determined by the regularities of the combustion of fuel in the cylinder and the law of displacement of the piston and depends, inter alia, on the composition of the working fluid, which continuously changes during combustion of diesel fuel, increasing volume and mass. Existing methods for calculating the heat dissipation characteristics consider a working body consisting of two components - a fresh charge and combustion products. Such an approach reduces the accuracy of calculations when determining the heat input from the diesel fuel indicator chart operating on fuels with modified chemical composition or on non-traditional fuels, since it does not take into account the change in the heat capacity and internal energy of the combustion products. In this article, a mathematical model to compute the heat dissipation in the cylinder of a diesel engine when operating on diesel fuel for the changes in the working fluid composition. The presented results of calculations for a diesel engine of 2CH10.5/12.0 when operating on diesel fuel at the nominal operating mode correspond to the results of the determination of the integral and differential heat dissipation rate obtained by the well known CNIDI method.

1. Introduction

Increase of thermodynamic efficiency of the internal combustion engine cycle, is an important research direction. This allows to solve problems of fuel efficiency and increase the efficiency of the indicator and efficient power plants. Indicator performance of the diesel directly depends on the organization of the combustion process and, ultimately, on the characteristics of heat supply to the working body (WB). The type of heat dissipation characteristic is evaluated on the basis of the desire to increase the efficiency and operation of the cycle and to obtain an acceptable maximum rate of rise in pressure, maximum pressure and temperature of the cycle [1-4]. The law and rate of heat release in each phase are determined by the features of the fuel supply and mixture formation process, the
chemical composition and physical and fuel properties, the organization the movement of air charge, the
design and features of the combustion chamber. To optimize the parameters that influence the
combustion process in the diesel cylinder, it is necessary to establish a connection and to ensure the
accuracy and simplicity of calculation of the heat dissipation characteristics by the indicator diagram,
taking into account the composition of the fuel and WB in the combustion process.

2. Experimental part
The working body in the combustion chamber (CC) of the diesel engine represents a mixture of gases
whose volume fractions continuously change during combustion. As the combustion of fuel injected
into the combustion chamber changes, the mass of the WB changes. It can be simplified to imagine
that the WB to the beginning of the combustion process consists of air and residual gases, and as the
fuel burns in the WB, the concentration of products of complete combustion - CO₂ and H₂O -
increases.

According to the first law of thermodynamics, the supplied heat \( Q \) to WB is consumed by changing
the internal energy \( U \) of the gas and by making the gas work \( L \) [5-7]:

\[
dQ = dU + dL.
\]

The internal energy of the gas mixture can be defined as the sum of products by expression [8]:

\[
U = \sum M_i \cdot C_{vi} \cdot T
\]

where \( M_i \) is the number the \( i \)-th gas in the WB; \( C_{vi} \) is the average molar heat capacity of gases at
constant volume, J/mole·K; \( T \) is the temperature of WB, K.

The average molar heat capacity is a function of temperature and is determined from the reference
data (figure 1). It can be seen from the figure that the heat capacity of gases increases with the increase
in the molar mass of the gas, therefore, with a high concentration of unburned hydrocarbons in the
exhaust gases of the diesel engine, neglecting their content in the WB leads to a significant error in
determining the internal energy of the combustion products.

![Figure 1. Heat capacity of gases that make up WB.](image)

The temperature of the gases can be determined from the equation, by the CNIDI method [10]:

\[
T = \frac{P \cdot \varepsilon \cdot T_a}{P_a \cdot \varepsilon_a},
\]

where \( P_a \) and \( T_a \) are the pressure and temperature at the end of the inlet; \( \varepsilon \) is the function of the
degree of compression in the angle of rotation of the crankshaft of the diesel engine; \( \varepsilon_a \) is the
compression ratio at the end of the intake.

If the pressure at the end of the intake can be determined from the indicator diagram, the
temperature of the working fluid at the time of closing the exhaust valve can only be set approximately
by measuring the temperature of the air at the inlet, taking into account the charge heating due to heat exchange with the diesel parts. The temperature of the WB can also be determined using the indicator diagram and the cylinder volume change equation depending on the angle of rotation of the crankshaft.

The mixture of gases obeys the equation of state [9]:

$$T = \frac{PV}{GR},$$

(4)

where $P$ is the gas pressure in the cylinder, Pa; $V$ is the volume of the cylinder, m$^3$; $G$ is the mass of the WB, kg; $R$ is the gas constant of the gas mixture, J/kg·K.

The gas constant of a mixture of gases is equal to the sum of the products of the mass fractions of each gas by its gas constant:

$$R = \sum g_i \cdot R_i,$$

(5)

where $g_i$ is the mass fraction of the $i$-th gas; $R_i$ is the gas constant of the $i$-th gas J/kg·K.

The mass fraction of gas in the mixture, like the mass of WB, varies during combustion, i.e. is a function of the angle of rotation of the crankshaft of the diesel engine. If the composition of the fuel is given by the mass fractions of the atoms, then when it is taken into account that the fuel consists of only carbon atoms $C$, hydrogen $\text{H}$ and oxygen $\text{O}$, we can write the Equation:

$$C + H + O = 1$$

(6)

Then the amount of combustion products in the WB wells defined by the Equation:

$$M_{\text{H}_2\text{O}} = \frac{q \cdot H}{2 \cdot m_H}$$

(7)

$$M_{\text{CO}_2} = \frac{q \cdot C}{m_C}$$

(8)

where $m_H$, $m_C$ are molecular weight hydrogen and carbon, respectively, g/mole.

Assuming that the air charge consists of 0.21 parts by volume of $\text{O}_2$ and 0.79 parts of nitrogen $\text{N}_2$, then the moles required for combustion of the incoming charge will be determined by the equation:

$$M_0 = \frac{q}{0.21} \left( \frac{C}{12} + \frac{H}{4} - \frac{O}{32} \right).$$

(9)

The theoretical coefficient of molecular variation of the mixture during the cyclic supply of fuel $q$ is determined from the Equation:

$$\beta_0 = 1 + \frac{8H + O}{32\alpha \cdot M_0}$$

(10)

where $\alpha$ is the excess air factor.

We accept the rate of formation of products of complete combustion proportional to the rate of heat release, then the functions of the components of the WB depending on the angle of the crankshaft rotation with the contents of residual gases in the cylinder can be determined by the Equations:

$$(M_{\text{H}_2\text{O}})_x = M_{\text{H}_2\text{O}} \left( x + \frac{\gamma}{\beta_0} \right)$$

(11)

$$(M_{\text{CO}_2})_x = M_{\text{CO}_2} \left( x + \frac{\gamma}{\beta_0} \right)$$

(12)
$$\left( M_{N_i} \right)_o = 0.79M_o \left( \alpha + \frac{\chi}{\beta} \right);$$  \hspace{1cm} (13)

$$\left( M_{\alpha_i} \right)_o = 0.21 \cdot M_o \left( \alpha + \frac{\chi}{\beta} \right) - \left( x + \frac{\chi}{\beta} \right);$$  \hspace{1cm} (14)

where $\gamma$ is the coefficient of residual gases; $\chi$ is the integral characteristic of fuel burn up in the combustion chamber of a diesel engine.

Setting the temperature as a function of the gas composition leads to unnecessary complication of the analytical determination of the rate of heat release. In this case, the internal energy of the WB will be determined by the equation:

$$U = \frac{PV \cdot \sum M_i \cdot C_u}{\sum M_i \cdot m_i \cdot R_i}.$$  \hspace{1cm} (15)

The main difficulty is to determine the heat capacity of the gas mixture components, provided that the heat capacity of the gases is a function of temperature, and therefore depends on the total gas composition in the cylinder. To simplify the expression for the derivative of internal energy, the temperature WB will be determined from the characteristic equation without taking into account the change in the composition of the gas mixture. To do this, we determine the pressure of the gases at the end of the compression by the indicator diagram and, knowing the mass of the WB and the current volume of the cylinder at the end of compression, we determine the temperature of the gases $T_u$. Then the derivative of the internal energy is determined:

$$dU = dT \cdot \sum M_i \cdot C_w + T \left( \sum M_i \cdot C_w + \sum C_w dM \right)$$  \hspace{1cm} (16)

The work of the cycle can be determined from the detailed indicator diagram for the differential Equation:

$$dL = \frac{V_i \cdot P \cdot \left( \sin \varphi + \frac{\lambda}{2} \sin 2\varphi \right)}{2}.$$  \hspace{1cm} (17)

where $\lambda$ is the ratio of the length of the connecting rod to the radius of the crank.

Part of the heat released during the combustion allotted through the cylinder wall due to convective heat transfer, can be approximately estimated from the differential equation [10,11]:

$$dQ_w = (a_2 + a_3 \cdot \varepsilon) \cdot \sqrt{P \cdot T \cdot (T_w - T)}$$  \hspace{1cm} (18)

where $Q_w$ is the heat removed from the WB due to heat exchange with the walls of the combustion chamber; $a_2, a_3, \varepsilon$ are design parameters of the engine; $T_w$ is the average equivalent wall temperature.

$$a_2 = \frac{0.234 \cdot 10^{-4} \cdot C_e \cdot (S \cdot n)^{\frac{1}{2}} \cdot D^2}{n}$$  \hspace{1cm} (19)

where $C_e$ is the heat transfer coefficient; $S$ is stroke of the piston; $n$ is rotational speed of the crankshaft of a diesel engine; $D$ is the diameter of the piston.

$$a_3 = \frac{2 \cdot a_2 \cdot S}{(\varepsilon_0 - 1) \cdot D}$$  \hspace{1cm} (20)

We define the derivatives of the functions for changing the composition of gases, then taking into account the heat exchange with the walls of the cylinder, the first law of thermodynamics can be written down:
\[ dQ = dL + dT \cdot \sum M_i C_{W_i} + T \cdot \sum M_i dC_{W_i} + dx \cdot T \left( C_{cc_i} \frac{q \cdot C}{m_c} + C_{atf,o} \frac{q \cdot H}{2 \cdot m_H} - 0.21 \cdot C_{atf,o} \cdot M_0 \right) - dQ_w \]  

(21)

The amount of heat supplied to the WB per cycle is determined by the product of the calorific value of the fuel and the value of the cyclic feed. We divide both sides of the equation by the heat supplied to the WB, and express the derivative of the combustion rate of the fuel. Then the rate of heat release for PT, consisting of the components listed above, is determined by the Equation:

\[
x = \frac{dL + dT \cdot \sum M_i C_{W_i} + T \cdot \sum M_i dC_{W_i} - q \cdot H \cdot dQ_w}{q \cdot H \cdot -T \left( C_{cc_i} \frac{q \cdot C}{m_c} + C_{atf,o} \frac{q \cdot H}{2 \cdot m_H} - 0.21 \cdot C_{atf,o} \cdot M_0 \right)}
\]

(22)

3. Results and considerations

Calculation of the heat release rate was performed for a diesel engine of 2CH×10.5/12.0 when operating on diesel fuel (DT) and compared with the result of calculation using the CNIDI method.

As a result of the numerical solution of equation 22 by the Runge-Kutta method, we find the rate of heat supply to the WB and the rate of change in the composition of WB by the derivatives of equations (11), (12) and (14). The volume concentrations of the WB components can be determined by the Equation (23) and are shown in figure 3.

\[ r_i = \frac{M_i}{\sum M_i} \]

(23)

Change in moles \( N_2 \) when forming both nitrogen oxides and other chemical compounds in this model is not taken into account, however, the volume concentration of \( N_2 \) falls with the release into the mixture of products of complete combustion. Since the content of water vapor and \( CO_2 \) in the air is small, the concentration of products of complete combustion of the beginning of the calculation determined on their content in the residual gases.

The current mass of the WB in the cylinder \( G \) will be equal to the sum of the products of the molar mass per mole of the i-th component:

\[ G = \sum M_i \cdot m_i \]

(24)

Taking into account Equations (4) and (5), the average temperature of the gases in the cylinder is determined:

\[ T = \frac{PV}{\sum M_i \cdot m_i \cdot R_i} \]

(25)
Figure 4 shows the results of calculation of the WB temperature by the CNIIDI Equation and by Equation (25), taking into account the change in the gas composition.

The error in the measurement and the mass of the air charge in the cylinder and the excess air ratio in the cylinder leads to an increase in the temperature difference defined by Equations (3) and (15), and error calculation WB internal energy and heat release rate. Therefore, after calculating the current gas composition in the cylinder, it is necessary to reconcile the calculations for the averaged WB temperature.

The results of calculating the heat release rate were compared with the results of determining the heat dissipation characteristic from the indicator diagram by the known CNIDI technique (figure 5). As we see in the figure, the characteristic sections of homogeneous and diffusive combustion, calculated by different methods, completely coincide. However, in the phase of burn-out of fuel portions, the heat release rate and the integrated characteristic calculated from the presented model are lower. This may be due to the difference in the heat capacities of the combustion products and the absence in the presented model of accounting for a mole of unburned hydrocarbons in the WB in the afterburning phase and further expansion.

![Figure 5. Integral and differential heat dissipation characteristics.](image)

4. Summary
The presented technique allows to estimate more accurately the combustion process in the diesel cylinder, including when working on unconventional fuels and fuels with a changed chemical composition, and to assess the effect of fuel composition and composition of WB on the indicator performance of the diesel engine, the heat dissipation characteristics.

Using the techniques presented can be determined I ratio of heat wasted on the work cycle, heat dissipation and a change in energy Cored oil WB with a predetermined gas composition, determine the influence of composition of exhaust gases indicated efficiency.

The rate of heat release during operation of a diesel engine by a diesel engine, calculated by the proposed method, is identical to the heat release characteristic determined by the known CNIDI technique, and therefore can be used for analysis of the combustion process.

Of considerable interest is the possibility of refinement of the proposed model by taking into account the evaporated fuel and other gases formed in the cylinder of the diesel engine in the combustion process as part of the WB, also by clarifying temperature WB in various areas of the CC, as well as taking into account the products of incomplete combustion of hydrocarbon fuel.

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