Numerical Simulation of Rotating Detonation under Variable Conditions

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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 the space between two coaxial cylinders. The inlet flow conditions, including stagnation pressure and temperature, have been artificially set as slowly changing during detonation rotation, in order to catch the influence of these conditions on the process of rotation.

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 three-dimensional flows the equations are as follows:

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

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

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

Here p and ρ are pressure and density of the mixture, u, v and w are the velocity components along the axes x, y and z 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.
The equations for the state of the mixture are of the form

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

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

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

where 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.

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 curvilinear surfaces into hexahedral 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 Statement of the Problem for Modeling of the Process in the Combustion Chamber

The combustor scheme selected for numerical studies is shown in Fig. 1. The combustion chamber is a space between two coaxial cylinders. The numbered points on the figure designate the places of flow parameters registration performed during calculations. The arrow shows the direction of propane-air mixture injection. The dimensions of the combustion chamber are as follows: length L = 100 mm, large radius R = 57.5 mm and small radius r = 47.5 mm. The width of the gap is $\Delta = R - r$ = 10 mm. All parameters of the flow are being registered in the whole domain while solving the problem numerically. This allows to visualize the dynamic parameters of the flow field and to examine detonation propagation in real-time. It is assumed that the combustible mixture is injected through the left end with parameters that depend on the stagnation parameters of the mixture in the tank, which contains quiescent pre-mixed propane with air.

We describe the inflow of the combustible mixture during detonation in a following way. First, the filling of the combustion chamber with a gas mixture without igniting is described. In our statement of the problem, the one-dimensional theory of the Laval nozzle is used, according to which it is possible to determine the parameters of the gas flowing out of the vessel in which it resides at rest under certain pressure, temperature and density (stagnation parameters). In a place where the gas escapes into the surrounding space, flowing through the respective channels, the stagnation parameters are sufficient to described the steady flow. The latter will occur if the pressure in the surrounding area is less than the pressure in the tank. In this case, a uniform flow will enter the combustion chamber, with known gas dynamic parameters that depend on the

stagnation parameters and the pressure in the outer space. Therefore, if the mixture does not ignite, the uniform steady flow will pass through the combustion chamber.

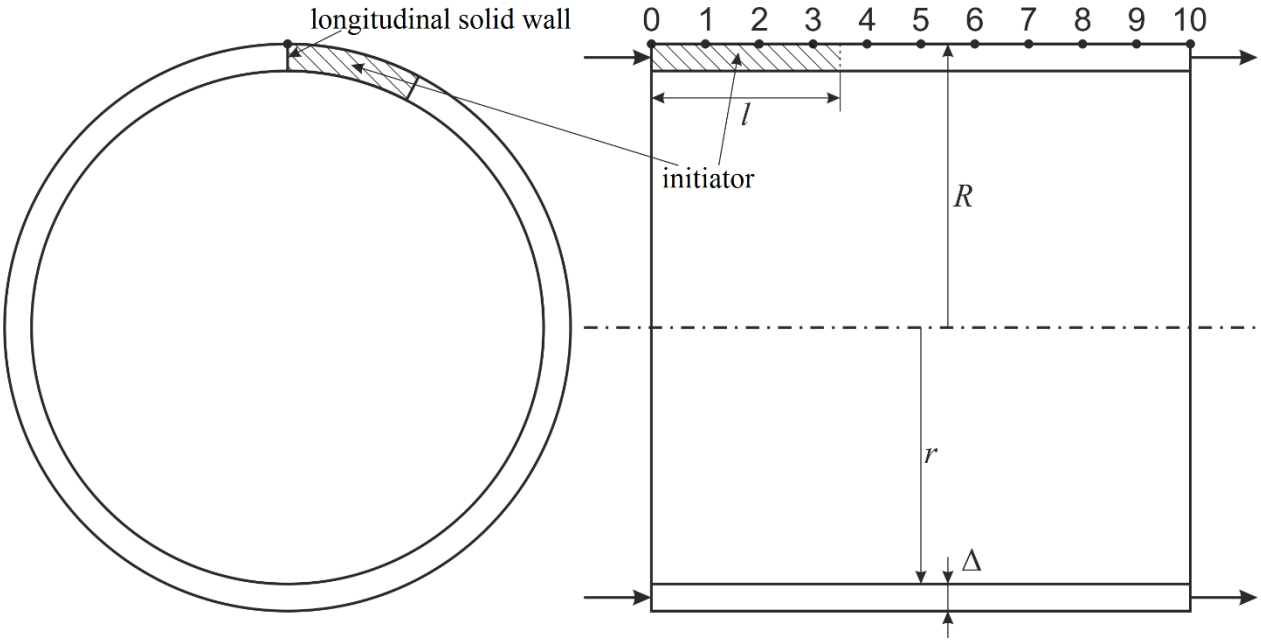

Figure 1. Scheme of the combustion chamber. Numbered points indicate positions of the "gauges"

In the case when rotating detonation is formed near the inlet, the inflowing mixture parameters will be nonuniform over the inlet face of the combustion chamber. This is due to the variability of the parameters of detonation products behind the rotating wave. In this case the parameters of gas flowing through various points of the inlet face are not dependent on pressure in the surrounding space, like it was without detonation, but rather on the state of detonation products. In this context, three cases are possible. If the static pressure near the inlet is greater than stagnation pressure P_0 of the mixture in the tank, the inflow is absent. If the static pressure of the detonation products is less than stagnation pressure P_0, but is greater than critical (sonic) pressure, the inflow is calculated using the local pressure and stagnation parameters. If the static pressure is less than the critical pressure, the mixture flows exactly with the sonic parameters calculated by the stagnation parameters. At each time step of the calculation and each point of the inlet, the case is selected (computed) automatically.

A special scheme was proposed to initiate rotating detonation. In this scheme the initiation is carried out with concentrated energy supply from one side of the wall of length l, placed longitudinally in the combustion chamber near its end (Fig. 1). To determine the parameters of the initiator, a series of calculations were performed, and the size of the energy zone, as well as the energy of initiation was obtained. It was assumed that the wall disappears (burns) after a certain time. According to the computational results, this time is a significant parameter that determines the formation of rotating detonation. Thus, at the initial time a homogeneous flow disturbance is introduced in a limited area near the end of the combustion chamber. The density of combustible mixture in this zone is equal to that in the rest of the combustion chamber, while the pressure and the temperature are calculated using the energy balance equation.

The following are some of the results of the rotating detonation computations carried out on the supercomputer "Lomonosov" of the Moscow State University. Several hundreds of rotation periods were simulated continuously in some of the calculations.

4 Numerical Results

Fig. 2 shows a temperature field during the rotation of the detonation wave. Fig. 3–4 show the computational results for constant stagnation parameters of combustible mixture: P_0 = 40 atm and T_0 = 3000 K. In this case the average Mach number at the outlet of the annular combustion chamber is M = 1.2. In order to study the rotating detonation under changing conditions of mixture injection, two processes were considered with a slow (changing by 0.15% over a period) linear decrease of the thermodynamic parameters in the tank with quiescent fuel mixture, specifically, one with decreasing pressure and constant temperature, and the second with decreasing temperature and constant pressure. It was found that under both laws of change of the stagnation parameters, the rotating detonation wave is formed in the combustion chamber. According to the computations in the case of variable pressure in the tank, the rotating detonation persists until the total pressure in the tank drops to the critical value. Therefore, the existence of the minimal critical total pressure at which the rotation is stopped, was discovered. In the case of a variable temperature, it is shown the rotating detonation does not stop for a long time.

Total pressure values were used to calculate the average values for the period of oscillations, required for the determination of the total pressure growth compared with the pressure in the tank. The resulting plots of gas parameters against time show that the process is complex, periodic and oscillatory. According to the computations, the highs and lows of the static and total pressure at the control points within the combustion chamber substantially change over time in the oscillatory mode. The obtained ratios of the total pressure to the stagnation pressure, averaged over the oscillation period, also oscillate slightly (Fig. 5 for changing stagnation temperature) in both cases during the process of detonation wave rotation. For decreasing pressure in the tank, the ratio of the averaged total pressure to the overall stagnation pressure increases slightly with time from 1.3±0.07 to 1.5±0.06. For decreasing temperature in the tank, the ratio of the total pressure to stagnation pressure, averaged over the period, substantially depends on time and increases from 1.3±0.07 to 1.83±0.17. The average value of this ratio during the whole computation oscillates, wherein the frequency and amplitude of the oscillation vary. The computational results indicate that a significant increase in the average value of the ratio of the total pressure to the stagnation pressure is possible.

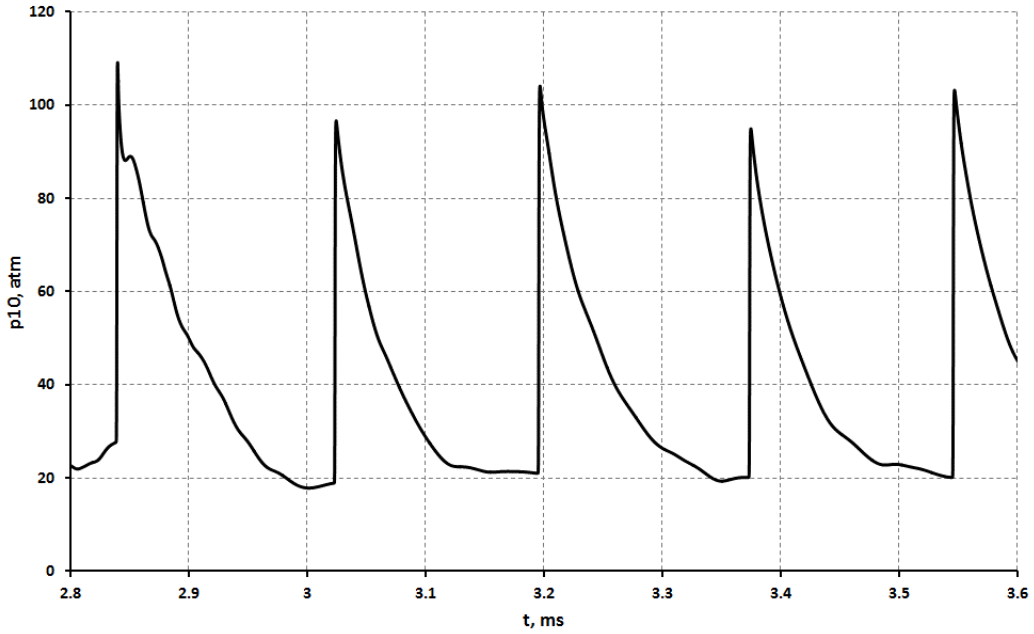

Figure 2. Static pressure as a function of time at 100 mm distance from the inlet (“gauge” 10) at P_0 = 40 atm

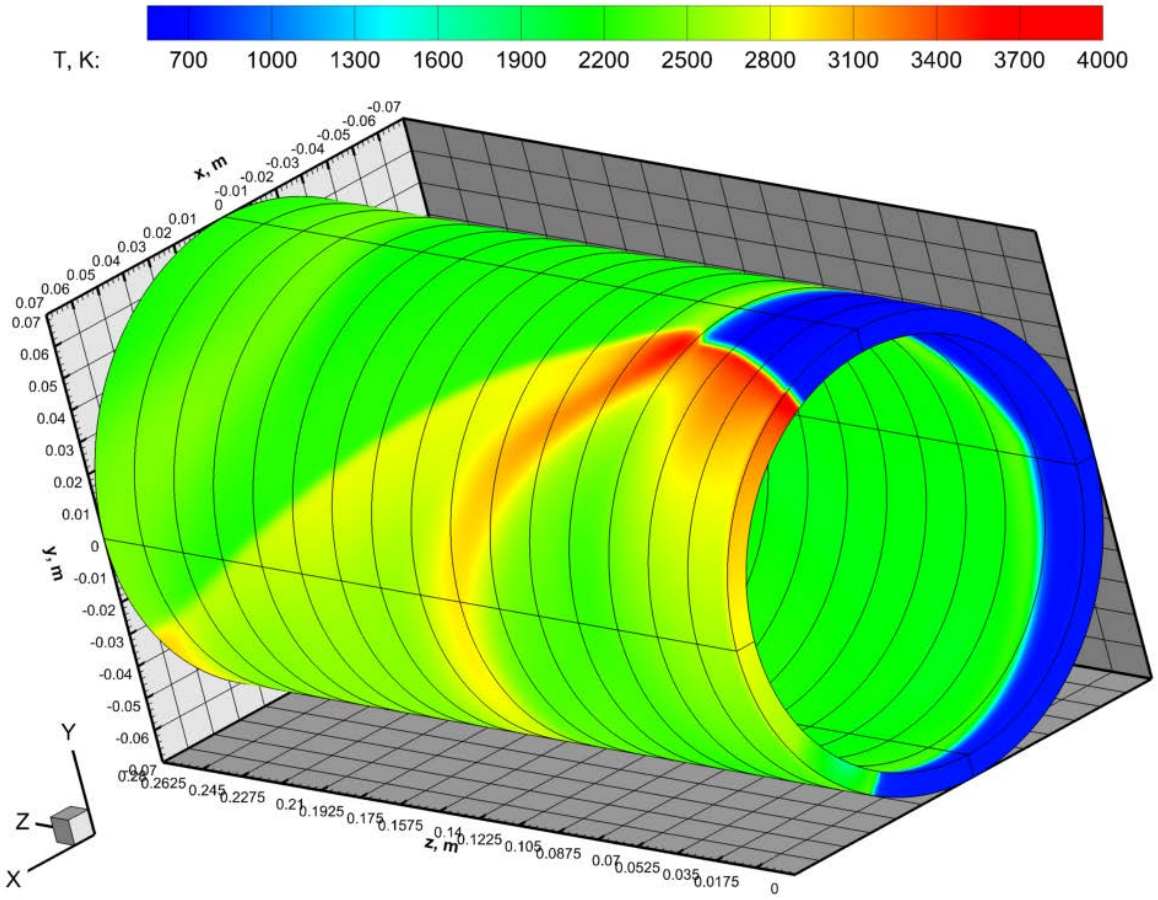

Figure 3. The temperature field during rotation of the detonation wave

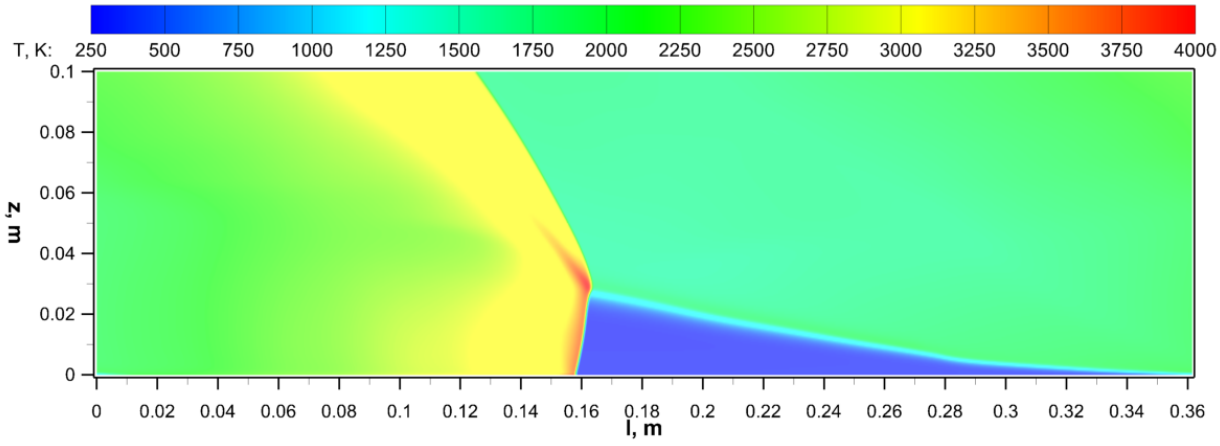

Figure 4. The temperature field on the outer lateral wall of the combustion chamber

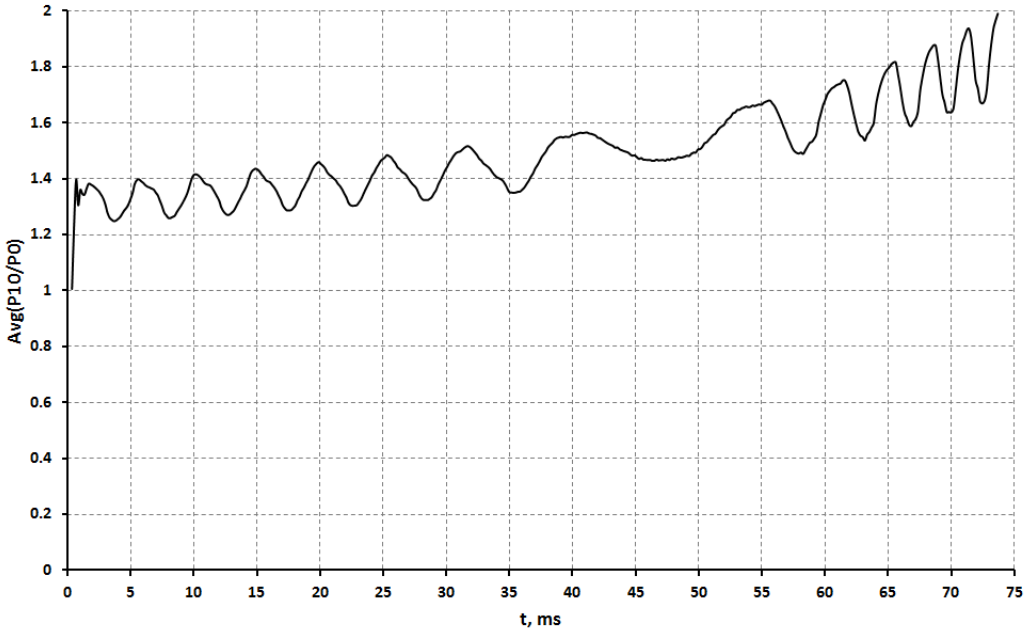

Figure 5. The total pressure at 100 mm distance from the inlet, averaged over the period and divided by constant stagnation pressure P_0, as a function of time for linearly decreasing stagnation temperature $T_0(t)$

4 Acknowledgements

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References

[1] S.K. Godunov, A.V. Zabrodin, M.Ya. Ivanov et al. Numerical solution of multidimensional problems in gas dynamics. Moscow: Nauka. 1976. 400 p.

[2] Westbrook C.K., Dryer F.L. Chemical kinetic modeling of hydrocarbon combustion // Prog. Energy Combust. Sci. 1984. V. 10. P. 1–57.

[3] Voevodin Vl.V., Zhumatiy S.A., Sobolev S.I., Antonov A.S., Bryzgalov P.A., Nikitenko D.A., Stefanov K.S., Voevodin Vad.V. Practice of “Lomonosov” Supercomputer // Open Systems J. – Moscow: Open Systems Publ., 2012, no.7. [http://www.osp.ru/os/2012/07/13017641/] (In Russian)