Modeling of detonation propagation in expansion channel in bidisperse mixture

Fedorov A V, Khmel’ T A and Lavruk S A

Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, Novosibirsk, Russia

E-mail: khmel@itam.nsc.ru

Abstract. The problem of detonation propagation in channels with linear expansion filled with two-fractional alumunium mixture dispersed in oxigen was investigated. Fractional composition of mixture with particle diameters 3.5 and 1 μm was varied. Transition from diffusion to kinetic regime of combustion was taken into account in the description of the chemical reactions for microsized aluminum particles. It was established that fractional composition of the mixture influence on propagation regimes and formation of transverse waves of cellular detonation.

1. Introduction

The combustion of nano-dispersed aluminum powders, including in the detonation mode, attracts great interest in view of the wide prospects for their use. The problems of detonations in aluminum particles gas suspensions have been extensively studied experimentally and theoretically for the micro-dimensional particle size range.

Propagation of shock waves behind a rectangular edge in a heterogeneous monodisperse mixture and influence of particle concentrations and sizes on flow patterns was analyzed in [1]. It was noted that main features that distinguish wave patterns of flow from flows in gas media are caused by presence of zones of velocity and thermal relaxation of the phases. Similar problems for detonation waves in gas – particles mixtures of aluminum in oxygen were considered in [2-6]. Two types of diffraction problem were analyzed for different initial conditions: for a flat detonation wave (the Chapman-Jouguet flow) and for cellular detonation. It was demonstrated in [2] that even with a flat detonation wave as the initial conditions, a flow with transverse waves develops in the wide part of the channel behind the edge that characterize cellular detonation.

In [3] description of wave patterns in different diffraction regimes on the backward step of a flat detonation wave is given. The channel width and particle size were varied from 0.01 to 0.15 m for channel and from 1 μm to 3.5 μm for particles. The results allow us to classify the diffraction regimes similar to those observed in gas detonation: supercritical, critical, and subcritical. The works [4, 5] presented results of numerical simulation data on propagation of cellular detonation in a half-space behind the backward ledge in a gas suspension of aluminum particles with sizes 1.5 - 3.5 μm where channel width varied from 0.5 to 4 detonation cells. Wave patterns were analyzed in the process of reorganization of cellular structures in different propagation modes.

Real aluminum powders are characterized by heterogeneity and certain dispersion in particle sizes. In [5-7] processes of initiation and propagation of plane and cellular detonation waves in bidisperse and polydisperse mixtures of aluminum were studied. Two-dimensional flows in flat channel and
channel with sudden expansion were analyzed in [5-6]. It was found that in mixtures with large dispersion in particle sizes or in bidisperse suspensions with equal partition of fractions the cellular detonations transform into plane detonation waves which propagate sustainably without transverse waves. It was established in [7] that the structures of plane waves refer to nonideal detonation and depend on the fractional composition of the mixture. Small additions of fine fraction lead to significant decreases in the initiation energy.

In the present work processes of propagation of detonation in a channel with section of linear expansion in bi-fractional aluminum suspensions of particles 3.5 μm and 1 μm are studied. The main goal of this work is to analyze effect of bidisperse fractional composition on propagation regimes and detonation flow characteristics.

2. Physical and mathematical model.

The Euler equations for two-dimensional flow in dilute gas particle suspensions follow from conservation laws for mass, momentum, and energy (the subscripts 1, 2, 3 indicate gas and reactive particles, respectively) [8]:

\[
\begin{align*}
\frac{\partial W}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} &= \Gamma, \\
W &= \begin{pmatrix} W_1 \\ W_2 \\ W_3 \end{pmatrix}, \\
F &= \begin{pmatrix} F_1 \\ F_2 \\ F_3 \end{pmatrix}, \\
G &= \begin{pmatrix} G_1 \\ G_2 \\ G_3 \end{pmatrix}, \\
\Gamma &= \begin{pmatrix} \Gamma_2 - \Gamma_3 \\ \Gamma_2 \\ \Gamma_3 \end{pmatrix},
\end{align*}
\]

\[
W_i = \begin{pmatrix} \rho_i \\ \rho_i u_i \\ \rho_i v_i \\ \rho_i E_i \end{pmatrix}, i = 1, 2, 3,
\]

\[
F_i = \begin{pmatrix} \rho_i u_i \\ \rho_i u_i^2 \\ \rho_i u_i v_i \\ \rho_i u_i E_i \end{pmatrix}, i = 1, 2, 3,
\]

\[
G_i = \begin{pmatrix} \rho_i v_i \\ \rho_i v_i^2 \\ \rho_i v_i E_i \end{pmatrix}, i = 1, 2, 3.
\]

The system is enclosed by the equations of state and relationships for mass, momentum, and heat exchange between the gas and the particles

\[
\dot{J} = \frac{\rho_i}{\tau_{\text{m}}} (\dot{u}_i - \dot{u}), \quad q_i = \frac{\rho_i c_{v_i} T_i}{\tau_{\text{n}}} (T_i - T), \quad J = \frac{\rho_i}{\tau_{\text{g}}} (\xi_i - \xi_k)
\]

\[
p = \rho_i R T_i, \quad E_1 = \frac{u_i^2}{2} + c_{v_{i}} T_i, \quad E_2 = c_{v_{2}} T + Q + \frac{u_j^2}{2},
\]

(2)

Here indexes 1, 2 and 3 refer to gas and particles, respectively. We use the following notations: \( p \) is pressure; \( \rho_i = m_i \rho_i, u_i, E_i, T_i, c_{ij}, m_i \) are mean densities, velocities, total energy per unit mass, temperatures, heat capacities, and volume concentrations of the components, \( \xi_i = \rho_i / \rho \) is mass particle concentration, \( \xi_k \) is fraction of unburnt particles, \( \rho_{it} \) are true densities, \( R \) is the reduced gas constant, \( Q \) is heat effect of particle combustion in the frame of reduced chemical kinetics.

The interphase interactions are presented by parameters \( J \) (the mass transfer), \( \dot{f} \) (the interphase interaction force), and \( q \) (the heat transfer):
the plane of symmetry there are separation of the shock wave front and combustion front (Figure 2b). Here, near
\eta=0.05, \text{time of 0.26 ms is 30 mm.}

In the Schlieren image (Figure 2a) the separation of the leading front of the shock wave (SW) and the lagging combustion front (CW) can be seen, the distance between the fronts at the time of 0.26 ms is 30 mm.

When 5\% large (3.5 \mu m) particles are replaced by smaller ones (1 \mu m) and the saturation parameter \eta=0.05, a transition to the critical mode of detonation propagation is observed (Figure 2b). Here, near the plane of symmetry there are separation of the shock wave front and combustion front (Figure 2b).
At the same time in the most part of channel detonation continues to propagate without a noticeable separation of the fronts. Transverse wave propagates along the front of the detonation wave which is formed as a result of re-initiation of detonation on the inclined wall. Pressure in the transverse wave reaches values of about 70 atm.

Further increase in the saturation parameter to $\eta = 0.1$ leads to a supercritical detonation propagation regime. Here the leading front propagates with stretching and without breakdown (Figure 2c). It also shows formation of transverse wave that moves along the leading front.

![Figure 2](image_url)

**Figure 2.** Detonation propagation modes depending on the saturation parameter $t=0.24$ ms: subcritical ($\eta=0$) a), critical ($\eta=0.05$) b), supercritical ($\eta=0.1$) c).

For the inclination angle 30º in Figure 3 shows the maximum pressure fields in the channel for different saturation parameters are presented. A critical regime is realized in a monodisperse mixture of 3.5 μm aluminum particles (Figure 3a). Partial detonation failure in Figure 3a can be observed as pressure drop of up to 20 atm in the region $0 < y < 0.04$ m on the leading edge near the plane of symmetry.

With increase in saturation parameter $\eta$ from 0 to 0.1, the transition to supercritical detonation propagation regime without failing is observed in the maximal pressure fields (Figure 3b). With further increase in the saturation parameter a supercritical detonation propagation regime takes place (Figure 3c $\eta = 0.3$). It is also worth noting that with increase in the saturation parameter the maximal pressure in collisions of the transverse waves which propagate along the leading edge decreases. For $\eta=0$ and $\eta=0.1$ the maximal pressure reaches the values up to 70 atm, while for $\eta = 0.3$ it does not exceed 55 atm. At the same time inhomogeneities are practically absent on the detonation front (Figure 3c).
Figure 3. The effect of the fractional composition on the cellular detonation formation: maximal pressure histories; $t=0.24$ ms, $\eta=0$ (a); $\eta=0.1$ (b); $\eta=0.3$ (c).

Further increase in concentration of small particles leads to formation of the regime of detonation propagation in which the surface of the leading front is almost completely smoothened. Figure 4 shows the pressure fields in area near the leading front of detonation wave. It can be seen that as the fraction of fine particles in the mixture increases, the pressure in the transverse wave decreases from 65 atm with $\eta=0.1$ to 45 atm with $\eta=0.5$. With predominance of the fraction of fine particles in the mixture the transverse waves are again produced ($\eta=0.7$). It is observed that the pressure at the front increases up to 65 atm with $\eta=0.7$. Also formation of inhomogeneities at the front of the detonation wave again occurs.

Figure 4. Pressure fields at the front of the detonation wave as a function of the saturation parameter.
With $\eta=0.7, 0.9, 1.0$, one can see the formation of cellular structure in the channel (Figure 5). In fields of maximum pressure (Figure 5), it can be seen that increase in the fraction of fine particles results in increase in the number of triple points and increase in maximum pressure in these regions. At $\eta=0.9, 1.0$ irregular cellular structures with relatively equal pressure values at triple points are formed in the channel. In general the structures of transverse waves in Figures 5b and 5c are similar.

The problem of weakening of transverse waves in cellular detonation in bidisperse and polydisperse suspensions was discussed in [5-7] in analysis of the propagation of detonation in plane channels and channels with a discontinuity of the cross section. Applying similar arguments we can explain the weakening of transverse waves with mean values of the saturation parameter and in problem of the detonation wave exit into a channel with linear expansion. According to [5-7] growth of small perturbations at front of the detonation wave and formation of secondary transverse waves agrees with the acoustic theory proposed by Bartel in [11] and developed in [7] for heterogeneous mixtures. The specific feature of bidisperse mixtures is that they form peculiar flow structure in the relaxation zone behind the leading shock wave front. In this flow the acoustic perturbations being formed by primary transverse waves either not come back to the leading front (and secondary transverse waves do not appear) or partly come back with overcompressed or weakened sections of the front. It leads to the dispersion of transvers waves (weakening) and the reduction of peak pressures until the steady propagation in the Chapman-Jouguet regime. It can be assumed that weakening of transverse waves in the processes of detonation propagation in a channel with a linear expansion filled with bidispersed particle suspension in gas is due to similar mechanisms.

**Figure 5.** Maximal pressure histories at $t=0.24$ ms, $\eta=0.7$ (a); $\eta=0.9$ (b); $\eta=1$ (c).
4. Conclusions
The problem of propagation of detonation in bidispersed mixtures in a channel with linear expansion was studied on the base of numerical simulations within the semiempirical model of detonation of microdispersed suspension of aluminum particles. The model takes into account the transition regime from diffusion to kinetic in the description of aluminum particle combustion. The flow patterns in the main propagation regimes in channels with inclination angle of the wall of 45 ° and 30 ° at $H_1 = 0.03$ m and variation of the fractional composition of particles with sizes of 3.5 and 1 μm are analyzed.

It is established that an increase in part of fine particles in the mixture leads to a change in the mode of propagation of detonation in the expanding channel. The transition from subcritical to critical regime occurs at $\eta = 0.05$ and from critical to supercritical at $\eta = 0.1$.

At close values of part of each fraction of bidisperse suspension the detonation propagation in channel is characterized by a weakening of transverse waves and a decrease in pressures peak in transverse waves. With the saturation parameter $\eta = 0.4-0.5$, the transverse waves are almost completely absent as in propagation of detonation in bidisperse suspensions in flat channels. With the subsequent increase in fraction of fine particles the transverse waves form again and with predominance of small particles similar pattern of transverse waves as in the monodisperse fine particle suspension is observed.

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