NUMERICAL SIMULATION OF DETONATION FORMATION IN POLIDISPERSE ALUMINUM PARTICLES SUSPENSIONS IN OXYGEN

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Introduction

Investigations of ignition, combustion, and detonation in aluminum particle suspensions in air or oxygen are related with explosion and fire safety in industries utilizing powder technologies or processes of aluminum wares. Recent developments of detonation propulsion systems stimulate analysis of gaseous suspensions of reactive particles considering them as working mixtures in the combustion chambers. Overwhelming majority of results on detonation processes in aluminum – air and aluminum – oxygen suspensions were obtained for monodisperse mixtures (see, for example, [1-4]). At the same time most of gaseous suspensions of aluminum particles are polydisperse and characterized by certain size distribution function. Numerical modeling of plane and cellular detonations in bi-dispersed mixtures of aluminum particles and oxygen revealed properties different from monodisperse mixtures. In particular, degeneration of cellular detonation structures and stable propagation of plane front in some cases were obtained in [5] numerically and confirmed on the base of acoustic analysis.

The present work focuses on numerical modeling of detonation initiation and propagation in polydisperse suspensions (on the model of thee- and five-fractional mixtures of aluminum particles in oxygen) in a plane channel. Problems of plane and cellular detonation initiation and propagation are considered and influence of the mixture content (particle size distribution) on the detonation characteristics is analyzed.

Formulation of the problem

A planar channel of infinite length is considered, which is filled with a mixture of aluminum particles and oxygen over the entire width and a halved length. The detonation initiation in gas-particle mixture is modeled as a result of the effect on the cloud of particles of a planar shock wave of explosion character (with adhering expansion wave) propagating in the gas.

The physical and mathematical model of detonation in stoichiometric monodisperse aluminum particle suspensions in oxygen based on equations of a mechanics of heterogeneous media with a reduced chemical kinetics of Arrhenius type has been proposed in [6-7, 3]. The application of the model to two-dimensional detonation flows is given in [4].

The advanced model takes into consideration several fractions with different particle sizes. The processes of interaction of each particle component with gaseous phase are described identically with regard for the particle diameters. The Euler equations follow from the laws of conservation of mass, momentum, and energy for the gas phase and each fraction of the disperse phase and have the form

\[
\begin{align*}
\frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho u_i)}{\partial x} &= \sum_{i=2}^{N+1} J_i, \\
\frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho u_i)}{\partial x} &= -J_i, \\
\frac{\partial (p + \rho u_i^2)}{\partial t} + \frac{\partial (p + \rho u_i^2 u_j)}{\partial x} &= \sum_{i=2}^{N+1} -f_i + J_i u_i, \\
\frac{\partial u_i}{\partial t} + \frac{\partial (\rho u_i)}{\partial x} &= f_i - J_i, \\
\frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho u_i)}{\partial x} &= \sum_{i=2}^{N+1} -q_i - f_i u_i + J_i E_i, \quad (1)
\end{align*}
\]

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The system is closed by equations of state of an ideal gas with ignored volume of particles, by relations that describe interphase interaction [the Stokes force in the flow around the particles in the gas flow behind the front of the shock (detonation) wave and heat transfer between the phases with allowance for the change in the Nusselt number], and by Arrhenius-type equations of reduced chemical kinetics; the description of combustion of aluminum particles takes into account incomplete combustion and involves the temperature criterion of ignition.

\[ p = \rho_i R T_i, \quad E_i = \frac{u_i^2}{2} + c_{v,i} T_i, \quad E_i = \frac{u_i^2}{2} + c_{v,i} T_i + Q, \]

\[ J_i = \frac{\rho_i}{\tau_\xi} \max(0, (\xi_i - \xi_{iw})) \exp\left( -\frac{E_{iw}}{RT_i} \right) \times \max[0, \text{sign}(T_i - T_{gw})], \]

\[ f_i = \frac{3m_i \rho_{11}}{4d_i^2} c_{D} |u_i - u_i|(u_i - u_i), \quad q_i = \frac{6m_i \lambda_i}{d_i^2} \text{Nu}(T - T_i), \]

\[ c_D(\text{Re}_i, M_{li}) = [1 + \exp\left( -\frac{0.43}{M_{li}^{4.85}} \right)] (0.38 + \frac{24}{\text{Re}_i} + \frac{4}{\sqrt{\text{Re}_i}}), \]

\[ \text{Re}_i = \frac{\rho_i d_i |u_i - u_i|}{\mu}, \quad \text{Nu}_i = 2 + 0.6 \text{Re}_i^{1/2} \text{Pr}^{1/3}, \quad M_{li} = \frac{|u_i - u_i| \sqrt{\rho_{11}}}{\sqrt{\gamma_i} p_i}, i = 2, 3. \]

Here the subscript 1 refers to the gas, 2, ..., N+1 denote the particles; \( p \) is the pressure, \( \rho_i = m_i \rho_{ia} \) is the mean density, \( \rho_{ia} \) is the true density of the \( i \)th component \( (i = 1, \ldots, N+1) \), \( u_i \) is the velocity, \( E_i \) is the total energy of the unit mass, \( c_{v,i} \) is the specific heat, \( T_i \) is the temperature, \( m_i \) is the volume concentration, \( Q \) is the heat release in the chemical reaction, \( d_i \) is the particle diameter, \( \lambda_i \) is the thermal conductivity of the gas, and \( \gamma_i = R / c_{v,i} \) is the ratio of specific heats of the gas. In Eqs. (2), \( \xi_i = \rho_i / \rho \) is the relative mass concentration of particles, \( \rho = \rho_1 + \rho_2 + \rho_3, \ E_{iw} \) is the activation energy, \( \xi_{iw} \) is the concentration of the corresponding component in the final equilibrium state (unburned particles and condensed aluminum oxide), \( T_{gw} \) is the ignition temperature, and \( \tau_\xi = \tau_0 (d_i / d_0)^2 \) is a constant determining the characteristic time of ignition. The values \( \tau_0 = 0.0024 \) msec and \( d_0 = 10 \) \( \mu \)m ensure the agreement with available data on combustion of aluminum particles in pure oxygen.

The initial-boundary problem is posed in a manner similar to [4, 5] as the problem of shock-wave initiation of plane detonation waves in a plane channel where the shock wave (SW) in the gas interacts with the cloud of the gas suspension:

\[ t = 0, \quad \varphi = \begin{cases} \varphi_{sw}(x), & 0 \leq x < X_{sw}, \\ \varphi_0, & X_{sw} \leq x < X_{cl}, \\ \varphi_{cl}, & X_{cl} \leq x < +\infty, \end{cases} \]

Here \( \varphi = \{\rho_1, \rho_2, \rho_3, \rho_{u1}, \rho_{u2}, \rho_{u3}, \rho_{E1}, \rho_{E2}, \rho_{E3}\} \) is the vector of the solution, \( \varphi_{sw}(x) \) are the parameters behind the SW front in the gas, \( X_{sw} \) is the initial location of the shock wave, \( \varphi_0 \) are the parameters of the initial state ahead of the SW front in the gas, and \( \varphi_{cl} \) are the parameters of the initial state.
of the mixture in the cloud; \( X_{cl} \) determines the cloud boundary. The density of particles outside the cloud equals zero (\( \rho_2 = \rho_3 = 0 \) for \( x < X_{cl} \)). The density of particles in the cloud corresponds to the stoichiometric point \( \rho_{p0} = 1.34 \text{ kg/m}^3 \). The gas and particles have zero initial velocities ahead of the SW front and in the cloud. The content of the polydisperse mixtures are characterized by the relative particle concentrations \( \eta_i = \frac{\rho_{i+1}}{\rho_{p0}} \), \( \rho_{p0} = \sum_{i=2}^{N_{i+1}} \rho_{i0} \), \( N \) is the number of fractions.

The Euler equations are solved with application of the TVD scheme for gas and the Gentry-Martin-Daly scheme for the particle fractions. The numerical techniques has been tested in [8, 9] on one-dimensional and two-dimensional problems of detonation initiation and propagation.

Formation of cellular detonation is modeled as a result of development of weak waves generated by a local perturbation of particle density on the particle cloud edge at interaction with the initiating shock wave in gas similarly [4, 5]. In this formulation stable propagation of the plane detonation front during long time in two-dimensional calculations is possible too.

### Cellular and planar detonations in three-fraction mixtures

The results of computations in the channel 0.66 m in width for three-fraction mixtures of particles with diameters of 1 \( \mu \)m, 2 \( \mu \)m, and 3.5 \( \mu \)m are shown in Figs. 1 and 2. Different values of the middle fraction saturation \( \eta_2 \) were considered (it remained dominant in all cases), it was also assumed that \( \eta_i = \eta_3 = 0.5(1 - \eta_2) \).

Figure 1 presents the maximum pressure patterns \( p_{\text{max}}(x,y) = \max_{t} [p(x,y,t)] \) for a steady regime of the cellular detonation propagation. The gray scale, which is the same for all patterns, is shown in Fig. 1, a. Comparing figures 1, a-d one can see that the reduction of the dominating fraction concentration leads to the cellular detonation degeneration similarly to the process occurring in bi-dispersed gas-particle mixtures. A reduction of the contrast of figures is observed, the maximum pressure monotonously drops with increasing \( \eta_2 \) at a collision of triple points. So it amounts to 147 at in the monodisperse gas-particle mixture of 2 \( \mu \)m particles and drops in three-disperse gas-particle mixtures to 113 at for \( \eta_2=0.8 \), to 85 at for \( \eta_2=0.6 \), and to 73 at for \( \eta_2=0.5 \). The cell size varies very weakly: in Figs. 1,b and 1,c the number of cells is the same as in Fig. 1,a, but they are nonuniform to a larger extent than in a monodisperse gas-particle mixture. In Fig. 1,d the cells are uniform, however, they are larger (3.5 cells per the channel width instead of 4).

![Cellular and planar detonations in three-fraction mixtures](image)

Fig. 1. Composition influence on cellular detonation patterns in three-fraction gas-particle mixtures of 1 \( \mu \)m, 2 \( \mu \)m, and 3.5 \( \mu \)m particles: \( \eta_2=1 \) (the monodisperse mixture 2 \( \mu \)m, a); \( \eta_2=0.8 \) (b); \( \eta_2=0.6 \) (c); \( \eta_2=0.5 \) (d).
Figure 2 shows the gas density profiles at the channel wall for two moments of time with the interval of 0.1 ms. The data in Fig. 2,a are shown for \( \eta_2 = 0.8 \) (dashed lines) and \( \eta_2 = 0.6 \) (solid lines), and in Fig. 2,b for \( \eta_2 = 0.5 \) (dashed lines) and \( \eta_2 = 0.4 \) (solid lines). One can see here the profile flattening (the reduction of fluctuation amplitude) at a reduction of the middle fraction concentration. The fluctuations are insignificant for \( \eta_2 = 0.5 \), and for \( \eta_2 = 0.4 \) they are absent completely, that is the profile corresponds to the one-dimensional flow of a planar detonation wave (the maximum pressure is 49.6 at). In this case, the transverse waves do not arise and the cellular detonation does not develop. Thus, at a considerable dispersion of particles, the complete degeneration of cellular detonation (as also in some bi-disperse gas-particle mixtures [5]) takes place.

Figure 3. Cellular detonation in a monodisperse gas-particle mixture of 3 \( \mu \)m particles (a) and in five-fraction gas-particle mixtures: \( \eta_3 = 0.7 \) (b); \( \eta_3 = 0.5 \) (c).
Cellular and planar detonations in five-fraction mixtures

Similar computations were carried out in the channel of the same width (0.066 m) also for five-fraction gas-particle mixtures with particles of 1 μm, 2 μm, 3 μm, 4 μm, and 5 μm diameters. The distribution function of particles over their sizes was also assumed symmetric: $\eta_1 = \eta_3$, $\eta_2 = \eta_4$, $\eta_5 = 1 - 2 \eta_1 - 2 \eta_2$, the $\eta_1$, $\eta_2$ values were varied. The trend of the cellular detonation degeneration with increasing dispersion of particles is quite similar to the case of the three-fraction gas-particle mixture, which is illustrated by the data presented in Figs. 3 and 4. Figure 3 shows the patterns of the maximum pressure history in the monodisperse mixture of particles with mean size of 3 μm, which are similar to Fig. 1 (Fig. 3,a) and in five-fraction mixtures for $\eta_1 = 0.05$, $\eta_2 = 0.1$, $\eta_3 = 0.7$ (Fig. 3,b) and for $\eta_1 = 0.1$, $\eta_2 = 0.15$, $\eta_3 = 0.5$ (Fig. 3,c). Here 2 nonuniform cells with the size of 3.3 cm are formed in the monodisperse gas-particle mixture, which takes place at a non-coincidence of the channel width and the multiple number of “natural” cells [4]. (The cell size at the detonation propagation in a fairly wide channel amounts to 3.9 cm according to the formula obtained in [4] by generalizing a large number of computed data.) The maximum pressure at the collision of triple points nevertheless amounts to 149.5 atm. When the particles of another size appear in the mixture composition (at a respective reduction of the middle-fraction share) the strength of transverse waves reduces, and the maximum pressure drops to 79 atm for $\eta_3 = 0.7$ (Fig. 3,b) and 64 atm for $\eta_3 = 0.5$ (Fig. 3,c). This manifests itself in a reduction of the contrast of the figures plotted by using the unified grayscale.

A further reduction of the share of 3 μm particles leads to a complete vanishing of cells and to a stable propagation of the planar detonation front similarly to detonation flows in bi-dispersed and three-disperse gas-particle mixtures. Figure 4 shows the pressure profiles on the channel wall with time step of 0.1 ms, solid lines correspond to the composition $\eta_1 = \eta_3 = \eta_4 = 0.2$, dashed lines correspond to $\eta_1 = 0.1$, $\eta_2 = 0.2$, $\eta_3 = 0.4$. In both cases, no signs of transverse wave flows are observed.

Thus, the cellular detonation from small perturbations does not develop in considered many-fraction gas-particle mixtures with the middle fraction share of no more than 40%.

Acoustic analysis of the detonation flows

Some foundation for this phenomenon may be derived from the acoustic analysis of the structure of detonation waves by the method of [10]. The method of [10] was applied in [4] for estimation of the detonation cell size in a monodisperse stoichiometric mixture of aluminum particles in oxygen and a good agreement with the data of numerical modeling of cellular detonation was obtained. A similar approach enabled in [5] the explanation of the phenomenon of the “degeneration” and “vanishing” of cells in bi-disperse gas-particle mixtures.

The method of [10] consists of determining the distance between the transverse waves following one another from the following considerations. The primary disturbance of the planar detonation...
wave front (the “hot point”) gives rise to a diverging cylindrical acoustic wave. Due to the diffraction, refraction, and partial reflection of this wave in a nonuniform flow field, part of disturbances returns to the front, giving rise to two “hot” points equidistant from the initial perturbation. The location of these points is determined from the solution of the corresponding acoustics problem. According to [10], the cell transverse size is the integral

$$\lambda_{ac} = 4 \int_{x_1}^{x_2} \frac{c_f}{\sqrt{\sigma^2 - (c_f^2 - u_1^2)}} \, dx.$$  

For a two-phase mixture with a low volume concentration of particles, $c_f$ is the frozen sound velocity (the velocity of the propagation of small disturbances in gas), $u_1$ is the gas velocity in the front-fitted system, $\sigma_*$ is a constant. The $x_1$ point coincides with the frozen shock wave front, the $x_2$ point corresponds to the condition $\sigma_* = c_f^2 - u_1^2$. The $\sigma_*$ value is determined as the value ensuring the minimum of the time integral

$$t(\sigma_*) = \min_{\sigma} \int_{x_1}^{x_2} \frac{c_f \sigma}{\sqrt{\sigma^2 - (c_f^2 - u_1^2)}} \, dx.$$  

The values of integrals are determined by the behavior of function $c_f^2 - u_1^2$. Examples of characteristic functions $c_f^2 - u_1^2$ for three-fraction (1 $\mu$m, 2 $\mu$m, and 3.5 $\mu$m) and five-fraction (1 $\mu$m, 2 $\mu$m, 3 $\mu$m, 4 $\mu$m, and 5 $\mu$m) mixtures are presented in fig. 5. The data for monodisperse gas-particle mixtures of the mean size 2 $\mu$m (fig. 5,a) and 3 $\mu$m (fig. 5,b) are shown by dashed lines for comparison. As can be seen, the dashed lines (monodisperse gas-particle mixtures) are characterized by two points of the local maximum. If the constant $\sigma_*$ coincides with the value of function $c_f^2 - u_1^2$ at one of them, then the integral diverges. In the interval, the integral is finite, and there is a value $\sigma_*$, at which the minimum is reached.

In Fig. 5, curves 1, 2, and 3 correspond to the mixtures with a decreasing value of the middle fraction concentration: $\eta_2 = 0.8, 0.6, \text{ and } 0.4$ for three-fraction (fig. 5,a), $\eta_3 = 0.7, 0.4 \text{ and } 0.2$ for five-fraction mixtures (fig. 5,b).

It is seen that with the increasing dispersion of particles (the reduction of the concentration of predominant middle fraction) the shape of curves changes. In fig. 5, a curves 1 and 2 have two points of the local maximum (the distance between transverse waves is determined), and the shape of curve 3 does already not enable the determination of the detonation cell size. The results completely agree here with the numerical modeling data: the cellular detonation forms for $\eta_2 \geq 0.5$ (fig. 1) and does not form for $\eta_2 = 0.4$ (solid lines in fig. 2, b).
In fig. 5,b all solid lines are characterized by a single point of local maximum. Thus, the distance at which the transverse waves following one another must form, is not determined. At the numerical modeling of the same five-fraction gas-particle mixtures the cellular detonation does not form here for $\eta_3 = 0.4$ and $\eta_4 = 0.2$ (fig. 4), although it develops in a degenerate form for $\eta_3 = 0.7$.

On the whole, both the numerical modeling data and the acoustic analysis results point to a difficulty in the cellular detonation formation in polydisperse gas-particle mixtures at a considerable dispersion in the distribution of particles over their sizes.

Conclusions
The cellular detonation formation in polydisperse mixtures of fine aluminum particles in oxygen has been investigated by the methods of numerical modeling and acoustic analysis of detonation flows. The following peculiarities have been established:

1. Cellular detonation formation is possible by the technique of the development of small disturbances at the planar detonation front

2. The cellular detonation degeneration takes place in polydisperse mixtures at a considerable dispersion in the distribution of particles over their sizes. This property is invariant under the number of fractions. In some mixtures, cellular structures do not form at a middle fraction content being not higher than the critical value (0.4 both for three-fraction and for five-fraction mixtures).

3. The results of numerical modeling are confirmed practically in all cases by the data of an acoustic analysis of corresponding detonation structures. This analysis enables one to establish the existence or absence of a reference scale determining the detonation cell size.

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