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Original Research Article

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SIMULATION OF LIQUID FUEL SPRAY FORMATION AND DISTRIBUTION IN A REACTING TURBULENT FLOW

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Abstract. *The paper presents the computational experiments of the liquid fuels spray and its droplets distribution in a turbulent reacting flow. Primary and secondary atomization of two types of liquid fuel droplets (isooctane and dodecane) in the presence of combustion was described by the equations of continuity, momentum, internal energy, concentration of components of reacting substances and a two-parameter model for calculating turbulent flow. The study results of the spray, dispersion and combustion of droplets of hydrocarbon liquid fuels in a model combustion chamber when changing the injector injection angle were obtained. The injection angle values varied from 2 to 10 degrees. Based on the computational experiment temperature profiles and concentration characteristics of combustion products and gas in the combustion chamber at various times were obtained. Numerical calculations of the droplets' Sauter mean diameter distributions have the same dispersion pattern for dodecane. This suggests that the accuracy and adequacy of developed complex model of the formation and distribution of spray in a reacting flow has been confirmed by its strong correlation and good agreement of the modeling results with experimental data from other researchers. This kind of modeling methods and the obtained computational experiments results from them are widely used not only in traditional thermal power engineering, but also in the study of technological processes in the new generation engines chambers, combustion of alternative types of fuels and optimization of their combustion.*

Keywords: fossil fuel, spray, simulation, combustion, injection angle, emissions.

1. Introduction

The increase in harmful emissions of combustion products into the environment is a consequence of the extended consumption of hydrocarbon fuels in the energy, industry and transport sectors. According to long-term monitoring, the volume of environmentally hazardous chemical compounds, wastes and substances emitted into the atmosphere as a result of fuel combustion doubles every 12-14 years. Thus, one of the major environmental problems of the modern world is environmental pollution due to anthropogenic impact. The quality and type of liquid fuel burned, the conditions for organizing its combustion and the technical condition of internal combustion engines affect the toxicity of gas emissions and soot into the surrounding atmosphere. Although the use of low-quality fuels reduces the costs spent on its purchase, it also increases the concentration of environmentally harmful substances that enter the air [1].

The internal combustion engines exhaust gases emitted into the air contain more than 70% carbon oxides, about 52% nitrogen oxides, up to 5.5% soot and water. A complex combination of physical and chemical, kinetic, thermodynamic and heat exchange processes influence the environmentally hazardous

pollutants formation dynamics during the various types of fuels combustion. However, despite the existing significant amount of research in this area, the mechanisms of such harmful substances' formation are still not fully understood [2, 3]. By actively influencing the harmful emissions formation, it is possible to reduce thermal and gas pollution of the air, which is the most promising way to eliminate them. Improvement of the technological cycle of fuel processing and supply, methods of modernization and updating of injection devices contributes to changing the conditions for the harmful pollutants' formation in the environment. At the current stage of energy development, environmental problems are becoming a priority. Since carbon dioxide is the most common indicator of harmful substances, reducing its production into the atmosphere and using up to 80% of renewable energy sources by 2050 is a long-term goal set for all countries by the International Energy Agency. In this regard, it becomes imperative to improve and increase the efficiency of devices and systems for supplying and burning various types of fuel, as well as minimizing harmful gaseous emissions into the atmosphere. Figure 1 shows the main specific pollutant emissions dynamics for 2019-2023 in Kazakhstan [4].

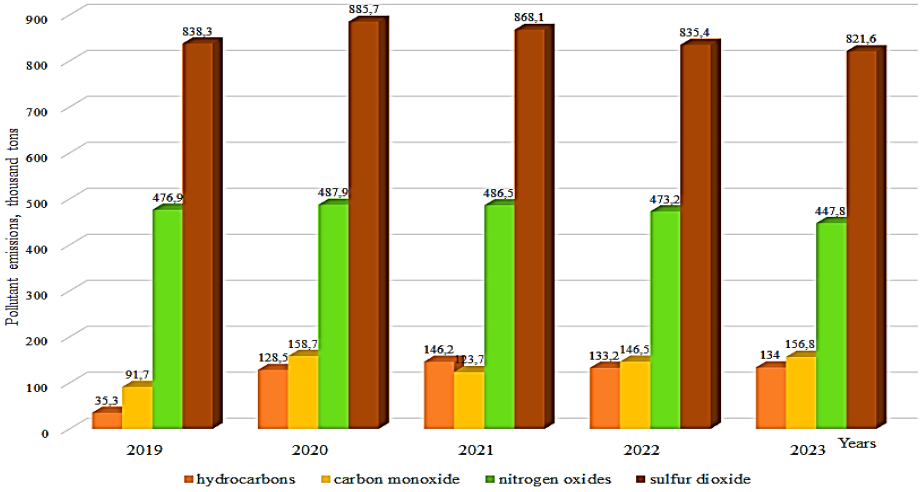

Fig.1. Emissions of main pollutants in Kazakhstan, thousand tons

In this paper, the study of thermophysical processes in heat engines is carried out, considering the geometry of the combustion chamber, methods of fuel supply, design parameters, and location of injection devices, and also identified effective technological mechanisms of the injection, allowing for rational fuel combustion optimization with minimal gaseous waste emissions.

2. Mathematical model of the problem and computational grid

During two-phase reacting flow modeling, the continuity, momentum, internal energy and reaction components concentration equations are solved by using numerical methods, taking into account chemical transformations, medium high turbulence, interphase heat and mass transfer and interfacial interaction [5-8].

The reacting components mass conservation in a two-phase flow is described by the continuity equation taking into account the atomized dispersed phase contribution:

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

where u is the fluid phase velocity, S_{mass} is source term describing the change in gas phase density as a result of liquid fuel droplets evaporation.

The particles movement in a two-phase reacting flow is determined by the gas phase momentum conservation equation:

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

where S_{mom} is source term describing the moving drops contribution to the gas phase momentum velocity change.

The two-phase reacting flow internal energy conservation with dispersed particles is as follows:

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

where **q** is isolated heat flow according to Fourier's law, S_{energy} is contribution to the change in the system's internal energy coming from atomized dispersed phase droplets.

The system's mass density is determined by the conservation equation for the component m:

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

where ρ_m is the m component mass density, ρ is the total mass density.

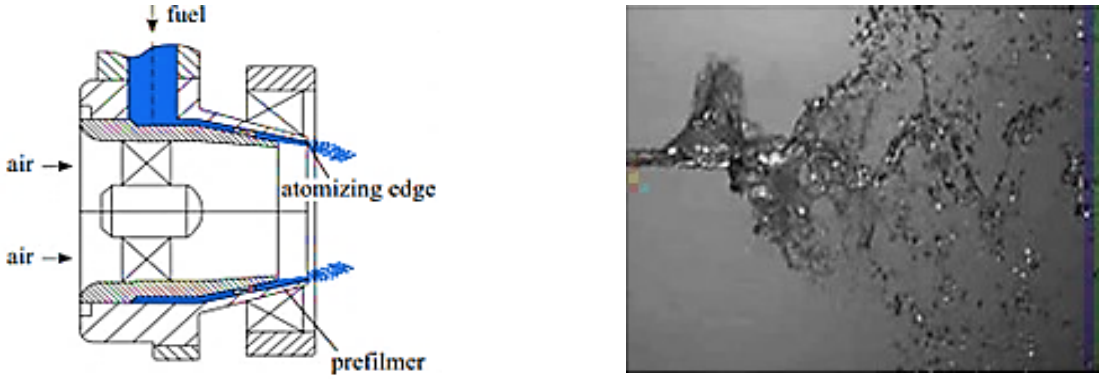
During the complex turbulent flows simulation, according to the turbulent kinetic energy cascade transfer law the high turbulence of the reacting two-phase flow was taken into account by two main parameters: the kinetic energy of turbulence k and its dissipation degree ε, which was expressed by an empirical turbulence model included in the mathematical model of the problem [9, 10]:

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

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

The constants c_{ε_1}, c_{ε_2}, c_{ε_3}, σ_k, σ_ε, used in the empirical turbulence model above are determined from experiment [11, 12].

Aircraft and rocket engines inject a liquid jet with a high-velocity co-current gas flow. When interacting with a co-current gas flow, the liquid jet breaks up into fragments, which is called primary atomization. When modeling the formation and evolution dynamics of liquid injections, the main attention was paid to the air-blast atomization process, which is most common in highly reactive jets. The air-blast atomization process configuration is shown in Figure 2 [13-15]. In such injection systems, a stream of liquid fuel is injected into thin liquid fragmentary sheets at low pressure. High-speed liquid jets surrounded by a co-current gas jet make a large contribution to the kinetic energy of the entire flow. Due to the presence of the jet-to-jet interaction phenomenon and intense interaction with co-current gas stream, liquid's layered sheets are torn on both sides into ligaments. Further downstream, these liquid ligaments break up into various size droplets. This phenomenon is called secondary atomization.

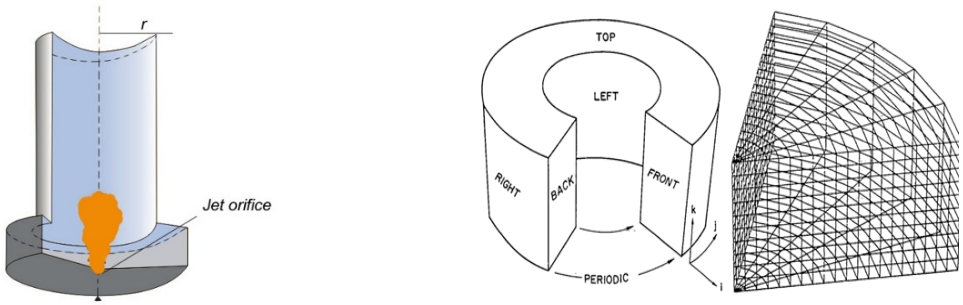


a) b)

Fig.2. Premixed air-blast atomizing scheme [13-15]

Using a calculation program, a cylindrical combustion chamber virtual prototype with a height of 15 cm and a diameter of 4 cm was built. Liquid fuel is sprayed throughout the entire volume of the chamber through a nozzle located in its lower part. Before the experiment, the fuel droplets had a temperature of 900 K. Two types of liquid fuels (isooctane and dodecane) injected droplets' mean radius was 25 μm. The optimal initial injection mass and pressure for isooctane were 6 mg and 100 bar, for dodecane were 7 mg and 80 bar. These optimal parameters for the combustion process of these fuels were obtained in previous studies by the authors [16, 17].

The combustion chamber general view and generated computational mesh template are presented in Figure 3. The computational domain is centered on a Cartesian coordinate 3D structured grid with various node configurations. The computational grid is divided into blocks of cells across the entire logical space.



a) model chamber b) computational mesh

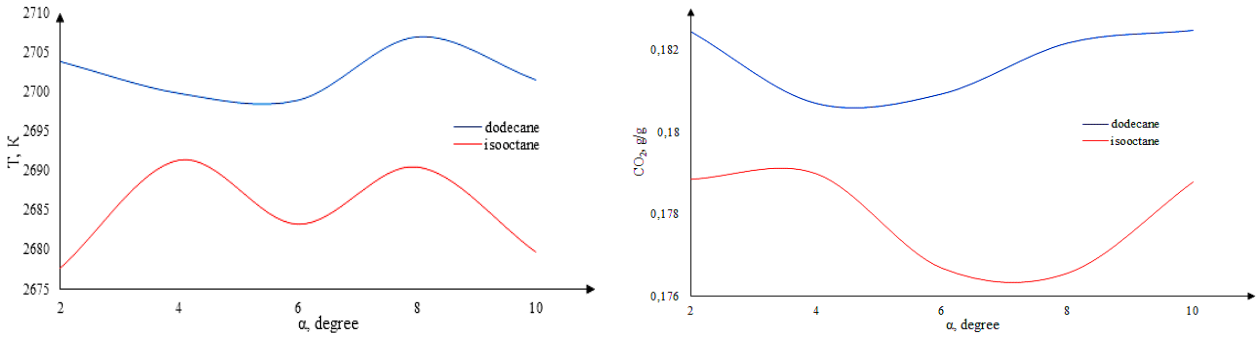
Fig.3. a) Model camera general view; b) Pseudo-polar grid and perspective view of the sector grid outline

Using the initial and boundary conditions of the problem, a three-dimensional mesh is formed from pseudo-polar blocks of cells. Although the program's functions cover broader areas of its application, our main goal was its targeted application for modeling thermal processes in reacting flows. Using an automatic mesh generator built into the SETUP subroutine, a three-dimensional cylindrical mesh was created to describe the different types of injectors and nozzles of gasoline and diesel thermal engines [6, 18].

3. Simulation results and analysis

Influence of the injection angle on the two types of liquid fuel (isooctane and dodecane) spray formation, droplets distribution, and combustion in a turbulent reacting flow in the cylindrical chamber was investigated. The values of the injection angle varied from 2 to 10 degrees. Figures below show the graphs for determining the fuels optimal combustion regime depending on the injector injection angle value.

The distribution of the maximum combustion temperature of the reacting mixture throughout the entire volume of the combustion chamber when the injection angle changes is shown in Figure 4 (a). As a result of a detailed analysis of the curves in the Figure 4 (a), it was found that the maximum combustion temperature of isooctane is 2690 K at 4 and 8 degrees of injection angle. Because diesel fuels have high surface tension, the interface between the two phases remains stable for a long time. In this regard, during the ignition and combustion of dodecane droplets, the highest temperature value of 2707 K is observed at 8 degrees of injection angle. Therefore, we can say with confidence that the greater the droplet spray angle, the more intense the fuel burns, the heat exchange between the two phases increases and the temperature rises to 3000 K.



a) combustion temperature b) CO_2 concentration

Fig.4. Dependences of the maximum combustion temperature and carbon dioxide concentration on the injection angle during the combustion of isooctane and dodecane

The influence of two types of fuels (isooctane and dodecane) droplets injection angle on the distribution of the carbon dioxide maximum concentration was investigated. As is known, CO_2 is the main component of greenhouse gases. The amount of carbon dioxide produced during the combustion of dodecane exceeds the

concentration of CO_2 released during the isooctane droplets combustion. The volume of carbon dioxide formed during the dodecane combustion varies between 0.180-0.182 g/g at injection angles of 4-10 degrees. The distribution of carbon dioxide concentration during combustion of isooctane is very different from that of dodecane, since its decrease is observed with increasing injection angle. For this reason, within 6-8 degrees, the volume of CO_2 released is 0.176 g/g, which is much less compared to dodecane. This difference in the behavior of fuels can be explained as follows: isooctane is a reference fuel with high octane number and lower concentration of impurities.

According to the distribution of temperature and CO_2 concentration in Figure 4, it was found that for the two types of liquid fuels most often used in internal combustion engines and included in gasoline and diesel, the effective injection angle is 8 degrees. With an effective injection angle, due to intensive mixing of the fuel jet with the co-current gas flow, the temperature in the combustion chamber increases, and the amount of carbon dioxide in the combustion products does not exceed environmental standards requirements.

Three-dimensional graphs of the temperature and concentration characteristics of the reacting flow of two types of liquid fuels (isooctane and dodecane) were obtained through a numerical CFD modeling experiment taking into account an effective injection angle of 8 degrees (Figures 5-7). Liquid fuel combustion is a heterogeneous process, since the interaction products are in the condensed phase due to phase separation and high temperatures of more than 2000 K, the role of plasma processes increases. The same picture of the formation of areas with high temperatures and its distribution over the entire combustion chamber height is observed during the combustion of solid fossil fuels in high-temperature energy, thermophysical and technological facilities [19]. At different times and combustion zones, isooctane and dodecane have similar temperature profiles with a monotonic spreading gradient (Figure 5).

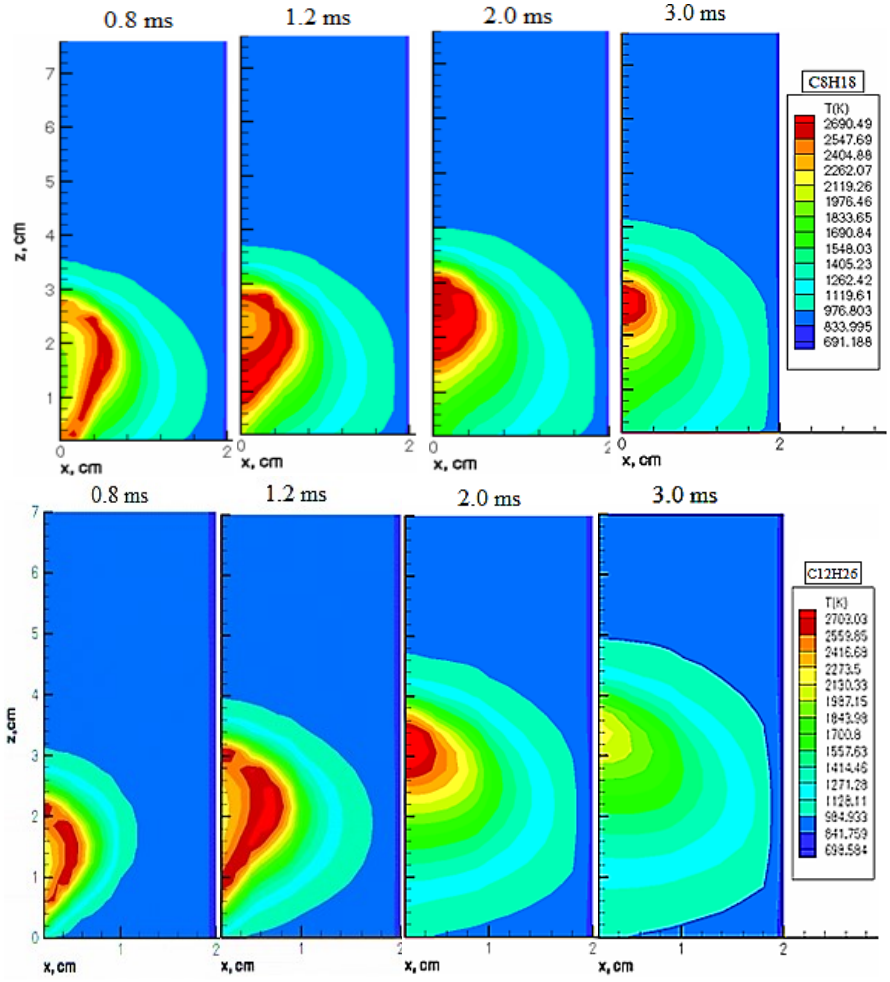


Fig.5. Temperature profiles during isooctane and dodecane combustion at different time moments in the combustion chamber

Due to the temperature gradient, intense heat exchange and mixing with the oxidizer, a high-temperature flame spreads throughout the entire volume from the central part of the combustion chamber. Spray areas remote from the flame core heat up to 975-985 K during combustion of both types of fuels. The core of the flame when burning isooctane occupies 3 cm in height, and 0.8 cm in width, and the temperature reaches 2690 K, for dodecane, it is much larger than 3.6 cm by 0.5 cm, respectively, but the maximum temperature is 2703 K. The concentration fields of consumed oxygen and carbon dioxide at an effective injection angle at a time of 3 ms are shown in Figures 6 and 7.

Oxygen consumption in various parts of the combustion chamber and its distribution across combustion zones for two types of fuels is shown in Figure 6. Since the fuel droplets intensive combustion process occurs in the flame core, the highest oxygen consumption is observed in the central part of the chamber. And in other parts of the combustion chamber, a high concentration of oxidizer remains for both isooctane and dodecane.

The amount of oxygen that has not reacted with the fuel for isooctane and dodecane is 0.22 g/g. The unconsumed oxidizer concentration located in the flame core was 0.015 g/g for both types of fuel. An intense reaction of isooctane with oxygen occurs in the area of 2.9-4.8 cm along the model combustion chamber height. When dodecane is burned, O2 consumption begins from a chamber height of 3.8 cm, which is an indicator of the high mobility and reactivity of its droplets. Since the region of high temperatures for dodecane begins at this height of the chamber, we can confidently say that oxygen molecules are focused in the plume core. This statement can be observed in Figure 6.

Numerical data on the concentration profiles of carbon dioxide formation during the combustion of isooctane and dodecane, depending on the effective injection angle, are presented in Figure 7. On the axis of the combustion chamber, where the temperature flame is formed and the highest fuel consumption, the maximum amount of carbon dioxide is produced, which confirms the fulfillment of the laws of chemical kinetics.

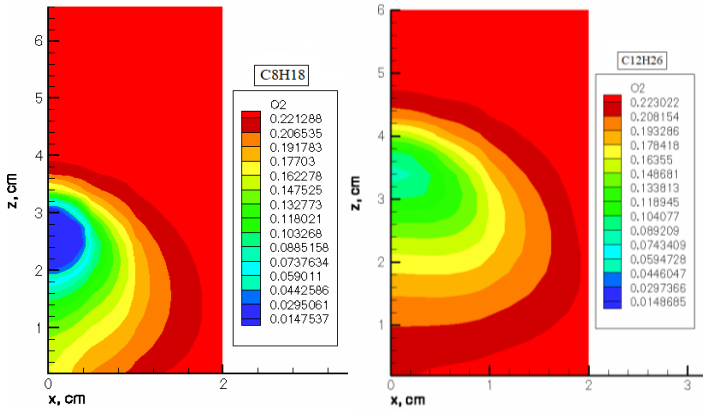


Fig.6. The oxidizer O_2 concentration profiles in a model combustion chamber at t=3 ms

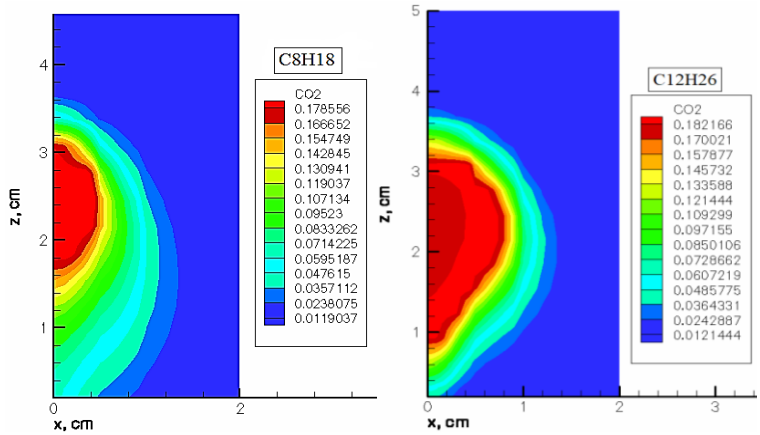


Fig.7. The carbon dioxide concentration properties in the combustion chamber at t=3 ms

The maximum concentration of CO_2 formed in the central part of the model chamber was 0.18 g/g for both isooctane and dodecane. At the combustion chamber exit, the amount of CO_2 gradually decreases, thereby at the final moment of fuel combustion it takes on minimum values for the two types of fuels. This phenomenon shows that the formation and distribution of greenhouse gases during the combustion of liquid hydrocarbon fuels is identical. At an effective injection angle of 8 degrees, the concentration of released carbon dioxide is 0.012 g/g. The efficiency of the combustion process of liquid fuel droplets in internal combustion engines directly depends on their spraying from the nozzle and breakup into small secondary droplets, including their size distribution. The isooctane and dodecane droplets' Sauter mean diameters (SMD) were measured at different distances from the injector nozzle edge at various times (Figure 8). Since the Sauter mean diameter is a volume-surface unit of droplets, this value is a parameter of the particle size distribution and is involved in the secondary atomization of liquid fragments. To verify the computer simulation data, a comparative analysis was carried out with experimental data taken from [20]. According to a thorough analysis of the calculated and experimental indicators presented in Figure 8, it was found that model calculations for the size distribution of dodecane droplets are similar to the experimental data.

In the experiment the dispersion of the droplets' Sauter mean diameter was measured at distances from 10 to 60 mm from the nozzle at various times [20].

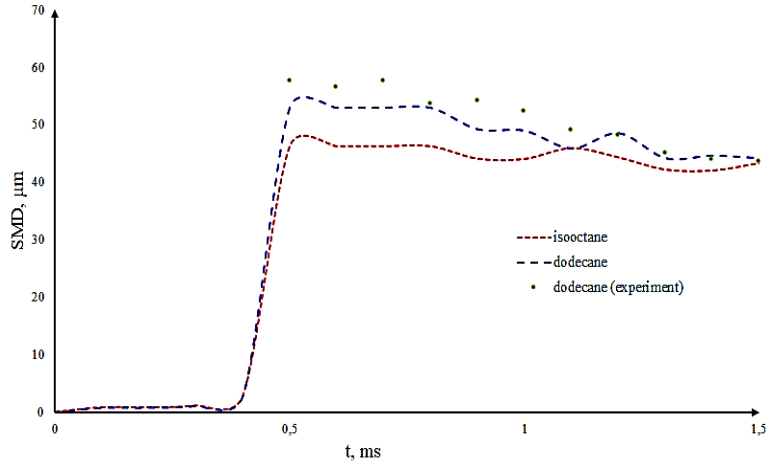


Fig.8. The isooctane and dodecane droplets Sauter mean diameter (SMD) dispersion at a distance of x=40 mm from the injector nozzle

Identical researches of the isooctane and dodecane droplets' Sauter mean diameter dispersion at various times were carried out in simulation at a distance of 40 mm from the injector nozzle. When comparing the relative data in Figure 8, it is established that the measured results of the numerical experiment are in good agreement with the experimental measurements belonging to the authors of [20]. Relying on this agreement between the numerical results and the experiment, we can state that the complex CFD model of the distribution, atomization and combustion of liquid fuel droplets in a cylindrical combustion chamber proposed in our work is adequate and can be applied to real processes and phenomena occurring in thermal power and thermophysical facilities with built-in injection systems.

4. Conclusion

The processes of distribution and atomization of two types of fossil fuels (isooctane and dodecane) in a highly turbulent flow in the presence of combustion were studied using a set of complex methods for modeling technological structural systems. The effective injection angle influence on the liquid fuels' droplets atomization and distribution in the presence of combustion was determined by simulation methods based on computational experiments in order to organize rational combustion of fuels with the least negative impact on the environment. From the analysis of computer experiments, it was found that for isooctane and dodecane, the optimal injection angle of the injector is 8 degrees. At this effective value of the injection angle, the fuel quickly reacts with the oxidizer, due to high temperatures, intermediate products of the chemical reaction are released in a minimal volume, and the concentration of carbon dioxide produced does not exceed environmentally acceptable standards.

The proposed numerical data in the work have practical significance and will serve as a background for their use in the design of various heat engines with injection devices and optimal structural parameters. The results obtained in the work will contribute to solving the problems of rational and efficient combustion of various types of fossil fuels with subsequent optimization of these processes and reducing the carbon footprint from their anthropogenic 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

Bolegenova S.A.: Conceptualization, Funding acquisition; Askarova A.S.: Supervision; Ospanova Sh.S.: Investigation, Writing-Original draft preparation, Writing Reviewing and Editing; Makanova A.: Resources, Software; Zhumagaliyeva S.: Data curation, Methodology; Nurmukhanova A. and Adilbayev N.: Investigation, Visualization; Akzhol Sh.: Software, Validation. The final manuscript was read and approved by all authors.

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