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LES modeling of gas particle dispersion and thermal characteristics in a reacting turbulent low

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This paper presents the results of a 3D computer simulation of the combustion processes of gas particles (methane) in turbulent flow by applying numerical methods for calculating complex turbulent flows. The numerical model for calculating turbulent reacting flow is based on the filtered equations of conservation of mass, momentum, and internal energy using a spatial filter for calculating and modeling complex vortex structures. Aerodynamic, temperature and thermal characteristics of the flow were obtained based on the study on the influence of the Sauter mean radius of methane particles on its distribution and combustion processes. 3D visualization of the reacting flow was obtained considering the degree of its turbulence and the intensity of methane particle collision on the area of its distribution. The obtained results can be used for a deep understanding of the theory of gas combustion, in combustion chambers of various thermophysical objects and as an alternative to liquid hydrocarbon fuels due to safety and low harmful load of methane on the environment.

Key words: combustion, gas, turbulent, filtering, combustion, Sauter radius.
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1 Introduction

Nowadays, much attention is paid to the scientific design of chemical reactors and installations in which chemical transformation phenomena complicated by turbulent heat and mass transfer processes take place. In the systems under consideration, there are complex physical and chemical processes, the components of which are: gas flow motion, mass transfer, heat transfer, and chemical transformation. At the center of attention of numerous researches of chemical transformation processes in turbulence conditions is the question of the influence of gas-dynamic characteristics of mixing turbulent flows on conditions of the course of chemical processes, and also on possibilities of control of these processes through various external influences [1].

It is known that knowledge only of average values of such pulsating quantities as velocity, temperature, concentrations of reacting components, and reaction products is insufficient for a complete description of complex processes of chemical transformation under conditions of non-exothermicity and turbulence even in those cases when the influence of the chemical reaction on the gas dynamic characteristics of the system can be neglected. The strong and ambiguous interaction between the chemistry and dynamics of liquids and gases seriously complicates both the experimental study of reacting flows and the creation of a more or less rigorous theory. Therefore, numerical simulations can be successfully used to predict and study the behavior of such complex systems.

Experimental observations and approximate theoretical models suggest laws that a physical system must obey. Using numerical experiments it is possible to check the fulfillment of these laws, obtain quantitative predictions, and compare these predictions with the results of known experiments. A rigorous quantitative calculation of a diffusive turbulent plume of finite size is very difficult, but this very task is of the greatest practical interest. As the analysis of scientific publications shows, a rigorous theory of turbulent combustion is far from being complete at the moment. There are various approaches to modeling turbulent reacting systems that require further development and refinement, as

well as their application for solving specific problems.

Modern fuel combustion modeling techniques are designed to determine high combustion efficiency and minimum emission of pollutants into the atmosphere. They are widely used in designing and optimizing practical combustion systems because, compared to experimental testing and prototyping, the development costs of mathematical and computer simulations are very low. Today, no real progress in design or optimization can be made without numerical or computer simulations [2, 3].

The work used a model of turbulent combustion, which is based on the density of the probability function, the theory of combustion of atomized fuel under combustion conditions in diesel engines. This approach, applied earlier by the authors of [4-6], takes into account the effects of turbulence and random dynamics of vaporized gas droplets, which affect the average rate of chemical kinetics of the processes. Also in the paper, a probability density function for the variables describing the gas medium is given, where vaporized gas-liquid mixture droplets are considered in terms of source terms.

Phenomenological models aim to represent the most significant characteristics of spray formation without consuming huge amounts of computational resources. The first category of phenomenological models consists of simple Lagrangian models, which have been frequently used in industrial numerical codes for the last thirty years. In such models, the precursor mechanisms for the initial breakup of a gas jet are surface instabilities [7, 8], particle distribution [9], spontaneous breakup [10], jet turbulence [11, 12], and cavitation [13-15].

The classical theory uses the assumption of the similarity of diffusion and thermal phenomena in the vicinity of gas particles. This assumption allows one to analytically determine the particle lifetime, flame temperature, distance from the particle surface to the flame front, and some other parameters. However, concerning modern problems, especially the problems of controlling the combustion of jets and reducing the output of harmful substances during combustion, such a simple model is not very effective. To solve such problems, data on the dynamics of physical and chemical processes in the particle itself and its vicinity are required. For example, [16] presents the results of the analysis of the vaporization of a single droplet using the model of independent diffusion of components – fuel vapors, oxygen, and nitrogen.

Efficient combustion of gaseous fuels in promising engines and power plants requires good mixing and, consequently, sufficient length of the burnout section. When burning hydrocarbons, it is necessary to consider that their kinetic properties are worse compared to hydrogen, which is reflected in the increase of chemical reaction times in the ignition and combustion processes by more than an order of magnitude.

Most of the 90% of harmful substances in the air of megacities are harmful waste emitted by vehicles, soot, smoke, toxic compounds emitted by burning petroleum fuels at thermal power plants, and heavy metals. Methane is considered an environmentally efficient fuel. In engines running on methane, the content of carbon monoxide is 2-3 times lower, and nitrogen oxides are emitted half as much. The amount of smoke is reduced by 9 times compared to liquid fuels, and it does not contain sulfur and lead. The high safety of methane also depends on its physical properties. In countries where natural gas vehicles are used, such as Italy and Germany, there is a reward when a vehicle is converted to natural gas. In many countries, methane vehicles also have a lower transport tax. The idea of lower taxation for owners of methane-fueled vehicles in many countries is being discussed by the Ministry of Energy.

The purpose of this research was to investigate the characteristics of methane particles in a reactive flowing gas. Numerical models for calculating complex turbulent flows were used to assist in their analysis of the intricate gas movement.

2 Numerical model of turbulent flow calculation

Direct numerical modeling of turbulent flows is inefficient and prohibitively expensive, as a significant number of computational resources are expended to capture small eddy structures that contain negligible amounts of turbulence kinetic energy. Large eddy modeling of turbulent flows is an intermediate method between DNS and RANS and is increasingly being used as a tool to study turbulence dynamics in technical applications.

The main difference between LES and DNS lies in the concept of the filtering procedure for LES, the separation of small-scale and large-scale structures [17-19]. In large eddy simulation, large eddies are directly resolved on the numerical grid and time, while the smallest subgrid-scale eddies are modeled.

In LES approach, large eddy structures are simulated, which depend on boundary conditions and consist of most of the kinetic energy of the flow. The basic premise of this approach is that the largest vortices carry the maximum Reynolds stresses and must be calculated. Small scales or SubGrid Scales (SGS) contain low values of Reynolds stresses, in addition, small-scale turbulence is close to isotropic and has near-universal characteristics that are more amenable to modeling.

Modeling of turbulent flows consists of four steps:

1. Spatial filtering;
2. Obtaining filtered Navier-Stokes equations;
3. Modelling of unresolved movements;
4. Numerical solution.

In LES, large scales are resolved, and only small-scale structures are simulated. Large scales are derived at the expense of the flow geometry and can change with changes in the flow geometry. Small scales, involving the dissipation of turbulence kinetic energy, are generally universal and easily simulated. The spatial filtering operation decomposes the flow field into two components, the first of which is resolvable (filtered) and the second is subgrid.

The filtered continuity, momentum, and mass equations are written as follows.

The filtered mass conservation equation is written as follows:

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho \tilde{u}_i}{\partial x_i}=\tilde{S}_{mass}. \quad (1)$$

The filtered momentum conservation equation looks like this:

$$\frac{\partial \rho \tilde{u}_i}{\partial t}+\frac{\partial \rho \tilde{u}_i \tilde{u}_j}{\partial x_j}=\rho g-\frac{\partial \tilde{p}}{\partial x_i}+\frac{\partial \tilde{\sigma}_{ij}}{\partial x_j}+\tilde{S}_{mom}. \quad (2)$$

The filtered equation of conservation of internal energy of the system is written as follows:

$$\frac{\partial \rho \tilde{E}}{\partial t}+\frac{\partial \rho \tilde{E} \tilde{u}_j}{\partial x_j}=-\frac{\partial \tilde{p} \tilde{u}_j}{\partial x_i}+\frac{\partial \tilde{u}_j \tilde{\sigma}_{ij}}{\partial x_j}+\tilde{S}_{energy}. \quad (3)$$

The anisotropic part of the Reynolds subgrid stress, whose value is unknown, can be modeled using the Boussinesq approach [20]:

$$\sigma_{ij}^s-\frac{1}{3}\delta_{ij}\tilde{\sigma}_{kk}^s=-\mu_t \tilde{S}_{ij}. \quad (4)$$

Here $\tilde{\sigma}_{ij}$ plays a similar role in the filtered equations as the Reynolds stress tensor in RANS. $\tilde{S}_{ij}$ denotes the strain rate tensor in the filtered scale:

$$\tilde{S}_{ij}=\left(\frac{\partial \tilde{u}}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x_i}\right). \quad (5)$$

The choice of the function for the filter is one of the central points in the modeling of large eddies. Some of the commonly used filters are given below [21].

Volume-averaged box filter is:

$$G(x-\xi;\Delta)=\begin{cases}1/\Delta, & |x_i-\xi_i|<\Delta x_i/2\\ 0, & |x_i-\xi_i|>\Delta x_i/2\end{cases}.$$

Gaussian filter is:

$$G(x-\xi;\Delta)=\left(\frac{6}{\pi\Delta^2}\right)^{3/2}\exp\left(-6\frac{|x_i-\zeta_i|}{\Delta^2}\right)^2.$$

The shortened Fourier filter is:

$$G(x-\xi;\Delta)=\frac{1}{\Delta^3}\prod_{i=1}^{3}\frac{\sin(x_i-\xi_i)/\Delta}{(x_i-\xi_i)/\Delta}.$$

3 Results of computer simulations

This paper presents the results of numerical modeling of the processes of atomization and combustion of gaseous methane at varying initial values of the Sauter mean radius of its particles in a

model combustion chamber. As a result of computer simulation, the graphs of particle size distribution, profiles of combustion temperature, and reaction products along the height of the combustion chamber at values of 25, 50, 75, 100, and 125 μm droplets' Sauter mean radius were obtained.

Figure 1 shows the distribution of the longitudinal component of the velocity during methane combustion in the combustion chamber at different values of the Sauter mean radius. As can be seen from the figure, at an initial value of 25 microns, the velocity will have a maximum value of 200 m/s. As the particle radius increases, the velocity decreases along the height of the chamber. At the last values of 100 and 125 microns, the velocity tends to a minimum (80 m/s).

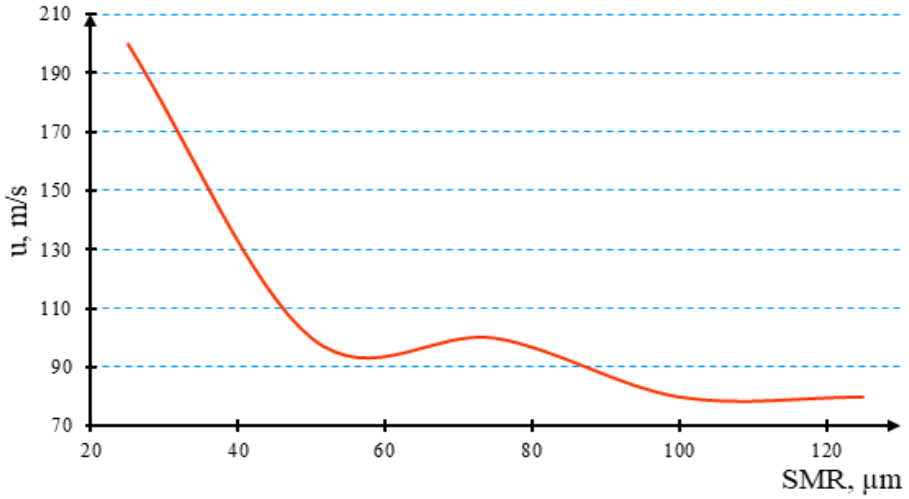


Figure 1 – Dependence of the velocity component in the longitudinal section in the combustion chamber on the Sauter mean radius of the particles

Figure 2 shows the dependence of the transverse velocity component on the Sauter mean radius of the particles. Even in this case, the velocity component decreases monotonically as the particle size increases. At the initial 100 microns, the maximum value of the velocity was 1250 m/s, and at 50 microns was 700 m/s. These values coincide with the results published in the works of some authors [22-24]. Similar behavior of the aerodynamic characteristics of the flow in the presence of combustion can also be observed during the combustion of hydrocarbon liquid fuels in the combustion chambers of thermal power facilities [25]. The only difference between liquid fuel and methane is that liquid fuel droplets go through a stage of evaporation and breakup, which affects the duration of their combustion process.

The following Figure 3 shows the value of the Nusselt number as a function of methane particle radius, which is one of the thermal criteria of the combustion process. At initial values of the radius, the Nusselt number will be low. As the particle size increases, its value also increases. Only at 100 microns a minimum of the Nusselt number can be observed. The maximum value of the Nusselt number was 1.9 at 125 microns.

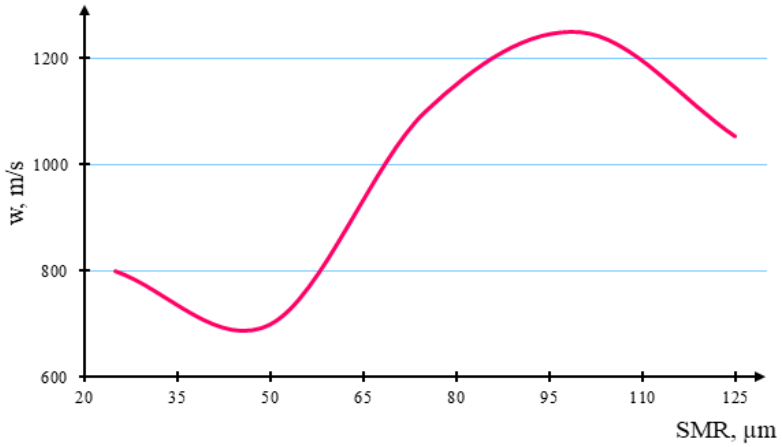


Figure 2 – Dependence of the transverse component of the velocity in the longitudinal section in the combustion chamber on the Sauter mean radius of the particles

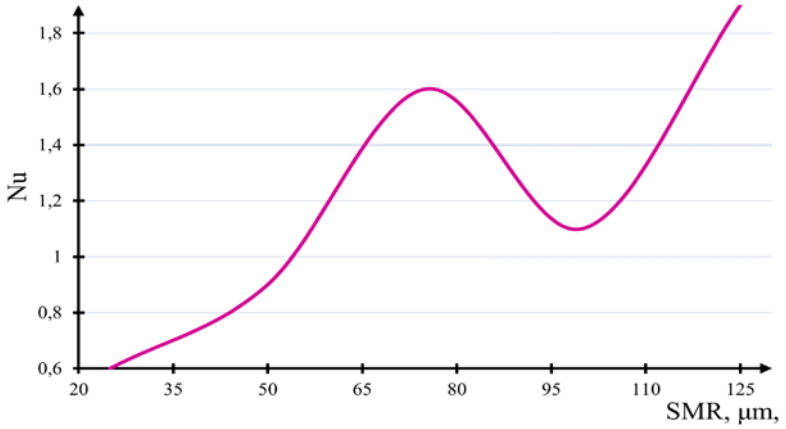


Figure 3 – Dependence of the Nusselt number on the mean Sauter particle radius

According to the results of the performed numerical simulation, the influence of different values of the Sauter mean radius of the particles on methane combustion was studied. As a result of the numerical simulation, it was found that 125 microns corresponds to the effective combustion mode. At this value, the particle size inside the chamber under combustion reaches a maximum value and particle velocities increase. A lot of oxygen is released in the middle of the combustion chamber, which helps the methane burn efficiently and evenly.

Since the numerical calculation program is designed for modeling not only liquid but also gaseous fuels, for the transition of the numerical calculation from liquid fuel to gas, changes were made in the values of the lines corresponding to the accounting of rupture, evaporation, and merging of liquid droplets:

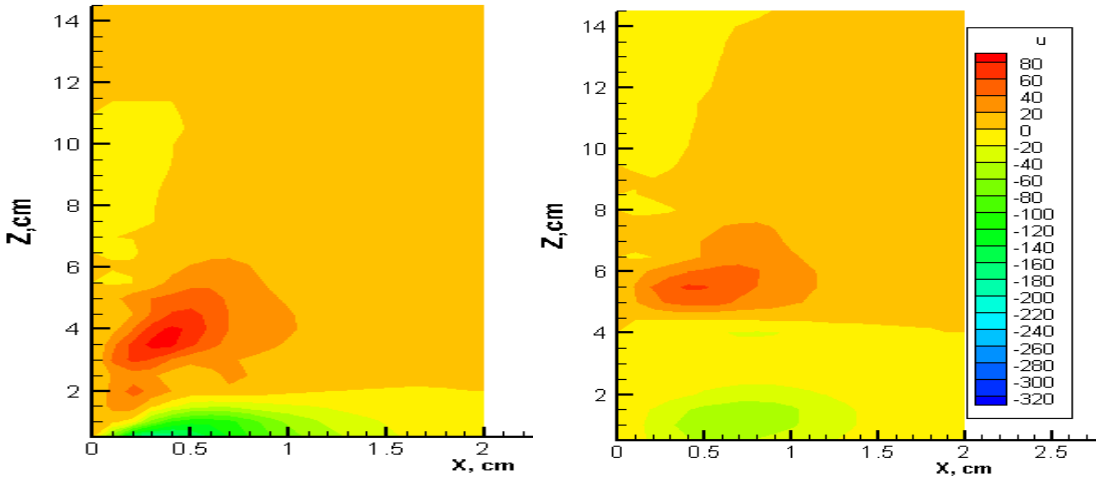
Table 1 – Modification of program sub-files for gas combustion

breakup 1.0	change to	breakup 0.0.
evapp 1.0		evapp 0.0
kolide 1		kolide 0

Through computer testing, 3D visualizations of the process of methane particle fragmentation and combustion were generated. To gain a better understanding of the combustion of methane and its specific physical and chemical characteristics was the goal of this work. Thermal, aerodynamic, and dispersion characteristics of methane particles in the combustion chamber under the efficient combustion mode were determined.

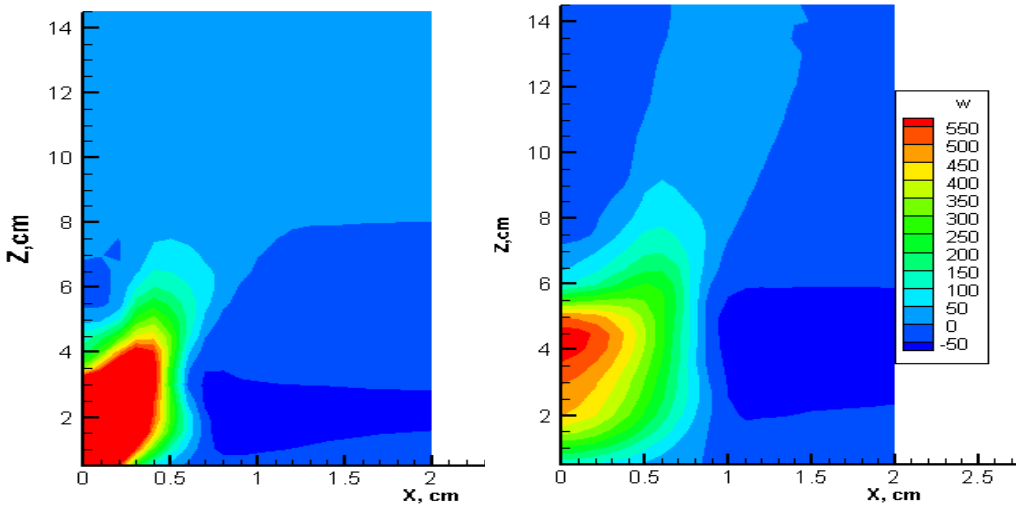
Figure 4 shows the distribution of the longitudinal component of the methane particle velocity in the combustion chamber at different time moments. At the initial time of 0.8 ms, the velocity of methane combustion in most of the combustion chamber is 20 m/s, and at time t=2.5 ms, its value reaches the maximum value of 80 m/s.

Figure 5 shows the distribution of the transverse velocity component inside the combustion chamber. At the axis of the combustion chamber, the velocity reaches its maximum value of 550 m/s. And in the rest of the combustion chamber, the velocity value was equal to 50 m/s.



a) t=0.8 ms b) 2.5 ms

Figure 4 – Distribution of the longitudinal component of methane particle velocity at the effective combustion mode



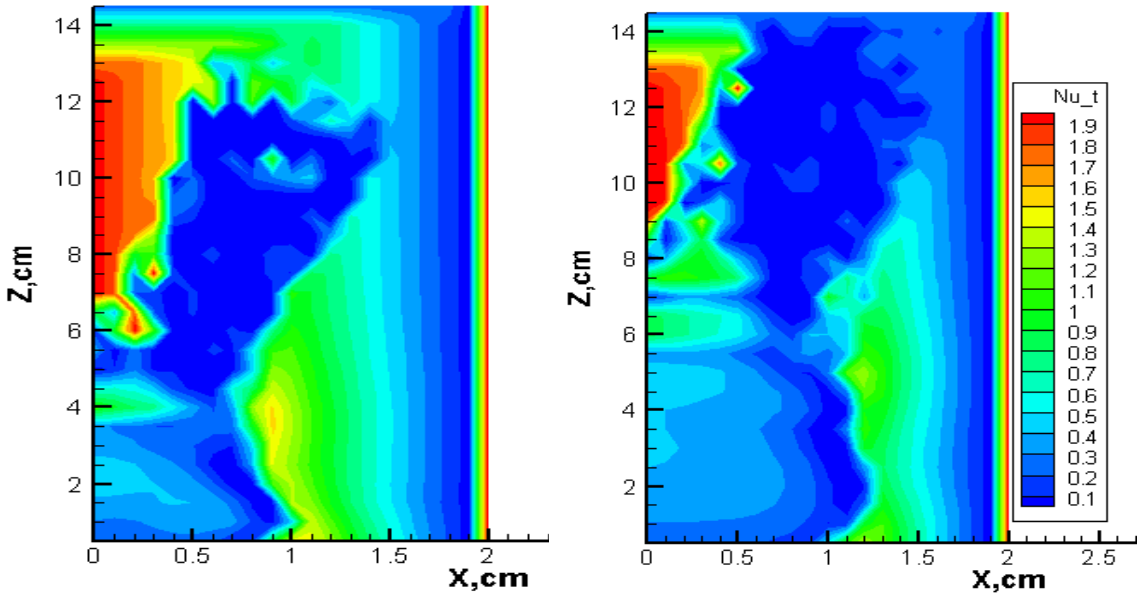
a) t=0.8 ms b) 2.5 ms

Figure 5 – Distribution of the transverse component of methane particle velocity at the effective combustion mode

Heat convection is always accompanied by thermal conductivity, since when a liquid or gas moves, individual particles of different temperatures inevitably come into contact. The combined transfer of heat by convection and conduction is called convective heat transfer.

Figure 6 shows the intensity of convective heat transfer between the body surface and the free gas flow, which is expressed by the Nusselt number. As can be seen from the figure, at the initial moment the heat transfer intensity slowly increases and becomes more intense upstream. With time, the value of the Nusselt number decreases because of the heat increase along the height of the combustion chamber.

Typically, laminar flows have a Nusselt number in the range of 1. That is, the heat flow due to convection always exceeds in magnitude the heat flow due to thermal conductivity. Large Nusselt numbers indicate strong convective heat flow, which is a characteristic of turbulent flows.



a) t=0.8 ms b) 2.5 ms

Figure 6 – Intensity of heat exchange due to convection and heat conduction in the free flow of methane particles

Thus, in this paper, computational experiments were carried out to determine the effective mode of gas combustion when the particle size changes at the beginning of the process. Based on the results obtained, it can be said with certainty that for methane the best size of the average Sauter droplet radius is 125 microns. Since at this value, methane combustion is intensive, its particles spread over long distances, due to the intensive collision of particles the heat exchange between the environment is improved and the aerodynamics of the flow becomes stable.

4 Conclusions

In this paper, computational experiments on 3D modeling were carried out to determine the thermophysical, aerodynamic, and dispersion characteristics of methane particles in a reacting gas flow in a model combustion chamber. The influence of different Sauter mean radii of methane particles on the processes of its atomization and combustion was investigated, considering the degree of flow turbulence.

The distribution of the longitudinal component of particle velocity during methane combustion in

the combustion chamber at different values of the Sauter mean radius was shown. The process of efficient combustion of methane particles occurs at SMR=125 μm.

The distribution of the transverse velocity component in the combustion chamber at different time moments is shown. At the initial time of 0.8 ms, the velocity of methane combustion in most of the combustion chamber was 20 m/s, while at the chamber extension, t=2.5 ms its value reached its maximum value of 80 m/s. The particles reach their maximum velocity of 550 m/s at the axis of the combustion chamber.

The intensity of heat transfer due to convection and conduction was shown by Nusselt number, which gradually decreased towards the exit of the combustion chamber.

This work has not only scientific but also used applications, as methane can be used as a substitute for liquid fuel in various internal combustion engines, as it has good physical and chemical properties and low harmful load on the environment.

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