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STUDY OF THERMOPHYSICAL DYNAMICS IN BIOFUEL DROPLET ATOMIZATION AND COMBUSTION

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Abstract. *The article presents a study of computer modeling of thermophysical processes occurring during atomization and turbulent combustion of biofuel (biodiesel) droplets in the combustion chamber of a direct injection engine. For this purpose, a complex computer model was developed, including mathematical, spatial, and numerical submodels for calculating a complex turbulent reacting flow. Using the developed model, computational experiments were performed to investigate the thermal and aerodynamic properties of the reacting fuel-air mixture of biodiesel, focusing on the effects of temperature and pressure variations in the combustion chamber. The research results made it possible to obtain a visualization of the reacting flow with temperature and concentration characteristics of harmful emissions during biodiesel combustion. The numerical data obtained during the modeling were compared with the results for traditional diesel fuel.*

Keywords: bioenergetics, biofuel, atomization, complex model, common rail system, visualization, harmful emissions.

1. Introduction

Biodiesel production is experiencing rapid growth globally, driven by the increasing demand for eco-friendly fuels. Derived from vegetable oils, animal fats, or waste, biodiesel is a renewable energy source. Key producers include the United States, Brazil, Germany, and Indonesia, where transesterification technologies are employed to convert oils into biodiesel [1-4]. The widespread adoption of biodiesel plays a crucial role in reducing dependence on fossil fuels and cutting greenhouse gas emissions, thereby contributing to the improvement of the global environmental landscape.

Biodiesel production in Kazakhstan is developing in response to the growing interest in renewable energy sources and environmentally friendly technologies. The country has significant agricultural potential, which allows the use of vegetable oils such as rapeseed and sunflower oil, as well as agricultural waste, to produce biodiesel. Biodiesel in Kazakhstan is used in such industries as transport and energy, helping to reduce dependence on fossil fuels and improve the environmental situation. However, the development of this sector faces several challenges, including high initial costs, insufficient infrastructure, and the lack of full legislative support. Nevertheless, given global trends in the field of ecology and energy, Kazakhstan is actively working to improve biodiesel production technologies and create conditions for its widespread implementation in the future.

In 2013, specific targets were set for the development of the renewable energy sector, which made it possible to determine the market size and potential for reducing greenhouse gas emissions. Within the framework of the Concept of Kazakhstan's Transition to a "Green" Economy and the "Kazakhstan-2050

Strategy", the desire was set to increase the share of alternative and renewable energy sources in the country's energy balance to 15% by 2030 and to 50% by 2050 (Figure 1) [5].

In this regard, BioOperations LLP is the flagship for deep grain processing in Kazakhstan. The company produces high-tech products: biodiesel, bioethanol, wheat gluten, and starch. The products are certified by FSSC 22000 and ISCC, and exported to India, the USA, Colombia, Norway, the CIS countries, and the EU. The plant is the largest producer of gluten and starch in Kazakhstan and bioethanol in the CIS [6].

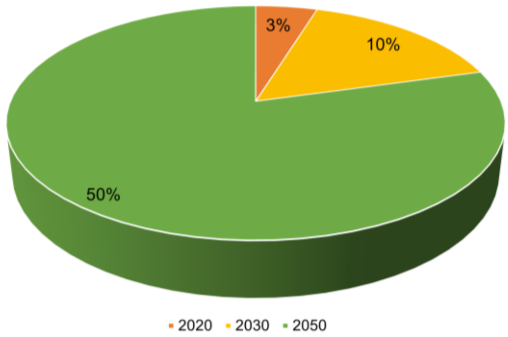

Fig.1. Development of renewable energy sources in Kazakhstan [5]

In this work, the thermophysical processes of atomization and combustion of biodiesel droplets in the model chamber of a direct injection engine are studied. Based on the developed complex computer model, studies of the thermal, aerodynamic, and concentration characteristics of biodiesel droplets during their spraying in a reacting flow were carried out.

2. Mathematical, spatial and physical models of the problem

The mathematical model of liquid fuel droplet combustion includes equations of continuity, momentum, energy, and concentration of reacting components in a two-phase flow [7-9].

The continuity equation for the gas phase of a dispersed system has the following form:

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \mathbf{u}) = S_{mass}, \tag{1}$$

where u fuel drop velocity, S_{mass} is a local change in gas density caused by evaporation or condensation processes in a two-phase flow.

The equation of conservation of momentum for a gas is written as follows:

$$\rho \frac{\partial u}{\partial t} + \rho(\mathrm{grad}\mathbf{u})\mathbf{u} = \mathrm{div}\xi + \rho \mathbf{g} + S_{mom}, \tag{2}$$

where S_{mom} represents the local rate of change of momentum in the gas phase caused by the movement of droplets.

The equation for the conservation of internal energy has the following form:

$$\rho \frac{\partial E}{\partial t} = \boldsymbol{\tau}:\mathbf{D} - \rho \mathrm{div}\mathbf{u} - \mathrm{div}\mathbf{q} + S_{energy}, \tag{3}$$

where **q** is the specific heat flux corresponding to Fourier's law of heat transfer, and S_{energy} means the contribution to the change in internal energy caused by the sprayed liquid or phase.

The equation for the conservation of concentration of component m is written in the following form:

$$\frac{\partial(\rho c_m)}{\partial t} = -\frac{\partial(\rho c_m u_i)}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\rho D_{c_m} \frac{\partial c_m}{\partial x_i}\right) + S_{mass}, \tag{4}$$

where ρ_m is the mass density of a component m, which denotes the amount of mass of this component contained in a unit volume, ρ is the total mass density, which is the sum of the masses of all components contained in a unit volume of the systemю

The k-ε turbulence model is used to simulate turbulent flow in various engineering problems, including fuel-air mixtures. In this model, two transport equations describe the turbulent kinetic energy (k) and its dissipation (ε), which allows the prediction of turbulence parameters such as the velocity and distribution of turbulent flows [10, 11]:

$$\rho\frac{\partial k}{\partial t}+\rho\frac{\partial \overline{u}_j k}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]\frac{\partial \overline{u}_i}{\partial x_j}+G-\frac{2}{3}\rho k\delta_{ij}\frac{\partial \overline{u}_i}{\partial x_j}-\rho\varepsilon, \quad (5)$$

$$\rho\frac{\partial \varepsilon}{\partial t}+\rho\frac{\partial \overline{u}_j \varepsilon}{\partial x_j}-\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]=c_{\varepsilon_1}\frac{\varepsilon}{k}G-\left[\left(\frac{2}{3}c_{\varepsilon_2}-c_{\varepsilon_3}\right)\rho\varepsilon\delta_{ij}\frac{\partial \overline{u}_i}{\partial x_j}\right]-c_{\varepsilon_2}\rho\frac{\varepsilon^2}{k}. \quad (6)$$

Constant parameters of the calculation model, such as c_{ε_1}, c_{ε_2}, c_{ε_3}, σ_k, σ_ε, are typically determined through experimental methods [12]. This is important for more accurate modeling of combustion, fuel atomization, and aerodynamic characteristics in engines.

In this study, a prototype of the common rail fuel injection system, commonly employed in modern diesel engines, was utilized. In such a system, fuel is supplied under high pressure to a common manifold, from where it is evenly distributed to the injectors, which spray it into the combustion chamber. This fuel system refers to direct injection injectors with multiple holes. The schematic design of this system is shown in Figure 2 [13]. Due to the precise dosage of fuel and the ability to change the injection time, the common rail system allows the reduction of harmful emissions such as nitrogen oxides and carbon compounds, which helps to comply with environmental standards.

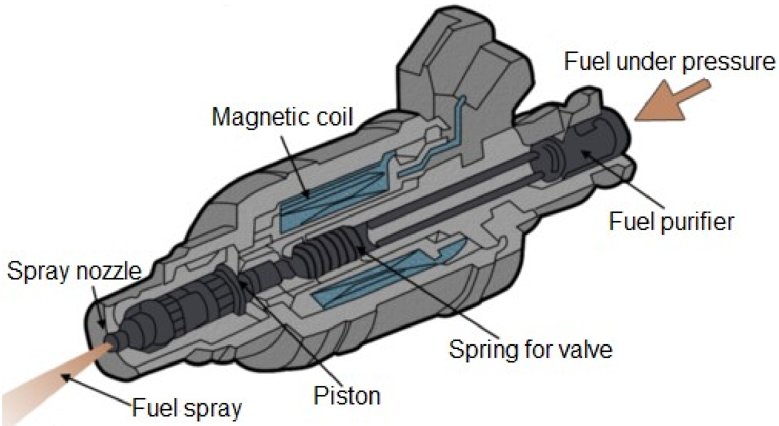

Fig.2. The cross-section of a common rail fuel injector [13]

The system uses a fuel filter to clean the fuel before it enters the system, and a high-pressure cylinder pump to increase the fuel pressure needed for the injectors to operate properly. All these components work together to ensure optimal combustion, increased power, and minimized harmful emissions in modern diesel engines. The CHEMKIN program was used to model the chemical kinetics of biodiesel combustion, which allows the creation of a reaction mechanism that describes the thermodynamics and kinetics of biodiesel combustion, as well as the interaction of fuel with an oxidizer [14, 15]. The system takes into account such parameters as temperature, pressure, and flow rate, which allows for accurate modeling of the combustion process, including the formation of pollutants (CO, CO_2) and evaluation of combustion efficiency.

In this work, pure rapeseed biodiesel Biofuel RME B100 was used as biofuel, which is a mixture of fatty acid methyl esters (FAME) obtained from rapeseed oil. The main component is methyl oleate ($C_{19}H_{36}O_2$) - a monounsaturated ester, which makes up to 90% of the total composition, with admixtures of saturated and polyunsaturated esters. The use of RME in the conditions of Kazakhstan is justified, since it has increased resistance to low temperatures, which is critically important for the northern regions of the country. In addition, the agroclimatic resources of Kazakhstan are favorable for growing rapeseed, which makes RME production sustainable and economically feasible at the national level.

Dodecane ($C_{12}H_{26}$) was used as a model diesel fuel because its combustion characteristics, as well as its physicochemical properties such as boiling point, viscosity and cetane number, are closest to those of biodiesel among simple hydrocarbons. Due to these properties, dodecane is widely used in research as a reference compound for modeling combustion processes of diesel fuel.

The equations for the complete combustion of biodiesel and petroleum diesel fuel under internal combustion engine conditions with the participation of air are presented as follows:

$$C_{19}H_{36}O_2+27O_2+101,52N_2=19CO_2+18H_2O+101,52N_2,$$

$$C_{12}H_{26}+18.5O_2+69.56N_2=12CO_2+13H_2O+69.56N_2.$$

In the engine, biodiesel burns with the formation of CO_2 and H_2O, releasing thermal energy sufficient for its operation, but having a slightly lower energy density compared to petroleum diesel fuel.

For comparison purposes, Table 1 presents the values of the physicochemical characteristics of the fuels (biodiesel and diesel fuel) used in the computational experiments [12].

Table 1. Physicochemical characteristics of biodiesel and diesel fuel

Parameter	Diesel fuel	Biodiesel
Chemical formula	$C_{12}H_{26}$	$C_{19}H_{36}O_2$
Chemical class	alkanes (paraffins)	esters (methyl esters)
Flash point	46°C	130°C
Viscosity (at t=20°C)	1.3–1.5 cSt	4.0–5.0 cSt
Density (at t=15°C)	0.752–0.765 g/cm^3	0.86–0.88 g/cm^3
Surface tension (at t=20°C)	~26.0–28.0 mN/m	~30.0–32.0 mN/m
Cetane number	52	52
Compression ratio	18	18

3. Modeling results and analysis

This paper presents a comprehensive study of computer modeling of the thermophysical processes of atomization and combustion of biodiesel droplets in a model combustion chamber. A comparatives analysis is conducted aimed to determine the efficient fuel combustion parameters that ensure maximum combustion efficiency. Figure 3 shows the temperature distribution of biodiesel and petroleum diesel droplets at 50 mm from the injector nozzle. The results of computer modeling showed that the maximum combustion temperature of the biodiesel fuel-air mixture reaches approximately 3000 K, while the highest combustion temperature of diesel fuel does not exceed 1400 K [16]. From these data, it follows that biodiesel has a significantly higher combustion temperature, which can lead to higher combustion efficiency and heat transfer. Because biodiesel has a high flash point, which makes it safer to handle than conventional diesel fuel.

During the study of the distribution of aerodynamic characteristics of fuels depending on the pressure in the combustion chamber, it was found that with increasing pressure, the velocities of biodiesel and diesel droplets also increase. It follows that an increase in pressure in the combustion chamber contributes to an increase in the droplet velocity, which can affect the combustion process and the efficiency of the heat engine. The results of computational experiments showed that at a pressure of 60 bar, the maximum velocity of biodiesel droplets reaches 33 m/s, while diesel droplets have a velocity of 25 m/s, which confirms the greater mobility of biodiesel droplets (Figure 4).

Increasing the pressure and temperature in the combustion chamber increases the speed of the fuel droplets. This can affect the atomization, mixing, and combustion processes of the fuel. Biodiesel has greater droplet mobility, confirmed by a higher droplet speed. This indicates better atomization and more efficient mixing with air, which can improve combustion processes and lead to more complete combustion. Also, the efficiency of a heat engine can be improved when using biodiesel due to better atomization of the droplets, which contributes to more efficient combustion of the fuel and, possibly, to a reduction in carbon emissions and other harmful substances.

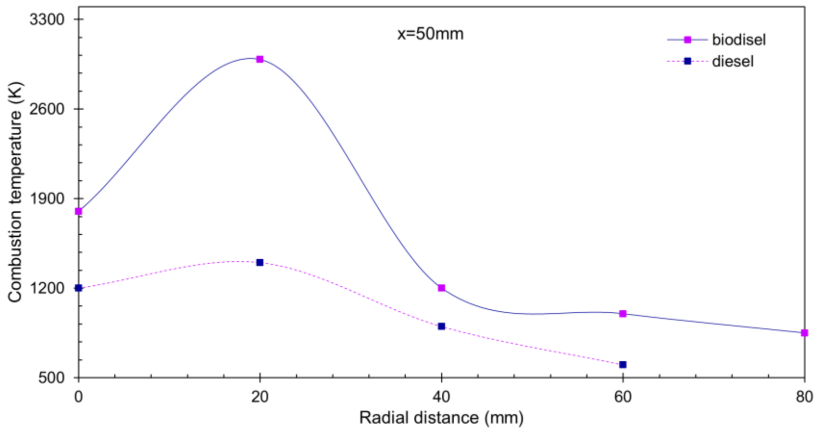

Fig.3. Combustion temperature distribution of fuel droplets

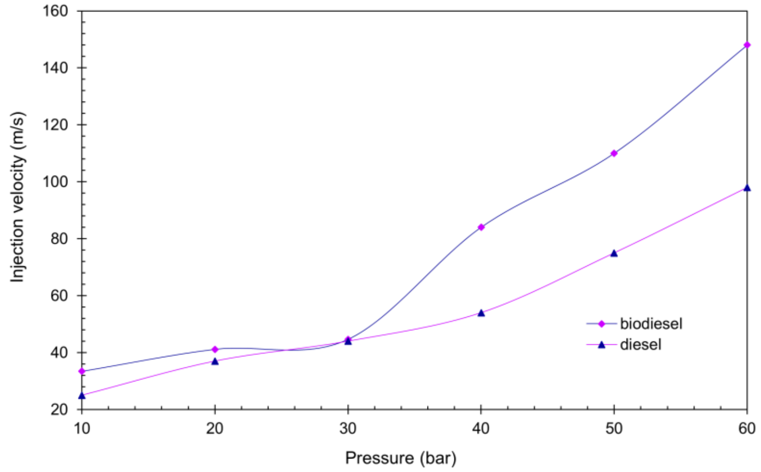

Fig.4. Distribution of biodiesel and diesel droplet velocities as a function of combustion chamber pressure

The spray area of both fuels is between 0.43 and 1.3 cm along the combustion chamber height (Fig.5). Since biodiesel droplets have a higher velocity, their spray area is located higher than that of petroleum diesel droplets. The reason for this phenomenon is that biodiesel droplets have a higher velocity, which allows them to travel a greater distance in the combustion chamber before they interact with air. The higher spray velocity contributes to the longer droplet spread, which leads to their location higher along the combustion chamber height compared to petroleum diesel droplets (Fig.5).

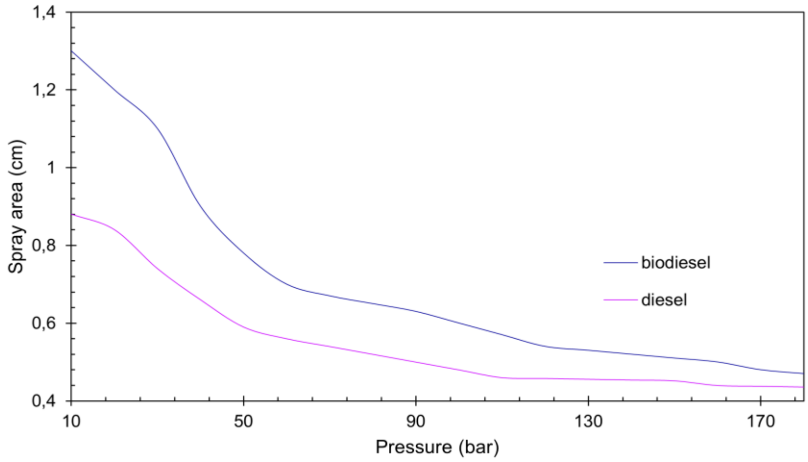

Fig.5. Spray areas of biodiesel and conventional diesel droplets

Based on the computational experiments conducted, a visualization of the reacting flow was obtained. Figure 6 shows the temperature profiles of biodiesel fuel at a time of 3 ms. It is evident from the figure that in the core of the torch the temperature reaches its maximum, about 3000 K. The height of the temperature torch is 4.2 cm of the combustion chamber, and in the rest of the chamber, the temperature remains within 2300-2500 K. Figure 7 shows the distribution of concentration fields of carbon dioxide CO_2 during combustion of biodiesel droplets at a time of 3 ms. The maximum concentration of CO_2 reached 0.183 g/g, while the minimum value was 0.012 g/g. The maximum concentration of carbon dioxide will be observed in the center of the combustion chamber, in the area where the main combustion of the fuel occurs. This is because, in the center of the torch, the temperature and density of the reactive substances are maximum, which contributes to the more intensive formation of carbon dioxide. However, at the exit from the combustion chamber, the concentration of carbon dioxide will be somewhat reduced since the processes of cooling and dilution of gases are already taking place here. Reducing CO_2 emissions from heat engines is an important step towards improving the environmental situation and combating climate change [17]. Biofuels emit significantly less carbon dioxide when burned than traditional fuels. Moreover, some biofuels can be carbon neutral if their production and use are optimized.

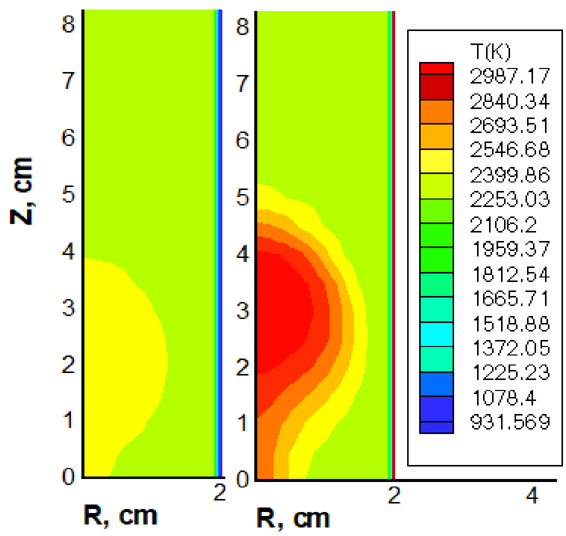

Fig.6. Temperature profiles of biodiesel droplets at t=3 ms

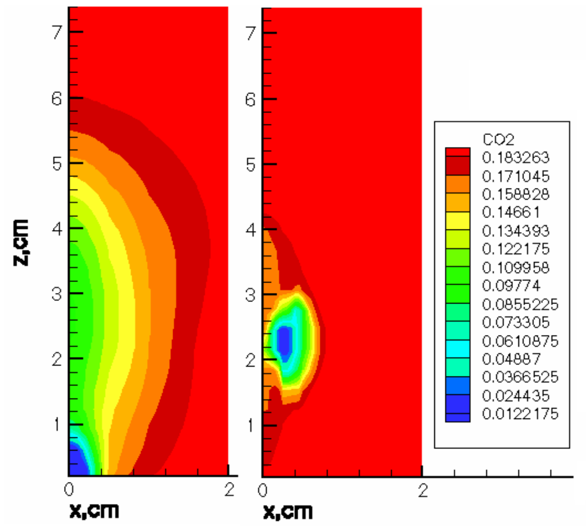

Fig.7. Concentration fields of carbon dioxide during combustion of biodiesel at t=3 ms

Figure 8 shows the dispersion of biodiesel droplets by specific temperature. In the upper part of the combustion chamber, the maximum specific temperature of biodiesel droplets reaches 655 K, while in the lower part, there are droplets with a temperature of 300-400 K.

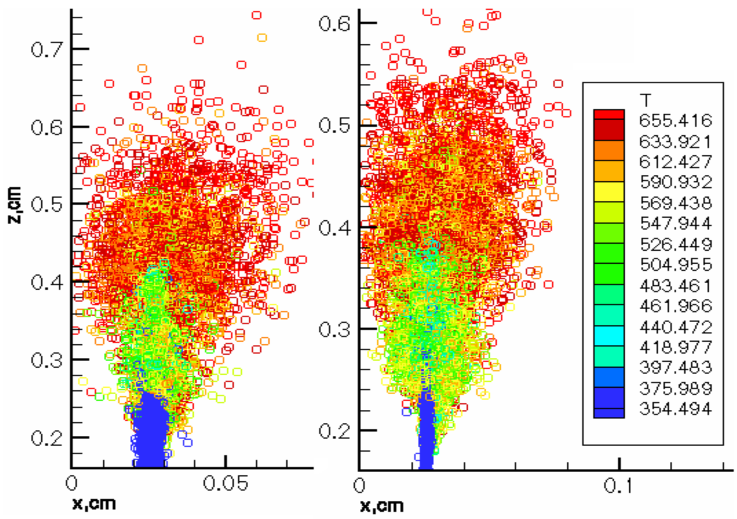

Fig.8. Dispersion of biodiesel droplets by specific temperature at t=3 ms

This is because, in the upper part of the combustion chamber, biodiesel droplets are exposed to a more intense effect of high temperatures formed in the core of the torch, where the main combustion occurs. While in the lower part of the chamber, the temperature is lower due to a more remote location from heat sources and less exposure to high-temperature gases.

Figure 9 shows the distribution of carbon monoxide concentration CO during biodiesel combustion. As can be seen, the concentration of CO remains low enough, which confirms the complete combustion of the fuel with the oxidizer without residual products. It follows that the combustion process of biodiesel occurs efficiently and completely, without the formation of significant amounts of intermediate products, such as carbon monoxide. This indicates high combustion quality and minimal emissions of harmful substances.

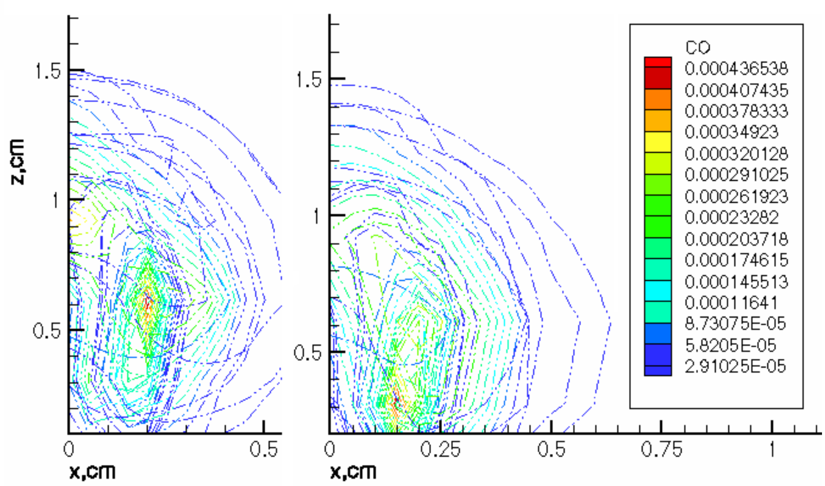

Fig.9. Concentration fields of carbon monoxide during biodiesel combustion at t=3 ms

Complete combustion of biodiesel with minimal emissions of carbon monoxide has a positive effect on the operation of the heat engine. This contributes to more efficient use of fuel energy, improves the thermal performance of the engine, and reduces environmental pollution [18]. In addition, the absence of incomplete combustion residues reduces the risk of carbon deposits accumulating in the combustion chamber, which can extend the service life of the engine and reduce the need for maintenance.

Figure 10 shows the results of computational experiments showing the change in the time distributions of the Sauter mean diameter (SMD) of diesel and biodiesel fuel droplets at 40 mm from the injector nozzle. The Sauter mean diameter is the average volume-surface diameter of the droplets. The same figure presents a comparison between the calculated data for diesel fuel [19] and the experimental results provided in [20].

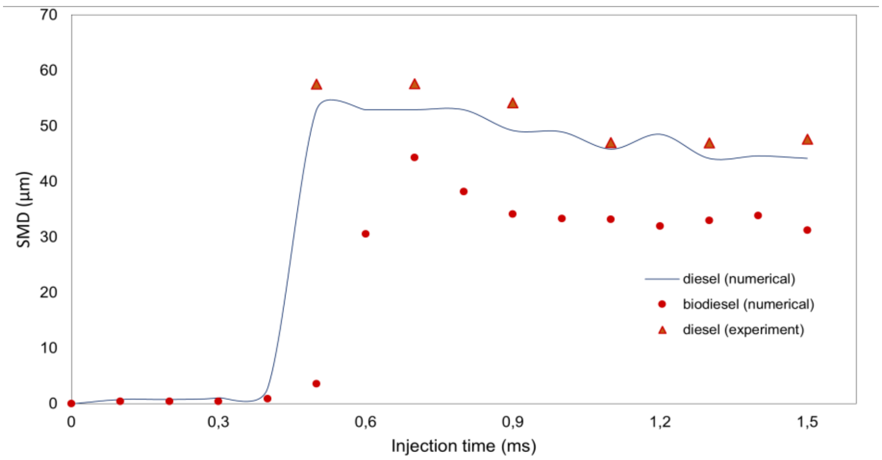

Fig. 10. Comparison of time distributions of the Sauter mean diameters (SMD) of diesel and biodiesel droplets with an experiment at 40 mm from the injector nozzle

As can be seen from the graph, the calculated data for diesel fuel is in good agreement with the experimental results. Biodiesel droplets exhibit a smaller volume-surface diameter compared to diesel droplets, which can be attributed to the lower surface tension coefficient and distinct molecular structure of biodiesel. These characteristics promote finer atomization. Additionally, biodiesel's improved flow properties contribute to the formation of smaller droplets during atomization. Together, these factors enhance atomization efficiency and result in a smaller Sauter mean droplet diameter.

4. Conclusions

Based on the research conducted on modeling of thermophysical processes of spraying and combustion of biodiesel fuel droplets, the following conclusions can be made:

1. The maximum combustion temperature of the fuel-air mixture of biodiesel reaches about 3000 K, while for diesel fuel this temperature does not exceed 1400 K. This indicates a higher combustion temperature of biodiesel, which can lead to improved combustion efficiency and heat transfer;
2. At a combustion chamber pressure of 60 bar, the maximum speed of biodiesel droplets is 33 m/s, while for diesel droplets it is 25 m/s. This confirms the greater mobility of biodiesel droplets, which contributes to better atomization and more complete mixing with air, which improves combustion processes and the efficiency of the heat engine;
3. The spray area for both fuels varies from 0.43 to 1.3 cm in the combustion chamber height. Biodiesel droplets, due to their higher speed, have a higher spray area, which allows them to reach more distant areas of the combustion chamber;
4. In the flame core, the temperature of the biodiesel fuel reaches a maximum value of about 3000 K. The temperature in the upper part of the combustion chamber flame is 2300-2500 K, which confirms the high combustion temperature in the center of the flame and lower temperatures in the rest of the chamber;
5. The concentration of carbon dioxide (CO_2) during biodiesel combustion reaches a maximum of 0.183 g/g in the center of the combustion chamber, where the temperature and density of the reactants are maximum, and a minimum of 0.012 g/g after the gases leave the chamber. At the same time, the concentration of carbon monoxide (CO) remains low, which confirms the complete combustion of the fuel with the oxidizer and the absence of significant carbon monoxide residues. These data indicate high efficiency of biodiesel combustion and minimal emissions of harmful substances;
6. From the computational experiments, it is evident that biodiesel droplets have a smaller Sauter mean diameter compared to diesel droplets. This is explained by the lower surface tension coefficient and molecular structure of biodiesel, which contributes to finer atomization and improved mixing with air. The computational results show that biodiesel has better atomization characteristics, which leads to more efficient combustion;
7. The reduction of CO_2 and carbon monoxide emissions from biodiesel combustion contributes to a better environmental situation. Biodiesel not only emits less CO_2 than diesel fuel, but can also be carbon neutral if its production and use are optimized. It also contributes to improved efficiency of heat engines and a lower environmental impact.

Conflict of interest statement

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

Credit author statement

Askarova A.S.: Supervision; **Bolegenova S.A.:** Conceptualization, Funding acquisition; **Ospanova Sh.S.:** Investigation, Writing Reviewing and Editing; **Maxutkhanova A.:** Resources, Software; **Bolegenova K.:** Data curation, Methodology, Investigation; **Baidullayeva G.:** Visualization, Validation. The final manuscript was read and approved by all authors.

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