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NUMERICAL SIMULATION OF ISOOCTANE AND BIODIESEL COMBUSTION PROCESS USING OPENFOAM

This paper presents a numerical simulation of the combustion process of two types of liquid fuels, isooctane and biodiesel, with application of the OpenFOAM software package. The relevance of this study is caused by the growing interest in alternative energy sources as well as the need to reduce harmful emissions when using traditional hydrocarbon fuels. Biodiesel or biofuel can be used as an alternative liquid fuel in internal combustion engines because it is renewable and produces fewer harmful emissions when burned. The numerical simulations were used to analyze the temperature fields and velocity profiles for two specified types of fuel, traditional and alternative. The performed analysis showed that the maximum combustion temperature of isooctane is 100-150 K higher than that of biodiesel which is due to the physical and chemical properties of the fuels. Analysis of the speed characteristics showed that when isooctane is burned, more intense but less stable combustion of the fuel is observed. Biodiesel exhibits a more stable and uniform combustion mode with a smooth speed distribution and smaller local fluctuations. The obtained results indicate the feasibility of using biodiesel as a renewable and environmentally friendly fuel that can replace traditional hydrocarbon types of liquid fuels. The numerical analysis performed in the article has practical significance in the design of fuel systems for internal combustion engines. The results can be used to develop strategies for the transition to alternative energy sources.

Keywords: biofuel, isooctane, combustion, numerical modeling, OpenFOAM, temperature fields.

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OpenFOAM қолданылуымен изооктанды және биодизельді жану процесін сандық модельдеу

Мақалада OpenFOAM бағдарламалық кешенін қолдана отырып, екі түрлі сұйық отынның - изооктан мен биодизельдің жану процесін сандық модельдеу нәтижелері ұсынылған. Зерттеудің өзектілігі баламалы энергия көздеріне деген қызығушылықтың артуымен, сондай-ақ дәстүрлі көмірсутек отынын пайдалану кезінде зиянды шығарындыларды азайту қажеттілігімен байланысты. Биодизель немесе биоотын іштен жанатын қозғалтқыштарда баламалы сұйық отын ретінде қолданылады, себебі ол жаңартылатын және жағылған кезде зиянды шығарындыларды азайтады. Алынған сандық модельдеу нәтижесінде отынның екі көрсетілген түрі, балама және дәстүрлі, үшін температура өрістері мен жылдамдық профильдерін талдау жүргізілді. Жүргізілген талдау нәтижесінде изооктанның максималды жану температурасы биодизельге қарағанда 100-150 К жоғары екені анықталды, бұл олардың физика-химиялық қасиеттерімен түсіндіріледі. Жылдамдық сипаттамаларын талдау изооктан жанған кезде отынның қарқындырақ, бірақ тұрақсызырақ жануы байқалатынын көрсетті. Биодизель бірқалыпты жылдамдық таралуы мен аз жергілікті ауытқулары бар неғұрлым тұрақты және біртекті жану режимін көрсетеді. Алынған нәтижелер биодизельдің дәстүрлі көмірсутекті сұйық отындарды алмастыра алатын жаңартылатын және экологиялық таза отын ретіндегі мүмкіндігін дәлелдейді. Мақалада жүргізілген сандық талдау іштен жанатын қозғалтқыштарда арналған отын жүйелерін жобалауда практикалық маңызға ие және баламалы энергия көздеріне көшу стратегияларын әзірлеуде қолданылуы мүмкін.

Түйін сөздер: биоотын, изооктан, жану, сандық модельдеу, OpenFOAM, температура өрістері.

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Численное моделирование процесса горения изооктана и биодизеля с помощью OpenFOAM

В данной работе представлено численное моделирование процесса горения двух видов жидкого топлива: изооктана и биодизеля с использованием программного пакета OpenFOAM. Актуальность исследования вызвана возрастающим интересом к альтернативным источникам энергии, а также необходимостью снижения вредных выбросов при использовании традиционных углеводородных видов топлива. Биодизель или биотопливо используется в качестве альтернативного вида топлива в двигателях внутреннего сгорания благодаря тому, что является возобновляемым, а также при его сгорании образуется меньшее количество вредных выбросов. В результате полученного численного моделирования был проведен анализ температурных полей и профилей скорости для двух указанных видов топлива, альтернативного и традиционного. Проведенный анализ показал, что максимальная температура горения изооктана больше на 100-150 К по сравнению с биодизелем, что связано с физико-химическими свойствами топлив. Анализ скоростных характеристик показал, что при горении изооктана наблюдается более интенсивное, но менее устойчивое сгорание топлива. Биодизель показывает более устойчивый режим горения с плавным распределением скоростей и меньшими локальными колебаниями. Полученные результаты говорят о целесообразности использования биодизеля в качестве возобновляемого и экологически безопасного топлива, который способен заменить традиционные углеводородные виды жидких топлив. Проведенный в статье численный анализ имеет практическую значимость при проектировании систем двигателей внутреннего сгорания. Результаты могут быть использованы при разработке стратегий по переходу на альтернативные источники энергии.

Ключевые слова: биотопливо, изооктан, горение, численное моделирование, OpenFOAM, температурные поля.

Introduction

Combustion is an important physical and chemical process that plays a key role in everyday life as well as in industry, transportation and energy. Combustion is an oxidation reaction that releases heat and light. This process underlies the operation of internal combustion engines, boilers, turbines and other similar devices. Without combustion, it is impossible to imagine the existence and operation of modern energy, transportation and industry.

The relevance of this research stems from the growing need to find and improve alternative energy sources amid increasing global consumption of traditional fuels. Traditional fuels (oil, natural gas) are limited natural resources. In Kazakhstan, oil fields are gradually are being depleted and their development is becoming increasingly difficult. According to the Minister of Energy: "A significant decline in oil production has been observed in the Mangistau, Aktobe and Kysylorda regions…by 2040, the trend of declining oil production at fields excluding the large ones will continue" [1]. Thus, conducting research aimed developing environmentally friendly and efficient alternative fuels is a relevant important scientific problem.

Literature review

Biodiesil or biofuel is an alternative fuel source for many fields. Biofuel is a promising replacement for petroleum diesel. It is a renewable and environmentally friendly fuel that can replace traditional petroleum fuel. Due to its compatibility with modern diesel plants, biodiesel can be adapted to existing energy infrastructure.

The use of biodiesel helps reduce emissions of carbon monoxide, carbon dioxide, soot and others. The article [2] presents results confirming the reduction of emissions when using biodiesel mixtures with polymer additives. The authors obtained a significant reduction in emissions of carbon monoxide, carbon dioxide and nitrogen oxides. Optimization of polymer oil waste concentration in biofuel improves fuel performance, such as specific fuel consumption and thermal efficiency. It has been shown that the use of biofuel leads to increase energy efficiency and reduced environmental pollution.

In the study [3] the authors analyzed the characteristics of engine emissions when using a mixture of biofuels based on cooking and sunflower oil in different proportions. Biodiesel mixture were tested in combination with conventional diesel fuel at concentrations of 5%, 10%, 20% and 50%. The biodiesel mixtures resulted in reduced emissions of carbon oxide, unburned hydrocarbons and carbon dioxide compared to diesel. CO_2 emissions decreased by approximately 9.38% for a fuel mixture containing 5% biodiesel from used cooking oil and by 8.59% for a fuel mixture containing 5% biodiesel from sunflower oil. Biodiesel mixtures up to 20% appear to be the most suitable providing a balance between the loss in power and the improvement in the emission characteristics. It has been shown that a biodiesel mixture can be used effectively in diesel engines without significant modifications.

The paper [4] studies the use of biodiesel as a fuel in a controlled jet ignition engine. Biodiesel was produced karanja oil (pangamia oil) [5]. The main objective of this study has been to evaluate how efficiently and environmentally friendly, this engine operates when a mixture of gasoline and biodiesel is used instead of diesel. The engine fueled with karanja biodiesel blends has demonstrated an improvement in brake thermal efficiency from 31% at a compression ratio of 16:1 to 35.9% at 18:1 with optimized injection timing. Compared to conventional diesel, biodiesel blends showed significant reduction in NO_x emissions exceeding 20% under full-load conditions. Overall, the use of biodiesel improved combustion efficiency while simultaneously decreasing pollutant emissions.

This work [6] explores the difference between conventional fuel and biofuel in application to aviation. Aviation kerosene as conventional fuel and hydrotreated vegetable oil as biofuel (alternative) were used in the study. The authors study the mean breakup lengths of conventional and alternative fuels, the droplet sizes. The authors concluded that biofuel can be an alternative to conventional gasoline for aviation from the point of view of spray and atomization and that is important for environmentally friendly aviation fuels.

This article [7] is about obtaining biofuel form the wood or forest residues of Madhuca longifolia using pyrolysis. This article contains a detailed information about characteristics of the obtained products like quality, content and the proportion of various fractions (oil, ash residue and gas)

This article [8] describes the possibility of obtaining biofuel (bioethanol) from blossom wastes as an alternative source of energy. The authors describe the technological cycle of receiving bioethanol from biomass containing sugars and hydrocarbons. This cycle includes raw material preparation, hydrolysis and fermentation and then distillation in order to obtain bioethanol.

The work [9] is also about possibilities of obtaining biofuel from different sources. This article examines environmental benefits of biofuels as alternative to conventional fossil fuels. Celluloid ethanol from biomass wastes can be produced on a large scale. This article emphasizes the role of biofuel as a renewable energy solution for the better future. This article [10] compares the combustion of two types of fuels – conventional and biofuel this research is related to the combustion process of solid fuels – charcoal and biofuel briquettes. This article compares the emissions of pollutants (CO2, CO, fine particles and etc.). The goal of this work was to evaluate the application of biofuel briquettes in comparison with conventional charcoal.

This study [11] examines cellulosic jet fuel produced by hydrothermal/hydrocondensation-hydrotreating method. The article includes a comparison of the emissions and combustion products of this biofuel with conventional kerosene under two conditions: laminar flame in the Bunsen burner and turbulent combustion in a jet engine. The article [12] describes an overview of modern technologies for energy recovery in the internal combustion engines. The study highlights specific application of these technologies when using biofuels.

The authors [13] study data on several biofuels like bioethanol, biodiesel and biogas. They made comparative analysis on their chemical and physical properties: density, viscosity, calorific value and so on. The article evaluates what biofuel can be preferable based on fuel properties and combustion performance. The article [14] shows that when using biofuel blends spray characteristics change significantly compared to traditional diesel fuel. The authors have concluded that the transition to alternative fuels requires a detailed analysis of spray process and have confirmed the relevance of modeling similar to that performed in this study. This article [15] studies the combustion of blends of biofuel and conventional fuels. The work shows improved emission characteristics of biofuel compared to pure fossil fuels and that makes blends of biofuels a better alternative when integrating biotechnology into existing engines.

Isooctane is a hydrocarbon widely used in gasoline. It is used as a standard for determining the octane number of gasoline as its octane rating is 100. Isooctane is often used as a model fuel to analyze combustion characteristics, ignition delay and emissions in internal combustion engine studies. In work [16] the combustion of fuel consisting of 92% isooctane and 8% heptane was studied experimentally and numerically. The authors studied the process of autoignition of liquid fuels at high injection pressure and using exhaust gas recirculation. The authors used the KIVA-3V program which showed good agreement with experimental data on heat generation, combustion chamber pressure and nitrogen oxide emissions.

Comparison of the combustion processes of isooctane and biodiesel has high scientific and practical significance. This type of research allows to understand the characteristics of heat and mass transfer during the combustion of liquid fuels and contributes to the development of effective solutions for improving the performance of internal combustion engines. Modern numerical modeling methods provide the opportunity for a detailed analysis of combustion processes of various types of liquid fuels.

The scientific novelty of this study is that a comparative analysis was conducted for two types of fuel, isooctane and biodiesel, and biodiesel is an alternative and renewable fuel. The aim of the work is to compare the combustion characteristics of isooctane as traditional fuel and biodiesel as an alternative fuel.

Methodology

The mathematical model is based on the equations of turbulent flow with fuel injections in a cylindrical combustion chamber. This model includes the equations of motion for the liquid phase of fuel, the mass conservation equation for the different components of the combustion reaction, as well as the energy equation and the *k-ε* turbulence model [17].

The mass conservation equation for a component m is as follows:

$$\frac{\partial \rho_m}{\partial t} + \vec{\nabla}(\rho_m u) = \vec{\nabla}\left[\rho D \vec{\nabla}\left(\frac{\rho_m}{\rho}\right)\right] + \dot{\rho}_m^c + \dot{\rho}^s \delta_{m1}, \tag{1}$$

where ρ_m is the mass density of component m, ρ is the total density, u is the flow velocity.

The momentum equation in this model:

$$\frac{\partial(\rho\vec{u})}{\partial t} + \vec{\nabla}(\rho\vec{u}\vec{u}) = -\frac{1}{a^2}\vec{\nabla}p - A_0\vec{\nabla}\left(\frac{2}{3}\rho k\right) + \vec{\nabla}\vec{\sigma} + \vec{F}^s + \rho\vec{g}, \tag{2}$$

where p denotes the fluid pressure.

The equation for conservation of energy is:

$$\frac{\partial(\rho I)}{\partial t} + \vec{\nabla}(\rho\vec{u}I) = -p\vec{\nabla}\vec{u} + (1 - A_0)\sigma\vec{\nabla}\vec{u} - \vec{\nabla}\vec{J} + A_0\rho\varepsilon + \dot{Q}^c + \dot{Q}^s. \tag{3}$$

The calculation of the heat flux vector J was carried out using the following relationship:

$$\vec{J} = -K\vec{\nabla}T - \rho D \sum_m h_m \vec{\nabla}\left(\frac{\rho_m}{\rho}\right), \quad (4)$$

where T is the liquid temperature, h_m is the enthalpy of component m, $\dot{Q}^c$is the amount of heat due to chemical reactions, $\dot{Q}^s$ is the amount of heat entering the combustion chamber during fuel injection.

The equations of the k-ε model, in which k is the turbulence kinetic energy and ε is the rate of dissipation of kinetic energy, are calculated using the following formulas [18]:

$$\frac{\partial \rho k}{\partial t} + \vec{\nabla}(\rho\vec{u}k) = -\frac{2}{3}\rho k\vec{\nabla}\vec{u} + \vec{\sigma}\vec{\nabla}\vec{u} + \vec{\nabla}\left[\left(\frac{\mu}{Pr_k}\right)\vec{\nabla}k\right] - \rho\varepsilon + \dot{W}^s, \quad (5)$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \vec{\nabla}(\rho\vec{u}\varepsilon) = -\left(\frac{2}{3}c_{\varepsilon_1} - c_{\varepsilon_3}\right)\rho\varepsilon\vec{\nabla}\vec{u} + \vec{\nabla}\left[\left(\frac{\mu}{Pr_\varepsilon}\right)\vec{\nabla}\varepsilon\right] + \frac{\varepsilon}{k}\left[c_{\varepsilon_1}\vec{\sigma}\vec{\nabla}\vec{u} - c_{\varepsilon_2}\rho\varepsilon + c_s\dot{W}^s\right]. \quad (6)$$

Biodiesel, or in other words biofuel, is a type of motor biofuel. It is obtained by chemical processing of animal fats or vegetable oils. The basis of biofuel is monoalkyl esters of fatty acids obtained as a result of chemical reactions with the formation of esters. In these reactions triglycerids, which are found in animal fats or vegetable oils, react with alcohols (methanol, ethanol, etc.) to form biofuel and glycerol (a by-product of the reaction). Biofuel formula is $CH_3(CH_2)nCOOCH_3$ [19] or it can be written in the short form as $C_{13}H_{24}O_2$.

The combustion reaction of biodiesel to form carbon dioxide and water is expressed by the following equation:

$$C_{13}H_{24}O_2 + 18O_2 = 13CO_2 + 12H_2O.$$

Isooctane is an organic compound with chemical formula C_8H_{18}. Possessing anti-knock properties, isooctane is used to create aviation fuel and it has a characteristic smell of gasoline and it also insoluble in water.

The chemical reaction of isooctane combustion is written by the following expression:

$$2C_8H_{18} + 25O_2 = 16CO_2 + 18H_2O.$$

Table 1 shows the main characteristics of isooctane and biofuel, such as molecular weight, boiling point, density and etc.

The numerical simulation was carried out using the free and open source software OpenFOAM. OpenFOAM is widely used in scientific research and industry due to its versatility and ability to solve various problems. OpenFOAM can simulate complex flows with heat transfer, chemical reactions and turbulence. New versions of OpenFOAM are released twice a year and the software undergoes rigorous testing before each release ensuring high quality. During the verification process various tests are launched. These tests are designed to evaluate the stability and efficiency of the code [22]. OpenFOAM was developed by Henry Weller and was originally intendent to solve strength problems, but can now be used in areas such as [22]: calculations of stress-strain states of structures, hydrodynamics of viscous fluids, simulation of various turbulence models, multiphase flows with chemical reactions and more. Thus, OpenFOAM is a powerful tool for numerical modeling in various engineering and scientific fields.

Table 1 – Main parameters of two fuels: isooctane [20] and biodiesel [21]

Parameter	Isooctane C_8H_{18}	Biodiesel $C_{13}H_{24}O_2$
Molecular weight	114 g/mole	270g/mole
Boiling point	99 °C	320-250°C
Density at normal conditions	688 g/m^3	880 g/m^3
Viscosity	Low	High
Evaporation rate	High	Low

To visualize the results of numerical simulation the ParaView program with open source was used [23]. This program can be used to analyze data from a numerical experiment. ParaView supports the OpenFOAM output format, it allows displaying temperature, pressure and velocity fields and works with large volumes of data [23].

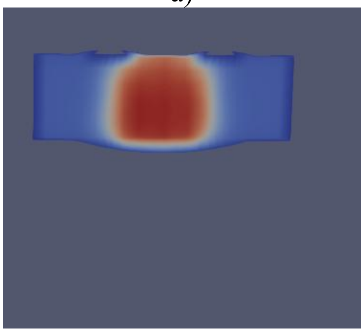
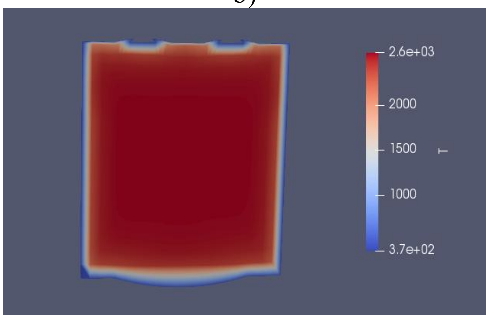
The calculations have been performed using engineFoam solver. A moving mesh model for the piston chamber was used for calculations. The numerical grid has 85 743 computational cells. Engine parameters: bore length is 0.092 m, stroke is 0.084 m, connecting rod length is 0.147 m.

Biodiesel combustion was calculated using the same model as for isooctane (Finite-Rate chemistry and PaSR) but the chemical reaction mechanism FAME fuel (FAME – kinetic scheme of fatty acid methyl esters). This model took into account the increased rate chemical conversion due to internal oxygen in the fuel molecule.

Results and discussion

The numerical experiment was performed for a cylindrical chamber with a height of 8.5 cmand a diameter of 9.2 cm. The initial gas temperature in the chamber is 373K, the initial pressure is 10^5 Pa. The injected fuel mass is 38 mg for both types of fuel.

As a result of the numerical experiment the temperature field in the combustion chamber during isooctane combustion was obtained. The data are presented in Figure 1 for three angles of the crankshaft position, where -180 means the beginning of the intake stroke, 45 is the end of intake and the beginning of compression, 180 is the bottom dead center. The combustion temperature reaches 2600K for the isooctane combustion process.

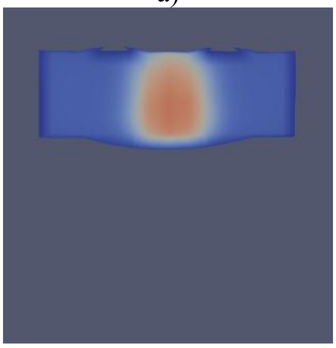
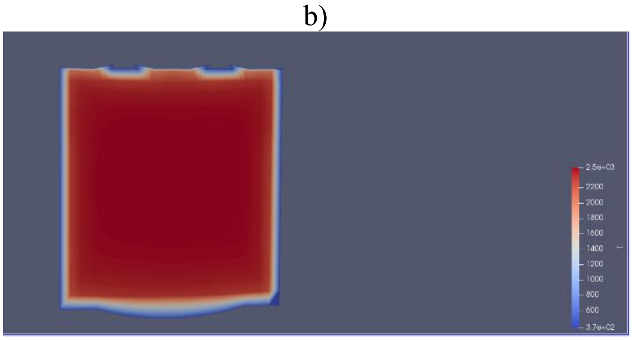

a)

b)


c)

Figure 1 – Temperature fields during combustion of isooctane: a) -180, b) 45, c) 180

Figure 2 shows the temperature fields for biodiesel combustion for the same angular positions. The maximum combustion chamber temperature is lower for biodiesel and the difference is 100K from the maximum of isooctane temperature of combustion. Both figures 1 and 2 show that by the 180 angle the whole chamber is heated to maximum temperature, which corresponds to the completion of the main combustion phase. The temperature fields are uniform, indicating the disappearance of the flame front. The cold boundary layer at the walls remains, consistent with heat transfer to the cylinder walls.

The results of the numerical simulation presented in figure 2 are in good agreement with the article [24], the authors obtained the biofuel temperature of 2390 K. The calculated biodiesel temperature is consistent with another study [25], where the authors reported peak temperature of soybean biodiesel of 2576K.


a)

b)


c)

Figure 2 – Temperature fields during combustion of biodiesel: a)-180, b) 45, c) 180

Figure 3 shows the temperature distribution along the cylinder axis at the center of the combustion chamber at the bottom dead center (crankshaft rotation angle is 180) during the combustion of two types of fuel: isooctane and biodiesel. A sharp increase in temperature at the beginning of the profile indicates an area of intense heat generation. When using isooctane, significant heating of the chamber is observed, the temperature in the most volume of the chamber is 2550-2600K. This graph indicates complete and uniform combustion of the fuel-air mixture. At the walls of the chamber (with the chamber height of 10 cm), a decrease in temperature is observed due to heat transfer to the cooled surfaces. The temperature for biodiesel reaches 2450 K, which is 100-150 K less than for isooctane. The obtained values are consistent with the characteristics of biodiesel: slow ignition, higher viscosity, lower flame temperature. The higher temperature of isooctane shows a more intense chemical combustion reaction with greater heat release. Although the combustion temperature of biodiesel is slightly lower than that of isooctane, this reduction is not significant, since both cases of combustion occurs at temperatures above 2400 K. The use of biofuel remains preferable as more environmentally friendly and renewable.

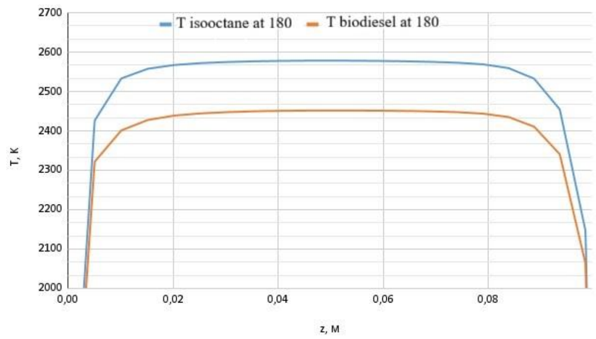


Figure 3 – Temperature distribution along the chamber height during the combustion of isooctane and biodiesel at 180

Figure 4 shows the velocity modulus (m/s) for isooctane and for biodiesel for bottom dead center (180). The graph shows the velocity profile with values ranging from 0 to 1.85 m/s. In the central part of the graph, the velocity remains virtually unchanged, indicating a stable gas flow regime. This is typical for uniform expansion of combustion products at the bottom dead center. The sharp drop in velocity at the ends of the graph is due to the boundary layer at the chamber walls.

Isooctane reaches a velocity of 1.8 m/s compared to biodiesel (up to 1.6 m/s). The isooctane profile has local maxima, which indicates uneven flows of liquid fuel distribution in the combustion chamber. The biodiesel profile has a smooth appearance, indicating a more uniform movement of biofuel within the combustion chamber. This also reflects the improved mixture homogeneity and more complete combustion of biodiesel compared to isooctane. This again emphasizes advantages of biofuel instead of traditional hydrocarbon fuels.

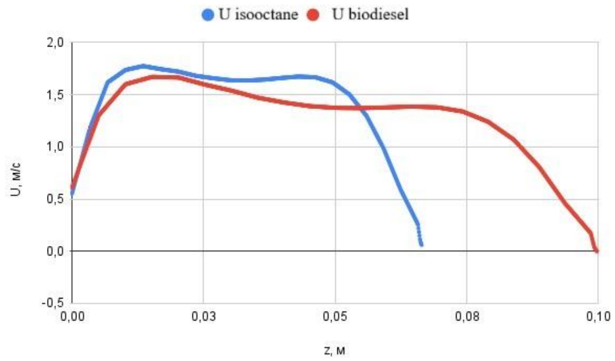


Figure 4 – The velocity module of isooctane and biodiesel along the chamber height during the combustion of isooctane and biodiesel at 180

In figure 4 in the decline section the rate of isooctane decreases sharply compared to biodiesel, the rate of biofuel decreases smoothly, which indicates a stable combustion phase in biodiesel. This, in turn, has a positive effect on the completeness of combustion of biodiesel. A smooth decline in the velocity profile at the combustion chamber walls in the case of biodiesel combustion compared to isooctane confirms the stability of combustion process and better heat and mass transfer in biofuels.

The obtained results of the numerical simulation demonstrate the potential of biodiesel as a stable smooth-burning fuel. This shows the ability of biodiesel to ensure efficient operation of an internal combustion engine.

Conclusion

The conducted numerical analysis of the combustion processes of isooctane and biodiesel allows formulating the following conclusions:

1. Complete combustion of the fuel mixture for two types of fuel (isooctane and biodiesel) occurs in the combustion chamber reaching high temperatures above 2400 K.

2. The difference between the maximum combustion temperatures of isooctane and biodiesel is only 100-150 K, which is due to the physical and chemical properties of fuels.

3. The maximum velocity is higher for isooctane than for biodiesel, indicating a more intense but less stable flow in the case of isooctane.

4. The velocity profiles show a more stable combustion mode in the case of using biodiesel, local velocity variations in isooctane indicate the presence of uneven flows, which can reduce the intensity of fuel combustion.

5. Thus, despite a slight reduction in maximum temperature the biofuel provides a more stable and even combustion. The use of biodiesel as fuel is preferable because biofuel promotes a sustainable combustion process and it is a renewable and environmentally friendly source of energy.

6. The obtained data can be useful in design of fuel systems for engines using alternative and renewable fuels taking into account energy efficiency and environmental requirements.

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