

Low-Gas Detonation in Low-Density Mechanically Activated Powder Mixtures

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Abstract—We have analyzed experimental data on supersonic self-sustained propagation of an energy-release wave in low-density mechanically activated mixtures. Various mechanisms that can be responsible for this process have been investigated, and the mechanism for detonation-like propagation of reaction in powder mixtures has been proposed. It is shown that under certain conditions, this process possesses all features of detonation and must be treated as a variety of detonation. It is demonstrated that this type of detonation basically differs from classical “ideal” detonation: instead of a shock wave, a compaction wave propagates in a powder mixture, in which powder compaction and not compression of particle material occurs due to mutual displacement of particles. In this case, a chemical reaction is initiated due to mutual friction of oxidizer and fuel particles in the powder compaction wave.

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INTRODUCTION

Detonation (in a generalized sense) is the term that can be applied to any self-sustaining energy-release process propagating in a reactive medium at a velocity exceeding the speed of sound in the initial material if the compression wave produced by the substance expanding in the energy-release zone ensures energy release in an amount and at a rate sufficient for maintaining its further propagation (i.e., compensating natural damping of the compression wave). The substance expanding in the energy-release zone plays the role of a piston pushing the compression wave in front of it.

Detonations in substances with different structures and chemical compositions can differ in the mechanism of initiation and physical origin of energy release at the shock wave front or behind it. Examples are

(i) Classical detonation in continuous media (liquids, gases, and solids) with gaseous combustion products; the adiabatic compression of such a medium in a shock wave initiates exothermal chemical reactions and creates conditions for their fast occurrence behind its wave front.

(ii) Detonation in heterogeneous porous explosives in accordance with the ballistic mechanism, when high-speed jets of hot products propagate in front of the compression wave [1].

(iii) Photo-detonation wave [2], in which the energy release behind the shock front is induced by absorption of high-power laser radiation in a compressed medium; the compression of the medium occurs in a conventional shock wave, while the change in its density and (mainly) ionization behind the shock wave sharply increase the laser radiation absorption coefficient as compared to the initial medium.

(iv) Solid-phase detonation without intermediate gaseous products (gas-free detonation), which is a hypothetical process that has not been realized so far in pure form but is theoretically possible in principle [3–7].

In true gas-free detonation, condensed reaction products play the role of the piston; for this, the volume of these products must substantially increase either due to thermal expansion or due to the formation of less dense (as compared to the initial substance) condensed products of synthesis.

Processes close to gas-free detonation were realized in low-density mechanically activated powder mixtures [8–13]. The role of the piston in such experiments is played by gaseous combustion products; in some cases, only intermediate combustion products are gaseous, while initial particles and final reaction products are in the solid state.

It should be noted that the speed of sound in a low-density powder as in a “continuous medium” amounts

to 100–300 m/s [9, 14, 15]; for this reason, any energy-release wave moving relative to the initial powder at a velocity lower than 300 m/s is supersonic. Obviously, the term “detonation wave” cannot be applied to any supersonic energy-release wave. For an energy-release wave propagating with a supersonic velocity in a powder mixture to be treated as a detonation wave, it must generate in front of it a powder compaction wave or a shock wave in gas filling pores, which directly initiates a reaction in powder particles. For a powder compaction wave to be able to directly initiate and accelerate chemical reactions in particles, its intensity must be quite high. To this end, the powder density in it must be increased substantially, which implies a high pressure in the powder and in the gaseous products of combustion of particles behind the compaction wave front. In addition, the powder mixture must exhibit a high chemical activity for a compaction wave to be able to initiate chemical reactions in it, and these reactions must occur at a high rate required for sustaining a compaction wave.

For increasing the energy release rate in mixtures of metals with solid oxidizers, preliminary mechanical activation of powders was used in [8–13]. It was shown that mechanical activation of Me/X mixtures (Me = Mg, Al, Si; X = MoO₃, fluoroplastic (–CF₂–CF₂–)_n, potassium perchlorate KClO₄ (PPC), ammonium perchlorate NH₄ClO₄ (APC), and potassium nitrate KNO₃ (PN)) increase the combustion rate by three orders of magnitude and facilitate the transformation of combustion in detonation.

For example, for a mixture of silicon nanopowder (average grain size of about 60 nm) with ammonium perchlorate (nSi/APC), uniquely high explosive combustion rates (~600 m/s) were obtained, and conversion of burning into detonation was observed in porous samples. For a porosity of 70–80% of the initial mixture, the conversion of burning into detonation occurred over a length of 20–60 mm; in this case, detonation velocities of 130–2000 m/s were attained. Upon an increase in silicon nanoparticle size (to above 150 nm) or a reduction of the fraction of active silicon in the powder, relatively low burning velocities (100–130 m/s) without a conversion into detonation were observed.

For Al/PPC powder charges (with a porosity of 70–80%) based on aluminum pyrotechnical powder (PP-2) in steel tubes of diameter 10 mm, the length of conversion to detonation varied from 1 to 7 cm, and the detonation velocity was 1000–1500 m/s (in some experiments, it was up to 2400 m/s with a conversion length of 1–2 cm). It was found that the length of conversion to detonation and the steady-state detonation velocity depend on the mixture composition and activation time [8–13]. For example, for an activation time of 2 min, the conversion to detonation was not observed, but explosive combustion with a velocity of 420 m/s was detected; the tube in this case was pre-

served without noticeable destruction. For activation times exceeding 5 min, a conversion of burning into detonation was observed. The maximal velocities were obtained for Al/PPC 30/70 mixtures. For activation times longer than 40 min, the velocity decreased, indicating a partial reaction of components during mechanical processing.

In mechanically activated Al/fluoroplastic mixtures (with a porosity of 70–80%), steady-state detonation with velocities of 700–1300 m/s was observed depending on the aluminum concentration in the mixture. The pressure in detonation products was estimated from measured values of pressure in the shock wave at fluoroplastic or aluminum plates arranged at the end of the charge, which were in the range 0.5–1.6 GPa; this corresponds to pressures of 0.1–0.3 GPa in the products.

Experiments [8–13] show that for a powder porosity lower than a certain limit (~60%), detonation in the studied mixtures is not observed, and only relatively slow combustion with velocities from several tens to several hundred meters per second occurs without conversion into detonation. It follows from experiments [8–13] that the initial density of the powder plays the fundamental role in this process, which is not quite clear.

1. MECHANISMS OF HEAT PULSE TRANSFER

Experimental data [8–13] lead to the conclusion that gas-free (both true and “low-gas”) detonation can be observed in low-density powder mixtures (with a porosity exceeding 60%) with high chemical activity of particles, which can be attained by increasing the area of the oxidizer–fuel contact surface in well-mixed nanosize mixtures, as well as using preliminary mechanical activation.

Theoretically, the powder porosity can affect the velocity of energy-release front propagation either via filtration of hot combustion products that can ignite still uninflamed particles at the detonation front (combustion front) or via the powder compression under the action of pressure of gaseous combustion products.

Obviously, the lower the initial density of the powder, the higher the possible degree of its compaction. Powder compaction during the supersonic propagation of energy release occurs in the form of a compaction wave in which the relative density of the powder may change by 2–3 times. Expanding gaseous combustion products of particles play the role of a piston that increases the density of the powder layer in front of it. Contacting particles transfer the compressive force to the next powder layers, which forms a compaction wave, viz., a relatively narrow zone with a powder density varying over the width. Such a compaction wave can propagate over the initial powder with a nearly constant velocity exceeding the velocity

of sound in the initial powder [14, 15]. The compaction wave in the powder is an analog of a shock wave in gases. This analogy becomes even more visual if we consider the fact that the width of a shock wave in a gas is on the order of several mean free paths of molecules, while the width of compaction wave (zone) in low-density powders is on the order of several sizes of pores between particles [14, 15] (average pore size is a sort of the “mean free path” of particles in the powder).

During adiabatic compression of the gas in a shock wave, its heating occurs due to conversion of mechanical energy of the gas flow into thermal energy. This is essentially the mechanism of a heat pulse transfer in a detonation wave in gases (as well as in liquids and continuous solids). In contrast to gases, the mechanism of heat pulse transfer from burning particles to unignited ones during “gas-free” detonation of a low-density powder mixture remains unclear.

The main candidates for such a mechanism are listed below.

1. *Conductive mechanism* in which heat is transferred to a particle through contacts between particles (contact heat conduction). As shown in [16, 17], the rate of burning of mechanically activated powders in the case of purely contact heat conduction between particles decreases upon an increase in the porosity of the powder mixture, which contradicts the results in [8–13]. This means that the conductive mechanism cannot play the leading role in fast burning and more so, in detonation of low-density powder mixtures.

2. *Convective mechanism* (impact filtration) in which hot gaseous combustion products are filtered through pores and ignite still unignited particles. This mechanism is obviously possible only when either the final or intermediate gaseous combustion products are present; in true gas-free detonation, this mechanism is not realized. In our opinion, the convective mechanism can be operative only in the case of explosive conduction of low-density powder mixtures investigated in [8–13], ensuring anomalously high combustion velocities (up to 600 m/s), as well as during the conversion of burning into detonation, ensuring the acceleration of the process at the initial stage and increasing pressure in combustion products to values at which other faster mechanisms of heat pulse transfer come into play. In the case of detonation of a low-density powder mixture, the convective mechanism of heat pulse transfer turns out to be too slow; simple estimates show that at a detonation velocity of about 1000 m/s, the particle heating due to filtration of hot gaseous combustion products during the passage of the detonation front through particle does not exceed a few tens of degrees.

3. *Jet (relay-race) mechanism* in which burning particles “scatter” incandescent fragments (drops) and jets in the surrounding medium. Hitting still unignited particles within “direct visibility,” these particles can ignite them, which ensures heat pulse transfer

to the next layers of the powder mixture. This mechanism is a variety of the relay-race mechanism. For such a process to determine the detonation velocity, the velocities of the jet and of fragments of burning particles must be substantially higher than the experimentally observed detonation velocity (i.e., a few kilometers per second). It should be noted that the role of porosity in this process is ambiguous: on the one hand, high porosity facilitates the formation and propagation of hot fragments and jets, but on the other hand, the higher the powder porosity, the longer (on the average) time is required for their flight through pores and the lower the bulk energy release. This means that the rate of heat pulse transfer in accordance with this mechanism must decrease upon an increase in powder porosity, which contradicts the results of observations [8, 13].

4. *Impact initiation* of chemical reactions [3–7], in which high stresses and strains emerging in particles during fast (impact) compacting of the powder initiates rapid exothermal reactions on the contact surfaces between fuel and oxidizer particles. The higher the porosity of the initial powder, the higher the relative velocities that can be acquired by particles in a compaction wave. Therefore, an increase in the powder porosity must facilitate impact initiation, which is in conformity with experimental data [8–13].

5. *Heating of oxidizer and fuel particles (predominantly in their contact region) due to friction* upon fast compression of powder in a compaction wave [18]. During powder compaction, friction emerges between contacting particles as well as particles and walls of the tube containing powder. The higher the powder porosity, the larger relative displacements of particles in a compaction wave, the larger the work done by friction forces, and, hence, the higher the temperature acquired by interacting particles. It was shown in [13] that mechanically activated composites nSi/APC, nSi/PPC, Al/MoO₃, and Mg/MoO₃ have a very high sensitivity to friction, which is comparable with the sensitivity of lead azide. The results in [13] indicate a certain correlation between the sensitivity of mechanically activated composites to friction and their detonation velocity. For example, composites nSi/APC exhibit a higher sensitivity and simultaneously a higher detonation velocity as compared to nSi/PPC; at the same time, the sensitivity of nSi/PN nanocomposites to friction is approximately 20 times lower than that of lead azide, and detonation could not be initiated for them (only fast burning with a velocity of 590 m/s was observed). A significantly nonequilibrium action of detonation products on the plate surface was observed only from imprints on witness plates. The strongest (both mechanical and erosion) action is observed at the plate periphery, indicating the nonuniformity of the detonation front: the detonation velocity and, accordingly, the velocity of detonation products at the periphery (near the tube wall) is higher than in its central part. This can be explained by the higher friction

between powder particles and tube walls than between contacting powder particles, which leads to a faster heating of particles during powder compression in the compaction wave at tube walls as compared to the central region. The results are higher detonation velocity and detonation pressure at tube walls. This pattern is completely opposite to that observed during the detonation of a gas mixture in a tube: the detonation velocity at tube walls is always lower than in its central part, which is associated with the gas viscosity and heat losses to the wall.

It can be expected that all aforementioned mechanisms participate to a certain extent in heat pulse transfer from burning particles to still uninflamed ones during the detonation of low-density powder mixtures and especially during conversion of burning into detonation. However, we can single out among these mechanisms the main one responsible for the regularities of the considered process, while the remaining mechanisms are secondary.

In most publications devoted to gas-free detonation, the impact mechanism of initiating chemical reactions is treated as the basis [3–7]. However, according to estimates [3–7], this mechanism requires very high pressures (on the order of 10 GPa), which are not realized during the detonation of mechanically activated low-density powder mixtures [8–13].

Above analysis shows that the most probable mechanism for initiating particles in gas-free detonation in low-density powder mixtures is friction between contacting particles of oxidizer and fuel, as well as between particles and walls of the tube into which the powder is pressed-in.

For describing gas-free detonation, the hydrodynamic approach is traditionally used, the result of which is the conventional Hugoniot adiabat [3–7]. Such an approach is justified only in the case when heating of the medium in a compaction wave in a powder mixture is associated with adiabatic compression of particle material as a continuous medium. If the relative powder density is substantially smaller than unity, its compacting is a complex multistage process [19]. Usually, three stages of powder compaction are usually singled out: (i) low relative density (less than 0.5); compaction of powder occurs due to special regrouping of particles as a results of their mutual displacement; resistance to powder compression is associated with mutual friction of the particles and with their inertia; (ii) moderate relative density (0.5–0.7); powder is compacted due to destruction (fragmentation) of particles and spatial regrouping of their fragments as a result of mutual displacement; (iii) high relative density (exceeding 0.7); powder compacting occurs due to plastic deformation of particles and their fragments.

Since the width of the compaction wave is on the order of several average pore sizes, we can estimate the residence of powder particles in a compaction wave

(up to their inflaming) using the expression $\tau \sim k \left(\frac{1}{\rho - 1} \right)^{1/3} \frac{d}{D}$, where d is the particle size, ρ is the relative density of the initial powder, D is the wave velocity, $k < 10$. For example, for $d \sim 1 \mu\text{m}$, $D = 1000 \text{ m/s}$, $\rho = 0.3$, and $k = 10$, we obtain $\tau \sim 0.1 \mu\text{s}$. During such a short time, particles cannot be noticeably deformed; therefore, we can expect that only the first stage of powder compacting is realized in the compaction wave.

2. MODEL OF GAS-FREE DETONATION

Let us consider the 1D model of a compaction wave in a powder mixture of an oxidizer and fuel reacting with the formation of final solid substances in the presence of intermediate gaseous products.

In contrast to shock waves in gases, a compaction wave in the powder should be treated not as a geometrical surface at which a jump of parameters occurs, but as a zone of a finite (albeit small) thickness, in which the powder mixture density, pressure in the powder, and temperature of particles vary continuously. In this case, the pressure in the powder and the pressure in the gas filling pores between particles must be distinguished.

Let us consider the case when the role of the gas filling pores between particles in the initial powder can be disregarded. Moreover, we assume that gaseous combustion products do not participate directly in heating and inflaming of powder particles; these products only play the role of a piston compacting the powder.

The equations of 1D motion of the powder as a medium being compressed has conventional form

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0, \quad (1)$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial \rho v^2}{\partial x} = -\frac{1}{\gamma} \frac{\partial \sigma}{\partial x}, \quad (2)$$

where γ is the density of the powder particle material, ρ is the relative density of the powder, v is the velocity of the powder as a continuous medium, and σ is the pressure (compressive stress) in the powder as a continuous medium. By definition, we have

$$\sigma = \frac{R}{F}, \quad (3)$$

where R is the force acting between powder particles separated by the cross section of area F . Stress σ is the pressure in the powder caused by the interaction of particles.

Equations (1) and (2) must be supplemented with the rheological equation describing the relation between the pressure in the powder and its density and the compaction rate (rate of density variation).

Let us consider a stationary compaction wave propagating relative to the initial (noncompacted) powder with velocity D . As usual, we will consider the frame of reference moving together with the compaction wave (its resting frame of reference). We direct the x axis towards the initial powder (in the direction of compaction wave propagation). In this frame of reference, the initial powder moves with velocity $-D$, and the powder parameters are independent of time. Then, Eqs. (1) and (2) assume form

$$\frac{d\rho v}{dx} = 0, \tag{4}$$

$$\frac{d\rho v^2}{dx} = -\frac{1}{\gamma} \frac{d\sigma}{dx}. \tag{5}$$

Considering natural boundary conditions (for $x = \infty$), these equations have solutions

$$\rho v = -\rho_0 D, \tag{6}$$

$$\gamma \rho v^2 + \sigma = \gamma \rho_0 D^2, \tag{7}$$

where ρ_0 is the relative density of the initial powder. Here, we assume that the pressure in the initial (non-compacted) powder equals zero:

$$\sigma(\infty) = 0. \tag{8}$$

Using Eq. (6), we can write relation (7) in form

$$\sigma = \gamma \rho_0 D^2 \left[1 - \frac{\rho_0}{\rho} \right]. \tag{9}$$

This relation, which is known as the Michelson (or Rayleigh) straight line, establishes the connection between the pressure and density of the powder in the compaction wave.

In contrast to continuous media (gases, liquids, and solids), in which compression is associated with overcoming of the thermal motion of atoms and molecules as well as the forces of interaction between them and is reversible, compaction in powders is associated (at least at the first stage) with mutual displacement of solid particles and, hence, with friction between them. For this reason, compaction of a powder is an irreversible process, and the work done during powder compaction is mainly the work of forces of friction between contacting particles.

The work of pressure forces done during compaction of a powder per its unit mass is given by

$$A = -\frac{1}{\gamma} \int_{\rho_0}^{\rho} \sigma d \frac{1}{\rho}. \tag{10}$$

Here, we consider the compaction of the powder from initial density ρ_0 to a certain density $\rho > \rho_0$.

Since the powder compaction in a compaction wave is a rapid (adiabatic) process, we can assume with a high degree of accuracy that at the first stage of powder compaction, friction forces lead to heating of pow-

der particles; in this case, the entire work (10) done by friction forces is converted into heat: $\Delta Q = A$, where ΔQ is the heat released during friction between particles.

This enables us to estimate the variation of temperature of particles in the powder during its compaction:

$$\gamma c_p \Delta T = \beta \int_{\rho_0}^{\rho} \frac{\sigma}{\rho^2} d\rho, \tag{11}$$

where c_p is the specific heat of the powder and β is the coefficient that considers on average the nonuniform friction in the powder and nonuniform heating of powder particles.

With allowance for relation (9), we obtain

$$c_p \Delta T = \frac{1}{2} \beta D^2 \left(1 - \frac{\rho_0}{\rho} \right)^2. \tag{12}$$

It should be noted that this relation replaces the Rankine–Hugoniot equation used in hydrodynamic theory of detonation of continuous media.

Here, we assume that entire amount of heat (10) released during friction of particles in the course of powder compaction is distributed uniformly between powder particles and that powder particles are heated uniformly. In fact, different powder particles are in different conditions due to the random structure of the powder. As a result, average amount of heat (10) released during powder compaction is distributed nonuniformly among particles (some particles receive more heat, while others receive, accordingly, less heat). In addition, powder particles are heated nonuniformly over their volume, and this nonuniformity is the higher the smaller the heat transfer coefficient of the particle material. These factors can be considered only using the statistical approach analogous to the kinetic theory of gases or direct numerical simulation of powder compaction, in which a detailed calculation of motion of each particle is performed considering its mechanical, thermal, and chemical interactions with other particles. Such an approach is most promising in our opinion and will be described in subsequent studies.

In this article, we disregard the nonuniformity of heat release during friction of different particles and assume that the thermal conductivity of particles is so high that the heat released during friction is distributed uniformly over the particle volume.

We assume that after the attainment of a certain temperature T_{ign} , ignition of a particle occurs. We assume that ignition temperature T_{ign} is a constant and preset characteristic of the powder. Note that in a more consistent model, instead of the ignition temperature, one can use, for example, Arrhenius kinetics of chemical reactions in powder particles. Then, the

ignition of a particle has the form of a thermal explosion initiated by friction between particles.

The approach considered here makes it possible to estimate the degree of compaction of the powder in a compaction wave, at which ignition of its particles occurs:

$$c_p \Delta T_{\text{ign}} = \frac{1}{2} \beta D^2 \left(1 - \frac{\rho_0}{\rho_{\text{ign}}} \right)^2, \quad (13)$$

where $\Delta T_{\text{ign}} = T_{\text{ign}} - T_0$, T_0 being the initial temperature of the powder, and ρ_{ign} is the density at which temperature T_{ign} is attained during powder compaction.

In the powder cross section in which condition (13) is created, burning on the contact surface between oxidizer and fuel particles begins with formation of intermediate gaseous products, which leads to an abrupt increase in pressure. This cross section will be referred to as the detonation front in the low-density powder mixture. We assume that $x = 0$ is the coordinate of the detonation front in the moving system of coordinates. It is assumed that there is no gas phase up to the detonation front ($x > 0$) and only the powder is present, while behind the detonation front ($x < 0$), the two-phase mixture (gaseous products of combustion of particles and burning particles themselves) is present. The powder particles behind the detonation front are not in contact because they are repelled from one another by gaseous combustion products flowing from the surface.

Gaseous combustion products behind the detonation front produce pressure on the powder layer located immediately at the detonation front. It is precisely the pressure transferred to other layers of particles at the detonation front that is responsible for the compaction of the powder. It can be expected that pressure $\sigma(0)$ in the powder at the detonation front is proportional to pressure p in the gaseous combustion products immediately behind the detonation front,

$$\sigma(0) = \eta \rho_{\text{ign}} p, \quad (14)$$

where coefficient η can weakly depend on ρ_{ign} . Here, we assume that this coefficient is constant. The dependence of $\rho(0)$ on ρ_{ign} takes into account the fact that the higher the density of the layer of particles at the detonation front, the larger the force of pressure exerted by gaseous combustion product on the unflamed powder.

Considering Eq. (9), we obtain

$$\eta \rho_{\text{ign}} p = \gamma \rho_0 D^2 \left[1 - \frac{\rho_0}{\rho_{\text{ign}}} \right]. \quad (15)$$

Let us introduce the degree of powder compaction at the detonation front:

$$\xi_{\text{ign}} = \frac{\rho_{\text{ign}}}{\rho_0}. \quad (16)$$

Then, we obtain from Eqs. (13) and (15)

$$p = p_0 (\xi_{\text{ign}} - 1)^{-1} \quad (17)$$

and

$$D = D_0 \frac{\xi_{\text{ign}}}{\xi_{\text{ign}} - 1}. \quad (18)$$

This gives

$$\xi_{\text{ign}} = 1 + \frac{1}{\pi} \quad (19)$$

and

$$D = D_0 (\pi + 1), \quad (20)$$

where

$$\pi = p/p_0 \quad (21)$$

is the dimensionless pressure of gases at the detonation front,

$$p_0 = \frac{2\gamma c_p \Delta T_{\text{ign}}}{\beta \eta} \quad (22)$$

is the characteristic detonation pressure, and

$$D_0 = (\eta p_0 / \gamma)^{1/2} \quad (23)$$

is the characteristic detonation velocity. Considering expression (22), we obtain

$$D_0 = (2c_p \Delta T_{\text{ign}} / \beta)^{1/2}. \quad (24)$$

Relations (19) and (20) establish the connection of the powder degree of compaction at the detonation front and the detonation velocity with the pressure of gaseous combustion products behind the detonation front. Note the linear dependence of the gas-free detonation velocity on the pressure behind the detonation front.

Figure 1 shows the dependence of the powder degree of compaction in the detonation wave on the dimensionless pressure behind the detonation wave front. It follows from expression (19) and Fig. 1 that the degree of compaction of the powder in the detonation wave decreases with increasing pressure behind the detonation wave front; at a very high pressure, $p_0 \gg 1$, the degree of powder compaction tends to unity. This strange (at first glance) result has a simple explanation: with increasing pressure, the detonation velocity increases in accordance with a linear law. As a result, the residence time of the powder in the compaction wave (up to ignition of particles) decreases upon an increase in pressure; the degree of compression of the powder that has not reached high densities also decreases simultaneously.

The relative density of the powder that can be attained only due to regrouping of particles without their deformation and fracture does not exceed a certain value ρ_{max} . Usually, $\rho_{\text{max}} \approx 0.5$. Therefore, the above results are valid as long as $\rho_{\text{ign}} < \rho_{\text{max}}$. The fol-

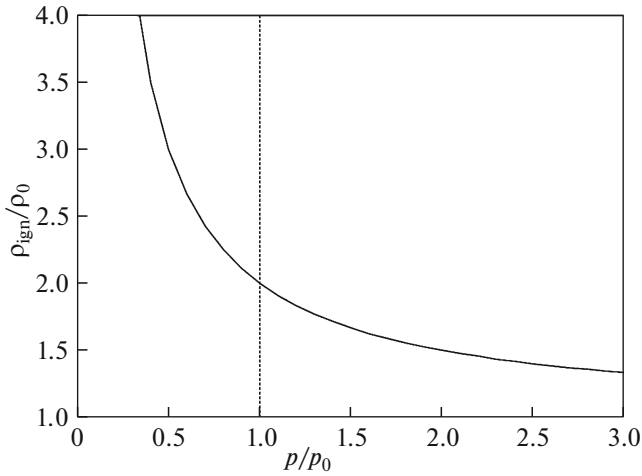


Fig. 1. Dependence of the degree of compaction of the powder in the detonation wave on dimensionless pressure behind the detonation front. Vertical dashed line corresponds to $p = p_0$.

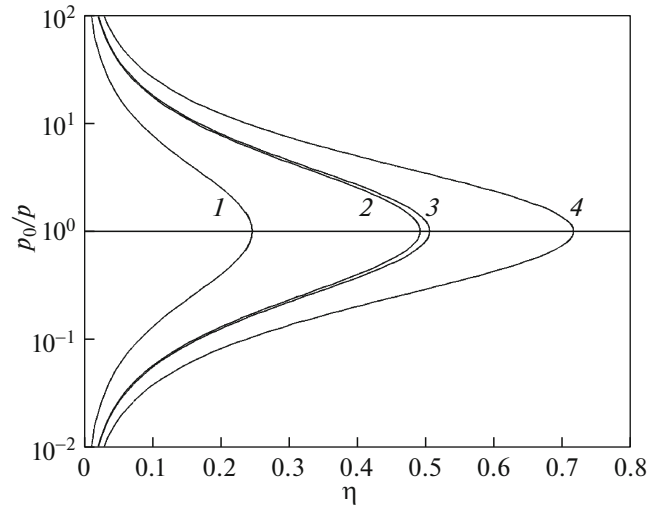


Fig. 2. Dependences of p_0/p on parameter η for different combinations of experimental values of (D, p) reported in [8–10]: (1) $D = 700$ m/s, $p = 1$ GPa; (2) $D = 700$ m/s, $p = 0.5$ GPa; (3) $D = 1100$ m/s, $p = 1.2$ GPa; (4) $D = 1000$ m/s, $p = 0.7$ GPa.

lowing interesting fact is worth noting: until now, we have not used any rheological law describing the behavior of powder medium; this means that the results above do not depend on the specific form of the rheological law.

Relations (20), (21), and (23) make it possible to estimate characteristic pressure p_0 from the values of the experimentally determined detonation velocity and pressure behind the detonation front.

Substituting relations (21) and (23) into (20), we obtain a quadratic equation in p_0 for p and D . This equation has two solutions,

$$p_0 = z^2, \tag{25}$$

where

$$z_{1,2} = \frac{1}{2}(\gamma/\eta)^{1/2} D \pm \sqrt{\frac{\gamma D^2}{4\eta} - p}. \tag{26}$$

It should be noted that

$$z_1 z_2 = p. \tag{27}$$

The most undetermined parameter in this expression is coefficient η , that must satisfy condition

$$\eta \leq \frac{\gamma D^2}{4p}. \tag{28}$$

According to the results in [8–10], the following values were obtained in experiments with mechanically activated Al/fluoroplastic mixture: $D = 700$ – 1300 m/s and $p = 0.5$ – 1.6 GPa. Figure 2 shows the dependence of p_0/p on parameter η for different combinations of experimental values of (D, p) from [8–10]. In our calculations, we assumed that $\gamma = 2000$ kg/m³. The upper branch in the figure corresponds to solution (26) with the plus sign, while the lower branch, to

solution (26) with the minus sign. Therefore, for the same value of parameter η , the preset combination of experimental values of (D, p) can correspond to two different characteristic detonation pressures p_0 (one higher than experimentally observed pressure p and the other lower than this value). Using formula (22), we can estimate the ignition temperature for particles in the detonation wave, which can be achieved due to friction between particles during powder compaction:

$$\Delta T_{ign} = \frac{\beta \eta p_0}{2\gamma c_p}. \tag{29}$$

Figure 3 shows dependences of ΔT_{ign} on parameter η for the same combination of experimental values of (D, p) . In our calculations, we assumed that $\gamma = 2000$ kg/m³, $c_p = 1$ kJ/(kg K), and $\beta = 1$.

Like pressure p , ignition temperature ΔT_{ign} , which can be achieved due to friction between particles in the powder compaction wave has two different values for the same value of parameter η . The upper branch of the curves in Fig. 3 (like in Fig. 2) corresponds to the solution (26) with the plus sign, while the lower branch corresponds to solution (26) with the minus sign. It can be seen that the detonation wave corresponding to the solution with the minus sign can exist only at an unrealistically low temperature of ignition of powder particles. Therefore, this type of detonation in a low-density powder mixture can correspond only to solution (26) of Eq. (25) with the plus sign,

$$p_0 = z^2, \tag{30}$$

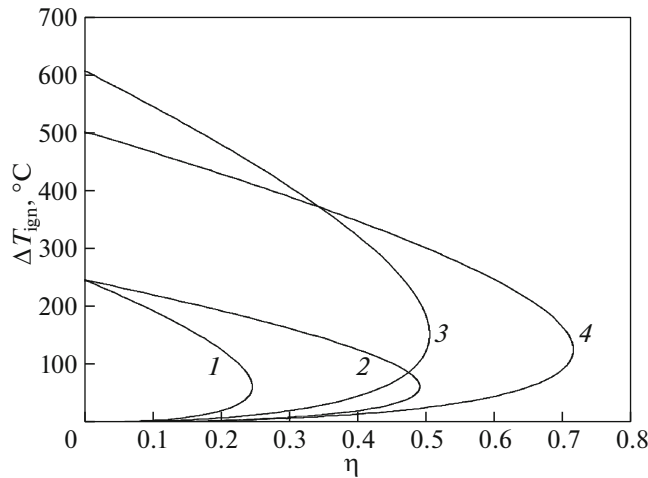


Fig. 3. Dependences of ΔT_{ign} on parameter η for the same combinations of experimental values of (D, p) . The notation of the curves is the same as in Fig. 2.

where

$$z = \frac{1}{2}(\gamma/\eta)^{1/2} D + \sqrt{\frac{\gamma D^2}{4\eta} - p}. \quad (31)$$

It can be seen from Fig. 3 that the increase in the temperature of particles on the upper branches of the curves due to mutual friction in the compaction wave can attain high values comparable with the ignition temperature for real powders. According to experimental data [8–13], mechanical activation substantially reduces the ignition temperature of powder mixtures. For example, the ignition of a conventional Al/MoO₃ mixture occurs at a temperature exceeding 600°C (which is close to the melting point of Al), while ignition of a mechanically activated Al/MoO₃ mixture occurs in air as a flash during contact with the heated surface at a temperature from 240 to 300°C (depending on the type of Al particles and activation dose). With a glance at Fig. 3, it is clear why the same powder mixture after mechanical activation is capable of detonation, while in the absence of mechanical activation, only its burning without a transition to detonation is observed.

In accordance with relation (24), characteristic detonation velocity D_0 is a monotonically increasing function of ΔT_{ign} . After mechanical activation, the ignition temperature of particles decreases, as well as characteristic detonation velocity D_0 . At the same time, according to the results from [8–13], the detonation velocity increases as a result of mechanical activation. In accordance with relation (20), the detonation velocity increases with pressure behind the detonation front; therefore, the increase in pressure in detonation products due to mechanical activation obviously “overrides” the decrease in D_0 associated with mechanical activation of the

powder increases its chemical activity (due to an increase in the specific contact surface of reagents as well as due to crystal structure defects of the oxidizer), which leads to an increase in the mass velocity of particle burning per unit mass; this in turn leads to an increase in pressure behind the detonation front.

Relation (13) makes it possible to explain why detonation according to this mechanism is impossible in high-density powders. At a preset ignition temperature of powder particles, we can determine the minimal degree of compaction of the powder in the compaction wave, at which this temperature can be attained:

$$\left(\frac{\rho_0}{\rho_{\text{ign}}}\right)_{\text{max}} = 1 - \frac{1}{D} \left(\frac{2c_p \Delta T_{\text{ign}}}{\beta}\right)^{1/2}.$$

Assuming that the relative density of the powder in the compaction wave attains values $\rho_{\text{ign}} < \rho_{\text{max}} \approx 0.5$, we can find the maximal initial density of the powder, at which detonation of low-density powder mixture is possible:

$$\rho_{0 \text{ max}} = \rho_{\text{max}} \left[1 - \frac{1}{D} \left(\frac{2c_p \Delta T_{\text{ign}}}{\beta}\right)^{1/2} \right].$$

For initial powder density $\rho_0 > \rho_{0 \text{ max}}$, detonation is ruled out. In this case, velocity D is either equal to the detonation velocity, or to the velocity of the compaction wave produced by the initial (initiating) pulse. For example, for $D = 1500$ m/s, $c_p = 0.8$ kJ/(kg K), $\Delta T_{\text{ign}} = 250^\circ\text{C}$, $\rho_{\text{max}} \approx 0.5$, and $\beta = 2$, we obtain $\rho_{0 \text{ max}} = 0.35$, which is in conformity with experimental data [8–13].

CONCLUSIONS

The process of fast propagation of a chemical reaction in low-density mechanically activated powdered mixtures, which was experimentally investigated in [8–13], exhibits all features of detonation and should be acknowledged as a variety of detonation: abrupt compaction of the powder occurs due to high pressure of intermediate gaseous combustion products; the compaction zone moves in space at a velocity exceeding the speed of sound in the initial powder. Upon fast compression of the powder in the compaction wave, powder particles are regrouped due to their mutual displacement without noticeable deformation of particles, which is accompanied by intense friction of contacting particles. As a result of friction, individual particles can be heated to high temperature at which their ignition (thermal explosion) occurs at the contact surface of reagents, followed by intense combustion. The formation of high-temperature gaseous combustion products as a result of rapid burning of powder particles sustains a high pressure behind the compaction front, compensating the pressure drop due to gas outflow to the surrounding medium. This ensures continuous propagation of the detonation wave over the powder.

The basic difference between a detonation wave in low-density powder mixtures and a detonation wave in gases, liquids, and continuous solid explosives lies in the mechanism of initiation of chemical reactions in the compaction wave: the increase in the temperature of the medium required for the initiation and acceleration of chemical reactions during classical detonation occurs due to adiabatic compression of the medium in a shock wave, while in low-density powders, this occurs due to friction between particles in the course of their mutual displacement in the compaction wave.

As mentioned above, detonation in mechanically activated low-density powder mixtures can be realized only in a very narrow range of control parameters (initial density of the powder mixture and chemical activity of powder particles). The chemical activity of a powder as a complex criterion includes the ignition temperature of powder particles and the rate of formation of intermediate gas-phase combustion products of the powder (mass of the gas released per unit time per unit mass of the powder). This activity can be increased by using nanopowders as well as due to preliminary mechanical activation of the powder.

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