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NUMERICAL MODELING OF TEMPERATURE PLUME FORMATION OF NON-ISOTHERMAL LIQUID INJECTIONS

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ABSTRACT

This paper presents the results of computational experiments to study the formation of a spray and a temperature plume of non-isothermal liquid injections under high turbulence. Numerical modeling of atomization and combustion of liquid fuel injections and the influence of the initial gas temperature in the combustion chamber on these processes has been carried out. The temperature in the combustion chamber varied from 700 K to 1500 K for two types of liquid fuels: octane and dodecane. The distributions of liquid fuel droplets along the radii and temperature at various points in time are constructed. The influence of the initial temperature on the concentration characteristics of various types of fuel is revealed. As a result, it was found that at a pressure of over 80 bar with high turbulence, the gas temperature equal to 900 K was taken as optimal. At this temperature, the chamber is heated to high temperatures and the concentration of the resulting reaction products is the lowest. The obtained results can be applied in the construction of the liquid fuels' combustion theory and will contribute to a deeper understanding of the complex physical and chemical phenomena that occur in combustion chambers.

Keywords: liquid fuel, spray, temperature flame, computational experiment, combustion.

1. Introduction

In the modern world, the limited resources of fossil fuels dictate the need to find more economical ways to burn it. The scale of industrial production is such that the problem of the formation of harmful substances during the combustion of organic fuels comes to the fore. In the total air pollution by waste from the production of thermal power plants and the activities of vehicles, dust emissions account for 20%, for sulfur dioxide – 50%, for nitrogen oxides – 30% [1-5].

Road transport is the most aggressive in comparison with other modes of transport in relation to the environment, which is a powerful source of its chemical, noise and mechanical pollution. It should be emphasized that, with an increase in the car park, the level of the harmful effects of vehicles on the environment is intensively increasing.

When designing engines of previous generations of cars, insufficient attention was paid to the problem of environmental friendliness, which led to increased emissions of toxic substances. Also, catalytic exhaust gas cleaning systems were not used in cars. For cities and industrial centers, the share of vehicles in the total volume of pollution is much higher and reaches 70% or more, which creates a serious environmental problem that accompanies urbanization. The largest share of chemical pollution of the environment by road transport is accounted for by the exhaust gases of internal combustion engines. Because of the physical and mechanical processes in the engine cylinders, the actual composition of the exhaust gases is very complex and includes over 200 components, a significant part of which is toxic.

The composition of the exhaust gases of engines on the example of passenger cars without their neutralization is shown in Figs. 1 and 2.

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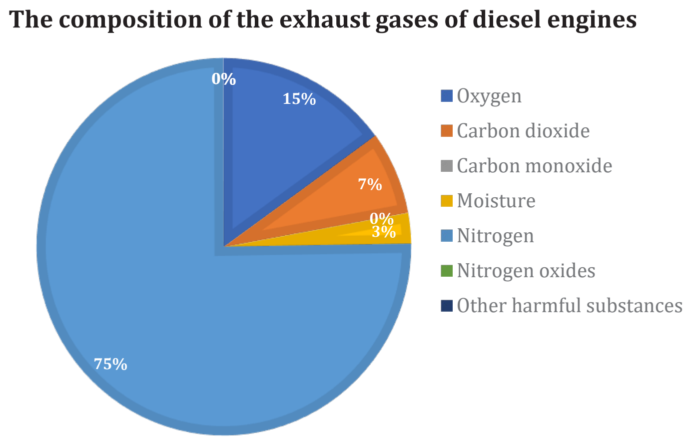


Fig. 1. The composition of exhaust gases on the example of diesel engines without neutralization.

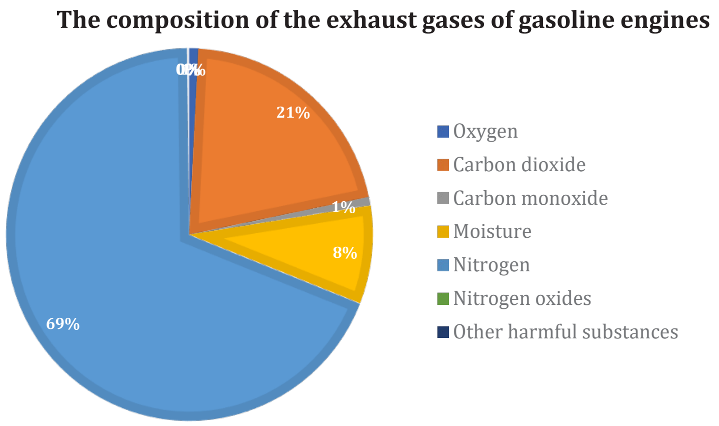


Fig. 2. The composition of exhaust gases on the example of gasoline engines without neutralization.

As seen from the figures, the composition of the exhaust gases of the considered engines differs significantly, primarily in the concentration of products of incomplete combustion of carbon monoxide, hydrocarbons, nitrogen oxides and soot. The difference in the composition of the exhaust gases of gasoline and diesel engines is explained by the large excess air coefficient of diesel engines and better fuel atomization.

New technologies and equipment are based on a deep scientific understanding of the laws of physical and chemical processes that determine the characteristics of the combustion of liquid hydrocarbons depending on their composition, dynamic and thermal conditions implemented in specific modes and devices. The development of promising injector jet devices for burning liquid hydrocarbons requires the study of several interrelated processes, such as fuel dispersion, the formation of a spatial structure of a two-phase reacting flow, interfacial heat and mass transfer, the formation of soot particles, mixture formation, ignition, gasification and burnout of fuel, the output of combustion products, including toxic components. These processes are the subject of many modern studies devoted to the development of scientific foundations and the creation of methods for intensifying heat and mass transfer processes in multiphase reacting systems [6-10].

Thus, one of the promising directions for reducing the volume of harmful automotive emissions into the atmosphere and optimizing the combustion process is the use of mathematical modeling methods for spraying non-isothermal liquid injections during the combustion of low-octane liquid hydrocarbon fuels. This allows, first of all, to reduce the concentration of toxic oxides of carbon (CO and CO_2) and nitrogen, which are released as a result of the operation of thermal engines and increase the efficiency of fuel combustion The study of the regularities governing the characteristics of the combustion of liquid fossil fuels is an urgent scientific and technical problem, the solution of which is of fundamental importance for the creation of promising technologies for energy production and engine building.

The solution of the tasks set contributes to the transition to an environmentally friendly and resource-saving «green» thermal power industry while expanding the raw material base, reducing the emission of harmful industrial emissions, and solving the problem of optimization and efficiency of fuel combustion.

2. Mathematical and physical statement of the problem

All heat and mass transfer processes taking place in combustion chambers of thermal machines are turbulent and the state of turbulence in the flow movement impresses the flow parameters such as momentum transfer, temperature, and concentration of substances in the mixture. In this paper, we have used a mathematical model of atomization and dispersion of liquid injections, which describes the process of ignition and combustion of liquid fuels based on equations of conservation of mass, momentum, energy, and concentration of components.

The mass conservation equation is planned as below [11-15]:

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

where *u* is the liquid velocity. If a gas-liquid mixture is considered, the source term S_{mass} represents the local change in gas density because of evaporation or condensation.

The momentum conservation equation for the gas is [13, 15]:

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho\left(\vec{u} \cdot grad\right)\vec{u} = div\vec{\vec{\xi}} + \rho \vec{g} + S_{mom} \tag{2}$$

If the one-phase gas flow is considered, $S_{mom}=0$; if the two-phase flow, S_{mom} represents the local rate of change of momentum in the gas phase because of droplet motion.

Equation of conservation of internal energy [12-16]:

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

where q is the specific heat flux, represents the Fourier law of heat transfer. The source term S_{energy} refers to the contribution to the change in internal energy because of atomized liquid or solid phase.

The concentration conservation equation for component m has the form [17, 18]:

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

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

Two liquid fuels were used in our work: octane and dodecane, which are liquid hydrocarbons of the alkane class and are found in large quantities in oil, straight-run gasoline (up to 10%), and also in large quantities in synthetic gasoline produced from CO and H_2. The oil of Kazakhstan is characterized by a predominance of normal paraffin hydrocarbons, so straight-run gasoline from it is characterized by low octane numbers.

Calculation experiments on atomization and temperature plume formation during octane and dodecane combustion were carried out in a model cylinder-shaped combustion chamber. A general view of the chamber is shown in Fig. 3. This Fig. also shows the model of the injector with multiple holes, which is most often used in modern internal combustion engines. Ratio Li/Di is a very important parameter for multi jet injectors, as it affects the formation of the internal flow at the outlet of the injector orifice and the spray formation. The computational domain comprises 650 cells. Liquid fuel is injected through a nozzle,

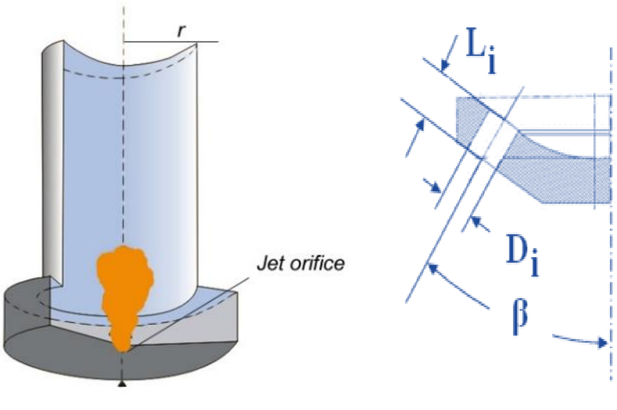


Fig. 3. General view of the combustion chamber and virtual prototype of a multi-hole injector of an internal combustion engine, where Li is injector's hole length, D_i denotes nozzle orifice diameter, and parameter β shows the injection angle from the central axis of the injector.

which is in the center of the lower part of the combustion chamber. The initial gas temperature in the combustion chamber is 900 K.

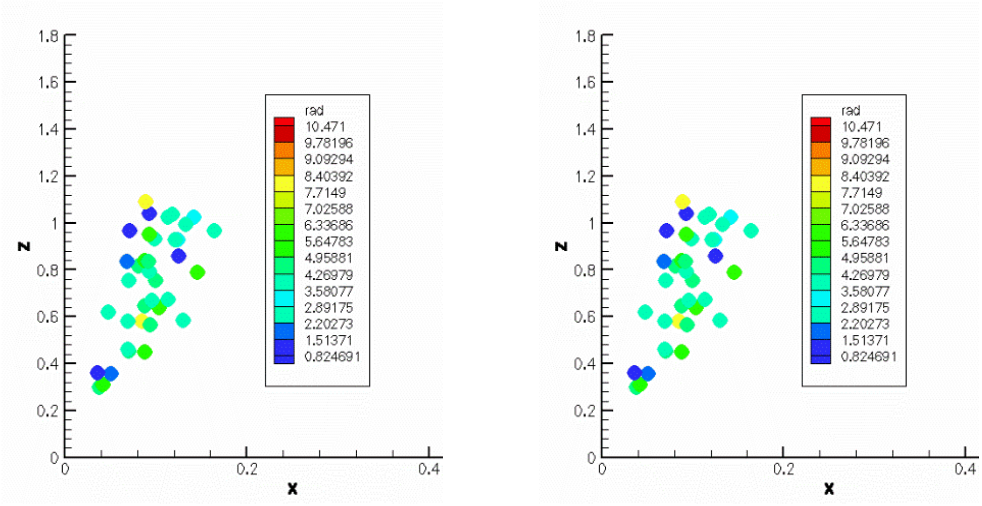
In this paper, we investigated the effect of initial gas temperature on the formation and evolution of the liquid injection temperature plume under high turbulence. The temperature in the combustion chamber varied from 700 K to 1500 K. The pressure in the combustion chamber was 100 bar for octane and 80 bar for dodecane and the injection velocity was 350 m/s in both cases. These values were taken from previous works of the authors [19-23].

3. Results and Discussion

Figures 4 and 5 show some results of computational experiments on the radius distribution of liquid fuel droplets (octane and dodecane), respectively. Analyzing the obtained data, we can say that with increasing temperature in the combustion chamber, the droplet size of the liquid fuel decreases, but is insignificant.

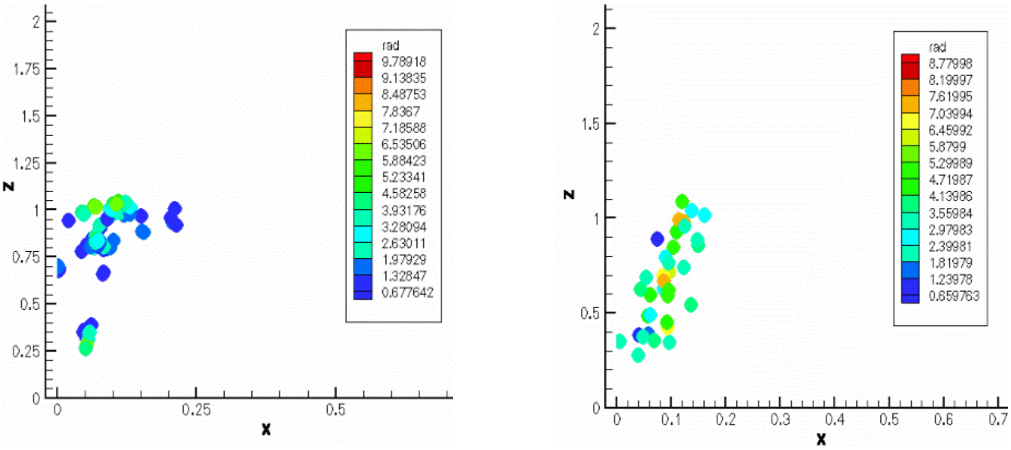
Comparing the behavior of octane and dodecane, it can be seen that droplets in both fuels spread within the same limits: they rise to the same height of 1.2 cm at a time and there is also uniform distribution of droplets up to 0.2 cm across the chamber width. Octane and dodecane vapors reach the same height and their concentration on the axis is approximately the same.

Consider the dispersion of liquid fuel droplets by specific temperature in the combustion chamber (Figs. 6 and 7). At the bottom of the chamber, both fuel droplets have a temperature of about 300 K, but the temperature of dodecane



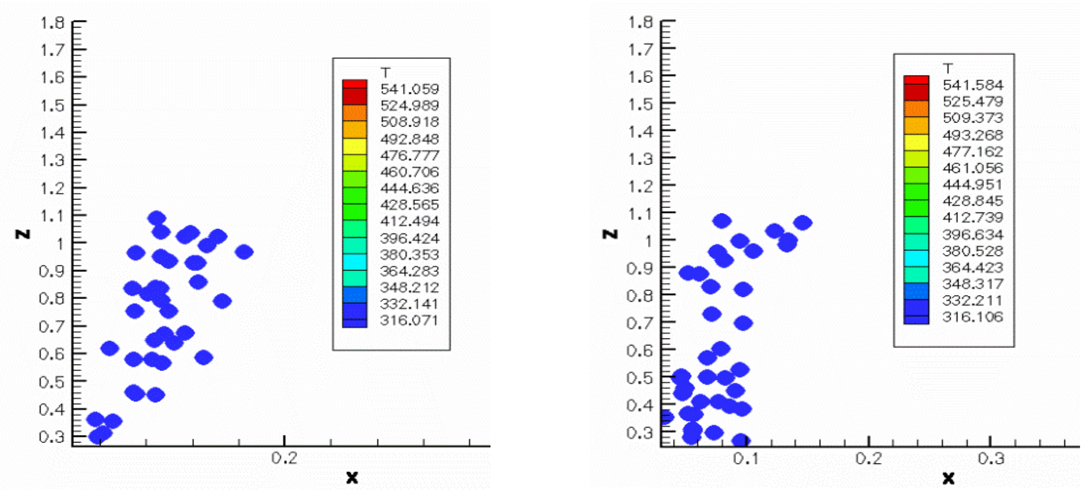
a) 1000 K b) 1500 K

Fig. 4. Distribution of octane droplets along the radii in the space of the combustion chamber at different initial temperatures.



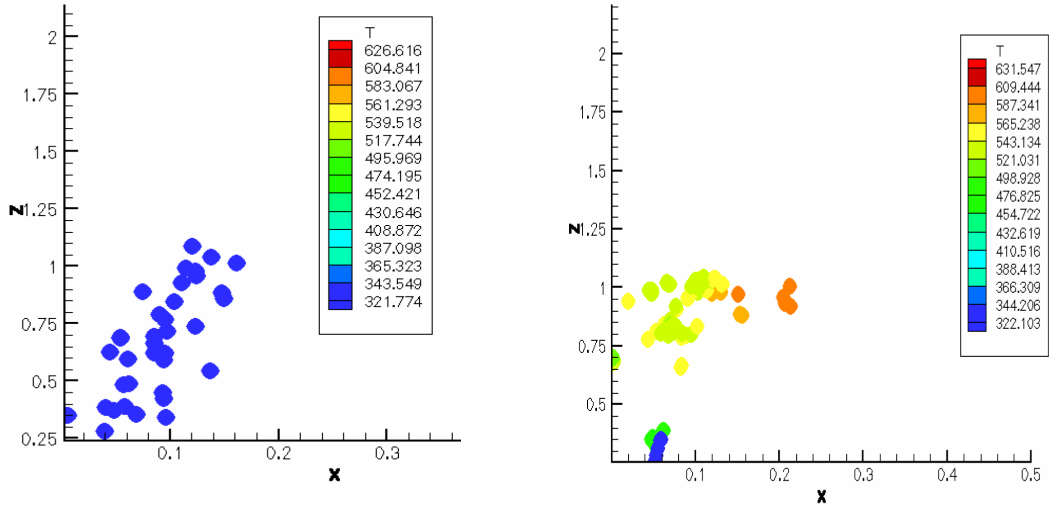
a) 1000 K b) 1500 K

Fig. 5. Distribution of dodecane droplets along the radii in the space of the combustion chamber at different initial temperatures.



a) 1000 K b) 1500 K

Fig. 6. Temperature distribution of octane droplets in the combustion chamber space at the different initial temperatures.



a) 1000 K b) 1500 K

Fig. 7. Temperature distribution of dodecane droplets in the combustion chamber space at the different initial temperatures.

droplets reaches 565 K. This indicates that a temperature of 1500 K is sufficient for evaporation and subsequent ignition of dodecane.

Because of a calculation experiment, it was found that no combustion occurred at pressures over 80 bar and temperatures of 800 K and below, as seen from the Fig. 8 showing the dependence of the maximum gas temperature on the initial temperature in the combustion chamber (Fig. 8). As the analysis of Fig. 8 shows, if the oxidizer in the combustion chamber has a temperature above 900 K, then liquid fuel combustion with high heat release and heating of the chamber is observed in this case.

Thus, during combustion of octane at T = 900 K, T_g = 1726 K is released and as a result, at T = 1500 K, T_g = 2208 K is released. The initial temperature in the combustion chamber has the greatest influence on the combustion of dodecane because an increase in the initial temperature from 900 to 1500 K leads to an increase in the maximum temperature from 2080 to 2685 K.

Figure 9 shows a graph of the distribution of the maximum concentration of CO_2 for the two fuels combusted as a function of the initial gas temperature in the combustion chamber. During dodecane's combustion, the concentration of formed carbon dioxide takes the highest value of 0.148 g/g at the initial gas temperature of 1000 K and the lowest one of 0.120 g/g at T = 900 K. When burning octane at T = 900 K and above, a slight increase in CO_2 concentration is observed, which is 0.085 g/g.

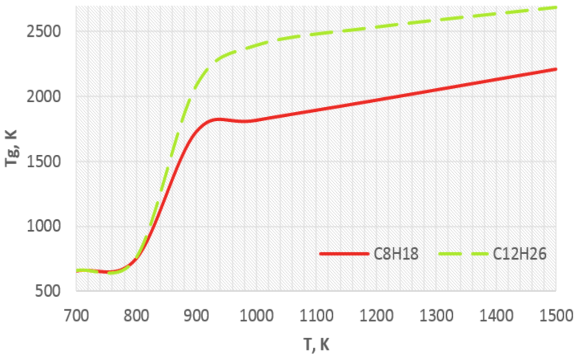


Fig. 8. Flame temperature distributionas a function of the initial gas temperature in the combustion chamber.

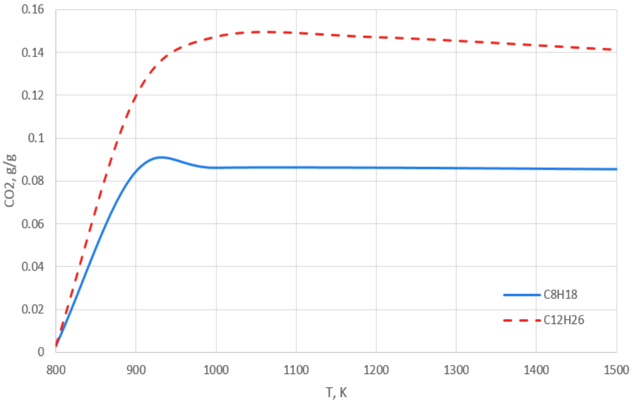


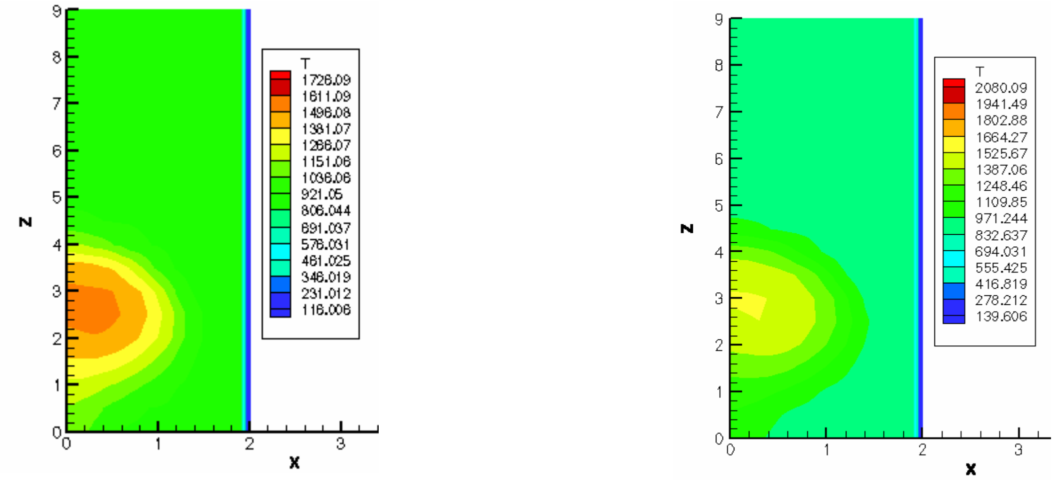
Fig. 9. Dependence of the formed carbon dioxide concentration on the initial gas temperature in the chamber.

Figures 10 and 11 show the change in temperature over time in the combustion chamber for two liquid fuels at an initial oxidizer temperature of 900 K. At the initial point in time in the fuel atomization area, the temperature decreases slightly because of the heat input for evaporation of the fuel droplets. An increase in pressure understandably reduces the high-temperature region and delays the ignition time, and most of the combustion chamber has a temperature of about 1000 K. When the fuel vapor/oxidizer mixture ignites, the fuel burns, and most of the chamber width is covered by the flame. At 100 bar, octane combustion proceeds with a heat release of 1726 K, while dodecane combustion reaches a maximum temperature of 2080 K.

As shown in Fig. 12, at high pressure the area of maximum oxygen consumption decreases as the fuel concentration decreases. At time 3 ms in octane combustion (Fig. 12 a), this region is in the flame’s core between 2.9 to 4.8 cm in height of the chamber and contains the least amount of oxidant 0.0125 g/g compared to dodecane combustion where the O_2 concentration is 0.05 g/g (Fig. 12 b) at 3.8 to 4.6 cm.

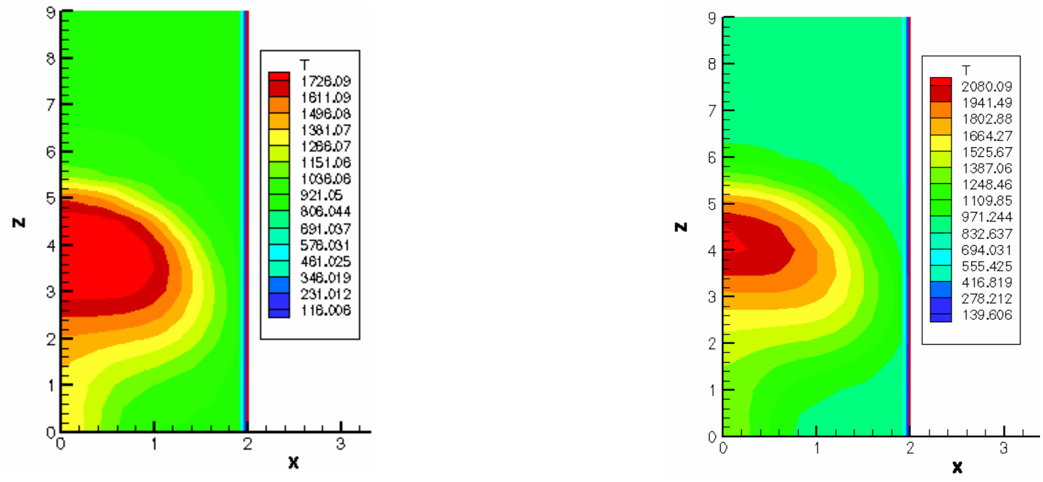
Also, during computational experiments, we considered the evolution of liquid injection vapors in the presence of evaporation, which gives a deep understanding of the propagation of spray drops, its structure, and the formation of a homogeneous combustible mixture.

Figure 13 shows the results of numerical simulation of the fuel vapor fraction (octane) in the vertical sections of the combustion chamber at two points in time after the injection starts. Fuel vapors are released in the center of the spray itself, their trajectories and shapes are well separated from each other. When moving downstream, the fuel vapors surrounding the torch merge with each other.



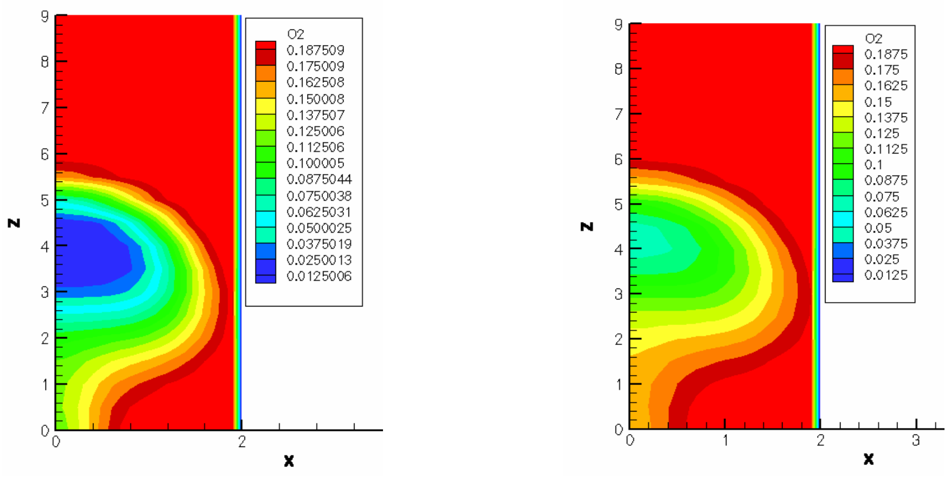
a) octane b) dodecane

Fig. 10. Temperature plume distribution during octane and dodecane combustion at time t = 2.5 ms.



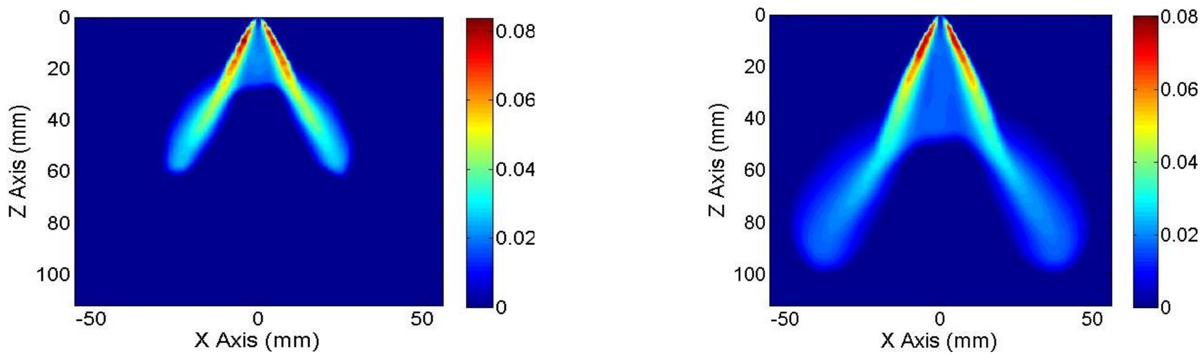
a) octane b) dodecane

Fig. 11. Temperature flare distribution during octane and dodecane combustion at time t = 3 ms.



a) octane b) dodecane

Fig. 12. Oxidizer concentration fields at time 3 ms.



a) t = 1.75 ms b) t = 3 ms

Fig. 13. Distribution of fuel vapors in the vertical section of the combustion chamber at various times after the injection starts.

Analyzing Fig. 13, one can see that at this stage of the atomization process itself, the fuel vapor fractions have the shape of a hollow cone. The spread of the spray jet can theoretically be divided into two regions: the first region is located near the nozzle and the second refers to the downstream region where a change in the spray angle is observed. At this point in time, depending on the location of the nozzle, the spray angle changes.

According to all obtained results, the gas temperature in the combustion chamber is taken as the optimum temperature equal to 900 K. Based on these results, the optimum combustion modes for octane and dodecane are determined: at high pressures and high turbulence, according to which at oxidizer temperature of 900 K the ignition and combustion process of fuel occurs, the chamber is heated to high temperatures.

4. Conclusion

Based on a mathematical model, computational experiments were carried out to study the atomization and combustion of liquid fuels depending on the initial temperature of the gas in the combustion chamber.

Computational experiments of the initial temperature influence on the processes of atomization and combustion of liquid fuels at high turbulence were carried out. Distributions of droplets for two types of liquid fuel (octane and dodecane) along the radii and specific temperature were plotted depending on the initial temperature of the gas in the chamber, which showed that octane and dodecane vapors reach the same height, and their concentration on the axis approximately coincides.

The distribution of the temperature flame depending on the initial temperature in the chamber showed that the maximum of 2080 K for octane and 2685 K for dodecane falls on T = 1500 K. The temperature profiles and concentration fields of the consumed oxygen at the moments of ignition (t = 2.5 ms) and intense combustion (t = 3 ms) were obtained.

The distribution of carbon dioxide concentration showed that, as expected, the more intense the reaction is, the more CO_2 is formed. At 900 K, a minimum amount of 0.120 g/g of carbon dioxide is released for dodecane and, for octane, an insignificant concentration of carbon dioxide is 0.085 g/g, which lies within the permissible limits.

The optimal temperature of the gas in the combustion chamber is taken to be 900 K at high pressures and high turbulence, at this temperature of the oxidizer, ignition and fuel combustion occurs, the chamber heats to high temperatures, with complete combustion of the fuel, the concentrations of the formed reaction products (CO_2) are the smallest.

In a numerical study of the evolution of fuel vapors during evaporation in vertical sections of the combustion chamber at different times, it was found that at the initial stage of the combustion process, fuel vapors gain a closed structure, which then turns into a hollow cone shape.

The obtained results of numerical simulation on the study of the physics of liquid injections provide a deeper understanding of the spray multiplication, the interaction of cocurrent air and liquid jets, the structure and formation of the mixture, the phenomenon of jet-to-jet interaction, which ultimately has a huge impact on the global injection structure.

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Численное моделирование образования температурного факела неизотермических жидких впрысков

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Аннотация

В данной работе представлены результаты вычислительных экспериментов по исследованию образования распыла и температурного факела неизотермических жидких впрысков при высокой турбулентности. Проведено численное моделирование распыла и горения жидких впрысков топлив и влияния начальной температуры газа в камере сгорания на данные процессы. Температура в камере сгорания менялась от 700 до 1500 К для двух видов жидких топлив: октана и додекана. Построены распределения капель жидких топлив по радиусам и по температуре в различные моменты времени. Выявлено оказываемое влияние начальной температуры на концентрационные характеристики топлива различного вида топлив. В результате установлено, что при давлении более 80 бар при высокой турбулентности за оптимальную принимается температура газа равная 900 К. При данной температуре камера прогревается до высоких значений температур и концентрация образующихся продуктов реакции наименьшая. Полученные результаты могут быть применены при построении теории горения жидких топлив и будут способствовать более глубокому пониманию сложных физико-химических явлений, которые происходят в камерах сгорания.

Ключевые слова: жидкое топливо, распыл, температурный факел, вычислительный эксперимент, горение

Изотермиялық емес сұйық бүркулердің температуралық алауының түзілуін сандық модельдеу

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Аңдатпа

Бұл жұмыста жоғары турбуленттіліктегі изотермиялық емес сұйық бүркулердің бүрку және температуралық алауының түзілуін зерттеу бойынша есептеуіш тәжірибелерінің нәтижелері ұсынылған. Отындардың сұйық бүркулерінің бүрку және жану процестеріне және осы процестерге жану камерасындағы газдың бастапқы температурасының әсеріне сандық модельдеу жүргізілген. Жану камерасындағы температура қос отын түрі – октан және додекан үшін 700 К-нен 1500 К-ге дейін өзгеріп отырды. Әр түрлі уақыт мезеттеріндегі сұйық отын тамшыларының радиусы және температурасы бойынша таралуы тұрғызылды. Бастапқы температураның әр түрлі отын түрлерінің концентрациялық сипаттамаларына әсері анықталды. Нәтижесінде 80 бар қысымда және жоғары турбуленттілікте 900 К-ге тең газ температурасы тиімді деп қабылданды. Аталған температурада камера жоғары температура мәндеріне дейін қыздырылады және түзілетін реакция өнімдерінің концентрациялары ең аз болады. Алынған нәтижелер сұйық отындардың жану теориясын қалыптастыруда қолданылады және жану камераларында жүзеге асатын күрделі физика-химиялық құбылыстардың терең түсінуге түрткі болады.

Кілт сөздер: сұйық отын, бүрку, температуралық алау, есептеуіш тәжірибе, жану.