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INVESTIGATION OF THE DROPLET DISPERSION INFLUENCE ON THE ATOMIZATION OF LIQUID FUEL PROCESSES IN VIEW OF LARGE-SCALE STRUCTURES FORMATION

This paper is devoted to an important research from the point of view of modern combustion physics of the problem of numerical modeling of spraying, ignition and combustion of liquid fuel at different values of the initial radius of the droplets. The need for a detailed study of the physicochemical processes taking place in the combustion of liquid fuels is determined by the increased requirements for the efficiency of various technical devices, the accuracy of the prediction of ignition, the burning rate and is because of modern environmental requirements for environmental protection. The efficiency of various technical devices, in particular internal combustion engines, is largely based on the results of a fundamental study of the processes of physics and combustion chemistry. Purpose of the work is to use methods of mathematical modeling, investigate the process of atomization, ignition and combustion of liquid fuel droplets at various initial radii, in the presence of turbulence, chemical transformations, and determine the optimal parameters for liquid fuel combustion. Computer simulation of the spray and combustion of liquid fuel injection was carried out using differential equations describing turbulent flow in the presence of chemical reactions.

The theoretical significance of the research is that the fundamental results, which are got in this work, can be applied in the combustion's construction theory to achieve a deeper understanding of complex physical and chemical phenomena, something in the combustion chambers. The practical significance of computational experiments is that the results obtained can be used in the design of various technical devices using combustion, which would solve simultaneously the problem of process optimization, increasing the efficiency of fuel combustion and minimizing emissions of harmful substances.

Key words: atomization, combustion chamber, liquid fuel, numerical simulation, high turbulence, harmful emissions.

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Исследование влияния дисперсности капель на процессы распыла жидкого топлива с учетом образования крупномасштабных структур

Данная статья посвящена исследованию проблемы численного моделирования распыла, воспламенения и горения жидкого топлива при различных значениях начального радиуса капель, которая является наиболее важной с точки зрения современной физики горения. Необходимость достоверного изучения физико-химических процессов, происходящих при сжигании жидких топлив, определяется предельно высокими требованиями к эффективности различных технических устройств, точности прогнозирования воспламенения, скорости горения и обусловлена современными экологическими требованиями по охране окружающей среды. Эффективность различных технических устройств, в частности двигателей внутреннего сгорания, в значительной степени базируется на результатах фундаментального исследования физики и химической кинетики процессов горения. Целью работы является исследование процессов распыла, воспламенения и горения жидкого топлива при различных значениях начального радиуса капель с учетом турбулентности и химических реакций посредством методов математического моделирования и определение оптимальных параметров горения жидкого

топлива. Компьютерное моделирование распыла и горения впрыска жидкого топлива выполнялось с использованием дифференциальных уравнений, описывающих турбулентный поток при наличии химических реакций.

Теоретическая значимость исследования заключается в том, что фундаментальные результаты, полученные в этой работе, могут быть применены в построении теории горения для достижения более глубокого понимания сложных физических и химических явлений, происходящих в камерах сгорания. Практическая значимость вычислительных экспериментов заключается в том, что полученные результаты могут быть использованы при проектировании различных технических устройств, использующих сжигание, которые одновременно решали бы задачу оптимизации процесса, повышения эффективности сжигания топлива и минимизации выбросов вредных веществ.

Ключевые слова: распыл, камера сгорания, жидкое топливо, численное моделирование, высокая турбулентность, вредные выбросы.

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Ірі масштабты құрылымдардың түзілуін ескергендегі тамшылардың дисперстілігінің сұйық отынды бүрку процесіне әсерін зерттеу

Берілген мақала заманауи жану физикасы тұрғысынан анағұрлым маңызды саналатын бастапқы радиустың әр түрлі мәндеріндегі сұйық отынның бүрку, тұтану және жануын сандық модельдеу мәселесіне арналады. Сұйық отындарды жағу барысында өтетін физика-химиялық процестерді сенімді зерттеу қажеттілігі түрлі техникалық құрылғылардың тиімділігіне тұтануды болжау дәлдігіне, жану жылдамдығына қойылатын талаптардың жоғарылығымен анықталады және қоршаған ортаны қорғау бойынша заманауи экологиялық талаптарға негізделеді. Түрлі техникалық құрылғылардың, оның ішінде іштен жану қозғалтқыштарының тиімділігі айтарлықтай дәрежеде жану процесінің физикасы мен химиялық кинетикасын іргелі зерттеу нәтижелеріне негізделеді. Жұмыстың мақсаты – математикалық модельдеу әдістері арқылы турбуленттілік пен химиялық реакцияларды ескергендегі тамшылардың бастапқы радиустарының әр түрлі мәндеріндегі сұйық отынды бүрку, тұтану және жану процестерін зерттеу және сұйық отынның жануының тиімді параметрлерін анықтау. Сұйық отынның бүркуі мен жануын компьютерлік модельдеу химиялық реакциялар бар кездегі турбулентті ағынды сипаттайтын дифференциалдық теңдеулерді қолдана отырып жүргізілді.

Зерттеудің теориялық құндылығы аталған жұмыста қол жеткізілген іргелі нәтижелерді жану камераларында өтетін күрделі физикалық және химиялық құбылыстарды терең түсіну үшін жану теориясын қалыптастыруда қолданылатындығымен анықталады. Алынған нәтижелерді процесті оңтайландыру, отынды жағудың тиімділігін арттыру және зиянды қалдықтардың мөлшерін азайту міндетін бірмезгілде шешетін жануға негізделген түрлі техникалық құрылғыларды жобалау барысында пайдалану мүмкіндігі есептеуіш тәжірибелердің практикалық маңыздылығын білдіреді.

Түйін сөздер: бүрку, жану камерасы, сұйық отын, сандық модельдеу, жоғары турбуленттілік, зиянды қалдықтар.

Introduction

Nuclear and thermonuclear energy in developed countries is only 20% of the total energy produced, and alternative and non-traditional energy is only 5% in the total volume of energy production worldwide. The main volume of energy produced, and this is over 70% of the generated energy, comes from the use of traditional fossil fuels [1-3]. Natural fuels of organic origin include peat, lignites, bituminous and anthracite coals, oil and natural gas. We often refer these fuels to as fossil fuels because they are the end products of the physicochemical transformations of fossilized plant remains. Various fossil fuels are used in the energy sector, but the main ones are gaseous, refined petroleum products and solid fuels.

Technologies for capturing and keep carbon dioxide and methane emissions control at all stages of the incremental cost of fossil energy. It can help meet the enormous objectives of reducing CO_2 emissions while fossil fuels are still part of the energy system. These measures allow fossil fuels to be part of the solution, rather than remain part of the

problem. Sustainable economics assigns an important role in energy systems to each technology.

Fossil fuels today account for 80% of global primary electricity demand; the energy system supplies about two-thirds of the world's CO_2 emissions [4]. The emissions of methane and other transient air pollutants are affecting the climate. It is believed to be seriously underestimated; it is likely that the processes of generation and consumption of electricity account for a large share of emissions. Nowadays, a significant proportion of biomass fuels are used for heating and small-scale cooking in the world. These are extremely inefficient and environmentally polluting processes; they are harmful to indoor air quality in many less developed countries. Using renewable biomass in this way presents a challenge from a sustainable development perspective.

If modern trends continue, the current share of fossil fuels is maintained and the demand for electricity nearly doubles by 2050. Emissions will far exceed the carbon limit for a global warming limitation of 2 degrees Celsius. This level of emissions would have catastrophic consequences for the planet. There are several opportunities in the energy sector to reduce emissions; the most significant among them are reducing energy consumption and reducing the carbon intensity of the energy industry by switching to other types of fuels and controlling CO_2 emissions. The need to reduce emissions does not prohibit the use of fossil fuels, but requires a significant change in approach. It does not combine the business as usual scenario with the reduction of emissions in global energy systems.

Energy efficiency and renewable solutions are often the only solutions. Climate goals in an energy context need to achieve, but they are not enough. It is impossible to uniformly use renewable fuels as a substitute for fossil fuels today in the energy sector. It is because of the distinct possibilities of different energy subsectors to switch from fossil fuels to renewable fuels. Alternative technologies that could replace existing methods are not yet available at the scale required, so current technologies are expected to continue in the short to medium term. CO_2 emissions are not the only fossil fuel issue that needs to be addressed. 110 million tons of methane is emitted annually into the atmosphere at all the stages of the increment in the value of fossil sources. This is a significant part of total methane emissions. Methane is a powerful greenhouse gas, emissions must be significantly reduced. An ongoing and critical challenge is to ensure a better quality of life and economic growth while reducing the energy sector's impact on the environment. The transition to a sustainable energy system represents an opportunity to improve energy efficiency all the way from source to use, minimize environmental impact, reduce energy and carbon intensity, and correct energy market gaps. Seizing this opportunity will require a coordinated review of strategies and reform across multiple sectors.

Figure 1 shows necessity of liquid and gaseous fuel in any spheres all over the World [5].

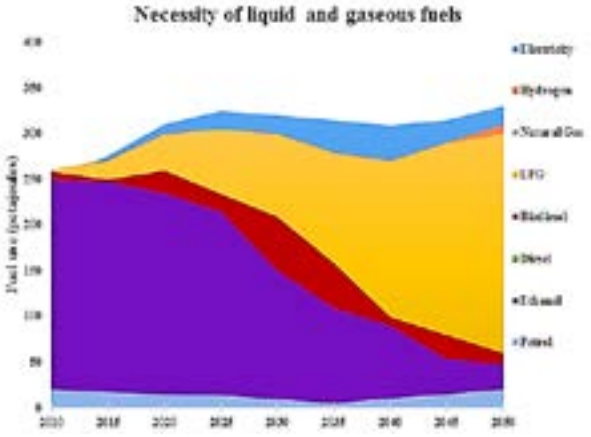


Figure 1 – Necessity of liquid and gaseous fuel in any spheres all over the World [5]

The combustion speed is determined by such process, which is the slowest. In the combustion's situation of uniform homogeneous mixtures of fuel-oxidant (air), this process is kinetics of chemical reactions. However, in case of heterogeneous mixtures, such processes are physical processes, vaporization and the mixing. The model of the combustion process of heterogeneous mixtures, in which it assumed that there is a mutual interaction of the phase gaseous and liquid and processes controlling the combustion are the slowest processes, was worked out.

Regarding liquid fuels, the slowest process is the decomposition process of the liquid phase. Combustion processes of liquid fuels are relative to the boundary layer, which then is relative to the speed and the character of the flow of the stream of gases.

Flow can be laminar, transient or turbulent. Speed of the stream of gases intensifies combustion processes. The speed and the stream of gases influence the thickness of the boundary layer. Influence of pressure on combustion processes of liquid fuels multiples, and is connected with the influence of the speed of the stream of gases, and is

depend on the fuel. Increase in pressure intensifies combustion processes in phase gaseous, but decreases intensity decomposition of the liquid phase, which controls the combustion. Increase in pressure causes decreasing of the distance to the flame front from surface of the fuel, which increases the heat stream delivered to surface of the fuel and intensifies decomposition process (vaporization) of the fuel [6-8].

Intensification decomposition process of the fuel connected with pressure increase moves away the flame front from surface of the fuel. In these three situations, as a result, the opposed influence of the pressure and decomposition of the liquid phase can appear. Flame front can decrease distance, increase distance or to stay in the same distance to surface of the liquid fuel. Most previous models concerning the combustion of liquid fuels assumed that the fuel was homogeneous, the combustion has a constant character, a temperature on border surface of phases is boiling temperature of liquid. Influence of the radiation, diffusion, changes of pressure, changes of physical characteristics and chemical fuel, air and exhaust gases were neglected. Two situations: the combustion under conditions of the lack of the convection and conditioned appearances of the convection can be distinguished.

Mathematical model and methods

Breakup model

To describe the droplet breakup process in term of the critical deformation of the oscillating droplet is used for modeling this process in KIVA II code. $y=2e/r_d$ is the normalized radial droplet deformation, where e-the extension of the droplet radius from its equilibrium position, r_d is the droplet radius.

The time evolution of this quantity is described by the force, damped linear harmonic oscillator [9, 10]:

$$\frac{\partial^2 y}{\partial t^2} = \frac{2\rho_2 U_m^2}{3\rho_1 r_d^2} - \frac{8\sigma}{\rho_1 r_d^3} y - \frac{5\mu_1}{\rho_1 r_d^2}\frac{dy}{dt}, \qquad (1)$$

where the external forcing comes from the relative motion of the drop, the restoring force is surface tension and the damping force is the fluid dynamic viscosity, μ_1. The solution for $y(t)$ can be found analytically, and breakup is modelled by assuming that $y=1$ at the moment of breakup.

The Sauter Mean Radius (SMR) of the droplets at the moment directly after breakup can be found from the conservation of droplet energy during breakup [11, 12]:

$$S = \frac{r_p}{\frac{7}{3} + \rho_1 r_p^3 \left(\frac{dy}{dt}\right)_{bu}^2 / 8\sigma}, \qquad (2)$$

where r_p is the radius of the parent droplet and $(dy/dt)_{bu}$ is the value of dy/dt at breakup, i.e. when $y=1$. The TAB model produces a distribution of droplet sizes after breakup, given by:

$$f(r_d) = \frac{3}{S}\exp\left(-\frac{3r_d}{S}\right). \qquad (3)$$

The results predicted by the TAB model for modelling fuel sprays agree well with the experimental results of [13-17]. This model, however, over-predicts the rate of breakup and tends to under-predict the droplet size close to the injector. Tanner changed it to enable it to describe breakup at larger Weber numbers, which is the dominating mechanism in the primary breakup region of liquid jets [18, 19].

The primary break-up of the jet column is then related to the Kelvin-Helmholtz instability induced by the relative velocity at the interface. Among the many wavelengths, the one, which grows faster is considered as the one responsible for the break up, that is the more unstable one: the dimension of this wavelength and its growing rate.

Regarding numerical implementation of the models and to their competition, a substantial difference lies because KH model, regarding RT model and to TAB model, is not limited to a liquid mass redistribution within each numerical particle, but requires creation of new numerical particles characterized by diameters, velocities, temperatures directly governed by the generating particle. Figure 2 below shows the phenomena of instability in two-phase flows and their interaction with each other.

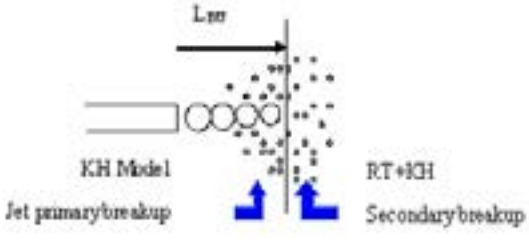


Figure 2 – KH-RT Interaction

A general conservation equation which governs the motion of a fluid in the Eulerian framework, based on the concepts of divergence theorem and Reynolds transport theorem, has been represented in equation (4) [20-24]:

$$\frac{dx}{dt} = P + S + F\,. \qquad (4)$$

In the equation above, a rate of change of physical quantity (X) is balanced by the production term P, supply term S and flux term F. Production term can be referred to source or sink term. Supply term S originates because of the body forces in the flow like gravity etc. Lastly, the flux term F comes into play because of the surface stresses on the fluid body or from heat flux through surfaces.

Similarly, the conservation equations for a specific physical quantity can easily be explained by the equations of the motion of a fluid with density (ρ), velocity ($\vec{u}$), and internal energy (e).

The total mass conservation equation [25, 26]:

$$\frac{d\rho}{dt} = \nabla(\rho\vec{u}) = \mathrm{S}_{mass}\,, \qquad (5)$$

S_{mass} is the change of mass density.

Momentum conservation equation for fluid mixture [25, 26]:

$$\frac{d\rho\vec{u}}{dt} + \nabla.(\rho\vec{u}\vec{u}) = \rho g - \nabla.(\tau) + \mathrm{S}_{mom}\,, \qquad (6)$$

S_{mom} is the rate of momentum exchange with spray per unit volume.

Energy conservation equation [25, 26]:

$$\frac{d\rho e}{dt} + \nabla.(\rho\vec{u}e) = -\nabla.(\vec{\mathrm{q}}) + (\nabla\,\vec{\mathrm{u}}/\,\tau) + \mathrm{S}_{energy}\,. \qquad (7)$$

Here $\vec{q}$ is the specific heat flux and can be explained by the simple Fourier law of heat transfer. The expression $\nabla u : \tau$ represents the double inner product of the gradient of u with Cauchy's stress tensor. The source term S_{energy} because of interaction with spray will be defined later.

Cauchy stress tensor, used in the above equations, is defined as:

$$\tau = -p\vec{I} - \mu[(\nabla\,\vec{\mathrm{u}} + \nabla\,\vec{\mathrm{u}}^{T}) - \frac{2}{3}\nabla\,\vec{\mathrm{u}}\vec{\mathrm{I}}]. \qquad (8)$$

Turbulence modelling

Statistic particles are injected one after another, thus yielding the random geometry of the liquid core; each particle trajectory ends after a length of time determined by kinetic energy transfer from the gas flow to the liquid.

The statistics of the core surface are used to get the size and position characteristics of the drops surrounding the core, sampled with the total mass rate equal to the inflowing liquid mass rate. RANS is used to simulating the gas flow and is conditioned by the liquid core. Such a conditioned flow of gas and subject to secondary atomization and coalescence, both modeled by an inter-droplet collision mechanism drags along the blobs formed around the core) (Figure 3) [27].

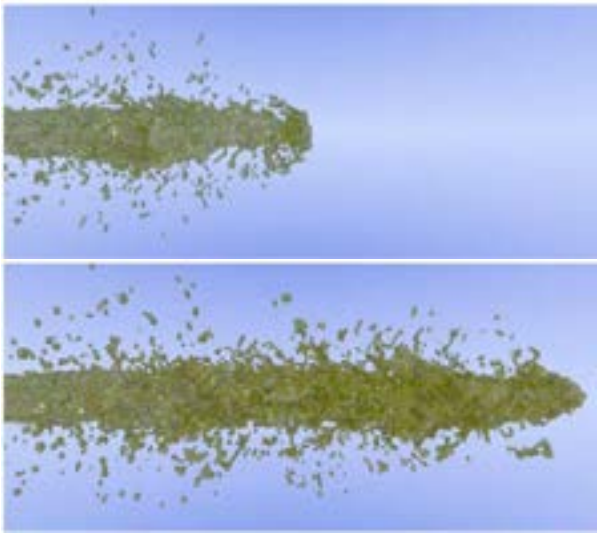


Figure 3 – Two successive snapshots of the turbulent atomization of a liquid diesel [27]

In this work, the model of combustion chamber as a cylinder was used, whose height is 15 cm, diameter 4 cm. General view of the combustion chamber is shown in Figure 4.

The computational domain comprises 650 cells. Fuel is injected using the nozzle, which is in the bottom center of the combustion chamber. Area of the nozzle is equal to $2 \cdot 10^{-4}$ см^2. Temperature of the walls of the combustion chamber is 353 K. The initial temperature of the gas in the combustion chamber 900 K, the fuel is injected at 300 K. Initial radius of the injected droplets 25 microns. Droplet

injection angle is 10^0. The pressure in the combustion chamber is 80 bar, injection speed of liquid fuel equal to 250 m/s.

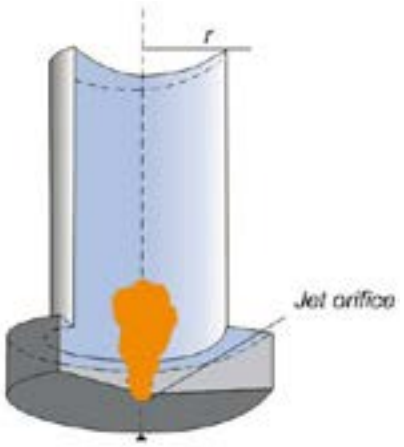
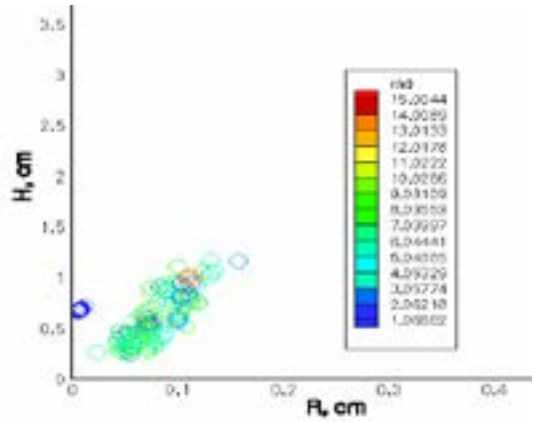


Figure 4 – General view of combustion chamber

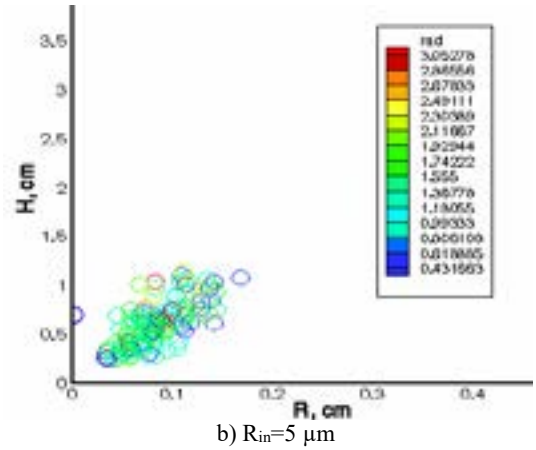
Results and Discussion

The computational experiment was performed, with high turbulence at 100 bar for an octane with a mass of 6 mg. The fuel was injected into the combustion chamber for 1.6 ms at 350 m/s. The droplet radius varied from 1 to 20 microns. Based on the results of the performed experiments, the size distributions of the liquid fuel droplets were obtained. The figures are presented for the initial drop radii of 1, 5, 10 and 20 microns. In all cases, the octane droplets are concentrated in an area up to 0.2 cm along the chamber radius and up to 1.5 cm in height.

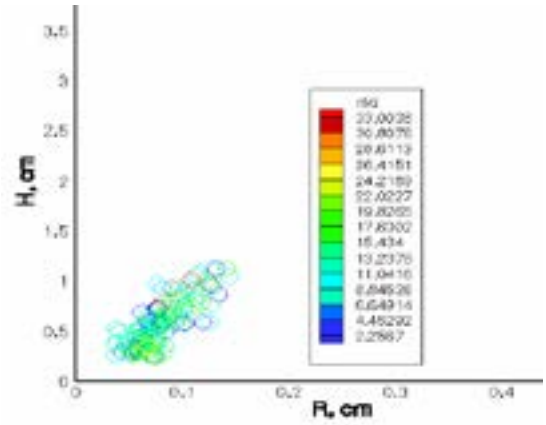
The initial radius affects the subsequent distribution of droplets in the combustion chamber space: when injecting droplets with an initial radius of 1 micron, droplets can reach over 3 microns in the chamber, at 20 microns – 57 microns respectively (Figure 5).



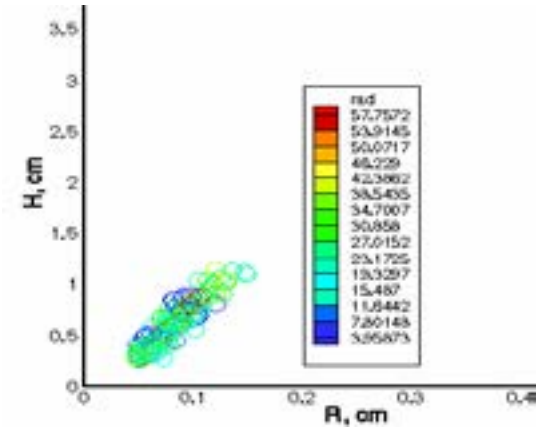
a) R_{in}=1 µm



b) R_{in}=5 µm



c) R_{in}=10 µm

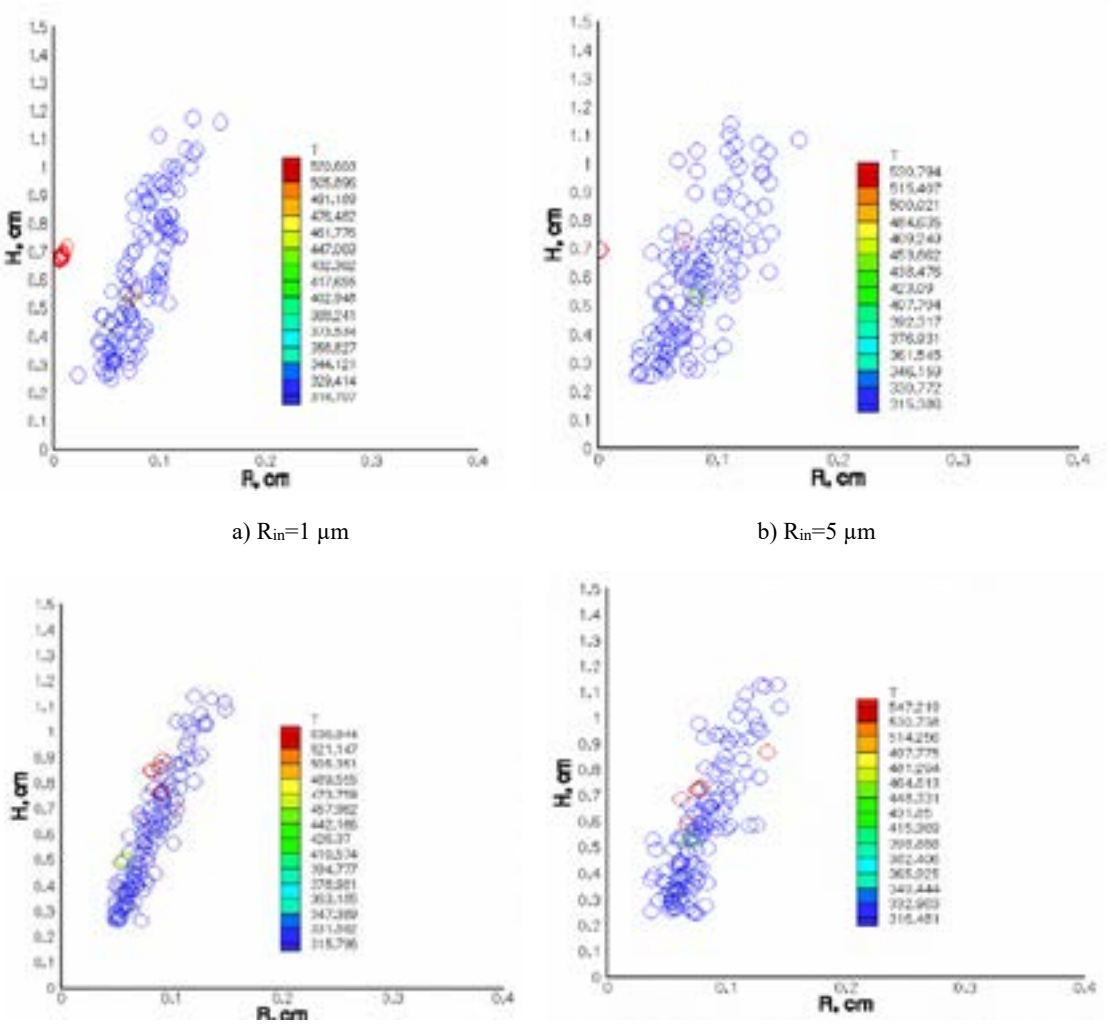


d) R_{in}=20 µm

Figure 5 – Octane droplet size distribution at different initial radii

Thus, the initial radius of the droplets affects the subsequent size of the formed droplets 3 – 57 microns for octane and has no significant effect on penetration of liquid particles into the combustion chamber.

The distribution of droplets by temperature when changing the initial radius of injected droplets showed that the temperature in the chamber during octane combustion reaches a value of 547 K (Figure 6). The zone of intense evaporation for octane is near 0.5-1 cm in the height of the combustion chamber and 0.2 cm in width. Thus, as the radius of the droplets increases, their temperature increases for octane.



a) R_{in}=1 μm

b) R_{in}=5 μm

c) R_{in}=10 μm

d) R_{in}=20 μm

Figure 6 – Distributions of octane droplets by temperature at different initial radii

Analysis of Figure 7 shows the dependence of the temperature plume height on the initial droplet radius during octane combustion. The flare height for octane at 1 μm reaches 7 cm over the height of the combustion chamber.

Based on the results of computational experiments, the temperature profiles during combustion t=4 ms and at the moment of ignition t=2.5 ms as a function of the initial radius of injected fuel droplets at high turbulence were plotted.

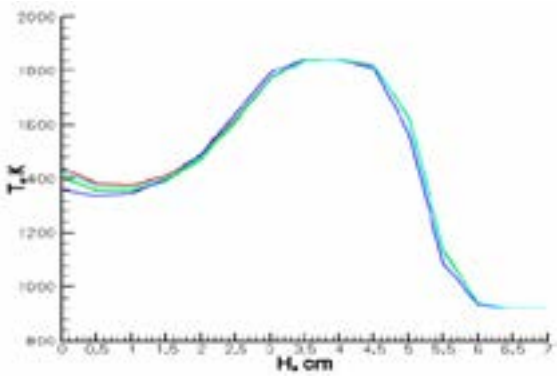
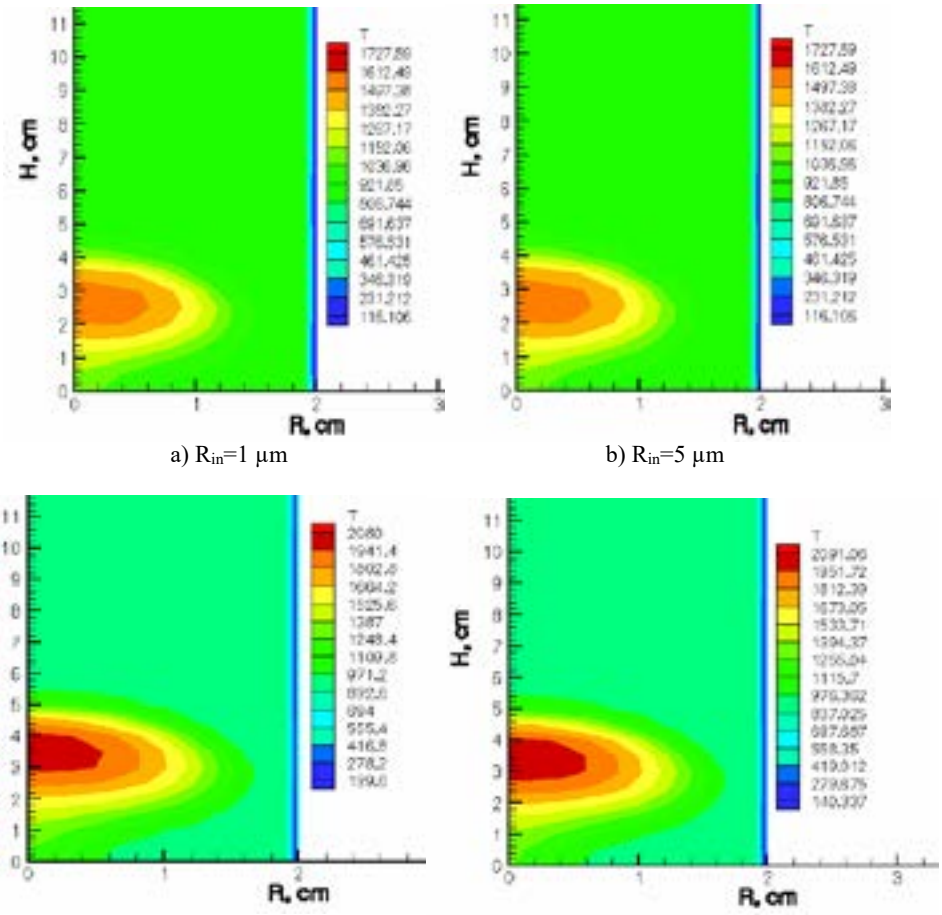


Figure 7 – Temperature distribution during fuel combustion (octane) over the combustion chamber height depending on the initial radius of the droplets

The ignition time for octane was 2.5 ms (Figure 8). As the temperature profiles show, octane burns with a small heat release, the temperature in the chamber during octane combustion reaches a value of 1728 K. However, comparing the data for 1 and 20 microns, it can be seen that the maximum temperature does not change much when burning octane. The zone of intense combustion for octane is in 1.5-3.5 cm in the height of the combustion chamber.



a) R_{in}=1 µm b) R_{in}=5 µm

c) R_{in}=10 µm d) R_{in}=20 µm

Figure 8 – Temperature profiles at the moment of octane ignition t=2.5 ms depending on different initial droplet radii

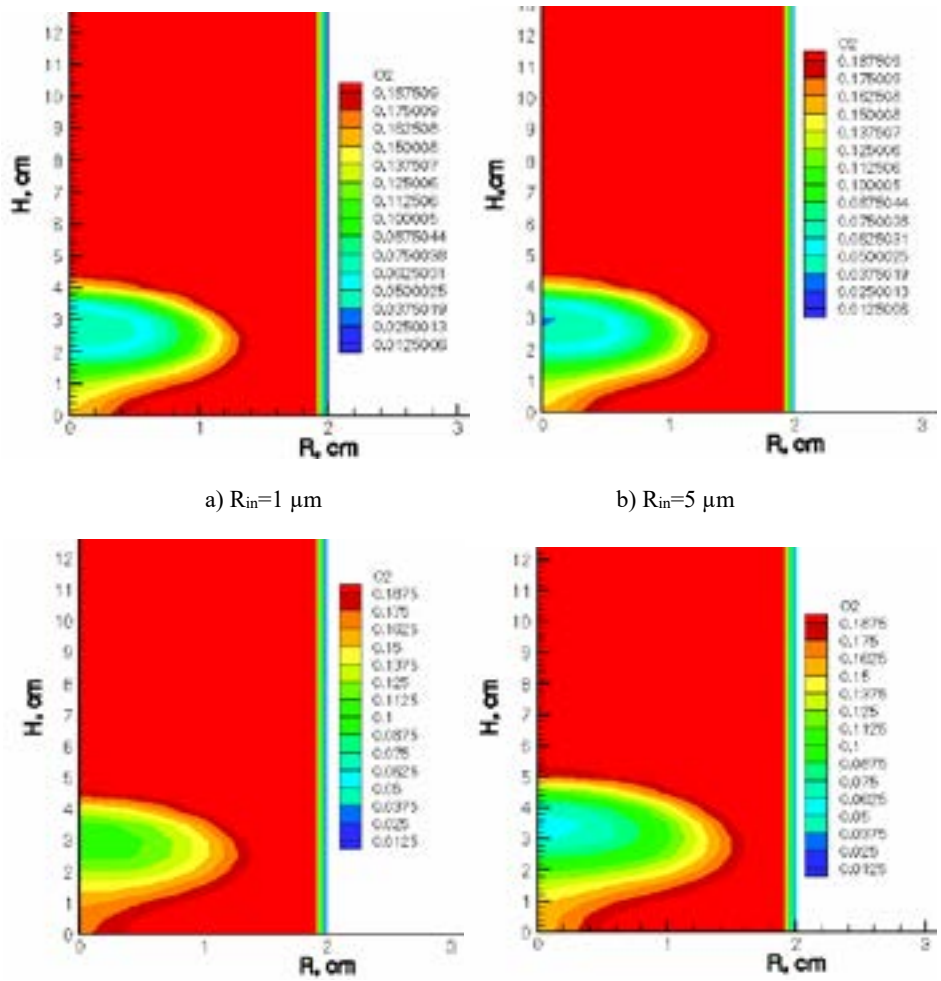
The comparative analysis shows that the initial droplet radius has no significant effect on the processes of ignition and combustion of liquid fuel in the combustion chamber.

The maximum concentration of the oxidizer in the combustion chamber relative to the fuel is 0.1875 g/g for octane (Figure 9). However, it can be seen from Figure 9 that, as the initial droplet radius increases, the area of maximum oxygen consumption increases.

As a result of computational experiments, the obtained results were generalized and the optimal parameters of atomization, combustion, and processes of liquid fuel under high turbulence were determined.

A graphical interpretation of the obtained results was performed. The dependences of the liquid fuel particle size and combustion temperature on the initial radius of the injected fuel were plotted. We completed optimization of liquid atomized fuel combustion processes.

Analysis of Figure 10 shows that the particle size grows rapidly as the initial radius of the injected droplets increases. The maximum value is reached at an initial radius of 20 μm.



a) R_{in}=1 μm b) R_{in}=5 μm

c) R_{in}=10 μm d) R_{in}=20 μm

Figure 9 – Oxidizer profiles at the moment of octane ignition t=2.5 ms at different initial radii

The most efficient combustion of liquid fuel occurs at an initial drop radius of 20 μm, as shown in Figure 11, at which the temperature in the chamber takes the maximum value. For octane, the maximum temperature is 1728 K. Thus, as the initial drop radius increases, the combustion temperature of the liquid fuel increases.

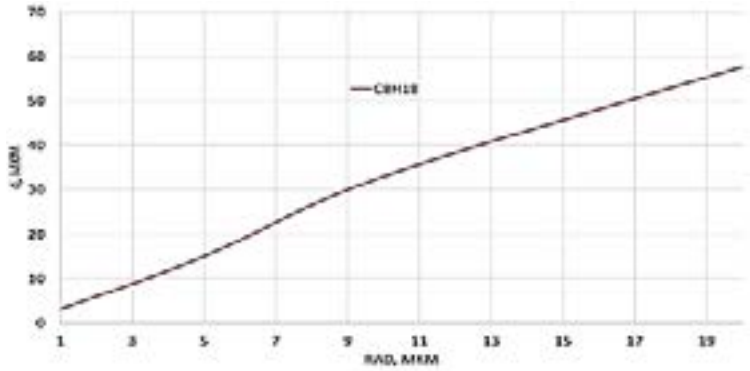


Figure 10 – Dependence of the octane particle size on the initial radius of its injected droplets

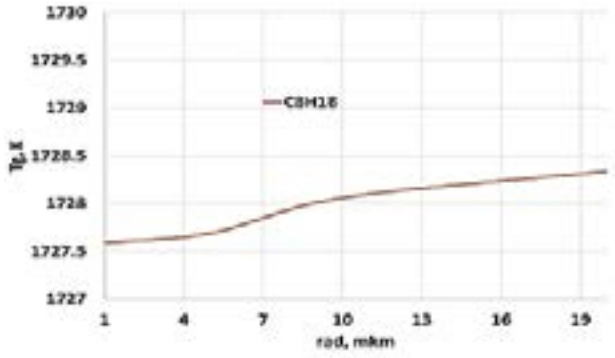


Figure 11 – Dependence of the combustion temperature of liquid fuel on the initial radius of its injected droplets

Conclusion

Because of the computational experiment, we found that, during high turbulence, the initial radius has the maximum effect on liquid particles of lighter molecular composition of fuels. With heavier molecules, the effect of the initial radius is insignificant. Combustion process of liquid fuel proceeds most effectively at an initial droplet radius of 20 μm, in which case the temperature in the chamber takes the maximum value for octane.

Obtained results are of fundamental and practical importance and can be used for the development of the theory of combustion of gas and liquid fuels. Obtained new knowledge contributes not only to increasing the level of scientific research and achievement of the world level in the priority direction of science, but also has a great applied value. This is due, first, to the fact that the continuous growth of our knowledge about the physical-mechanical and chemical properties of matter causes the observed technological explosion in the world. In this view, it is not unexpected that the vast majority of modern technologies used in almost all major industries are based on the principle by using the mechanical, thermodynamic, electro physical and other properties of gaseous, solid and liquid fuels.

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