Rotating Detonation in Annular Gap

Vladimir A.Levin[1,2], Ivan S.Manuylovich[1,2], Vladimir V.Markov[1,2]
[1]Institute of mechanics of the Moscow State University, Moscow, Russia
[2]Central aerohydrodynamic institute, Zhukovsky, Russia

1 Introduction

To date, research of rotating detonation is fully transferred to practical implementation, for which one must correctly choose the operating conditions, ensuring possibility of wave rotation and optimizing its parameters. This paper presents the results of numerical investigation of the process of propane-air mixture combustion in a rotating detonation wave enclosed in a combustion chamber of special configuration. The problem is formulated in three-dimensional nonstationary way. The rotating detonation is generated in the annular gap of an axisymmetric device between two parallel planes perpendicular to its axis of symmetry. It is assumed that a homogeneous combustible propane-air mixture, resting in a reservoir with predetermined stagnation parameters, is injected in the annular gap through its outer cylindrical surface towards the axis of symmetry and its parameters depend on the pressure in the reservoir and the static pressure in the gap. The incoming fresh mixture is continuously burning in rotating detonation wave and the detonation products flow out of the gap into space, bounded on one side by an impenetrable wall-the continuation of the side of the gap.

2 Mathematical model and calculation method

For the description of unsteady gas-dynamic flows the system of Euler equations is used for ideal multicomponent reactive mixture in fixed Cartesian coordinates. For the case of three-dimensional flows, the equations are as follows:

$$\frac{\partial \rho_i}{\partial t}+\frac{\partial(\rho_i u)}{\partial x}+\frac{\partial(\rho_i v)}{\partial y}+\frac{\partial(\rho_i w)}{\partial z}=\omega_i, \quad \frac{\partial(\rho u)}{\partial t}+\frac{\partial(p+\rho u^2)}{\partial x}+\frac{\partial(\rho uv)}{\partial y}+\frac{\partial(\rho uw)}{\partial z}=0,$$

$$\frac{\partial(\rho v)}{\partial t}+\frac{\partial(\rho uv)}{\partial x}+\frac{\partial(p+\rho v^2)}{\partial y}+\frac{\partial(\rho vw)}{\partial z}=0, \quad \frac{\partial(\rho w)}{\partial t}+\frac{\partial(\rho uw)}{\partial x}+\frac{\partial(\rho vw)}{\partial y}+\frac{\partial(p+\rho w^2)}{\partial z}=0,$$

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

Correspondence to: ivan.manuylovich@gmail.com

Here p and ρ – pressure and density of the mixture, u, v and w – velocity components along the axes x, y and z respectively, N – the number of mixture components, ρ_i and h_i – density and enthalpy of the i-th component, ω_i – rate of ρ_i change due to chemical reactions, H – full enthalpy.
The equations of state of the mixture are of the form

$$p = \sum_{i=1}^{N} \frac{\rho_i}{\mu_i} R_0 T, \quad h_i = c_{0i} + c_{pi} T, \quad i = 1, \dots, N,$$

where T is temperature of the mixture, μ_i – molar masses of the components, R_0 – universal gas constant, and c_{0i}, c_{pi} – constant coefficients obtained from approximation of table values.
The boundary conditions being set on the solid walls are the impermeability conditions, on the outlet – "exhaust" condition of outflow to normal pressure region, on the inlet – special condition (explained below). Study of the flow of combustible hydrocarbon mixture is conducted in framework of a one-step kinetics model [1], in which combustion is described by one irreversible reaction. The propane-air mixture is considered as a combustible mixture with the stoichiometric reaction equation

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

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

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

where indexes i are replaced by symbols of the mixture components. A, E, a, b and β are constants.
As discussed below the air is considered as a mixture of oxygen and nitrogen in a molar ratio $\nu_{O2}:\nu_{N2} = 1:4$, and propane-air mixture is defined by ratio $\nu_{C3H8}:\nu_{O2}:\nu_{N2} = 1:5:20$.
The study is carried out numerically using the original software package in which the modified S.K. Godunov's [2] method for multi-block grids is implemented. This complex has a graphical user interface that allows definition and modification of the computational domain boundaries, provides functions to perform decomposition of the domain by curvilinear surfaces to hexahedral calculation blocks, define the multi-component mixtures, initial and boundary conditions. Calculations can be performed both on the PC and on a supercomputer using code parallelization based on MPI. This paper presents the results of calculations performed on the MSU supercomputer "Lomonosov". The maximum computational cell size did not exceed 0.05 mm. Such grids give sufficient resolution of chemical reaction zone.

3 Statement of the Problem for Modeling of the Process in the Combustion Chamber

An axially symmetric chamber is considered; the shape of its cross section is shown in Fig. 1. Thick black lines represent solid walls. In the three-dimensional space, the solid walls are given by a flat circular disk, a flat ring parallel to the disk, a part of a conical surface with a half-opening angle of 45°, and a flat ring near the outlet of the combustion chamber. The disk and the ring parallel to it form a gap of the annular nozzle into which a combustible mixture is injected. The radius of the disk is 3.76 cm, the inner radius of the parallel ring is 3.32 cm, the width of the annular nozzle is 0.44 cm, and the height of the conical section is 1.5 cm. We used a special computational grid that did not densify near the symmetry axis.
On the solid boundaries of the computational domain that correspond to the walls of the chamber, the impermeability conditions were imposed. On the "output" boundary of the computational domain, the

parameters are determined from the solution of the Riemann problem with pressure $p_0 = 1$ atm and temperature $T_0 = 300$ K beyond the boundary of the computational domain.

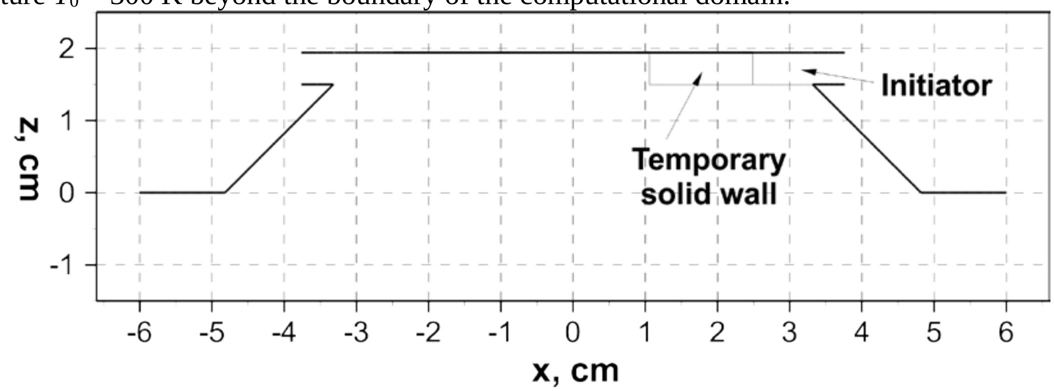

Figure 1. Axial section of the combustion chamber

In this statement of the problem, the combustible mixture flows into the chamber near the external ring. The inflow process is described by a special boundary condition under which the combustible mixture with constant composition flows from the reservoir with given pressure p_s and temperature T_s (also called stagnation parameters) into a zone with variable pressure in the chamber. It is assumed that if the static pressure at the inlet exceeds the stagnation pressure, then there is no reverse flow in this place because the channel is choked as if by a valve. Otherwise, the outflow occurs according to the one-dimensional theory of the de Laval nozzle. According to this theory, in the place where the gas flows out into the surrounding space through inlet channels, all the parameters of the gas are determined by the pressure, temperature, and density (stagnation parameters) in the reservoir from which the outflow occurs. If the static pressure near the inflow point is higher than the critical (sound) pressure calculated by the pressure in the reservoir, then the outflow parameters are calculated by the stagnation parameters for this local value of the static pressure. If the static pressure near the point under consideration is less than the critical pressure, then gas-dynamic choking of the flow occurs, and the inflow parameters are assumed to be constant and equal to the critical values in the de Laval nozzle. At every point of the chamber, the flow parameters are variable during the whole process of development; therefore, at every point of the external ring through which the combustible mixture flows in, the inflow regime varies with time. During steady rotation of detonation along the indicated ring, high values of pressure are reached immediately behind the front and the outflow stops for a while. Then, as pressure drops to the stagnation pressure, the inflow of the fresh combustible mixture starts according to the theory of the de Laval nozzle. Further, for strong rarefaction, the inflow of the combustible mixture with sound parameters occurs.

We have developed a special procedure to form rotating detonation. It consists of two stages: the formation of a convergent axially symmetric flow of the combustible mixture, and the stage of detonation initiation. At the initial time, before the first stage of the process, the space of the chamber is filled with air with pressure p_0 and temperature T_0. At this moment, the air with given stagnation parameters starts to flow into the chamber along the whole annular section. Since air in the chamber is quiescent, this leads to the formation of two shock waves that converge to the symmetry axis. After a short time Δt_1, the combustible mixture with the same parameters starts to flow into the combustion chamber. At this moment, there is no discontinuity of gas-dynamic parameters in the inlet boundary section, and the flow of combustible mixture propagates to the symmetry axis just behind the "trailing" shock wave. Then, after time Δt_2, the stage of formation of a convergent flow of the combustible mixture ends, and detonation is initiated by an instantaneous uniform energy supply. To obtain a rotating detonation, we model the initiation on one side of a solid wall placed in a plane passing through the symmetry axis. The wall has a rectangular shape (Fig. 1) with width equal to the width of the annular nozzle and with length equal to a given value l_1. One of the sides of the wall is located at the boundary of the computational domain through which the combustible mixture flows in (external ring). The wall is needed to separate, for a short period, the hot detonation products on one side from the cold combustible mixture on the other side. In this case, detonation due to energy supply starts to propagate from the wall in a certain direction along the annular nozzle, and after a short time delay Δt_3 the solid wall disappears, allowing the propagation of rotating detonation along a circle. In practice, the disappearance of the wall can be implemented by making it burnable under high temperature of detonation products. The boundary of the energy-supply region that lies on the temporary solid wall has a rectangular shape (see Fig. 1) with width equal to the width of the annular nozzle and with length equal to a given value $l_2 < l_1$. The opposite side of the energy-supply zone has the same shape but is located in a plane passing through the symmetry axis and inclined at a certain angle α to the plane of the temporary wall. The remaining four surfaces of the energy-supply zone are parts of two parallel planes and two coaxial cylinders. To determine the initiation parameters, we have performed a series of calculations and chosen appropriate values of the parameters Δt_1, Δt_2, Δt_3, l, α, and the initiation energy E. According to these calculations, all the above parameters are important for the formation of rotating detonation.

4 Results of Calculations

The detonation propagates through a layer of the combustible mixture that has not yet been burnt. According to the inflow condition, the parameters in this layer near the inlet section are critical. Temperature is about 268 K, and pressure is 22.3 atm. The rotation of detonation in a steady-state regime occurs at an angle to a straight line tangent to a section of the annular nozzle, because detonation propagates through the mixture flowing at large velocity (305 m/s) equal to the velocity of sound in the fresh mixture with critical parameters. In about 100 μs after the initiation of detonation, the rotation is stabilized. On a flat surface perpendicular to the symmetry axis, a flow pattern is formed with a series of shock waves and a curved convex detonation wave propagating through the fresh mixture (Fig. 2).

The left part of Fig. 3 demonstrates the pressure field on a flat surface in the exponential scale at 337 μs after initiation. By this moment, all shock-wave structures rotate uniformly counterclockwise with an angular velocity of 78000 rad/s and completely preserve their shape. In this figure, $\log p = 0$ corresponds to a pressure of $p = 1$ atm, and $\log p = 1$, to a pressure of $p = 10$ atm. The main shock and detonation waves that form the flow structure are marked with Latin letters. The wave **a** is the main curved rotating detonation wave. The wave **b** propagates through the combustible mixture but is a shock wave, because temperature behind it turns out to be lower than the ignition temperature of the mixture. The wave **b** is also strongly curved; moreover, its intensities at different points are significantly different. The wave **c** is a detonation wave. It propagates in the layer of the combustible mixture heated by the wave **b**. The shockwave **d** is attached to the detonation wave **c** and propagates through the combustion products of the mixture. The waves **c** and **d**, just as the gases ahead of them, are separated by a combustion wave, which is not seen in the pressure field in view of its continuity. In this case, the combustion wave is a contact surface or a stream line separating the gas from the combustion products. Near this line, the gases flow with identical velocity along the tangent to the line. The indicated contact surface is situated between the shock wave **b** in the combustible mixture and the shock wave **e** propagating through the detonation products. Near the waves **d** and **e**, there is a shock wave **f**. These three waves have a common intersection point, at which the intensities of all waves decrease to zero. This point is the center of a vortex zone in which the detonation products rotate clockwise and intersect three shock waves on their way. Fig. 3 also shows the shock wave **g**, which propagates through the detonation products. It is a shock wave reflected from the inflow surface, which is formed due to the inclination of the “incident” detonation wave **a**.

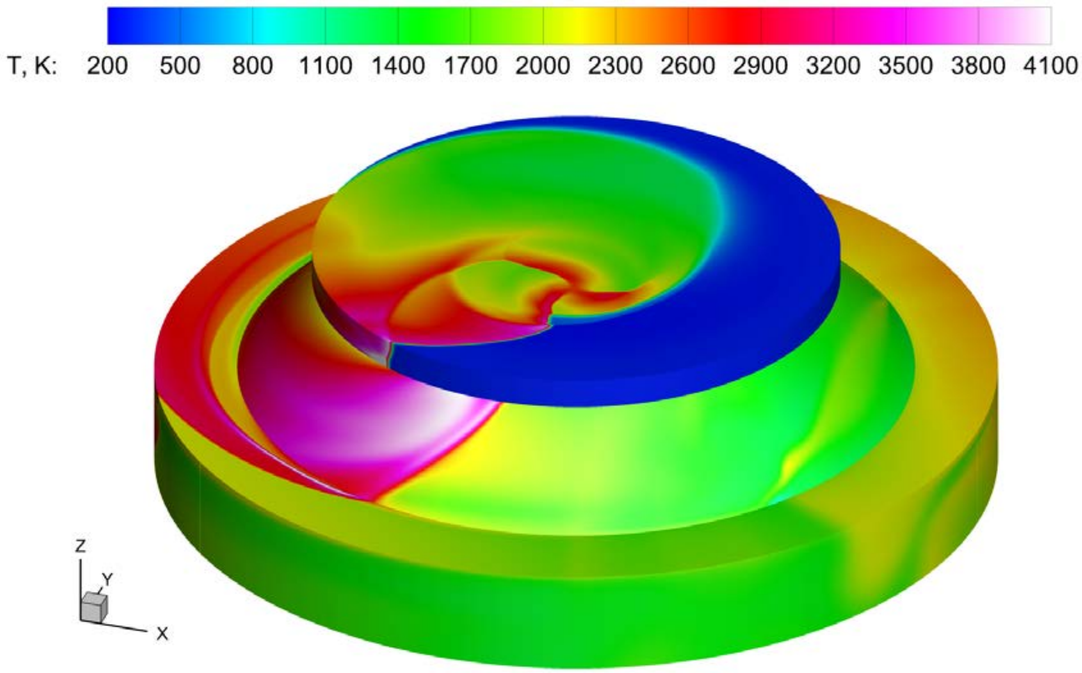

Figure 2. Pressure field in the exponential scale for steady counterclockwise rotating detonation

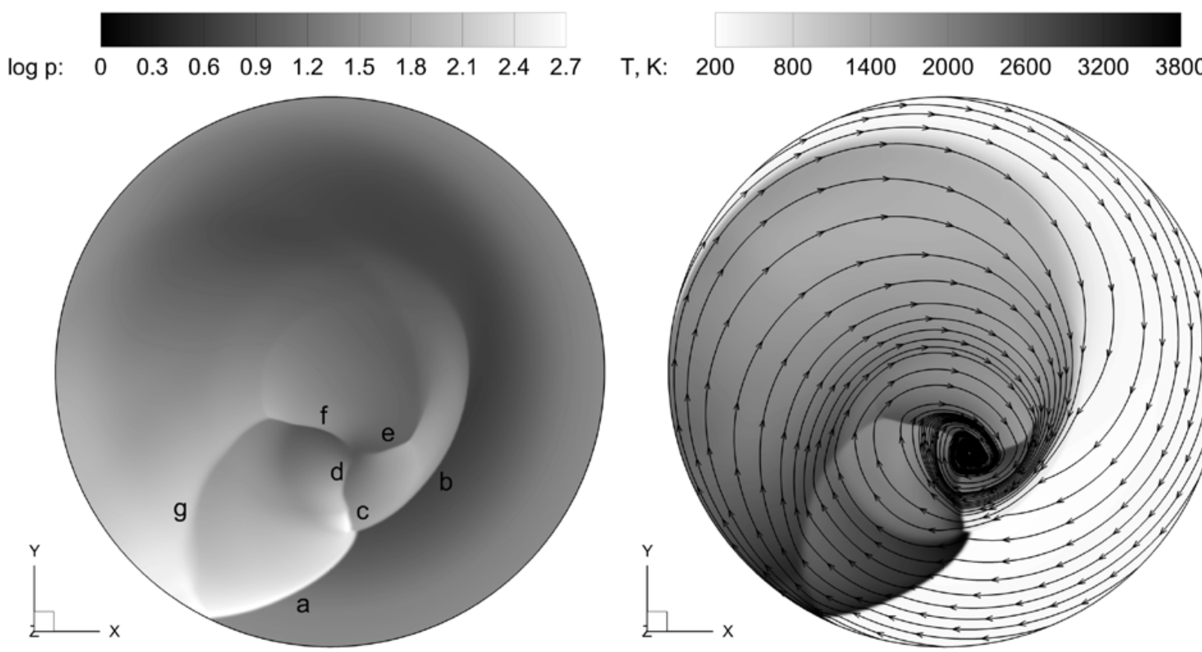

Figure 3. Pressure field (left) and temperature field (right) in the exponential scale for steady counterclockwise rotating detonation. The streamlines on the right figure are presented in the coordinate system rotating with the wave

The right part of Fig. 3 shows the temperature field for steady-state rotation of the detonation. The streamlines presented here were constructed in a coordinate system rotating with the detonation wave. In this figure, a vortex zone is visible and the streamlines on shock waves are refracted. All streamlines emerge from the boundary circle at the same angle, determined by the ratio of the leak-in rate and the linear velocity during the rotation of the detonation. In the restricted zone, there is no inflow behind the detonation wave and the streamlines are parallel to the boundary circle. In the figure, the contact surface between the shock waves **b** and **e** is visible. It separates a dark zone with an elevated temperature and a dense arrangement of streamlines and a light zone of a heated mixture in which the streamlines are sparser. It is clearly seen that the contact surface in question coincides with one of the spiral streamlines ending at the center of the vortex zone.

Note that in the region occupied by the cold combustible mixture, the gas-dynamic parameters are nonconstant due to the convergence of the flow to the symmetry axis. The temperature and pressure of the mixture are slightly higher near the center. Note also that according to the calculations, the flow pattern in the zone between the planes between which the combustible mixture flows in depends weakly on z. As z decreases and the outlet of the combustion chamber becomes nearer, the flow pattern in the perpendicular plane deforms and detonation waves transform into shock waves. Here the three characteristic central waves are also observed. In the three-dimensional space, these waves are curved and slightly twisted with respect to their common connecting line. At the same time, this line, being the centerline of the vortex zone, turns out to be nonparallel to the symmetry axis (z-axis): near the outlet of the combustion chamber, this line deviates from the symmetry axis by a significant distance.

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