

INFLUENCE OF PARTICLE ON GAS DETONATION BY SHOCK**V.P. Efremov**

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There exist evidence, that the gaseous detonation passing through a cloud of solid particles could be attenuated or even suppressed. Contrary to these known works, in the present article, we have found that just one single 160-micron particle can serve as a trigger for the detonation onset. By numerical simulation, we have obtained that there are the concentration ratio limits, in which single particle is enough to initiate gaseous detonation, although without particle the detonation is not ignited in the same conditions in a tube of restricted size. In other words, the presence of a solid particle in the combustible mixture could decrease significantly the ignition delay time. Using of temperature pattern visualization, we have demonstrated that the ignition arises in the subsonic region located between the particle and the bow shock front. The approximations of the used model are discussed. It is shown that used assumptions are valid within investigated time intervals

Keywords

Combustion, detonation, gas, particle, ignition, initiation, shock wave

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Introduction. Detonation wave incombustible gases in sufficiently long channels can be initiated by a shock wave due to the mechanism proposed in Ref. [1]. With the accumulation of combustible gases during the operation of various technical systems used in various industries, there is a real danger of explosion and detonation of these gases. Explosion protection requires an understanding of the physical mechanisms of ignition and detonation, as well as numerical describing of the initiation of combustion [2]. Detonation can occur in a limited range of conditions (pressures, mixtures, etc.) [3]. Any deviation of the analyzed problem of initiating detonation from the use of a one-dimensional

model of a stationary shock wave [1] can cause a change in the limiting values, both in the direction of deceleration and in the direction of facilitating ignition, as shown in Ref. [3]. For example, the walls of the channels on which the adhesion condition is fulfilled may contribute to earlier ignition during the passage of the shock wave. A numerical calculation performed in Ref. [4] showed that taking into account friction on the walls, the induction time could be much shorter than the induction time in the one-dimensional approximation without friction.

Safety requirements for technological processes can be tightened if solid particles are present in the gas since in this case the ignition limits can be shifted, including towards their expansion. Changes in the ignition and detonation limits in gaseous mixtures containing solid-state particles can be associated both with the processes of evaporation or combustion of these particles [5] and with their gas-dynamic effect on the reacting flow, which takes place even in the case of chemically inert particles [6].

The phenomena of attenuation and suppression of detonation in a mixture of hydrogen and oxygen, in which the detonation velocity decreases due to the addition of inert solid particles of sand to the combustible mixture, were considered in Ref. [7]. In work [7], it was shown that with decreasing particle size and with an increase in their volume concentration, the detonation velocity decreases significantly. The considered process is useful for the purposes of the supporting of the explosion hazardous objects safety.

The role of particles in the initiation of gas detonation was studied in Ref. [8], where a review of experiments on shock wave initiation of combustion of dust — combustible mixtures is presented. The ignition of dust particles under conditions created behind the incident and reflected by shock waves is considered. In particular, the relevance of this work is confirmed by the indication formulated in Ref. [8] on the opacity of the flashing mixture, which makes it impossible to experimentally clarify the details of the process of single ignition of particles.

In experiments on ignition in fast compression machines [9], it was found that before ignition of the gas mixture, microparticles that were randomly distributed in the combustible mixture are ignited.

The appearance of ignition regions in the shock tube also occurred in the presence of particles specially added by experimenters to the gas mixture [10]. Since additional energy can be locally released in the flow due to friction or catalytic reactions on the surface of the particles, in this way these particles can create local hot spots of ignition.

The influence of the size of the computational grid and the kinetics of chemical reactions on ignition due to the incidence of a shock wave on a poorly

streamlined body was studied in detail in Ref. [11]. A stage was found numerically at which the reaction zone noticeably approaches the surface of the body, which leads to additional heat release from high-temperature reactions. With a further increase in resolution, temperature fluctuations intensify and can noticeably perturb the flow.

A mathematical model for calculating the initiation of detonation by a small particle moving in combustible mixtures at supersonic velocity was proposed in Ref. [12]. In this work, stationary and non-stationary calculations are compared with experimental data and a conclusion is made about the advantage for problems with a moving particle of non-stationary calculations with the dynamic adaptation of numerical grids.

The gas heating caused by particles suspended in a non-reacting gas behind the shock wave front was numerically investigated earlier in Ref. [13]. The temperature fields formed in the vicinity of the particle are visualized. It is shown that an inert gas mixture containing one particle is heated in the region between the forehead particle surface and the front of the shock wave reflected from it, i.e., in the region of the subsonic flow. Next, the heated gas fell into the region behind the particle. The consideration of gas heating in the vicinity of the particle was supplemented in Ref. [14] by modeling chemical reactions in flow to reveal the effect of particles on the initiation of gas detonation. It is numerically confirmed that particles play the role of detonation promoters, and it is shown how ignition occurs near a particle.

This work is a development of the approaches proposed in Ref. [13, 14]. Here, the phenomenon of acceleration of ignition in the presence of a particle in mixtures of various mixture compositions is investigated.

Statement of the problem and model specification. To achieve a clear understanding of the effect of an individual particle on the ignition of a gaseous mixture, the following idealized formulation of the problem is used. In the work, the process of ignition of a hydrogen-oxygen mixture in a stream behind an incident shock wave was simulated as a result of the deceleration of the stream by 160-micron particle placed in it. The geometry of the problem is shown schematically in Fig. 1.

The shock tube is divided into a high-pressure chamber and a low-pressure chamber by an infinitely thin diaphragm. The opening of the diaphragm occurred instantly at a time $t = 0$. The gases in both parts of the pipe were initially at a temperature $T_1 = 300$ K. The low-pressure chamber was filled with a hydrogen-oxygen mixture of a given composition, and the high-pressure chamber was filled with helium. Two series of calculations were carried out at different values of the

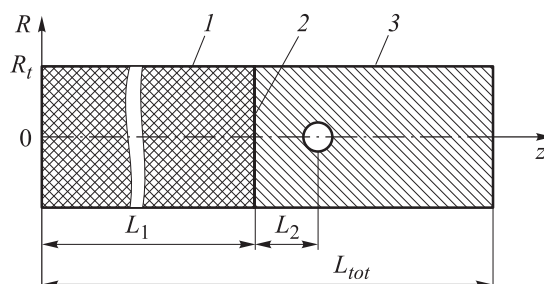
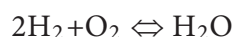


Fig. 1. The geometry of the problem:

L_1 is the length of the high pressure chamber; L_2 is the distance from the diaphragm to the particle; L_{tot} is pipe length; R_t is the radius of the pipe; 1 is high pressure chamber; 2 is aperture; 3 is low pressure chamber

pressure of the reacting mixture in the low-pressure chamber: $p_1 = 0.1$ MPa and $p_2 = 0.01$ MPa. The shock tube model is not critical for considering the possibility of gas ignition under conditions of a supersonic flow seeded with particles. However, the statement of the problem of the development of the process in the shock tube allows us to see the realism of achieving the studied parameters in laboratory conditions.

In the framework of the stated statement of the problem, shock-heated gas flow was formed under the solution of the problem of the decay of an arbitrary discontinuity. The characteristic profiles of pressure (Fig. 2, *a*), temperature (Fig. 2, *b*) and shock wave velocity (Fig. 2, *c*) are shown in Fig. 2. The value ν denotes the ratio $\frac{[\text{O}_2]}{2[\text{H}_2]}$ — of the number of moles of oxygen to twice the number of moles of hydrogen. With this choice of the variable ν in the stoichiometric mixture $\nu = 1$, which corresponds to the reaction



To identify the features of ignition and the formation of detonation in the presence of 100-micron particles, two classes of problems were solved: 1) the problem of ignition in a stream behind an incident shock wave in the absence of particles in a one-dimensional formulation; 2) the problem of igniting a mixture in a stream with 160 micron particle placed in it in a two-dimensional axisymmetric approximation. In the first case, ignition for natural reasons occurred directly on the contact gap between the shock-heated combustible mixture and the pushing gas. In the second case, ignition modes were considered before the contact discontinuity entered the cross-section in which the particle was placed. The pipe length is fixed for the same task classes.

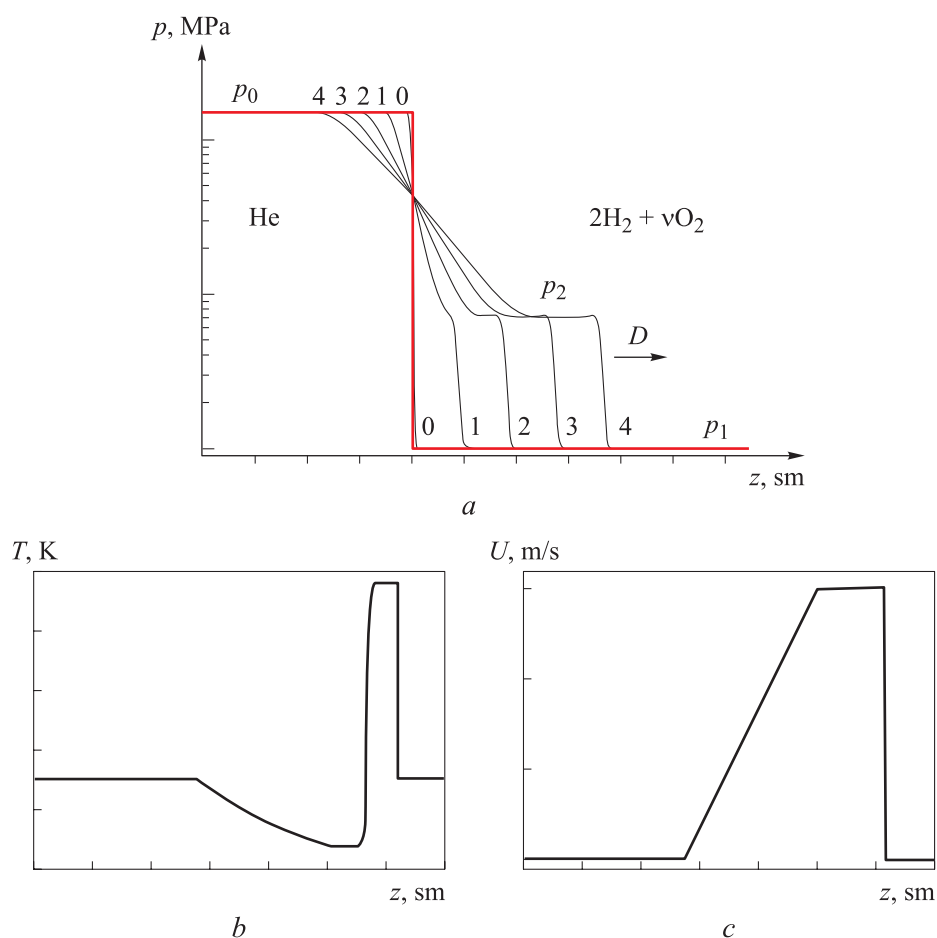


Fig. 2. Characteristic profiles of pressure (a), temperature (b) and shock wave velocity (c) (the numbers 0–4 indicate the pressure profiles corresponding to consecutive moments of time separated by the same time intervals)

The choice of particle radius is the compromise between the two requirements. On the one hand, it is necessary to study the effect on the ignition and the possibility of initiating detonation of micron-sized particles characteristic of conditions realized in laboratory experiments and in event of emergencies at industrial facilities. On the other hand, a decrease in the size of the model particle leads to the need to increase the resolution of the computational grid and significantly increase the computation time and corresponding computer resources.

Earlier in Ref. [14], a similar study was performed concerning to a stoichiometric hydrogen-oxygen mixture. It should be noted here that the stoichiometric mixture of hydrogen with oxygen is the most chemically active gaseous mixture, which under conditions typical for the compression ratios

considered in shock [14] ensures detonation even when very small spatial scales of local heating regions (ignition foci) are formed). In addition to detonation itself, a certain danger in the development of an emergency scenario with the release and subsequent ignition of a gaseous mixture is also represented by waves of deflagration combustion, which are formed when the ignition focus is not large enough. The ignition process can get such a development when using less active combustible mixtures, for example, containing a lower fraction of hydrogen.

The study of the characteristics of ignition and the formation of detonation in depleted compositions of hydrogen-containing mixtures is of particular interest for applications in the field of fire and explosion safety and, in particular, for determining the concentration limits of ignition and detonation of combustible mixtures. In this regard, in the framework of this study, the problem of ignition in a stream behind a shock wave containing a microparticle was solved for hydrogen-oxygen mixtures with different hydrogen contents.

In the framework of the accepted statement of the problem, the particle was considered motionless on the considered time scales. The particle surface was assumed adiabatic. The adiabaticity approximation is acceptable only for times not exceeding the temperature relaxation time $t_t \approx R^2/\chi$, where R is particle radius; χ is the thermal diffusivity of the particle material. The particle immobility approximation is permissible for times shorter than the velocity relaxation time $t_U = m/(6\pi\eta R)$, where m is particle mass; η is the dynamic viscosity of the gas. In the framework of the problem statement considered in this work, processes that develop approximately a particle on time scales much shorter than both relaxation times are studied. In this formulation, the thermal conductivity and specific heat of the particle are excluded from consideration. To verify the accepted assumptions, we estimated the amount of heat absorbed by the particle from the stream to analyze how much the temperature field pattern will change taking into account the indicated properties of the particle. The calculations presented in Ref. [13] showed that the heat absorbed by the particle during a time of the order of the relaxation time of the particle velocity to the flow velocity is much less than the heat additionally released in the flow during the same time due to the deceleration of the flow in the presence of the particle. Therefore, the picture of the temperature field, taking into account the thermal conductivity and heat capacity of the particle, does not significantly change in this time.

The radius of the computational domain is chosen to avoid the influence of oblique shock waves reflected from the sidewall on processes developing near a 160-micron particle. Equations and calculation methods are traditional and do not require additional lighting and analysis.

For calculations, a computer code was used, which is widely used to solve the problems of gas dynamics of combustion, for example, in Ref. [15], and which implements the solution of the equations of gas dynamics of a reacting gas using the Euler — Lagrange approach, also known as the “large-particle” method [16]. In the process of calculations, the physical quantities characterizing the flow are determined at the centers of the cells of the Eulerian grid, and their change in a time step is calculated in three stages. The implementation of the “large particles” method used here has the first order of accuracy in time and a second order of accuracy in space [17]. The mathematical model itself is a standard notation of balanced equations for a compressible reactive gas, taking into account viscosity, thermal conductivity, and diffusion. A detailed record of equations in Euler variables is given, for example, in Ref. [18]. The size of the counting cells was $0.016 \times 0.016 \text{ mm}^2$.

The equations of state of the fresh mixture and combustion products were set based on *NASA* tables by interpolation [19]. The kinetics of combustion of a hydrogen-oxygen mixture was described according to the well-established kinetic mechanism [20], which reproduces both qualitative and quantitative features of ignition and combustion of a hydrogen-oxygen mixture with good accuracy.

To test the applicability of the code used for calculating temperature fields and other flow parameters, the code was tested on the problem of estimating the maximum heating obtained when the flow completely stops when it flows onto a rigid wall [13]. The results obtained showed good agreement with analytical estimates for an ideal gas [21]. Numerical and analytical data coincided. The calculated temperature values turned out to be slightly (about 5 %) lower than analytically predicted, which is associated with the use of the table equation of state in calculations [13].

The computer code used in the statement of the problem was previously applied to solve a wide class of problems of combustion gas dynamics, such as the flame acceleration problem [18]; the problem of flame propagation in confined spaces filled with reactive mixtures of various compositions [22]; the task of initiating the combustion of a hydrogen-air mixture near the lower concentration limit of ignition [23]; the problem of the influence of thermal radiation of combustion products on flame propagation in a dispersed medium [17], etc.

Results. In a simple one-dimensional calculation of the effect of a shock wave on a combustible gas, gas ignition occurs not at the shock front, but behind it. When considering the decay of a fracture at a specific time after the opening of the diaphragm, it is obvious that the combustible gas near the interface between the combustible and pushing gases is in a compressed and heated state for a longer

time than the gas directly behind the front of the shock wave. At each subsequent moment, the shock wave captures the unreacted mixture, and the combustible gas near the contact surface is exposed to an ever-longer exposure to elevated temperature. As a result of the difference in the duration of the reaction in different regions of the pipe, the exothermic stage of the reaction occurs near the contact surface earlier than in the regions into which the shock wave arrives later.

If a particle is placed in the flow, then when a shock wave falls on it, a reflected shock wave departs from the particle (Fig. 3). Between the front of the reflected shock wave and the surface of the particle, a region is formed in which the gas is additionally compressed and heated — the region of the heated and denser gas I. Heating is associated with the deceleration of the flow on the particle. A region of heated gas is also formed behind the particle. It should be noted that heat in supersonic flow is mainly released in the region of a slow subsonic flow, in Fig. 3, this region is limited by a sound line that closes regions I and II within itself [13]. The sound line shows the place in the stream where the local Mach number is 1.

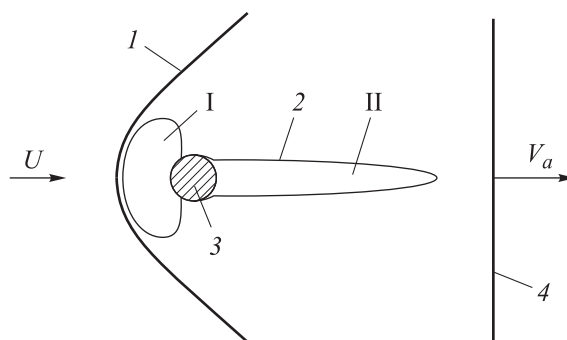


Fig. 3. Design of interaction of a supersonic gas and particle flow behind the front of the shock wave:

I, II are areas; V_a is velocity of the front of the transmitted shock wave; U is gas velocity behind the front of the transmitted wave; 1 is reflected shock wave; 2 is Mach line; 3 is particle; 4 is previous shock wave

The change in the critical pressure in the high-pressure chamber depending on the volumetric concentration of hydrogen is shown in Fig. 4, *a*. The critical pressure is the smallest pressure p_0 at which detonation was initiated in the calculations, i.e., at pressures above the critical level, detonation is initiated, below detonation does not occur. The volumetric concentration of hydrogen in the calculations was determined by the percentage of moles of hydrogen in the combustible mixture:

$$[H_2] = \frac{2}{2 + \nu} \cdot 100, \%$$

where ν is the number of moles of oxygen in a non-stoichiometric mixture. Two lines (Fig. 4) correspond to different pressures in the low-pressure chamber p_1 . The pressure in the high-pressure chamber p_0 is normalized to p_1 to show both graphs on the same coordinate grid. Rich combustible mixtures during the formation of a shock wave flash with a greater degree of compression (i.e., at a higher pressure in the high-pressure chamber). However, in the process of calculating the search for the shock wave of the lowest critical intensity for a given composition of the combustible mixture, detonation is initiated under close thermodynamic conditions behind the shock wave front, as shown in Fig. 4, *b* and 4, *c*, for examples of the lowest pressure p_2 and temperature T_2 , at which detonation is initiated in a pipe of a fixed length.

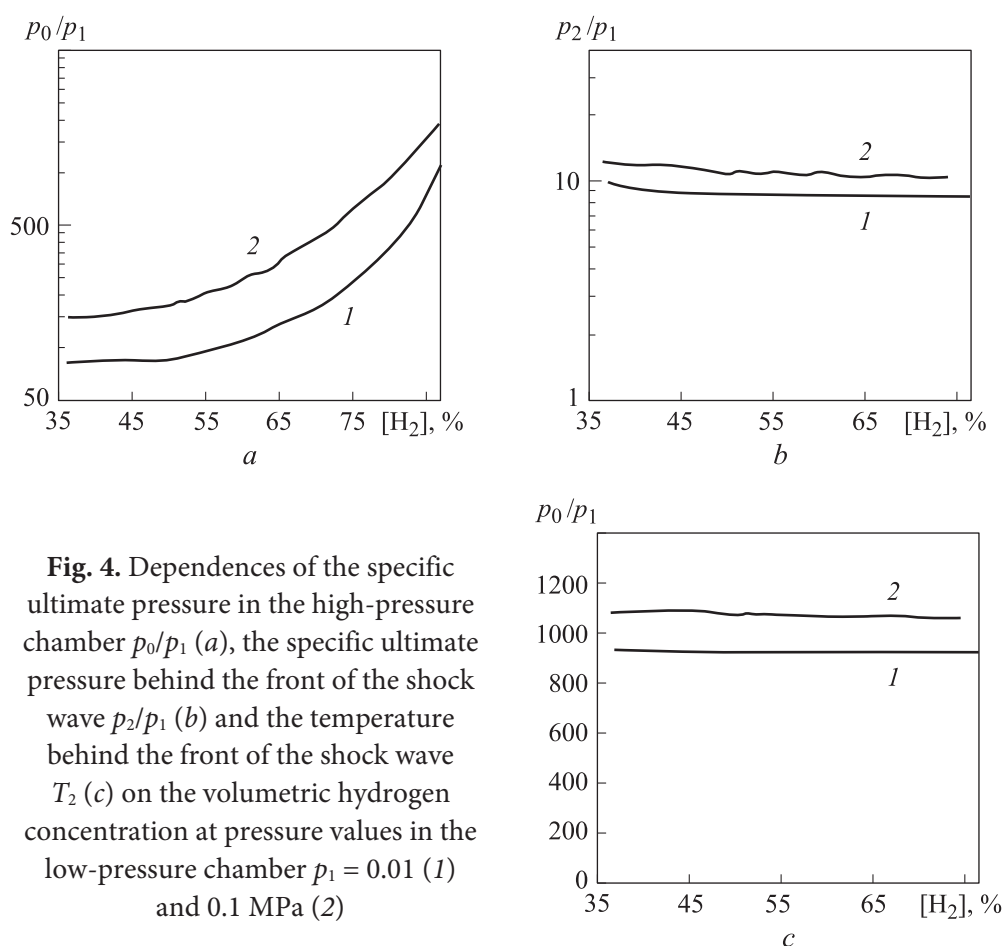


Fig. 4. Dependences of the specific ultimate pressure in the high-pressure chamber p_0/p_1 (*a*), the specific ultimate pressure behind the front of the shock wave p_2/p_1 (*b*) and the temperature behind the front of the shock wave T_2 (*c*) on the volumetric hydrogen concentration at pressure values in the low-pressure chamber $p_1 = 0.01$ (*1*) and 0.1 MPa (*2*)

The pressure behind the front of the shock wave for ideal gases can be obtained numerically from the solution to the disintegration problem, which can be calculated using the nonlinear equation obtained at the point of

intersection of the shock adiabat of the pushed gas and the isentropic discharge of the push gas [21]:

$$p_2 = p_0 \left(1 - \frac{\gamma-1}{2} \frac{(p_2 - p_1) \sqrt{\frac{2V_1}{(\gamma-1)p_1 + (\gamma+1)p_2}}}{C_0} \right)^{\frac{2\gamma}{\gamma-1}}, \quad (1)$$

where γ is adiabatic exponent; C_0 is sound velocity; V_1 is initial specific volume. Index “2” indicates that the values refer to the conditions in the hydrogen-oxygen mixture behind the shock wave, “1” indicates that the values refer to the initial parameters in the hydrogen-oxygen mixture in the low-pressure chamber, “0” indicates that the values refer to the characteristics of helium in the high-pressure chamber.

In the framework of the proposed work, the time interval between the opening of the diaphragm and the estimated time when the gas temperature approximately the particle exceeds $1.05T_2$ is taken as the induction time. The values of the induction time for different values of the pressure in the low-pressure chamber, the composition of the mixture and the model used are given in the Table. Each of the two pressures in the low-pressure chamber includes four columns. The first column shows the number of moles of oxygen per two moles of hydrogen, the remaining three columns show the induction times for different calculation models. Column 0D shows the values of induction time obtained in a simplified calculation for a stationary combustible mixture in a thermodynamic state (p_2, T_2) , column 1D shows the time values determined in a one-dimensional calculation of a shock wave without a particle, and column 2D shows the results of calculations of the time of induction in conditions behind the front of the shock wave in the presence of a particle. The calculations for the stoichiometric composition of the mixture are highlighted in bold.

According to the data given in Table, the induction time in the presence of a particle decreases by an order of magnitude. In this case, the time of induction during ignition by a shock wave of an initially cold mixture (approximation 1D) corresponds to the time of induction of a stationary combustible mixture located at a temperature and pressure behind the front of the shock wave (approximation 0D). The results for the 1D model are only slightly underestimated due to the inclusion of dissipative processes in the contact discontinuity region.

The value of the induction time depending on the pressure in the low-pressure chamber, mixture composition and model used

v	[H ₂], %	t _{inds} S			v	[H ₂], %	t _{inds} S		
		0D	1D	2D			0D	1D	2D
p ₁ = 0.01 MPa									
0.4	83.33	9.11E - 04	5.26E - 04	3.74E - 05	0.5	80.00	4.15E - 05	1.70E - 05	2.44E - 05
0.8	71.43	8.17E - 04	6.46E - 04	5.00E - 05	0.6	76.92	4.25E - 05	1.21E - 05	2.62E - 05
1.0	66.67	6.50E - 04	4.52E - 04	4.30E - 05	1.0	66.67	4.63E - 04	4.32E - 04	3.41E - 05
1.1	64.52	7.34E - 04	5.70E - 04	5.10E - 05	1.3	60.61	6.10E - 04	5.94E - 04	3.67E - 05
1.8	52.63	8.68E - 04	6.87E - 04	7.00E - 05	2.0	50.00	6.62E - 04	6.53E - 04	3.57E - 05
2.5	44.44	8.72E - 04	5.92E - 04	6.55E - 05	2.5	44.44	4.77E - 04	4.52E - 04	5.12E - 05
3.0	40.00	1.02E - 03	6.11E - 04	6.83E - 05	3.0	40.00	5.49E - 04	5.66E - 04	5.26E - 05
3.5	36.36	1.30E - 03	8.19E - 04	7.06E - 05	3.5	36.36	6.48E - 04	6.69E - 04	5.46E - 05

The formation of a detonation wave is shown in Fig. 5. It is possible to trace how the flow is heated near the particle due to the deceleration of the gaseous medium. The visualization of the calculation of the chemically active hydrogen-oxygen mixture is shown in Fig. 5, *a*, visualization of the calculation with the same initial data, but under the assumption of a chemical inertness of the mixture is shown in Fig. 5, *b*. In the case of a reactive mixture, the figure shows the formation of a detonation wave as a result of additional heating. With further passage of the front, its distortion caused by the interaction with the particle is smoothed and disappears when the particle is 3–4 times apart along with the flow.

Let us consider in detail the development of the detonation initiation process as a result of the interaction of a compressed gas stream with a particle. The dependence of the front velocity of the shock wave U_f reflected from the particle on the time elapsed after the front of the incident shock wave propagated is shown in Fig. 2 in two cases (the medium is reactive or neutral) in Fig. 6. At the moment of arrival of the shock wave in front of the particle, the gas is braked and accumulated. In the absence of chemical reactions, the speed at which the boundary of the compressed and heated gas moves opposite the flow tends to zero. In other words, within the relaxation time, the structure of the flow near the particle stabilizes. If chemical reactions take place in gas, then the velocity of the front of the reflected wave monotonically increases due to the release of energy in the region of the chemical reaction to the velocity of the front of the detonation wave.

The dependences of the additional energy released because of deceleration and the additional mass accumulated in the region of deceleration of the flow in front of the particle are shown in Fig. 7. The data for the reacting mixture (ΔE^+ and ΔM^+) are indicated by the superscript “+”, and for the non-reacting mixture (ΔE^- and ΔM^-) are indicated by the superscripts “-”. The additional energy of the reacting mixture increases linearly from the moment the shock wave arrives. In contrast, for a non-reacting mixture, the additional energy, not including the heat generated by chemical reactions, but produced by the action of hydrodynamic laws alone, varies slightly with time.

Conclusion. It is shown that in the presence of a particle in a combustible mixture, the induction time is decreased by order of magnitude. The effect of a particle on the fields of temperature, pressure, and velocity near a particle is determined.

Ignition of the mixture and the formation of detonation occur in the field of flow inhibition near the front surface of the particle, in the subsonic region.

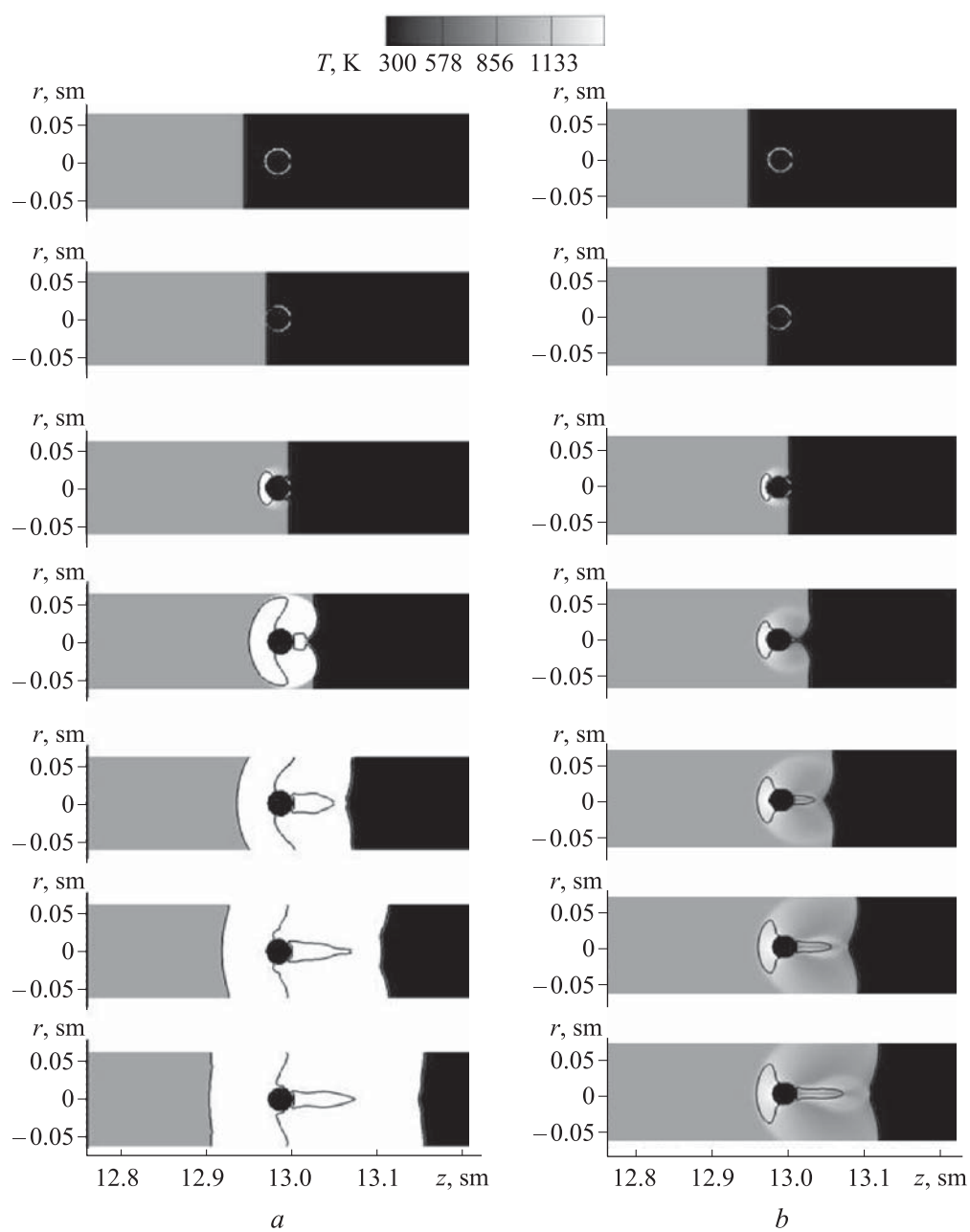


Fig. 5. The formation of a detonation wave:

a sequence of frames for a chemically active combustible mixture; *b* for similar conditions, but in the approximation of the absence of chemical reactions (frames correspond to temperature fields at successive times, the interval between frames is $0.1 \mu s$; the black line corresponds to the position in the stream, where the local flow velocity is equal to the speed of sound)

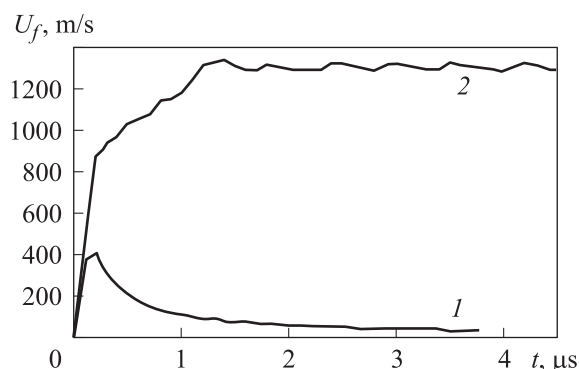


Fig. 6. Dependence of the front velocity of the shock wave reflected from the particle on the time elapsed after the front of the incident shock wave passed, without taking into account reactions (1) and taking into account the reactions (2)

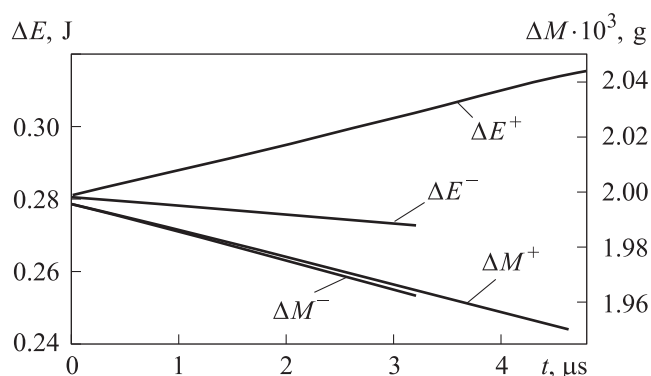


Fig. 7. Dependences of the additional energy ΔE , released before the particle, the additional mass ΔM , accumulated before the particle, on time (the index “+” corresponds to the reacting mixture, the index “-” corresponds to the neutral mixture)

Evaluation of the ignition parameters of mixtures of various compositions indicates a relatively weak dependence on the composition. Moreover, to achieve critical parameters in rich hydrogen-air mixtures, a significantly more intense effect on the medium is required.

Translated by K. Zykova

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