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On Analogy of 2D and 3D Combustible Mixture Flows

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ABSTRACT
The results of numerical simulations are presented for planar air flows in a bounded volume of square cross section diminishing due to a uniform motion of the walls, for a flow of a propane-air mixture under sinusoidal variation of the size of the square domain, for three-dimensional (3D) supersonic air and propane-air flows in channels of variable square cross section. The flows inside and outside the rotating elliptical cylinder, inside helical 3D channel of elliptic cross section were investigated. Specific features of shock-wave processes that are associated with the piston effect and focusing are established. The hypersonic analogy between planar and spatial flows is confirmed, which allows one to use 2D solutions in estimating 3D flows. The equations of a multi-component ideal perfect gas and one-stage kinetics of chemical reactions are used to describe the flows. The method of numerical simulations is based on S. K. Godunov's scheme and implemented within an original software package.

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Introduction

The logic of the development of gas dynamics leads to the complication of mathematical models due to the necessity to take into account the real properties of a medium and various fast physicochemical processes and to consider flows in spatial domains of complex geometry. Today, the main research tool capable of solving the fundamental problems of science and practice is a computational experiment, which, owing to the recent progress in the fields of computer science and computer technology, opens up virtually unlimited possibilities for specialists. It is the numerical methods that allowed the scientists from the Institute of Mechanics (Moscow State University) and the Steklov Mathematical Institute (Russian Academy of Sciences) to obtain pioneering results in the field of detonation theory (Korobeinikov et al, 1972).

Among the problems addressed by scientists who study wave processes in reacting gas mixtures, of special importance is the formation of a self-sustained mode of detonation propagation. The increased interest in this problem is due, in particular, to the practical application of detonation in various fields of human activity. Recently, interest in detonation has grown in connection with attempts of its application to jet engines and various-purpose power plants. Among the relevant problems, the most

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important one is that of detonation initiation. There are two traditional approaches to it. The first one is related to igniting a mixture by a weak source of energy and then transforming the combustion into detonation by means of special devices that intensify combustion. In this way normal slow combustion develops into detonation combustion. In the second approach, called a direct initiation of detonation, detonation is formed due to a shock wave generated by an external source of energy, e.g., by the explosion of explosives or electrical or laser breakdown. The role of the initiator of detonation can be played by a shock wave either ahead of a body flying with supersonic velocity in a combustible mixture or ahead of a fixed body streamlined by a supersonic flow.

Slightly more than 10 years ago, a new method of initiation was investigated in the one-dimensional (1D) approximation in which the focusing of an originally weak shock wave occurs near the axis or the center of symmetry (Levin et al., 2001, 2002). This approach has been extended to 2D planar and axially symmetric flows, which has resulted in an original method of shaped pipes (Levin et al., 2010; Semenov et al., 2008, 2009; Tunik, 2010). The idea of the method is that a sufficiently weak shock wave propagates in a channel and, due to its interaction with the pipe walls and focusing, favorable conditions for the ignition and transformation of the shock wave into a detonation wave are formed near the axis. According to the hypersonic analogy (Chernyi, 1959; Il'yushin, 1956), a flow in a pipe is similar to a 1D axially symmetric unsteady flow arising under the action of a piston whose radius varies in time and reproduces the profile of the pipe. The results of the study of the initiation of detonation by a piston show that this process is efficient from the viewpoint of minimization of both energy expenditure and formation time of detonation (Levin et al., 1990).

In the present article, we describe the results of recent studies of the fundamental problems of detonation that are related to the substantiation of new methods of detonation initiation without abundant power supply from outside, and in which the decisive role is played by the interaction of gas mixtures with solid boundaries of the flow region, focusing phenomena, and the formation of complex shock-wave structures.

The purpose of this study is to show the applicability and possibilities of hypersonic analogy to the 3D studies of the process of initiation of detonation by 2D calculations. It is widely known that this analogy is valid for non-viscous flows. The influence of the boundary layer is a separate challenge, which will be considered in the future.

Mathematical model and numerical method

To describe gas-dynamic flows, we apply the system of Euler equations for an ideal multicomponent reacting mixture in a fixed Cartesian system of coordinates. In the case of 2D planar flows, the equations have the form:

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial(\rho_i u)}{\partial x} + \frac{\partial(\rho_i v)}{\partial y} = \omega_i$$
$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(p + \rho u^2)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} = 0$$
$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho u v)}{\partial x} + \frac{\partial(p + \rho v^2)}{\partial y} = 0$$
$$\frac{\partial(H - p)}{\partial t} + \frac{\partial(H u)}{\partial x} + \frac{\partial(H v)}{\partial y} = 0$$
$$H = \sum_{i=1}^{N} \rho_i h_i + \rho \frac{u^2 + v^2}{2}, \quad \rho = \sum_{i=1}^{N} \rho_i$$

Here, p and ρ are the pressure and density of the mixture, u and v are the velocity components along the x and y axes, N is the number of components of the mixture, ρ_i and h_i are the density and enthalpy of the ith component, ω_i is the variation rate of ρ_i under chemical reactions, and H is the total enthalpy. The equations of state of the mixture are:

$$p = \sum_{i=1}^{N} (\rho_i/\mu_i) R_0 T \qquad h_i = c_{0i} + c_{pi} T \qquad i = 1, \ldots, N$$

where T is the temperature of the mixture, μ_i are the molar masses of the components, R_0 is the universal gas constant, and c_{0i} and c_{pi} are constant coefficients obtained by approximating tabular data.

Unsteady 3D flows are described by the following system of equations:

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial(\rho_i u)}{\partial x} + \frac{\partial(\rho_i v)}{\partial y} + \frac{\partial(\rho_i w)}{\partial z} = \omega_i$$
$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(p + \rho u^2)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} + \frac{\partial(\rho u w)}{\partial z} = 0$$
$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho u v)}{\partial x} + \frac{\partial(p + \rho v^2)}{\partial y} + \frac{\partial(\rho v w)}{\partial z} = 0$$
$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho u w)}{\partial x} + \frac{\partial(\rho v w)}{\partial y} + \frac{\partial(p + \rho w^2)}{\partial z} = 0$$
$$\frac{\partial(H - p)}{\partial t} + \frac{\partial(H u)}{\partial x} + \frac{\partial(H v)}{\partial y} + \frac{\partial(H w)}{\partial z} = 0$$
$$H = \sum_{i=1}^{N} \rho_i h_i + \rho \frac{u^2 + v^2 + w^2}{2}, \quad \rho = \sum_{i=1}^{N} \rho_i$$

Here, w is the velocity component along the z axis, and the other notations coincide with those given above.

As the boundary conditions on solid boundaries, we use the impermeability condition.

The flows of a combustible mixture of hydrocarbons with air are studied within the model of one-stage kinetics (Westbrook and Dryer, 1984), in which combustion is described by a single irreversible reaction. As a combustible mixture, a propane-air mixture is used, for which the reaction occurs in accordance with the stoichiometric equation:

$$C_3H_8 + 5O_2 + 20N_2 \rightarrow 4H_2O + 3CO_2 + 20N_2$$

Here, $N = 5$, and the reaction rate determines all ω_i according to the equalities:

$$\frac{\omega_{C_3H_8}}{\mu_{C_3H_8}} = \frac{\omega_{O_2}}{5\mu_{O_2}} = -\frac{\omega_{H_2O}}{4\mu_{H_2O}} = -\frac{\omega_{CO_2}}{3\mu_{CO_2}} = AT^{\beta}\exp\left(-\frac{E}{R_0 T}\right)\left(\frac{\rho_{C_3H_8}}{\mu_{C_3H_8}}\right)^a\left(\frac{\rho_{O_2}}{\mu_{O_2}}\right)^b \quad \omega_{N_2} = 0$$

where the subscripts i are replaced by the symbols of mixture components and A, E, a, b, and β are constants.

In the problems considered below, air is regarded as a mixture of oxygen and nitrogen with a molar ratio of $\nu_{O_2} = \nu_{N_2} = 1:4$, and a propane-air mixture is defined by the ratio $\nu_{C_3H_8} = \nu_{O_2} = \nu_{N_2} = 1:5:20$. In the case of air flows in the absence of fuel, we have $N = 2$ and $\omega_1 = \omega_2 = 0$.

Parameters used in single-step reaction mechanism have been adjusted using the private data to correctly describe the thermal effect of reactions, the induction heat, and time. As a result, it was possible to reproduce in the calculations 2D and 3D cellular structures and spin detonation. This one-step mechanism is widely used by different authors. We emphasize that we are able to use sophisticated models of chemical kinetics, but in this article we have used consciously simplified models. In the future we plan to use a complicated chemical kinetics model to show the limits of applicability of simplified models in the simulation.

The study is carried out by a modified Godunov's method (Godunov et al., 1976) of first-order accuracy in both space and time. The method is implemented in an original software package designed for solving a wide range of 1D, 2D, and 3D problems of unsteady dynamics of gaseous combustible mixtures.

Adequate calculation of flows of reacting gas mixtures requires high spatial resolution such that a sufficiently large number of cells are always contained in the reaction zone. Computational algorithms were tested and validated on problems with the exact solution. In addition, the validation was carried out on 2D and 3D calculations, which reproduced the experimentally observed cellular structure of detonation. Therefore, the numerical analysis requires large resources of multiprocessor supercomputers. The software package developed and used by the authors in the present study is parallelized on the basis of MPI and is capable of performing calculations for problems with up to a few billion computational cells. In the present study, calculations have been carried on the Lomonosov supercomputer (Voevodin et al., 2012) at Moscow State University, with computational grids containing from 50 to 100 million cells.

Below, we consider a number of 2D and 3D problems in which shock and detonation waves arise either due to the action of the moving boundaries of the 2D flow region or under the interaction of a 3D supersonic flow with the walls of the channel. Below we will show that all of these problems are closely related to each other.

Air flow in a square chamber of decreasing size

Consider a square chamber with side length H that contains, at the initial instant of time, still air at temperature T_0 and pressure p_0. The opposite sides of the square start to move toward each other with given constant velocity W, so that the side length of the square decreases according to the linear law $h = H - 2Wt$, while the center of the square remains fixed (Figure 1).

It follows from the statement of the problem that at every instant of time the arising flow is symmetric with respect to the "horizontal," "vertical," and "diagonal" axes of symmetry of the square. The moving sides of the square play the role of a piston and generate, at the initial instant of time, plane shock waves propagating in still air at constant velocity depending on W. As $W \to 0$, the velocity of shock waves tends to the sound velocity in unperturbed air, and the jump in the gas-dynamic parameters on the shock waves tends to 0. For larger values of W, both the velocity of the shock waves and the jump in the gas-dynamic parameters on the front of the shock waves increase. Immediately after the beginning of motion, the shock waves interact with each other near the diagonals of the square. Due to the symmetry, the diagonals can be considered as solid walls from which shock waves incident at an angle of 45° are reflected. This reflection is of irregular character; it gives rise to Mach waves that propagate along the diagonals. At the initial stage of motion of the shock waves from the sides of the square, these waves form an octagon with four plane sides P strictly parallel to the sides of the square and the other four sides D that separate the plane regions of P (see Figure 1). According to the results of calculations, the D waves are not rectilinear.

The diagonal D waves, which result from the interaction of the P waves, propagate with greater velocity than the P waves; therefore, the density, pressure, and temperature

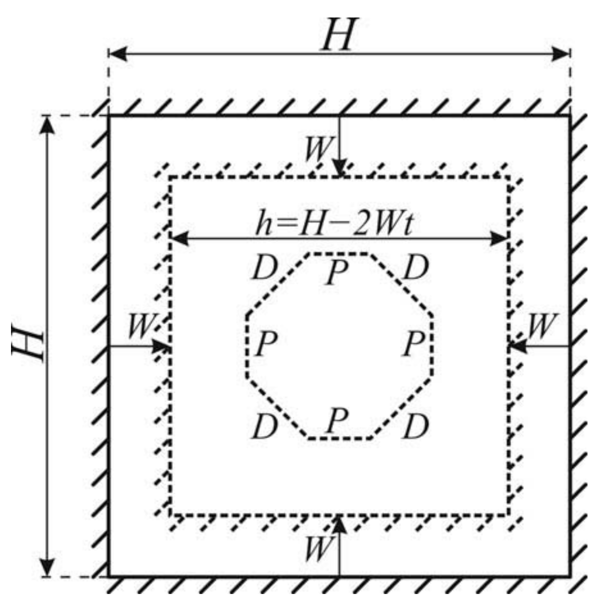

Figure 1. Scheme illustrating the statement of the problem and the shape of a shock wave at the initial stage of a flow.

behind these waves are higher. As the shock waves propagate, the length of the P wave regions decreases, while the length of the D wave regions increases. At some instant of time, the P waves disappear, and the shape of the composite shock wave becomes close to a square with somewhat curvilinear sides situated along the diagonals of the original square. After this instant of time, the D waves interact with each other near the horizontal and vertical axes of symmetry of the square. The further development of the flow may occur in various scenarios, depending on the principal defining parameter of the problem, the velocity W of the sides. The relevant non-self-similar flows can be analyzed only numerically.

Results of calculations

In view of the symmetry of the problem, we carried out the calculations in the first quadrant in the coordinate system with the origin at the center of the square and axes x and y parallel to the sides of the square. On all boundaries of the computational domain, we imposed impermeability conditions. We used a moving uniform orthogonal computational grid whose deformation is determined by the motion of the solid boundaries of the square. Below we present the results obtained for $H = 0.06$ m under the initial conditions $T_0 = 20°C$ and $p_0 = 1$ atm.

The calculations confirmed the above-described dynamics of the shock-wave flow pattern. Figure 2a shows the temperature field for $W = 1500$ m/s at an instant of time when the shock waves form an octagon consisting of alternating P and D waves.

The interaction between P and D waves leads to a complex shock-wave structure of the flow in the perturbed domain. For instance, in this case, in the flow behind the composite shock wave, which separates the flow and rest regions, one observes a regular reflection of secondary shock waves from the sides of the square. Here, jets along the diagonals of the square are formed in which air flows toward the center. These jets lead to significant bending of the D waves. The degree of bending related to the intensity of jets increases with the velocity W. Figure 2b shows the temperature field for a small velocity of $W = 500$ m/s. One can see that there is almost no bending of the D waves, and the Mach reflection of the secondary waves from the sides of the square takes place.

Of special interest is the flow at time instants when the shock wave approaches the center of the square. As we pointed out above, starting from some instant of time, the P waves, which are parallel to the sides of the square, disappear, and the diagonal D waves start to interact with each other. According to the calculations, at velocity W greater than a certain critical value $W = 750$ m/s, the interaction of the D waves has a regular character, and up to the moment of arrival at the center of the square, the wave has the shape of a symmetric curvilinear quadrangle. Moreover, even for $W < W_*$, a regular reflection can be observed for a long period of time as the waves travel to the center of the square. The aforesaid is illustrated by Figure 2c, which shows the temperature field for $W = 700$ m/s. For $W < W_*$, during the time interval when the Mach interaction of the shock D waves occurs, the Mach shock waves are curvilinear due to the effect of flows directed to the center along the coordinate axes. This situation is illustrated in Figure 2d, which demonstrates the temperature field for $W = 400$ m/s. Notice the qualitatively different character of the flows near the center of the square for super- and subcritical values of the velocity W.

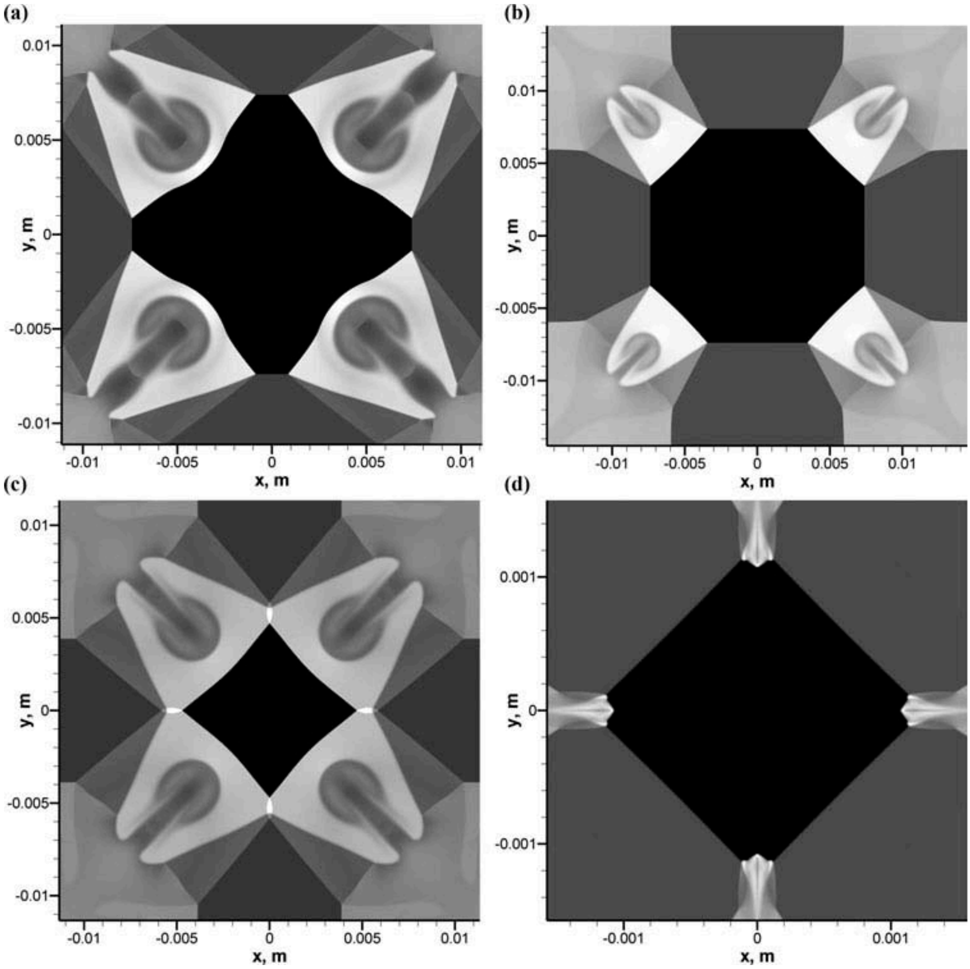

Figure 2. Temperature field in air for the following values of W: (a) 1500 m/s, (b) 500 m/s, (c) 700 m/s, and (d) 400 m/s.

The results obtained for air flows allow one to reveal the specific features of the shock-wave pattern and to determine high-temperature areas in which ignition sites can be formed that lead to the formation of detonation. At the same time, it may occur that for the initiation of detonation it is more efficient to use a more complicated motion of walls, for instance, according to the harmonic law rather than a uniform motion.

Formation of detonation of a propane-air mixture in a variable-size square chamber

Consider a square chamber that contains, at the initial instant of time, a still stoichiometric propane-air mixture at temperature T_0 and pressure p_0. It is assumed that at the subsequent instants of time the center of the chamber remains fixed, while the length of its side varies according to the sinusoidal law $h = H - A[1 - \cos(2\pi t/\mathcal{T})]$, where H is the

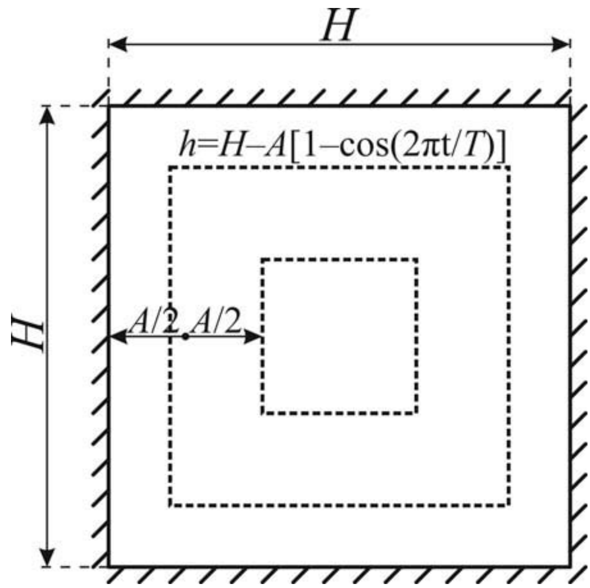

Figure 3. Scheme illustrating the statement of the problem.

side length at the initial instant of time, $\mathcal{T}$ is the oscillation period, and $A < H/2$ is the oscillation amplitude of each of the sides (Figure 3).

The velocity of the sides of the square in this case is equal to $2\pi A\mathcal{T}^{-1}\sin(2\pi t/\mathcal{T})$. It vanishes at the initial instant of time and attains its maximum of $2\pi A/\mathcal{T}$ after a quarter of the oscillation period. After a half oscillation period, the side length attains its minimum value of $H - 2A$.

At every instant of time, the walls of the chamber act as a piston, thereby giving rise to a shock wave or a rarefaction wave in the gas, depending on the direction of motion of the wall. When the wall moves toward the gas, the intensity of the shock waves increases with the velocity of the wall, and, in some range of values of A and $\mathcal{T}$, the motion of the wall may lead to a rapid initiation of detonation during the first reduction of the chamber size. For small intensity of the initial shock waves, detonation may arise in finite time due to the interaction of shock waves, focusing at the center of the chamber, or generation of new shock waves during further oscillation periods. The flow pattern becomes still more complicated due to the focusing of shock waves at the corners of the chamber. A detailed analysis of the processes can be carried out only numerically. Just as in the case of air, the numerical simulation is based on a modified Godunov's scheme with a moving uniform orthogonal computational grid fixed to the deforming boundary, and the calculations are carried out in the first quadrant.

The main defining parameters in the problem under consideration are the amplitude A and oscillation period $\mathcal{T}$. The arising flow pattern significantly depends on these parameters. To classify and construct the diagrams of the flow regimes, we carried out 200 calculations for various values of the pair $(A, \mathcal{T})$ with $T_0 = 20°\text{C}$, $p_0 = 1$ atm, and $H = 0.06$ m.

Results of calculations

When constructing the diagram of flow regimes, we took the parameter A in the full range (0, $H/2 = 30$ mm) with a step of $\Delta A = 2$ mm. The value of the period $\mathcal{T}$ was defined in the range (0, 140 μs] with a step of $\Delta \mathcal{T} = 10$ μs.

The results of calculations allowed us to reveal various modes of detonation initiation separated by critical curves in the "amplitude–oscillation period" plane (Figure 4). The higher the oscillation amplitude and the smaller the period, the more intense the formation of detonation. Detonation may either not arise or arise along the entire perimeter, at the corners, or at the center after one or several oscillation periods. In some cases, a combustible mixture was ignited after five or more oscillation periods. In this case, the initiation of detonation occurred owing to "pumping" energy into the combustible mixture due to the work of the walls of the combustion chamber. One can also observe some resonance phenomena consisting in the ignition of the mixture at a certain oscillation period for smaller values of the amplitude or for greater values of the oscillation period due to the generation of shock waves by the walls of the chamber in a way consistent with the propagation of the shock waves formed at the preceding oscillation periods.

In all flow regimes, in the first oscillation period, one observes a characteristic wave structure near the corners of the square. The structure is formed by plane shock or detonation waves P parallel to the sides of the square and by diagonal shock or detonation waves D. In view of the symmetry of the flow with respect to the diagonals of the square, the D waves can be considered as Mach waves that arise when the P waves impinge on the diagonals as on solid surfaces. The intensity of the diagonal D waves is higher than the intensity of the P waves; therefore, a detonation initiation mode is possible only at the

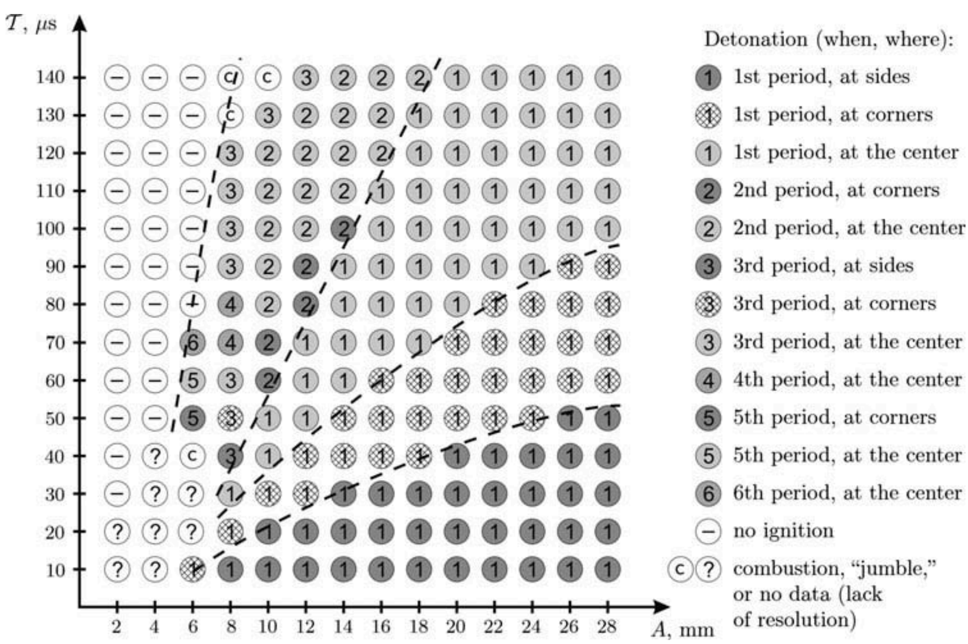

Figure 4. Flow regime diagram on the "amplitude–period" plane.

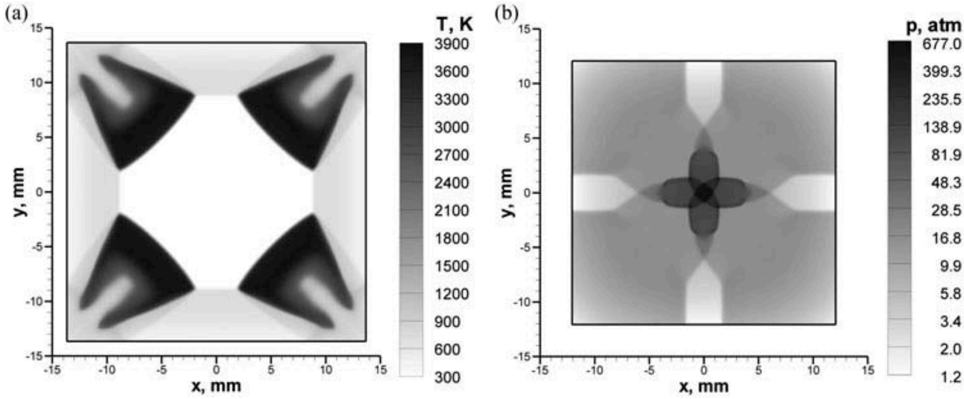

Figure 5. (a) Temperature field for $t = 24$ μs, $A = 18$ mm, and $\mathcal{T} = 60$ μs and (b) pressure field for $t = 38$ μs, $A = 18$ mm, and $\mathcal{T} = 80$ μs.

corners. In this case, the diagonal detonation waves border on plane shock waves parallel to the sides of the square. Figure 5a illustrates this situation. It shows the temperature field for the case of $A = 18$ mm and $\mathcal{T} = 60$ μs.

Modes with detonation initiation at the center on the first period occur at smaller values of the amplitude or for greater values of the oscillation period. In this case, a complicated wave structure of the flow arises at the center, and focusing stimulates the initiation of detonation (Figure 5b).

Note that one can use the above-described results of calculations of 2D wave processes in air and in a combustible mixture for estimating the parameters of 3D flows when studying the initiation of detonation in 3D channels with variable square cross section along the channel axis. This can be done on the basis of the hypothesis of plane sections (Chernyi, 1959; Il'yushin, 1956).

Air flow in a 3D channel of square cross section of variable area

Consider a 3D channel whose surface is obtained by a simultaneous linear reduction of the size of the square and its motion with constant velocity along the rectilinear axis of the channel. Such a channel has four side walls inclined to the channel axis at an angle α. In this case, $\tan\alpha$ is the coefficient of the linear dependence chosen when designing the shape of the channel.

Suppose that homogeneous air with temperature T_0 and pressure p_0 flows into the channel along its axis with given supersonic velocity U. Let x and y be the coordinates along the sections of the channel and z be the coordinate along the channel axis measured from the input section $z = 0$. For sufficiently high velocity of the flow, the air flow is stabilized, and a certain distribution of all gas-dynamic parameters is settled in any cross section of the channel.

According to the hypothesis of plane sections, for sufficiently large values of U, the distributions of parameters on a channel section with coordinate z are close to the distributions at $t = z/U$ in an unsteady 2D flow caused by a change in the shape of the cross section.

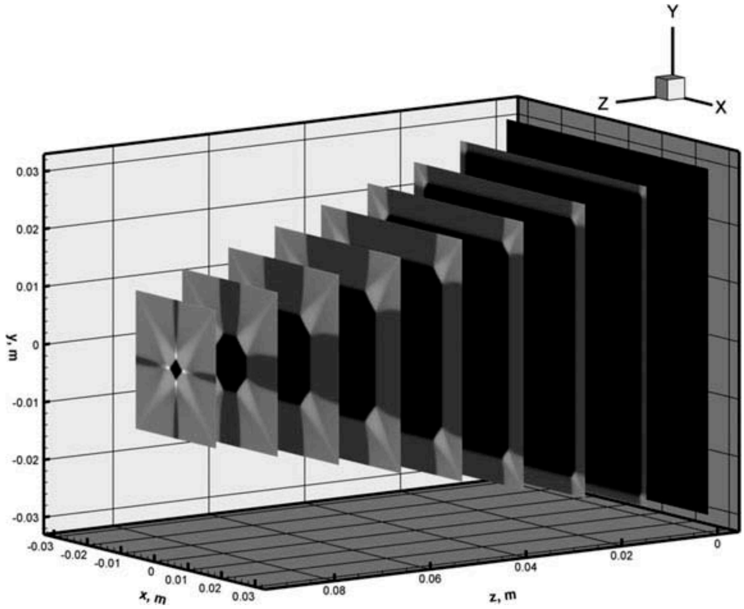

Figure 6. Sections of the temperature field in a 3D steady air flow; $U = 2000$ m/s, $\tan\alpha = 1/5$, and $H = 0.06$ m.

In this case, in the 2D problem, the initial condition ($t = 0$) corresponds to still homogeneous air with the parameters at the input cross section of the 3D channel ($z = 0$). In addition, the square cross section of the channel varies along the z axis, and so the corresponding region of the 2D flow decreases in size and its boundaries move toward each other with velocities $W = U\tan\alpha$. Due to these properties, a steady air flow in the 3D channel for large H is analogous to the indicated 2D air flow in a square of decreasing size.

Results of calculations

The calculations of the 3D air flow were based on Godunov's method with a fixed computational grid. At $t = 0$, as before, air was homogeneous and still. For $t > 0$, a supersonic flow ran into the channel through the input section $z = 0$ at a given velocity U, and the flow became steady in a while.

The calculations fully confirmed the hypothesis of plane sections. Figure 6 presents the temperature fields in several channel cross sections in a steady air flow with velocity $H = 2000$ m/s for a channel with $\tan\alpha = 1/5$ and the input section width $H = 0.06$ m. One can see a good agreement with the 2D flow patterns.

Detonation in a 3D channel of square cross section of variable area

Now, consider a 3D channel of special shape whose surface is obtained under simultaneous variation of the size of the square according to the harmonic law and its translation with constant velocity along the channel axis. Such a channel has curvilinear side walls, and its cross section varies periodically along the channel axis. We will call this period a pitch of the channel by analogy with the pitch of a screw. If a homogeneous combustible mixture flows into the channel at a given velocity U directed along the axis, then the perturbation of the flow caused by the interaction with the channel walls may produce favorable conditions for the formation of detonation. If the channel pitch is much greater than the size of the channel cross section, then one can apply the hypothesis of plane sections. In this case, the shape of the channel is determined by the velocity U of the combustible mixture and by the parameters A and $\mathcal{T}$. In the plane that is perpendicular to the channel axis and moves along this axis at a given velocity H defined at the input, the size of the flow region varies and the flow pattern corresponds to the 2D one in a variable-size square chamber. Here, the results of calculations performed for certain specific values of A and T can be applied to a whole spectrum of channels with different values of step $L = UT$ and with different inclinations of the side walls to the incoming flow. At every point of the side wall of a 3D channel with inclination angle α, shock or detonations waves arise in the same way as in the case of a flow impinging on a wedge. The inclination angle α of the channel walls corresponds to the motion of the walls in a 2D unsteady flow at the velocity $W = U \tan \alpha$, and this value determines the intensity of a local piston effect. Analogs of the 2D P and D waves in 3D supersonic flows are the surfaces of interacting skew steady shock or detonation waves that converge to the axis of the channel downstream of the flow.

Results of calculations

The calculations of a 3D flow of a propane-air mixture were based on Godunov's method with a fixed computational grid. It was assumed that at $t = 0$ the channel contains homogeneous still air. For $t > 0$, a supersonic air flow ran into the channel through the input section $z = 0$ at a given velocity U; the flow was almost completely stabilized in time Δt. For $t > \Delta t$, a stoichiometric propane-air mixture ran into the channel at the same velocity. Under appropriate conditions, a detonation arose, and later the flow became steady.

Calculations for large values of H confirmed the hypothesis of plane sections. Figure 7 shows the temperature fields in several cross sections of a channel in a steady air flow with velocity $H = 6000$ m/s for a channel of length $l = 0.09$ m and cross-section width $h = H - A[1 - \cos(\pi z/l)]$ with $H = 0.06$ m and $A = 0.012$ m. In this case, there is good agreement with 2D flow patterns. One can see skew shock waves attached to the sides of the input section and detonation waves representing curvilinear surfaces in the form of angles with vertices at the corners of the input cross section of the channel.

Note that when considering flows with detonation, the limits of application of the hypothesis of plane sections are shifted toward higher velocities of the incoming flow. According to calculations, for insufficiently high velocity of this flow, an increase in the flow energy due to the heat release in chemical reactions leads to a choking phenomenon and to the propagation of the detonation wave toward the input cross section. This situation is illustrated in Figure 8, which shows the temperature field in several cross sections of the channel for $H = 3000$ m/s.

Detonation initiation inside and outside of rotating elliptic cylinder

We also considered an elliptical cylinder with semi-axes lengths a and b, which was coaxially aligned in a circular cylinder of radius r. A combustible mixture under standard

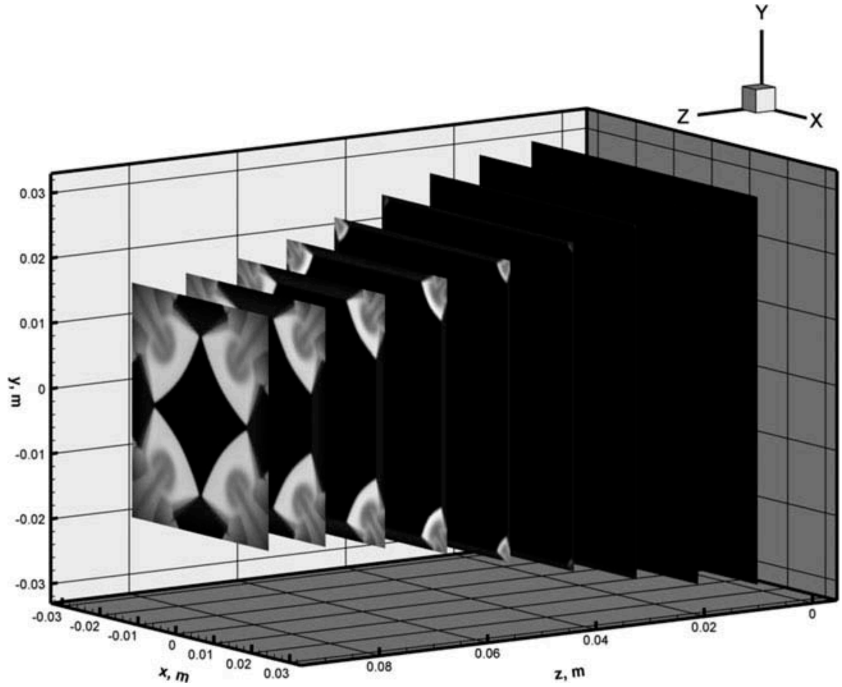

Figure 7. Stationary detonation near dihedral angles of the 3D channel; $H = 6000$ m/s.

conditions was located in the elliptical cylinder and outside of it. It was assumed that the internal cylinder instantaneously acquires a constant angular velocity ω with respect to the cylinder axis at the initial time ($t = 0$). As a result, a 2D flow depending on the x and y coordinates in the base plane is formed in the combustible mixture. Cylinder rotation induces both shock waves near the cylinder surface regions moving toward the mixture and expansion waves near the cylinder surface regions moving in the opposite direction, because each element of the cylinder surface acts as a piston.

The results calculated at $a = 0.2$ m, $b = 0.1$ m, $r = 0.25$ m, and different angular velocities ω are described below. For angular velocities greater than the critical value $\omega_{**} = 13,000$ rad/s, detonation is almost instantaneously (within the induction period) induced near two regions of the ellipse boundaries symmetric with respect to the ellipse center. At $\omega = \omega_{**}$, initiation occurs at ellipse points whose location corresponds to the peak points of the normal component of velocity. As ω increases, the initiation zone gradually expands and transforms to two symmetric regions between the ends of the major and minor semi-axes.

According to calculations, no detonation is formed at all if the angular velocity is smaller than the critical value $\omega_{*} = 6000$ rad/s, because there are no flow regions where elevated parameters exist within a sufficiently long time for ignition. In the interval of velocities $\omega_{*} < \omega < \omega_{**}$, detonation formation requires a long time, after which the complex interaction of shock waves with each other and with the cylinder wall creates the most favorable conditions for detonation initiation at the ends of the major axis of the ellipse because the curvature and linear velocity have the maximum values at these points in the case of cylinder rotation. In some regions of symmetric shock waves generated at the initial time, the intensity increases with time; as a result, shock waves transform to detonation waves.

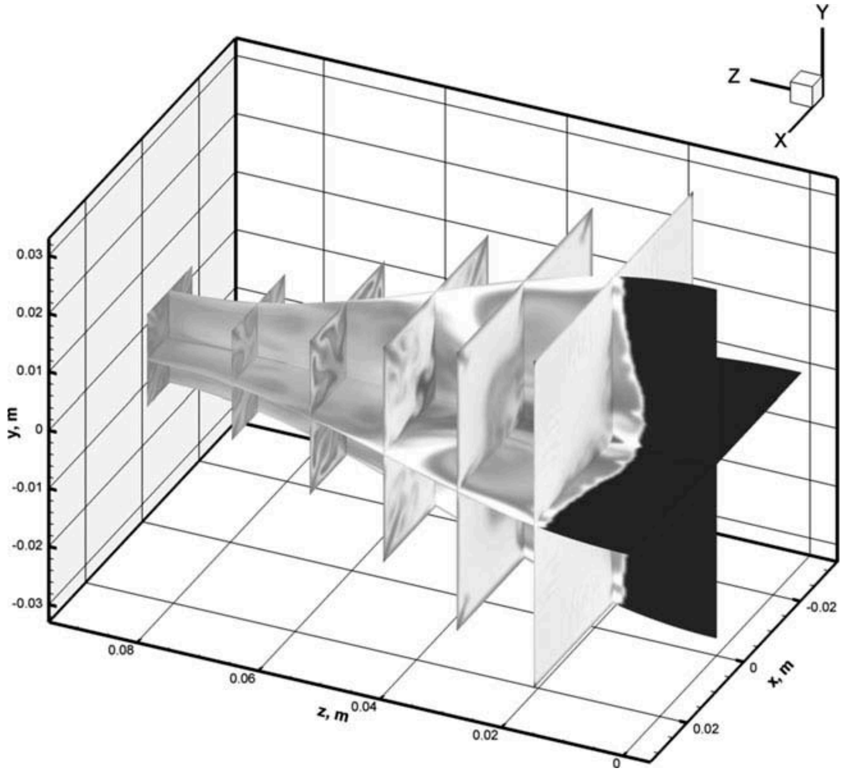

Figure 8. Temperature field in cross sections of the channel in the case when the plane sections hypothesis is inapplicable due to flow choking; $H = 3000$ m/s.

It should be noted that initiation occurs within one quarter of the cylinder revolution even at the minimum angular velocity ω_* sufficient for detonation initiation. Moreover, by virtue of the similarity criterion, a proportional increase in the ellipse axes lengths leads to a decrease in ω_* and ω_{**} in accordance with the equalities $\omega_* a = \text{const}$ and $\omega_{**} a = \text{const}$.

Detonation outside the rotating elliptical cylinder arises during the induction period at angular velocities greater than ω_{**}. According to calculations, at fixed values of $\omega < \omega_{**}$ and different radii r of the circular cylinder, detonation occurs in the combustible mixture at values of r smaller than the critical value r_*. Moreover, as the gap $r - a$ between the elliptical and circular cylinders decreases, the critical angular velocity ω_* also decreases. In the case of a small gap, detonation is formed owing to the effect of "choking" of the combustible mixture flow in this gap. Figure 9 shows the temperature field in an elliptical cylinder with $a = 0.2$ m, $b = 0.1$ m, $r = 0.25$ m at $\omega = 12,000$ rad/s, where detonation arises both inside and outside the cylinder.

Detonation in a supersonic flow in 3D channels of special shapes

It should be noted that the results obtained for a 2D flow can be used for estimating the parameters of 3D flows in studying detonation initiation in channels of special shapes. This can be done by using the hypersonic analogy (Chernyi, 1959; Il'yushin, 1956).

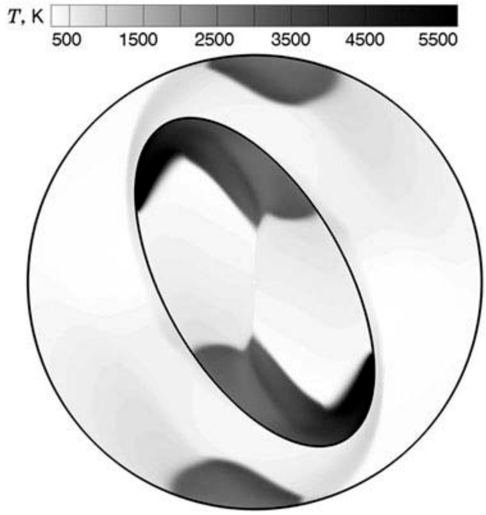

Figure 9. Temperature field in the case of detonation of the mixture inside and outside a rotating elliptical cylinder enclosed into a circular cylinder.

Let us consider a 3D channel of a special helical shape whose surface is obtained owing to simultaneous uniform rotation of an ellipse and its constant-velocity motion along the straight axis of the channel. If a homogeneous combustible mixture enters such a channel with a prescribed velocity U directed along the channel axis, favorable conditions for detonation formation can be created because of flow perturbation due to its interaction with the channel wall. If the helix pitch is much greater than the ellipse size, it is possible to use the hypothesis of plane cross sections. In this case 2D calculation data can be compared with corresponding 3D data obtained for the channel shape determined by the velocity U of the incoming flow. Figure 10 shows that for $U = 2400$ m/s and $H = 2.25$ m the temperature fields in the channel cross sections are close to the temperature fields in the 2D nonstationary problem at the corresponding time instants.

Conclusions

The numerical simulation of planar air flows that arise in a region bounded by an impermeable square contour with the opposite sides moving toward each other at a constant velocity has revealed the laws of development of the shock-wave pattern for various velocities and has allowed us to determine the areas of energy concentration in which detonation can be initiated.

In the problem of detonation initiation of a propane-air mixture under sinusoidal variation of the size of the square region, we have classified the modes of detonation formation depending on the amplitude and period of oscillations of the side length of the square.

The calculations of 3D supersonic flows in channels of variable square cross section have confirmed the hypersonic analogy between planar and spatial flows, which allows one to use 2D solutions to evaluate the parameters of 3D flows as applied to the problems of

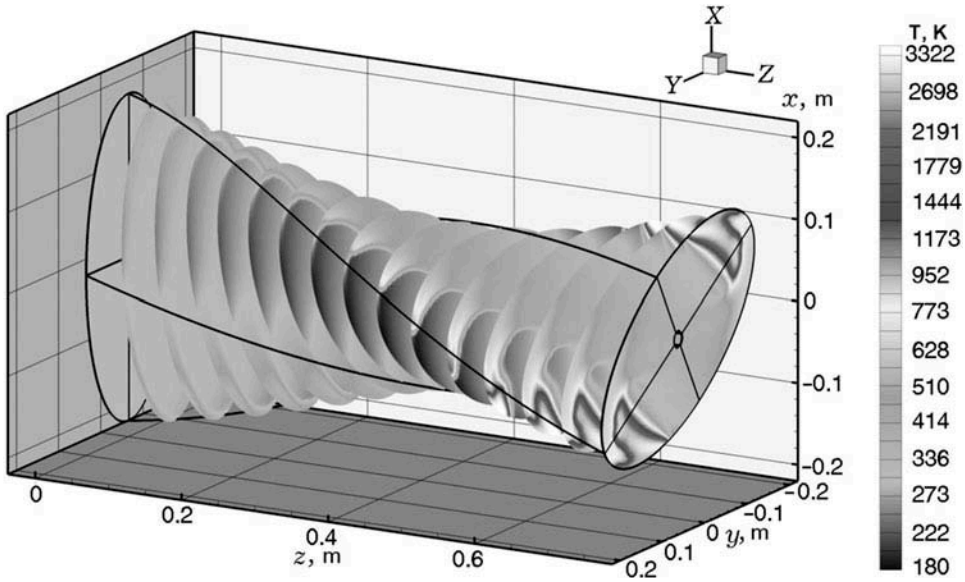

Figure 10. Cross sections of the stationary temperature field in the case of detonation in a helical channel of elliptical cross section ($U = 2400$ m/s and $H = 2.25$ m).

initiation, propagation, and stabilization of detonation waves. At the same time, we have established that the choking phenomenon limits the applicability of this analogy.

The numerical study of detonation initiation in a combustible mixture inside and outside a rotating elliptical cylinder enclosed into a circular cylinder revealed a possibility of detonation formation. The existence of two critical angular velocities of cylinder rotation were found, which determine the qualitative and quantitative pattern of the flow.

Formation of steady 3D detonation in a supersonic flow injected to a helical channel of elliptical cross section was obtained in numerical calculations. It was demonstrated that results of 2D calculations can be used for estimating the possibility of detonation formation in helical 3D channels.

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