Numerical and Experimental Investigation of Detonation Initiation in Multifocused Systems

Pavel S. Utkin[1,2], Alexander I. Lopato[1,2], Anatoly A. Vasil'ev[3]
[1]Moscow Institute of Physics and Technology
Dolgoprudny, Moscow region, Russia
[2]Institute for Computer Aided Design RAS
Moscow, Russia
[3]Lavrentyev Institute of Hydrodynamics SB RAS
Novosibirsk, Russia

1 Introduction

The problem of reactive mixture initiation is important as the interdisciplinary problem from the scientific, applied and ecological safety aspects points of view. The main goal is the determination of the critical conditions of initiation and its optimization due to the spatial distribution of the energy input and the time characteristics. The effect of combustion and detonation excitation usually has a "threshold" (yes – no) character for any initiator. The minimum energy of the initiator that ensures the excitation of combustion or detonation is usually called the critical energy of combustible mixtures. At the same time, experimental and numerical studies (see, for example, [1, 2]) with varying the duration of the energy release while maintaining the spatial dimensions of the supply region showed that the critical initiation energy is the only criterion parameter of the mixture only for the case when the duration of the initiating discharge does not exceed a certain critical value. Otherwise, the longer the discharge duration, the greater the energy required for detonation wave (DW) initiation. It was also found that upon the variation of the size and shape of the energy input domain with the energy input being unchanged the minimum critical energy can be significantly (by an order of magnitude or more) reduced as compared with the value determined by varying only the temporal characteristic of the input energy.

Among different initiators the shock wave (SW) has the special role. The SW is able to compress and heat rapidly and uniformly the reactive mixture under the high pressure and temperature. But even under the condition of uniform parameters of the mixture behind the SW the ignition occurs spontaneously at the separate points. In reactive mixtures where the instability development is typical the fact of ignition is determined not by the average temperature but by the "hot spot" temperature. Such "hot spots" can be created with the use of boundary conditions, for example due to the interaction of SW with obstacles, curved walls, periodical structures etc. Due to such non-one-dimensional SW patterns it is possible to create "hot spots" and noticeably reduce the critical energy (in comparison with one-dimensional models).

Correspondence to: pavel_utk@mail.ru

Many researchers investigated the problem of gaseous detonation initiation as a result of relatively weak SW interaction with the profiled end-wall of the channel. In the experimental study [3] the reflectors in the form of two-dimensional (2D) wedges, semi-cylinder and parabola were considered. The peculiarities of mild and strong ignition inside the reflector cavity were visualized. It was shown that the mild ignition inside the reflector cavity can lead to detonation initiation outside the cavity. In the recent paper [4] containing both numerical and experimental results the reflector in the form of three-dimensional cone was considered. Several different flow scenarios were detected in reflection of shock waves all being dependent on incident SW intensity: reflecting of SW with lagging behind combustion zone, formation of DW in reflection and focusing, and intermediate transient regimes. Semi-circular geometry of the reflector was investigated experimentally in [5]. For the hydrogen-oxygen mixture and for the range of incident SW Mach number 2.2 – 2.8 the ignition delay times were measured for the case of semi-circular reflector and compared with the delays for the case of normal reflection of the SW.

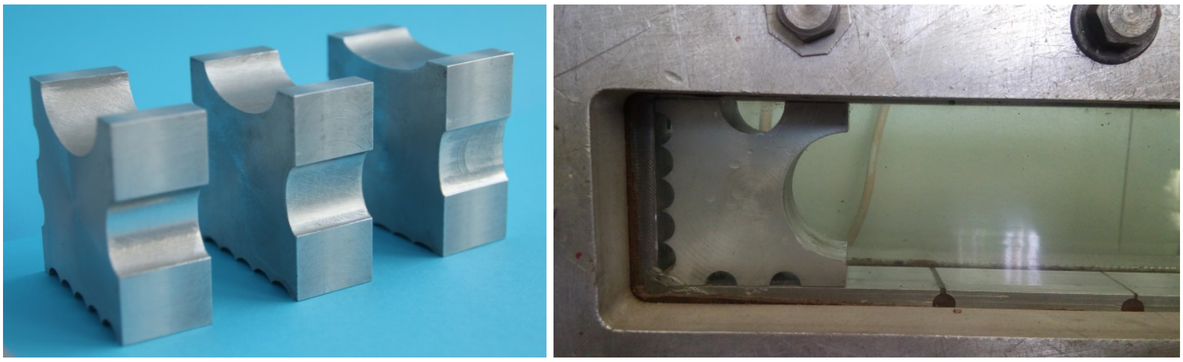
The system of reflectors was considered in [1] and named the "multifocused system". The multifocused system follows the concept of minimization of detonation initiation energy due to the time-spatial factors that is due to the usage of spatially distributed initiators that ignites non-simultaneously. The concept was realized in different solutions. It was shown in numerical studies [2] that it is possible to initiate detonation with the use of several discharges with the total energy input less than the energy of direct initiation. In [6] DW was formed as a result of successive actions of the distributed ignition pulses on the passing relatively weak SW. The close idea was realized in [7] both numerically and experimentally but without additional energy input due to the special regular parabolic profile of channel walls.

The goal of the work is the investigation of the mechanisms of the detonation initiation in the multifocused systems [1] using the numerical technology based on the fully unstructured computational grids [8].

2 Experimental Setup

The experiments were carried out in the two-section shock tube with a thin cellophane membrane. The high-pressure section was filled with the helium or a mixture of H_2-O_2 with such an excess of hydrogen that after the rupture of the membrane, the detonation products could only provide ignition of the mixture and the propagation of a low-speed flame, but could not ensure the transition of combustion to detonation behind the incident wave along the entire length of the working section. The working section is filled with the quiescent stoichiometric hydrogen-oxygen mixture under the initial pressure 0.04 atm and with the temperature 298 K. Reflectors were fabricated by means of milling. The milling cutter angles were 90° (semi-circular reflectors), 45°, 30° and 15° (semi-elliptical ones), see Fig. 1a. The classical semi-elliptical reflectors of different sizes were investigated as well as the multifocused systems. In the latter case the individual reflectors were positioned so that their leading edges were in contact with the edges of neighboring reflectors, or the edges of neighboring reflectors were shifted by some distance, forming a jumper with flat reflective surface. Reflectors were installed at the end of the measuring section with transparent windows (see Fig. 1b). Registration of the process was carried out with the help of an optical shadow installation and a high-speed camera coupled with it, operating in the scan mode. The propagation velocities and gas-dynamic flow parameters are determined by the known scanning speed, the reduction coefficient of the optical system and the measured angles of the trajectories of all waves.

In the paper we will consider two most non-trivial geometries from Fig. 1a. Namely, the cases of two and five reflectors (the milling cutter angle is 45°). The experimental critical values of the incident SW Mach number for the detonation initiation are 2.48 for the geometry with five reflectors and 2.44 for the geometry with two reflectors.



(a) (b)

Figure 1. Multifocused systems: (a) the examples of the insertions for the different angles of the milling cutter, (b) insertion with the semi-circular reflectors in the shock tube

3 Mathematical Model and Numerical Algorithm

Computational domain is the plane square channel with the length and the height 30 mm. The incident SW location is x = 28 mm. The SW Mach numbers M = 2.4, 2.5 and 2.6 are considered. At the initial time moment in the area $x \leq 28$ mm the parameters behind the SW are set. Slip-conditions are set at the bottom, upper and right boundaries, and the inflow conditions at the left boundary. The simulations last up to the moment of DW (or reflected SW in case of unsuccessful initiation) arrival at the left boundary. For the sake of computational cost diminishing the computational domain corresponds to one half of the channel.

Mathematical model is based on 2D system of Euler equations written in the Cartesian frame supplemented by one-stage chemical kinetics model [9]. The simulations were carried out with the resolution about 5 cells per half reaction length in the Zeldovich-von Neumann-Doring solution. The grid convergence study revealed that the usage of more detailed computational grid did not lead to the changes in the main features of the detonation initiation mechanism. The main difference was that for the twice finer grid the stages of the process took place with a delay of one microsecond.

The main feature of the computational technique is the usage of completely unstructured computational grids with triangular cells. A Delaunay triangulation is carried out to construct the grid. The computational algorithm is based on the Strang splitting principle in terms of physical processes. At the gas dynamics stage of the algorithm the spatial discretization is carried out using the finite volume method. The numerical flux is calculated using AUSM scheme extended for the case of a two-component mixture. For the approximation order increase the reconstruction of the grid functions [10] is applied. Time integration is carried out using explicit Runge-Kutta method of the second approximation order. The time step is chosen dynamically from the stability condition. On the second stage of the algorithm the system of ordinary differential equations of chemical kinetics for the progress variable and temperature in each computational cell of the grid is solved. The estimation of the practical approximation order of the algorithm on the problem of isentropic vortex evolution gave the value near 2. The details of the numerical approach could be finding elsewhere [8].

4 The Mechanisms of Detonation Initiation in the Multifocused Systems

For the lowest considered Mach number M = 2.4 the initiation didn't occur during the time of simulations.

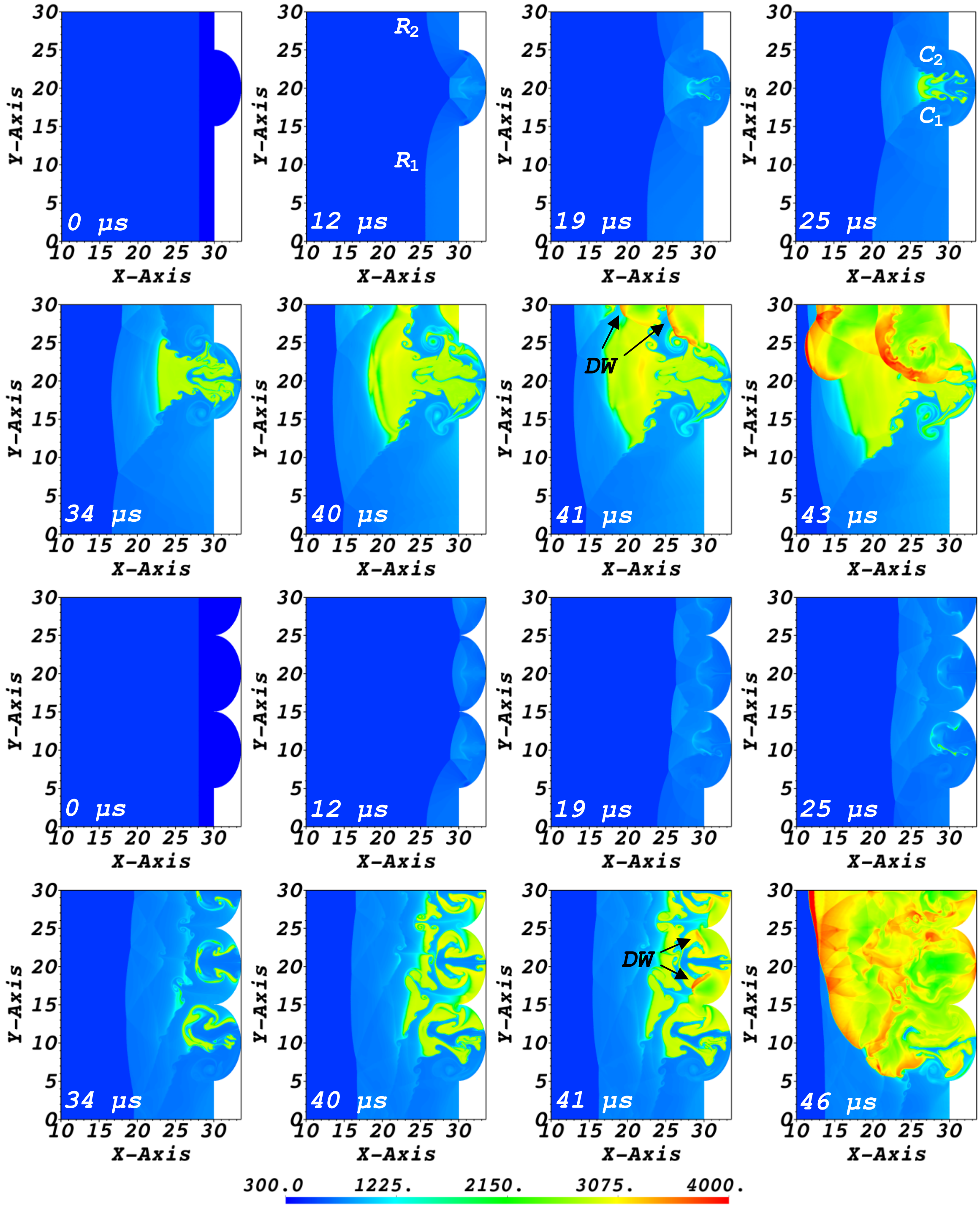


Figure 2. Predicted temperature distributions at the successive time moments for two geometries of multifocused systems: with two reflectors (the first and the second rows) and with five reflectors (the third and the fourth rows). *M* = 2.5. Axes are in mm, temperature is in Kelvin degrees.

Fig. 2 illustrates the main stages of the process for M = 2.5. For two reflectors with the parts of flat wall the waves R_1 and R_2 reflected from these parts amplifies the parameters inside the reflector cavity in contrast to the geometry with five adjoining reflectors. Ignition occurs in the region of focusing of the flow at about 20 μs. The combustion area gradually occupies the cavity of the reflector and spreads outwards primarily in the area between the contact surfaces C_1 and C_2. Detonation initiates at about 41 μs in several points at the symmetry axis of the channel outside the cavity of the reflector. For the geometry with five reflectors without flat wall parts between them the combustion area is non-uniform and is characterized by a number of unreacted layers. Nevertheless detonation is initiated almost at the same time as for the geometry with two reflectors. Taking into account the dependence of the initiation time on the grid resolution within one microsecond, we can say that the initiation times for both geometries are the same. Initiation occurs inside the cavity of one of the reflectors.

For the higher incident SW Mach number M = 2.6 the geometry with two reflectors provides distinct smaller shock-to-detonation transition time. Initiation occurs at about 20 μs as a consequence of gas dynamics focusing of the flow in one reflector without interference effect as in case of M = 2.5 (see Fig. 3a). For the geometry with five reflectors initiation occurs at about 25 μs as a result of interference of the combustion zones and pressure waves of two lower reflectors (see Fig. 3b).

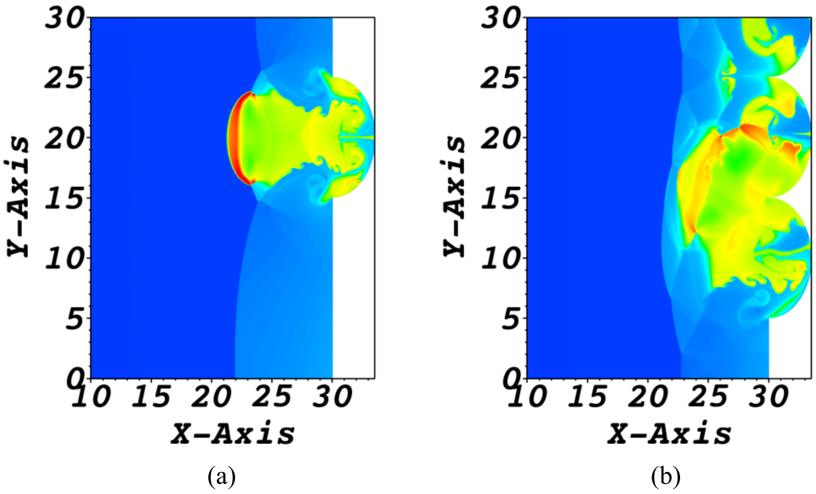


Figure 3. Predicted temperature distributions at the moments of DW initiation. M = 2.6. Axes are in mm, the scale is the same as in Fig. 2.

5 Conclusions

The mechanisms of detonation initiation in the multifocused systems of two types – with two semi-elliptical reflectors with the part of flat wall and with five adjoin semi-elliptical reflectors – are investigated. Mathematical model is based on two-dimensional Euler equations and one-stage chemical kinetics model. Simulations are carried out on fully unstructured computational grids. The spatial diversity of the reflectors and the presence of a flat wall part for the geometry of the first type gives different modes of initiation for the larger (without interference) and the smaller (with interference) Mach numbers of the incident wave.

For the lowest considered Mach number M = 2.4 the initiation didn't occur during the time of simulations. For M = 2.5 both multifocused systems provides initiation. For M = 2.6 the geometry with two reflectors works better. The numerics are in correspondence with the experimental data: M_{crit} = 2.48 for the geometry with five reflectors and M_{crit} = 2.44 for the geometry with two reflectors. The simulations for the intermediate incident shock wave Mach numbers between 2.4 and 2.5 for the considered geometries as well as the simulations for other semi-elliptical reflectors are to be carried out.

References

[1] Vasil'ev AA. (2015). Cellular structures of a multifront detonation wave and initiation (review). Comb., Expl. Shock Waves. 51: 1.

[2] Levin VA, Markov VV, Zhuravskaya TA, Osinkin SF. (2005). Nonlinear wave processes that occur during the initiation and propagation of gaseous detonation. Proc. Steklov Inst. Math. 251: 192.

[3] Gelfand BE, Khomik SV, Bartenev AM, Medvedev SP, Gronig H, Olivier H. (2000). Detonation and deflagration initiation at the focusing of shock waves in combustible gaseous mixture. Shock Waves. 10: 197.

[4] Smirnov NN, Penyazkov OG, Sevrouk KL, Nikitin VF, Stamov LI, Tyurenkova VV. (2017). Detonation onset following shock wave focusing. Acta Astron. 135: 114.

[5] Achasov OV, Labuda SA, Penyaz'kov OG. (1996). Initiation of detonation by gasdynamic methods. J. Eng. Phys. Thermophys. 69: 807.

[6] Frolov SM. 2006. Initiation of strong reactive shocks and detonation by traveling ignition pulses. J. Loss. Prev. Proc. Industr. 19: 238.

[7] Frolov SM, Semenov IV, Komissarov PV, Utkin PS, Markov VV. (2007). Reduction of the deflagration-to-detonation transition distance and time in a tube with regular shaped obstacles. Dokl. Phys. Chem. 415: 209.

[8] Lopato AI, Utkin PS. (2018). Numerical study of detonation wave propagation in the variable cross-section channel using unstructured computational grids. J. Combust. 3635797.

[9] Schultz E, Shepherd J. (2000). Validation of detailed reaction mechanisms for detonation simulation. Report No. FM99-5, CalTech Explosion Dynamics Lab.

[10] Chen G, Tang H, Zhang P. (2008). Second-order accurate Godunov scheme for multicomponent flows on moving triangular meshes. J. Sci. Comput. 34: 64.