On Analogy of 2D and 3D Combustible Mixture Flows

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1 Introduction

This study was carried out to examine the new methods of detonation initiation and to analyze the possible use of solutions of 2D non-stationary flows of combustible mixture to evaluate the stationary supersonic flows in 3D channels of variable cross-section. The results of numerical simulation of detonation in flat chambers with movable walls and detonation in 3D helical channels or 3D channels of square section, blown by supersonic flows of combustible mixture, are presented and compared. The study is carried out in a framework of one-step combustion kinetics by 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 case of three-dimensional flows the equations are as follows:

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

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

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

Here p and ρ are 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 have the form

$$p = \Sigma^{N}_{i=1} (\rho_i / \mu_i)R_0T, \qquad h_i = c_{0i}+c_{pi}T, \qquad i = 1, \ldots, N,$$

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 on the solid walls used the impermeability condition.

The 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 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. 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 Flows in a plane square chamber decreasing in size

The flows in a contracting square chambers filled with air were studied for different constant values of square sides velocity. Complicated wave patterns of the flows were obtained (Fig. 1).
The problem of detonation initiation in a square region with sinusoidally varying length of the side was studied. The dependence of the side length on time was defined as $h=H-A[1-\cos(2\pi t/T)]$, where H=0.06 m is the initial side length, A – amplitude and T – period. In order to identify all possible flow regimes, 196 simulations for different pairs (A, H) have been performed (Fig. 2). A changed from 2 to 28 mm with 2-mm step. T changed from 10 to 140 μs with 10 μs step. Several different flow regimes were found. Detonation may occur instantly in the 1st period along the whole perimeter of the square or in the 1st period in the corners (Fig. 3). Initiation of detonation can take place after some time at the center in the 1st period or after several periods. As calculations showed, in the latter case detonation may occur also on the sides, in the corners or at the center. The calculations revealed flow regimes with initiation of detonation only after 6 periods of square size oscillations. All possible flow regimes are divided in a plane “amplitude-period” by critical curves.

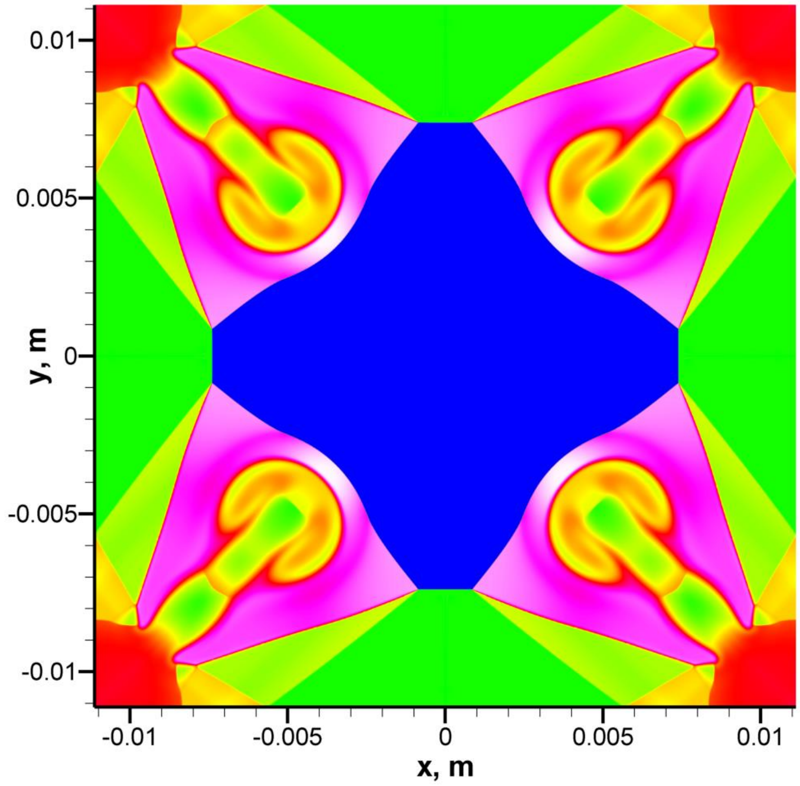

Fig. 1. Temperature field in air inside the contracting square chamber. The velocity of sides is 1500 m/s.

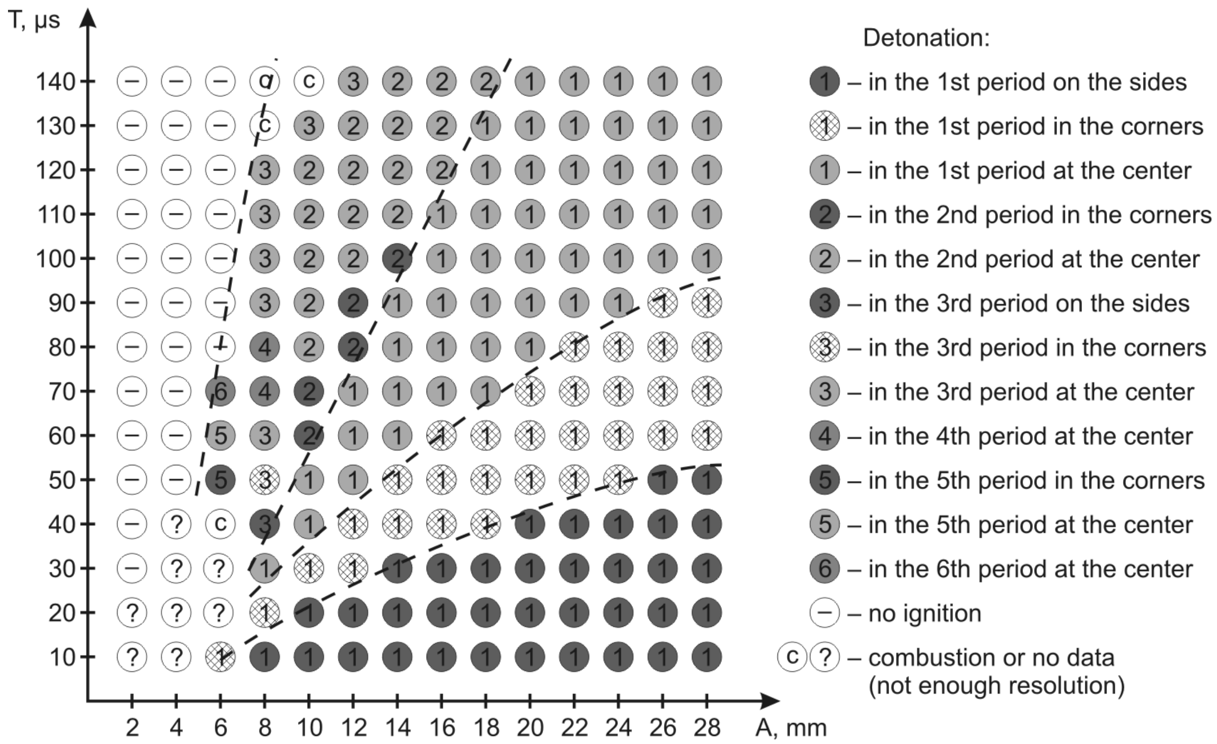

Fig. 2. Diagram of flow regimes in a plane “amplitude-period”.

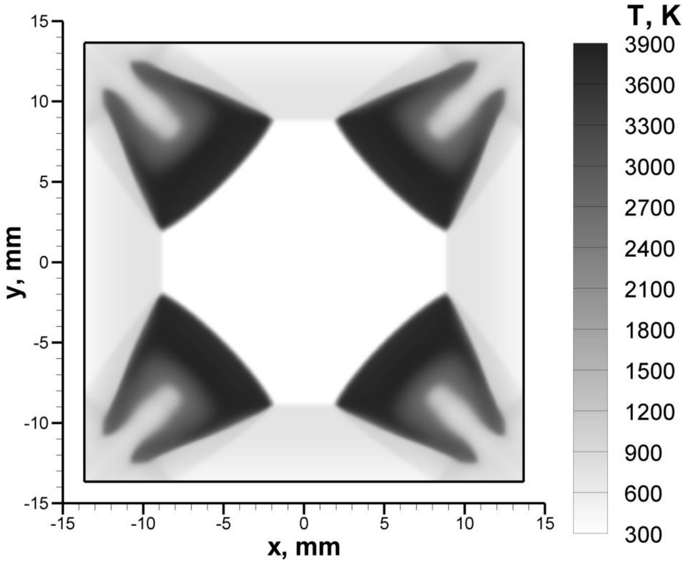

Fig. 3. Temperature field for regime with detonation in the 1st period in the corners.

4 Supersonic flows in 3D channels of variable square cross-section

In the problem of the formation of detonation in three-dimensional channel with square variable cross-section detailed stationary (Fig. 4) and unsteady flow patterns with and without detonation have been found. The critical values of gas-dynamic parameters separating different flow regimes were obtained. Hypersonic analogy of flat and three-dimensional flows, allowing the use of two-dimensional solutions to estimate the parameters of three-dimensional supersonic flows, have been confirmed. The limitations of the analogy have been determined. It was shown that the “chocking” of the burning flow (Fig. 5) is the main limitation.

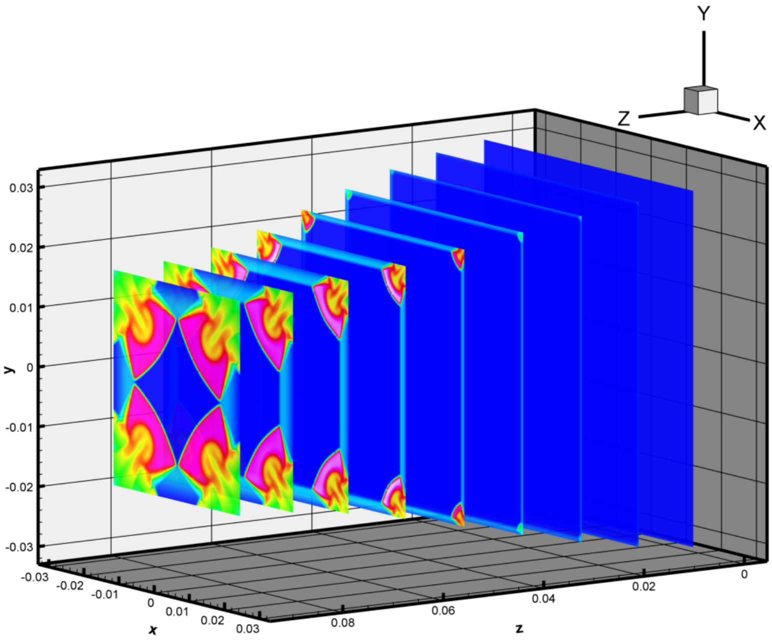

Fig. 4. Temperature field slices in the case of stationary detonation of supersonic combustible mixture flow in 3D channel.

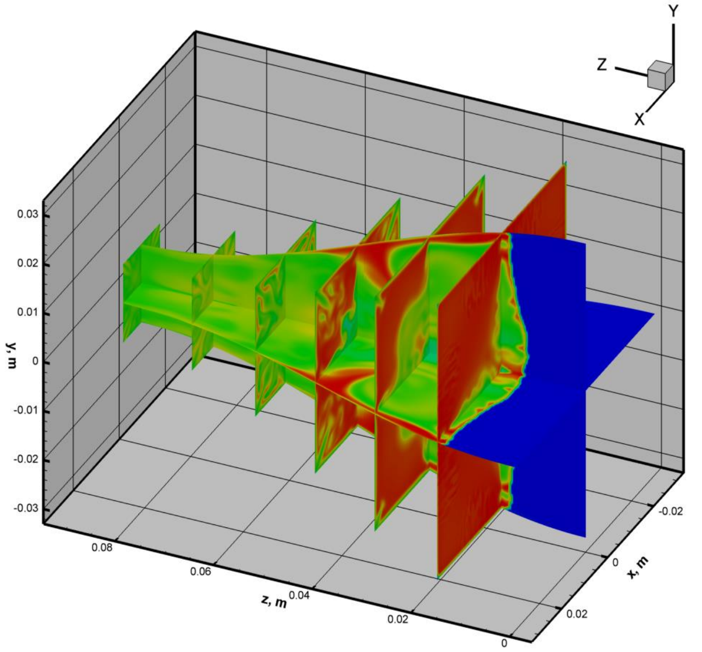

Fig. 5. Temperature field slices for detonation in supersonic combustible mixture flow with choking effect and inapplicability of hypersonic analogy.

5 Detonation initiated by rotation of plane chambers filled by mixture

Detonation initiation using rotation of the elliptic cylinder enclosed in the circular cylinder, both filled with stoichiometric propane-air mixture, was numerically investigated. The feasibility to form detonation both inside, and outside the elliptic cylinder was stated. Two critical angle velocities of cylinder rotation, which govern the quantitative and qualitative flow pattern, were found. The possibility of rapid detonation initiation by rotating parabolic blades was studied in two configurations (Fig. 6a, 6b).

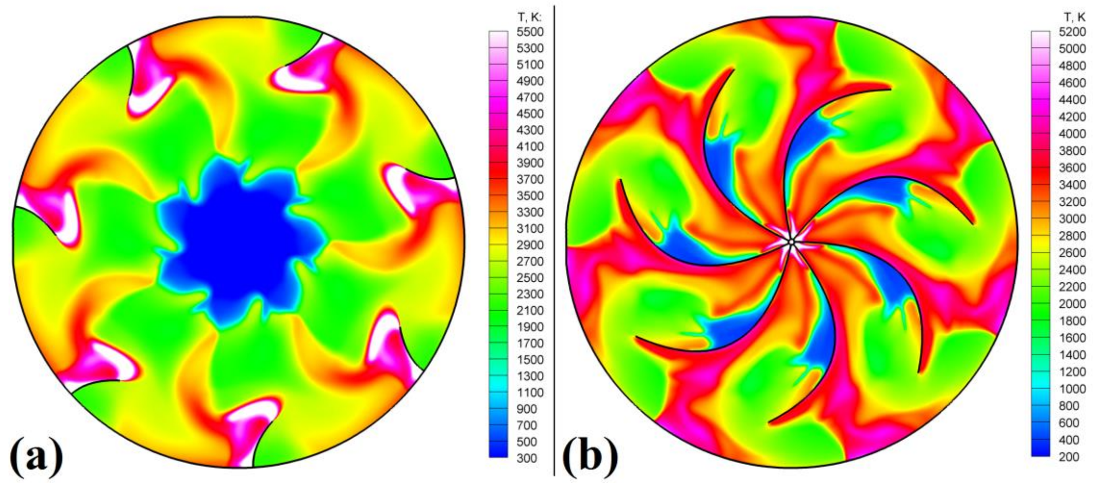

Fig. 6. Formation of detonation inside the rotating cylinder with parabolic blades (a) and inside the cylinder with rotating star in the center.

6 Detonation initiated by rotation of plane chambers filled by mixture

The method to estimate parameters of the supersonic flows in 3D helical channels is proposed based on the plane-sections hypothesis. The comparison with 3D simulation is presented (Fig. 7, 8).

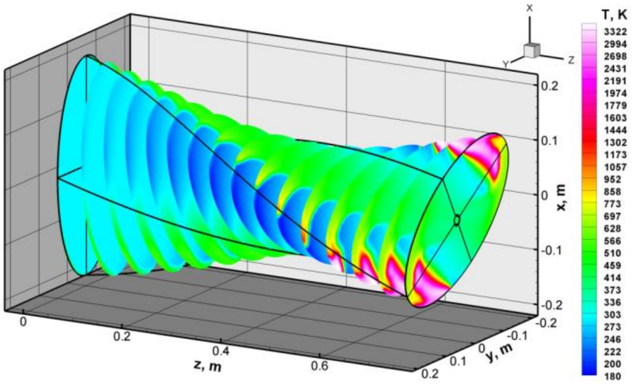

Fig. 7. Slices of stationary temperature field under detonation in helical channel of elliptic cross-section.

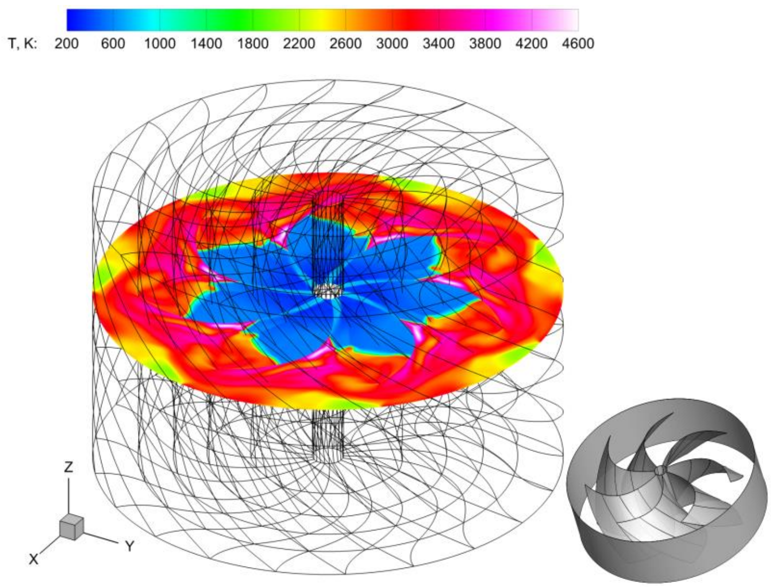

Fig. 8. A slice of stationary temperature field with detonation in channel with blades (shown at right).

7 Acknowledgements

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