Generation of Detonation in a Supersonic Flow of Combustible Mixture with use of Bended Channel

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1 Introduction

The recent increasing interest in the calculations of channel flows with detonation waves is due to the possible application of their results in developing detonation engines and other power plants, more effective than the equipment, where fuel combustion occurs in the normal combustion regime. They have a simple design with the least possible number of movable details and are intended for flight vehicles on a wide range of velocities, from subsonic to hypersonic. Different versions of detonation engines were proposed, with both continuous detonation and its cyclic repetition. From the standpoint of the detonation application to hypersonic jet engines, of great interest is detonation initiation without supplying the energy from outside but only at the expanse of the kinetic energy of a high-velocity combustible mixture flow. In this study, flows in plane channels of constant cross-section with a bend playing the role of both the initiating and stabilizing detonation device are numerically investigated.

2 Mathematical Model and Calculation Method

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

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

$$\frac{\partial(\rho v)}{\partial t}+\frac{\partial(\rho u v)}{\partial x}+\frac{\partial(p+\rho v^2)}{\partial y}=0, \quad \frac{\partial(H-p)}{\partial t}+\frac{\partial(Hu)}{\partial x}+\frac{\partial(Hv)}{\partial y}=0,$$

$$H=\sum_{i=1}^{N}\rho_i h_i+\rho\frac{u^2+v^2}{2}, \quad \rho=\sum_{i=1}^{N}\rho_i\,.$$

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

Unsteady three-dimensional flows are described by the equations

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

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

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

Here w is the velocity component along the axis z, and the remaining symbols are the same as those given above. The boundary conditions being set on the solid walls are the impermeability conditions. The equations for the 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 are molar masses of the components, R_0 are universal gas constant, and c_{0i}, c_{pi} are constant coefficients obtained from approximation of table values.

The boundary conditions set on the solid walls are the impermeability conditions. On the outlet we set “exhaust” condition of outflow to normal pressure region, while on the inlet a special condition (explained below) is prescribed. Study of the combustible hydrocarbon mixture flow is conducted in the framework of a one-step kinetics model [2], in which combustion is described by one irreversible reaction. The propane-air mixture is considered as a combustible one 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 every ω_i according to equalities

$$\frac{\omega_{C_3H_8}}{\mu_{C_3H_8}}=\frac{\omega_{O_2}}{5\mu_{O_2}}=-\frac{\omega_{H_2O}}{4\mu_{H_2O}}=-\frac{\omega_{CO_2}}{3\mu_{CO_2}}=AT^{\beta}e^{-\frac{E}{R_0T}}\left(\frac{\rho_{C_3H_8}}{\mu_{C_3H_8}}\right)^{a}\left(\frac{\rho_{O_2}}{\mu_{O_2}}\right)^{b}, \quad \omega_{N_2}=0,$$

where indices 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 $v_{O2}:v_{N2} = 1:4$, and propane-air mixture is defined by ratio $v_{C3H8}:v_{O2}:v_{N2} = 1:5:20$. In the case of air flows in the absence of fuel $N = 2$, $\omega_1 = \omega_2 = 0$.

The study is carried out numerically using the original software package in which a modified Godunov's method for multi-block grids is implemented. This complex has a graphical user interface that allows to define and modify the boundaries of the computational domain, perform decomposition of the domain by curves and curvilinear surfaces into calculation blocks, and define multi-component mixtures as well as initial and boundary conditions. Calculations can be performed either on a PC or a supercomputer using parallel code based on MPI. This paper presents the results of calculations performed on the MSU supercomputer “Lomonosov”. The maximal computational cell size did not exceed 0.05 mm. Such grids give sufficient resolution of chemical reaction zone.

3 Formulation of the 2D Problem

We will consider a plane channel of constant width with a bend formed by circular arcs joined with the rectilinear channel walls (Fig. 1). The centers of the arcs coincide, while the rectilinear regions of the channel boundaries are tangent to the arcs.

We will denote the channel turn angle by α, its width by h, and the greater and smaller radii of curvature by R and r, respectively. Then $r = R - h$. The coordinate system is so introduced that the region of the "lower" wall near the entry is parallel to the x axis and has the coordinate $y = 0$. The common center of the circular arcs is at the point with the abscissa $x = 0$.

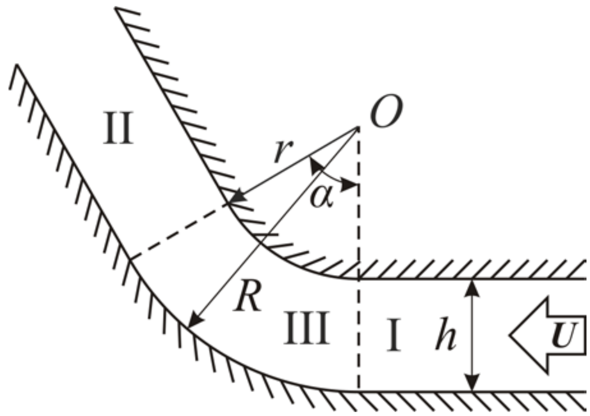

Figure 1. Schematics of the channel; I and II are the regions with plane walls and III is the bend region; α is the turn angle, O is the center of the circular arcs, R and r are their radii, and h is the channel width

The right and left ends of the channel are open. It is assumed that a supersonic flow arrives into the channel from right and flows out of the channel through the left end into a reservoir of large volume, whose walls are impermeable. It is made in the shape of a square, 150h in side length. The orifice in the reservoir is in the middle of one square sides. The following calculations showed that the presence of the reservoir with the above-noted dimensions has no effect on the channel flow for the time interval under consideration.

Let the channel and the reservoir be filled with the air at rest at the pressure p_0, the density ρ_0, and the temperature T_0 and at $t = 0$ a uniform supersonic gas flow start to arrive through the right channel end at a constant velocity U. As a result, a time-dependent flow occurs in the channel, which can stabilize, depending on the values of the parameters α, U, h, and R. At first, a steady air flow is injected and established. After a steady air flow has been formed in the channel, the propane-air mixture with the same parameters p_0 and T_0 starts to arrive in the channel through the entry section instead of the air . The question of interest being numerically investigated is the influence of the mentioned governing parameters on the possibility of initiation and stabilization of detonation.

4 Numerical Results

The rectilinear entry section of the channel had the fixed length of 6 cm which made it possible to observe the detonation wave exiting from the channel if it propagated upstream. The rectilinear exit region length was chosen in such a way that the longer lower channel boundary had a fixed length of 21 cm.

Below we present the results of the calculations for $p_0 = 1$ atm and $T_0 = 300$ K. For the purpose of constructing the flow regime diagram it was originally taken that $h = 2$ cm and R = 3 cm, while the parameters U and α were varied. The velocity U took the values from the range [1000, 3000] m/s with the step $\Delta U = 200$ m/s and the turn angle α from the range (0, 90°] with the step $\Delta\alpha = 5°$.

The results obtained made it possible to reveal different flow patterns separated by critical curves in the U, α plane. The flow pattern diagram constructed from the calculated results is presented in Table 1.

Table 1. The flow pattern diagram in the (U, α) parametric plane

α, deg U, m/s	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90
1000	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
1200	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
1400	X	X	X	X	X	X	X	D	D	D	D	D	D	D	D	D	D	D
1600	X	X	X	X	D	D	D	D	D	D	D	D	D	D	D	D	D	D
1800	X	X	X	X	D	D	D	D	D	D	D	D	D	D	D	D	D	D
2000	X	X	X	X	S	S	S	S	D	D	D	D	D	D	D	D	D	D
2200	X	X	X	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
2400	X	X	X	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
2600	X	X	X	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
2800	X	X	X	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
3000	X	X	X	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
3200	X	X	X	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
3400	X	X	X	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S

Here h = 2 cm and R = 3 cm; X means the regime without mixture ignition, D is the regime with a detonation wave going out of the entry section of the channel, and S is the regime with steady-state detonation. In accordance with the calculations, at any values of U and α the air flow attained the steady state for a finite time. At the flow turn angles α and the velocities U greater than certain critical values a typical wave pattern associated with flow separation was formed near the upper wall of the channel (Fig. 2, left). At the center of this wave configuration there is a vortex zone. At fairly small turn angles or at low oncoming- flow velocities this configuration changes for a single rarefaction wave. At a fairly high flow velocity a compression wave is formed near the lower wall; this is due to the smooth turn of the wall. In this case, in the vicinity of the lower wall a pressure maximum is observable at a certain point, whose position depends on the control parameters (Fig. 2, right). The interaction of these waves leads to the generation of an internal curvilinear shock wave. At low flow velocities it begins near the lower wall, at the point $x = 0$ of the beginning of the channel turn, and overlaps almost the entire channel width.

If the flow turn angle or the flow velocity are fairly large, the temperature behind the shock waves near the channel bend is greater than the ignition temperature and detonation is generated in the propane-air mixture. The further flow development depends on the flow velocity. In accordance with the calculations, if the velocity is smaller than a certain critical value dependent on the angle α, then the detonation wave leaves the channel through the entry section (Fig. 3, left).

If the flow velocity is greater than the critical velocity, then the detonation wave stabilizes (Fig. 3, right). The calculations show that at neither values of the control parameters the detonation wave is carried away by the flow and leaves the channel through the exit section. An increase in the flow velocity results only in a slight downstream displacement of the detonation wave. In accordance with the calculations, the flow structure and the maximum temperature in the air flow near the channel weakly depend on R (Fig. 4).

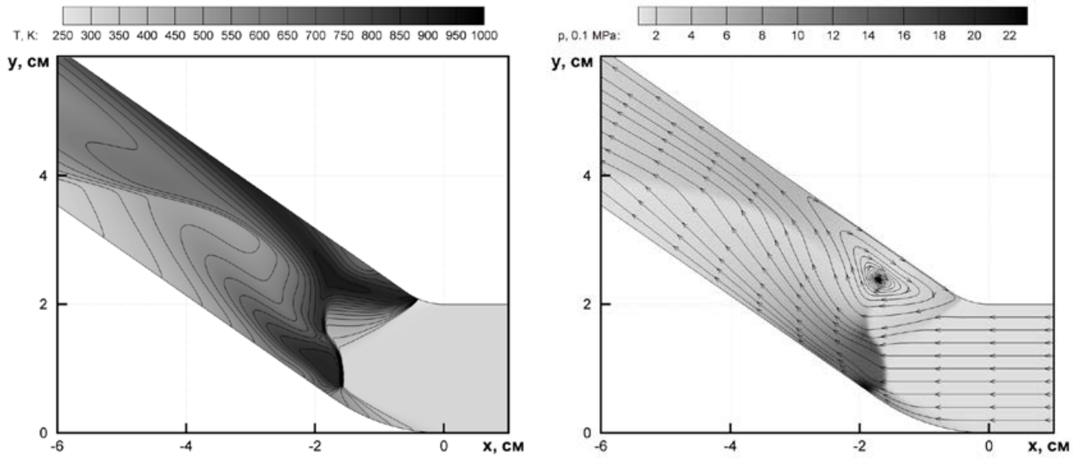

Figure 2. Temperature field (left) and pressure field with streamlines (right) in the steady air flow; U = 1.2 km/s, α = 35°, R = 3 cm

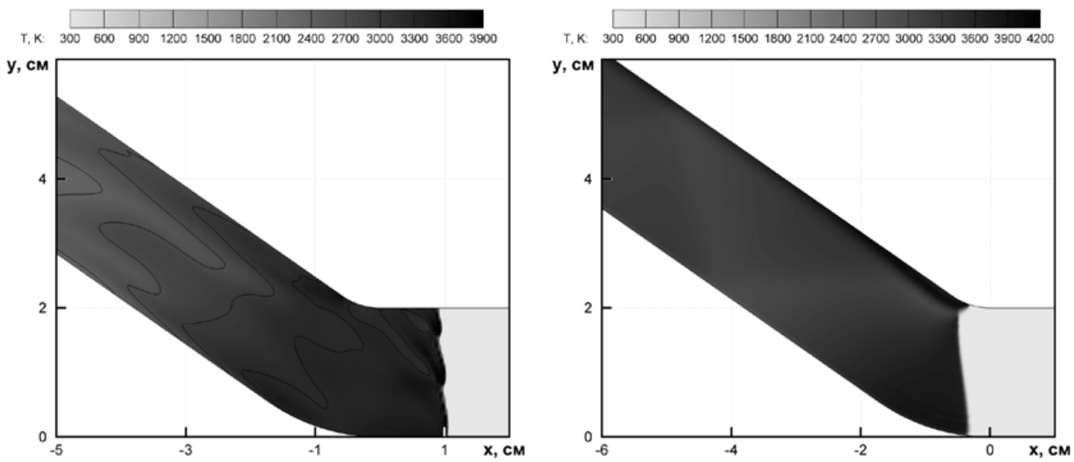

Figure 3. Temperature fields for α = 35°, R = 3 cm, U = 1.6 km/s (left, detonation exits from the channel) and U = 2.2 km/s (right, steady detonation)

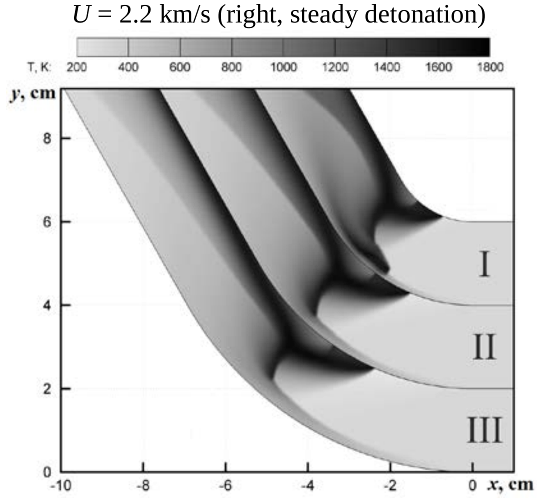

Figure 4. Temperature fields in the steady air flows; U = 1.8 km/s, α = 35°, h = 2 cm, and R = 4, 6, and 8 cm (I–III)

5 3D Problem

The similar problem of detonation initiation and stabilization was considered for a 3D bended tube of circular cross section. Simulations in this case also revealed 3 different flow regimes – without detonation, with detonation exiting channel through inlet and with stationary detonation. Fig. 5 shows a case with stationary air flow transforming to stationary detonation after mixture injection.

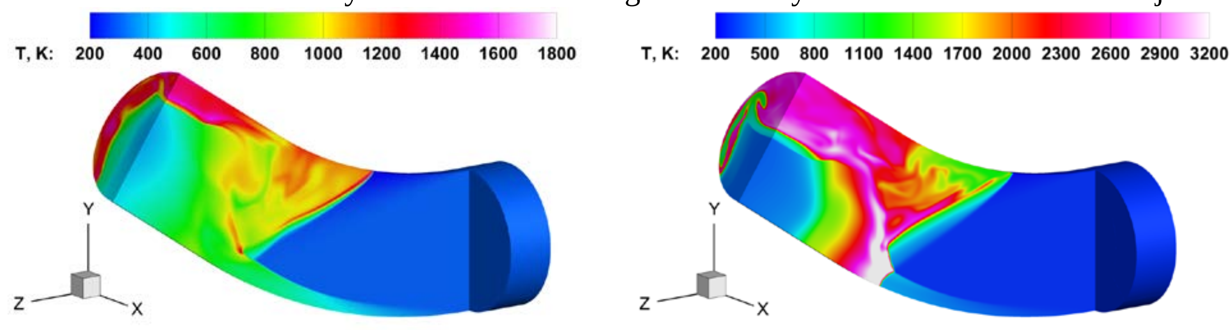

Figure 5. Stationary temperature field (left) before mixture injection and dynamic temperature field (right), transforming to steady field after detonation initiation behind the shock wave; U = 1.8 km/s

6 Conclusions

The problem of detonation initiation in a supersonic flow of stoichiometric propane-air mixture occupying the entire cross-section of a plane or 3D bended channel is considered. Detonation is initiated as a result of the formation of shock wave configurations associated with the flow turn in the channel. The time-dependent flow patterns are obtained and the their dependence on the problem parameters (incoming flow velocity, channel width, channel turn angle, and radii of curvature of the walls at the bend location) is investigated. The flow regime diagram is constructed in the velocity-channel turn angle plane. The numerical calculations show that the radius of curvature of the channel bend has almost no effect on the position of the critical curves separating different flow regimes. It is established that the detonation propagation pattern depends on the ratio of the channel width to the radius of curvature. The investigation is carried out using the special software package intended for solving the problem considered.

7 Acknowledgements

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