Modeling the detonation propagation in nanodisperse mixture of aluminum particles in channels with expansion

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Abstract. The problem of detonation propagation in channels with linear expansion filled with nano-sized aluminium mixture dispersed in oxygen was investigated. Transition from diffusion to kinetic regime of combustion with variation of the activation energy was taken into account in the description of the chemical reactions. Specific features of detonation failing in subcritical regimes and propagation in critical regimes have been revealed. The detonation propagation was found to be more unstable than in microdisperse aluminum suspensions.

1. Introduction
Studies of the propagation of detonation waves in volumes of complex geometry are of interest both from the standpoint of preventing the consequences of explosions and in application to the development of detonation engines. Detonation capacity of oxygen and air suspensions of aluminum powders is confirmed experimentally in [1], [2]. The properties of detonation were studied in a variety of theoretical and numerical studies, for example, [3], [4], [5], [6], [7]. Essential differences in the critical propagation properties behind the backward step from analogous gas detonation flows were analyzed in [8], [9], [10]. The peculiarities of the propagation of detonation of microdispersed powders in channels with linear expansion were discussed in [11], [12]. The physicochemical properties of ultradisperse aluminum powders strongly depend on the particle size. An overview of data on the ignition and combustion of microsize and nanosized aluminum particles is given in [13]. According to the data given in [13], when the particle size is less than 1 μm, aluminum combustion occurs in a transition mode from diffusion-limited combustion (inherent to coarse particles) to the kinetic combustion of nanoparticles. This transition is accompanied by a change in the dependence of the burning time of the particle on its diameter, and also on the temperature and pressure of the surrounding gas. On the basis of number of data presented in [13], a model of detonation of nanodispersed aluminum suspensions was constructed in [14], where, in particular, the activation energy of the reduced combustion kinetics of particles of the order of 50 - 100 nm is determined to be 60 kJ/mol, and data on stationary structures were obtained. In [15], [16], cellular detonation flows in plane channels were analyzed, where differences were also found from microdispersed suspensions, in particular, the irregularity of cellular structures and the enlargement of the cell. It is of interest to study the propagation of this type of detonation in expanding volumes.
2. Physical and mathematical model

Euler equations for two-dimensional flows of a two-phase medium follow from the laws of conservation of mass, momentum, and energy, and are presented in [15]. The closing relations express the equations of state of an ideal gas, the laws of interphase interaction and the laws of detonation combustion of aluminum suspensions. For this, the previously developed semiempirical models of detonation of microsized [4, 5] and nanosized [14], [15] suspensions of aluminum particles in oxygen are used. Combustion is described within the framework of reduced Arrhenius-type kinetics. The change in the combustion regime of aluminum particles from the diffusion-limited to the kinetic regime is taken into account. As in [16], the dependence of the characteristic burning time of aluminum particles in the submicron range from 135 nm to 1 μm is taken as:

\[ \tau_d = \tau_0 (d / d_0)^{0.3} \exp(E_a / RT_1)(p / p_0)^{-m}, \]  

(1)

where \( m = -0.25 \ln d [\mu m] \), \( E_a = 0.5 \{ E_{micro} (2 + \ln d[\mu m]) - E_{nano} \ln d[\mu m] \} \), and \( E_{micro} \) is the activation energy for micron particles (32 kJ/mol [5, 7-10]), \( E_{nano} \) is the activation energy for nanoparticles (60 kJ/mol [14, 15]), \( p \) is pressure, and \( d \) is the particle diameter.

3. Formulation of the problem

The channel geometry is shown in Fig. 1. We consider a plane detonation wave, which is located at the initial instant at a distance \( L_1 \) from the left boundary of the region under consideration. The initial gas pressure is 0.1 MPa, gas temperature is 300 K, the detonation velocity in stoichiometric mixture of aluminum particles in oxygen is 1.6 km/s. The position of the expansion angle is at a distance \( L_2 \). The magnitude of the expansion angle varied from 15 to 60 degrees.

![Figure 1. Scheme of the computation domain.](image)

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. The step of the finite-difference grid was determined according to the scale of the relaxation zones, varied in the test calculations. For calculations in the region shown in Fig. 1, the grid was constructed in such a way that the nodes hit exactly on the boundary, including the inclined wall.

4. Numerical results

As in previous analogous studies for micro-sized suspensions [8], [10], [11], [12] in the expanding region, depending on the geometric parameters of the channel, three propagation modes are possible:
subcritical (detonation failure), critical (with reconstruction in transverse waves) and supercritical (continuous propagation).

![Figure 2](image)

**Figure 2.** Detonation development in the channel with \( H=0.02 \) m, \( \alpha=45^\circ \), \( d=200 \) nm. \( t=0.08 \) ms (a), 0.12 ms (b), 0.21 ms (c), 0.3 ms (d). Schlieren images: (a) – (c); maximal pressure fields (d).

*The subcritical regime* is realized in a monodisperse mixture of particles with a diameter of 200 nm at \( H = 0.02 \) m and a wall angle of 45°. The Schlieren images (Figure 2) show that at initial moments of time, transverse waves develop in the plane of symmetry (Figure 2a), and in the region near the inclined wall the combustion fronts and the shock wave are separated. Subsequently, transverse waves continue to develop in the plane of symmetry, but on a greater part of the leading front of the DW (detonation wave), the combustion front lags behind the shock wave (Fig. 2b). At the moment of 0.21 ms (Figure 2c), the combustion front is separated from the shock wave over the entire section. On the surface of the combustion front, it can be seen that there are pronounced curvatures due to the action of transverse waves and the development of Richtmyer-Meshkov instability. These transverse waves can be seen in the picture of maximum pressures (Figure 2d) in the plane of symmetry at the beginning
of the expansion section. However, none of the sections of the combustion front interacts with the leading front of the shock wave, re-initiation of detonation does not occur, and the transverse waves decay rather rapidly.

**Critical regime.** As the channel width increases to $H = 0.06 \text{ m}$, a transition to the critical flow regime occurs (Fig. 3). Here, the development of transverse waves initially occurs according to the same scenario as in the subcritical regime, but they do not attenuate. It leads to the formation of cellular structures in the plane of symmetry. Later on, a separation of the fronts of combustion and the shock wave takes place at a section near the inclined wall, but in the middle part of the channel in sufficiently strong transverse waves, detonation is restored. Here it can be noted that unlike microdispersed suspensions, in the areas between divergent transverse waves there is no generation of a set of secondary transverse waves. This is due to higher values of the activation energy of the combustion reaction and the enlargement of the detonation cell (Fig. 3a). Nevertheless, the propagation of detonation in the regime of alternation of breakdown and re-initiation areas continues. In Fig. 3b, the propagation of the transverse wave in the region $x = 0.24 \text{ m}$ moving toward the wall is clearly visible, which propagates and re-initiates detonation in the given region, and at a small distance from the transverse wave, the detonation occurs near the center of the region and the combustion front lags behind the shock wave.

![Figure 3. Detonation development in the channel with $H=0.06 \text{ m}$, $\alpha=45^\circ$, $d=200 \text{ nm}$, $t=0.3$ ms. Maximal pressure field (a), Schlieren image (b).](image)

In general, a similar mechanism is observed for the channel at $30^\circ$ and $60^\circ$. Re-initiation of the DW occurs in transverse waves, which are formed in the plane of symmetry (Fig. 4). For an inclination angle of $30^\circ$ in the fields of maximum pressure, it is seen that a cellular structure is formed near the plane of symmetry (Fig. 4a), due to a sufficiently strong transverse wave, re-initiation of detonation occurs on the inclined wall. And on the leading front, transverse waves are formed. For the channel $H = 0.1 \text{ m}$, $\alpha = 60^\circ$ (Fig. 4b), the cellular structure is observed in the plane of symmetry, and the propagation of detonation waves occurs near the inclined wall. From the plane of symmetry, transverse waves propagate at the leading edge of which the re-initiation of the DW occurs. At some points, transverse waves collide and the triple points, where the pressure exceeds 150 atm form.
The mechanism closest to the detonation propagation in micron particles was obtained at a wall inclination angle of 15°. The width of channel $H$ was 0.02 m. Figure 5 shows the maximal pressure field in the channel. It can be seen that at the beginning of the expansion a transverse wave forms on an inclined wall, after which re-initiation of detonation in the plane of symmetry occurs. At $0.13 < x < 0.16$ m, the pressure in the plane of symmetry is below 50 atm, which indicates a partial detonation detachment. Re-initiation occurs in a transverse wave and it is seen that in the plane of symmetry at $x = 0.18$ m, the pressure rises to 150 atm and higher, which indicates intense combustion of aluminum particles. Later in transverse waves the pressure is more than 100 atm, while in the channel an irregular cellular structure is formed. The propagation of this detonation wave is unstable. It can be seen that on the leading front there are sections where the pressure does not exceed 50 atm, which indicates the detonation failure. Re-initiation here will occur in strong transverse waves propagating along the surface of the leading detonation front.

Figure 4. Maximal pressure fields: $H=0.05$ m, $\alpha=30^\circ$, $d=200$ nm, $t=0.19$ ms (a); $H=0.1$ m, $\alpha=60^\circ$, $d=200$ nm, $t=0.25$ ms (b).

Figure 5. Maximal pressure fields, $H=0.02$ m, $\alpha=15^\circ$, $d=200$ nm, $t=0.23$ ms.
5. Conclusions
Numerical modeling of two-dimensional detonation flows reveals the peculiarities of heterogeneous detonation propagation in flat channels with a linear expansion area. Monodisperse suspensions of aluminum particles in oxygen in the range of particle sizes from 200 nm to 1 μm are considered. It is established that the propagation patterns generally correspond to the detonation of microdispersed suspensions. The following propagation modes are revealed: subcritical (with detonation failure) and critical (with disruption and recovery in transverse waves). The supercritical regime (with continuous propagation) is not obtained with the parameters considered. In subcritical regimes, the development of a decaying detonation is characterized by the appearance and amplification of fluctuations in the shape of the combustion front behind the shock wave, which indicates the development of instability. In critical regimes, the initial number of transverse waves is reduced, the detonation cell is enlarged and the detonation is highly unstable. The propagation of detonation in the expanding channel is accompanied by numerous disruptions with a significant weakening of the leading shock wave. The restoration to the amplitude values exceeding the values of the Chapman-Jouguet waves occurs only in strong transverse waves after their reflection from the walls. These properties are due to transition from the diffusion regime of aluminum particle combustion to the kinetic one with a decrease in particle size, which is accompanied by an increase in the activation energy of the reduced kinetics.

Acknowledgements
The work was supported by the Russian Science Foundation (grant No. 16-19-00010).

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