2D and 3D Detonation in Layered Reacting Mixtures

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1 Introduction

The paper considers problems of detonation initiation in the supersonic flow of stoichiometric propane-air mixture, which partially or fully fills in the channel cross-section. The initiation in the flow takes place due to a “bench” or a wall, which fully blocks the channel, and in the medium at rest it is caused by explosion. The investigation is performed within the framework of single-stage combustion kinetics by the numerical method based on the S.K. Godunov scheme [1].

2 Mathematical model and calculation method

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

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

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

$$H=\sum_{i=1}^{N}\rho_i h_i+\rho\frac{u^2+v^2}{2}=0, \quad \rho=\sum_{i=1}^{N}\rho_i .$$

Here p and ρ – pressure and density of the mixture, u and v – velocity components along the axes x and y 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 have the form

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

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.

Unsteady three-dimensional flows are described by the equations

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

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

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

Here w is velocity component along the axis z, and the remaining symbols are the same as those given above. The boundary conditions on the solid walls used the impermeability condition.

Study of the flow of combustible hydrocarbon mixture is conducted in 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 mixture with the 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

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

where 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 $\nu_{C3H8}:\nu_{O2}:\nu_{N2} = 1:5:20$. 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 the modified S.K. Godunov's method for multi-block grids is implemented. This complex has a graphical user interface that allows to define and to modify the boundaries of the computational domain, 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 in 3D calculations did not exceed 0.05 mm. Such grids give sufficient resolution of chemical reaction zone.

3 Results of numerical simulation

Critical detonation conditions connected with the inflow velocity and explosion energy were determined. In all the discussed processes one can find then unknown detonation propagation mechanism, which is conditioned by formation of complicated wave flow structure, characterized by shock wave penetration in the inert gas to the layer in front of the detonation wave, with the resulting warmup and combustion. The process is periodic in nature, and differs from standard cellular detonation in the uniform medium. The existence of critical inflow velocities was established upon which qualitative and quantitative flow pattern is dependent. In the uniform flow two different detonation modes were obtained – with stationary wave on the bench and with the wave propagating to inlet channel section. In the combustible mixture layer we found three detonation modes, i. e. with stationary wave on the bench (Fig. 1) and with the wave propagating to the inlet channel section in the form of stationary wave complex or in the mode of galloping layered detonation (Fig. 2 for the channel with a bench, Fig. 3 for the channel with a wall blocking the channel).

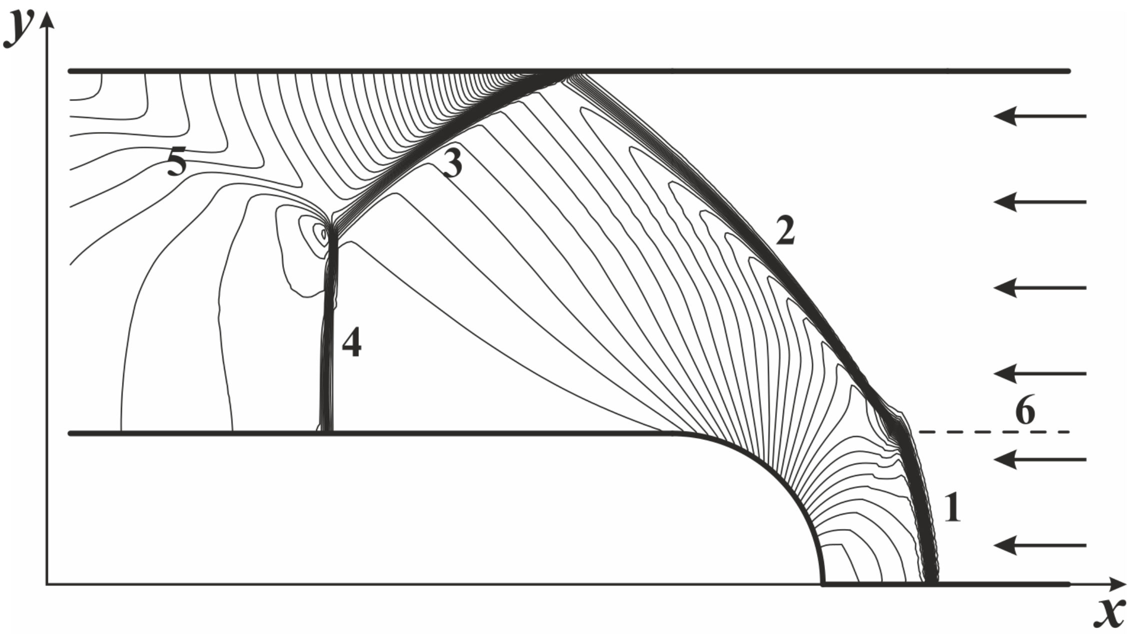

Fig. 1. Stationary detonation in the combustible mixture layer (temperature isolines).

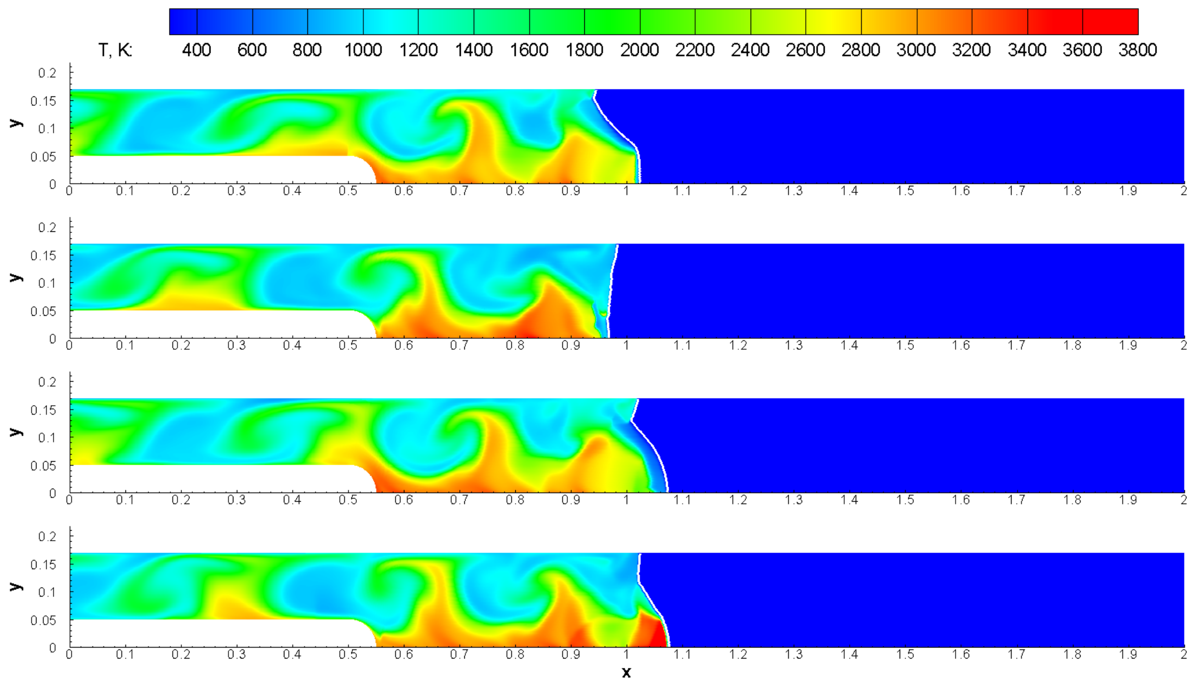

Fig. 2. Phases of galloping layered detonation in a channel with bench (temperature fields).

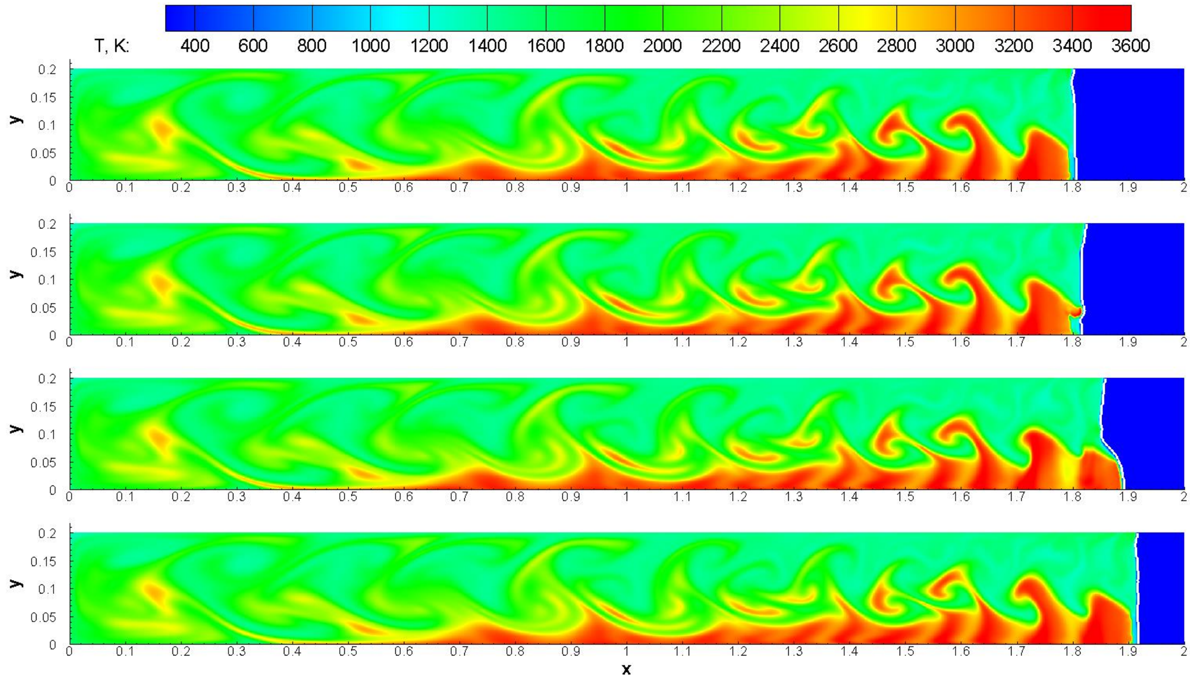

Fig. 3. Phases of galloping layered detonation in a channel with blocking wall (temperature fields).

As the flow rate increases, the rate of wave travel in direction of the inlet section decreases and at the rate equal to the critical one the wave turns to the stationary mode.
2D and 3D supersonic flows have been examined in several configurations. 2D channels were plane or axisymmetric (Fig. 4) with different widths and forms of the bench in the plane case and the central rod in axisymmetric case. The width of the jet as well as the inflow velocity was also variable.

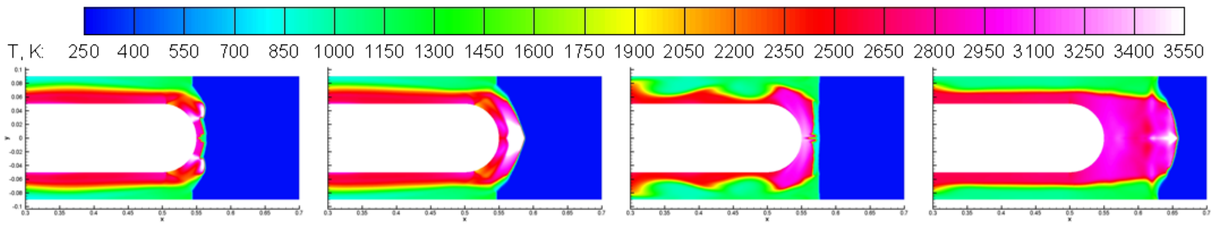

Fig. 4. Galloping layered detonation in a circular channel with a rod in the center.

3D channels differed by forms and sizes of a bench, cross-section forms and sizes (rectangular or circular) and combustible mixture jet cross-section form and location. For several configurations the obtained patterns of the flow were similar to patterns of 2D flows. Particularly, the 2D galloping regime of detonation was observed in 3D calculations. In some cases the unsteady wave structure of the flow was much more complicated as compared with 2D galloping detonation due to propagation of strong transverse shock waves. Fig. 5 shows the scheme of the 3D channel with a bench inclined respect to incoming flow. For this channel a range of incoming flow velocities was found, for which galloping detonation occurs. Fig. 6 and 7 illustrate pressure and temperature fields under 3D galloping layered detonation in the channel with incoming flow velocity equal to 1450 m/s.

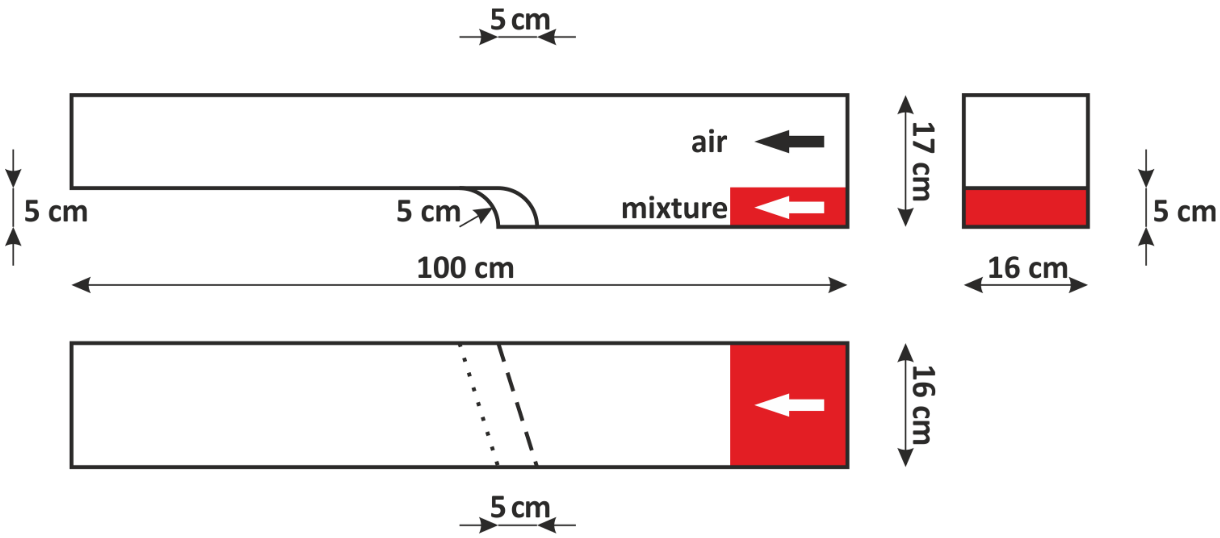

Fig. 5. Three projections of the 3D channel with sizes, air and mixture jet shown.

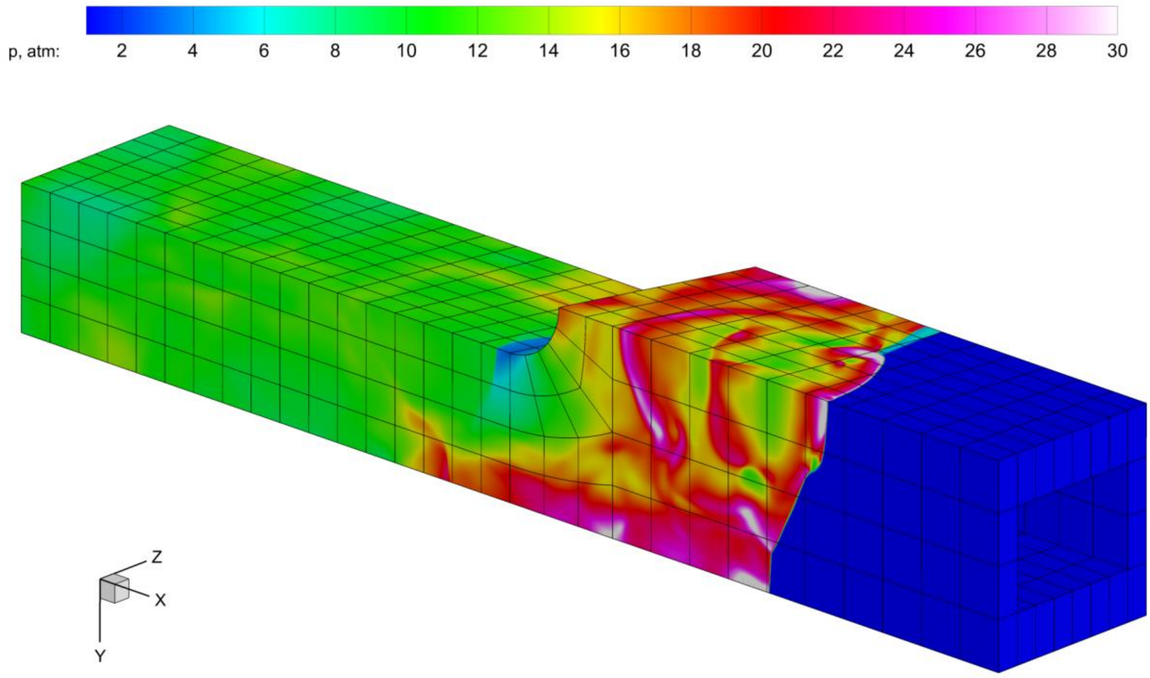

Fig. 6. Pressure field under 3D galloping layered detonation in a channel with inclined bench. The layer is located near the upper wall.

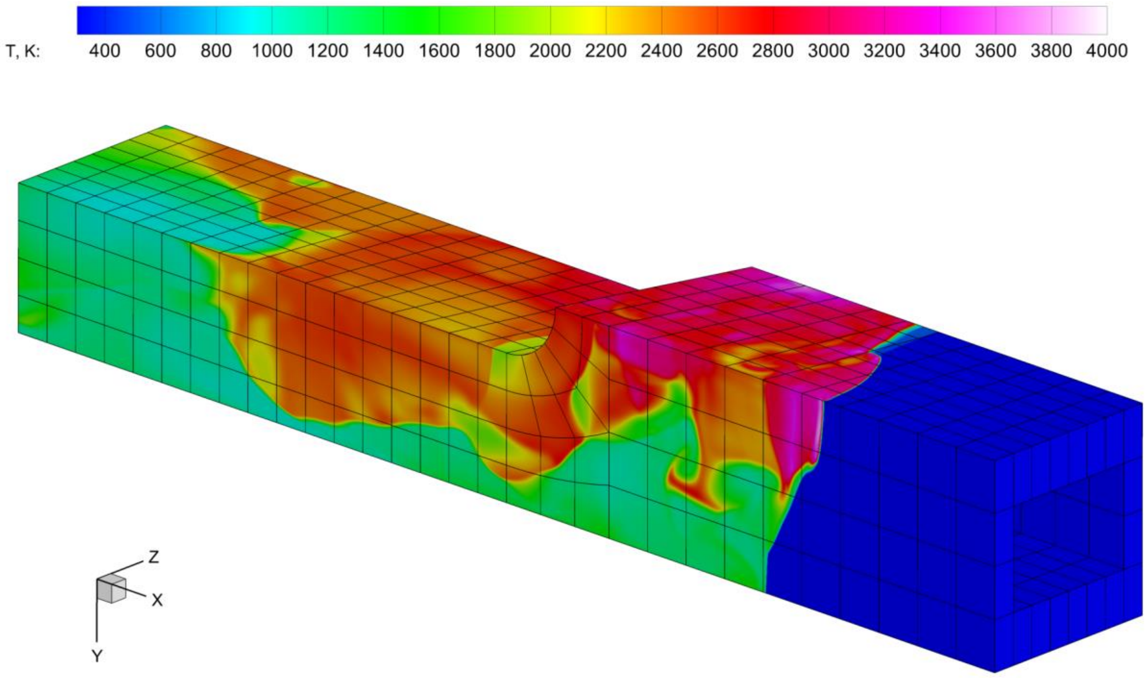

Fig. 7. Temperature field under 3D galloping layered detonation in a channel with inclined bench. The layer is located near the upper wall.

4 Acknowledgements

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