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DETONATION INITIATION BY ROTATION OF AN ELLIPTIC CYLINDER INSIDE A CIRCULAR CYLINDER AND DEFORMATION OF THE CHANNEL WALLS

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The possibility of initiating detonation in a closed field due to motion of its boundaries for a one-step kinetic model is studied by numerical simulation of the problems of flow of a propane–air mixture inside and outside a rotating elliptic cylinder enclosed in a circular cylinder; in rotation of a circular cylinder with parabolic blades uniformly distributed along its boundary, or in rotation of a star-shaped figure with parabolic rays originating from the center of rotation; and in a plane chamber with deformable walls. Critical parameter values for which detonation occurs are determined. A method of approximate description of the processes occurring in three-dimensional helical channels is considered. In the numerical study of these processes, software based on the Godunov scheme was used.

Key words: *initiation, detonation, rotation, numerical method, one-step kinetics, propane–air mixture.*

Introduction. Among the problems of wave processes in reactive gas mixtures, self-sustained detonation propagation holds a special place. Continuing attention to this problem is due, in particular, to the use of detonations in various human activities. Increased interest in detonation in the last decade has been motivated by attempts to use detonation in propulsion units. Estimates show that the thermal efficiency of engines using detonation combustion is much higher than the efficiency of conventional combustion devices. In this case, the main problem is detonation initiation. Traditionally, there are two approaches to solving this problem. The first involves the ignition of a mixture by a weak energy source with subsequent deflagration-to-detonation transition implemented by special devices boosting combustion. This leads to transition from normal combustion to a detonation mode. The second approach, called direct initiation of detonation, consists of detonation initiation by a shock wave propagating from an external energy source, for example, igniting of an explosive or electrical or laser breakdown. Detonation can be initiated by a shock wave propagating ahead of a body moving at hypersonic velocity in a combustible mixture or ahead of an immovable body in hypersonic flow. In the late 1990s, a new method of initiation using the cumulation effect of an initially weak shock wave near the axis or center of symmetry [1, 2] was studied in a one-dimensional approach. An extension of this approach to two-dimensional plane and axisymmetric flows is the original method of contoured tubes [3, 4], according to which a weak shock wave moving in a channel interacts with the walls, resulting in cumulation near the axis creation of favorable conditions for ignition and transformation of the shock to a detonation wave. According to the hypersonic analogy [5, 6], the tube flow is similar to the axisymmetric one-dimensional unsteady flow produced by a piston whose radius varies with time according to the shape of the tube contour. Investigations of the detonation initiation by a piston have led to the conclusion that it is effective from the point of view of minimization of both power inputs and the time required for detonation initiation [7].

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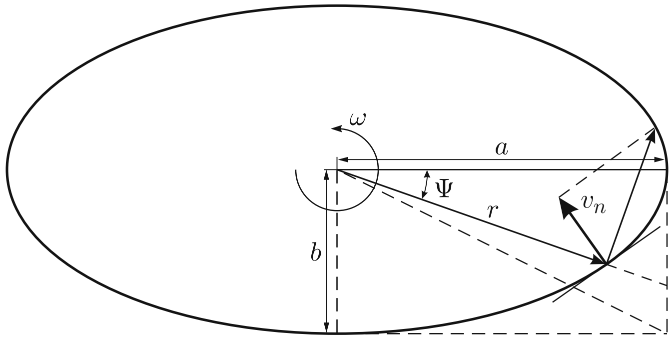

Fig. 1. Diagram of the problem.

The present paper reports the results of a study of the fundamental detonation problems involved in the design of advanced engines based on detonation combustion. These results can be used in the development and validation of new methods of detonation initiation.

Mathematical Model. The ideal perfect gas model is used in the study. It is assumed that the gas is a mixture of chemically reactive components in which exothermic and endothermic chemical reactions can proceed. The motion of the mixture is considered in a two-dimensional approximation.

The plane unsteady flows of the reactive gas mixture are described by the system of equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0, \qquad \frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho_i u)}{\partial x} + \frac{\partial (\rho_i v)}{\partial y} = \omega_i,$$

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (p + \rho u^2)}{\partial x} + \frac{\partial (\rho u v)}{\partial y} = 0, \qquad \frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho u v)}{\partial x} + \frac{\partial (p + \rho v^2)}{\partial y} = 0,$$

$$\frac{\partial (H - p)}{\partial t} + \frac{\partial (H u)}{\partial x} + \frac{\partial (H v)}{\partial y} = 0,$$

where x and y are Cartesian coordinates, u and v are the corresponding velocity components, t is time, ρ, p, and H are the density, pressure, and total enthalpy of the mixture, respectively, and ρ_i and ω_i are the density of the ith component of the mixture and the rate of its change due to chemical reactions.

For the mixture treated as a perfect multicomponent gas, the equations of state are written as

$$p = \sum_{i=1}^{N} \frac{\rho_i}{\mu_i} R_0 T, \qquad H = \sum_{i=1}^{N} \rho_i h_i + \rho \frac{u^2 + v^2}{2}.$$

Here T is the temperature, R_0 is the universal gas constant, μ_i is the molecular weight of the ith component, and and N is the number of components of the mixture. Temperature dependences of the partial enthalpies h_i are obtained by approximation of the data contained in the NASA database.

A stoichiometric mixture of propane with air is considered. The chemical transformations are described by one-step kinetics according to the following stoichiometric equation for five components [8]:

$$\mathrm{C_3H_8} + 5\mathrm{O_2} + 20\mathrm{N_2} \rightarrow 4\mathrm{H_2O} + 3\mathrm{CO_2} + 20\mathrm{N_2}.$$

Here air is considered a mixture of oxygen with nitrogen in a molar ratio of 1 : 4. Then, the rate of change in the density of the mixture components is determined from the relations

$$\frac{\omega_{\mathrm{C_3H_8}}}{\mu_{\mathrm{C_3H_8}}} = \frac{\omega_{\mathrm{O_2}}}{5\mu_{\mathrm{O_2}}} = -\frac{\omega_{\mathrm{H_2O}}}{4\mu_{\mathrm{H_2O}}} = -\frac{\omega_{\mathrm{CO_2}}}{3\mu_{\mathrm{CO_2}}} = A T^{\delta}\, \mathrm{e}^{-E/(R_0 T)} \left(\frac{\rho_{\mathrm{C_3H_8}}}{\mu_{\mathrm{C_3H_8}}}\right)^{\alpha} \left(\frac{\rho_{\mathrm{O_2}}}{\mu_{\mathrm{O_2}}}\right)^{\beta}, \qquad \omega_{\mathrm{N_2}} = 0.$$

The study is performed using a modified Godunov method of the first order in space and time [9], which is effective for calculations of various problems of shock and detonation waves [10–17].

Flow in a Rotating Elliptic Cylinder. We consider an elliptic cylinder with the semiaxes of the base of length a and b (Fig. 1). The cylinder is filled with a propane–air mixture at pressure p_0, density ρ_0, and temperature T_0. At the initial time $t = 0$, let the cylinder begin to rotate instantaneously with constant angular velocity ω around the axis through the center of the base parallel to the generator. The rotation gives rise to two-dimensional flow of the combustible mixture in the base plane. Below, instead of the term elliptic cylinder we use the term ellipse. Shock waves are formed near the sites of the cylinder walls which move in the direction of motion of the mixture, and rarefaction waves are formed near the sites moving in the opposite direction. It is obvious that powerful shock waves can cause detonation. The intensities of the shock waves and rarefaction waves arising from the rotation of the ellipse depends on the positions of the point on its boundary. At the ends of the minor and major axes of the ellipse, the intensity of the waves is equal to zero because of the vanishing of the normal velocity component of the boundary at these points which divide the boundary of the ellipse into parts, in each of which a shock wave or a rarefaction wave is formed. In addition, there are two points on the ellipse boundary which are symmetric about its center and at which the maximum of the normal velocity component of the boundary is reached. At these points, the intensity of the shock waves formed at the initial time is maximal. Generally, for a cylinder with base of any shape, the position of the maximum points can be determined from the condition $d^2r^2/ds^2 = 0$, where r is the distance from the point on the boundary of the cylinder to the point of intersection of the axis of the cylinder with the base; and s is the arc length. In the polar coordinates (r, φ), the positions of the maximum points can be determined from the equivalent condition $r^3\, d^2r/d\varphi^2 + (dr/d\varphi)^4 = 0$. In the case of ellipse, the maximum of the normal velocity component of the boundary is equal to $\omega(a - b)$ and is reached at the ends of the radius vector oriented at an angle $\Psi = \arctan\,[(b/a)^{3/2}]$ to the major semi-axis; the angle is reckoned in a direction opposite to the rotation direction. The above-mentioned points correspond to the best conditions of rapid initiation of detonation at high rotation velocities. However, for small values of ω, detonation can occur not immediately, but after a certain time interval, due to the complex interaction of shock waves with the ellipse wall and with each other.

The results of the studies performed agree with the scenarios of the process presented above. Below, we give the results of calculations of the flow for values of the determining parameters $a = 0.2$ m, $b = 0.1$ m, $p_0 = 1$ atm, and $T_0 = 20°$C and various values of the angular velocity ω. For angular velocities exceeding the critical velocity $\omega_{**} = 13{,}000$ rad/sec, detonation occurs near two sites of the ellipse boundary which are symmetric about its center. For $\omega \to \infty$, these sites increase to sizes close to 2/4 of the ellipse, and for $\omega = \omega_{**}$, they degenerate to points. The calculated position of these points agrees with analytical conclusions on the position of the points at which the maximum of the normal velocity components is reached. At angular velocities lower than the critical velocity $\omega_* = 6000$ rad/sec, detonation does not occur in the rotating cylinder. At velocities between ω_* and ω_{**} detonation occur not immediately, but after a certain time interval, because of the complex interaction of the shock waves. In some regions, the shock waves formed at the initial time become more intense with time. After the intensity of these waves reaches the threshold value, they transform to detonation waves. In this case, the most favorable conditions for detonation initiation take place near the ends of the major axis of the ellipse because at these points, the curvature and linear velocity are maximal. We note that even for the minimum angular velocity of rotation ω_* leading to detonation, initiation occurs fairly rapidly — after the time required for the cylinder to perform 1/4 rotation.

It should be noted that the plane problem considered has the following three-dimensional analogy, which is important from a practical point of view. We consider a channel of a special helical shape produced by uniform rotation of an ellipse with simultaneous motion along the channel axis at constant velocity. If a combustible mixture flows in this channel along the axis with specified hypersonic velocity, the interaction of the flow with the wall leads to a complex three-dimensional flow pattern, resulting in the creation of conditions for detonation initiation. If the helix pitch is much greater than the sizes of the ellipse, then, based on the hypothesis of plane sections [5, 6], the results of the above problem in a plane formulation can be used for an approximate description of three-dimensional processes at hypersonic velocities of the inflowing mixture. Calculated data obtained for a definite value of ω can be used to study flows in channels with various helix pitches $H = 2\pi U/\omega$.

Detonation Initiation outside an Elliptic Cylinder. Let a quiescent propane–air mixture at the same temperature and pressure as in the problem considered above be outside an elliptic cylinder. According to the hypothesis of plane sections, the flow outside the rotating elliptic cylinder can be treated as hypersonic flow around a helical body. We consider flows for various values of the angular velocity of rotation of the ellipse ω. As one might expect, at an angular velocity exceeding the previously obtained critical velocity ω_{**}, instantaneous initiation of detonation occurs. At lower velocities, detonation is absent. The results obtained above for the case of flow inside

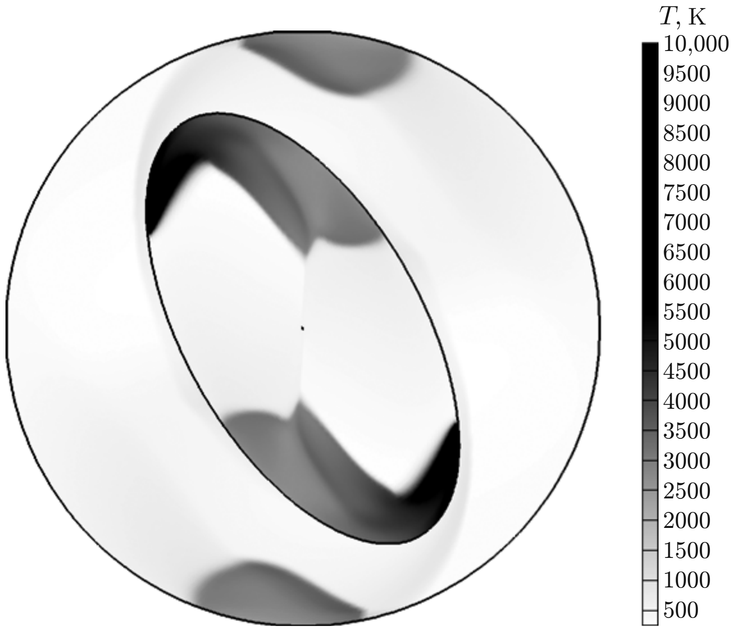

Fig. 2. Temperature field for detonation of the mixture inside and outside a rotating elliptic cylinder enclosed in a circular cylinder.

an ellipse imply that, for $\omega < \omega_{**}$, detonation initiation occurs within a certain time interval after the beginning of rotation as a result of interaction of shock waves with the ellipse walls and with each other. In this case, the concavity of the cylinder walls play a leading role. This suggests that to initiate detonation in the case of external flow, it is necessary to prevent the propagation of divergent shock waves, by restricting the flow region. As the restriction we consider a circular cylinder whose axis coincides with the axis of the elliptic cylinder. Calculations performed for fixed $\omega < \omega_{**}$ and various values of the radius r of the circular cylinder showed that detonation in the gas mixture occurs if the radius of the circular cylinder r is smaller than the critical value r_*. The critical angular velocity ω_* required to initiate detonation decreases with decreasing difference between r and the length of the major semi-axis of the ellipse a, i.e., with decreasing gap between the cylinders. With a small size of the gap, detonation initiation is promoted by the blocking of the gas mixture flow in the gap relative to the reference frame attached to the elliptic cylinder. Figure 2 shows the temperature fields outside and inside (for comparison) an elliptic cylinder for $\omega = 12{,}000$ rad/sec, $a = 0.2$ m, $b = 0.1$ m, and $r = 0.25$ m. The flows inside and outside the cylinder are independent, and their simultaneous calculation allows one to compare the angular velocities necessary for detonation initiation and flow patterns as a whole.

Detonation Initiation during Rotation of Rough Cylinders. Investigation of cylindrical surfaces with fractures or any roughness is motivated by the possibility of rapid detonation initiation due to cumulation effects at the points of surface fracture. Below we give the results of solution of two problems which show the flow features and the mechanisms involved in detonation initiation.

Let obstacles in the form of parabola segments be uniformly distributed in a circular cylinder along its inner boundary. The parabola is constructed in Cartesian coordinates whose origin is at a point on the circle, the x axis is directed along the outside normal, and the y axis along the tangent to the circle in the rotation direction. The parabola segment starts at the coordinate origin and ends at the point ($x_0 = -0.04$ m, $y_0 = 0.02$ m). We consider flows at various velocities of rotation. The results considered below were obtained for a cylinder of radius $r = 0.2$ m for the initial pressure and temperature specified above. Figure 3 gives the temperature field at a rotation velocity $\omega = 7000$ rad/sec. The upper half of the circle corresponds to time $t = 81$ μsec, and the lower half to $t = 119$ μsec. In this case, detonation occurs directly ahead of the obstacle in the neighborhood of the point of its intersection with the cylinder. At lower velocities of rotation, rapid initiation was not observed. Thus, $\omega = 7000$ rad/sec is the critical velocity ω_{**} which decreases with increasing r, according to the equality $v_{**} = \omega_{**} r = 1400$ km/sec.

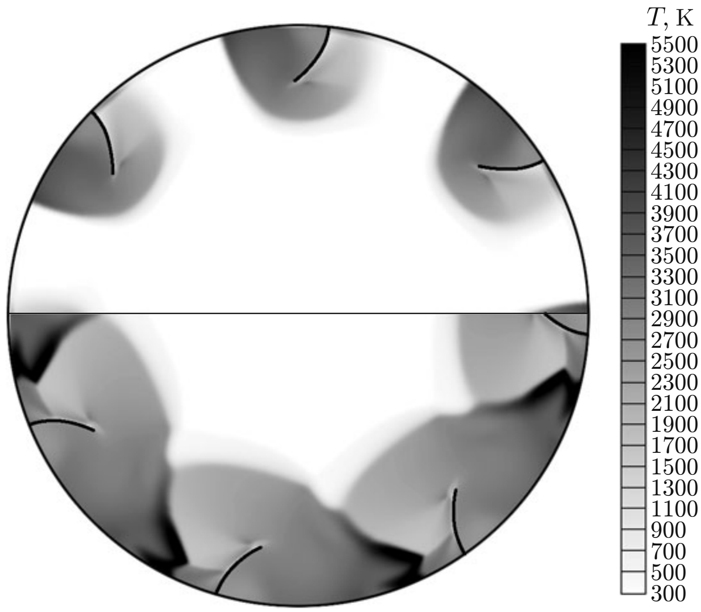

Fig. 3. Temperature field in a rotating circular cylinder with steps of parabolic shape uniformly distributed over its inner boundary for $t = 81$ (at the top) and 119 μsec (at the bottom).

The quantity v_{**} is a linear velocity of rotation of the cylinder boundary. It should be noted that the rotation of the cylinder results in a shock wave occurring at the point of intersection of circle with the parabola segment and moving at a velocity of 1640 m/sec. Under the conditions considered, the ideal Chapman–Jouguet wave velocity is 1880 m/sec. This indicates that in this case, the mechanism of detonation initiation is similar to the mechanism of soft initiation of detonation by a piston responsible for Chapman–Jouguet detonation. With time, the detonation wave propagates along the cylinder surface and is amplified due to centrifugal forces. Flow is gradually formed with a detonation wave converging to the center and having the shape of a curvilinear heptagon (according to the number of obstacles), followed by inhomogeneous flow.

A different flow pattern is observed in the case of rotation of a star-shaped figure with rays in the form of parabola segments stating at the center. This figure consists of seven parabola segments obtained by rotation transformation through an angle of $2\pi/7$ of a segment of the parabola defined by the formula $y = 0.2(x/0.16)(1.1 - x/0.16)$ in Cartesian coordinates with origin at the center of rotation. This parabola segment is specified by the points $(0, 0)$ and (0.16 m, 0.02 m). Figure 4 shows the temperature field at a velocity $\omega = 7000$ rad/sec. The upper semicircle corresponds to the time $t = 245$ μsec, and the lower semicircle to $t = 350$ μsec. In this case, detonation occurs not immediately, but after a fairly long time interval during which the cylinder makes 1/4 rotation. The rotation generates shock waves which diverge from the center and interact with the parabolic rays and with each other. Originally. detonation occurs near the ends of the rays, where the linear velocity is maximal. Subsequently, the detonation wave diverges from the initiation site. It spreads in the form of a thin layer along the ray toward the center and, with intensely diverging front, moves to the cylinder boundary. The powerful shock wave generated after the interaction of the detonation wave with the cylinder transforms to a convergent detonation wave with a broken front, thus initiating reactions in the unburned mixture in the space between the rays (the lower semicircle in Fig. 4).

Flows in a Plane Chamber with Deformable Walls. Below we give the results of investigation of detonation initiation in regions of simple configuration bounded by deformable walls. It is assumed that the volume can vary due to deformation. The investigated plane problems can be used for an approximate description of three-dimensional high-velocity flows in channels with cross section varying along the length.

Below we give temperature fields for the case where the upper wall of the channel deforms sinusoidally with specified frequency and amplitude, retaining parabolic shape, and the remaining three walls are rectilinear and immobile. The effect of the vibration frequency on the detonation initiation is studied. The side walls are 0.05 m high and 0.1 m wide, and the maximum amplitude in the middle of the deformable wall is 0.02 m. Figure 5

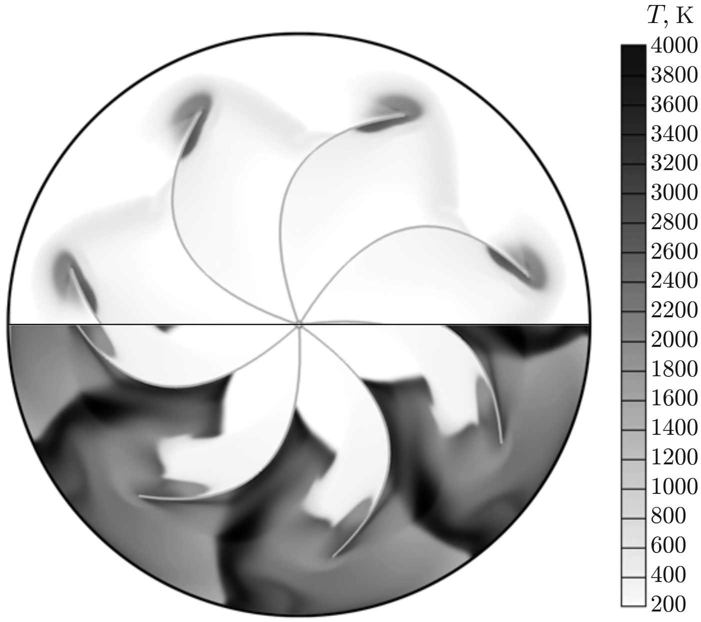

Fig. 4. Temperature field in a circular cylinder inside which a star-shaped figure is rotated for $t = 245$ (at the top) and 350 μsec (at the bottom).

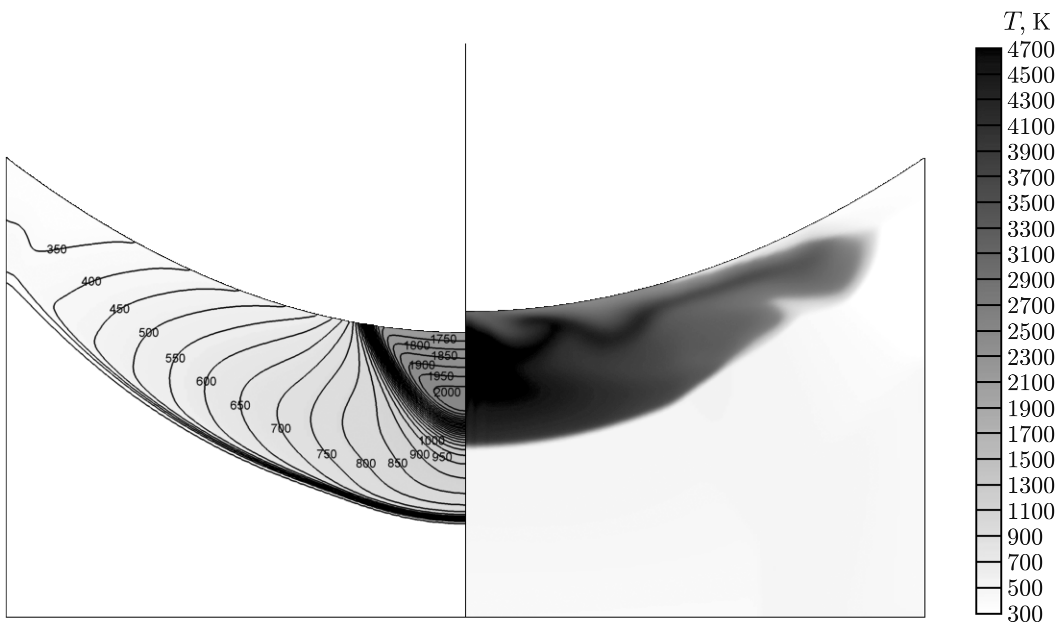

Fig. 5. Temperature field and isotherms in the region with a parabolic wall subjected to harmonic vibrations: $t = 27$ (at the left) and 104 μsec (at the right).

corresponds to the case where the vibration period is 90 μsec. The time $t = 27$ μsec corresponds to the left half of the circle and $t = 104$ μsec to the right half. In this case, the shock wave formed due to the motion of the wall produces a hot spot near the vertex of the parabolic wall but detonation does not occur. Detonation initiation occurs in the beginning of the second vibration period. According to the calculations, the critical vibration period at which there is rapid detonation initiation is equal to $T_{**} = 85$ μsec. For $T > T_* = 300$ μsec, detonation is absent. If T is in the range (T_*, T_{**}), detonation occurs on any of the walls.

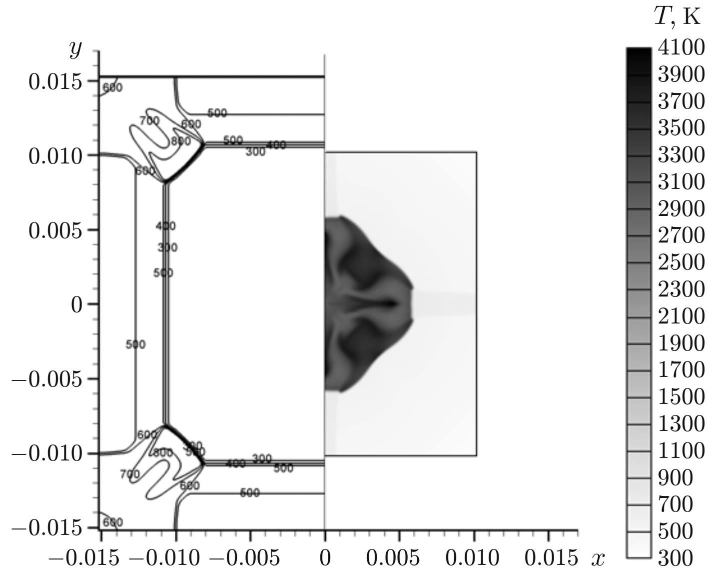

Fig. 6. Temperature field and isotherms in a square region with sinusoidally varying side length: $t = 33$ (at the left) and 47 μsec (at the right).

The problem of detonation initiation in a square region with sinusoidally varying length of the side was studied. Critical values of the vibration periods were obtained. Figure 6 gives the temperature field for two times $t = 33$ and 47 μsec at $T = 100$ μsec for the case where the vibration amplitude of the square side length is 0.02 m (mean length of the square side is 0.04 m). In this case, the critical values of the vibration period were found to be equal to $T_{**} = T_* = 85$ μsec.

A similar study of detonation initiation in a circle whose radius varies sinusoidally at a vibration amplitude of 0.01 m (mean radius of the circle is 0.02 m) shows that the critical values T_{**} and T_* are smaller than the values obtained for the square. For example, at $T = 100$ μsec, the detonation in the circle does not occur.

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REFERENCES

1. V. A. Levin, V. V. Markov, S. F. Osinkin, and T. A. Zhuravskaya, "Determination of critical conditions for detonation initiation in a finite volume by a converging shock wave," *Combust., Expl., Shock Waves*, **38**, No. 6, 693–699 (2002).
2. T. A. Zhuravskaya, V. A. Levin, V. V. Markov, and S. F. Osinkin, "Effect of a collapsing shell on detonation formation in a finite volume by a converging shock wave," *Khim. Fiz.*, **22**, No. 8, 34–37 (2003).
3. I. V. Semenov, P. S. Utkin, and V. V. Markov, "Numerical simulation of two-dimensional detonation flows on a multiprocessor computer," *Vychisl. Met. Program.*, **9**, No. 1, 123–132 (2008).
4. I. V. Semenov, P. S. Utkin, and V. V. Markov, "Numerical simulation of detonation initiation in a contoured tube," *Combust., Expl., Shock Waves*, **45**, No. 6, 700–707 (2009).
5. A. A. Il'yushin, "Law of plane sections in the aerodynamics of high hypersonic velocities," *Prikl. Mat. Mekh.*, **20**, No. 6, 733–755 (1956).
6. G. G. Chernyi, *High Hypersonic Velocity Gas Flows* [in Russian], Moscow, Fizmatgiz (1959).
7. V. A. Levin, V. V. Markov, and S. F. Osinkin, "Initiation of detonation by a piston in a hydrogen–air mixture," *Dokl. Akad. Nauk SSSR*, **258**, No. 2, 288–291 (1981).
8. C. K. Westbrook and F. L. Dryer, "Chemical kinetic modeling of hydrocarbon combustion," *Progr. Energ. Combust. Sci.*, **10**, 1–57 (1984).

9. S. K. Godunov, A. V. Zabrodin, M. Ya. Ivanov, A. N. Kraiko, and G. P. Prokopov, *Numerical Solution of Multidimensional Problems of Gas Dynamics* [in Russian], Nauka, Moscow (1976).
10. V. V. Markov, "Numerical simulation of the formation of the multifront structure of a detonation wave," *Dokl. Akad. Nauk SSSR*, **258**, No. 2, 314–317 (1981).
11. L. I. Sedov, V. P. Korobeinikov, and V. V. Markov, "Theory of shock-wave propagation," *Tr. Mat. Inst.*, **175**, 178–216 (1988).
12. V. A. Levin, V. V. Markov, and S. F. Osinkin "Direct initiation of detonation in a hydrogen–oxygen mixture diluted with nitrogen," *Izv. Akad. Nauk SSSR, Mekh. Zhidk. Gaza*, No. 6, 151–156 (1992).
13. V. A. Levin, V. V. Markov, and S. F. Osinkin "Detonation initiation in a hydrogen–air mixture by explosion of a spherical TNT charge," *Combust., Expl., Shock Waves.*, **31**, No. 2, 207–210 (1995).
14. V. A. Levin, V. V. Markov, and S. F. Osinkin "Restoration of detonation by means of a collapsing shell," *Dokl. Akad. Nauk*, **352**, No. 1, 333–335 (1997).
15. T. A. Zhuravskaya, V. A. Levin, V. V. Markov, and S. F. Osinkin, "Calculation of initiation of gaseous detonation by an electrical discharge," *Khim. Fiz.*, **23**, No. 9, 52–55 (2004).
16. V. A. Levin, V. V. Markov, T. A. Zhuravskaya, and S. F. Osinkin "Nonlinear wave processes during initiation and propagation of gaseous detonation," *Tr. Mat. Inst.*, **251**, 200–214 (2005).
17. V. A. Levin, I. S. Manuilovich, and V. V. Markov, "New effects of layered gaseous detonation," *Dokl. Ross. Akad. Nauk*, **430**, No. 2, 35–43 (2010).