On the possibility of gaseous fuel self-ignition in a cylindrical or vortex detonation chambers

D.V.VORONIN

Lavrentyev Institute of Hydrodynamics of SB RAS,
Lavrentyev str, 15, 630090 Novosibirsk
RUSSIA
Phone: +7 383 333 26 06;
Fax: +7 383 333 16 12;
E-mail: voron@hydro.nsc.ru, dvvoronin@bk.ru

Abstract. - The numerical calculations of the flowfield in a planar vortex or cylindrical chambers have been performed. The model is based on conservation laws of mass, momentum and energy for non steady two (in case of swirl axial symmetry) and three dimensional compressible gas flow. The processes of viscosity, heat conductivity and turbulence have been taken into account. It was found that transition of kinetic energy of gas into heat due to processes of dissipation generates "hot spots" in boundary layers at the chamber walls. The gas temperature at the spots may exceed the temperature of gas ignition, while the surrounding regions remain still cold. It may be the reason of cold gas self-ignition observed in experiments.

Key words: - modeling, turbulence, compressible flows, hot spots, self-ignition

1 Introduction.

The increased interest to a problem of detonation burning of fuels is revealed recently in connection with idea of creation of the detonation engine. The facility of the jet engine with a continuous detonation for the first time is offered in [1]. The detailed analysis of experimental and theoretical works on the problem contains in [2]. One of problem here is the determination of optimum modes of operations of installation. It requires, in particular, creation of mathematical models and determination of fields of the basic thermodynamic parameters inside the combustion chamber of the detonation engine. The works [3, 4] are devoted to the problem, for example. In experiments [5] it was found that the stable work of installation can be interrupted by regular self-ignition of a combustible gas mix in conditions, when average temperature of gas, acting inside of the chamber, is much less than temperature of self-ignition. The nature of this phenomenon is not quite clear till now. Detailed mathematical modeling of processes inside the installation with the description of the most essential factors determining gas dynamics of the flow is necessary.

The present work is devoted to numerical modeling of a gas flow in the plane vortex or cylindrical chambers. The geometry and main physical characteristics correspond to experimental data [5].

2 Problem Formulation

Let's consider gas flow in the vortex chamber (fig. 1). Here S_1 is the entrance surface of the chamber (lateral surface of the circular cylinder by a diameter of 204 mm and height of 15 mm), the reacting gas penetrates through it inside the chamber from collectors, S_2 is the surface of gas exit from the chamber (circle by a diameter of 40 mm). S_3 is lateral surface of the central branch pipe of the chamber (circular cylinder of height 42 mm along an axis z), which serves for release of products in an atmosphere. All external surfaces of the vortex

chamber except for S_1 and S_2 represent rigid impenetrable walls. Initially internal volume of the facility is filled with nitrogen or air at initial pressure of gas $p_0 = 1$ bar and temperature $T_0 = 300$ K. The initial velocity of the flow is equal to zero. The gas in collectors is at the increased meanings of pressure p_r and density ρ_r, temperature T_0 and zero velocity. At the initial moment of time $t_0 = 0$ gas from the collectors starts to propagate inside the chamber through the surface S_1 at the angle of 45^0 with respect to the surface, that provides rotary motion of the flow around of an axis z. It is required to determine the values of parameters of gas in the chamber at $t > 0$.

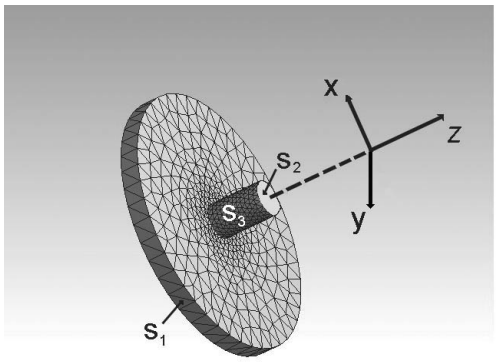


Fig. 1. The scheme of the vortex chamber

As the velocity of gas in the chamber is close to sound velocity, and the values of Reynolds numbers for compressed air in various areas of the chamber considerably exceed critical, $\mathrm{Re} = \rho u L/\mu >> 10^4$ [6], the description of the flow needs to be carried out with the effect of turbulence taken into account.

Unsteady motion of viscid compressible turbulent fluid was described by Reynolds equations [7]:

$$\frac{\partial Q}{\partial t} + \frac{\partial U}{\partial x} + \frac{\partial W}{\partial y} + \frac{\partial F}{\partial z} = 0, , \qquad (1)$$

where *x, y, z* – space Cartesian coordinates. The vectors *Q, U, W, F* are defined by the equations

$$Q = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e \end{pmatrix}, \quad U = \begin{pmatrix} \rho u \\ \rho u^2 + p - \tau_{xx} \\ \rho uv - \tau_{xy} \\ \rho uw - \tau_{xz} \\ (\rho e + p)u - u\tau_{xx} - v\tau_{xy} - w\tau_{xz} + q_x \end{pmatrix},$$

$$W = \begin{pmatrix} \rho v \\ \rho uv - \tau_{yx} \\ \rho v^2 + p - \tau_{yy} \\ \rho vw - \tau_{yz} \\ (\rho e + p)v - u\tau_{yx} - v\tau_{yy} - w\tau_{yz} + q_y \end{pmatrix}, \quad F = \begin{pmatrix} \rho w \\ \rho uw - \tau_{zx} \\ \rho vw - \tau_{zy} \\ \rho w^2 + p - \tau_{zz} \\ (\rho e + p)w - u\tau_{zx} - v\tau_{zy} - w\tau_{zz} + q_z \end{pmatrix},$$

here the components of the shear stress tensor have the form

$$\tau_{ij} = \mu_e\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3}\frac{\partial v_k}{\partial x_k}\delta_{ij}\right),$$

The components of heat flux vector are

$$q_i = -\lambda_e \frac{\partial T}{\partial x_i},$$

Here the velocity vector V has the components u, v, w along x, y, z axis respectively; e, p, ρ, T and $\gamma = c_{p,l}/c_{v,l}$ are the full energy per mass unit, pressure, density, temperature and the ratio of specific heats, respectively; μ_e and λ_e are the effective viscosity and effective thermal conductivity of the gas. μ_e is a sum of molecular μ and turbulent μ_t viscosity, $\lambda_e = c_p\left(\mu / \mathrm{Pr} + \mu_t / \mathrm{Pr}_t\right)$, Pr and Pr_t are molecular and turbulent Prandtl numbers.

The law of Sazerland is used for the values of molecular viscosity

$$\frac{\mu}{\mu_*} = \left(\frac{T}{T_*}\right)^{3/2} \frac{T_* + S_0}{T + S_0}$$

where $\mu_* = 1.68\times10^{-5}$ kg/(m·s), $T_* = 273$ K, $S_0 = 110$ K for air.

The processes of turbulence were described according to two-parametric k-ε model [8]:

$$\frac{\partial \rho k}{\partial t} + (\rho V \cdot \nabla)k = \nabla\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\nabla k\right] + P^* - \rho\varepsilon,$$

$$\frac{\partial \rho \varepsilon}{\partial t} + (\rho V \cdot \nabla)\varepsilon = \nabla\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\nabla \varepsilon\right] + \frac{\varepsilon}{k}\left(C_{\varepsilon 1}P^* - C_{\varepsilon 2}\rho\varepsilon\right).$$

with values $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.92$. Here k is turbulence kinetic energy, ε is its rate of dissipation, term P^* represents the production of turbulence kinetic energy, $P^* = \mu_t S^2$, $S = \sqrt{e_{ij}e_{ij}}$.

Turbulent viscosity was defined according to Kolmogorov-Prandtl formula:

$$\mu_t = \frac{C_\mu \rho k^2}{\varepsilon}, \quad C_\mu = 0.09.$$

The change of concentration of components of gas was described with the help of the diffusion equation:

$$\frac{\partial(\rho C)}{\partial t} + \frac{\partial(\rho u C)}{\partial x} + \frac{\partial(\rho v C)}{\partial y} + \frac{\partial(\rho w C)}{\partial z} = \rho D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right), \qquad (3)$$

Where D is the diffusion coefficient.

To complete the system the equation of perfect gas is assumed to be valid:

$$p = (\gamma - 1)\rho\left(e - \frac{1}{2}\left(u^2 + v^2 + w^2\right)\right)$$

As boundary conditions on rigid impenetrable walls of the chamber the condition of a constancy of temperature $T = T_0$ and sticking condition is put: $u = v = w = 0$.

On the input surface S_1 a condition of adiabatic expiration of gas from collectors [9] is fair

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

Where V is a velocity of the expiration, c_0 is a sound velocity of gas in the collector.

On the output surface S_2 the soft boundary conditions (equality to zero first derivative on z of required functions) are valid.

3 Numerical solution of the problem

The calculations were performed for the following initial values of air: p_0 = 1 bar, ρ_0 = 0.1225 kg/m^3, γ = 1.4, $u = v = w = 0$; initial values of air pressure p_r and density ρ_r in the receiver : $p_r / p_0 = 10$, $\rho_r/\rho_0 = 10$. The problem stated above, was solved numerically with the help of the method of large particles [5].

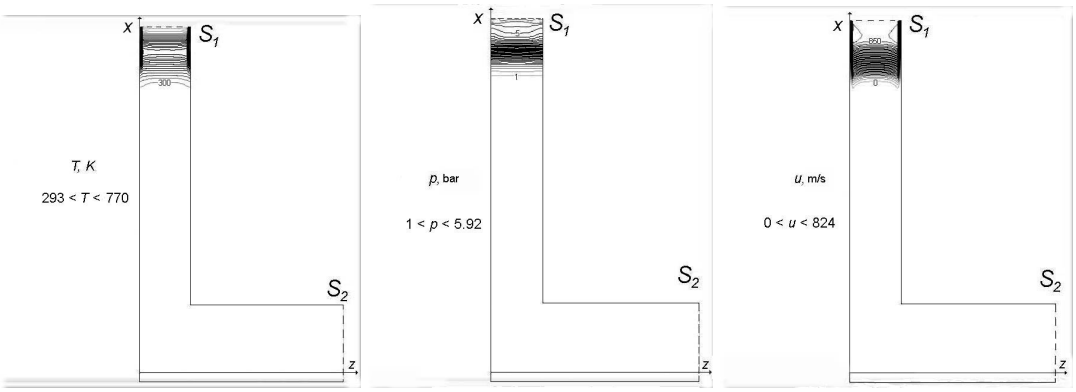


Fig.2. Flow field of the main thermodynamic parameters in the chamber at initial stage of the processes, $t = 1.0 \cdot 10^{-4}$ s.

The initial stage of numerical simulations is presented in Fig. 2. Here $U = \sqrt{u^2 + v^2 + w^2}$. It could be seen that a compression wave starts to propagate from the inlet surface to the symmetry axis z. The pressure amplitude in the wave is up to 5.92 bar. The flow friction at the chamber walls results in mass growing of gas at the walls due to processes of dissipation, and subsequent transition of gas kinetic energy into heat starts. The values of temperature in generated boundary layers is growing up to 770 K (z = 0), while in the center of the channel it is equal to 520 K (at the same x and z = 8 mm).

The subsequent stage of the processes is presented in Fig. 3. The compression wave continues to propagate nearly at the same amplitude. The sizes of hot boundary layers are growing along with temperature values in them. The giant vortex is generated in the chamber at the walls. Its axes is the axes of symmetry A. The vortex is gradually coming down to the axes z. In recent simulations the initial pressure in the receiver p_r = 10 bar. In the experiments [5] it may be up to 100 bar. Then the temperature in the boundary layers (in the vortex) exceeds the ignition temperature T_{ig} = 1200 K. That results in self-ignition of gas in a whole volume observed in the experiments [5].

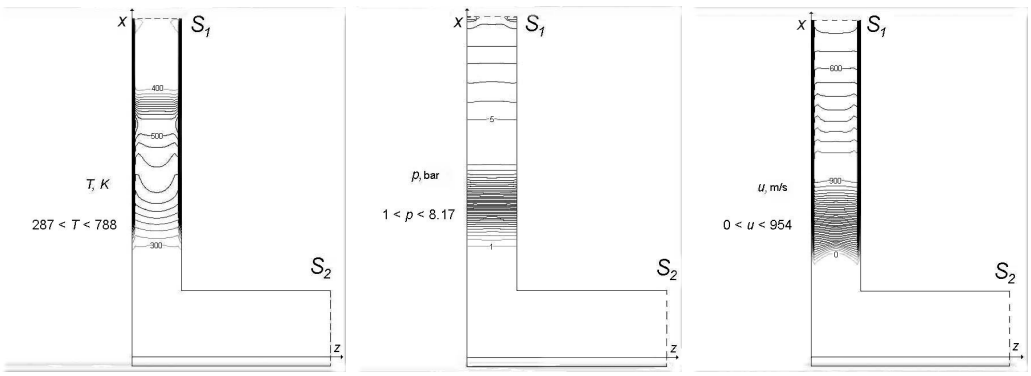


Fig. 3. The maps of the main thermodynamic parameters in the chamber at $t = 5.0 \cdot 10^{-4}$ s.

When the vortex comes down to the axes z, and gas masses collide (Fig. 4), the temperature amplitude reaches the value of 1480 K, that initiates the processes of gas self-ignition even at present p_r = 10 bar. But the maximum of temperature takes place not at the axes of symmetry z but in the heated spot at the chamber corner (x = 20 mm, z = 15 mm), where the boundary layer tearing off from the chamber walls occurs.

Interaction of the heated spot with reflected shock waves (from the symmetry axes z) and gas acceleration in the spot (due to rarefaction wave) from the outlet surface result in subsequent temperature growth. At the course of time the temperature values in the spot exceed 2000 K (Fig. 5).

Dynamics of the maximum values of gas temperature we can see in Fig. 6. The dotted line in the figure corresponds to the value of ignition temperature T_{ig}. We can determine six stages of the processes. The initial stage *1* is a temperature growth from 300 *K* to 800 *K,* when the shock wave starts to propagate from the receiver to the chamber through the inlet surface. The stagnation period *2* corresponds to the shock wave propagation to the center of the chamber (the symmetry axes *z*). The temperature growth at the stage *3* is a result of shock waves collision at the symmetry axes *z*. Here the gas temperature at the axes is increased up to 1500 *K* and exceeds the value of T_{ig}. That may result in gas self-ignition in the region. The interval *4* is the processes discharge in the direction of the outlet surface. The stage *5* is a temperature growth in the tearing off boundary layer at the chamber corner at its interaction with reflected shock wave. The temperature here exceeds here the value of 2100 *K*. The stage *6* lasts till rarefaction wave from the outlet surface appearance at the corner.

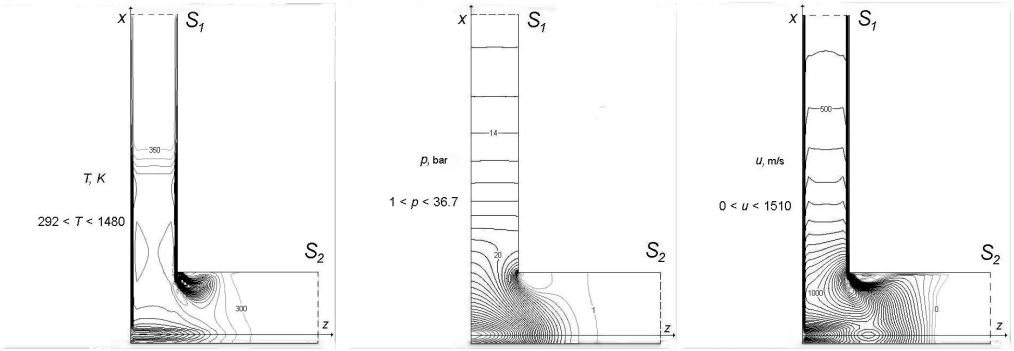


Fig. 4. The maps of the main thermodynamic parameters in the chamber at $t = 9.0 \cdot 10^{-4}$ s.

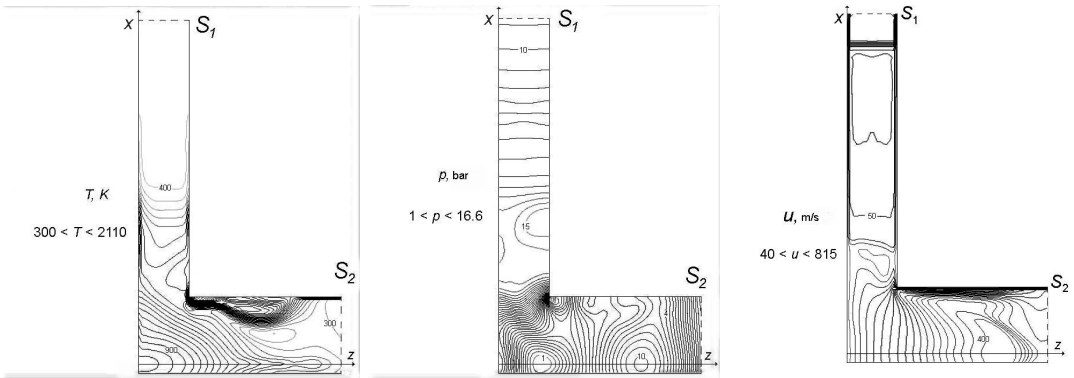


Fig. 5. The maps of the main thermodynamic parameters in the chamber at $t = 1.4 \cdot 10^{-3}$ s.

To appreciate the influence of turbulence on the gas self-ignition, the numerical simulations of laminar flow were performed on the base of Navier-Stokes equations (Fig. 7) at the same initial values of the problem parameters. It could be seen from the figure that for laminar flows the mixture self-ignition may occur as well. Although the maximum value of temperature in laminar hot spot T = 1370 K is significantly less than turbulent T = 2110 K at the same instant.

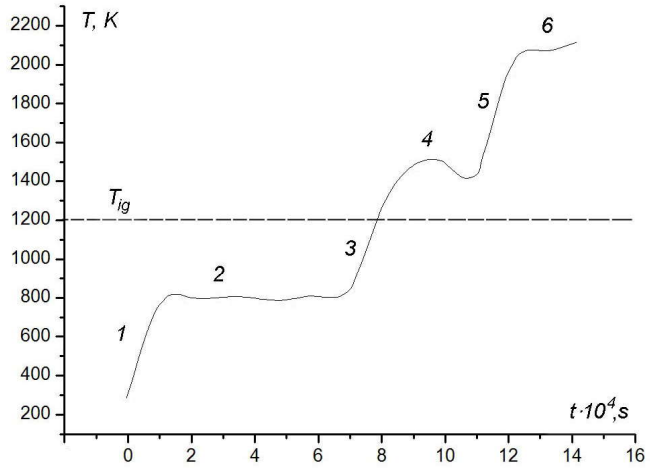
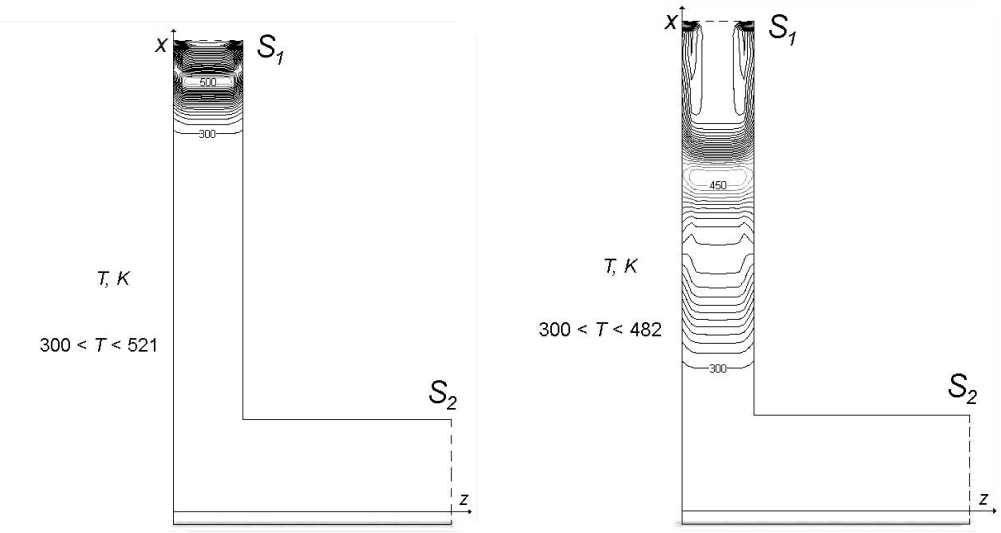


Fig. 6. Dynamics of the temperature maximum in the chamber



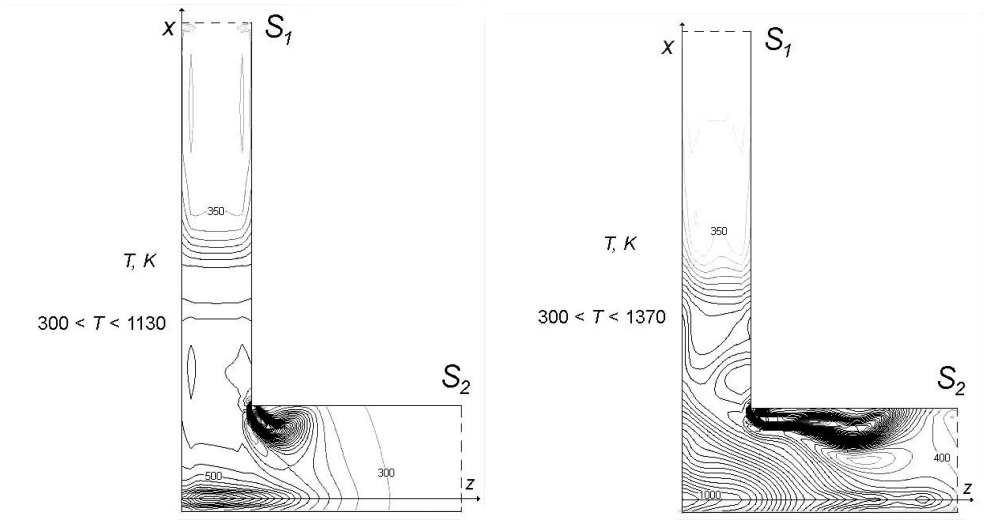


Fig. 7. The temperature maps in the chamber for laminar flow at $t = 1.0 \cdot 10^{-4}$ s, $5.0 \cdot 10^{-4}$ s, $9.0 \cdot 10^{-4}$ s, $1.4 \cdot 10^{-3}$ s respectively.

As it is visible from stated above numerical simulation, the ignition of a gas mix can take place already at the moment of compression waves collision in a vicinity of an axis of symmetry z. It is fair, first of all, for the preliminary mixed combustible gas. However in experiments [5] fuel and oxidizer move in the chamber separately, and the self-ignition takes place in an average part of a cylindrical part of the chamber with a surface S1 at later stages of process. For clearing this effect we should carry out modeling with separate submission of fuel and oxidizer from collectors into the chamber. Let suppose that at the initial moment of time the chamber is filled with nitrogen at $p_0 = 1$ bar, $T_0 = 300$ K, $u = v = w = 0$. At $t = 0$ through different holes of a surface S_1 the submission of fuel and oxidizer in the chamber begins. The specific charges of hydrogen and oxygen at the entrance of the chamber per unit of the hole area are 353 kg / (м^2·s) and 1443 kg /(м^2·s) respectively. The maps of distribution of concentration H_2, O_2 and N_2 in the facility in view of mixing and diffusion of substance are submitted in fig. 8. It is known, that the concentration limits of ignition of hydrogen in oxygen is from 4 up to 94 % of volume [11]. It is visible, that the concentration of hydrogen (necessary for ignition) originally arises in the region approximately on 1/3 of distance from the input surface up to an axis of symmetry. That corresponds to the data of experiment [5].

A space dimension of the mathematical model may play decisive role in determination of the hot spots as well. As it could be seen from fig. 9 micro vortexes appear at the wall of the chamber, where values of temperature is gradually growing. The vortexes are the origins of subsequent hot spots. The structure of such a vortex could not be described within the two-dimensional approach

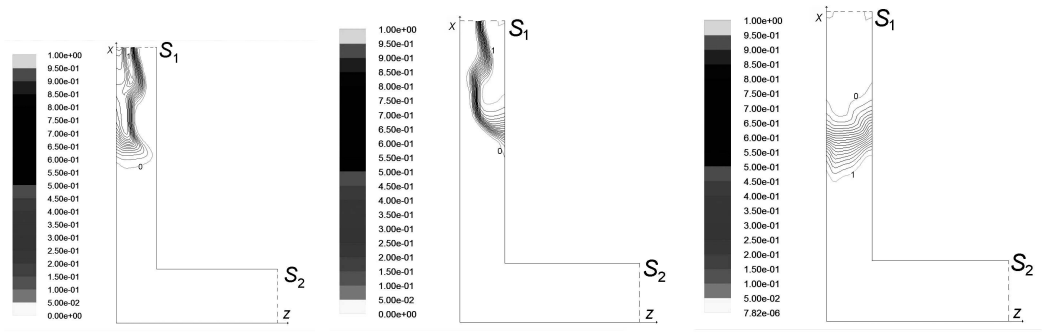


Fig. 8. The maps of hydrogen, oxygen and nitrogen volumetric concentration in the chamber at $t = 1.4 \cdot 10^{-3}$ s

4 Conclusion

The numerical calculations of the flowfield in a planar vortex or cylindrical chambers on the base of Reynolds equations have been performed. The model is based on conservation laws of mass, momentum and energy for non steady two-dimensional compressible gas flow in case of swirl axial symmetry. The processes of viscosity, heat conductivity and turbulence have been taken into account. It was found that transition of kinetic energy of gas into heat due to processes of dissipation generates “hot spots” in boundary layers at the chamber walls. The gas temperature at the spots may exceed the temperature of gas ignition, while the surrounding regions remain still cold. It may be the reason of cold gas self-ignition observed in experiments. The flow turbulence, species mixing and diffusion, three dimensional approach may play decisive role in possibility of gas self-ignition.

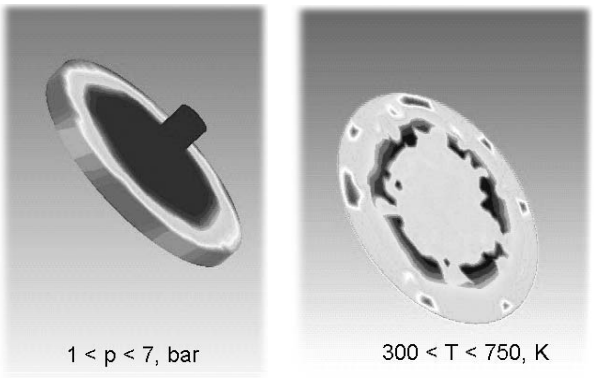


Fig. 9. Maps of pressure and temperature in the chamber for three dimensional simulations.

References.

1. Voitsechovskii B.V. A stationary detonation // Dokl.. AN SSSR. 1959. V. 129, № 6. P. 1254 - 1256.

2. Bykovskii F.A., Zhdan S.A. A continuous spin detonation. Novosibirsk. SO RAN Publ. 2013..

3. Frolov S.M., Dubrovskii A.V., Ivanov V.S. Three-dimensional numerical modeling of working process in the chamber with a continuous detonation // Chemical physics. 2012. V. 31, № 3. Pp. 32 - 45.

4. Frolov S.M., Dubrovskii A.V., Ivanov V.S Three-dimensional numerical modeling of working process in the chamber with a continuous detonation at separate submission of fuel and oxidizer // Chemical physics. 2013. V. 32, № 2. Pp. 56 - 65.

5. Bykovskii F.A., Zhdan S.A , Mitrofanov V.V., Vedernikov E.F. Research of self-ignition and features of the flow in the plane vortexl chamber // Physics of burning and explosion. 1999. V. 35, № 6. Pp. 26 - 41.

6. Vargaftik N.B. The directory on thermo physical properties of gases and liquids. Moscow. Nauka. 1972.

7. Anderson D., Tannehill J., and Pletcher R. Computational Fluid Mechanics and Heat Transfer. Hemisphere. New York. 1984.

8. Launder B.T., Spalding D.B. The numerical computation of turbulent flows // Computer Methods in Applied Mechanics and Engineering. 1974. V.3, № 2. Pp. 269 - 289.

9. Loytsianskii L.G. The mechanics of a liquid and gas. Moscow, Nauka, 1987.

10. Belotsercovskii O.M., Davydov Yu.M. Method of large particles in gas dynamics, Moscow, Nauka, 1984.

11. Staskevich N.L., Severinets G.N., Vigdorchik D.Ya. The directory on gas supplying and using of gas. L.: Nedra, 1990.