



CFD Analysis of Gas-Dynamic and Heat Transfer Processes in a Propulsion System Using Polymer Fuel

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ABSTRACT

In the presented work, a computer model of thermodynamic and gas-dynamic processes in a rocket engine of a new type, which uses solid polymers as fuel is considered. The design feature is the presence of a central body - a gasification chamber, where solid polymer fuel is decomposed into volatiles. To conduct the research, a preliminary thermodynamic analysis of the combustion of gasification products was carried out. Based on the results of the thermodynamic analysis using the mathematical model of the turbulent flow of viscous compressible gas, the processes of gas dynamics and heat transfer in the chamber and nozzle of the rocket engine were simulated. Analyses are made for the geometry of a real experimental sample of a polymer-fuelled rocket engine developed at Oles Honchar Dnipro National University (Ukraine), which has passed the first successful tests. As a result of CFD simulation, dynamic and thermal fields in the combustion chamber and engine nozzle were obtained, and ways of further improvement of the design were determined.

1. Introduction

Fierce competition in the space launch services market requires engineers and designers to look for new solutions to increase the efficiency of propulsion systems, for example original ideas, including alternative fuel engines, were presented by several authors in works [1-7].

It is known that the use of polymers of petrochemical origin as fuel is possible due to the high calorific value of such substances as showed by Kumar *et al.*, [8]. Currently, many technologies have been developed for the conversion of polymers, in particular polyethylene, into liquid fuel. A review of these approaches was presented by Kumar *et al.*, [9]. Al-Salem *et al.*, [10] demonstrate that the liquid fuel obtained this way is quite suitable, for use as a diesel fuel. The use of high-density polyethylene as one of the fuel components for hybrid rocket engines is considered by several

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authors in works [11-13]. Kositsyna *et al.*, [14] substantiate the use of polymer fuels in rocket engines from an ecological point of view.

A concept of an engine operating on polyethylene fuel was proposed at Oles Honchar Dnipro National University (Dnipro city, Ukraine). Yemets *et al.*, [15], report the results of the first successful tests. The concept is garnering growing interest among researchers today. For example, Bdzyk *et al.*, [16] have shown how polyethylene fuels can be utilized in engines operating on the autophagy principle. Nonetheless, the pioneering work in developing the autophagy engine and its subsequent research is attributed to Yemets *et al.*, [17]. The engine is designed for new promising ultralight rockets made of polymer materials, which discussing Dreus *et al.* in [18]. Using polymer as fuel for polymer rockets involves the transfer of fuel from a solid to a gaseous state. This requires a specific design of a rocket engine. In particular, it requires the presence of a gasification chamber, where, under the influence of high temperature, thermal destruction of polymeric fuel occurs and decomposition products form. Then the decomposition products are delivered to the combustion chamber with a gaseous oxidizer.

Similar designs are known as a nozzle with a central body. Even though such propulsion systems may have certain advantages, they have not been widely used in aerospace. Effective operation modes of engines with a central body have not been sufficiently studied. CFD is a powerful research tool, that allows to determine effects that are difficult to establish even experimentally, as shown Alekseyenko *et al.*, [19], or Khan *et al.*, [20]. The primary contribution of presented work is the analysis of dynamic and thermal fields in the propulsion system chamber, which includes a central body and uses polyethylene as fuel. By examining these aspects, we can establish crucial design parameters for the chamber for applications. To accomplish this goal, two objectives were addressed: the creation of CFD models and the numerical investigation of gas dynamics and mass transfer processes within the propulsion chamber.

2. Brief overview of the problem

The quality of the engine's operation, its cost-effectiveness, as well as the performance of the engine as a whole depends on the thermo- and gas-dynamic processes in the combustion chamber and engine nozzle, where the thermal energy from the fuel is converted into the kinetic energy of the movement of combustion products.

There are two main types of design schemes for propulsion systems that use polymer fuel: with a round or an annular nozzle. In a scheme with a round nozzle, it is possible to use a traditional combustion chamber and a de Laval nozzle, which is an advantage of this implementation scheme. The disadvantage of this scheme is the need for a special heating circuit of the gasification chamber, which should ensure the process of polymer fuel destruction. The scheme with an annular nozzle makes it possible to accommodate the gasification chamber directly into the combustion chamber and combine them into one unit. This significantly simplifies the pneumohydraulic scheme and makes the design easier. Based on these considerations, a scheme with an annular nozzle is appropriate for an engine operating on polymer fuel. So, the design feature consists in supplying the gasified fuel mixture into the combustion chamber from the gasification chamber, which is symmetrically located in the central part of the engine. Figure 1 shows a 3D model of a chamber of LV engine on polymer fuel mentioned above.

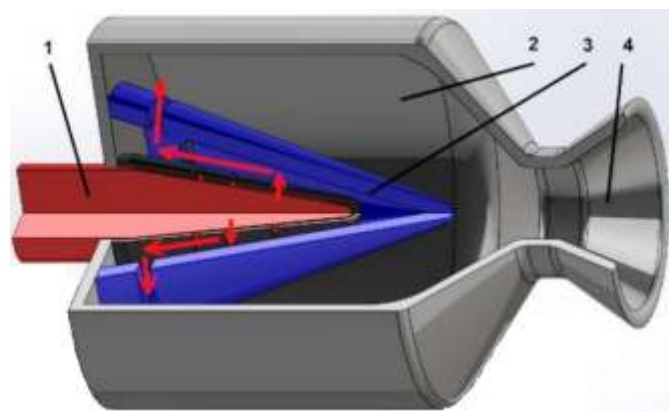


Fig. 1. Scheme of LV engine on polymer fuel: 1 – fuel rod; 2 – combustion chamber; 3 – gasification chamber; 4 – nozzle

In aerospace engineering, such nozzles are called nozzles with a central body, for example Khare *et al.*, in work [21]. The main purpose of the central insert (central body) is to control the thrust vector. Nozzles with a central body make it easier to improve aerodynamic characteristics due to more even and parallel flow at the exit, as Hamaidia *et al.*, demonstrate in study [22], and Hagemann *et al.*, in [23]. So, the advantages of such nozzles are: the ability to stabilize the flow in the required direction; engine thrust control by adjusting the cross-section area of the nozzle. The use of such engines allows you to adapt the thrust depending on the flight altitude.

The use of a central body significantly complicates the design and requires an additional cooling system for the central insert. Therefore, today such nozzles are not widely used in LV engines. Nozzles with a central body are used in cavitation devices or burners, Yang *et al.*, [24], which work at low-temperature loads. At the same time, the potential advantages of using such nozzles in aerospace stimulate the research into LV propulsion systems using a central body. In particular, in works Ferlauto *et al.*, [25] and Wang *et al.*, [26], the advantages of liquid fuel engines with a central body and an annular nozzle are presented, and the current state of research in this direction is described, including launching single-stage LVs into orbit. On the other hand, in contrast to the known designs of nozzles with a central body, in the presented work, the nozzle is not intended for adjusting thrust but is a necessary structural element.

3. Mathematical model and algorithm for computing thermo- and gas-dynamic processes in the combustion chamber

An algorithm for computing thermo- and gas-dynamic processes in the combustion chamber of a polymeric LV engine includes two stages.

At the first stage, the thermodynamic parameters of the polymer fuel combustion process (fuel + oxidizer) are calculated based on the universal thermodynamic method of determining the characteristics of heterogeneous systems, after Williams [27], which is based on the principle of maximum entropy. Ammonium perchlorate and polyethylene were chosen as fuel for the study.

The initial data on the engine geometry and the fuel charge were chosen following the data from laboratory tests of the polymer fuel engine prototype presented by Yemets: a fuel charge consisting of a polyethylene pipe with an outside diameter of 20 mm and an inside diameter of 16 mm, and a solid rod of ammonium perchlorate with a diameter of 16 mm placed inside the pipe. The speed of the fuel charge is taken to be 12 mm/s, the density of ammonium perchlorate: 1.95 g/cm³; density of polyethylene: 0.92 g/cm³; mass rate of fuel: 6 mg/s.

The combustion process of lithium perchlorate with polyethylene is computed in Astra-4 program. The following initial data are selected for this program according to Table 1.

Table 1
 Initial data for computing the combustion process

Parameter	Value
Pressure in the combustion chamber	31.8 atm
Coefficient of expansion of the nozzle	9.61
Chemical formula of fuel	C ₂ H ₄
Chemical formula of the oxidizer	NH ₄ ClO ₄
Enthalpy of polyethylene formation	52.3 kJ/mol
Enthalpy of formation of ammonium perchlorate	-295.3 kJ/mol

As a result of the computation, the parameters of the gas mixture of the combustion products were determined for three characteristic sections of the engine: in the combustion chamber, at the critical section of the nozzle and at the outlet section of the nozzle. The computation results are shown in Table 2. The estimated stoichiometric ratio of oxidizer to fuel is 10.05.

Table 2
 Computation results of parameters of the mixture of polymer fuel combustion products

Parameter	Parameter name	In the combustion chamber	At the critical section	At the outlet section of the nozzle	Dimensionality in SI
P	Pressure	3.12	18.03	0.47	MPa
T	Temperature	3010.20	1850.70	1855.70	K
V	Specific Volume	0.31	0, 49	11.88	m ³ /kg
S	Entropy	10,16	10,16	10,16	kJ/(kg·K)
I	Enthalpy	-2116.30	-2624.40	-5258.90	kJ/kg
U	Internal energy	-30727.00	-3521.00	-5818.10	kJ/kg
M	The total number of moles of components	37,11	37.83	36,24	mol/kg
Cp	Specific heat capacity at constant pressure (frozen)	1.78	1.85	1.71	kJ/(kg·K)
K	K = Cp/Cv	1.21	1.21	1.21	-
Cp''	Specific heat capacity at constant pressure (equilibrated)	1.39	4.18	2.06	kJ/(kg·K)
k''	K' = Cp'/Cv'	1.15	1.15	1.19	-
A	Equilibrium speed of sound	1041.30	1008.00	813.69	m/s
μ	Dynamic coefficient of viscosity	9.08·10 ⁻⁵	8.74·10 ⁻⁵	6.35·10 ⁻⁵	N·s/m ²
λ	Thermal conductivity coefficient	0.23	0.25	0.16	W/(m·K)
Lt''	Full coefficient of thermal conductivity	0.56	0.75	0.22	W/(m·K)
Mm	Average molar mass	26.94	26.44	27.59	g/mol
R _g	Gas constant	317.73	314.52	301.35	kJ/(kg·K)
W	Flow rate		1008.00	2507.00	m/s
Ma	Mach number		1.00	3.08	-
I _{spec}	Specific thrust (impulse) in a vacuum		193.51	278.40	s

The computation results of parameters of the mixture of combustion products are used at the second stage to model the processes of gas dynamics in the engine.

The mathematical model of the processes studied at the second stage includes a system of non-separable differential equations, momentum transfer for the washing liquid, heat transfer for turbulent transfer:

$$\frac{\partial u_j}{\partial x_j} = 0, \quad (1)$$

$$\frac{\partial u_i}{\partial \tau} + \frac{\partial}{\partial x_j} (u_j u_i) = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left((v + v_t) \frac{\partial u_i}{\partial x_j} \right), \quad (2)$$

$$\frac{\partial T}{\partial \tau} + \frac{\partial}{\partial x_j} (u_j T) = \frac{\partial}{\partial x_j} \left((\lambda + \lambda_t) \frac{\partial T}{\partial x_j} \right), \quad (3)$$

where u_i – are components of the velocity vector of combustion products in the directions of Cartesian coordinate system, indexes "i" and "j" from 1 to 3 means the corresponding direction of the Cartesian coordinate system, τ – time; p – pressure; T – temperature, ρ – density, v – kinematic viscosity, λ – thermal conductivity coefficient, index "t" means turbulence parameters.

System (1)-(3) is supplemented by appropriate initial and boundary conditions:

$$\left\{ \begin{array}{l} \text{at the inlet } u_1 = G/S_{\text{inlet}}, u_2 = u_3 = 0, T = T_{\text{comb}}, \\ \text{at the nozzle outlet } \partial u_1 / \partial x_1 = 0, u_2 = u_3 = 0, q = 0, \\ \text{on solid walls } u_j = 0, q = 0, \end{array} \right. \quad (4)$$

where G is the fuel mass consumption, S_{inlet} is the inlet cross-section square, q is the heat flux, T_{comb} , is the temperature of the combustion products at the entrance to the chamber.

Finite element analysis software ANSYS Fluent was used to solve the system Eq. (1)–(4). The k-omega SST turbulence model was selected for the analysis. A preliminary comparative analysis with computed data based on other turbulence models proved the absence of fundamental differences in the results.

Geometric characteristics of the modeling area are:

- outside diameter of the inner body (gasifier): 26 mm;
- inside diameter of the combustion chamber: 34 mm;
- diameter of the critical section of the nozzle: 2 mm;
- diameter of the outlet section of the nozzle: 6.2 mm;
- nozzle expansion coefficient: 9.6 mm;
- dimensions of the modeling area according to the outlet section: diameter - 78 mm, length - 102 mm.

Figure 2 shows the geometric model of the simulation area made in ANSYS Fluent preprocessor.

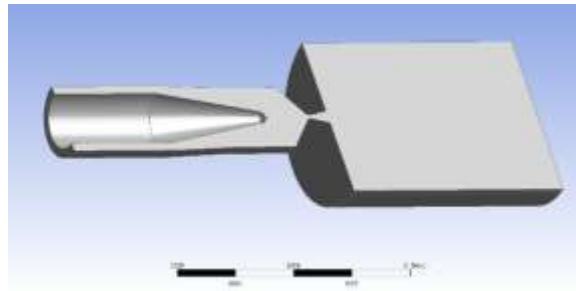


Fig. 2. Calculation area

The combustion chamber has injection holes for fuel mixture components. To simplify the mesh of the model, instead of individual inlet holes, a strip with the same area as the total area of injection holes was used. The following conditions are set on the inlet surface: inflow of a gaseous mixture of combustion products with a flow rate of 3 g/s (for the half of the geometric model), at a temperature of 3100 K.

In the outlet section, a pressure of 101.3 kPa (normal atmospheric pressure) and a temperature of 300°K are set. The parameters of the gas mixture are given in Table 3 below.

Table 3

Initial parameters for the gas mixture

The law of density change	An ideal gas
Specific heat capacity, C_p	4650,7 J/(kg·K)
Thermal conductivity	0.885 W/(m·K)
Coefficient of dynamic viscosity	$9 \cdot 10^{-5}$ Pa·s
Molecular weight	26/074 kg/kmol

An important step in solving the task is applying the adequate finite element mesh. Figure 3 shows the design mesh with thickenings in the nozzle area, and with larger elements in the cylindrical area. Mesh thickening was performed on solid walls for correct modeling of the boundary layer.

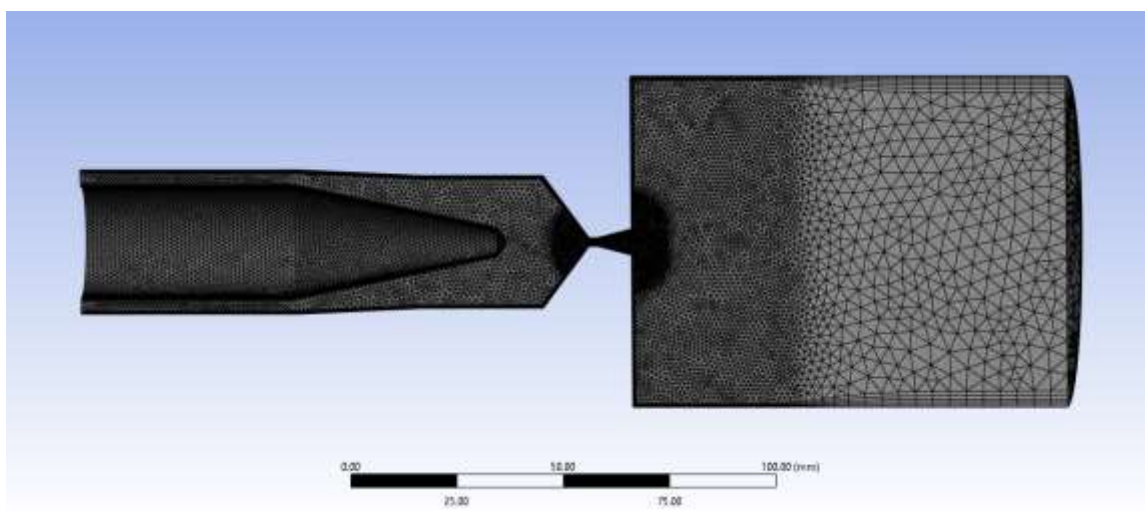


Fig. 3. General view of the meshed model

The tetrahedral type elements were selected for the analysis. The tetrahedral finite element meshes is motivated by their ability to efficiently represent complex geometries, and their

effectiveness in capturing boundary layer effects in fluid flow simulations. ANSYS provides robust automatic meshing algorithms that can generate high-quality tetrahedral meshes. The statistical characteristics of the mesh are 486.000 nodes and 2.4 million elements. The mesh elements are smaller in areas where the largest gradients of design values are expected, in particular, in the zone of the nozzle block and the critical section of the nozzle.

3. Results and discussion

The simulation results are presented in the form of fields, which illustrate the physical processes in the engine. The efficiency of LV depends on the mode of outflow of the gas jet from the nozzle. As it is known [21], there are two outflow modes: on-design and off-design, which in turn is divided into a mode with underexpansion of the jet and overexpansion of the jet. Off-design modes depend on the value of the pressure at the nozzle exit. If the atmospheric pressure at the nozzle exit exceeds the pressure in the jet, then there is a mode with underexpansion and, accordingly, energy loss. If the pressure in the jet at the nozzle exit exceeds atmospheric pressure, we have a mode with overexpansion.

Figures 4-10 present the simulation results. The velocity field is presented in Figure 4. It can be seen that the gas flow accelerates in the engine nozzle and in the critical section of the nozzle the velocity reaches the value of the speed of sound, after which the flow speeds up in the supersonic part of the de Laval nozzle, which is confirmed by the data in Figure 5, where the contour is presented on Mach numbers.

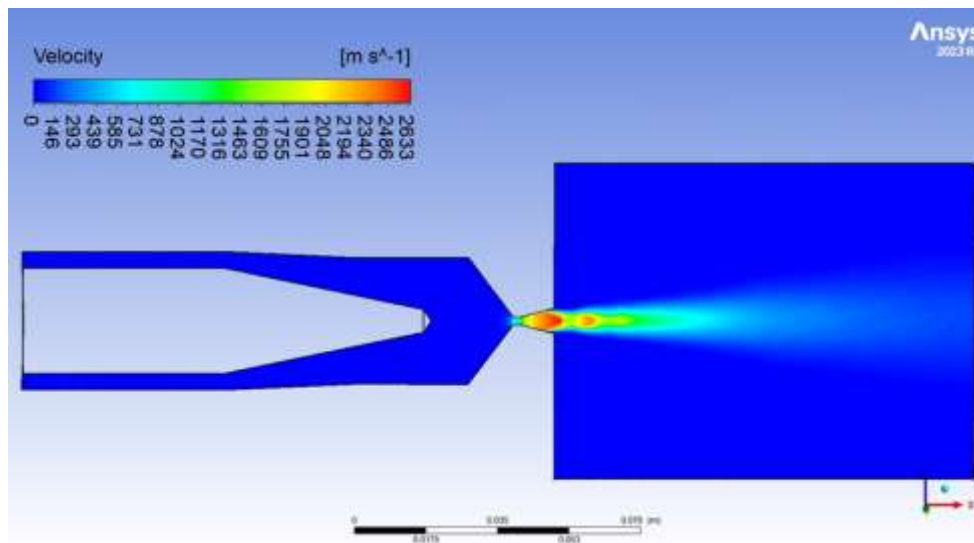


Fig. 4. Velocity field

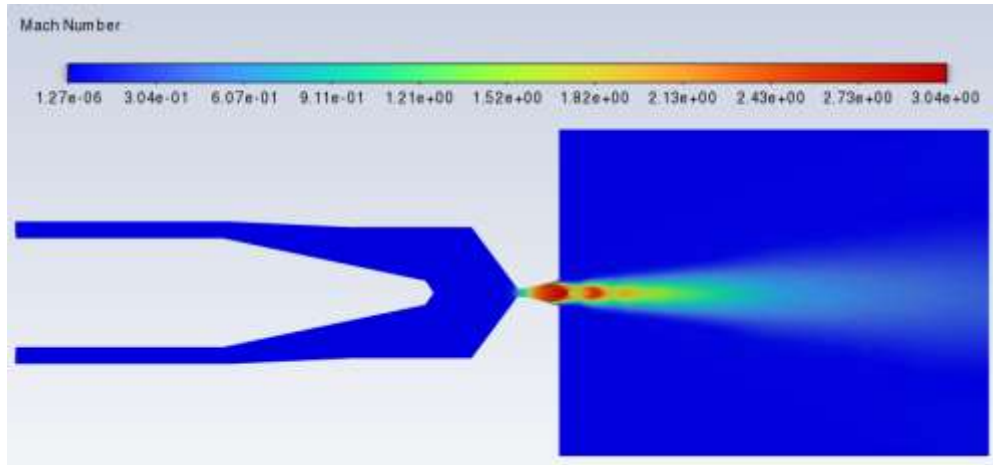


Fig. 5. Mach numbers

The pressure and temperature fields that were obtained as a result of computations for the specified input parameters are shown in Figure 6 and 7.

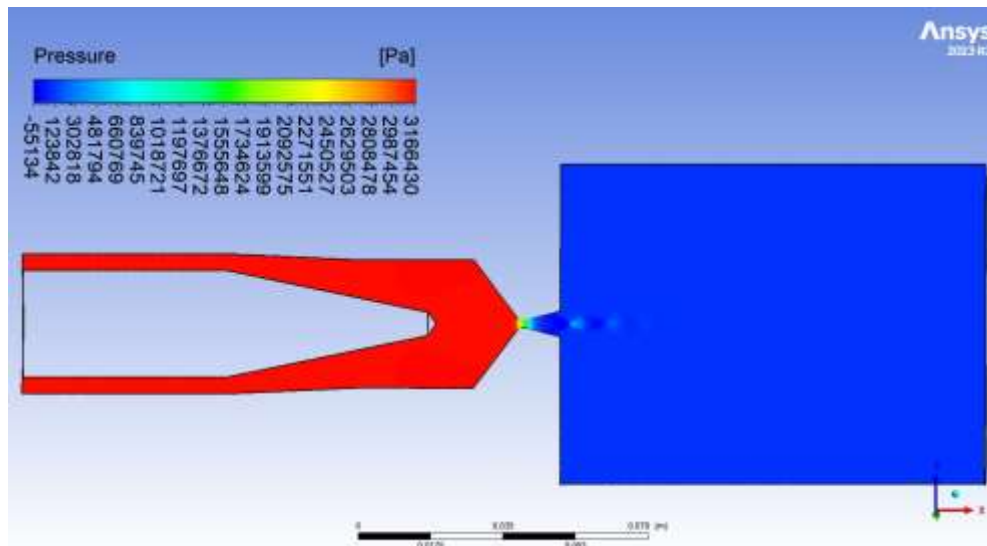


Fig. 6. Pressure field

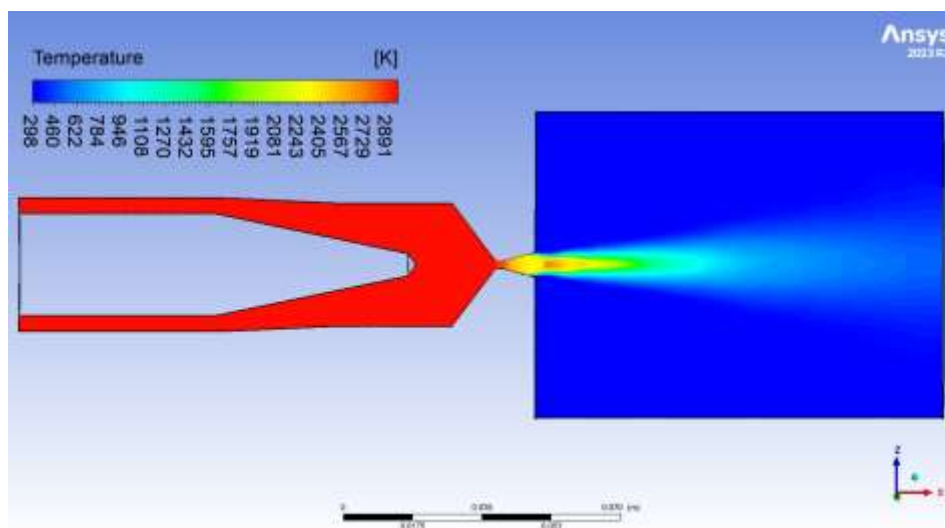


Fig. 7. Temperature field

Figure 8 shows the distribution of velocity, pressure, and temperature along the chamber axis.

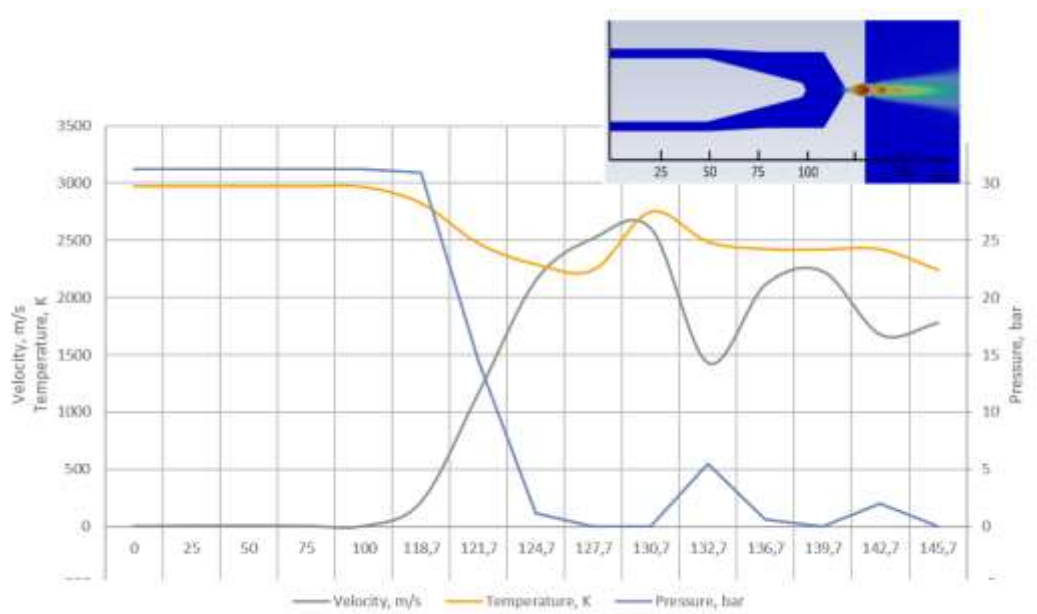


Fig. 8. Velocity, pressure, and temperature along the chamber axis

There is nonuniform the scale along the axial coordinate in Figure 8. Extremes in the supersonic path of the graphs are associated with local shock waves in jet. The temperature in the combustion chamber and the nozzle block reaches sufficiently high values, approaching 3100 K, which, on the one hand, indicates the high energy characteristics of the polymer fuel, and, on the other hand, requires the use of heat-resistant structural materials for the manufacture of the engine. The analysis of the results presented in Figures 4-8 shows that a system of shocks is formed in the output jet, which limits areas with a periodic increase in pressure, velocity, and temperature. This picture is typical for the outflow of a supersonic jet from the de Laval nozzle. The Mach number at the nozzle exit is equal to 3.

Table 4 presents the numerical values of computed parameters in the characteristic sections that were obtained as a result of the simulation.

Table 4
 Jet parameters computed in ANSYS Fluent

Parameter	Value
Temperature in the critical section of the nozzle, °K	2862.68
Temperature in the outlet section of the nozzle, °K	2295.49
Pressure in the combustion chamber, MPa	3.18
Pressure in the critical section of the nozzle, MPa	1.76
Pressure in the outlet section of the nozzle, Pa	-27891
Flow velocity in the critical section of the nozzle, m/s	1007.94
Flow velocity in the outlet section of the nozzle, m/s	2507.53

In the case under consideration, the value of the specific impulse was 273.6 with a stoichiometric coefficient of 10. At the same time, the obtained results indicate that under the selected parameters, the engine operates in the mode with underexpansion of the jet, since there is small back pressure at the nozzle exit. Therefore, the flow separation from the nozzle walls reduces the efficiency of its operation in a certain way. Figure 9 shows the area of the nozzle where the flow separation occurs.

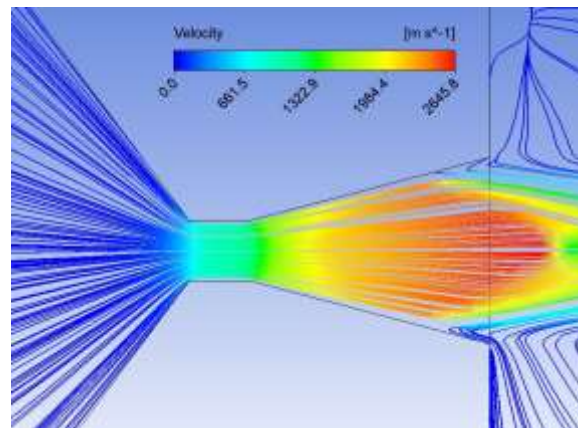


Fig. 9. Separation of the jet from the nozzle wall

The parameters in the section where the flow separation occurs are given in Table 5, respectively.

Table 5

Jet parameters in the section of jet separation from the wall

Parameter	Value
Temperature, °K	2373
Pressure, Pa	4579
Flow speed, m/s	2397
Cross-sectional area of the nozzle exit, mm ²	30,19
Cross-sectional area of jet separation, mm ²	20,91

In this case, as a result of jet energy loss, the thrust of the engine will decrease. The engine thrust is determined by the formula

$$P = GV_c + F_B(p_B - p_a), \quad (5)$$

where V_c is the velocity at the nozzle exit, F_B is the cross-sectional area, in which the flow separation occurs, p_B is the pressure in the section where the flow separation occurs, p_a is the external pressure (at the nozzle exit). The calculation according to formula (5), taking into account the numerical data given above, shows that the engine thrust is reduced by 4% compared to the case of the design mode.

4. Conclusions

The study of gas dynamics and heat transfer in the chamber of a novel propulsion system using a polymeric fuel is presented herein for the first time. The chamber's design is highlighted for its originality, owing to the presence of a central body. As a result of the performed computational experiments, the fundamental possibility of using polymer fuel (polyethylene) together with an oxidizer (ammonium perchlorate) as a solid rocket fuel, which allows creation of a high-energy gas jet and obtaining proper thrust (at least 273,6 m/s), has been proven. The operability of the engine design with a central body, where a gasification chamber is used as the central body, is shown. Structural materials for the engine must take into account the high temperatures (exceeding 2900 K in the critical cross-section and 2300 K at the nozzle) generated in the chamber. The jet's outflow velocity at the nozzle exit corresponds to a Mach number of 3. CFD modeling made it possible to establish the effect of jet separation from the nozzle wall. Therefore, the design of the nozzle of the polymer fuel engine requires further refinement, because under the specified parameters, the mode of jet outflow with underexpansion occurs, which leads to a loss of thrust by 4%.

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