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The effect of adding nanodispersed aluminum particles on characteristics of detonation of hydrogen-air mixtures

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The results of two-dimensional numerical simulation of detonation of poor hydrogen-air gases mixtures with additives of aluminum particles with a diameter of 150−300 nm are presented. The influence of particles on the character of cellular detonation (cells become regular) and cell size (significantly decreases with increasing load). The influence of particles on the detonation velocity was determined: in the range of the fuel equivalent ratio 0.6−1 speed increase can be up to 15%.

Keywords: detonation, numerical methods, hydrogen-air mixture, hybrid detonation.

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First of all study of detonation processes of fine dust of metals and non-metals relates to processes of explosion and fire safety. Explosions of dust clouds can result in damages in buildings and facilities, and to fatalities [1]. From other side, the fine powders of metals and non-metals can be used as additives to fuel to control the combustion processes and to improve the pulse and energy characteristics.

The experiments [2] stated the detonation velocity increasing upon presence of aluminium particles in mixtures of reacting gases, and double pressure jumps were also observed. Studies of the hybrid detonation were executed theoretically [3,4] and experimentally [5]. In [3,4] models were developed, they described double-front structures of detonation progress, in [5] the effect of reacting particles on the structure of detonation flow was studied, including the cellular detonation. In [6,7] the processes of the hybrid detonation in hydrogen-oxygen diluted by argon were studied under the physical and mathematical model of continuum mechanics and using equations of reduced kinetics. All previous theoretical studies of the hybrid detonation were limited to particles of micron size. Submicron and nanodisperse suspensions are of interest due to the aluminium particles combustion transition, when their size decreases, from diffusion-limited mode to the kinetic mode [8]. During heterogeneous detonation this was observed in the increase in degree of irregularity and size of the detonation cell at particles size of abut 100 nm [9]. In present paper we discuss the poor hydrogen-air mixtures with additives of aluminium particles 150−300 nm in diameter. The study objective is analysis of particles influence on speed and structure of the detonation wave for mixtures with different ratio of oxidizing agent and fuel.

A flat channel is considered, it is filled with premixed mixture of hydrogen, air and dispersed aluminum particles. The high pressure chamber filled with the combustion products (water vapors and air) is used to initiate the detonation. Quick development of the transverse waves is ensured by small inclination of the separating diaphragm. The chamber parameters are selected such that after the diaphragm rapture in gas a slightly overcompressed detonation is formed, it transits to the self-sustaining mode with the cellular structures formation. The combustible gaseous mixtures with fuel equivalent ratio (by hydrogen) $\varphi = 0.6-0.9$ were considered, the dust density of aluminum particles ρ_{20} varied from 10 to 150 g/m^3.

The physical and mathematical model and its parameters, numerical technology and model testing are described in [6,7]. The model of aluminium combustion is used [9,10] with equation of reduced kinetics of Arrhenius type. Applied to the hybrid detonation, it is expected that during the particle combustion either condensed nanoparticles of aluminium oxide at temperature close below 3500 K, or gaseous combustion products at temperature above 3500 K are formed. Combustion of the hydrogen-air mixture is described under frames of model of reduced kinetics [11], tested in detonation suppression problems in [12,13]. For the stoichiometric hydrogen-air mixtures in [13] we accepted $Q_{\mathrm{H}ox0} = -0.13$ MJ/mol — energy release during the gas mixture combustion. Corrections for hydrogen poor compositions are determined by us as $Q_{\mathrm{H}ox} = -0.19 + 0.06\varphi$ MJ/mol, which ensures correspondence of the experimental dependence of the detonation velocity on fuel equivalent ratio [14] in range $0.4 \leqslant \varphi \leqslant 1$. The thermal effects of aluminium combustion are taken as follows: during formation of aluminium oxide particles $Q_{\mathrm{Al}} = 15$ MJ/kg, during formation of gaseous suboxides $Q_{2\mathrm{Al}ox} = 4.5$ MJ/kg ($Q_{\mathrm{Al}ox} = \mu_{\mathrm{Al}}(Q_{\mathrm{Al}} - Q_{2\mathrm{Al}ox})/\mu_{\mathrm{Al}ox} = 9.34$ MJ/kg, respectively, where μ_{Al}, $\mu_{\mathrm{Al}ox}$ — molecular mass of aluminium and its suboxides).

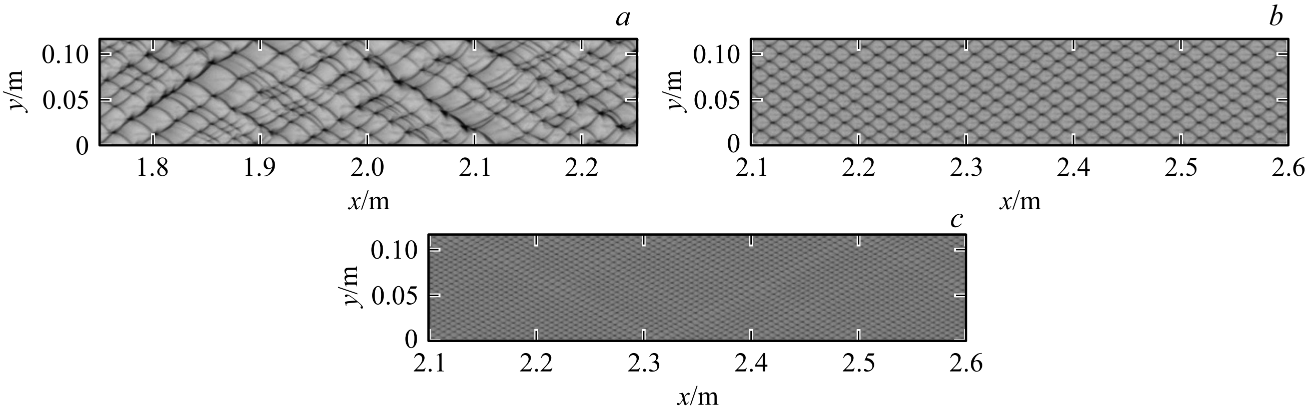

Figure 1. Patterns of triple points of gas detonation (a), hybrid detonation ($d = 300$ nm) for $\rho_{20} = 20$ (b) and $100\,\mathrm{g/m^3}$ (c).

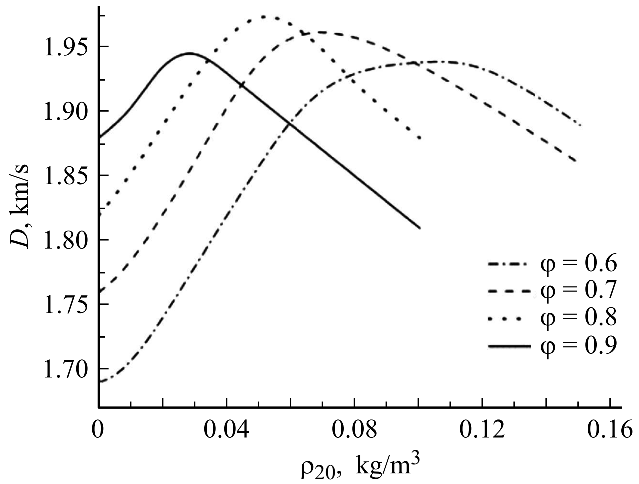

Figure 2. Leading front velocity vs. dust density of aluminium particles with diameter $d_{20} = 300$ nm.

The calculation results for the combustion mixture with $\varphi = 0.7$ at different values of dust density of particles ρ_{20} are given in Fig. 1. As can be seen the pure gas detonation (Fig. 1, a) is characterized by moderate cellular structure, where average cell size is 1–2 cm (five-six cells per channel width). If even small dust density $\rho_{20} = 20\,\mathrm{g/m^3}$ is added (Fig. 1, b) the cellular structure regularization occurs with seven uniform cells per channel width. Increasing ρ_{20} to $100\,\mathrm{g/m^3}$ results in increase in number of regular cells to 19 (Fig. 1, c). Note that at the same time the pressure decreases in triple spots (to ~ 100 atm), which is significantly less than during gaseous detonation (where it can reach 200 atm) (Fig. 1, a). Note also that in nanodisperse hybrid mixtures the double-front structures, observed in calculations with particles with diameter over $3.5\,\mu$m, are not observed. This can be associated with the abrupt decrease in time of speed and thermal relaxation as compared with such for similar processes in gas suspensions of micron-sized particles, as result the particles ignite already in combustion zone of gas mixture, which state did not reach the Chapman–Jouguet equilibrium. However, at the same time, submicron particles ensure stabilization of the cellular structure and acceleration of leading detonation front propagation.

Influence of particles addition on the detonation velocity is shown in Fig. 2, where speed of leading front vs. ρ_{20} is shown for particles 300 nm in diameter at different values of fuel equivalent ratio φ. All dependences have clearly visible maximum, i.e. for each φ there is optimal concentration of particles. Further increase in particles concentration decreases the detonation velocity, which is associated with lack of oxygen to ensure combustion of aluminium (aluminium interaction with water vapors in model is not considered). Besides, the optimal concentration decreases with stoichiometry approaching: if for $\varphi = 0.6$ speed maximum was observed at $\rho_{20} = 100–120\,\mathrm{g/m^3}$, than at $\varphi = 0.9$ the maximum was reached at $\rho_{20} = 30\,\mathrm{g/m^3}$. The maximum detonation velocity is achieved at $\varphi = 0.8$ and $\rho_{20} = 50\,\mathrm{g/m^3}$, i.e. there is also optimal value of fuel equivalent ratio φ. So, during hybrid detonation the fuel equivalent ratio and dust density of particles are the control parameters.

Effect influence of particles size on the patterns of developed cellular hybrid detonation is shown in Fig. 3 for $\rho_{20} = 50\,\mathrm{g/m^3}$. Here we see, that decrease by two times in particles size (from 300 to 150 nm) does not result in any qualitative changes: one can see only insignificant increase in cell size due to change in combustion kinetics of aluminium. Wave speed vs. density of particles 150 nm in diameter qualitatively coincide with the results shown in Fig. 2.

So, it was identified that addition of insignificant mass of submicron aluminium particles to the combustible gas mixture ensures stabilization of flow and regularization of cells, and can result in increase in the detonation velocity at $\varphi = 0.6$ by 15% (from 1.7 to 1.94 km/s). The effect is less visible in mixtures with large fuel equivalent ratio. Besides, in the considered suspensions of submicron particles no double-front modes are formed, which are typical for

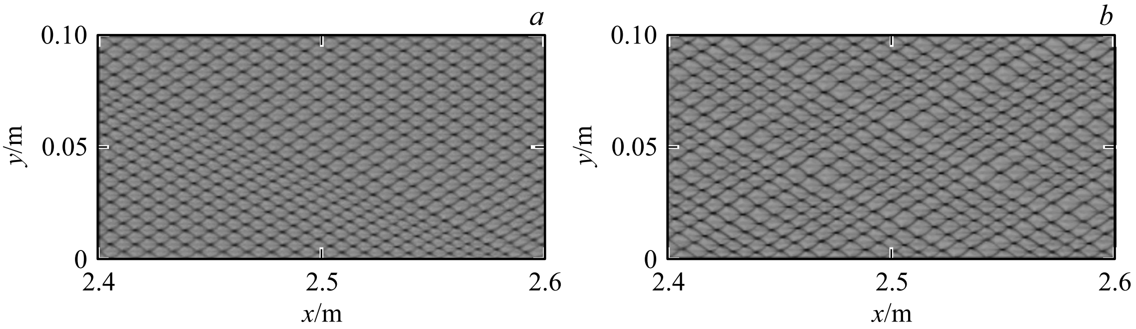

Figure 3. Patterns of triple points of stable hybrid detonation for $\rho_{20} = 50\,\mathrm{g/m^3}$. $d = 300$ (a) and 150 nm (b).

the hybrid mixtures with micron particles over $3.5\,\mu$m in diameter.

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Conflict of interest

The authors declare that they have no conflict of interest.

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