Numerical Modelling of Shock-to-Detonation Transition in Methane – Air Mixture

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1 Introduction

Detonation of natural gas-air mixture is very important and promising problem from the sense of energy plants effectiveness increasing. Besides the importance of investigation of detonation initiation critical conditions in natural gas-air mixtures is connected with explosion hazards in coal-mining industry and natural gas production.

Current work is the continuation of the series of works in which the authors firstly within two-dimensional (2D) approach [1] and then three-dimensional (3D) approach [2] investigated shock-to-detonation transition (SDT) in stoichiometric propane-air (PA) mixture due to the tube walls profile.

Propane was used in [1, 2] because propane is known to be one of the simplest hydrocarbons that could be representative of higher hydrocarbons used in practical applications. PA mixture is hardly-detonated mixture so the development of tube walls profile that provides SDT transition in such a mixture gives a hope that similar geometry will work for a number of heavier hydrocarbon fuels. Methane-air (MA) mixture is much more hardly-detonated than PA mixture. The detonation cell size for MA mixture under normal conditions is several times larger than for PA mixture [3, 4]. So the investigation of SDT in MA mixture demands significantly larger tube sizes that leads to dramatic increase of computational time costs.

The goal of the current work is 2D and 3D modelling of SDT in stoichiometric MA mixture under normal conditions and finding the tube geometry which provides detonation initiation for incident shock wave (SW) Mach number about 3.0. SW with such intensity could be generated before the accelerated flame front after for example Shelkin spiral [5] but it is not sufficient for deflagration-to-detonation transition on the short distance without additional means such as walls profiling.

2 Statement of the problem

The round tube of diameter D comprises five sections: Section 1 with constant cross-section, parabolic contraction (Section 2), the connecting Section 3 of constant narrow diameter, conical expansion (Section 4) and outlet Section 5 with constant cross-section (see Fig. 1). Initially, the tube is filled with homogeneous, quiescent, stoichiometric MA mixture under normal conditions (here and further the notation conventions are common standard):

$$\rho_{0,\mathrm{CH_4}} = 0.061\ \mathrm{kg/m^3},\ \rho_{0,\mathrm{O_2}} = 0.245\ \mathrm{kg/m^3},\ \rho_{0,\mathrm{N_2}} = 0.808\ \mathrm{kg/m^3},\ p_0 = 1\ \mathrm{atm},\ T_0 = 298\ \mathrm{K}.$$

It is considered that multisectional tube is determined by the following geometric parameters:

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$$D = 9.4 \cdot 10^{-2} \text{ m}, L_1 = 24 \cdot 10^{-2} \text{ m}, L_3 = 8 \cdot 10^{-2} \text{ m}, L_5 = 7 \cdot 10^{-2} \text{ m}.$$

The wall profile in Section 2 is given by the parabolic curve $z(r)$. The parabolic shape $z(r)$ was chosen to meet the following constrains: (i) the focus of the parabola should lie at the tube symmetry axis, (ii) the blockage ratio of contraction, $BR = 1 - (d/D)^2$, should not exceed a certain maximum value; and (iii) angle φ should not exceed a certain limiting value.

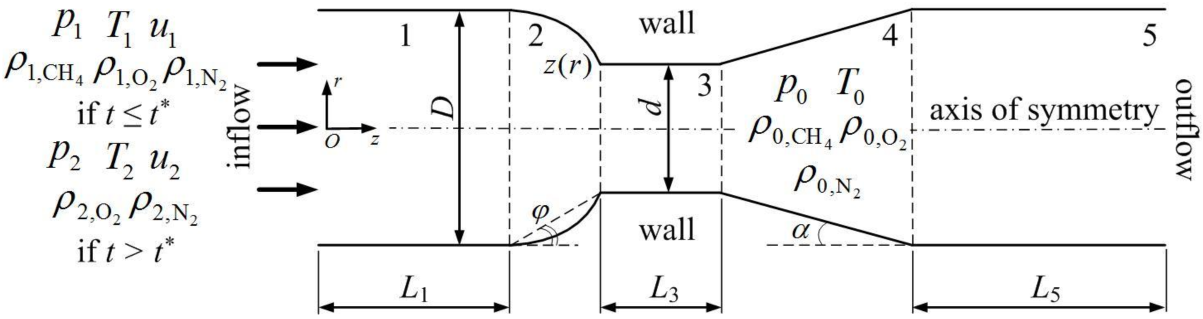


Figure 1. Scheme of the tube with profiled walls (longitudinal section).

The principle difference between the tube geometry under consideration the one from [1, 2] is the existence of connecting Section 3 of constant narrow diameter. The role of Section 3 which was introduced to support divergent blast wave from local explosion on the tube symmetry axis was discussed elsewhere [6].
The four test cases were investigated (see Table 1).

Table 1: Test cases for investigation

Number	φ, °	d, m	BR	α, °	Dimension
1	45	$6 \cdot 10^{-2}$	0.6	5	2D
2	30	$6 \cdot 10^{-2}$	0.6	5	2D
3	45	$4.7 \cdot 10^{-2}$	0.75	5	2D
4	45	$4.7 \cdot 10^{-2}$	0.75	2.5	2D/3D

The motion in the tube is assumed to be initiated by an incident SW with zero gradients of parameters directly behind the SW front. Therefore, the boundary condition imposed on the left end of the tube from the initial time to the time t^* = 300 μs is the gas inflow with the following parameters of the combustible mixture corresponding to parameters behind the SW with the Mach number 3.0:

$$p_1 = 10.11 \text{ atm}, T_1 = 706 \text{ K}, u_1 = 791 \text{ m/s},$$

$$\rho_{1,CH_4} = 0.262 \text{ kg/m}^3, \rho_{1,O_2} = 1.048 \text{ kg/m}^3, \rho_{1,N_2} = 3.449 \text{ kg/m}^3.$$

At the time t^*, the boundary condition is changed to the boundary condition for an inert gas with the following parameters:

$$p_2 = p_1 = 10.11 \text{ atm}, T_2 = 2500 \text{ K}, u_2 = u_1 = 791 \text{ m/s},$$

$$\rho_{2,O_2} = 3.268 \text{ kg/m}^3, \rho_{2,N_2} = 10.758 \text{ kg/m}^3.$$

Other boundary conditions were slip condition on the wall and zero-gradient outflow condition on the right boundary.

3 Mathematical model and numerical procedure

The mathematical statement of the problem is based on the set of equations for 2D axisymmetric [1] or 3D [7] transient flow of inviscid, compressible, multicomponent, explosive gaseous mixture. Methane oxidation is modeled with a single-stage overall reaction with the expression for the reaction rate w proposed by Dr. V.Ya. Basevich from Semenov Institute of Chemical Physics RAS:

$$CH_4 + 2O_2 + 7.524N_2 \rightarrow CO_2 + 2H_2O + 7.524N_2 + Q,$$

$$w = -4 \cdot 10^{14} \cdot p[\mathrm{atm}]^{-1} \frac{\rho_{CH_4}}{\mu_{CH_4}} \left(\frac{\rho_{O_2}}{\mu_{O_2}} \right)^2 \exp\left(-\frac{E}{RT} \right) \frac{\mathrm{mole}}{\mathrm{l \cdot s}},\ Q = 50\ \frac{\mathrm{MJ}}{\mathrm{kg\ of\ methane}},\ E = 50\ \frac{\mathrm{kcal}}{\mathrm{mole}},$$

where Q is the combustion heat of methane and E is the activation energy. The model of chemical kinetics was validated on experimental data [8]. The ZND structure of detonation wave (DW) yields half-reaction length about 2 mm. It should be noted that in spite of apparent simplicity one-stage kinetic models of chemical reactions are widely used at present for investigations of multidimensional flows with DWs and ignition problems [9 – 11].

The numerical procedure for solving Euler equations is based on the principle of splitting various physical processes and the finite volume approach. The fluxes through the computational cells faces are calculated with Godunov's method.

For 2D investigations time integration is performed by the explicit Euler scheme with the first-order approximation. The second order of spatial approximation is reached by means of piecewise-linear reconstruction of the cell functions with the use of minmod limiter. The multistep implicit Gear method is used to solve the system of ordinary differential equations of chemical kinetics (see [1] for detailed description of numerical algorithm for 2D approach).

To enhance the accuracy of 3D investigations the MUSCL approach is used with upwind-biased third order scheme (on uniform grids for one dimensional problems) of interpolation of values at cell centers to faces. The gradient of the solution vector is computed with the moving least squares method. Time integration is performed using the explicit predictor-corrector scheme with the second-order approximation (see [7] for detailed description of numerical algorithm for 3D approach).

The numerical algorithms are adapted for investigations to be performed on advanced multiprocessor computational systems with teraflops performance. Parallelization is performed by means of multidimensional decomposition of a computational domain.

4 Results of numerical investigations

Test case 1. In the first and second test cases computational grids with about 850 000 cell were used with spatial resolution from 0.2 mm to 0.1 mm. Fig. 2 illustrates predicted fields of gas temperature in successive time moments. As a result of interaction of leading shock wave (LSW) with parabolic contraction walls double Mach reflection is formed (see Fig. 2, 250 μs). Cumulation of SW reflected from parabolic contraction walls leads to local explosion on the symmetry axis (see Fig. 2, 290 μs). Fig. 2, 315 μs corresponds to the time moment when the blast wave from explosion reaches the wall of connecting Section 3 and reflects from it. The temperature behind reflected from tube walls in Section 3 SW is about 1300 K. This value is not sufficient for autoignition of methane-air mixture and in conical expansion the jet of hot products from explosion expands with the velocity about 1500 m/s. At the same time the retonation wave spreads upstream. The spatial grid resolution is enough to resolve large vortex structures on the contact boundary between combustion products and fresh mixture (see Fig. 2, 405 μs). It should be also noted that as a result of multiple reflections of secondary SWs in conical expansion the amplification of LSW is observed. This amplification from theoretical point of view can lead to detonation reinitiation in conical expansion.

Test case 2. For the purpose of tube geometry optimization with respect to detonation initiation it was decided to decrease the value of φ with the aim of local explosion place movement further inside the connecting Section 3 (compare Fig. 2, 290 μs and Fig. 3, 295 μs). Nevertheless the effort was fail (see Fig. 3, 335 μs).

Test case 3. The following progression was connected with increase of tube blockage ratio. For BR = 0.75 detonation reinitiation occurred in Section 3 but the divergence angle of conical expansion appeared to be too large for DW to come successfully into Section 5 (see Fig. 4).

Test case 4. Finally, the divergence angle of conical expansion was decreased twice and DW successfully came into outlet Section 5 and spreaded with the velocity about 2000 m/s. The value of divergence angle of conical expansion 2.5° (see Table 1) caused the increasing of the total tube length up to 1.08 m. The computational grid provided spatial resolution from 0.2 mm to 0.1 mm and included about 1.5 mln. cells. So the whole numerical experiment (about 100 000 computational time steps) lasted for about 6 hours with the use of 117 processor cores of MVS-100k supercomputer at Joint Supercomputer Center RAS.

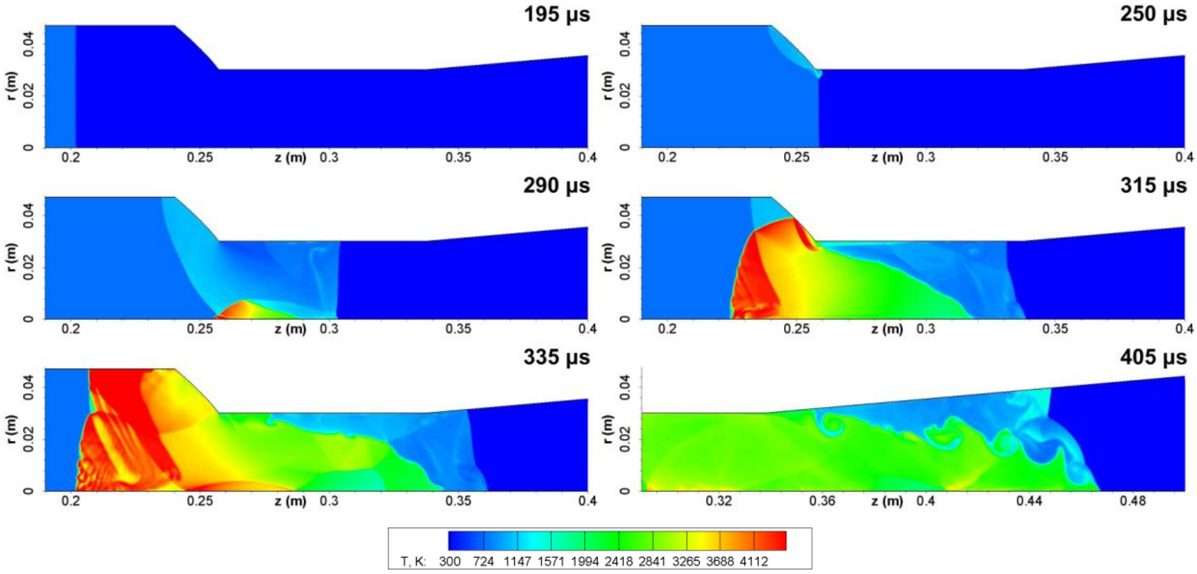


Figure 2. Predicted fields of gas temperature in test case 1. Detonation failure.

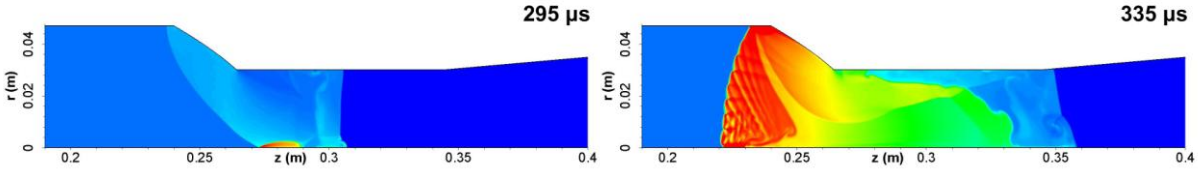


Figure 3. Predicted fields of gas temperature in test case 2. Detonation failure.

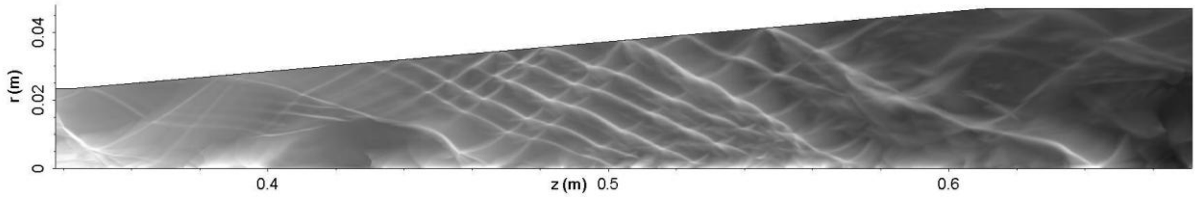


Figure 4. «Numerical soot footprint» in test case 3. Detonation failure.

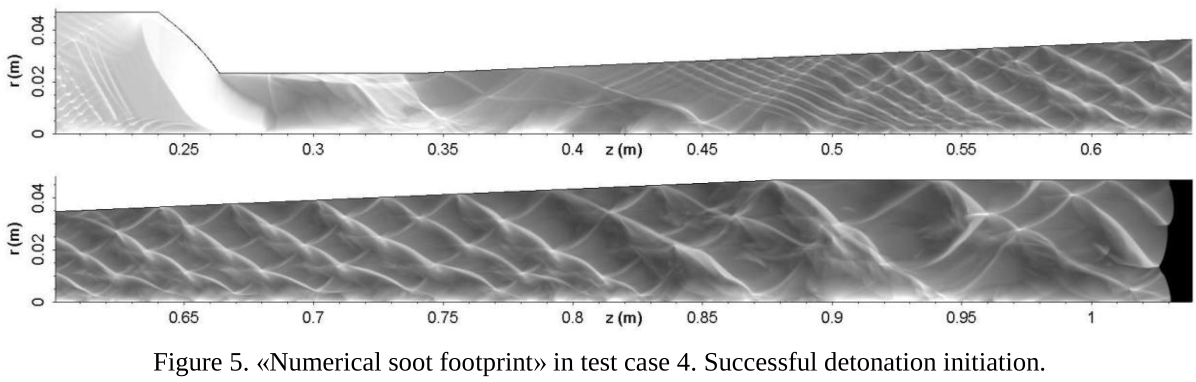
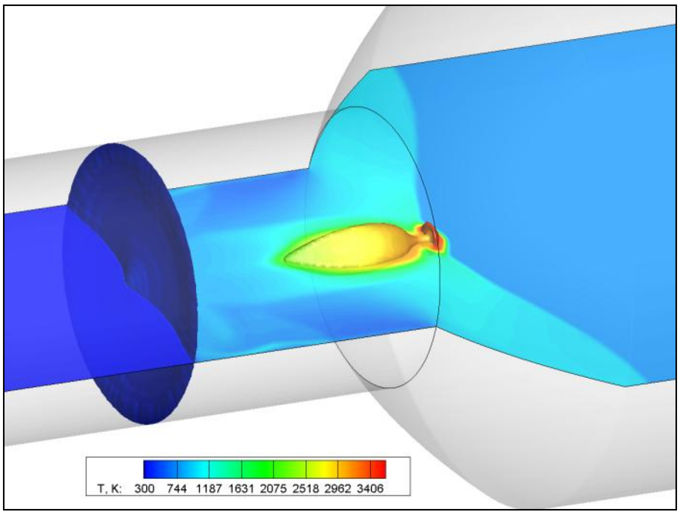


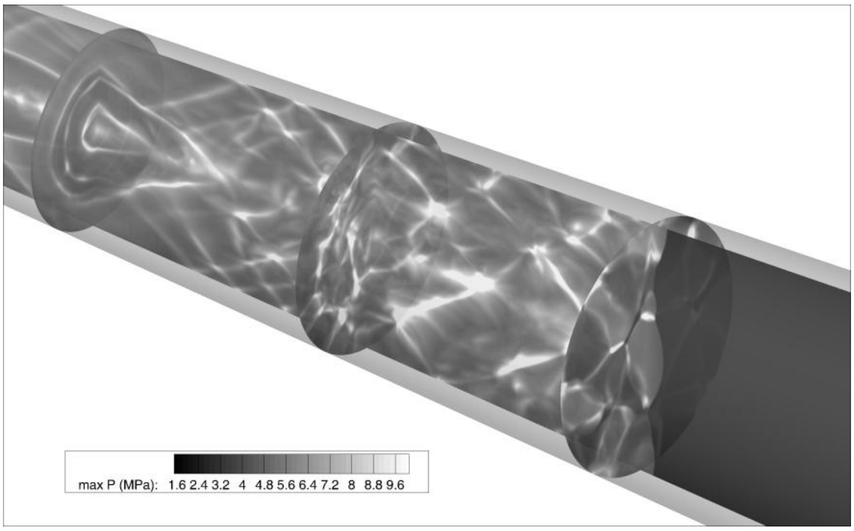
Figure 5. «Numerical soot footprint» in test case 4. Successful detonation initiation.

The estimations of characteristic length scales for reactive mixture in consideration show that the resolution of about 0.1 mm is well enough to describe the main features of detonation initiation in methane-air mixtures. Nevertheless, grid resolution simulations show that reasonable increasing or decreasing computational cell size doesn't lead to the changing of the mechanism of detonation initiation but only slightly changes the critical initiating shock wave Mach number necessary for detonation initiation either to the larger value or to the smaller one.

The numerical experiment corresponded to the test case 4 was carried out in 3D statement also. The computational grid provided spatial resolution from 0.3 mm to 0.1 mm and included more than 100 mln. cells. Fig. 6 gives an inside to the 3D pattern of the flow. Fig. 6a illustrates local explosion formation (yellow surface) at some distance after the LSW (blue surface) as well as the formation of retonation wave (red cap of a yellow surface). The results of 3D numerical investigation confirm in whole the results of 2D findings. However, 3D case indicates decay of initially axial symmetric flow structure associated with instability of DW front (Fig. 6b). More detailed qualitative analysis of the effects of three dimensionality in the tube of similar geometry could be found in [7].



(a)



(b)

Figure 6. Test case 4. (a) Isosurface of methane density of $0.07 \cdot 10^{-3}$ g/cm^3 with the gas temperature distribution over it and predicted gas temperature in longitudinal section of the tube. (b) «Numerical soot footprint» in the conical section for some slices.

5 Concluding remarks

The multidimensional 2D and 3D numerical experiments on SDT in methane-air mixture under normal conditions in tubes with parabolic contraction, connecting section of narrow diameter and conical expansion are performed. The shape of parabolic contraction and divergence angle of cone expansion are found which provide SDT for the incident SW Mach number 3.0. The results of 3D numerical investigation confirm in whole the results of 2D findings. It is important to note that the findings reported in the paper are in good agreement with the recent experimental investigation [12].

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