

Cellular detonation diffraction in gas-particle mixtures

A. V. Fedorov · T. A. Khmel ·
Y. V. Kratova

Received: 29 October 2009 / Revised: 16 April 2010 / Accepted: 20 October 2010 / Published online: 16 November 2010
© Springer-Verlag 2010

Abstract Diffraction of cellular heterogeneous detonation out of a channel into open half-space in a mixture of aluminum particles and oxygen is investigated numerically. The flow is found to be very similar to gas detonation diffraction. The detonation weakening behind the step results in combustion front deceleration and decoupling from the leading shock wave. Subsequent re-initiation takes place in a transverse wave. New transverse waves are generated along the expanding front. The computations that were performed show that the critical number of cells is several times less than that for gases. This is confirmed by theoretical estimates based upon the Mitrofanov–Soloukhin approach.

Keywords Cellular detonations · Diffraction · Gas suspensions · Numerical modeling

1 Introduction

There is an urgent need of investigations on detonations in gas suspensions of small solid particles, both because of safety issues, and potential development of useful technologies. Industrial dust explosions are accompanied by shock and detonation wave propagation in spaces with complex

Communicated by L. Bauwens.

This paper is based on work that was presented at the 22nd International Colloquium on the Dynamics of Explosions and Reactive Systems, Minsk, Belarus, July 27–31, 2009.

A. V. Fedorov · T. A. Khmel (✉) · Y. V. Kratova
Khristianovich Institute of Theoretical and Applied Mechanics,
SB RAS, Institutskaya 4/1, 630090 Novosibirsk, Russia
e-mail: khmel@itam.nsc.ru

A. V. Fedorov
e-mail: fedorov@itam.nsc.ru

geometry, such as rooms, conveyors, transporters, channel, shafts, etc. One possible application of detonations is in propulsion. A new generation of engines could use dust suspensions as components of the working fluid. Therefore, analysis of the specific features of detonation wave propagations in confined volumes with complex geometry is of interest. The typical configuration is a channel with sudden expansion.

The problems of detonation transmission into an unconfined volume and propagation through channels or tubes with cross-section change have been studied extensively for gaseous mixtures. Discussion and analysis of theoretical and experimental results can be found in reviews [1–3].

Conditions for survival of the detonation process, while coming out of a tube or channel into an open space are expressed in terms of the tube diameter (or width of a rectangular channel) and the transverse size of the detonation cell. The experimentally obtained relation between critical tube diameter and cell size in gases is $n = d/\lambda = 10 \div 13$ [1]. A theoretical basis for this estimate has been provided by Mitrofanov and Soloukhin [4]. The initial statement is that the reaction behind the curved shock front decays when a change in the ignition delay time becomes of the order of the delay time itself. This results in the following relation on the minimal number of the transverse waves:

$$n < \left| \frac{d\tau}{dT} \right| \frac{4Tc}{\tau D}. \quad (1)$$

Here, c is the speed of sound and D is the detonation velocity. When the Arrhenius dependence of an ignition induction time on temperature $\tau = \tau_0 \exp(E/RT)$ is applied the decaying condition takes the form of $n < 4Ec/RTD$, which yields $n \sim 10$ in [4].

In [5], an expression for the critical channel width for a cylindrical re-initiation is proposed

$$l = \sqrt{\pi}d/4 \approx 0.4d. \quad (2)$$

The relationship (2) is confirmed by comparison with experimental results on detonation exit from a tube and a channel closed by a diaphragm with a rectangular orifice. Experiments in which both mixture properties and exit orifice parameters were varied have shown that when the detonation exits through a rectangular orifice with reduced size, the parameter $n = l/\lambda$ may decrease down to a magnitude of order $2 \div 3$.

A number of papers on numerical simulation of detonation wave diffraction in abrupt rectangular channel expansion (in plane 2D geometry) [6–9] confirms the mechanism of the re-initiation in the transverse waves of the cellular detonation is responsible for the detonation reconstruction behind the diffracted wave. The critical number of cells per channel width obtained in these computations is about three, which agrees both with estimations [5] and theoretical predictions [10]. The results of the calculations coincide also with [8] experimental data.

Other possible mechanisms for detonation propagation beyond area expansion are discussed in [11, 12]. In [11], on the basis of numerous experimental results for different mixtures an attempt to reveal a connection between the critical tube diameter and a critical radius of the initiation and propagation of spherical detonation is made. It has been shown theoretically that the re-initiation energy when a plane detonation exits a tube is comparable to the initiation energy of a spherical detonation. But the influence of the transverse waves characteristic of cellular detonations on the process was not investigated. In [12], results of theoretical and experimental study of the cellular detonation exit from a tube into an open half-space are presented. It turns out that the critical conditions for detonation process preservation for cellular detonation are very close to those obtained numerically in [13] for the similar problem of plane detonation exit. Therefore, the authors conclude that the interaction of the reaction zone with the rarefaction wave and the unsteadiness of the process also plays an important role in detonation propagation and failure, together with the transverse waves.

A large number of experimental and numerical studies on detonation propagation in confined volumes with variable geometry were performed in the context of the pulse detonation engine. Review and discussion of these investigations can be found in [14]. New experimental and numerical data on detonation propagation in channels with variable cross-section and obstacles have been obtained in recent papers [15–19].

Detonation propagation in gaseous suspensions of solid particles is characterized by a more complex wave structure than in gaseous mixtures. The interphase processes inherent

to heterogeneous detonations affect both detonation initiation and propagation in the diffraction process. The wave structure in heterogeneous detonation essentially differs from gas detonation due to different relations between induction and combustion zone length, and because of the processes of temperature and velocity relaxation. Therefore, identifying similarities and differences of corresponding diffraction processes in gases and gas-particle mixtures is interesting.

Numerical modeling of detonation propagation in gaseous suspensions of unitary fuel particles in a tube with variable cross-section has been performed in [20, 21]. Both continued detonation propagation, and detonation decay can take place. Transition conditions were obtained relating diameter ratios between narrow and wide parts of the tube, and mixture fraction.

In [22], the process of planar shock and detonation waves exit from a plane channel into unconfined volume was investigated numerically within the limits of proposed physical and mathematical models for heterogeneous detonation in aluminum particle oxygen suspensions. A comparative analysis with results of [13] has been performed, where the corresponding problem for gaseous detonations was considered. Existence of three different regimes of propagation of the heterogeneous detonation, also present in gaseous mixtures has been established: subcritical (detonation failure), critical (partial failure with subsequent re-ignition), and supercritical (continuous detonation propagation). Detailed analysis of the flow in each regime was performed in [23]. Essential differences of the flow structure behind the backward step in gas particle mixtures compared with gas mixtures, in particular, different configurations of the combustion front shape were revealed. These differences are related to the influence of the relaxation processes of phase interactions, with scales determined by the particle sizes. Therefore, the transition from one regime to another depends not only on geometrical parameters (width of the channel), but also on particle sizes. It has been established that in some cases there is a transition to a cellular detonation mode.

In [24], similar research was performed taking into account the effects caused by the presence of the walls in a wide part of the channel, and also influence of distribution of particle sizes in polydisperse mixtures. Possible scenarios of the flow evolution after reflection of the diffracted wave from the wall in different regimes was described and analyzed in [22, 23] and the influence of the geometrical parameters and particles sizes were studied.

The present work is an extension of the studies [22–24] and focuses on investigation of propagation of the cellular detonation in monodisperse aluminum particle oxygen suspensions in channels with an abrupt cross-section expansion. The purpose of the work is the analysis of cellular heterogeneous detonation diffraction on a backward step, including: (1) identification of detonation propagation scenarios; and

(2) analysis of the influence of particle size and geometrical channel parameters on the flow development in different regimes.

2 Problem formulation

The problem considers a flat channel with an abrupt expansion of the cross section, filled with a homogeneous stoichiometric monodisperse mixture of oxygen and fine aluminum particles. The channel is assumed to be symmetric with respect to the x axis; therefore, it is sufficient to consider its upper or lower part (Fig. 1). An established cellular detonation wave propagates along the channel in the gas-particle mixture. Passage of this wave from the narrow part of the channel to the wide part is investigated. The channel geometry is shown in Fig. 1: H_1 is the channel width.

We use the same model and numerical method as in [22–24]. The mathematical model for detonation of aluminum particles in oxygen was developed in [25, 26] and verified by comparison with experimental data [27]. The model is based upon the concept of a two-velocity two-temperature continuum of the mechanics of heterogeneous media. Aluminum combustion is described in the frame of a reduced chemical kinetic model that allows for incomplete particle burning due to the oxide film growth. The reaction initiates when particles achieve a critical temperature, i.e., the ignition temperature. The parameter values (ignition temperature, activation energy, heat release, and chemical reaction velocities) were determined from the experimental data which includes detonation velocity, ignition zone length, and combustion duration. Detailed descriptions of the physical and mathematical model and governing equations are given in [22, 28].

The initial cellular detonation is obtained numerically from the problem of cellular detonation formation under the action of an explosive shock wave on the particle cloud [28]. Consider a plane channel of infinite length filled on a half of length with a mixture of aluminum particles and oxygen. The

other part of the channel is filled with pure oxygen. The planar shock wave accompanied with the adjacent rarefaction wave propagates in the gas and interacts with the mixture resulting in a planar detonation wave. Non-uniformity of particles density in the transverse direction on the cloud edge results in weak transverse waves. Reinforcement and regularization of these transverse waves lead to a cellular detonation with an average propagation velocity equal to the CJ value for a self-sustained detonation. The dependence of the detonation cell size on the channel width and the particle size has been analyzed in [28]. The numerical values of detonation cell width correlate with known experimental and calculated data for aluminum–oxygen and aluminum–air suspensions [29–31] taking into account the particle size and the type of oxidizer. In addition, the calculated results are confirmed by the acoustic analysis estimations obtained in [28] using the method by [32].

Part of that numerical solution ($0 \leq x \leq L_1 \leq y \leq H_1$), including the developed cellular detonation flow in the undisturbed section, the leading shock wave and the detonation structure, with part of the adjacent rarefaction wave is used as initial conditions in the current detonation diffraction simulation (Fig. 1).

Sufficient values of L_1 are used that allow implementation of an outflow condition on the left boundary. The channel walls are considered to be impenetrable and heat-insulated. The initial mixture properties are imposed on the right boundary.

The calculations have been performed for monodisperse stoichiometric mixtures of aluminum particles and oxygen with initial mass concentration of 0.55 (mean particle density 1.34 g/cm^3). A parametric study varying channel width H_1 from 0.0165 to 0.066 m and particle diameter from 1.5 to $3.5 \mu\text{m}$ has been carried out. The channel width contains from 0.5 to 8 detonation cells.

The numerical method includes the Harten TVD scheme for the gaseous phase and the Gentry–Martin–Daly upwind difference scheme for the solid phase dynamics. For convenience of numerical implementation of the two-dimensional TVD scheme for the current geometry, a planar channel of maximum width is used as the computational domain. At each time step, the computation is performed in the entire region with following re-imposition of the boundary conditions on the walls of both the narrow and wide parts of the channel. The numerical method has been tested previously including grid refinement and convergence, for the problems of detonation initiation and propagation [33, 34], cellular detonation formation [28], and planar shock and detonation wave diffraction [22, 23]. Test calculations with grid steps $1.5 \times 10^{-4} \text{ m}$, $2 \times 10^{-4} \text{ m}$, $3 \times 10^{-4} \text{ m}$, and $4 \times 10^{-4} \text{ m}$ were carried out for each of detonation diffraction regimes in the mixtures of 2 and $3.5 \mu\text{m}$ particles. The results for all supercritical and critical regimes and also for subcritical

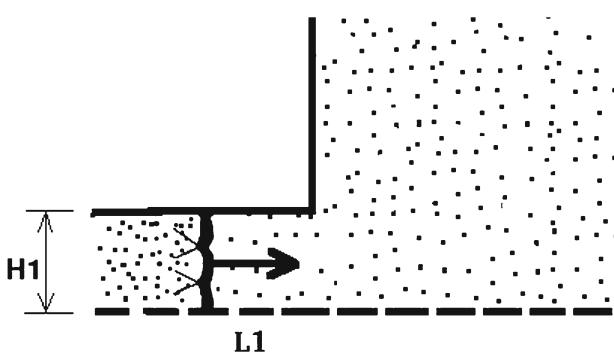


Fig. 1 Flow scheme

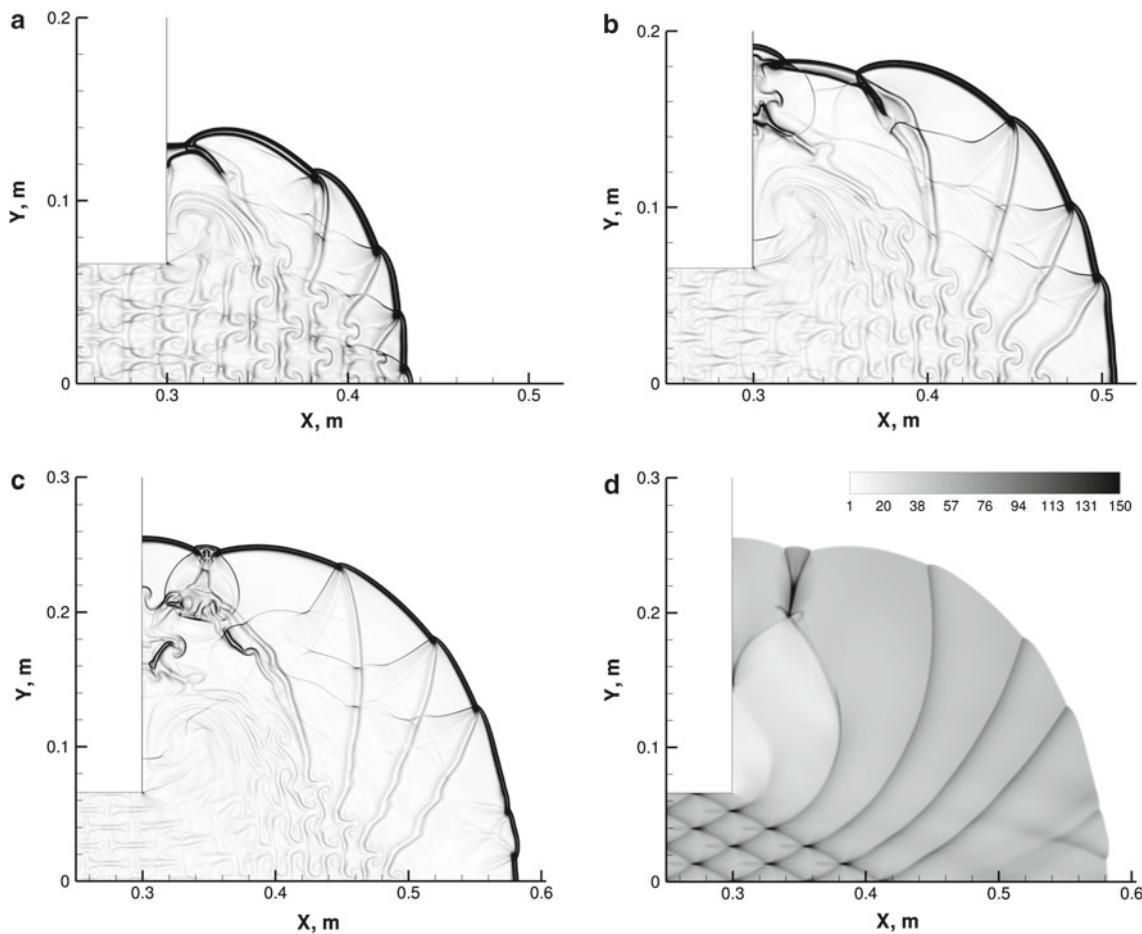


Fig. 2 Detonation flow development behind a backward step for $H_1 = 0.066$ m, $d = 2 \mu\text{m}$: numerical Schlieren images of gas density, $\Delta t = 0.05$ ms (**a–c**); maximal pressure history (**d**)

regime in the mixture of $3.5 \mu\text{m}$ particles agree qualitatively and quantitatively. Only for $2 \mu\text{m}$ particle mixture and $H_1 = 0.009$ m does the increase of the mesh size from 2×10^{-4} m to 3×10^{-4} m or to 4×10^{-4} m cause a switch from subcritical regime to critical. Thus, results are sensitive to the grid resolution for the limiting values of mixture properties and the channel width in the current regime. A similar influence resolution on the number of cells in plane channels has been discussed in [28]. In the present study as in [22, 23], the grid was chosen to provide agreement in all regimes considered. Thus, a uniform grid with 2×10^{-4} m mesh was used, providing more than 20 points per minimum relaxation scale ($1 \mu\text{m}$ particle combustion zone).

3 Characteristic features of the cellular detonation diffraction in gas-particle mixtures

Typical detonation pictures in a mixture with $2 \mu\text{m}$ particles are shown in Fig. 2 ($H_1 = 0.066$ m). Here, 2.5 cells occupy half of the narrow channel width and the detonation cell size

is 2.66 cm. This value correlates with the power-law dependence of the detonation cell size on the particle diameter for aluminum-oxygen mixtures obtained in [28] taking into account dispersion of the numerical results in narrow channels. In [28], the value of exponent is 1.6 and the character cell size for $10 \mu\text{m}$ particles is 27 cm.

The channel width and the number of the detonation cells in Fig. 2 are sufficient to provide continuous detonation propagation on the major part of the diffracted front. The front expansion leads to non-uniformity and transformation of the cellular structure. Interaction of the rarefaction wave zone behind the backward step with the detonation front leads to separation of the shock wave and the combustion front in a region adjacent to the confining wall. The separated section consists of two parts separated by a transverse wave (Fig. 2a). This transverse wave reaches the confining wall, on which it reflects, providing re-initiation near the wall. The second transverse wave joins the separated section of the front with the section of continuous detonation propagation. Figure 2c shows their interaction, which leads to full re-initiation. The averaged front propagation velocity in

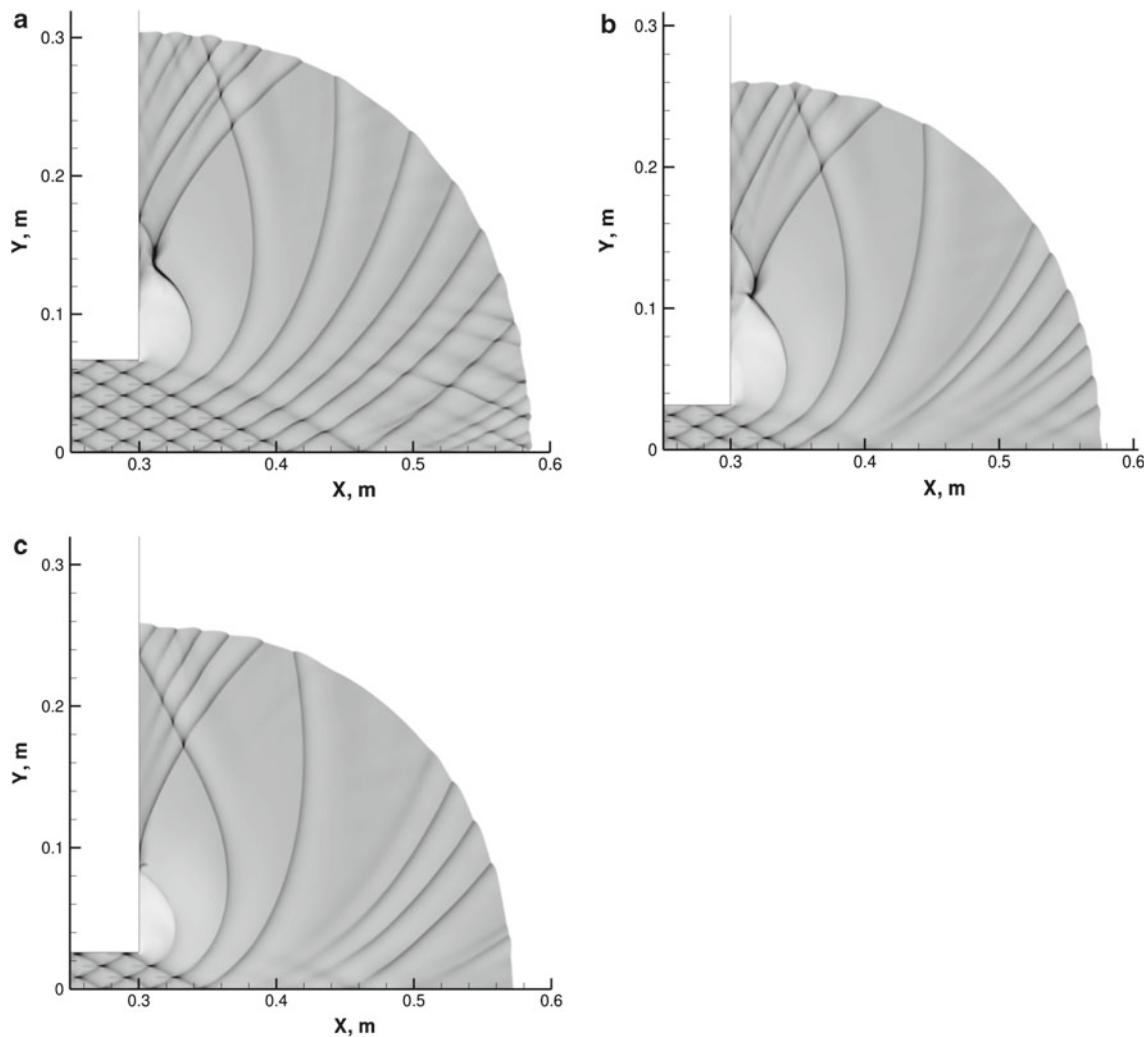


Fig. 3 Channel width effect on cellular detonation development: maximal pressure history, $d = 1.5 \mu\text{m}$, $H_1 = 0.066\text{m}$ (a); 0.033m (b); 0.025m (c)

Fig. 2a–c rises from 1,480 to 1,510 m/s in x direction and from 870 to 1,440 m/s in y direction. Thus, this case belongs in the critical regime of detonation propagation. In the section of the front adjoining the axis of symmetry, new transverse waves appear to originate (Fig. 2c) due to fluctuations along the detonation front. Corresponding maximal pressure history images $p_{\max}(x, y) = \max_t [p(x, y, t)]$ show the hot point tracks (Fig. 2); the same gray scale is used in all similar subsequent images).

Figure 3 presents results for $1.5 \mu\text{m}$ particles, with different numbers of cells across the channel, i.e. varying the channel width. These pictures confirm the non-uniformity and transformation of the cellular structure and appearance of new transverse waves, both in the near-wall region and near the plane of symmetry (Fig. 3a). Figure 4 evidences time-development of the process corresponding to Fig. 3a. The averaged propagation velocity in the case presented in

Fig. 4 is constant in the plane of symmetry (1,550 m/s) and rises along the backward step wall from 1,130 m/s (a–b) to 1,450 m/s (b–c) and to 1,560 m/s (c–d). Emergence of the new transverse waves that are clearly seen in Figs. 3a and 4 is related to instability of the detonation front with respect to disturbances, leading to its curvature (in the case of the Arrhenius-type reaction) and to propagation of acoustic waves in the flow behind the front. A detailed explanation of this phenomenon of gaseous detonation based on the methods of linear acoustics was offered in [32]. Application of the method to heterogeneous detonation in aluminum–oxygen mixtures proposed in [32] allowed confirming the detonation cell size dependence on particle diameter in [28] and the detonation degeneration in bi-dispersed mixtures in [35]. Appearance of a new transverse wave has been obtained in numerical simulations of diffraction of planar detonation wave in gases [13] and in gas–particle mixtures [22, 23].

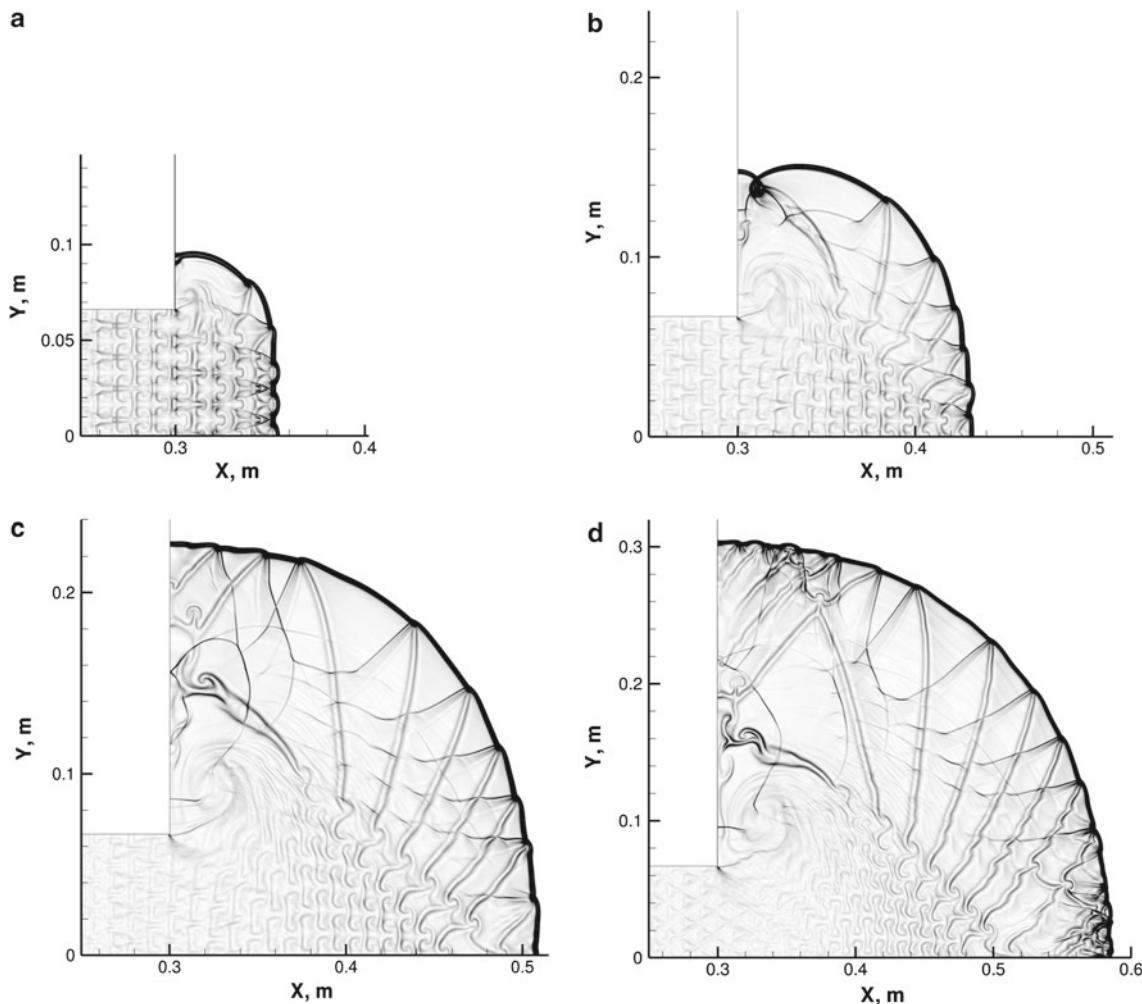


Fig. 4 Formation of new transverse waves on the diffracted detonation front, $d = 1.5 \mu\text{m}$, $H_1 = 0.066 \text{ m}$: Schlieren images of gas density, $\Delta t = 0.05 \text{ ms}$

Thus, as a whole the scenario of detonation propagation in the critical regime corresponds to gaseous detonation flows, where re-initiation of detonation at diffraction on a backward facing step is connected with the triple point collisions [9]. Therefore, the reinitiation mechanisms in the critical regime of propagation in gases and gas particle suspensions are similar. However, in our calculations on suspensions of aluminum particles in oxygen, the number of cells where re-initiation behind the backward step can occur is less than in gaseous mixtures. The numerical calculations show the detonation remaining only for the case of one detonation cell in the channel, which is significantly less than that in gaseous mixtures (10–13 for tubes and 2–3 for rectangular channels).

For a small number of transverse waves across the channel, the scenario may depend upon the position of the transverse waves in the exit plane. Figure 5 illustrates two cases of detonation development with one cell per half channel width or

two cells in the channel ($d = 3.5 \mu\text{m}$, $H_1 = 0.066 \text{ m}$) and different shock wave configurations at the moment of passage through the exit plane. In the first case, due to the transverse wave reflections from the wall and from the plane of symmetry and their collisions behind the exit plane, two strong transverse waves leave their marks (Fig. 5a1). Decoupling between the leading shock wave and the combustion front occurs only in a narrow zone near the wall (Figs. 5a2–a4). The average of 0.05 ms propagation velocities in x direction is 1,280 (a2–a3), 1,400 (a3–a4), 1,340, and 1,540 m/s (last moments are not presented in Fig. 5). Corresponding values in y direction are 1,130, 1,210, 1,150, and 1,410 km/s. This confirms that the detonation has been restored on a major part of the diffracted front.

In the second case, the transverse waves collide in the plane of symmetry and go around the corner. Reflection on the vortex structure generates weak dispersive shock waves, which reinforce after collisions in the plane of symmetry

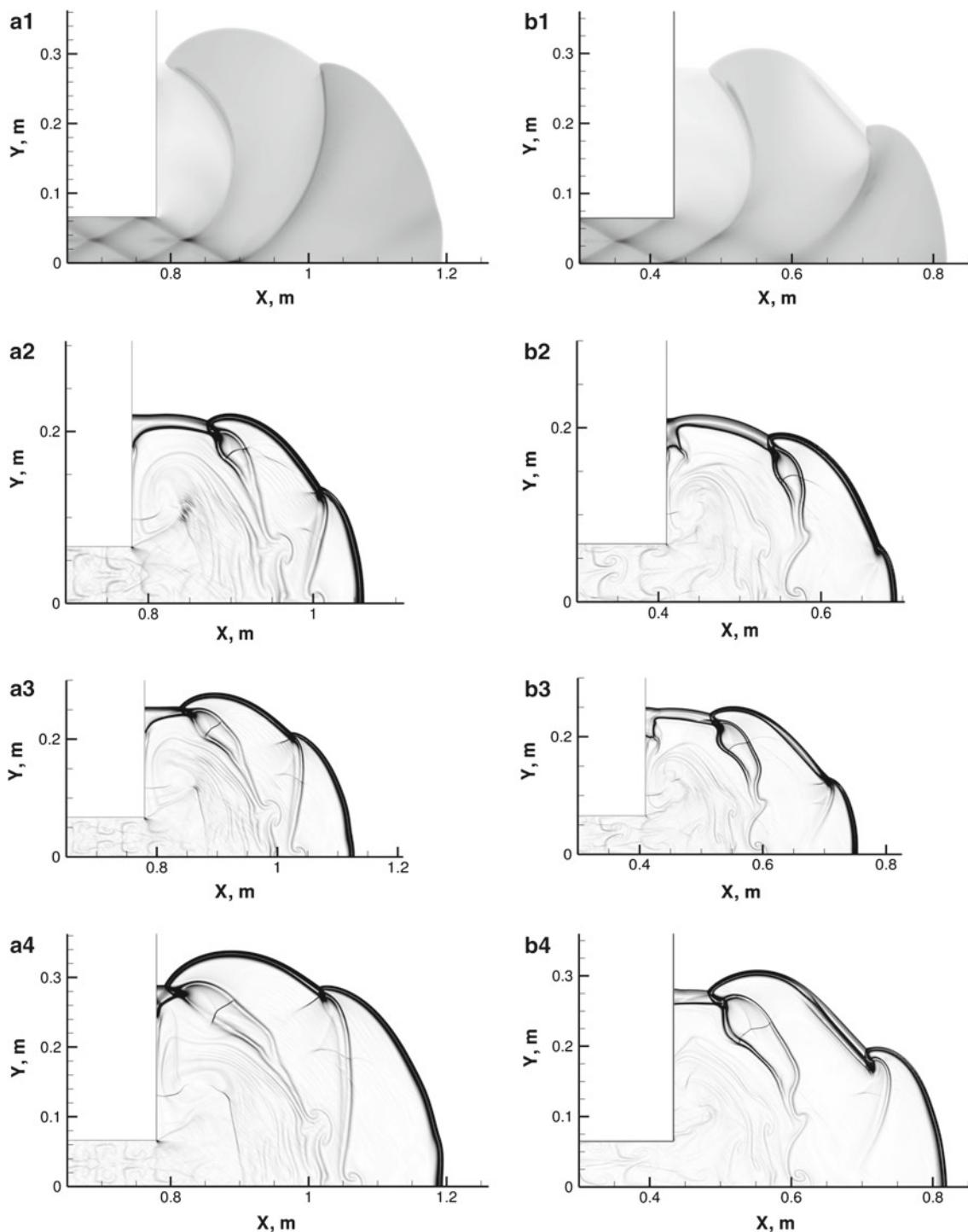


Fig. 5 Influence of transverse wave configurations (**a**, **b**) at the exit plane on detonation development, $d = 3.5 \mu\text{m}$, $H_1 = 0.066 \text{ m}$. Maximal pressure history (1), Schlieren images of gas density, $\Delta t = 0.05 \text{ ms}$ (2–4)

(the triple point tracks are evident in Fig. 5b1). Here, a significant part of the front shows decoupling between the weakened shock and the combustion front. The re-initia-

tion process delay is shorter (Fig. 5b2–b4 compared with Fig. 5a2–a4) and the detonation front covers less distance than in the previous case. The corresponding propagation

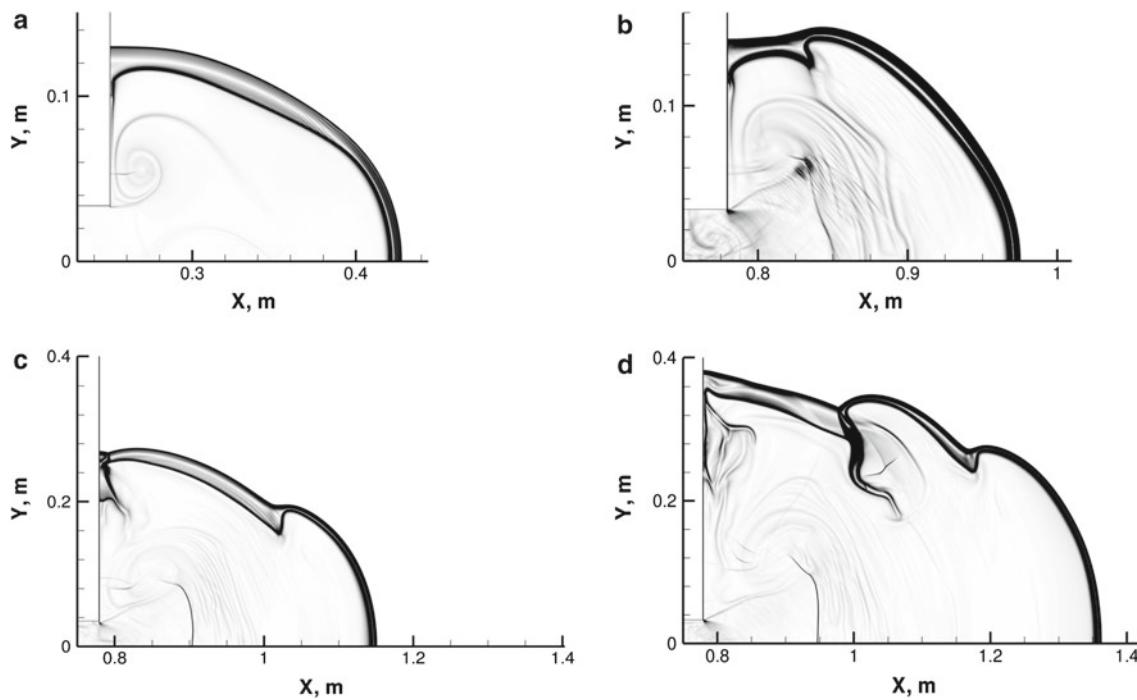


Fig. 6 Comparison of planar (**a**) and cellular (**b–d**, $\Delta t = 0.15\text{ ms}$) detonation diffraction: Schlieren images of gas density, $d = 3.5\text{ }\mu\text{m}$, $H_1 = 0.033\text{ m}$

velocities in x - and y -directions are only 1,190 and 760 m/s (b2–b3), 1,260 and 610 m/s (b3–b4), respectively. The detonation most likely reappears in the transverse wave which is formed on the front bow ($x \sim 0.7$ in Fig. 5b4), as in the critical regime for planar detonation wave diffraction [22].

Figure 6 shows how results differ for planar and cellular detonation diffraction in the same channel ($H_1 = 0.033\text{ m}$) in a mixture with $3.5\text{ }\mu\text{m}$ particles. The initial self-sustained planar detonation wave propagating, with adjacent rarefaction wave, was obtained from the initiation problem described in Sect. 2, but without a 2D perturbation. In this case, the formation of the cellular structure in 2D calculations is considerably delayed therefore when the detonation wave crosses the exit plane it is still planar.

Failure of the planar detonation wave due to diffraction is observed in Fig. 6a in a way similar to the results of [22] and [23] for $3.5\text{ }\mu\text{m}$ particles and $H_1 \sim 3\text{ cm}$. The detonation decays so that no transverse wave forms along the diffracted leading shock front. Formation of transverse waves in different regimes for planar detonation diffraction has been analyzed in [23].

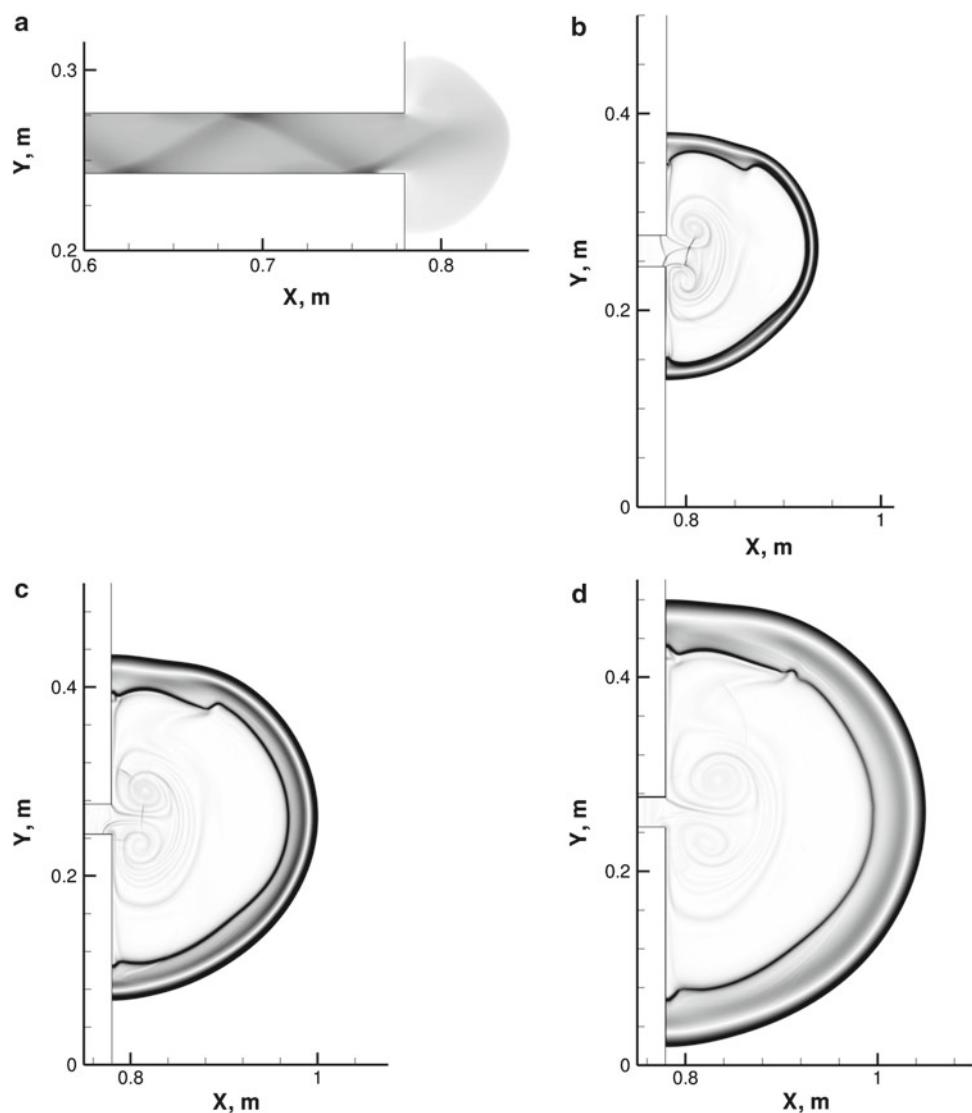
Cellular detonation diffraction shows the detonation process conservation (Figs. 6b–d). Here, a structure with only one transverse wave per half a channel (one detonation cell in the 0.066 m channel) forms in the narrow part, which does not contradict known criteria of cellular detonation propagating limits. The detonation cell size also correlates with data of [28].

The averaged propagation velocity rises monotonically from 1,100 to 1,450 m/s in the plane of symmetry, but varies non-monotonically between 730 and 1,040 m/s along the backward step wall. The flow patterns presented in Figs. 6b–d reveal that the primary transverse waves are not sufficient to reinforce the detonation (Fig. 6b–c). Re-initiation starts from the central section of the front due to new transverse waves formed as in the critical regime of plane detonations, in which the detonation reinforcement always takes place [22, 23].

Different results for planar and cellular detonation diffraction in this case may be explained by the influence of local overcompression in the central part of the detonation wave which is proper to a certain phase of cellular detonation propagation. Thus, the results presented in Figs. 5 and 6 confirm the influence of the transverse waves on evolution of the process after the detonation front exit into an open space. Cellular detonations provide in general better conditions of detonation propagation than plane detonations. At the same time the critical channel width for plane and cellular detonations are close, which agrees with results obtained for gaseous mixtures as discussed in [12].

Cellular detonation failure is obtained in the numerical results only in the case with one transverse wave in the channel, which corresponds to a half a cell channel width (Fig. 7, $d = 3.5\text{ }\mu\text{m}$, $H_1 = 0.0165\text{ m}$). In this case, the flow cannot be symmetric in y -direction. The interaction between transverse wave and the vortex structure behind the backward

Fig. 7 Cellular detonation failing at $d = 3.5 \mu\text{m}$, $H_1 = 0.0165 \text{ m}$: maximal pressure history (**a**) and numerical Schlieren images, $\Delta t = 0.1 \text{ ms}$ (**b–d**)



facing step is weakening, and it is too weak to re-initiate detonation even on the upper side of the domain, as displayed in Fig. 7.

As mentioned above the mean velocity of the detonation wave propagating in the narrow part of the channel is close to the CJ velocity (1,560 m/s). After the expansion, the velocity drop can be estimated from the time evolution images (Fig. 7). The velocity in the central part decreases linearly, with values 880, 650, and 490 m/s in Fig. 7b–d, respectively. In this case, the mixture and channel properties correspond to the subcritical regime of planar detonation wave diffraction [23]. In critical regimes, characterized by front acceleration in the process of re-initiation, a minimal propagation velocity of about 1,100–1,200 m/s was obtained in [23] for $d = 2 \mu\text{m}$, $H_1 = 0.015$ to 0.02 m. In the subcritical regime in Fig. 6a, the propagation velocity goes down to

751 m/s and lower. Thus, the regime in Fig. 7 is really also subcritical.

4 Discussion

Numerical results show that heterogeneous detonation propagation without failure still occurs in channels narrower compared with cell width than in gaseous mixtures. This is due to significant differences in conditions and mechanisms of aluminum particle ignition, compared with the ignition and induction processes in gaseous mixtures.

The approach of Ref. [4] applied to a gaseous suspension of solid particles results in a critical number of detonation cells. The minimum number of cells per channel width is also given by Eqs. (1, 2). However, it has to be taken into

account that the processes taking place behind the shock front in gaseous suspensions differ considerably from the ignition and induction process in gaseous mixtures. The particles are accelerated by the gas flow, giving rise to an additional heat generation due to the friction force. The particle heat rate and ignition conditions are determined not only by the ambient gas temperature, but also the Nusselt number dependence on relative particle velocity. In the ignition process of suspended aluminum particles behind the shock the dynamics of initial particle heating influences the ignition delay more strongly than the Arrhenius reaction of the surface oxidation. Therefore, in the proposed model the low-temperature reaction of oxidation of aluminum has been neglected during the heating stage and transition to combustion is defined by a critical temperature of about 900 K (called the “ignition temperature”). For particle temperatures of the order of 800 to 900 K an rapid acceleration of the oxidation rate takes place which leads to a heat equilibrium breakdown [36].

In a rough approximation, one can assume that the Nusselt number is constant, in which case particle heating in the phase of initial heating is described by the equation

$$\frac{dT_2}{dt} = \frac{1}{\tau_T} (T - T_2). \quad (3)$$

Here, T and T_2 are the gas and particle temperatures and τ_T is the characteristic time of thermal relaxation. The initial stage of the particle heating is characterized by non-monotonic behavior of the gas temperature [26], conditioned by two opposite processes, namely, heat generation due to particle acceleration in the flow, and heat transfer from the gas phase to the particles. The gas temperature at this stage varies in a range between 1,500 and 2,000 K. For estimation purpose we consider a simple approximation $T = \text{const}$, but the two extreme temperature values will be verified. The solution (3) for this condition takes the form $T_2 = T - (T - T_0) \exp(-t/\tau_T)$ and the ignition delay time is defined by $\tau = \tau_T \ln[(T - T_0)(T - T_{\text{ign}})]$. Substituting these relations in Eq. (1) leads to a condition for decay of the diffracted wave for spherical heterogeneous detonation:

$$n < \frac{(T_{\text{ign}} - T_0) 4Tc}{(T - T_0)(T - T_{\text{ign}}) \ln[(T - T_0)/(T - T_{\text{ign}})] D}. \quad (4)$$

For $D = 1,560$ m/s, $c = \sqrt{\gamma RT}$, $T_0 = 300$ K, $T_{\text{ign}} = 900$ K, Eq. (4) gives a critical value of about 3 (3.4 and 3.2 for gas temperature values of 1,500 and 2,000 K). Taking Eq. (2) into account the plane channel condition is written as $n = l/\lambda \sim 1.5$. Therefore, the simple estimates show that for heterogeneous detonations the critical conditions differ significantly from those for gaseous mixtures. This is confirmed to some extent by the numerical results above.

Wave flow pictures of the gas phase are similar and the propagation mechanism associated with re-initiation in the transverse waves exists, but there are several qualitative

differences in the fine detonation structure, such as non-monotonic behavior of the gas temperature, and the critical conditions for particle ignition. This leads to different critical conditions for propagation by the diffraction in gaseous mixtures and in suspensions of reacting particles. These differences appear to be mainly related to velocity and thermal relaxation, and they require an additional research.

5 Conclusions

A two-dimensional numerical simulation of cellular detonation propagation in stoichiometric suspension of aluminum particles and oxygen by diffraction on a backward facing step has been performed. In general terms, the process of detonation propagation in suspensions is similar to gaseous detonations, with re-initiation taking place in transverse waves behind the step. Also new transverse waves are generated along the expanding front.

Results for different particle size and channel width show that the critical number of the cells is much lower than for the gas detonation. For one or two detonation cells in the channel width the scenario depends upon the transverse wave configuration at the exit plane. Detonation failure has been obtained in numerical simulations only in the case of one transverse wave, i.e. half a cell, in the channel width.

The observed decrease of the critical number of the cells in heterogeneous detonations is confirmed theoretically by estimates obtained for aluminum particle mixtures, based upon the Mitrofanov–Soloukhin approach. This decrease is most likely due to the influence of velocity and temperature relaxation processes in the two-phase detonation structure.

Acknowledgments The work has been financially supported by Ministry of Education and Sciences of the Russian Federation, AVC Program “Development of Scientific Potentials of Higher School”, grant #2.1.1/4674 and by the program of fundamental investigation of branch of power industry, machine building, mechanics and control processes RAS #1.

References

1. Vasil'ev, A.A., Mitrofanov, V.V., Topchian, M.E.: Detonation waves in gases. *Combust. Explos. Shock Waves* **23**, 605–623 (1987)
2. Nettleton, M.A.: Recent work on gaseous detonations. *Shock Waves* **12**, 3–12 (2002). doi:[10.1007/s001930200134](https://doi.org/10.1007/s001930200134)
3. Bazhenova, T.V., Golub, V.V.: Use of gas detonation in a controlled frequency mode (review). *Combust. Explos. Shock Waves* **39**, 365–381 (2003)
4. Mitrofanov, V.V., Soloukhin, R.I.: The diffraction of multi-front detonation waves. *Sov. Phys. Doklady* **9**, 1055–1058 (1965)
5. Vasil'ev, A.A.: Critical conditions for initiation of multifront cylindrical detonation. *Combust. Explos. Shock Waves* **34**, 220–225 (1998)

6. Jones, D.A., Oran, E.S., Sichel, M.: Reignition of detonation by reflected shocks. *Shock Waves* **5**, 47–57 (1995)
7. Jones, D.A., Kemister, G., Oran, E.S., Sichel, M.: The influence of cellular structure on detonation transmission. *Shock Waves* **6**, 119–129 (1996)
8. Pantow, E.G., Fischer, M., Kratzel, Th.: Decoupling and recoupling of detonation waves associated with sudden expansion. *Shock Waves* **6**, 131–137 (1996)
9. Jones, D.A., Kemister, G., Tonello, N.A., Oran, E.S., Sichel, M.: Numerical simulation of detonation reignition in H₂–O₂ mixtures in area expansions. *Shock Waves* **10**, 33–41 (2000)
10. Liu, Y.K., Lee, J.H., Knystautas, R.: Effect of geometry on the transition of detonation through an orifice. *Combust. Flame* **56**, 215–225 (1984). doi:[10.1016/0010-2180\(84\)90038-5](https://doi.org/10.1016/0010-2180(84)90038-5)
11. Sochet, I., Lamy, T., Brossard, J., Vaglio, C., Cayzac, R.: Critical tube diameter for detonation transmission and critical initiation energy of spherical detonation. *Shock Waves* **9**, 113–123 (1999)
12. Pintgen, F., Shepherd, J.E.: Detonation diffraction in gases. *Combust. Flame* **156**, 665–677 (2009). doi:[10.1016/j.combustflame.2008.09.008](https://doi.org/10.1016/j.combustflame.2008.09.008)
13. Arienti, M., Shepherd, J.E.: A numerical study of detonation diffraction. *J. Fluid Mech.* **529**, 117–146 (2005). doi:[10.1017/S0022112005003319](https://doi.org/10.1017/S0022112005003319)
14. Roy, G.D., Frolov, S.V., Borisov, A.A., Netzler, D.W.: Pulse detonation propulsion: challenges, current status, and future perspective. *Prog. Energy Combust. Sci.* **30**, 545–672 (2004). doi:[10.1016/j.pecs.2004.05.001](https://doi.org/10.1016/j.pecs.2004.05.001)
15. Weng, Ch., Gore, J.P.: A numerical study of two- and three-dimensional detonation dynamics of pulse detonation engine by the CE/SE method. *Acta Mech. Sin.* **21**, 32–39 (2005). doi:[10.1007/s10409-004-0004-8](https://doi.org/10.1007/s10409-004-0004-8)
16. Canteins, G., Franzetti, F., Zoclonska, E., Khasainov, B., Zitoin, R., Desbordes, D.: Experimental and numerical investigations on PDE performance augmentation by means an ejector. *Shock Waves* **15**, 103–112 (2005). doi:[10.1007/s00193-006-0006-5](https://doi.org/10.1007/s00193-006-0006-5)
17. Levin, V., Markov, V., Zhuravskaya, T., Osinkin, S.: Initiation and propagation of detonation in channels of complex shape. In: Roy, G.D., Frolov, S.M. (eds.) *Pulse and Continuous Detonation Propulsion*, pp. 97–106. Torus Press, Moscow (2006)
18. Levin, V., Markov, V., Zhuravskaya, T., Osinkin, S.: Propagation of cellular detonation in the plane channel with obstacles. In: Hannemann, K., Seiler, F. (eds.) *Shock Waves*, vol. 1. 26th International Symposium on Shock Waves, vol. 1, Part IV, pp. 347–351. Springer, Berlin Heidelberg (2009). doi:[10.1007/978-3-540-85168-4_55](https://doi.org/10.1007/978-3-540-85168-4_55)
19. Sorin, R., Ratiba, Z., Khasainov, B., Desbordes, D.: Detonation diffraction through different geometries. *Shock Waves* **19**, 11–23 (2009). doi:[10.1007/s00193-008-0179-1](https://doi.org/10.1007/s00193-008-0179-1)
20. Kutushev, A.G., Shorokhova, L.V.: Numerical investigation of burning and detonation of monofuel mixtures suspensions in sharply extended tubes. In: Roy, G.D., Frolov, S.M., Santoro, R.J., Tsyganov, S.A. (eds.) *Advances in Confined Detonations*, pp. 161–166. Torus Press Ltd., Moscow (2002)
21. Kutushev, A.G., Shorokhova, L.V.: Numerical investigation of the processes of combustion and detonation of air-fuel mixtures of unitary fuel in abruptly expanding pipes. *Chem. Phys.* **22**(8), 94–99 (2003)
22. Fedorov, A.V., Kratova, Yu.V., Khmel, T.A.: Shock and detonation wave diffraction at a sudden expansion in gas-particle Mixtures. *Shock Waves* **18**, 281–290 (2008). doi:[10.1007/s00193-008-0162-x](https://doi.org/10.1007/s00193-008-0162-x)
23. Kratova, Yu.V., Fedorov, A.V., Khmel, T.A.: Diffraction of a plane detonation wave on a back-facing step in a gas suspension. *Combust. Explos. Shock Waves* **45**(5), 591–602 (2009)
24. Fedorov, A.V., Khmel, T.A., Kratova, Yu.V.: Cellular detonation formation and propagation in polydisperse mixtures. In: *Proceedings of 7th international symposium on hazards, prevention, and mitigation of industrial explosions*, vol. II, p. 238 (2008)
25. Fedorov, A.V.: Structure of heterogeneous detonation of aluminum particles dispersed in oxygen. *Combust. Explos. Shock Waves* **28**(3), 277–286 (1992). doi:[10.1007/BF00749644](https://doi.org/10.1007/BF00749644)
26. Fedorov, A.V., Khmel, T.A., Fomin, V.M.: Non-equilibrium model of steady detonations in aluminum particles-oxygen suspensions. *Shock Waves* **9**, 313–318 (1999). doi:[10.1007/s001930050191](https://doi.org/10.1007/s001930050191)
27. Strauss, W.A.: Investigation of the detonation of aluminum powder-oxygen mixtures. *AIAA J.* **6**(12), 1753–1761 (1968). doi:[10.2514/3.4855](https://doi.org/10.2514/3.4855)
28. Fedorov, A.V., Khmel, T.A.: Numerical simulation of formation of cellular heterogeneous detonation of aluminum particles in oxygen. *Combust. Expl. Shock Waves* **41**(4), 435–448 (2005). doi:[10.1007/s10573-005-0054-7](https://doi.org/10.1007/s10573-005-0054-7)
29. Ingignoli, W., Veyssiére, B., Khasainov, B.A.: Study of detonation initiation in unconfined aluminum dust clouds. In: Roy, G. et al. (eds.) *Gaseous and Heterogeneous Detonations*, pp. 337–350. ENAS-Publishers, Moscow (1999)
30. Zhang, F., Gronig, H., Van de Ven, A.: DDT and detonation waves in dust-air mixtures. *Shock Waves* **11**, 53–71 (2001)
31. Benkiewicz, K., Hayashi, A.K.: Two-dimensional numerical simulations of multi-headed detonations in oxygen-aluminum mixtures using an adaptive mesh refinement. *Shock Waves* **13**, 385–402 (2003)
32. Barthel, H.O.: Predicted spacings in hydrogen–oxygen–argon detonations. *Phys. Fluids* **17**(8), 1547–1553 (1974)
33. Khmel, T.A.: Numerical simulation of two-dimensional detonation flows in reactive particle gas suspensions. *Matematicheskoe Modelirovaniye* (in Russian) **16**(6), 73–77 (2004)
34. Fedorov, A.V., Khmel, T.A.: Numerical technologies for investigations of heterogeneous detonations of gas particle suspensions. *Matematicheskoe Modelirovaniye* (in Russian) **18**(8), 49–63 (2006)
35. Fedorov, A.V., Khmel, T.A.: Cellular detonations in bi-dispersed gas-particle mixtures. *Shock Waves* **18**(4), 277–280 (2008)
36. Fedorov, A.V., Kharlamova, Yu.V.: Ignition of an aluminum particle. *Combust. Explos. Shock Waves* **39**(5), 544–547 (2003). doi:[10.1023/A:1026109801863](https://doi.org/10.1023/A:1026109801863)