Shock wave and detonation flow regimes in gas suspension of reacting gases and inert particles

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Abstract. In this research, the interaction of shock waves (SW) with clouds of chemically inert solid particles of silica with a diameter of 100 μm in a hydrogen-air mixture is considered. Depending on the initial volume concentration of particles, three shock wave and detonation flow regimes are realized: 1. attenuation of the SW by a cloud of inert particles, 2. initiation of detonation behind the front of the SW reflected from the rigid wall, 3. initiation of detonation in a cloud of inert particles.

1. Introduction
In the modern world, great attention is paid to the study of the behavior of reacting gas mixtures, since they can be dangerous to humans. For example, they can self-ignite, followed by the initiation of detonation. The danger of reacting gas mixtures in industrial production in which gas mixtures are used as working substances should be highlighted. Therefore, it is worth developing a theory of explosion and fire safety.

2. Formulation of the problem
Studies on the suppression of detonation waves by clouds of inert particles have already been investigated in researches [1], [2]. A shock wave comes out from a cloud of inert particles after the detonation wave was suppressed by the cloud of particles. This shock wave is dangerous because it can transform into a detonation wave due to geometric obstacle (it’s shown in figure 1). Figure 1 shows the pressure distribution in the shock tube. The gas parameters in the high-pressure chamber at the initial time: \( p = 100 \, \text{atm}, \, T = 3000 \, \text{K} \), as a gas O\(_2\) is used. The gas and particle parameters in the low-pressure chamber at the initial time: \( p = 1 \, \text{atm}, \, T = 300 \, \text{K} \), gas mixture – hydrogen and air, coordinates of a cloud of inert particles \( 0.5 \, \text{–} \, 0.75 \, \text{m} \), the volume concentration of particles \( 2 \times 10^{-3} \), particle diameter – 100 μm. The bold line in figure 1 shows the distribution of pressure in a shock tube after a SW exits from the cloud of inert particles. Next the shock wave reaches the rigid wall, it is reflected from the rigid wall with the subsequent initiation of detonation. Therefore, it is important to study shock wave attenuation. One of the ways to attenuate shock waves is considered to be the addition of a cloud of inert particles in gas mixtures, but there is currently little research on the interaction of shock waves in reactive gas mixtures with clouds of inert particles. Therefore, the interaction between a shock wave and clouds of inert particles should be studied.
In this study, the interaction of SW in a hydrogen-air mixture with clouds of chemically inert solid particles of SiO$_2$ with a diameter of 100 μm is considered and the resulting shock wave and detonation flow regimes are determined. The mathematical model of the mechanics of reacting gas mixtures (hydrogen and air) and inert particles is a system of ordinary differential equations of the mechanics of heterogeneous media and has the form presented in [3]. The detailed kinetics model [4], which takes into account 38 reactions of 8 components, will be used to describe chemical reactions in reacting gas mixtures.

3. Calculations

Initial conditions in the shock tube for all calculations: gas mixture – hydrogen and air; the gas parameters before the accident shock wave front: p – 1 atm, T – 300 K; the velocity of the incident shock wave front is 1120 m/s (the maximum velocity at which self-ignition of the gas mixture doesn’t occur behind the front of the incident shock wave).

The first emerging regime is the regime of SW attenuation by a cloud of chemically inert particles (figure 2). A cloud of inert particles with a volume concentration of $5 \times 10^{-3}$ is located between 0.49 m (the coordinate where the rarefaction wave catches up with the shock wave) and 0.6 m. The shock wave is attenuated, when it passes through the cloud of inert particles, because of interaction between the shock wave and the cloud of inert particles. Ignition with subsequent initiation of detonation isn't observed both behind the front of a passing shock wave and after its reflection from a rigid wall (bold line in figure 2).

**Figure 1.** Pressure distribution in the shock tube in the presence of a shock wave.

**Figure 2.** Pressure distribution in the shock tube in the presence of a shock wave with a rarefaction wave. The regime of SW attenuation by a cloud of inert particles.
The second regime is the initiation of detonation behind the front of the shock wave reflected from the rigid wall (figure 3). A cloud of inert particles with a volume concentration of particles $10^{-4}$ is located near a rigid wall in the interval from 0.35 m to 0.5 m. In the interaction of the SW with a cloud of chemically inert solid particles, part of the shock wave passes into the cloud, and part is reflected from the cloud of particles. The shock wave as it passes through a cloud of particles is weakened by it. The bold line in figure 3 shows the moment of reflection of a shock wave from a rigid wall. Further, behind the front of the reflected shock wave, the mixture ignites, followed by the initiation of detonation.

![Image](image.png)

**Figure 3.** The pressure distribution in the shock tube with a cloud of inert particles with a volume concentration of $10^{-3}$. The regime of initiation of detonation behind the front of the SW reflected from the rigid wall.

With an increase in the initial volume concentration of particles to $2.5 \times 10^{-3}$, the third regime is realized — initiation of detonation in a cloud of inert particles (figure 4). In this case, the interaction of the shock wave with a cloud of particles and a rigid wall ignition of the mixture isn’t observed behind the fronts of the transient and reflected shock waves. Ignition of the mixture with subsequent initiation of detonation occurs in the cloud of inert particles (thick line in figure 4(a)). Figure 4 (b) shows the temperature distribution in the shock tube. Figure 4(b) shows the cause of the initiation of detonation in a cloud of inert particles. The thick line shows the temperature distribution at the moment of gas ignition in a cloud of inert solid particles. It can be seen from the figure that the temperature of the gas in the cloud has increased and this temperature is enough for the self-ignition of the gas. The gas temperature increases due to friction between the gas and the cloud of inert particles.

**4. Conclusion**

The interaction between SW and clouds of inert particles of SiO$_2$ with a diameter of 100 μm in a hydrogen-air mixture is considered. As a result of research, three shock-wave and detonation flow regimes were obtained, which is depend on the initial volume concentration of particles. First regime — attenuation of the SW by a cloud of inert particles, second regime — initiation of detonation behind the front of the SW reflected from the rigid wall, third regime — initiation of detonation in a cloud of inert particles.
The pressure distribution in the shock tube with a cloud of inert particles with a volume concentration of \(3.25 \times 10^{-3}\). The regime of initiation of detonation in a cloud of inert particles (a).

The temperature distribution in the shock tube with a cloud of inert particles with a volume concentration of \(3.25 \times 10^{-3}\). The regime of initiation of detonation in a cloud of inert particles (b).

**Figure 4.** The pressure distribution in the shock tube with a cloud of inert particles with a volume concentration of \(2.5 \times 10^{-3}\). The regime of initiation of detonation in a cloud of inert particles (a). The temperature distribution in the shock tube with a cloud of inert particles with a volume concentration of \(2.5 \times 10^{-3}\). The regime of initiation of detonation in a cloud of inert particles (b).

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