Estimation of the initiation energy of detonation excited by a fast moving body

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Abstract. The results of numerical study of the detonation initiation by small diameter spherical supersonic projectile in reacting mixture are presented. A stoichiometric hydrogen and oxygen mixture diluted with argon was used as a reacting medium. The reduced kinetic scheme of chemical reactions was used in our study. The flow regimes and the detonation cell size obtained numerically and experimentally were compared and showed good agreement. Calculations for various sphere diameters at fixed pressure were carried out. The detonation initiation energy for the calculated data was estimated.

1. Introduction
The study of detonation initiation and stabilization by high speed body is important both from the scientific and technical points of view. This field of study covers a wide area of science connected with explosion safety, and studying the issues of initiating and re-initiating detonation.

Currently, there are a lot of works devoted to this issue, which indicates the relevance of this problem for the whole world. To model the phenomena considered it is necessary to familiarize themselves with a certain number of experimental and theoretical works devoted to detonation processes.

In work [1], an experimental study of the detonation initiation during the high-speed body passage through a combustible mixture is presented. The mixture of C2H2 + 2.5O2 and a cylindrical body with a rounded or blunt nose, propelled at a speed of about 800-1400 m/s were used. A new mechanism for the conversion of shock waves into detonation waves in near-critical regimes was observed. An analytical correlation between the aerodynamic characteristics of a high-speed body and the physicochemical parameters of a combustible mixture as a criterion for initiating gas detonation was proposed.

In [2], the initiation and stabilization of three-dimensional oblique detonation waves by spheres 4.76 mm in diameter with velocities 1.06–1.31 times higher than the Chapman – Jouguet velocity in stoichiometric mixtures of oxygen with acetylene, ethylene, or hydrogen diluted with argon were experimentally studied. The development of an oblique detonation wave was investigated. It was found that the radius of curvature needed to stabilize the oblique detonation wave, referred to the size of the detonation cell, is 8-10 for mixtures diluted by 50%, and 15-18 for mixtures diluted by 75%.

In article [3], the initiation and stabilization of detonation combustion in a supersonic flow of hydrogen-air mixtures in an axisymmetric nozzle with a central body installed in it was numerically
studied. Two geometric configurations of the central body are considered: “cone – cylinder – cone” and “cylinder – cone”. Modelling was carried out in a two-dimensional, axisymmetric formulation. The Euler equations for a multicomponent gas mixture taking into account chemical reactions were used as a mathematical model. It is shown that the central body can serve as an effective tool for initiating and stabilizing detonation, which provides a thrust at free-stream Mach numbers from 7 to 9.

One of the most important problem of fire and explosion safety today is the assessment of the energy necessary for detonation initiation. There are a number of theoretical models that can be used to predict the initiation of detonation and evaluate the effects of an explosion. So, for example, in the work [4] a criterion for initiating detonation by a fast-flying body was proposed. It is assumed that in order to initiate gas detonation by a body flying at a high speed, it is necessary that the work of the aerodynamic drag forces per unit length of the body would be not less than the minimum initiation energy of cylindrical detonation in the mixture under given conditions (pressure, temperature).

The present work considers the detonation initiation of a hydrogen-oxygen mixture by high speed spherical particles and estimation of detonation initiation energy.

2. Problem formulation
A schematic of the simulation is shown in Figure 1. A premixed stoichiometric hydrogen–oxygen mixture diluted with argon (2H₂ + O₂ + 3Ar) having a velocity \( V = 1.24 \pm 0.03 \) \( V_{CJ} \), a static temperature \( T_{st} = 295 \) K, and an initial pressure \( P_{st} = 121 \) kPa was supplied to the inlet of the simulation domain. The diameter of the sphere was varied \( d = 3.18 \div 3.8 \) mm.

3. Mathematical model
A Favre-averaged Navier-Stokes equations for multicomponent gas mixture supplemented by an SST modification of the \( k-\omega \) turbulence model were used as a mathematical model. The ANSYS Fluent software package was used as a solver. An implicit second-order scheme was used for temporal approximation, and the AUSM flux vector splitting method with a second-order upwind scheme for spatial approximation. The reduced Arenius kinetic scheme including one gross reaction of hydrogen burning in air was used for the chemical kinetics simulation. In the work [5], this kinetic scheme was
verified according to the experimental data on the ignition delay and the propagation velocity of the detonation wave under different conditions.

A detailed quadrangular orthogonal grid was used. For convenience, the computational grid was divided into blocks in which the grid was constructed separately. Such way allows us to avoid unnecessary condensations, reduce the total number of grid nodes without increasing the grid step.

In work [6], the mathematical model and the calculation algorithm were subjected to additional verification against experimental data [7] on the detonation cell size and detonation modes. Comparative analysis showed that the approach used allows us to model complicated detonation processes, and in addition to qualitative agreement between the calculated and experimental flow pictures we achieved a quantitative agreement between detonation cell sizes.

4. Calculations results
In previous studies [6], we numerically obtained various detonation modes observed in experiments [7]. Figure 2 shows these modes.

![Figure 2](image)

**Figure 2.** The results of the verification. Density fields.
(a) – Oblique detonation wave at $P_{st} = 141$ kPa;
(b) – Straw-hat mode with oblique detonation wave at $P_{st} = 136$ kPa;
(c) – Straw-hat mode with attenuated oblique detonation wave at $P_{st} = 136$ kPa;
(d) – Shock-induced combustion at $P_{st} = 121$ kPa.

For these calculations, the detonation initiation energy was estimated using the formulas from [4]. Figure 3 shows the input energy deviation (work of the aerodynamic drag forces per unit length) from the critical initiation energy of detonation under given conditions.

In this study the detonation initiation at constant pressure $P_{st} = 121$ kPa is considered. By increasing the diameter of the sphere starting from 3.18 mm, the same regimes were obtained as in the works [6] and [7]. The results of the simulations are shown in Figure 4.
Figure 3. The input energy deviation from the critical detonation initiation energy for data [6] and [7].

Figure 4. The results of the calculations at pressure $P_{st} = 121$ kPa. Density fields.
(a) – Shock-induced combustion at $d = 3.18$ mm;
(b) – Straw-hat mode with attenuated oblique detonation wave at $d = 3.3$ mm;
(c) – Straw-hat mode with oblique detonation wave at $d = 3.4$ mm;
(d) – Oblique detonation wave at $d = 3.8$ mm.

Figure 5 shows the input energy deviation (work of the aerodynamic drag forces per unit length) from the critical initiation energy of detonation at pressure $P_{st} = 121$ kPa for various diameter of the sphere.

For the sphere diameter $d = 3.18$ mm, shock-initiated combustion is carried out. For $d = 3.3$ mm, we can see straw-hat mode with attenuated oblique detonation. For $d = 3.4 - 3.6$ mm, straw-hat mode with oblique detonation wave is carried out. For sphere diameter from $d = 3.8$ mm we can see stabilized oblique detonation wave.
Figure 5. The input energy deviation from the critical detonation initiation energy at $P_{st} = 121$ kPa for various diameter of the sphere.

5. Conclusions
The problem of detonation initiation and stabilization by various diameter high speed body was solved using a previously developed mathematical model and mathematical technology for its implementation based on the ANSYS Fluent package.

The input energy deviation (work of the aerodynamic drag forces per unit length) from the critical initiation energy of detonation under given conditions was found for experimental and calculated data.

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Nomenclature
$T_{st}$ - static temperature;
$P_{st}$ - static pressure;
$V_{CJ}$ - Chapman-Jouguet velocity;
d - diameter of the sphere;
$\Delta$ - the input energy deviation from the critical detonation initiation energy.

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