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Control of hydrogen-air mixture detonation processes by adding microdispersed aluminum particles

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The results of numerical modeling of cellular detonation of hydrogen-air mixtures with additives of dispersed micron-sized aluminum particles are presented. The effect of particle size and loading on the process characteristics is established. The variety of cellular detonation forms is shown: with a regular and irregular cell, with oblique cells and an inclined front, depending on the distribution of particles in space. The development of combined instability with a layered distribution of particles is demonstrated. The obtained results allow us to consider additives of aluminum particles as a control factor for the implementation of different detonation modes in hydrogen-containing hybrid mixtures.

Keywords: Detonation, gas suspensions, hydrogen-air mixture, aluminum particles, numerical modeling.

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The addition of finely dispersed aluminum powders is of interest in the context of accelerating the process of ignition and enhancing the heat of combustion of fuel mixtures. The potential for a significant increase in detonation velocity of hydrogen-oxygen and hydrogen-air mixtures with aluminum particles was noted in experiments [1,2], where two-front structures were also observed. The influence of particle size distribution and loading on the characteristics of cellular hybrid detonation was investigated experimentally in [3], and a relation between the detonation velocity and the cell size was established. Aluminum particles provide ample opportunities for flow control via the adjustment of their size distribution (since the combustion time depends on the particle size), fractional composition, and distribution of particle clouds in space. A physicomathematical model and certain calculated data for detonation in dilute hydrogen-oxygen and hydrogen-air suspensions of aluminum particles with a low loading factor and a homogeneous composition were discussed in [4–6]. In the present study, we use an extended model that incorporates the reaction of aluminum with water vapor and is applicable to mixtures with fairly high loading factors (up to $500\,g/m^3$) and a non-uniform spatial distribution of aluminum particles. The aim is to evaluate the factors controlling the detonation process: the influence of particle loading and spatial and size distributions of particles on the qualitative properties of cellular detonation of hybrid mixtures.

The object under study is a planar channel with a gas mixture of the $2\varphi H_2 + O_2 + 3.82N_2$ type in which a certain cloud of aluminum particles is dispersed. This cloud may occupy the entire space or only a certain fraction of the channel cross section. The distribution of particles in a cloud may be either uniform or non-uniform. The scenarios with a transverse gradient or discontinuity of the average particle density are considered. Detonation and development of transverse waves are triggered by the rupture of an inclined diaphragm separating the high-pressure chamber. The steady-state cellular detonation mode after weakening of the initiated over-compressed wave by rarefaction waves is analyzed.

The physicomathematical model is an extension of the model presented in [4]. The flow of a two-phase mixture is characterized using the methods of mechanics of heterogeneous media. Gas and two discrete components (aluminum particles and forming nanosized particles of aluminum oxide) are taken into consideration. Hydrogen, oxygen, nitrogen, water vapor, and a mixture of gaseous products of aluminum combustion (dominated by AlO, Al_2O, and AlOH), which is regarded as a single component, are taken into account in the gas phase. The combustion of a hydrogen-air mixture is characterized within the reduced kinetics model [7]. Although the single-stage model [7] is quite simple, it provides close agreement with experimental data on ignition delays, detonation velocities, and detonation cell sizes in stoichiometric hydrogen-oxygen and hydrogen-air mixtures diluted with argon. This model has been applied successfully to a number of problems [8,9]. We have introduced a correction for hydrogen-poor mixtures: the integral heat release depends linearly on the fuel excess coefficient: $Q_1 = -0.19 + 0.06\varphi$ [MJ/mol], $0.4 \leqslant \varphi \leqslant 1$ [5]. This approximation ensures compliance with the experimental dependence [10] of the detonation velocity on φ. The combustion of aluminum is characterized by Arrhenius-type reduced kinetics equations. It is assumed that the interaction of aluminum with oxygen results in the formation of either condensed aluminum oxide nanoparticles (below the boiling point of aluminum, which depends on pressure) or gaseous suboxides. The stoichiometric coefficients of

heterogeneous and homogeneous reactions of interaction with oxygen correspond to relations $2Al + 1.5O_2 \rightarrow Al_2O_3$ and $2Al + O_2 \rightarrow 2AlO$, respectively. The condition for transition from a heterogeneous reaction to a homogeneous one has the form of the pressure dependence of the boiling point of aluminum (T_{2b}): $T_2 = T_{2b} = 2960p^{0.087}$, where T_2 [K] and p [atm] are the aluminum particle temperature and the gas pressure [11]. The heat of aluminum combustion in a hydrogen-air medium was set to $Q_{23} = 15$ MJ/kg and $Q_{21} = 4.5$ MJ/kg for the formation of aluminum oxide particles and gaseous suboxides, respectively [5]. The interaction with water vapor ($Al + H_2O \rightarrow AlOH + H$) results in the formation of gaseous products; the heat of this reaction is $Q_{22} = 4$ MJ/kg. The calculated dependences of the detonation velocity on particle concentration fall within the interval between the experimental data [3] for $\varphi = 0.87$ and the data of thermodynamic calculations for $0.4 < \varphi < 1$ performed using a computer program [12]. The calculated patterns of cellular detonation in gas and hybrid mixtures with $\varphi = 0.87$ [5] are also a close match to the experimental ones [3].

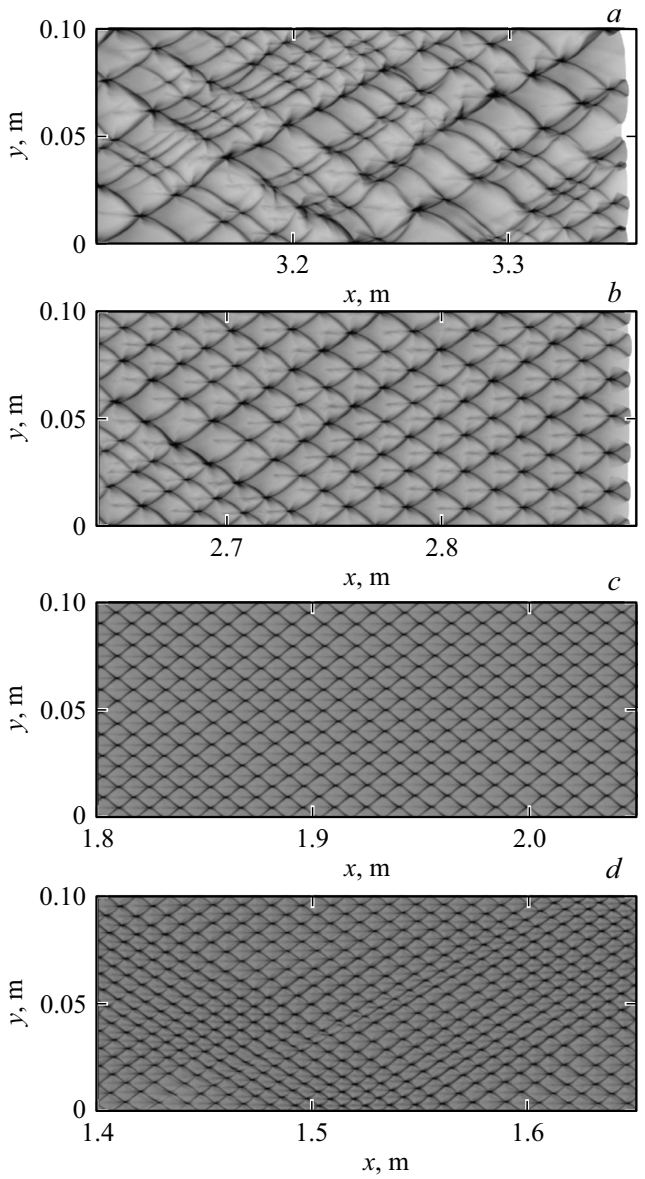

Figure 1. Triple point patterns of gas (a) and hybrid (b–d) detonation at $\varphi = 0.6$, $d = 1\,\mu$m. $\rho_{20} = 10$ (b), 50 (c) and 100 g/m^3 (d).

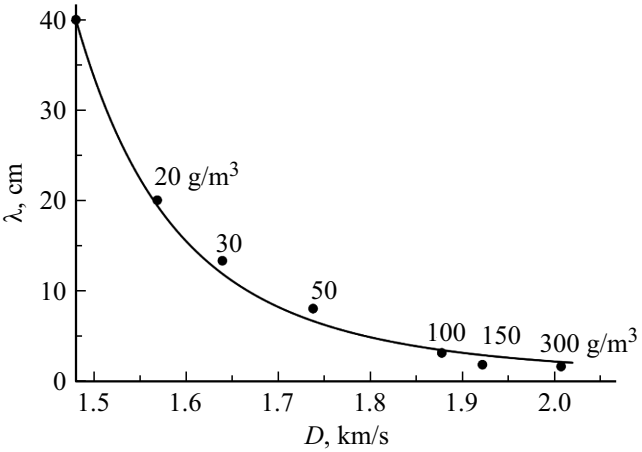

Figure 2. Dependence of detonation velocity and cell size on particle loading in a hybrid mixture with $\varphi = 0.4$. The solid curve represents the approximation dependence [3].

Lean hydrogen-air mixtures ($\varphi = 0.6,\ 0.4$) with their detonation characterized by an irregular cell are examined. In the mixture with $\varphi = 0.6$, the addition of even a small amount (10 g/m^3) of aluminum particles 1 μm in diameter ensures flow stabilization and regularization of the cellular structure (Fig. 1, $p_{\max}(x, y) = \max_t p(x, y, t)$ parameter fields). In the case of gas detonation, the cellular structure is irregular (Fig. 1, a). With an increase in particle loading, the detonation velocity increases, the cell shrinks in size, and the distance (and time) of formation of a homogeneous regular structure is shortened from 2.8 m at 10 g/m^3 (Fig. 1, b) to 1.8 m at 50 g/m^3 (Fig. 1, c). At a loading of 100 g/m^3, a slightly heterogeneous structure with fine cells forms within 1.4 m and remains unchanged afterward (Fig. 1, d).

The data on steady-state detonation velocity and cell size for the mixture with $\varphi = 0.4$ and different particle loading factors are presented in Fig. 2. In a gas mixture, detonation is characterized by a large cell (approximately 40 cm [13]); a structure with one transverse wave forms in calculations in a 20 cm channel (Fig. 3, a). The detonation velocity increases noticeably following the addition of 50–100 g/m^3 of aluminum particles; after that, the dependence curve flattens out and reaches a „plateau“The relation between the detonation velocity (D) and the cell size (λ) corresponds to the following functional dependence given in [3]: $\lambda = \lambda_0 \delta \exp[E/RT_{\mathrm{ZND}}(\delta^{-2} - 1)]$, $\delta = D/D_0$, where λ_0, D_0 are the detonation cell size and the detonation velocity for a gas mixture and T_{ZND} is the gas temperature at the Chapman–Jouguet point of gas detonation; $E/RT_{\mathrm{ZND}} = 7.1$ was determined for $\varphi = 0.4$ (solid curve in Fig. 2).

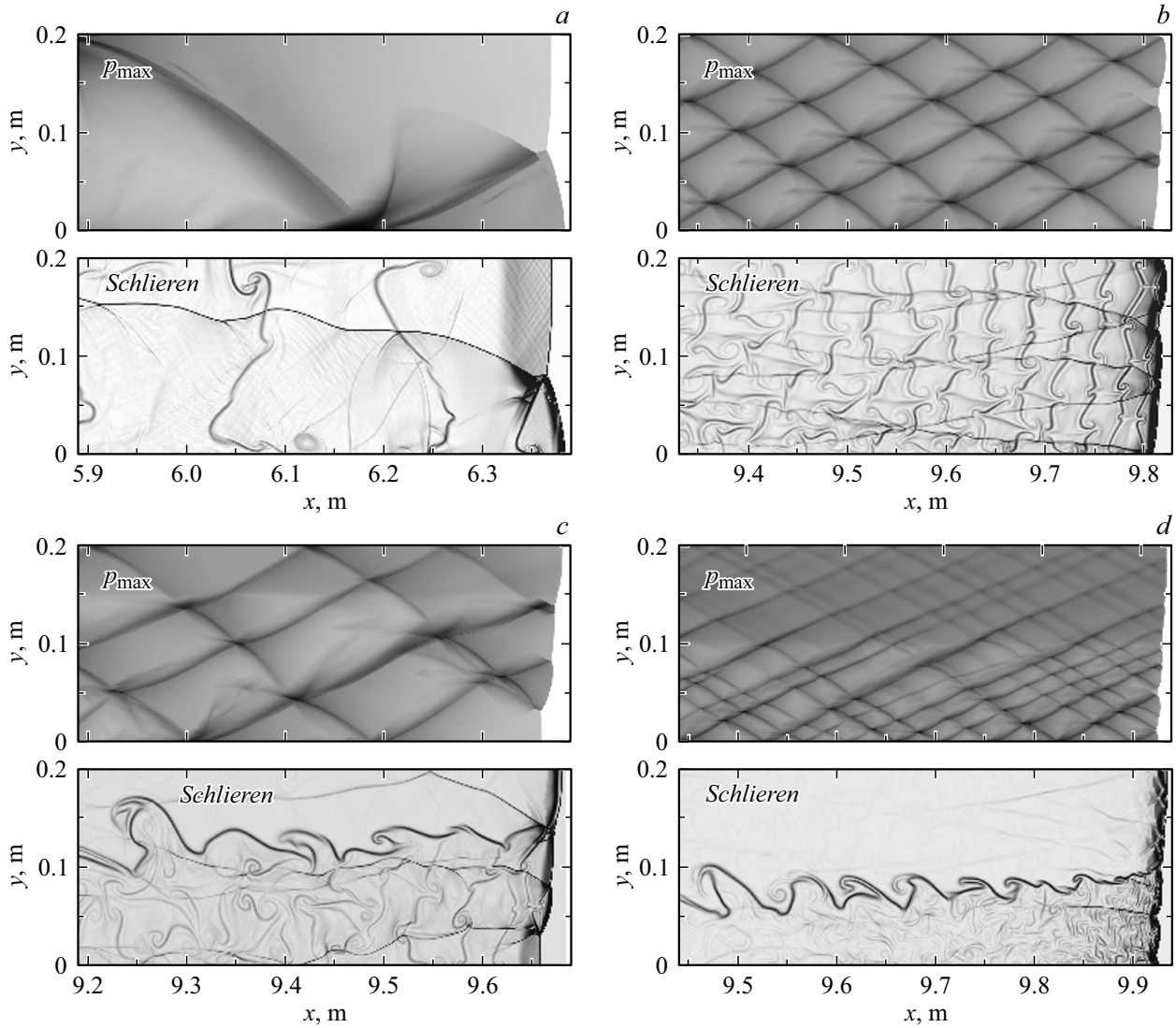

Figure 3. Patterns of cellular detonation in a gas mixture with $\varphi = 0.4$ (a) and in a mixture with a gradient particle distribution: $\rho_{2bot} = 0$, $\rho_{2top} = 100\,\mathrm{g/m^3}$ (b); with layered particle loading ($\rho_{20} = 300\,\mathrm{g/m^3}$) at $h/H = 0.25$ (c) and 0.5 (d).

The influence of heterogeneity of a particle cloud was analyzed by examining the following two types of particle distribution in a planar channel: with a gradient of average density from the bottom to the top (with the particle density varying gradually from ρ_{2bot} in the bottom part of the channel to ρ_{2top} at the top wall) and with a density discontinuity (layered distribution). The most significant deviations from a uniform distribution of particles are seen at concentrations ranging from $\rho_{2bot} = 0$ to $\rho_{2top} = 100\,\mathrm{g/m^3}$. With a gradient distribution, oblique cells with an inclined leading front (Fig. 3, b), which are similar to the patterns of heterogeneous detonation with a transverse concentration gradient [14], are formed.

With a layered distribution of particles, various cellular structures may form depending on the loading factor and the relative layer height. Examples for a lean hydrogen-air mixture with a high particle loading factor and different heights of the layer (adjacent to the top wall of a 20 cm channel) are presented in Figs. 3, c, d. Two oblique cells are formed at $h/H = 0.25$ (Fig. 3, c), and an irregular structure with cells of different sizes (larger at the bottom and smaller at the top) emerges at $h/H = 0.5$ (Fig. 3, d). As can be seen from Fig. 3, d, transverse waves in the top part of the channel are „blurred,“, which is indicative of their reduced intensity and dispersed nature. Having analyzed the pressure profiles on the top wall at different moments in time in the mixture with aluminum particle loading $\rho_{20} = 300\,\mathrm{g/m^3}$, we noted a reduction in the amplitude of oscillations relative to the mixture with particle loading $\rho_{20} = 100\,\mathrm{g/m^3}$. A similar phenomenon of cell „degeneration“ was reported and substantiated in [15] via acoustic analysis of the structure of heterogeneous detonation in bidispersed suspensions of aluminum particles. Figures 3, c and d also make it clear that an instability developing at the boundary of the gas suspension layer is a combination of Kelvin–Helmholtz (due to the difference in flow velocities

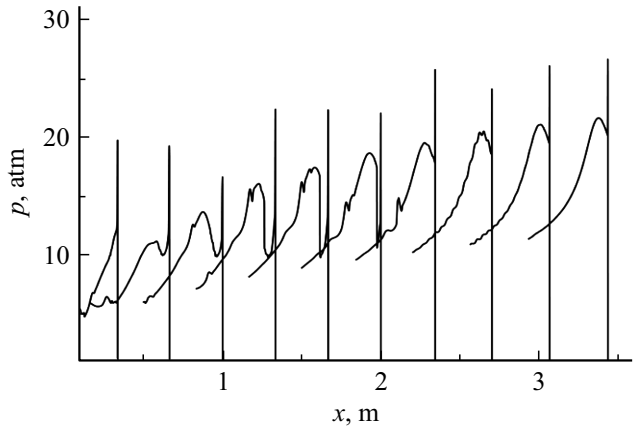

Figure 4. Scenario of intermediate formation of two-front configurations in a hybrid mixture with $\varphi = 0.6$, $d = 5\,\mu$m. Pressure profiles in 0.2 ms steps.

behind the front in gas and the gas suspension) and Richtmyer–Meshkov (due to the influence of transverse waves on the layer surface) instabilities.

As in [4], the steady-state structures and velocities of detonation were affected only slightly when the particle size was varied within the range of $1-5\,\mu$m. However, as in hydrogen–oxygen–argon mixtures, the formation scenarios include two-front configurations that persist for a limited time, eventually merging into a standard structure with one leading front and a system of transverse waves. An example of such a scenario is shown in Fig. 4, where a two-front structure is seen in three profiles within the 1.25–2 m interval. It is evident that the distance between the leading and secondary fronts becomes shorter. When the fronts merge, the propagation velocity and pressures increase sharply at the chemical peak (the point of maximum energy release in the chemical reaction, as evidenced by an increase in pressure at $x > 2.3$ m in Fig. 4).

Thus, the variation of cellular detonation patterns in a mixture of reacting gases (hydrogen-air mixture) and reacting particles (finely dispersed aluminum particles) with composition of this mixture, particle loading, and spatial distribution of particles was demonstrated. The obtained data suggest that the addition of aluminum particles to hydrogen-oxygen and hydrogen-air gas mixtures is a possible means of controlling the characteristics of detonation.

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Conflict of interest

The authors declare that they have no conflict of interest.

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