Problems of Detonation Wave Suppression in Hydrogen-Air Mixtures by Clouds of Inert Particles in One- and Two-dimensional Formulation

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1 Introduction

It is known that detonation waves in gas and heterogeneous combustible mixtures have a cellular structure [1-2]. It has also been established that the addition of inert particles to an explosive mixture contributes to the suppression of detonation [3-9]. The interaction between detonation waves and inert particles have been studied mainly in one dimension, resulting in estimates of the effect of volume concentration, particle diameter, and their thermophysical properties on the ability to attenuate and suppress detonation. However, the nonuniform structure of the detonation cell undoubtedly influences the parameters of mixtures of explosive gases with chemically inert particles and the limiting detonation characteristics. It can be noted that the interaction of cellular detonation waves in gases and mixtures of gas with inert particles has been the subject of a few studies, e.g., [4, 10]. Thus, it is of both theoretical and practical interest to investigate the critical detonation-wave parameters in mixtures of combustible gases and inert particles and compare results of one- and two-dimensional calculations.

2 Physical and mathematical formulation of the problem

Let's consider a shock tube filled with the mixture of hydrogen and air at atmospheric conditions ($p_0 = 1$ atm, $T_0 = 296\,\mathrm{K}$). Plane (in one-dimensional formulation) and cellular (in two-dimensional formulation) detonation wave (DW) was used as the initial data and located at the left boundary of shock tube. At some distance from the detonation wave the semi-infinite cloud of inert particles (Al_2O_3) is located. After the start of the calculation, the detonation wave moved from left to right and was attenuated by the particles. Mathematical model of the mechanics of the reacting gas mixtures and inert particles represents the system of equations of the dynamics of the gas mixture and solid particles and has the form shown in [6, 10]. To describe the chemical reactions in hydrogen-air mixture we will use the reduced kinetic model [11]. In [11], this kinetic scheme was verified by experimental data on the ignition delay time and the velocity of propagation of the detonation wave under various conditions. In [12], the model

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of reduced chemical kinetics was verified by the size of the detonation cell and the modes of oblique detonation waves.

In the calculations, a computational grid was used, which dynamically adapted on the density gradient to the gas-dynamic features of the flow. An implicit second-order scheme was used as an approximation in time. For approximation of convective terms in space the following methods were used: in 1-D formulation – van Leer flux-vector splitting and third order TVD scheme; in 2-D formulation – AUSM flux-vector splitting and the second-order backflow scheme.

3 Results of calculations of the interaction of a detonation wave with a cloud of inert particles. One-dimensional analysis

First of all, let's consider the interaction of a one-dimensional detonation wave with a semi-infinite cloud of inert particles. In this case, the cloud boundary was located in the coordinate $x = 1$ m. Fig 1 shows the pressure distribution at different times along the channel length (a) and the velocity of the detonation wave over time (b) for particles with a diameter of $d = 10^{-4}$ m and a volume concentration $m_2 = 10^{-4}$. It can be seen that after entering in the particles cloud the detonation wave attenuates and its further propagation through the cloud of particles occurs at stationary attenuated mode. When the particle diameter decreases to $d = 10^{-6}$ m at the same volume concentration, it leads to a strong development of its one-dimensional instability of detonation wave (Fig. 2, a). This leads to a significant irregularity of the detonation wave velocity (Fig. 2, b). In this case, we have a precritical mode of detonation propagation. With an increase in the volume concentration of particles with a diameter of $d = 10^{-4}$ m to $m_2 = 5 \cdot 10^{-4}$, a critical regime is observed — the detonation process is failed (Fig. 3). In this case, the detonation wave splits into a frozen shock wave and the front of ignition and combustion lagging behind it.

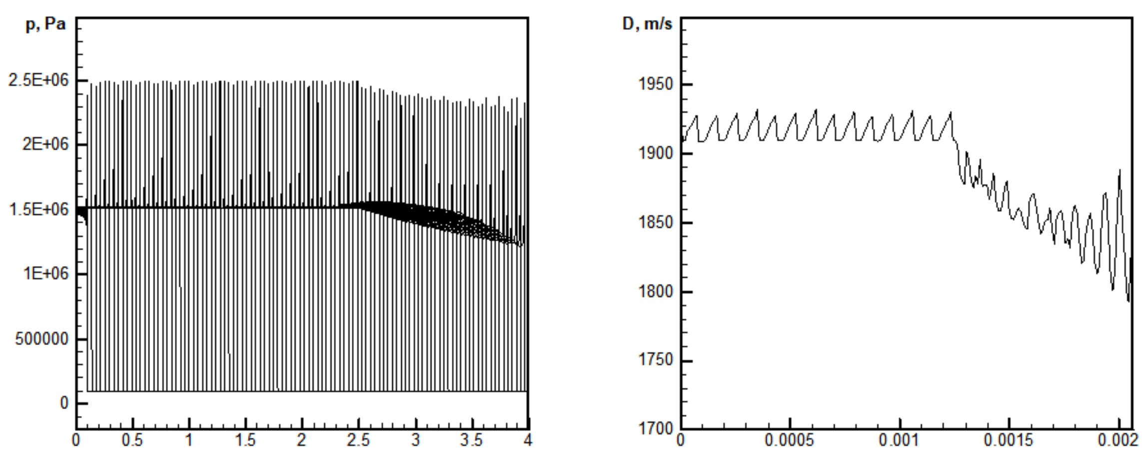

Figure 1. Left: (a) Pressure distributions at different points in time along the length of the channel, right: (b) the velocity of the detonation wave against time. $d = 10^{-4}$ m, $m_2 = 10^{-4}$.

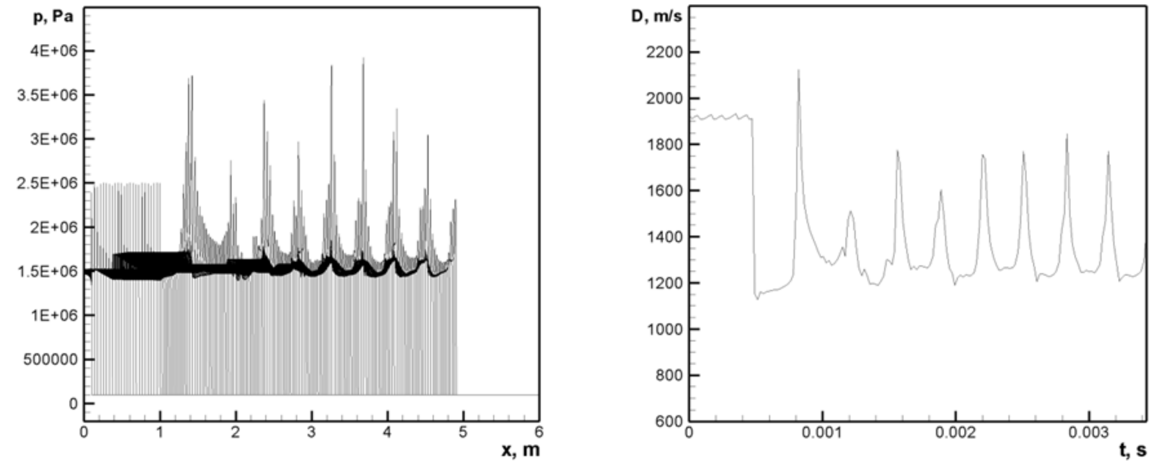

Figure 2. Left: (a) Pressure distributions at different points in time along the length of the channel, right: (b) the velocity of the detonation wave against time. $d = 10^{-6}$ m, $m_2 = 10^{-4}$.

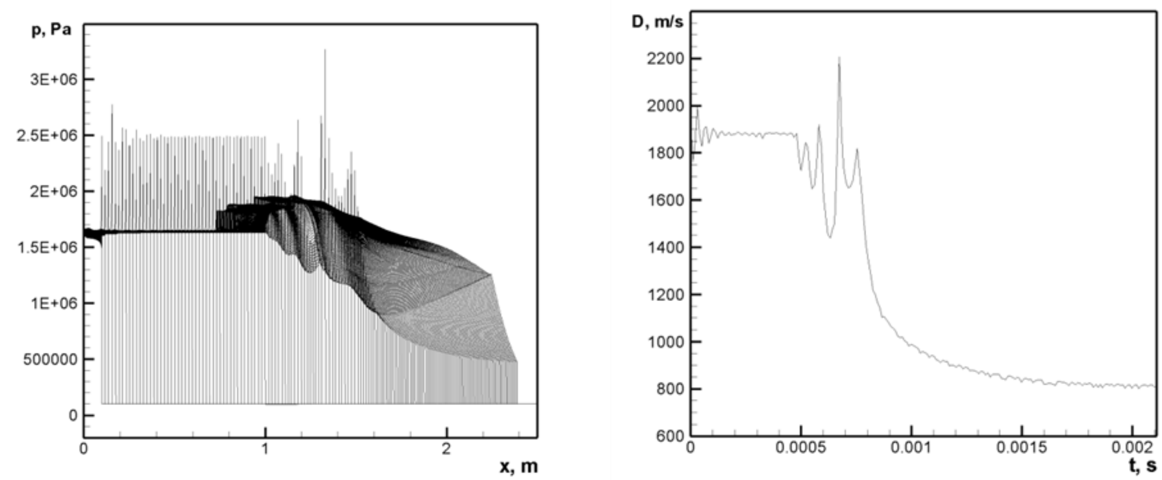

Figure 3. Left: (a) Pressure distributions at different points in time along the length of the channel, right: (b) the velocity of the detonation wave against time. $d = 10^{-4}$ m, $m_2 = 5 \cdot 10^{-4}$.

4 Results of calculations of the interaction of a detonation wave with a cloud of inert particles. Two-dimensional analysis

Let's now consider the problem of the interaction of a cellular detonation wave with a cloud of inert relaxing particles. The left boundary of the cloud was located at the point $x = 0.2$ m. Fig. 4 shows the maximum pressure field over time for a volume concentration $m_2 = 10^{-4}$ of $d = 10^{-4}$ m particles. For this concentration, there is no significant change in the structure of the cellular wave. The number of cells is preserved along the entire length of the cloud. The normalized detonation wave velocity for these conditions equals to $\eta = \dfrac{D}{D_{CJ}} = 0.97$. Here, D is detonation wave velocity in gas suspension, D_{CJ} is detonation wave velocity in pure gas mixture without particles.

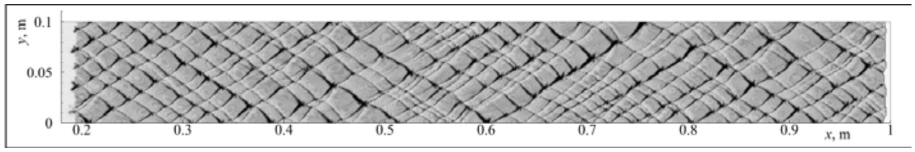

Figure 4. The maximum pressure field in time. $d = 10^{-4}$ m, $m_2 = 10^{-4}$.

Decreasing the diameter of the particles leads to the enlargement of the detonation cell. Fig. 5 shows the maximum pressure fields in time when a detonation wave interacts with a cloud of 1 μm particles with volume concentration $m_2 = 10^{-4}$. The figure allows to see the structure of cellular detonation and a gradual increase in the cell as the detonation wave passes through the cloud. In the cross section of the channel up to $x = 0.6$ m, restructuring and enlargement of the cell is observed, and in the future, one and half cells fit the width of the channel. The normalized detonation wave velocity is $\eta = 0.71$. It should be noted that for a given volume concentration of the particles decreasing of the diameter do not leads to a detonation quenching.

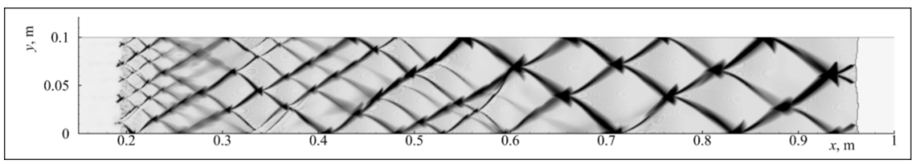

Figure 5. The maximum pressure field in time. $d = 10^{-6}$ m, $m_2 = 10^{-4}$.

An increase in the volume concentration of particles by an order of magnitude makes it possible to achieve detonation failure already for particles with a diameter of 10 μm. Fig. 6 shows the dynamics of detonation failure for this case. It can be seen from the figure that already at a distance of just over 0.1 m from the boundary of the cloud of particles, the detonation wave splits into a frozen shock wave and the front of ignition and combustion lagging behind it.

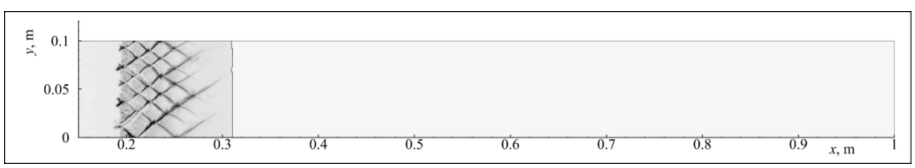

Figure 6. The maximum pressure field in time. $d = 10^{-5}$ m, $m_2 = 10^{-3}$.

5 Results of calculations of the interaction of a detonation wave with a cloud of inert particles. Comparison of one-dimensional and two-dimensional formulation.

Fig. 7 shows the dependences of the normalized detonation velocity on the particle diameter for both one-dimensional and two-dimensional calculations. Comparison of one-dimensional and two-dimensional approaches showed a quantitative similarity of the integral dependences of the normalized velocity and the correspondence of the values of volume concentration and particle diameters at which detonation failure is occurs. On the limiting modes of interaction in the one-dimensional and two-dimensional approaches, a different behavior of the passing detonation wave is observed. In the one-dimensional case, when approaching the critical volume concentration of particles, leading to detonation failure, a galloping detonation mode is observed. In the case of the interaction of a cellular detonation wave with inert particles with an increase in the volume concentration of particles, the detonation cell is enlarged, and then detonation failure is observed. In this case the galloping detonation was not obtained. In general, it can be noted that estimates of the limiting concentrations and particle diameters necessary for detonation failure, obtained in a one-dimensional formulation, can be applied in practice.

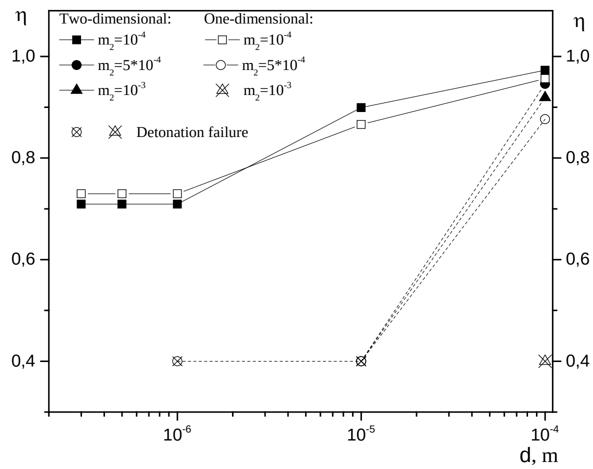

Figure 7. The dependences of the normalized detonation velocity on the particle diameter for both one-dimensional and two-dimensional calculations.

6 Conclusions

The interaction of a plane (one-dimensional) and cellular (two-dimensional) detonation wave with a semi-infinite cloud of inert particles was calculated. The integral dependences of the normalized detonation wave velocity for various volume concentrations and particle diameters were calculated. Volume concentrations and corresponding particle diameters, resulting to detonation wave failure in a hydrogen-air mixture were obtained. Comparison of one-dimensional and two-dimensional approaches showed a quantitative similarity of the integral dependences of the normalized detonation velocity and the correspondence of the values of volume concentration and particle diameters at which detonation failure is occurs.

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