ESTIMATION OF THE ENERGY OF DETONATION INITIATION IN A HYDROGEN-OXYGEN MIXTURE BY A HIGH VELOCITY PROJECTILE

by

Igor BEDAREV [*] ***and Valentin TEMERBEKOV***

Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, Novosibirsk, Russia

Original scientific paper
https://doi.org/10.2298/TSCI210115180B

The paper presents the results of a numerical study of the initiation of oblique detonation modes by a high velocity projectile moving in an argon-diluted hydrogen-oxygen mixture. The simulation of oblique detonation wave modes showed that calculated and experimental flow patterns agree. The calculated detonation cell size agreed with experimental data. For the initial pressure P_{st} = 121 kPa and P_{st} = 141 a series of calculations were carried out for a different projectile diameters. The detonation initiation energy was estimated, and the results were compared with theoretical models.

Key words: *detonation initiation energy, supersonic flow, numerical simulation, detonation cell, hydrogen-oxygen mixture*

Introduction

Studies of the combustion and detonation initiation in high velocity flows of combustible gases under various conditions are of great fundamental importance. Primarily, these studies focused on understanding the nature of detonation processes and identifying the criteria and conditions needed for combustion and explosion. This focus is due to the practical significance of explosion and fire safety, accident consequences and methods of prediction, and for the design of advanced engines with fuel combustion in detonation waves.

Much research effort was applied to the study of occurring and stabilizing detonations initiated by a supersonic flow of a combustible gas mixture around various objects or by a projectile moving with high velocity in a quiescent gas mixture, as well as to examination of the detonation structure and limits. These issues were extensively developed since the middle of the last century. Zel'dovich and Shlyapintokh [1] pioneered in implementing this method of ignition. They studied the combustion initiation by a shock wave generated by a high velocity bullet. In an inert medium, the spatial configuration of the ballistic wave near the head of a streamlined projectile is determined by the geometric profile of the projectile, and downstream this wave is transformed into an acoustic Mach wave. Behind the ballistic wave front, the gas is compressed and heated, so that chemical combustion reactions can occur in the reacting mixture. Almost every known combustion mode, from a slow laminar flame to hypersonic overdriven detonation, is observed behind the wave in accordance with the characteristics of the streamlined projectile and mixture parameters. There are a lot of work devoted to this phenomena. It is worth noting a number of such studies which were pablished the last century

[*] Corresponding author, e-mail: bedarev@itam.nsc.ru

[2-7]. Also, it is useful to note the research of Vasil'ev and coworkers [8-13] addressed to the geometric limits and critical regimes of detonation propagation in gas mixtures and detonation initiation by a high velocity projectile.

Despite 70 years of research, the issues related to the combustion and detonation initiation in supersonic flows or by a high velocity projectile, as well as the structure, limiting regimes, and critical energy of detonation initiation are still receiving considerable attention. For example, in work [14] the detonation limits of stoichiometric mixtures of $H_2/O_2/Ar$ and H_2/O_2 were experimentally studied. The initiation and stabilization of 3-D oblique detonation waves (ODW) by spheres with velocities higher than the Chapman-Jouguet velocity in stoichiometric mixtures of oxygen with acetylene, ethylene or hydrogen diluted with argon were experimentally studied in [15]. Special attention should be paid to the works devoted to the numerical study of the detonation structure. The results of a numerical study of the oscillatory instability in a shock-induced combustion around a hypervelocity spherical projectile are presented in [16]. A cellular structure of detonation wave in an $H_2/O_2/Ar$ and H_2-Air mixtures was numerically investigated in works [17-20]. The numerical simulation of the detonation waves interaction with a set of particles at the microlevel was carried out in [19]. The results of the numerical simulation of detonation initiation in a stoichiometric propane-air mixture are presented in work [21].

Thus, the researches of the detonation initiation and estimation of detonation initiation energy are still relevant today. In addition the fundamental issues of criteria for initiation, reinitiation and suppression of detonation, such studies are related to the problem of explosion and fire safety. This paper presents an investigation of detonation initiation for the argon-diluted hydrogen-oxygen mixture. Hydrogen is an environmentally friendly and highly efficient advanced fuel, and this has motivated the investigation of criteria for hydrogen combustion and detonation for its successful use.

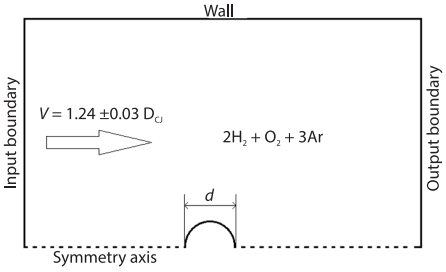

Figure 1. Simulation domain schematic

Problem formulation

The numerical simulation presented in this paper is based on the experimental work [22]. Figure 1 shows a schematic of the simulation domain. A premixed stoichiometric hydrogen-oxygen mixture diluted with argon ($2H_2 + O_2 + 3Ar$) entered the inlet of the computational domain, the velocity $V = 1.24 \pm 0.03 D_{CJ}$, the static temperature $T_{st} = 295$ K, and the different initial static pressure $P_{st} = 121$ kPa, $P_{st} = 131$ kPa, $P_{st} = 136$ kPa, and $P_{st} = 141$ kPa.

In [22], a spherical projectile with a diameter $d = 3.18$ mm was used. In our work, in addition the calculations based on experimental data, a series of calculations was performed with varying projectile diameter at $P_{st} = 121$ kPa and $P_{st} = 141$ kPa. For the initial pressure $P_{st} = 121$ kPa, the charge diameter increased from $d = 3.18$ to $d = 3.8$ mm. For the initial pressure $P_{st} = 141$ kPa, the charge diameter decreased to $d = 3$ mm. An increase or decrease in the sphere diameter at a constant pressure corresponded to an increase or decrease in the input energy, the parameter which determines the resulting combustion and detonation modes.

Mathematical model and calculation method

The mathematical model involves the solution of the Favre-averaged Navier-Stokes equations for a multicomponent gas mixture. These equations are supplemented by the equation of state and the SST modification of the k-ω turbulence model [23]. In this work, the chemical

kinetics was modeled using a reduced kinetic scheme containing one overall combustion reaction for the mixture of hydrogen and oxygen diluted with argon or nitrogen. In [24], this kinetic scheme was validated against the experimental data on the ignition delay and the propagation velocity of the detonation wave under various conditions.

The problem was solved using the ANSYS Fluent software designed to simulate complex liquid and gas-flows. A structured computational grid consisting of quadrangular elements was used, fig. 2(a). The dynamic adaptation was applied to the computational grid along the density gradient, which significantly increased the grid resolution, fig. 2(b).

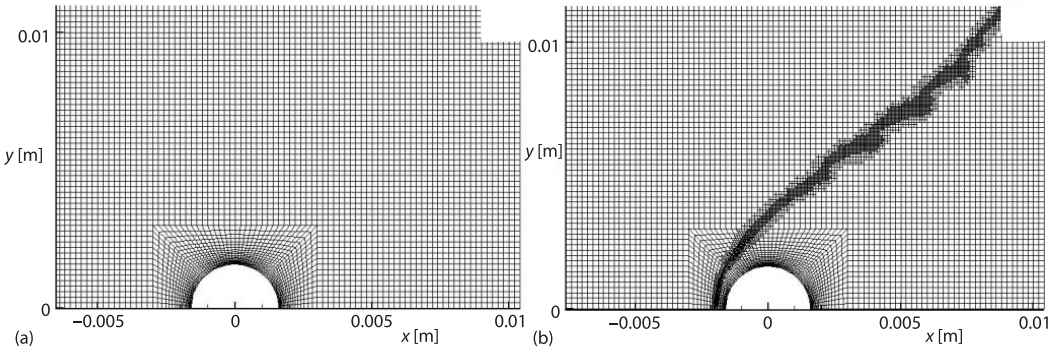

Figure 2. Fragments of the computational grid; (a) initial grid and (b) adapted grid

The purpose of this adaptation is to increase the number of grid elements in regions of high density gradients. This increase is achieved by reducing the grid spacing. For an adaptation coefficient $k = 1$, the grid spacing in regions of high density gradient is halved; for $k = 2$, it is reduced fourfold; for $k = 3$, it is reduced eightfold, and so on. Figure 3 shows the results of checking the convergence of the solution on the grid for the adaptation coefficient $k = 1$-4.

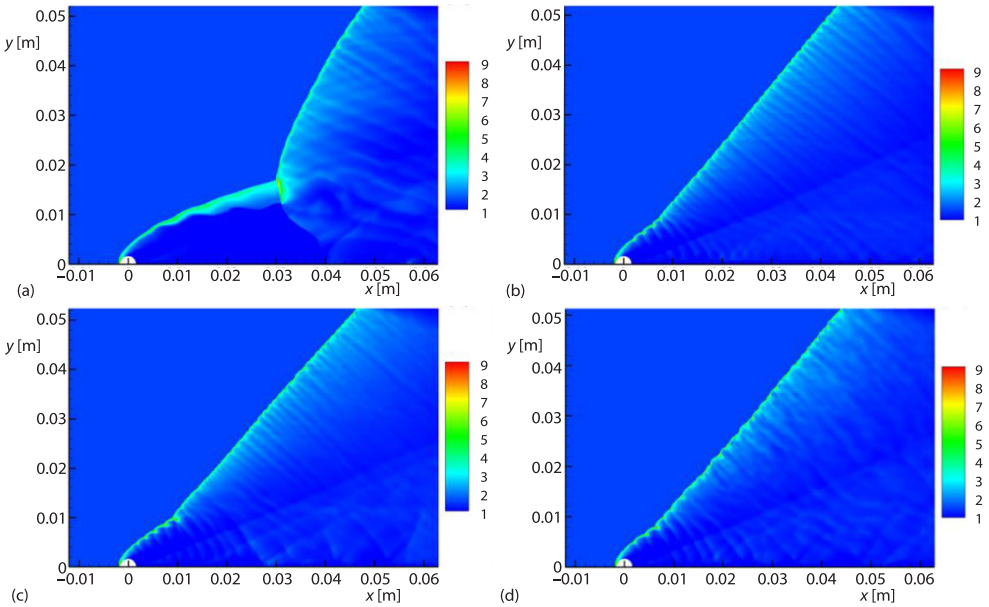

Figure 3. Calculated density fields for $P_{st} = 141$ kPa, $d = 3.18$ mm and $t = 70$ μs; (a) $k = 1$ (b) $k = 2$, (c) $k = 3$, and (d) $k = 4$

The simulation results show that for the adaptation coefficient $k = 1$, it is impossible to reproduce a stabilized oblique detonation mode; for $k = 2$, it is possible to obtain a flow pattern similar to the experimental one; for $k = 3$, the flow pattern does not change significantly, and the average detonation cell size slightly decreases. A further increase in the adaptation coefficient does not lead to a decrease in the detonation cell size, with the cell becoming less regular.

The problem was solved in an unsteady, 2-D axisymmetric formulation. An implicit second-order scheme was used in the temporal approximation, and the AUSM flux vector splitting method with a second-order upwind scheme for spatial approximation.

Method for estimating the detonation initiation energy

The present work considers the case of the cylindrical detonation initiation by a high velocity projectile. In [25], the following criterion for this case was formulated: when a high velocity projectile moves through an explosive mixture, the work of aerodynamic drag forces per unit length should exceed the minimum energy of cylindrical initiation of multifront detonation:

$$\frac{c_x \pi d^2 \rho_0 \omega^2}{8} \geq \beta E_{2*} \tag{1}$$

where c_x is the aerodynamic drag coefficient, d – the projectile midsection diameter, ρ_0 – the initial mixture density, ω – the projectile flight velocity, E^{2*} – the critical energy of initiation of cylindrical detonation, and β – the equivalence coefficient between the point and non-point initiators.

The critical initiation energy of cylindrical detonation can be defined:

$$E_{2^*} = A_2 \rho_0 D_0^2 b^2 \tag{2}$$

where D_0^2 is the ideal Chapman-Jouguet detonation velocity, and b – the length of the detonation cel, and A_2 – the dimensionless coefficient that depends on the explosive mixture.

To determine the coefficient A_2, one should refer to [26]. The detonation initiation energy is a certain number of times higher than the collision energy of transverse waves, which has the meaning of the initiation energy in the unit cell. Therefore, it can be assumed that the ratio of the detonation initiation energy to the initiation energy of the unit cell E_1 is equal to the ratio of the area of a circle (cylindrical case) with the critical diameter to the area of the unit cell:

$$E_{2*} = \frac{E_1 \pi d_*^2}{2ab} \tag{3}$$

where d_* is the critical diameter, a – the diameter of the detonation cell, and b – the length of the detonation cell.

The initiation energy of the unit cell E_1 can be defined:

$$E_1 = 4\varepsilon\alpha\rho_0 D_0^2 b^2 \tag{4}$$

where ε is the dimensionless initiation energy in the cell and α – the coefficient determined from the energy conservation law in the self-similar problem of a strong point explosion in an inert medium. The coefficients α and ε depend on the gas mixture and vary slightly.

It should be noted that according to [25, 26], this method is suitable only for estimation. However, in view of the problem formulation in the present work, this method is most appropriate.

We also calculated the deviation of the input energy, left side of inequality, eq. (1), from the critical energy required to initiate detonation, right side of inequality, eq. (1):

$$\delta = \frac{\frac{c_x \pi d^2 \rho_0 \omega^2}{8 - \beta E_{2*}}}{\beta E_{2*}} \times 100\% \tag{5}$$

Results

Previously [27], we simulated the ODW modes for the problem under study. It was found that the problem should be solved in an unsteady formulation using a dynamic adaptation of the computational grid along the density gradient. This approach allows not only obtaining all the modes observed experimentally, but also identifying the unsteady cellular detonation structure.

Figure 4 shows a comparison of the numerically obtained modes of ODW, figs. 4(a)-(c), and shock-induced combustion fig. 4(d) and the experimental shadow images given in [22] for a sphere with a diameter of 3.18 mm.

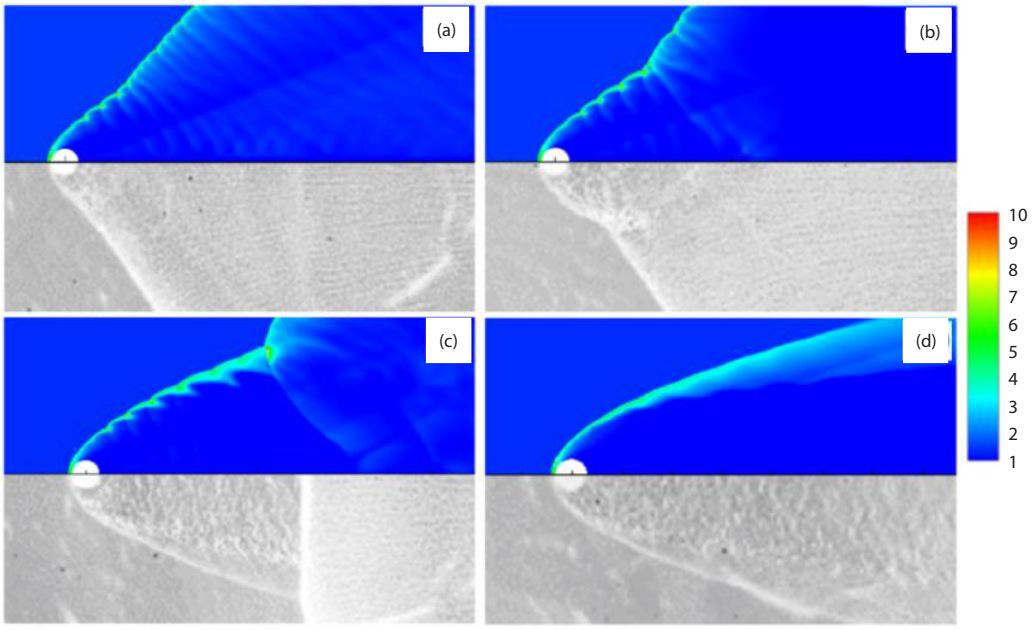

Figure 4. Calculated density fields (top). Experimental shadow images (bottom); (a) ODW at P_{st} = 141 kPa, (b) straw-hat mode with a stabilized ODW at P_{st} = 136 kPa, (c) straw-hat mode with an attenuated ODW at P_{st} = 131 kPa, and (d) shock-induced combustion at P_{st} = 121 kPa

In the modelling, good qualitative agreement was obtained between the calculated and experimental data. In addition the similarity of the flow patterns, the calculated dimensions of the detonation cell are close to the experimental values for each initial pressure, figs. 5 and 6. Figure 5 shows the fragments of the detonation wave front for different modes.

Figure 5 proves that the detonation cell size increases with decreasing initial pressure. The detonation cell size is very sensitive to changes of the initial pressure. It is important to correctly model such sensitivity for the detonation initiation energy estimating, as well as for detonation flows modelling. A similar trend is observed in the map of modes for numerical and experimental data, fig. 6.

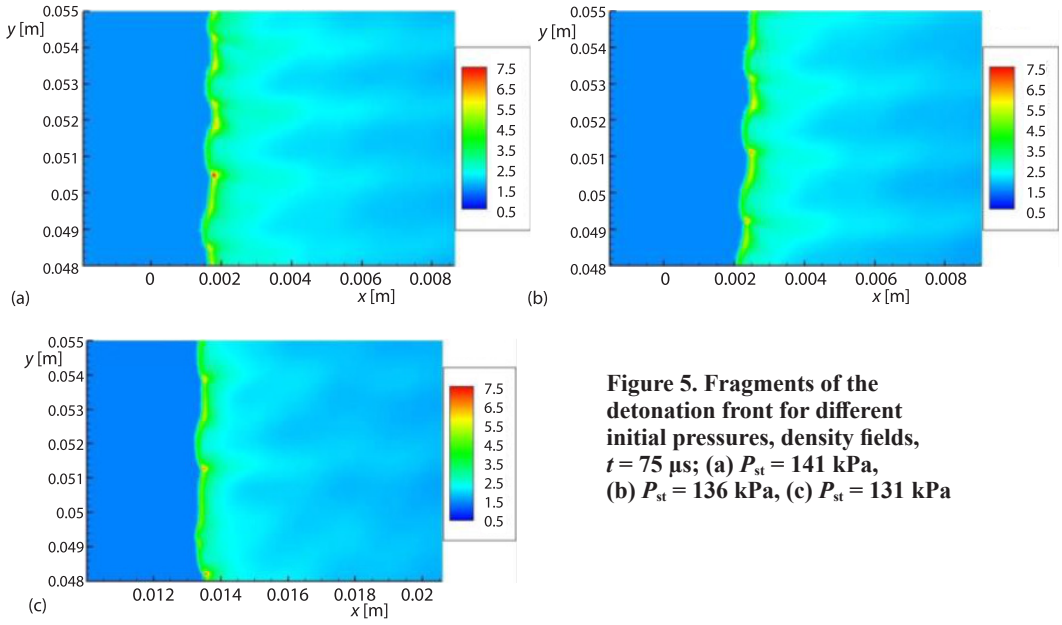

Figure 5. Fragments of the detonation front for different initial pressures, density fields, t = 75 μs; (a) P_{st} = 141 kPa, (b) P_{st} = 136 kPa, (c) P_{st} = 131 kPa

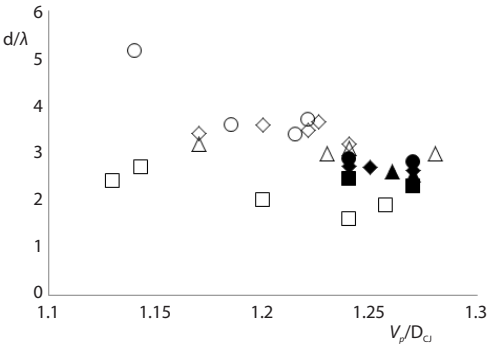

Figure 6. Map of modes; (○●) ODW, (◇◆) straw-hat mode with a stabilized ODW, (Δ▲) straw-hat mode with an attenuated ODW, and (□■) shock-induced combustion

The modes are presented as functions of the ratio of the projectile diameter to the detonation cell size and the ratio of the flight velocity to the Chapman-Jouguet detonation velocity. Null symbols refer to the experimental data [22], and filled symbols to the present calculations. Figure 6 shows that the calculated and experimental points for the corresponding detonation modes are close to each other. This agreement once again confirms the accordance of the calculated and experimental detonation cell size values. For shock-initiated combustion mode, the experimental points lying below the calculated ones. In experiments, this mode is formed at an initial pressure of P_{st} = 121 kPa. Straw-hat mode with an attenuated ODW at a pressure of P_{st} = 131 kPa is a transient mode and borders on the shock-initiated combustion mode.

As is known, the kinetic scheme of chemical reactions plays an important role in detonation process modelling. As was mentioned previously, in this work we used the Arrhenius type one-stage kinetic scheme. A lot of studies show that, to obtain a more accurate result, detailed kinetic mechanisms are necessary. For example, [28] shows that for simulation of the detonation initiation and the deflagration detonation transition, it is preferable to use complex models of chemical transformations. However, the results of this study enable to conclude that the used of the one-stage kinetics adequately describes the combustion of hydrogen in air, as will be shown later by the agreement between the experimental data [22] and the theoretical model [25].

The initiation energy for each of the detonation modes was estimated from the calculated data by the eqs. (1)-(4). In our previous work [29] we also tried to estimate the detonation initiation energy, but the results of the calculations did not correlate well enough with the theoretical model [25]. In this work, the dimensions of the detonation cell were refined. It permitted to carry out a more accurate energy estimation, both for the calculations based on experimental data [22], fig. 7, and for our own calculations, (figs. 2 and 3. Figure 7 shows the deviation of the input energy from the critical value calculated by the eq. (5) for each initial pressure for a projectile diameter d = 3.18 mm.

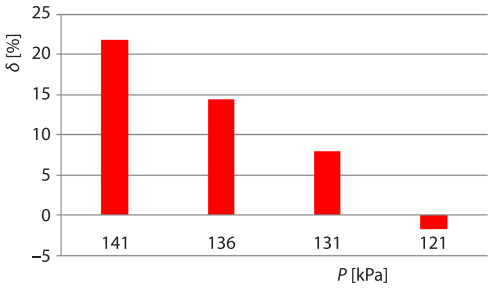

Figure 7. Deviation of the input energy from the critical value for d = 3.18 mm and P_{st} = 121-141 kPa

It can be concluded from fig. 7 that, to initiate the stabilized oblique detonation, fig. 3(a), the input energy should be significantly (about 20%) higher than the critical value. Increasing the initial pressure leads to a decrease in the detonation cell size, both in the numerical study and experiment. Decreasing the detonation cell size decreases the initiation energy in this cell, eq. (4), and the cylindrical detonation initiation energy, eq. (3). As a result, for an initial pressure P_{st} = 136 kPa, the deviation of the input energy from the critical value is about 16%, and deformation of the detonation wave, straw-hat mode with a stabilized ODW, fig. 3(b), is observed in the calculations and experiment. For the initial pressure P_{st} = 131 kPa, the deviation of the input energy from the critical value is 11%, but this is not sufficient to initiate the stable detonation. The unsteady straw-hat mode with an attenuated ODW is observed, fig. 3(c). For the lowest pressure P_{st} = 121 kPa, the input energy is about 2% lower than the critical value. Insufficient energy input leads to the shock-induced combustion, fig. 3(d).

For the initial pressure P_{st} = 121 kPa, a series of calculations were carried out for a projectile diameters d = 3.18−3.8 mm. In addition the shock-induced combustion regime obtained earlier for d = 3.18 mm, all regimes observed in the experiment were obtained. Figure 8 shows the deviation of the input energy from the critical value for the calculated data.

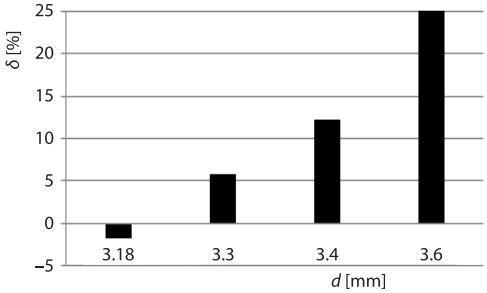

Figure 8. Deviation of the input energy from the critical value for d = 3.18-3.6 mm and P_{st} = 121 kPa

In this case, the critical energy remained constant, since the initial pressure did not change. The input energy (the work of aerodynamic drag forces) was increased by increasing the projectile diameter. To switch from the shock-induced combustion mode to the straw-hat mode with the attenuated ODW, it is sufficient to increase the sphere diameter to 3.3 mm. For this diameter, the input energy exceeds the critical value by about 6%. A further increase in the diameter leads to the establishment of the straw-hat mode with the stabilized ODW; in this case, the deviation of the input energy from the critical value is 12%. Then, as the diameter increases, the detonation wave flattens out, and for d = 3.6 mm, stabilized oblique detonation is observed.

For an initial pressure P_{st} = 141 kPa, a series of calculations were carried out for projectile diameters d = 3.1 mm and d = 3 mm. As a result, for d = 3.1 mm, a mode similar to

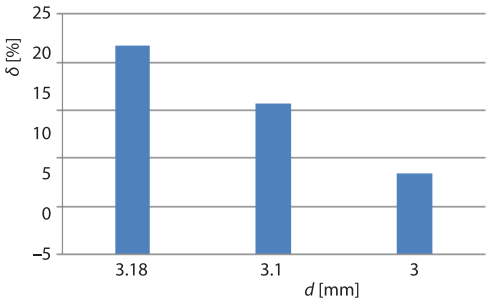

Figure 9. Deviation of the input energy from the critical value for d = 3-3.18 mm and P_{st} = 141 kPa

the straw-hat mode with the attenuated ODW is observed. The flow pattern corresponds to fig. 3(c). For d = 3 mm, the shock-induced combustion mode similar to that in fig. 3(d) is observed.

Figure 9 shows the deviation of the input energy from the critical value for a constant initial pressure P_{st} = 141 kPa and projectile diameters d = 3-3.18 mm.

As in the previous calculations, the critical energy remained constant, since the initial pressure did not change. The input energy decreased with the decreasing projectile diameter. In this case, a 16% excess of the input energy for a diameter of d = 3.1 mm does not lead to a stable detonation. Here, the straw-hat mode is observed with the attenuated ODW. For the diameter d = 3 mm, the input energy exceeds the critical value by 8%; however, as a result, the shock-induced combustion mode occurs. Note that such a difference in the modes at the same ratio of the input energy and the critical value is also observed in the experiment. Figure 4 shows different detonation modes for very close values of the detonation cell size and projectile flight velocity.

Conclusions

The mathematical model based on ANSYS FLUENT software was developed to calculate the initiation and stabilization of detonation by a supersonic projectile. This method was used to obtain all combustion and detonation modes observed in experiments.

This mathematical model was used to develop a computational method for estimating the detonation initiation energy in a hydrogen-oxygen mixture. It can also be used for other combustible gases.

The detonation initiation energy was estimated as a function of the initial pressure and projectile diameter. Predictions of the mathematical model agree not only with experimental data [22], but also with the theoretical model [25].

Acknowledgment

The research was partly carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (project No. 121030500163-4) and was partly supported by the Russian Foundation for Basic Research (Grant No. 20-38-90178).

References

[1] Zel'dovich, Y. B., Shlyapintokh I. Y., Ignition of Explosive Gas Mixtures in Shock Waves, *Dokl. Akad. Nauk SSSR, 115* (1949), 6, pp. 871-874
[2] Samozvantsev, M. P., On the Stabilization of Detonation Waves Using Blunt Bodies, *Journal Appl. Mech. Tech. Phys., 5* (1964), 4, pp. 126-129
[3] Gilinskii, S. N., *et al.,* Supersonic Flow of a Combustible Gas Mixture Past a Sphere, *Fluid Dynamics, 1* (1966), 5, pp. 4-8
[4] Chernyi, G. G., *et al.,* Supersonic Flow of Hydrogen-Air and Hydrogen-Oxygen Mixtures Past a Sphere, Report No. 987, Institute of Mechanics of Moscow State University, Moscow, Russia, 1969
[5] McVey, I. B., Toong, T., Mechanism of Instabilities of Exothermic Hypersonic Blunt-Body Flows, *Combustion Sciences and Technology, 3* (1971), 2, pp. 63-76
[6] Alpert, R. L., Toong T., Periodicity in Exothermic Hypersonic Flows about Projectiles, *Acta Astronautica, 17* (1972), 5, pp. 539-560

[7] Lehr, H. F., Experiments on Shock-Induced Combustion, *Acta Astronautica, 17* (1972), pp. 589-597
[8] Vasil'ev, A. A., Geometric Limits of Gas Detonation Propagation, *Combustion, Explosion, and Shock Waves, 18* (1982), 2, pp. 245-249
[9] Vasil'ev, A. A., Near-Limiting Regimes of Gaseous Detonation, *Combustion, Explosion, and Shock Waves, 23* (1987), 3, pp. 358-364
[10] Vasiljev, A. A., Initiation of Gaseous Detonation by a High Speed Body, *Shock Waves 3* (1994), 4, pp. 321-326
[11] Vasil'ev, A. A., Critical Conditions for Initiation of Cylindrical Multifront Detonation, *Combustion, Explosion, and Shock Waves*, *34* (1998), 2, pp. 220-225
[12] Nikolaev, Yu. A., *et al.,* Gas Detonation and Its Application in Engineering and Technologies (Review), *Combustion, Explosion, and Shock Waves, 39* (2003), 4, pp. 382-410
[13] Vasil'ev, A. A., *et al.,* Analysis of the Cell Parameters of a Multifront Gas Detonation, *Combustion, Explosion, and Shock Waves, 13* (1977), 3, pp. 338-341
[14] Gao Y., *et al.,* An Experimental Investigation of Detonation Limits in Hydrogen-Oxygen-Argon Mixtures, *International Journal of Hydrogen Energy, 41* (2016), 14, pp. 6076-6083
[15] Maeda, S., *et al.,* Initiation and Sustaining Mechanisms of Stabilized Oblique Detonation Waves around Projectiles, *Proceedings of the Combustion Institute, 34* (2013), 2, pp. 1973-1980
[16] Matsuo, A., Fujiwara T., Numerical Investigation of Oscillatory Instability in Shock-Induced Combustion around a Blunt Body, *AIAA Journal, 31* (1993), 10, pp. 1835-1841
[17] Liu, Y. F., *et al.,* Relationship between Ignition Delay Time and Cell Size of H_2-Air Detonation, *International Journal of Hydrogen Energy, 42* (2016), 16, pp. 11900-11908
[18] Hu, X. Y., *et al.,* The Cellular Structure of a 2-D H_2/O_2/Ar Detonation Wave, *Combustion Theory and Modelling, 8* (2004), 2, pp. 339-359.
[19] Bedarev, I., Micro-Level Modelling of the Detonation Wave Attenuation by Inert Particles, *Thermal Science*, *23* (2019), 2, pp. 439-445
[20] Taylor, B. D., *et al.,* Numerical Simulations of Hydrogen Detonations with Detailed Chemical Kinetics, *Proceedings of the Combustion Institute, 34* (2013), 2, pp. 2009-2016
[21] Wang, Z., *et al.,* Ignition Energy Effect on Detonation Initiation by Single and Two Successive Ignitions, *Thermal science, 24* (2020), 6, pp. 4209-4220
[22] Maeda, S., *et al.,* Scale Effect of Spherical Projectiles for Stabilization of Oblique Detonation Waves, *Shock Waves, 25* (2015), 2, pp. 141-150
[23] Menter, F. R., Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications, *AIAA Journal, 32* (1994), 8, pp. 1598-1605
[24] Bedarev, I. A., *et al.,* Application of Detailed and Reduced Kinetic Schemes for the Description of Detonation of Diluted Hydrogen-Air Mixtures, *Combustion, Explosion, and Shock Waves, 51* (2015), 5, pp. 528-539
[25] Vasil'ev, A. A., Detonation Combustion of Gas Mixtures Using a Hypervelocity Projectile, *Combustion, Explosion, and Shock Waves, 33* (1997), 5, pp. 583-597
[26] Vasil'ev, A. A., *et al.,* Critical Energy of Initiation of a Multifront Detonation, *Combustion, Explosion, and Shock Waves, 15* (1979), 6, pp. 768-775
[27] Bedarev, I. A., *et al.,* Simulating the Regimes of Oblique Detonation Waves Arising at Detonation Initiation by a Small-Diameter Projectile, *Thermophysics and Aeromechanics, 26* (2019), 1, pp. 59-68
[28] Liberman, M., *et al.,* Influence of Chemical Kinetics on Spontaneous Waves and Detonation Initiation in Highly Reactive and Low Reactive Mixtures, *Combustion Theory and Modelling, 23* (2019), 3, pp. 467-495
[29] Bedarev, I. A., Temerbekov V. M., Estimation of the Initiation Energy of Detonation Ex-Cited by a Fast Moving Body, *Journal Phys. Conf. Ser., 1404* (2019), pp. 012054-012059

Paper submitted: January 15, 2021
Paper revised: April 8, 2021
Paper accepted: April 8, 2021