NUMERICAL MODELING OF DETONATION PROPAGATION IN GAS-PARTICLE MIXTURES IN THE DUCT WITH A CROSS-SECTIONAL BREAKDOWN

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Introduction

A combustible dust explosion hazard may exist in a variety of industries, including: wood, coal, metals, etc. Finely dispersed airborne organic or metallic dust can be especially explosive when confined in a duct or building, since ignition is able to initiate a detonation process that intensifies due to repeated wave reflections from the walls. All this generates a necessity to investigate a behavior of detonations in gas-particle mixtures in confined vessels (ducts). Another field of application of the problem is concerned with development of detonation engines based on utilization of fine-dispersed suspensions in combustion chambers. Thereby investigation of detonation regimes in channels of complex geometry and influence of the mixture parameters on detonation characteristics present great interest.

Diffraction of detonation waves is one of the fundamental problems in gas dynamics and mechanics of multi-phase media. The diffraction of a detonation wave at a sudden expansion of a planar channel is of especial interest since such a configuration is typical of technological devices.

The processes of diffraction of shock waves in gas-particle mixtures are more complex than in gas mixtures. The flow pattern is characterized by an influence of the processes of relaxation of velocities and temperatures of both phases. Typical extensions of these relaxation processes are determined by the particles size.

Detonation flows are characterized by additional geometric scales, which are determined by chemical processes – the ignition delay (induction) and combustion. It is pointed out in [1] that the chemical processes occurring in the detonation wave lead to a loss of self-similarity of the flow in gaseous mixtures unlike similar processes of shock-wave diffraction in inert media.

It is also known for gases that the variation of the ratio of reaction zone length and the reference geometric parameter of the configuration gives rise to qualitatively different flow regimes. In the regimes with detonation failure behind the backward-facing step, a re-initiation is possible at the expense of the diffracted wave reflection from the wall of a channel wide part with a further merging of the shock wave and combustion front. Detailed flow patterns in such a regime, which agree well with experimental Schlieren photographs, were obtained in [2] by the numerical modeling methods. Three regimes of detonation propagation at a diffraction of a planar detonation wave on the backward-facing step were analyzed numerically in [3]. These regimes were termed as a subcritical one (complete detonation failure), critical one (a partial failure with re-initiation), and a supercritical one (continuous propagation). The passage from one regime to another was associated with the variation of the amount of activation energy (which causes also a variation of the reaction zone length). A possibility was indicated for the formation of a system of transverse waves at the detonation front in one of the regimes.

The results of similar investigations for gas-particle mixtures are very scarce. The detonation propagation processes in gas-particle mixtures of the particles of a unitary fuel in pipes with a sudden expansion were analyzed in [4]. A considerable influence of the mass load of the mixture on the value of critical ratio of pipe diameters for detonation failure prevention was found. A detailed structure of the two-phase mixture flow was, however, not presented, and the influence of the particle mass loading on the process was not studied. Detonation wave diffraction processes in a
two-phase medium were studied numerically in [5] on a backward-facing step, including also a rectangular one. A powder-like explosive characterized by a high detonation speed (7600 m/s) was considered. Results showed the flow patterns qualitatively similar to gaseous mixtures, although the authors determined the mean parameters of the mixture without identification of phases. Thus, the propagation of shock and detonation waves in heterogeneous media in regions of complex geometry was practically not investigated, especially from the viewpoint of the influence of relaxation processes of interphase interaction.

In the present work, we investigate by the numerical modeling methods the processes of the diffraction of detonation waves on the cross-sectional jump of a planar channel in the mixtures of fine aluminum particles and oxygen. In view of the absence of reacting components of gaseous mixture, the detonation is due to only a heterogeneous reaction of the oxidation of aluminum particles.

The purpose of the work is determination of the influence of particles size and of the channel geometric characteristics on the wave pattern and the detonation flow development at a diffraction of detonation waves.

**Formulation of the problem**

Consider a flat duct with an abrupt expansion of the cross section filled with a homogeneous mixture of oxygen and fine aluminum particles. Assume that the duct is symmetric with respect to the $X$ axis, therefore, it sufficient to consider its upper or bottom part (Fig. 1). A self-sustained planar detonation wave with an adjacent rarefaction wave propagates in the gas-particle mixture along the duct. We investigate the process of a passage of this wave from the narrow part of the duct into the wide part assuming its large transversal size. In the flow scheme (Fig. 1): $L_1$ is the location of wave front at the initial moment of time, $L_2$ is the length of the duct narrow part, $L$ is the computational region length, $H_1$ is the transverse size of the duct narrow part, $H_2$ is the transverse size of the duct wide part, $H_2 >> H_1$.

![Fig.1. The flow scheme](image)

The mathematical model of the detonation of aluminum particles in oxygen, which was developed in [6, 7], was verified by experimental data of [8]. The model is based on the concepts of a two-velocity two-temperature continuum of the mechanics of heterogeneous media. The aluminum combustion is described in the form of a reduced reaction initiated after the particle achieves a critical temperature (the ignition temperature) and accounting for an incomplete combustion of particles (due to the oxide film growth). The values of involved parameters (ignition temperature, activation energy, heat release, and chemical reaction velocities) were determined from the agreement with experimental data on detonation velocity and the length of zones of the ignition and combustion delay. The model agrees with data of [8] on the dependence of the stationary detonation velocity on particle concentration. The characteristic time of the aluminum particle combustion in oxygen agrees with the data presented in [9, 10]. The ignition temperature value determining the induction time was set to be close to the value adopted in [11]. A theoretical analysis of steady detonation structures was carried out in [6, 7, 12], the results computed for parameters in the Chapman—Jouguet plane agree with experimental data of [8] also in terms of the

The flows in gas-particle mixtures are governed by the system of Euler equations following from the laws of conservation of mass, momentum, and energy of each phase:

\[
\frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho_i u_i)}{\partial x} + \frac{\partial (\rho_i v_i)}{\partial y} = (-1)^{i-1}J
\]

\[
\frac{\partial \rho_i u_i}{\partial t} + \frac{\partial [\rho_i u_i^2 + (2-i)p]}{\partial x} + \frac{\partial [\rho_i v_i u_i]}{\partial y} = (-1)^{i-1}(-f_x + Ju_2)
\]

\[
\frac{\partial \rho_i v_i}{\partial t} + \frac{\partial (\rho_i u_i v_i)}{\partial x} + \frac{\partial [\rho_i u_i^2 + (2-i)p]}{\partial y} = (-1)^{i-1}(-f_y + Jv_2)
\]

\[
\frac{\partial \rho_i E_i}{\partial t} + \frac{\partial (\rho_i u_i (E_i + (2-i)p/\rho_i))}{\partial x} + \frac{\partial (\rho_i v_i E_i + (2-i)p/\rho_i)}{\partial y} = (-1)^{i-1}(-q - f_x u_2 - f_y v_2 + JE_2)
\]

The model is closed by equations of state with allowance for the fact that the volume concentration of particles is small

\[
p = \rho_i RT_1, E_i = (u_i^2 + v_i^2)/2 + c_v,iT_i + (i-1)Q,
\]

the laws of velocity and heat exchange between the phases

\[
\bar{f} = \frac{3m_2P_{11}}{4d} c_D \left[ \bar{u}_1 - \bar{u}_2 \right] \left[ \bar{u}_1 - \bar{u}_2 \right], \quad q = \frac{6m_2\lambda_1}{d^2} Nu(T_1 - T_2),
\]

and the equation of reduced chemical kinetics

\[
J = \frac{\rho_i}{\tau_\xi} \max(0,(\xi - \bar{\xi})) \exp(-E_a / RT_2) \text{ at } T_2 \geq T_{ign};
\]

\[
J = 0 \text{ at } T_2 < T_{ign}.
\]

The interphase interaction processes are described by the correlation matched with experimental data on the trajectories of particles motion behind shock waves [15]. The approximation \( \text{Nu} = 2 + 0.6 \text{Re}^{1/2} \text{Pr}^{1/3} \) is accepted for the Nusselt number versus the Reynolds and Prandtl numbers, and the formula

\[
c_D(\text{Re}, M_{12}) = \left( 1 + \exp \left( -\frac{0.43}{M_{12}^{4.67}} \right) \right) \times \left( 0.38 + \frac{24}{\text{Re}} + \frac{4}{\sqrt{\text{Re}}} \right)
\]

is used for the drag coefficient, where Reynolds and Prandtl numbers are defined as

\[
\text{Re} = \frac{\rho_{11}d |u_1 - u_2|}{\mu}, \quad M_{12} = \frac{|u_1 - u_2|}{\sqrt{\gamma_1 p}}.
\]

(The drag coefficient determined by formula (5) is shown by computations to differ little in detonation flows from the one determined by the known Henderson formula [16]).
In formulas (1)–(5), \( p \) is the pressure; \( \rho_i, u_i, v_i, T_i, E_i \), and \( c_{v,i} \) are the mean density, the longitudinal and transverse velocity components, the temperature, the total energy per unit mass, and the specific heat of the \( i \)th phase \((i = 1, 2)\), respectively. The relative mass concentrations of gas (subscript 1) and particles (subscript 2) are defined as
\[
\xi_i = \frac{\varphi_i}{\rho_i}, \quad \rho = \sum_i \rho_i, \quad \rho_i = \rho_0 m_i,
\]
where \( \rho_i \) and \( \rho_0 \) are the mean and true density of each phase, respectively, \( m_i = \frac{\rho_i}{\rho} \) is the volume concentration of the \( i \)th phase, \( \xi_i \) is the minimally allowed (remaining after the burn-out) fraction of particles, \( d \) is the particle diameter, \( c_D \) is the drag coefficient of particles, \( \lambda_t \) is the thermal conductivity of gas, \( \text{Re}, \text{Nu}, \text{Pr} \) are the Reynolds, Nusselt, and Prandtl numbers, \( \mu \) is the gas viscosity, \( \gamma_1 \) is the gas adiabatic exponent, \( E_a \) is the activation energy, \( T_{ign} \) is the ignition temperature, \( \tau_\xi \) is the typical combustion time.

The initial values of parameters of the mixture were taken identical to those used in [12, 13]:
\[
\rho_0 = 1 \text{ atm}, \quad T_0 = T_{20} = 300 \text{ K}, \quad \text{Pr} = 0.7, \quad c_{v,1} = 914 \text{ J/(kg·K)}, \quad c_{v,2} = 880 \text{ J/(kg·K)}, \quad T_{ign} = 900 \text{ K}, \quad E_a = 10^6 \text{ J/kg}, \quad Q = 2.94 \times 10^6 \text{ J/kg}, \quad \xi_0 = 0.55, \quad \rho_{20} = 1.34 \text{ kg/m}^3.
\]
The particle size was varied within 1–5 \( \mu \)m. For the constant determining the reaction rate of particle combustion, we use the formula \( \tau_\xi = \tau_0 (d/d_0)^2 \) with \( \tau_0 = 0.0024 \text{ msec}, \quad d_0 = 10 \mu \text{m}, \quad E_a = = 10^6 \text{ J/K} \) in accordance to [13]. The quadratic dependence of combustion time on the particle diameter for combustion of aluminum in oxygen is confirmed by the data presented in survey [10]. The value \( \tau_0 \) ensures the agreement with data of [9] on the duration of aluminum particle combustion in pure oxygen.

The system (1) – (5) is solved under the following initial conditions:
\[
t = 0, \quad \phi = \begin{cases} \phi_l, & 0 < x < L_1, \\ \phi_0, & L_1 < x \leq L, \end{cases}
\]
where \( \phi = \{\rho_1, \rho_2, \rho_1 u_1, \rho_2 u_2, \rho_1 v_1, \rho_2 v_2, \rho_1 E_1, \rho_2 E_2\} \) is the solution vector, \( \phi_l \) is the solution corresponding to a steady planar detonation wave, \( \phi_0 \) is the initial state ahead of the front.

**Computational method**

To solve the equations a numerical method which was tested on 1-D and 2-D problems of detonation initiation and propagation in [17, 18] and applied successfully in [13, 19] was taken as the basic method for computation. The method includes the Harten TVD scheme for the gaseous phase equations and the Gentry—Martin—Daly upwind difference scheme for the solid phase dynamics. For convenience of numerical realization of the two-dimensional TVD scheme in the volume of combined geometry, a planar channel of maximum width is taken as the computational domain. At each time step, the computation is performed in the entire region. After that, the boundary values on the walls of the channel narrow and wide parts are re-determined according to the slip and thermal insulation conditions.

The channel narrow part length is assumed to be rather extended. Here in the region near the left boundary the flow corresponding to the expansion wave is nearly one-dimensional and directed outside the region \((u_{1,2} < 0)\), which enables the use of "soft" boundary conditions. The initial state is specified at the right boundary, the computation is continued until this boundary is reached by the front.

A uniform two-dimensional finite-difference grid with a step corresponding to \(2 \times 10^{-4} \text{ m}\), was used for computation, which ensures about 2 dozens of points per the minimum relaxation scale (the zone of particle combustion \(1 \mu \text{m}\) in diameter). The influence of grid parameters on the solution was analyzed in [17, 18].
Numerical results

Three different scenarios of detonation wave propagation in gas mixtures at a diffraction on a backward-facing step are established experimentally and described theoretically in [1-3]. A continuous propagation of the detonation front is possible (the supercritical propagation regime), a complete detonation failure (the subcritical regime) as well as a partial detonation failure with a subsequent re-initiation (the critical regime). The passage from one regime to another in the same gaseous mixture depends on the channel geometric parameters.

In heterogeneous detonation of a gas-particle mixture, the combustion zone scale is determined by the particles size. Besides, there are the zones of the velocity and thermal relaxation of phases in shock-wave and detonation structures. Therefore, the particles size may also affect the realization of this or that regime.

The problem of detonation wave diffraction on a backward-facing step in the gas-particle mixture was studied on the model of stoichiometric mixture of aluminum particles in oxygen with the particle diameter 1 $\mu$m, 2 $\mu$m, 3.5 $\mu$m. The channel width $H_1$ was varied from 0.01 m to 0.03 m.

Computation showed that similar three regimes are also possible in the gas-particle mixture: the regime with a complete detonation failure, with a partial failure, and with a continuous detonation propagation. The examples of detonation structures for each regime are presented in Fig. 2 (the supercritical regime), Fig. 3 (the subcritical regime), and Fig. 4 (the critical regime). The numerical schlieren images constructed from the gas density gradients are shown for several sequential moments of time.

![Detonation behaviour in the supercritical regime:](image)

d=1 $\mu$m, $H_1=0.01$ m, $t=0.14$ msec (a); 0.15 msec (b); 0.16 msec (c); 0.18 msec (d).

The detonation wave structure in a gas-particle mixture includes the leading SW, the zones of the velocity and thermal relaxation of phases, and the combustion zone. At continuous detonation propagation, the width of the detonation front structure does not change with time (although it depends on the particles size). At a partial detonation failure (in critical regimes) or at a complete detonation failure (in subcritical regimes, a separation of the combustion front and the leading SW
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occurs. In the critical regime, the temporal lag of combustion front takes place in an interval of the front (Fig. 4). In the subcritical regime, the separation of combustion front from the leading SW occurs along the entire front and has a constant character (Fig. 3).

As can be seen from the comparison of Figs. 2-4, the elements of the flow wave pattern are similar in the neighborhood of the expansion angle. The flow corresponds here also to similar flows of gaseous mixtures [3] since the particle concentration (remaining after their burn-out) is very low.

We also note that the general characteristics of the front behavior in each regime are similar with similar detonation flows in gases.

The formation of the primary transverse wave in critical regimes is also revealed in the diffracted wave interval (Fig. 2) as a consequence of a Mach configuration development near the wall. The appearance of secondary transverse waves related to peculiarities of the propagation of disturbances in flow structure is discussed in [3].

A separation of the leading front and the combustion front in subcritical regimes leads to the shock-wave weakening and the detonation process decay.

In critical regimes (Fig. 4), the wave front behind the expansion corner is subdivided into two intervals: the detonation one (in the neighborhood of symmetry plane) and the shock one with a lagging combustion front (adhering to the lateral wall). The wave propagation in transverse direction slows down, and the flow structure in the region behind the backward-facing step is similar to the subcritical regime case. The detonation front interval expands, becomes convex, and its part starts propagating towards the wall of the backward-facing step, involving the region of the non-burnt mixture between the diffracted SW and the lagging combustion front. After this
transverse wave reflects from the wall of the backward-facing step, the front propagation acquires the supercritical regime features.

Note the differences in wave pattern of the detonation flow from the gaseous detonation structures, which are related to the influence of processes of the relaxation of phases.

The flow patterns in a near-wall region behind the backward-facing step are different for mixtures with different particle sizes. This leads to differences in the combustion front formation. Figure 5 shows the instantaneous streamlines patterns for the mixtures with different particle sizes, in which the contours of the leading edge of combustion front (the contours of particle temperature \( T_2 = \text{ign} \)) are shown by thick lines. In the mixture of particles with \( d=3.5 \, \mu m \) (Fig. 5,a, \( H_1=0.03 \, m \), the subcritical regime) the width of the detonation wave structure is comparable with the forming vortex size. Part of gas and particles, which have not reached the ignition temperature, is entrained in the vortex motion in the reverse direction, which leads to a bend in the combustion front along the backward-facing step wall. As can be concluded from the comparison of Fig. 5,a and Fig. 3, the near-wall bend of the combustion front is preserved in the further development dynamics and leads to its stretching along the wall.

In the mixture with \( d=2 \, \mu m \) for \( H_1=0.005 \, m \), the regime is also subcritical, but the flow pattern in the near-wall region is different. The vortex zone and the complex of the leading SW with an adhering relaxation and combustion zone develop here separately. The combustion front does not stretch along the wall but sets against it (Fig. 5,b), although a small bend of the front forms. The contact discontinuity adhering to the bend point of the combustion front, which can be seen in Fig. 4, represents a remainder structure of a relaxation reflection of the near-wall wave (relaxation type of the SW reflection from the wall was noted in numerical computations in [20]).

![Fig. 5. Particles size influence on the wave pattern behind the backward-facing step: d=3.5 \, \mu km, H_1=0.03 \, m, t=0.14 \, ms (a); d=2 \, \mu m, H_1=0.005 \, m, t=0.16 \, ms (b).](image)

The influence of the particles size on transition from one regime to another is demonstrated in Fig. 6,a, where a map of the regimes of detonation propagation is presented in the plane of parameters: the channel width – the particle size. For each fraction of particles there exist theoretically the values of the channel width at which the given propagation regime realizes. For example, for the gas-particle mixture of 1 \, \mu m, the critical regime is identified in numerical computations for the channel width of 0.001 \, m, for 2 \, \mu m at the channel width of 0.015 \, m. Figure 6,b shows the graphs of the envelopes of the maximum pressure in the symmetry plane. Curves 1-2 point to detonation decay, and curves 3-5 point to the detonation process preservation. A temporary relaxation of detonation due to its interaction with the fan of expansion waves emanating from the expansion corner manifests itself in a temporal reduction of the peak values on curves 3-5. A subsequent growth serves the sign of a re-initiation of the detonation process. As can be concluded from the analysis of computational results, the realization of this or that propagation regime of the detonation wave depends on the ratio of scales of the channel geometry and scales of the zones of
relaxation processes (the velocity, thermal, and chemical relaxation) determined by the particles size.

![Diagram of parameters influence on detonation propagation regime](image)

**Fig.6.** Parameters influence on detonation propagation regime: detonation regime map (a); envelops of the maximum pressure (b), \(d=2 \, \mu m\), \(H_1= 0.005 \, m\) (curve 1), 0.01 m (2), 0.015 m (3), 0.02 m (4), \(H_1=0.03 \, m\) (5).

Thus, the difference of detonation propagation in gas-particle mixtures at their exit from the channel into ambient space from a similar process in gaseous mixtures lies in both the influence of mixture dispersion on propagation regimes and in the differences in flow structure behind the backward-facing step. These characteristic features are related with the effect of interphase interaction processes.

**Conclusions**

The processes of detonation wave diffraction in the gas-particle mixture on a backward-facing step at the exit of a planar channel were studied numerically. The following was established:

- As in gases, three regimes of detonation propagation are possible: the subcritical one (detonation failure), critical one (a partial failure with subsequent re-initiation), supercritical one (a continuous detonation propagation).
- The passage from one regime to another depends not only on the channel width but also on the particle size in the gas-particle mixture.
- There are differences in flow structures behind the backward-facing step, which are related to the influence of relaxation processes. In particular, the interaction of relaxation zones with the vortex zone in subcritical regimes at the expansion corner gives rise to various configurations of the combustion front bend in the region behind the backward-facing step.

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