Study of propagation of heterogeneous detonation in a layer of aluminium particles

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Abstract. The propagation of heterogeneous detonation along a channel partially filled with a reacting mixture is considered using numerical simulation methods. Two different regimes of propagation are observed. Flow patterns and fields of maximum pressure are analyzed. It is found that decrease of the cloud thickness leads to decreasing velocity of detonation propagation.

1. Introduction

The problems of lifting, ignition and detonation of reacting dust remain relevant, due to the ongoing explosions in industry and coal mines [1, 2]. Investigation of dust lifting after interaction with shock wave was studied both theoretically [3–7] as experimentally [8–10]. Mainly researches were made for coal dust while detonation initiation in aluminum powders was investigated poorly [4]. Data as for flow fields as for critical regimes of detonation propagation in aluminum dust layer, is not enough. In this study the interaction of the shock wave with a heterogeneous mixture of aluminum particles in channel with next detonation propagation is investigated. The main goal is to investigate the influence of the thickness of the reacting layer on critical conditions and flow fields.

2. Physical and numerical model

Main equations follows from laws of conservation of mass, momentum and energy for each phase similar to [11, 12]. The system is closed by the equation of state of an ideal gas; particles are assumed to be incompressible. Relations for the processes of mass transfer between components (evaporation, condensation, combustion), momentum exchange (resistance forces) and heat transfer between gas and particles are presented in [13]. The model of aluminum detonation burning is used the same that is described in [12, 14, 15]. Aluminum burning is described within reduced Arrhenius-type chemical kinetic with taking into account incomplete combustion of the particles and ignition temperature criterion. Transition from diffusion to kinetic combustion of the aluminum macro- and nanoparticles is also taken into account [16–18], unlike to [4].

We consider a channel partially filled with pre-mixed stoichiometric mixture of aluminum particles in oxygen (figure 1). Shock wave with Mach number M=5 propagates in the channel. During the interaction of the shock wave with the particles cloud the aluminum particle ignites and the detonation initiates. The combination of the detonation-like structure in the layer and a shock wave in the gas over the layer propagates along the channel. Structure of the flow fields behind propagating combined detonation / shock wave is analyzed by the methods of mathematical and numerical modelling.
Boundary conditions on the top and bottom channel walls correspond to impermeability and thermal insulation. Taking into account that the velocity on the left boundary is negative (a rarefaction wave is specified as the initial conditions), some soft boundary conditions were accepted on the left boundary of computational domain in the form of \( \frac{du_1}{dx} = 0, \frac{d\rho_1}{dx} = 0, \frac{dT_1}{dx} = 0, v_1 = 0 \).

The numerical technique is based on the conservative flux-splitting schemes: the TVD scheme by Harten for gas and the Gentry-Martin-Daly scheme for particles. The numerical method has been tested earlier and applied for 2-D numerical simulations of the shock wave and detonation flows in [4, 11, 12].

\[ \text{Figure 1. Scheme of simulating area.} \]

3. Results of calculations

Numerical results for the channel height \( H=20 \text{ cm} \) and particle diameter \( d=3.5 \mu m \) are presented in figures 2 – 5. For the width of the reacting area \( h=10 \text{ cm} \) there is supercritical regime of detonation propagation. This regime of propagation is characterized by the lack of detonation failure. The detonation front expands with constant velocity that can be observed in maximum pressure history fields (figure 2). In area where the dust layer is situated there is a cellular structure with one cell on the reacting layer. The pressure values in the transverse waves are about 70 atm, that correlates with the results obtained earlier in [11]. Pressure values in the triple points reach 110 – 120 atm. It should be pointed out that these values are lower in comparison with the case when the mixture fills whole channel. Outside of the reacting layer the pressure values are less than 20 – 30 atm and only in the points of transverse waves collisions or reflections from upper wall they are about 40 atm. The average propagation velocity of combination of the detonation and shock wave in the channel in this regime is about 1.5 km/s. This value is close to the Chapman-Jouguet velocity in the stoichiometric aluminum-oxygen mixture.

\[ \text{Figure 2. Maximum pressure history, } h=10 \text{ cm, } H=20 \text{ cm, } d=3.5 \mu m, t=0.80 \text{ ms.} \]

The schlieren picture (figure 3a) and the field of mean density of the discrete phase (figure 3b) at time moment \( t=0.45 \text{ ms} \) demonstrate full burnout of aluminum particles in the area behind the front of the detonation wave. From the schlieren pictures it can be seen that detonation wave begin to overtake shock wave that propagate in upper part of the channel (figure 3a). The Kelvin-Helmholtz instability develops on the on the contact surface behind the shock wave. One can see the vortex structures forming in this area (figure 3a, figure 3b: \( 0.4<\chi<0.6, 0.1<y<0.18 \)).
Figure 3. Flow fields $h=10$ cm, $H=20$ cm, $d=3.5$ μm, $t=0.45$ ms. (a) schlieren pictures of the flow, (b) particles density.

With thickness of the reacting layer decreased to $h=5$ cm the regime of the detonation propagation is close to critical. This regime is characterized by partial detonation failure in the reacting layer and following re-initiation in the transverse waves. The area with unburned particles behind the detonation wave can be seen in the flowfields of the particle mean densities (figure 4). In whole the vortex structures behind the detonation front are similar to those for $h=10$ cm (figure 3b). The reaction products and unburned particles form complicated vortex structures behind the shock wave (figure 4: $0.8<x<1$, $0.08<y<0.2$).

Figure 4. Particles density, $h=5$ cm, $H=20$ cm, $d=3.5$ μm, $t=0.72$ ms.

From the analysis of the maximum pressure fields (figure 5), it can be concluded that in this case ($h=5$ cm) the detonation in the reacting mixture initiates and propagates from the left part of the channel. Then the detonation decays and the maximum pressure decreases to 30 – 35 atm in this area. The detonation front stays flat. Subsequently, the transverse wave initiation and propagation occur, where maximum pressure exceeds the Chapman–Jouguet value (55 atm). After going out of the reacting mixture the transverse waves propagate upward in the channel and reflect from the upper wall. Also the reflection of transverse waves occurs on contact surface that enforce detonation in reacting layer (figure 5). One can see the re-initiation of detonation in the plane of symmetry where pressure rises to 110 atm ($x=0.95$, $y=0$). In the end of the computational domain the detonation fails and the pressure does not exceed 40 atm. In this regime the average propagation velocity is about 1.3 km/s, that’s less than the Chapman–Jouguet velocity (1.56 km/s).
4. Conclusions

Two different propagation regimes were obtained by numerical simulation of heterogeneous detonation in a channel partially filled with a reacting mixture. Based on the analysis of flow patterns and the maximum pressure field, it was found that with a decrease of cloud thickness, a decrease in the velocity of detonation propagation occurs. In the considered cases, complete detonation failure was not observed.

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