Investigation of the heterogeneous detonation suppression by clouds of inert particles and droplet suspension

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Abstract. Using the methods of mechanics of heterogeneous media, we studied the process of suppressing heterogeneous detonation by clouds of inert particles and using a droplet suspension. The main flow regimes obtained as a result of modeling are described.

1. Introduction
Issues of explosion and fire safety of industrial production attract great attention. So, when using homogeneous and heterogeneous reacting media in production, accidental explosions may occur, that lead to great destruction. Therefore, the attenuation and suppression of explosive and detonation waves is one of the priority areas of research in this area. One of the ways to weaken or suppress detonation is to create clouds of solid inert particles or a suspension of inert liquid droplets in the flow field. In [1–6], the effect of chemically inert solid particles on the parameters of detonation waves in reacting gas mixtures was shown. Various regimes of detonation propagation during interaction with a cloud of inert particles were obtained: detonation propagation in the same regime, partial decrease in the velocity of detonation propagation, partial detonation failure, followed by re-initiation of the detonation wave, and complete detonation failure with separation of the shock front and the combustion wave. Galloping mode of detonation propagation was also obtained, in which a detonation propagation intensity decreases in a cloud of inert particles, next re-initiation followed by a decrease in the detonation wave intensity and repetition of the cycle [5,7]. In [3], a comparison of the one-dimensional and two-dimensional approaches to the description of the suppression of gas detonation is given. The suppression of detonation by droplet suspension was considered in [8–12]. In [8], a review of the available experimental work on the suppression of explosions of gas mixtures (hydrogen - air, methane - air, etc.) using water fog, as well as water sprays, was carried out. Numerical modeling of detonation suppression processes was considered in [10–12]. In the calculations, the authors considered the relations on the detonation wave, and investigated how the evaporation of liquid droplets behind the front of the detonation wave occurs.

In [13–15], the investigation of suppressing heterogeneous detonation in a flat channel by clouds of inert particles was considered. In [13,14], critical conditions were obtained for suppressing detonation with allowance for diffusion combustion of aluminum particles. In [15], the model took into account the collision between particles and the refinement of the flow patterns behind the front of the shock/detonation wave was obtained.

Previously, a diffusion-controlled combustion model was used to describe the heterogeneous detonation of aluminum particles. However, in [16] it was shown that, in the range of diameters of aluminum particles close to 3.5 μm, a transition occurs from the diffusion to the kinetic-controlled
combustion. In this work, we studied the interaction of detonation waves in gas-suspended aluminum particles with a diameter of less than 1 μm in air by clouds of inert particles of aluminum oxide and a suspension of inert liquid water droplets, taking into account the transition regime of combustion from diffusion to kinetic.

2. Physical and numerical model
The mathematical model of the detonation of aluminum particles in oxygen is based on the concepts of multi-velocity multi-temperature continua. In a two-dimensional unsteady flow, the basic equations describing detonation processes in monodisperse gas-suspended aluminum particles are presented in [13]. In this work, we use a mathematical model of a bi-dispersed heterogeneous medium, one fraction of which is reactive (index \( i=2 \)), and the second is inert (\( i=3 \)). A model of the combustion of aluminum particles taking into account the transient combustion regime was presented in [17].

With using water droplets as an inert phase, it is necessary to take into account their evaporation and crushing during interaction with a shock or detonation wave [10,12]. The breakage of droplets is described by the formula for detachment of the boundary layer [12]:

\[
\frac{dm_{br}}{dt} = \frac{3\sqrt{2} \rho_3 \left( \frac{\rho_{11}}{\rho_{33}} \right)^{\frac{1}{3}} \left( \frac{v_3}{v_1} \right)^{\frac{3}{2}} (u_3 - u_1)}{d_{31} \text{Re}^{0.2}}.
\]

And the evaporation of drops is described by the formula [10,18]:

\[
\frac{dm_{ev}}{dt} = -(4\pi)^{\frac{2}{3}} \frac{1}{3} \rho_3 m_3^3 K_v \left( 1 + 0.27 \text{Re}^{0.5} \right),
\]

where \( \rho_3 \) is water density, \( v_1, v_3 \) are gas and liquid viscosity, \( u_1, u_3 \) are gas and liquid velocity, \( K_v \) is evaporation constant, \( \text{Re} \) is Reynolds number. More detailed information on the model of droplet breaking is presented in the works [10,18].

The interaction scheme of the detonation wave with a cloud of inert phase is shown in Fig. 1. A cellular detonation wave propagates through the channel and interacts with a cloud of inert phase that consist of aluminum oxide particles or water droplets and reacting mixture of aluminum in oxygen. The cloud occupies the entire width of the channel.

![Figure 1. Scheme of computational area.](image)

3. Estimation of times of thermal and velocity relaxation of alumina particles and water droplets
Thermal and velocity relaxation times of an individual particle and a droplet behind the detonation wave front are estimated. The method of such estimation is described in detail in [4]. In fig. 2 shows the dependences of times of velocity and thermal relaxation of water droplets and aluminum oxide particles on droplet/particle size. It is seen that times of velocity and thermal relaxation of water droplets are lower than the corresponding times for alumina particles with the same droplet and particle sizes. Thus, liquid droplets will accelerate and warm up in the gas stream behind the detonation wave front faster than aluminum oxide particles. Thus, rates of impulse and energy take off from the reacting mixture will be higher in the case of the interaction of the detonation wave with liquid droplets. It can be assumed that the efficiency of detonation waves attenuation by liquid droplets will be higher than by solid particles.
Figure 2. Dependences of times of velocity (blue curves) and thermal (red curves) relaxation of water droplets (solid lines) and aluminum oxide particles (dashed lines).

4. Suppression by inert particles

After the interaction of a detonation wave with clouds of inert particles, various regimes of detonation propagation were obtained. At a volume concentration of inert particles of $m_3=10^{-4}$, regardless of their diameter, detonation combustion is continue to propagate with the same velocity, the cellular structure remains unchanged (Fig. 3). The maximum pressure patterns show that the cellular structure does not change when the detonation wave enters the cloud of inert particles. For this case a cloud of inert particles is located at a point $x=0.3$ m. The pressure value at triple points also remains in the same range as before a cloud of inert particles (about 220 atm).

Figure 3. History of maximum pressure $d_2=1$ μm, $d_3=1$ μm, $m_3 = 1\cdot10^{-4}$.

With an increase in the concentration of inert particles $m_3$ to $5\cdot10^{-4}$, the flow is rearranged, the cellular structure changes and the sizes of detonation cells increase. This is clearly seen in the schlieren images (Fig. 4). The inert cloud is at the point $x = 0.1$ m. Before interaction with a cloud of inert particles or at the initial stage of interaction, many transverse waves propagate along the leading front (Fig. 4a). When propagating through the cloud, the cellular structure is rearranged and the number of transverse waves decreases to 2–4 per channel width (Fig. 4b). Figure 4c shows that in some cases there is a partial separation of the combustion front and the shock front, and re-initiation occurs in transverse waves.
Figure 4. Detonation propagation $d_2=200$ nm, $d_f=5$ μm, $m_3=5 \cdot 10^{-4}$ at moment, a) 0.04 ms, b) 0.2 ms, c) 0.3 ms.

In the pictures of maximum pressure for this case shown in Fig. 3 there is a decrease in pressure values at triple points, as well as a rearrangement of the cellular structure (Fig. 5). The pressure at triple points drops from 250 atm to 170-180 atm.

Figure 5. History of maximum pressure $d_2=200$ nm, $d_f=5$ μm, $m_3=5 \cdot 10^{-4}$.

Detonation failure in gas suspensions of aluminum submicron particles is observed with an increase in the concentration of inert particles to $m_3=10^{-3}$ and higher. As the result the failure of the cellular structure that can be seen from the history of maximum pressure (Fig. 6a). Splitting of the detonation wave into a frozen shock the wave and the combustion front lagging behind can be seen on the schlieren image (Fig. 6b). Behind the combustion front, the so-called “bundles” begin to form, which were obtained in [14].

Figure 6. Flow fields $d_2=200$ nm, $d_f=1$ μm, $m_3=1\cdot 10^{-3}$. a) History of maximum pressure, b) schlieren images.
5. Conclusions
Three different propagation modes are obtained by numerical simulation of heterogeneous detonation in a channel filled with a mixture of reacting and inert particles. Based on the analysis of the flow patterns and the maximum pressure field, it was found that with an increase in the volume concentration of the inert phase, the velocity of detonation propagation decreases and a complete or partial detonation failure can be observed.

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