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Numerical Simulation of Turbulent Combustion of Liquid Fuels: Comparative Analysis of Benzene and Tridecane

The work presents a numerical simulation of the combustion process of two liquid fuels (benzene and tridecane) with the application of KIVA-II computational program. The research is focused on evaluation of the effect of fuel mass and spray angle on the combustion process and temperature distribution in a cylindrical combustion chamber. The fuel mass is varied from 5 to 20 mg and the spray angle ranges from 2° to 15°. Temperature fields are analyzed over time to determine heat release characteristics and flame structure for both fuels. The results demonstrate that increasing the injection mass leads to a significant rise in flame height and combustion temperature, which is attributed to enhanced heat energy release. The effect of spray angle is found to be significant only at small values, while at higher values it has little influence on the temperature fields of both fuels. Comparative analysis between benzene and tridecane shows that benzene combustion occurs more intensively and at higher temperatures than the combustion process of tridecane fuel. These findings are essential for optimizing fuel injection parameters and improving the design of combustion systems in internal combustion engines. The results of the study can be applied to enhance combustion efficiency and reduce harmful emissions into the environment.

Keywords: numerical combustion modeling, liquid fuels, benzene, tridecane, mass of injected fuel, spray characteristics, temperature field, concentration fields

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Introduction

Combustion of liquid fuels is characterized by complex physical and chemical reactions. The process of combustion of liquid fuels can depend on various factors such as initial parameters, chemical properties of a fuel or parameters of turbulence. If one can optimize these factors, it is possible to increase the combustion efficiency and to minimize emissions of harmful substances. In this work the object of numerical research is the combustion process of benzene and tridecane in a closed cylindrical combustion chamber.

The relevance and practical significance of this study are determined by the widespread use of liquid fuels in power plants, in industry and in vehicles. The problem of environmental pollution from combustion products of various fuels and fuel mixtures also remains important. In addition, the processes of combustion and turbulence are complex physical and chemical processes. When modelling it is necessary to take into account multiphase flows with sprays, the presence of chemical reactions and turbulence process.

The importance of modeling the combustion process of liquid fuels is confirmed by modern research. For example, in work [1] it is considered how the injection rate affects the combustion of liquid heptane. The authors conducted the analysis of the concentration fields of reacting substances in the combustion zone of liquid heptane.

In the study [2] the authors analyzed how the excess air ratio affects the combustion and atomization of benzene. As the result of numerical modeling the authors have shown that complete oxidation of the fuel does not occur when rich fuel mixtures burn. This results in increased fuel consumption and reduced combustion efficiency due to the presence of unburned hydrocarbons in the exhaust gases.

The work [3] demonstrates the features of liquid fuel combustion when the initial air temperature in the combustion chamber is changed. A numerical study has allowed to obtain temperature fields of fuel, concentration fields of liquid fuel combustion reaction products for different initial temperatures of the oxidizer in the combustion.

In the article [4] the authors have examined the influence of the temperature on the vortex combustion of liquid fuel. It has been found that flame oscillations appear due to the uneven flow of liquid fuel droplets

at low temperatures. As the result of the analysis the authors have demonstrated that increasing the temperature helps to stabilize and to improve the fuel combustion.

In the work [5] a numerical study of the combustion of fuel mixture of ammonia and hydrogen has been performed to assess the posibility of using this mixture as an alternative fuel. The authors have examined the combustion process of this mixture and have studied the combustion temperature as well as the fuel burning rate. The authors of the article have concluded that the addition of hydrogen improve the combustion process of the mixture by increasing the combustion temperature and by making the process more uniform which helps reduce the emission of harmful substances into the atmosphere.

Study [6] is dedicated to the comparison of various turbulence models. It includes the simulation of dodecane combustion with multiple injections. The numerical experiment has been conducted at different ambient temperatures. The results obtained by the authors have shown good agreement with experimental data.

The scientific novelty of this work lies in the comparative analysis of the influence of spray mass and angle of two different types of fuel (benzene and tridecane) in the combustion chamber using the KIVA-II computational program.

The aim of this study is to identify the optimal combustion conditions for two types of fuel (benzene and tridecane) through numerical simulation by varying the fuel mass and the spray angle of the liquid fuel.

Methods and materials

A mathematical model based on the equations of turbulent flow with fuel spray into a cylindrical combustion chamber has been used for the numerical simulation in this study. This model includes the equations of motion for the liquid phase of the fuel, the mass conservation equations for the various combustion reaction components and the k-ε turbulence model [7].

The mass conservation equation for the component *m* is expressed as follows [7]:

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

where ρ_m is the density of the mixture, 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 is the pressure of the fluid.

The parameter A_0 takes the value 1 for turbulent flow and 0 for laminar flow.

The energy conservation equation:

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

The calculation of the heat flux vector J is carried out according to the following relation:

$$\vec{J} = -K\vec{\nabla}T - \rho D\sum_m h_m \vec{\nabla}(\rho_m / \rho), \tag{4}$$

where T is the temperature of the fluid, h_m is the enthalpy of m. $\dot{Q}^c$ is the amount of heat generated by chemical reactions, $\dot{Q}^s$ is the amount of heat supplied to the combustion chamber during fuel injection.

The equations of the k–ε model where k is the turbulent kinetic energy ε is the kinetic energy dissipation rate are calculated using the following formula:

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

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

The standard k–ε model was chosen because of its reliable performance for engine turbulent flows. Moreover, it has full integration with KIVA-II code. The standard k–ε model gives reliable results and requires less computational resources. This model is commonly used for spray combustion simulations and it

has shown good performance in previous studies [1–3]. Other models like RNG k–ε model may be applied but they are computationally expensive.

Numerical simulation of liquid fuel combustion has been performed in a cylindrical burner chamber with a height of 15 cm and diameter of 4 cm. Initial conditions of the numerical experiment: air temperature is 900 K, wall temperature is 353 K, pressure is 4×10^6 Pa.

The computational domain consisted of 600 cells. Parameters are as follows: $nx = 20$ (number of cells along x axis, $ny = 1$ (axisymmetric task usual for cylinder), $nz = 30$ (along z axis, z is a height of chamber). The minimum cell size is 1 mm in the radial direction and 5 mm along z axis. The minimal time step is 1 microseconds. A grid and time step were selected based on established practices in KIVA-II modelling. The mesh and time step were found to provide consistent and stable results [1–3, 7].

The KIVA-II software package has been used for numerical simulation, detailed information about this software is provided in the source [7]. In this article, the authors have examined the combustion of two types of fuel: benzene and tridecane. The fuel mass has been varied from 5 to 20 mg. The influence of the spray angle (from 2° to 15°) has also been studied.

The reaction of benzene combustion producing water and carbon dioxide:

$$2C_6H_6 + 15O_2 \rightarrow 12CO_2 + 6H_2O \quad (7)$$

Benzene is a flammable hydrocarbon with a boiling point of 80,1 °C and a density of 0.7 g/cm^3. Benzene is used as a feedstock for engines and has a freezing point of –60 °C [8].

The combustion reaction of tridecane which also results in the formation of water and carbon dioxide:

$$C_{13}H_{28} + 20O_2 \rightarrow 13CO_2 + 14H_2O \quad (8)$$

Tridecane is a colorless liquid from the alkane group with a density of 0.7568 g/ml and it is used as a component of diesel fuel [9].

The formation and oxidation of soot during the fuel combustion are described using a global multi-step chemical reaction [10–12]:

$$C_nH_{2m} + O_2 \xrightarrow{k_q} 2R^* \quad (9)$$

In this reaction, the fuel reacts with oxygen leading to the formation of radical, branching agents and intermediate reaction products.

$$R^* + (\Gamma + 1)\left(\frac{1}{m}C_nH_m + pO_2\right) \xrightarrow{k_p} gP + f_1B + f_4Q + R^* \quad (10)$$

$$R^* + Q \xrightarrow{f_2k_p} R^* + B \quad (11)$$

$$B^* \xrightarrow{k_B} 2R^* \quad (12)$$

where R^* is radical, B is branching agent, Q is intermediate reaction product.

Coefficients Γ, p, g are formulated as follows:

$$\Gamma = \frac{f_1M_B + f_4M_Q}{\frac{M_{RH}}{m} + pM_{O_2}},\ p = \frac{n(2-\lambda)+m}{2m},\ g = \frac{n}{m} + 1. \quad (13)$$

The coefficient λ characterizes the ratio between the components of the reaction products $CO/CO_2 = \lambda/(1-\lambda)$, $\lambda = 0.67$ [10]. The molecular masses of the global components M_B, M_Q are calculated based on the mass balance equation.

During the reaction intermediate compounds are formed and they can be described as follows:

$$Q \xrightarrow{k_Q} \frac{M_Q}{M_{Pr_s}}Pr_s,\ Q \xrightarrow{k_S} \frac{M_Q}{M_S}S,\ S \xrightarrow{k_{OX}} \frac{M_S}{M_{Pr_s}}Pr_s, \quad (14)$$

where S defines soot particles (soot), Pr_s is global soot oxidation products, M_S is molecular weight of soot particles.

Results and discussion

The results of the numerical study of the influence of fuel injection mass on the combustion process of liquid fuels are shown in the figures below.

The temperature fields obtained as a result of tridecane combustion simulation are shown in Figure 1 for three time points from the start of the fuel injection. Data analysis has shown that by 4 ms the most of the chamber has warmed up to temperatures above 2000 K.

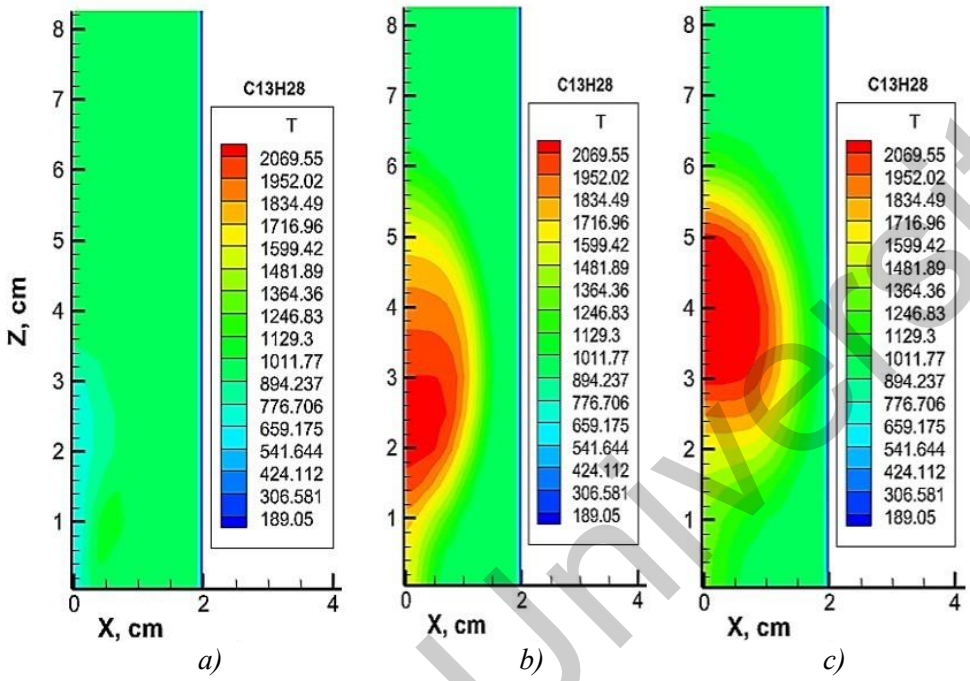

Figure 1. Temperature field during combustion of tridecane for times: *a* — 1.5 ms; *b* — 2.5 ms; *c* — 4 ms

The data in the Figure 2 show the change in temperature in the combustion chamber at three different time intervals for the case of liquid benzene spray. The maximum temperature is observed in the center of the temperature flame and reaches 2385 K. From graphs 1 and 2 it can be seen that benzene burns with a high heat release despite the smaller size of the temperature flame.

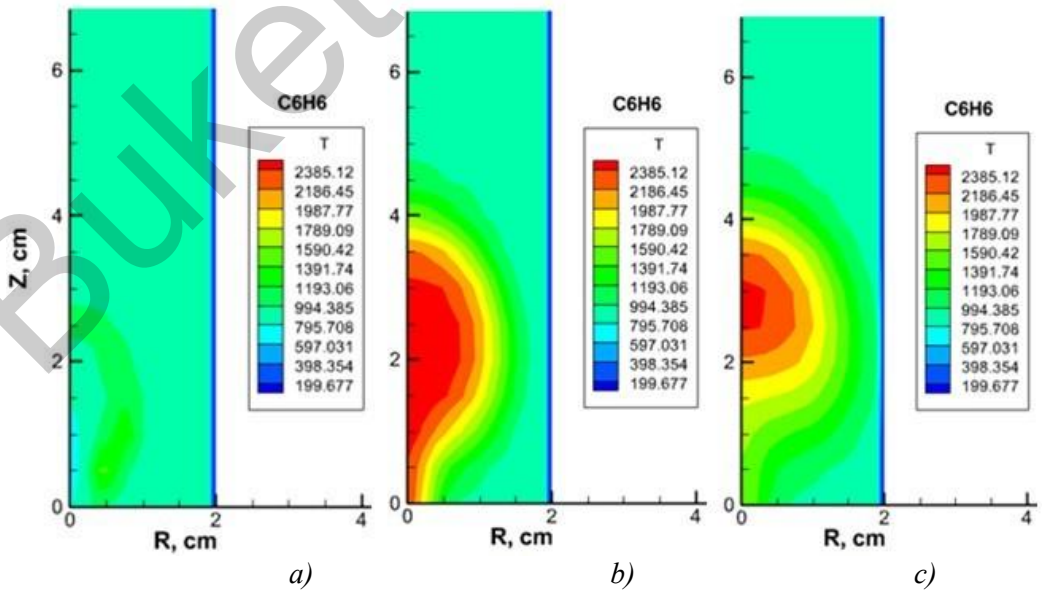

Figure 2. Temperature field during benzene combustion for times: *a* — *t* = 1.5 ms; *b* — *t* = 2.5 ms; *c* — *t* = 4 ms

Figure 3 shows the height of the temperature flame depending in the injection mass of tridecane. The greater the mass of the fuel the greater the height of the temperature flame. The increase in the height of the flame is associated with the increase in the amount of heat released during the fuel combustion. All of this also leads to a raise in the high temperature zone where intense combustion is observed. The graph also demonstrates small fluctuations due to the influence of spray and mixing of the combustion mixture.

The growth in the height of the temperature flame with the raise in the injection mass indicates the increase in the rate of combustion product outflow and the intensity of thermal convection, which is typical for diffusion combustion with the increase in the supplied fuel mass.

Thus, the dependence presented in the Figure 3 demonstrates the characteristic nonlinear dynamics of the temperature development with variations in the mass of the injected fuel which can be used too diagnose the combustion mode and optimize injection parameters in practical fuel supply problems.

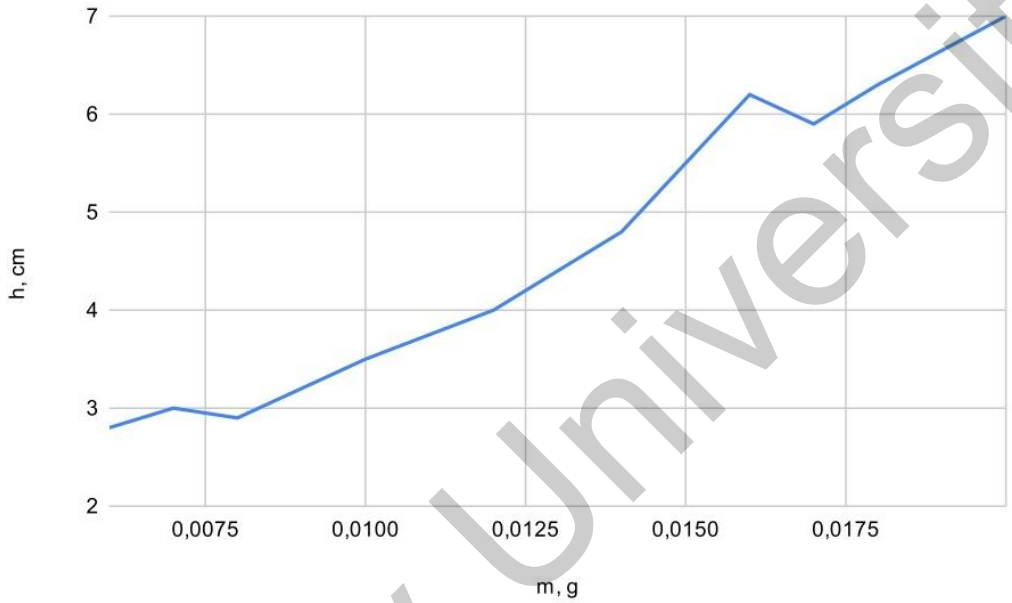

Figure 3. Effect of fuel mass on the height of the temperature flame

Figure 4 shows the effect of tridecane fuel mass on the formation of carbon dioxide in the combustion chamber. At low masses, a sharp increase in carbon dioxide is observed and then the influence of mass is already insignificant. At a mass of 10 to 20 mg the concentration of formed CO_2 stabilizes and this indicates that the limit of its formation during the combustion of tridecane has been reached.

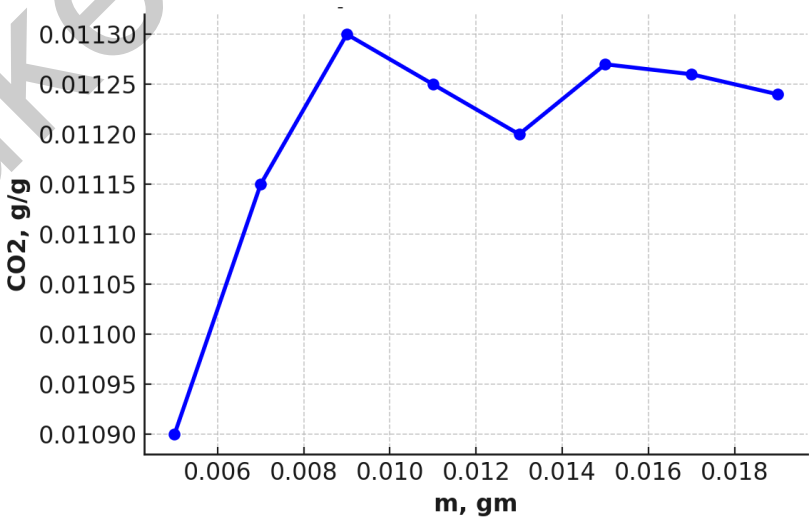

Figure 4. Effect of tridecane mass on carbon dioxide formation

Figure 5 shows how the injection mass of tridecane fuel affects the formation of soot during its combustion. Analysis of graph 5 demonstrates that increasing mass leads to a raise in the amount of soot. At a mass of up to 10 mg, the increase of soot concentration is insignificant; at a mass of more than 10 mg, a sharp increase in soot concentration is observed. Thus, the increase in mass leads to a raise in the formation of soot during the combustion of tridecane.

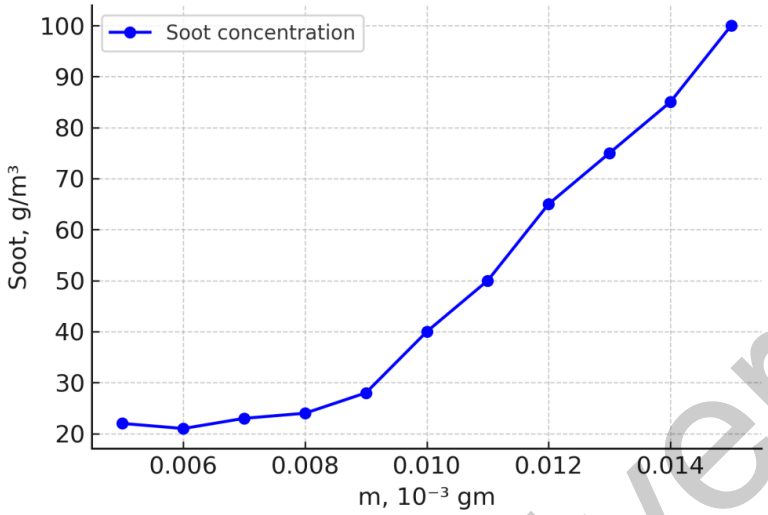

Figure 5. Dependence of the concentration of formed soot on the mass of tridecane injection

To validate the reliability of the simulation results the comparison with the experimental data available in the literature has been done. The calculated ignition time is within reasonable agreement with the experimental results presented in. The comparison confirms that the combustion model accurately reproduces the behavior of tridecane.

The results of the numerical calculation have shown that the optimal injection mass for liquid tridecane is 9 mg according to the graphs 4 and 5. Further increase in fuel mass leads to the raised formation of soot and carbon dioxide, which are harmful products of the chemical combustion reaction. At the same time, the mass of unburned particles also increases and this reduces the efficiency of fuel combustion.

A study on the influence of the spray angle on the combustion process of benzene and tridecane in the combustion chamber has also been conducted. The results of the numerical experiment for benzene (Fig. 6) show that the temperature change occurs at small spray angles. The subsequent increase (5–6°) has virtually no effect on the temperature field in the combustion chamber. It can be concluded that only at low values this parameter can influence the process of atomization and combustion of liquid fuel.

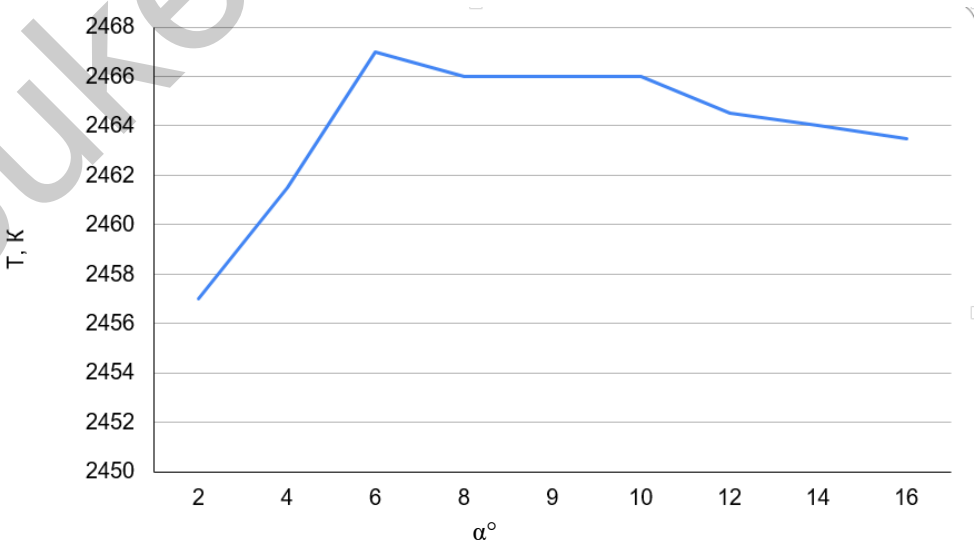

Figure 6. Effect of spray angle α on the maximum temperature during benzene combustion

From the analysis of the graph of the dependence of the maximum temperature during the combustion of tridecane (Fig. 7), it follows that the spray angle has no effect on the process of combustion and temperature changes remain insignificant.

Thus, it can be concluded that the spray angle does not have a significant effect on the process of mixing and combustion of liquid fuel, compared to other processes such as the concentration of fuel and oxidized or turbulence.

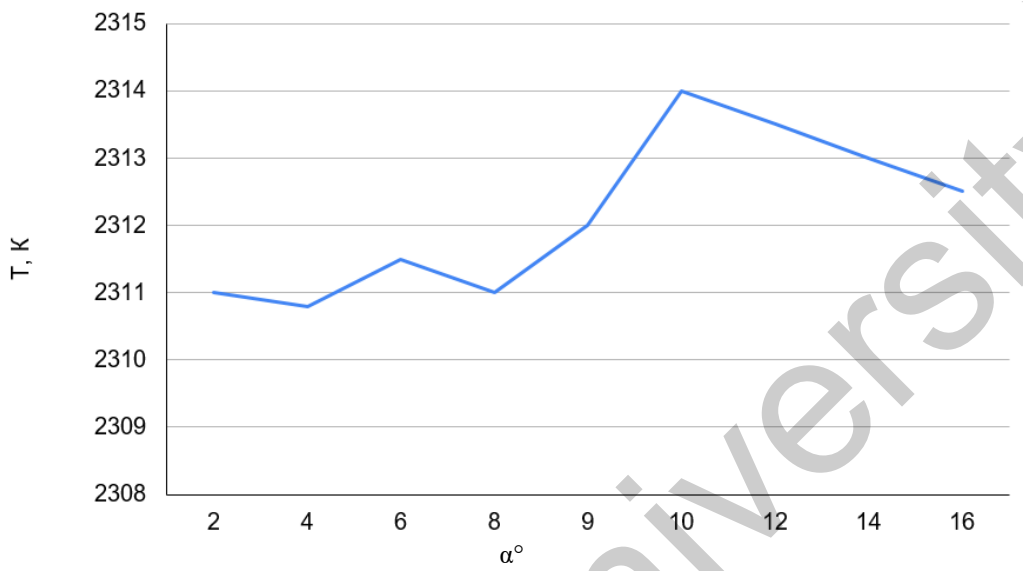

Figure 7. Distribution of maximum temperature for tridecane with changing spray angle α

Conclusion

In this article the authors have performed a numerical calculation of combustion of two types of liquid fuels: benzene and tridecane. A study has been conducted to investigate the influence of fuel mass and spray angle on the process of atomization and combustion of these fuels. Based on the results of numerical experiment the following conclusions can be drawn:

1. With the increase in the mass of fuel injection, a raise in the height of the temperature flame is observed which is associated with the increase in the amount of heat released during the chemical reaction of fuel combustion. There is also an increase in the high temperature zone where the most intense combustion occurs.

2. When adding small amounts of fuel, an increase in the amount of produced carbon dioxide is observed. When the injection mass reaches more than 10 mg, the process of carbon dioxide production stabilizes. Its concentrations remain practically unchanged with a further increase in the mass of fuel supplied to the chamber.

3. The mass of the fuel has a significant impact on the formation of soot in the combustion chamber, with a mass less than 10 mg the increase in soot concentration is insignificant; with a mass of more than 10 mg, a sharp increase in soot concentration is observed.

4. The analysis of the results has shown that the spray angle of liquid fuel droplets from 2 to 15° has little effect on the combustion parameters of the studied types of fuel. However, an increase in the injection mass of these fuels leads to a raise in heat exchange and temperature during the combustion of fuels.

The significance of the presented work is the possibility of practical application of the results for improving combustion and spraying processes in internal combustion engines operating on different types of fuel.

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М. Рыспаева, И. Березовская

Сұйық отынның турбулентті жануын сандық модельдеу: бензол мен тридеканды салыстырмалы талдау

Жұмыста KIVA-II есептік бағдарламасын қолдану арқылы екі сұйық отынның (бензол мен тридекан) жану процесінің сандық модельдеуі ұсынылған. Зерттеу жану процесіне, температураның цилиндрлік жану камерасындағы таралуына отын массасы мен бүрку бұрышының әсерін бағалауға бағытталған. Отын массасы 5-тен 20 мг-ға дейін, ал бүрку бұрышы 2°-тан 15°-қа дейін өзгертілді. Екі отын түрі үшін жылу бөлу сипаттамаларын және жалын құрылымын анықтау мақсатында температуралық өрістер уақыт бойынша талданды. Нәтижелер отын бүрку массасының артуы жалын биіктігі мен жану температурасының айтарлықтай өсуіне әкелетінін, бұл жылу энергиясының бөлінуінің артуымен байланысты екенін көрсетті. Бүрку бұрышының әсері тек аз мәндерде елеулі екені анықталды, ал үлкен мәндерде оның екі түрлі сұйық отынның температуралық өрістеріне әсері шамалы болды. Бензол мен тридекан арасындағы салыстырмалы талдау бензолдың жану процесі жоғары температурада және қарқындылығы жағынан тридеканнан басым болатынын көрсетті. Бұл тұжырымдар іштен жанатын қозғалтқыштарда қолданылатын жану жүйелерінің құрылымын жетілдіру және отын бүрку параметрлерін оңтайландыру үшін маңызды. Зерттеу нәтижелері жану тиімділігін арттыруға және қоршаған ортаға зиянды заттардың шығарылуын азайтуға қолданылуы мүмкін.

Кілт сөздер: жануды сандық модельдеу, сұйық отындар (бензол, тридекан), айдалатын отынның массасы, бүрку сипаттамалары, температура өрісі, концентрация өрістері

М. Рыспаева, И. Березовская

Численное моделирование турбулентного горения жидких топлив: сравнительный анализ бензола и тридекана

В работе представлено численное моделирование процесса сгорания двух жидких топлив (бензола и тридекана) с применением вычислительной программы KIVA-II. Исследование сосредоточено на оценке влияния массы топлива и угла распыла на процесс сгорания, а также на распределение температуры в цилиндрической камере сгорания. Масса топлива варьируется от 5 до 20 мг, а угол распыла – от 2° до 15°. Анализируются температурные поля во времени с целью определения характеристик тепловыделения и структуры пламени для двух видов топлива. Результаты показывают, что увеличение массы впрыска приводит к значительному увеличению высоты пламени и температуры сгорания,

что определяется увеличением выделения тепловой энергии. Показано, что влияние угла распыла значимо только при малых значениях, в то время как при больших значениях оно мало влияет на температурные поля обоих типов жидких топлив. Сравнительный анализ между бензолом и тридеканом показывает, что горение бензола происходит более интенсивно и при более высоких температурах, чем процесс сгорания тридекана. Эти выводы необходимы для оптимизации параметров впрыска топлива и совершенствования конструкции систем сгорания в двигателях внутреннего сгорания. Результаты исследования могут быть применены для повышения эффективности сгорания и снижения вредных выбросов в окружающую среду.

Ключевые слова: численное моделирование горения, жидкие топлива (бензол, тридекан), масса впрыскиваемого топлива, характеристики распыления, температурное поле, поля концентрации

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