Modeling of detonation processes in propulsion engine

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Abstract: - Numerical modeling of chemically reacting gas flow in the propulsion chamber using the Navier-Stokes equations has been performed. The simplest form of the chamber has been used, when the last one represents axially symmetrical plane disk. Fuel and oxidant were fed into the chamber separately with outflow to the periphery. The directions of fuel and oxidizer jets are not at right angles to the inflow surface and not parallel one to another to supply better mixing of species. The detonation triggering depends on the values of angles between fuel and oxidizer jets. At parallel directions of the jets significant part of not reacted gas components leaves the chamber. This type of the propulsion chamber is more effective than one studied before, because of absence of stagnation zones and good mixing of species before burning. The diameter of the chamber may be done less, since the largest part of fuel reacted at the inlet surface.

Key words: - modeling, turbulence, compressible flows, heat release, detonation, mixing
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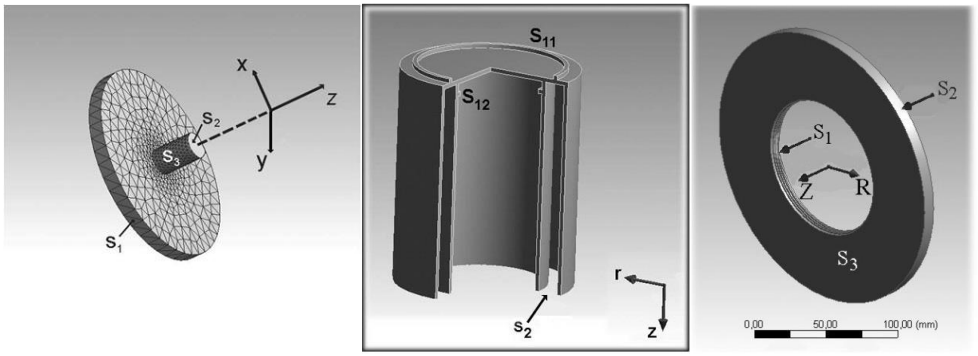
1 Introduction

Modern rocket engines of different classes and types, operated in various fields, use the so-called isobaric cycle or deflagration. In their combustion chambers constant value of pressure is maintained (at which there is a slow burning of fuel). The engine on deflagration principles does not need in particularly strong aggregates, but is limited in maximum performance. Increasing of the main characteristics is very difficult problem, starting from a certain level. System with so called detonation mode of a fuel burning is an alternative to an isobaric cycle engine in the context of performance enhancement. In this case, the reaction of fuel oxidation occurs behind a shock wave moving at a high velocity through the combustion chamber. This imposes special requirements on the design of the engine, but at the same time gives obvious advantages. In terms of fuel combustion efficiency, detonation combustion is 25% better than deflagration. It also differs from the burning with constant pressure by the increased heat release per unit of surface area of the reaction front. In theory, it is possible to increase this parameter by three or four orders of magnitude. As a result, the velocity of reactive gases can be increased by 20-25 times. Thus, the detonation engine, characterized by an increased efficiency, is able to develop more thrust with less fuel consumption. Its advantages over traditional designs are obvious, but until recently, progress in this area left much to be desired.

Possibility of such an engine was theoretically described in [1]. Detailed description of modern theoretical and practical investigations can be found in [2]. Paper [3], for example, is devoted to creation of such an engine as well. Determination of the optimal operating modes of the chamber requires the creation of detailed mathematical models describing the combustion process of fuels in the chamber. One of the most important aspects of the problem is geometrical form of the chamber. In fig.1 we can see three different possible types of the combustion chamber. Detonation processes for cases 1.a and 1.b were theoretically and numerically investigated in papers [4, 5]. One of the main problems here is the creation of the stagnation regions within the camera and not full burning of the mixture in the device.

Advanced theoretical and numerical investigations require creation of detailed mathematical models taking into account complicated physical and chemical processes within the regions like in papers [6, 7] for example.

This paper is devoted to the theoretical study of the initial stage of detonation excitation in the plane simple chamber of the form 1.c with inflow of reacting gas in the inner ring and outflow to the periphery (outer ring).



(a) (b) (c)

Fig. 1. Different types of the propulsion chamber

2 Formulation of the problem

Consider the gas dynamic flow in the propulsion chamber (Fig. 1c). The chamber itself is a plane ring body with inner diameter of 100 mm (empty hole in the body) and outer diameter of 200 mm. The zone of chemical reactions is a volume between two plane rings (S_3 sufaces), the distance between them is 10 mm. Surface S_1 is a wall, where three round inlet slots are disposed. Middle slot is inlet nozzle for oxidizer (oxygen), two other slots are inlet nozzles for fuel (hydrogen). Surface S_2 is outlet zone of the chamber (exit of detonation products into open space). Surfaces S_3 are walls of the chamber. Z-axis is the axis of symmetry of the body, R-axis is at right angle to Z-axis. Combustion of the mixture takes place inside the chamber. Oxygen in the channel is supplied from the receiver through the slot in surface S_1. The total area of the nozzle is 61 mm^2. The fuel came in through the nozzle at the same surface S_1. The total area of the nozzle is 35 mm^2. The fuel and oxidizer enter the chamber separately and mix already inside the chamber. Initially, the internal volume of the installation is filled with nitrogen at an initial gas pressure of p_0 = 1 atm and temperature of T_0 = 300 K. The initial velocity of the medium has zero value. The gas in the receivers is at elevated pressure values of 30 atm, temperature T_0 and zero velocity. The direction of oxygen jet is at right angle to the surface S_1. The jets of hydrogen are directed to meet the oxygen jet at the angle of 45^0 to the surface S_1 . Such a disposition of slots is required for better mixing of reacting materials. At the initial instant t_0 = 0 the valves are removed and the gas flows from the receivers into the chamber. Detonation was initiated by a concentrated release of energy in the mixing zone. It is necessary to determine the values of the gas parameters in the chamber after ignition at t > 0.

The geometric parameters of the installation and the nature of the boundary conditions allow us to model the flow within the framework of the axial symmetry approximation. Since the velocity of gas entering the chamber is close to the sound one, and the values of the Reynolds numbers for compressed air in various areas of the chamber significantly exceed the critical value, $\mathrm{Re} = \rho u L/\mu >> 10^4$ [8], the description of the motion of the medium should be carried out taking into account turbulence. The flow of a viscous heat-conducting compressible medium inside the chamber was described by non-stationary two-dimensional Navier-Stokes equations for the laws of conservation of mass, momentum, and energy, taking into account the effects of turbulence [6]:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{U}}{\partial r} + \frac{\partial \mathbf{F}}{\partial z} = \mathbf{G} \quad (1)$$

where the vector functions **Q, U, F, G** are described by the equations:

$$Q = \begin{pmatrix} r\rho \\ r\rho u_r \\ r\rho u_\theta \\ r\rho u_z \\ rE \\ r\rho\mu \\ r\rho Y \end{pmatrix}, \quad U = \begin{pmatrix} r\rho u_r \\ r(\rho u_r^2 + p - \tau_{11}) \\ r(\rho u_r u_\theta - \tau_{12}) \\ r(\rho u_r u_z - \tau_{13}) \\ r(E+p)u_r - r(u_r\tau_{11} + \\ u_\theta\tau_{12} + u_z\tau_{13} + q_r) \\ r\rho\mu u_r \\ r\rho Y u_r \end{pmatrix},$$

$$F = \begin{pmatrix} r\rho u_z \\ r(\rho u_r u_z - \tau_{13}) \\ r(\rho u_\theta u_z - \tau_{23}) \\ r(\rho u_z^2 + p - \tau_{33}) \\ r(E+p)u_z - r(u_r\tau_{13} + u_\theta\tau_{23} + \\ + u_z\tau_{33} + q_z) \\ r\rho\mu u_z \\ r\rho Y u_z \end{pmatrix},$$

$$G = (0, \rho u_\theta^2 + p - \tau_{22}, -\rho u_r u_\theta + \tau_{12}, \mu\rho u_z - \rho r W_\mu, \rho r W_Y + Y\rho u_z),$$

$$E = \rho(e + q^2/2),$$
$$e = p/((\gamma - 1)\rho), q^2 = u_r^2 + u_\theta^2 + u_z^2 \quad (2)$$

Here ρ, u_r, u_z, u_θ, p, E, μ, Y is the density, components of mass velocity of the gas in the direction of the coordinate axes r and z, the circumferential component of gas velocity, pressure, total energy per unit of mass, the average molecular mass of the gas and the part of induction period, respectively; W_Y, W_μ are velocities of changing of the induction period and changing of the molecular mass of the gas due to chemical reactions, γ is ratio of specific heats.

The aim of the numerical simulations is propagation of the detonation wave in the chamber. This wave is a complex of a leading shock wave, followed by a flame front and a zone of chemical transformations. Therefore, the compressibility of the medium is an important factor taken into account when constructing the model.

The components of the viscous stress vector τ_{ij} and the components of the heat flow vector q_r, q_z are defined similarly to [4]. The turbulence was described using a two-parameter k - ε model [8].

The purpose of this work is not to verify and compare different models of descriptions of turbulence effects, but only to take into account the influence of turbulence on the detonation process in the chamber. Therefore, the traditional k-ε model of describing this phenomenon was used. A detailed description of the model is also provided in [4].

The change of the concentration of the i-th gas component due to space-time diffusion and chemical reactions was determined using the second Fick's law:

$$\frac{\partial(r\rho C_i)}{\partial t}+\frac{\partial(r\rho u_r C_i)}{\partial r}+\frac{\partial(r\rho u_z C_i)}{\partial z}= \\ =r\rho D_i\left(\frac{\partial^2 C_i}{\partial r^2}+\frac{1}{r}\frac{\partial C_i}{\partial r}+\frac{\partial^2 C_i}{\partial z^2}\right)+r\rho H_i, \quad (3)$$

Where D_i is the diffusion coefficient and H_i is the intensity of the substance sources due to chemical reactions.

To describe possible chemical reactions, a two-stage model of chemical kinetics was used, when chemical reactions occur after the end of chemical ignition delay t_{chem} , calculated after reaching the ignition temperature of the medium. The detailed model of chemical reactions can be found in [4, 5].

At the inlet (surface S_1), the condition of adiabatic gas flow from the collectors is valid [8]:

$$V=\sqrt{\frac{2}{\gamma-1}c_0^2\left(1-\left(\frac{p_0}{p_r}\right)^{\frac{\gamma-1}{\gamma}}\right)}, \quad (4)$$

where V is the flow rate and C_0 is the velocity of sound in the collector gas; at the output (surface S_2) "soft boundary conditions" (the first z-derivatives of the main functions are equal to zero) are satisfied.

3 Numerical solution of the problem

The calculations were performed for the following initial air parameters: p_0 = 1 atm, γ = 1.4, $u_{r0} = u_{z0} = u_{\theta 0}$ = 0; initial values of pressure p_r and gas density ρ_r in the collector: p_r/p_0 = 30, ρ_r/ρ_0 = 30. Initial oxygen density ρ_{01} = 1.3 kg / m^3, initial hydrogen density ρ_{02} = 0.08 kg/m^3, initial gas density in the chamber ρ_0 = 0.1225 kg/m^3.

The system of equations (1) – (4) formulated above was solved numerically using the large particle method [9]. The calculations used a rectangular grid with a step of h = 0.01 mm. Further step reduction did not significantly affect the results of numerical simulation.

To verify the reliability of the calculation algorithm, test calculations of gas jet propagation in the chamber for inert media were performed using Comsol Multiphysics and Ansys software systems. The coincidence of the obtained results with the calculations based on the algorithm used in this work indicates the reliability of the latter.

Ignition of a gas mixture of hydrogen and oxygen is possible if the mass concentration of the fuel is in the range (0.45; 0.95) [10]. Therefore, the energy supply to the chamber for detonation initiation should be carried out when a region with the necessary parameters of the combustible gas mixture arises due to turbulent mixing.

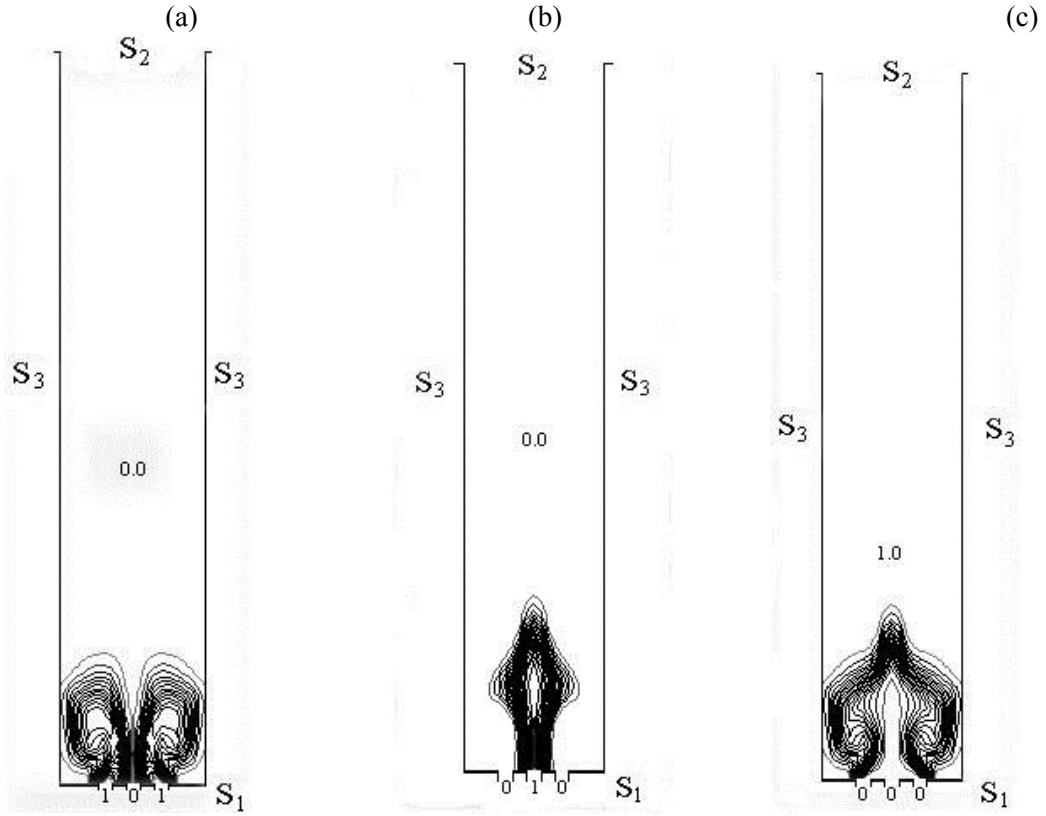


Fig. 2. Maps of mass concentrations of reagents in the chamber at initial stage of the process: (a) H_2, (b) O_2, (c) N_2.

The initial stage of numerical simulations at instant $t = 3.0 \cdot 10^{-4}$ s is represented in Fig. 2, where we have maps of mass concentration of hydrogen (a), oxygen (b) and nitrogen (c) at the cross section of the chamber with 20 levels of isolines of constant levels of concentration. One can see that jets of fuel and oxidize propagate inside the camera from inlet surface S_1 at the bottom of the figure up to the outlet surface S_2. The maximal gas velocity here is close to sound value (at the nozzles on the surface S_1). They generate shock waves with amplitude up to 15 atm. The process of intense turbulent mixing of reagents between themselves and with nitrogen occurs in the chamber. The mass concentrations of reacting gas components are changing from 1 (inside the jet) to zero (outside the jet). The greatest part of the chamber is still filled with N_2. The gas temperature in the camera doesn't exceed 600 K. The initiation of detonation has not occurred by this instant because of poor mixing so we have not chemical reactions within the device.

By the instant $t = 1.0 \cdot 10^{-3}$ s the zone of turbulent mixing of fuel and oxidizer becomes great enough for creation of self sustained detonation wave and initiation of detonation process takes place with the help of additional heat release inside the chamber (Fig. 3). Here jets of oxygen (b) and hydrogen (a) become very close to the outlet surface S_2. Inert gas N_2 gradually leaves the chamber through the surface S_2. But the concentration of N_2 is still quite great in some regions of the chamber (Fig. 3,c). The zone of chemical transformation is filled with mixture of water vapor and nitrogen (Fig. 3,d). Reacting materials occupy approximately 45% of the whole volume The maximum value of water mass concentration achieves the value of 0.84, and the gas temperature in the zone of reaction is up to 2390 K.

Subsequent stage of the process is represented in Fig. 4. The concentration of N_2 rapidly decreases here. Although at the exit surface S_2 it reaches still the value of 0.94, at the inlet surface S_1 we have maximum values below 0.29. Excessive nitrogen leaves the camera through the surface S_2. Reacting materials occupy approximately 87% of the whole volume. The size of the reaction zone increases twice as much in comparison with the instant $t = 1.0 \cdot 10^{-3}$. That results in whole growth of temperature and pressure values in the area. The maximum value of water mass concentration achieves the value of 0.91, and the gas temperature in the zone of reaction is up to 2510 K. Stabilization of gas pressure occurs, The amplitude of pressure changing is less than 21 atm.

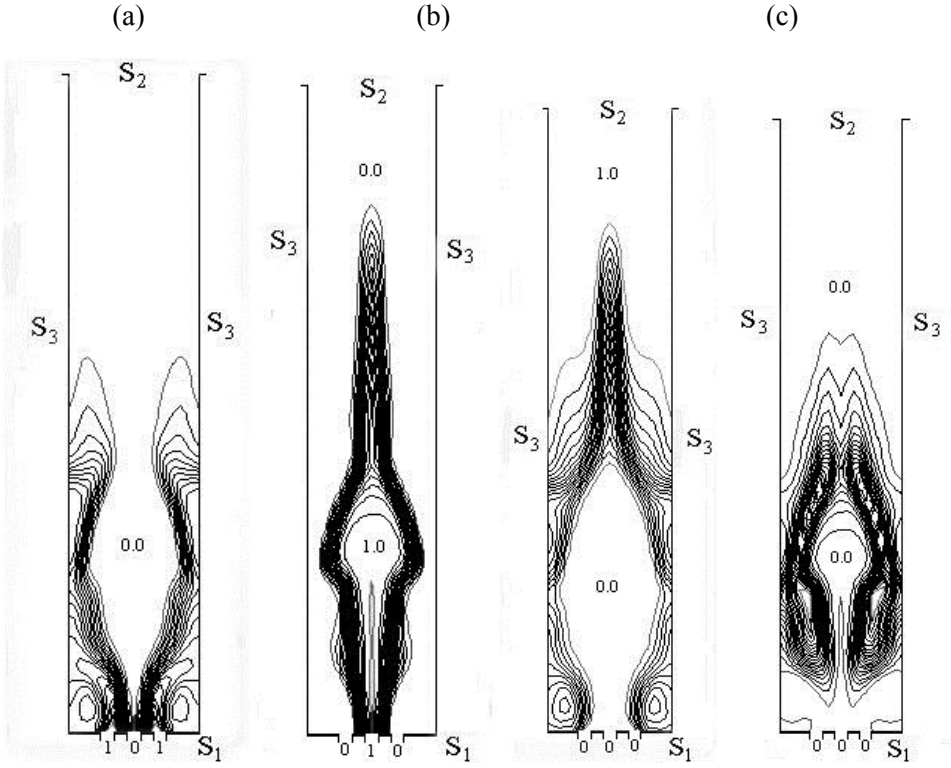


Fig. 3. Maps of mass concentrations of reagents in the chamber at instant $t = 1.0 \cdot 10^{-3}$ s : (a) H_2, (b) O_2, (c) N_2, (d) H_2O.

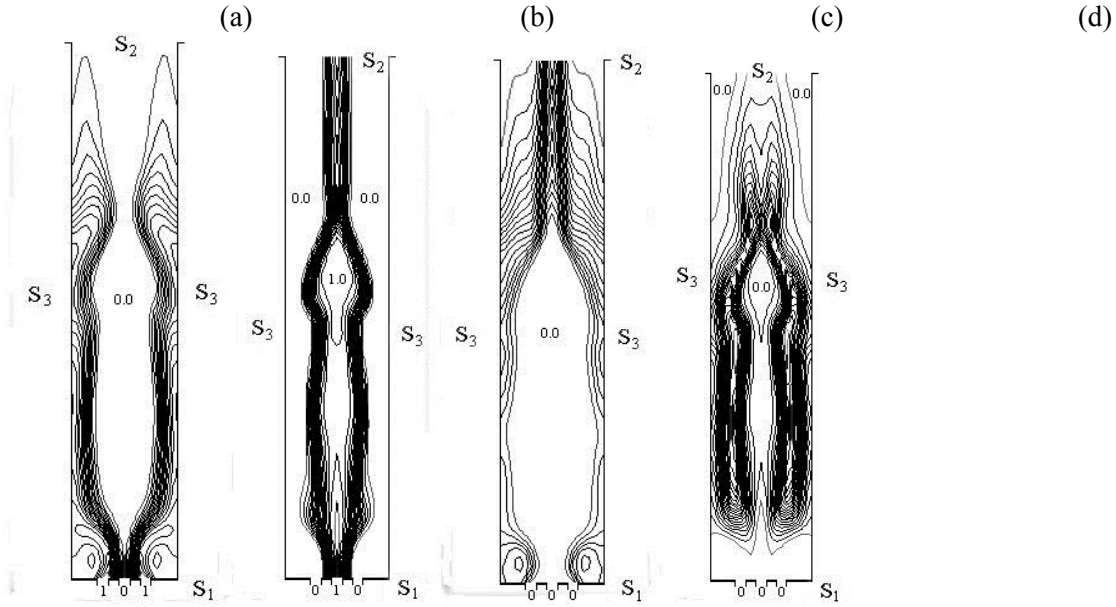


Fig. 4. Maps of mass concentrations of reagents in the chamber at instant $t = 1.7 \cdot 10^{-3}$ s : (a) H_2, (b) O_2, (c) N_2, (d) H_2O.

Stabilization of detonation processes occurs by instant $t = 2.5 \cdot 10^{-3}$ s (Fig. 5, 6). Leading shock wave of detonation complex is generated close to the surface S_1 with amplitude of 21 atm. The maximum value of water mass concentration achieves the value of 0.98, and the gas temperature in the zone of reaction is up to 2560 K. We may see secondary burning wave at the exit surface S_2, where remaining part of the fuel can react (Fig. 5c). This way is weaker than the detonation wave at the S_2. For example, the rate of reaction here achieves the value of $6.8 \cdot 10^2$ kg·moll/(m^3 s), for the main wave we have the value of $2.2 \cdot 10^3$ kg·moll/(m^3 s). Maximal value of nitrogen concentration is at surface S_2 and reaches 0.47. It is interesting that for this type of the propulsion chamber we have no significant stagnation zones where concentration of initial nitrogen keeps large values for course of time and portions of water vapor remain in some parts of the chamber. The mass concentration of not reacted hydrogen at the exit S_2 is less than 0.4, so this type of the propulsion chamber is more effective than studied in [4, 5]. Concentration of water vapor here behind a reaction front is very close to maximum value 1 (in the middle of the chamber).

So we have generation of detonation in the chamber. The failure of detonation can occur due to temporary cessation of reagents coming in the chamber due to the large pressure values in the reaction zone. The diameter of the chamber may be less, since the largest part of fuel is reacted at the inlet surface.

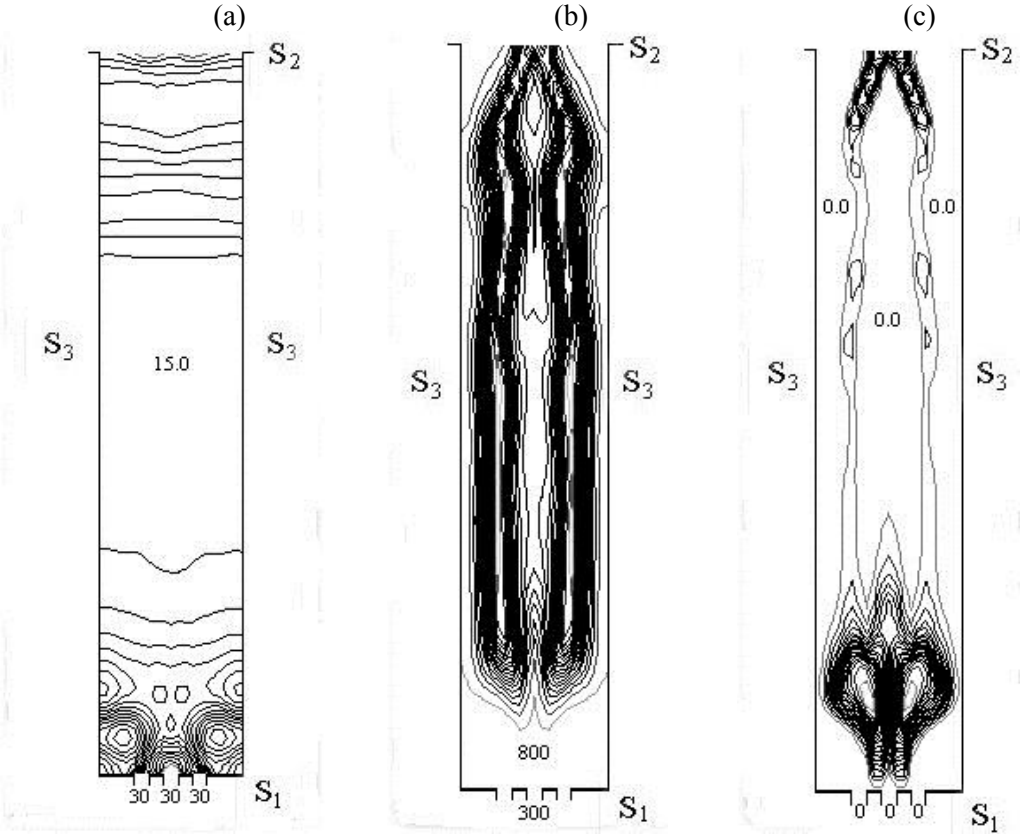


Fig. 5. Maps of gas pressure (a, atm), temperature (b, K) and rate of chemical reaction (c, kg·moll/(m^3 s)) in the chamber at instant $t = 2.5 \cdot 10^{-3}$ s.

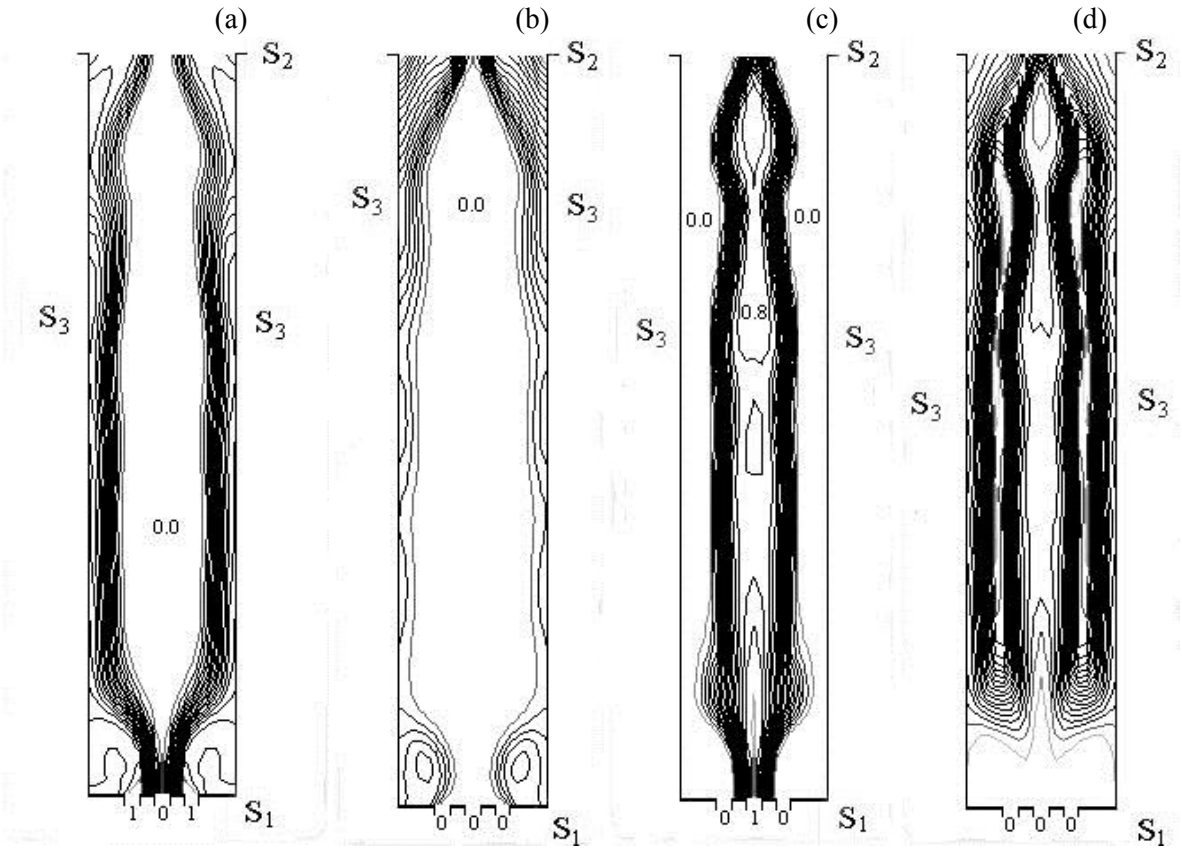


Fig. 6. Maps of mass concentrations of reagents in the chamber at instant $t = 2.5 \cdot 10^{-3}$ s : (a) H_2, (b) O_2, (c) N_2, (d) H_2O.

4 Conclusions

Numerical modeling of chemically reacting gas flow in the propulsion chamber using the Navier-Stokes equations has been performed. The simplest form of the chamber has been used, when the last one represents axially symmetrical plane disk. Fuel and oxidant were fed into the chamber separately with outflow to the periphery. The directions of fuel and oxidizer jets are not at right angles to the inflow surface and not parallel one to another to supply better mixing of species. The model is based on conservation laws of mass, momentum and energy for non steady two-dimensional compressible gas flow in case of axial symmetry. The processes of viscosity, thermal conductivity, turbulence and diffusion of species have been taken into account. Heat release was described on the base of two stage model of chemical kinetics. The possibility of detonation way of combustion of the mixture in the chamber was numerically demonstrated. Leading shock wave of detonation complex is generated close to the inlet surface. Secondary weak burning wave at the exit surface may appear. The detonation triggering depends on the values of angles between fuel and oxidizer jets. At parallel directions of the jets significant part of not reacted gas components leaves the chamber. This type of the propulsion chamber is more effective than one studied before, because of absence of stagnation zones and good mixing of species before burning. The diameter of the chamber may be less, since the largest part of fuel is reacted at the inlet surface.

Further investigations can be concentrated on using different types of fuels in the chamber (not only hydrogen) and simulations of subsequent stages of detonation processes with self-sustained regime.

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