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ORIGINAL ARTICLE

Cellular detonations in bidispersed gas-particle mixtures

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Abstract Formation of cellular detonation in bi-fractional stoichiometric mixtures of aluminum particles and oxygen is investigated numerically. The detonation cell size depends on the particle diameters and relative concentration of the fractions. Certain degeneration of cellular detonation is obtained when compared to the monodisperse mixtures. It is characterized by maximal pressure decrease, transverse wave relaxation, and detonation front rectification. Complete degeneration of cellular detonations and stable propagation of a plane detonation front is found in some bi-fractional mixtures. The numerical results are confirmed by acoustic analysis of the detonation structures.

Keywords Cellular detonations · Gas suspensions · Numerical modeling

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1 Introduction

The propagation of detonation waves in heterogeneous mixtures can occur in the cellular detonation regime [1–4]. It was shown in [4] numerically and by methods of acoustic analysis that in monodisperse gas-particle mixtures the distance between transverse waves (the transverse size of detonation cells) is related to the geometric characteristics of the detonation wave structure and depends on particle size. Analysis of data from numerical experiments provided an approximation formula for the detonation cell size in stoichiometric gas-particle mixtures of aluminum particles in oxygen

$$\lambda = \lambda_0 \, (d/d_0)^{\theta} \, , \tag{1}$$

where $\theta = 1.6$, $\lambda_0 = 27\,\mathrm{cm}$, $\mathrm{d}_0 = 10\,\mu\mathrm{m}$.

The actual mixtures are, as a rule, polydisperse and are characterized by a function of the particle size distribution. It is of interest to study the possibility of cellular detonation existence in polydisperse gas-particle mixtures and the influence of the mixture fractional composition on the detonation character and the cell size. The paper is devoted to an analysis of cellular detonation formation in bi-disperse mixtures of aluminum particles in oxygen.

The conditions for initiation of planar detonation waves in bi-disperse stoichiometric oxygen–aluminum particle mixtures and some preliminary results of cellular detonation formation were obtained in [5]. In the present work, the influence of the saturation parameter on cellular detonation characteristics is investigated. The formation of cellular structures is modeled numerically as a result of shock-wave initiation of detonation in a flat duct and a subsequent development of transverse waves. Results of numerical experiments compare with the estimates of cell size obtained within the framework of the acoustic approach [6] developed for gas-particle mixtures in [4].

2 Formulation of the problem

The physical and mathematical model of the non-ideal detonation of a stoichiometric gas-particle mixture of aluminum

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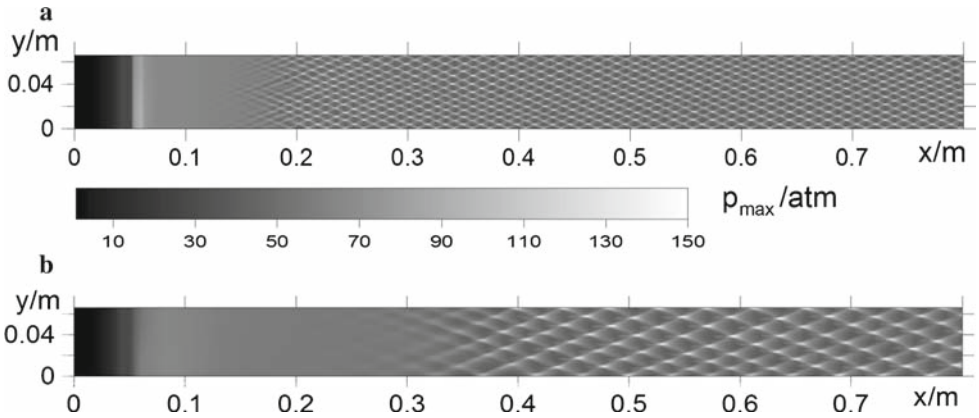

Fig. 1 Cellular detonation formation in monodisperse gas-particle mixtures: $d = 1\,\mu$m (**a**), $d = 2\mu$m (**b**)

particles in oxygen was developed earlier. A comprehensive description of the model is presented in [4]. The Euler equations for the mixture follow from the laws of conservation of mass, momentum, and energy for each phase. The system is completed by the equations of state and the relations for interphase interaction taking into account particle drag coefficient in supersonic flow behind the shock. The equation of the reduced chemical kinetics of the Arrhenius type takes into account an incomplete burning of aluminum particles in accordance with experimental observations of about 10% unburnt particles in the detonation products [7]. The combustion law agrees with known experimental data on the dependence of the burning time on the particle diameter of aluminum particles in pure oxygen. A temperature criterion for ignition is adopted with a value close to the conventional accepted value in [8] for detonations in aluminum-oxygen mixtures. The model provides agreement with the experimental data of [7] on the detonation velocity and the CJ gas pressure value. The theoretical analysis of the stationary detonation structures obtained in the frame of the model was performed in [9]. The model was applied to computation of cellular detonation flows in monodisperse aluminum–oxygen mixtures in [4]. The calculated values of detonation cell size agree with the data of [3] obtained for two values of particle diameters (3.5 and 1 μm) in the framework of a different kinetic model of aluminum particle combustion.

The numerical technology is based on the use of a scheme of the TVD class for the gaseous phase and the Gentry–Martin–Daly scheme for the discrete phase. The initial- and boundary-value problem is posed as a problem of the shock-wave initiation of detonation in a cloud of the gas-particle mixture occupying the half-space of a flat duct similarly to [4]. The values of the parameters of the initiating explosion shock wave are chosen in such a way that the conditions for detonation initiation in the mixture cloud are ensured. As in [4], a small perturbation of particle density at the cloud boundary $\rho_{p0}(x, y) = \rho_{st}(1 + \beta\cos(\pi y/Y))$ for $X_{cl} \le x \le X_{cl} + \delta X$, $\rho_{p0}(x, y) = \rho_{st}$ for $X_{cl} + \delta X < x < +\infty$ is taken as an initiator of transverse waves. Here X_{cl} is the cloud boundary coordinate, δX is the perturbed layer thickness, Y is the duct width, β is a small parameter, $\rho_{st} = 1.34\,\mathrm{kg/m^3}$ is the particles density in the mixture of stoichiometric composition. The computations were carried out for a duct 0.066 m in width and the gas-particle mixtures consisting of particles with size 3.5, 2 and 1 μm.

The bi-disperse mixture composition is characterized by saturation parameter $\eta = \rho_{s0}/(\rho_{s0} + \rho_{l0})$. The subscripts s and l refer to the fractions of fine and large particles, respectively. The values $\eta = 0$ and $\eta = 1$ correspond to monodisperse suspensions of large or fine particles.

3 Results of calculations and acoustic analysis

As was stated in [4], cellular detonation develops in monodisperse aluminum particle oxygen suspensions for all values of particle size within the range 1–12 μm and is similar to cellular gaseous detonation. At a divergence of transverse waves, a considerable decay of the front occurs. The pressure at the chemical peak point drops to 40 atm, which amounts to about 70% of the value corresponding to the CJ regime. The collision of transverse waves is Similar to an explosion (the pressure increases up to values of the order of 140 atm). The numerical soot foil (maximal pressure history $p_{\max}(x, y) = \max_t[p(x, y, t)]$) is shown in Fig. 1 for mixtures with 1 μm (Fig. 1a) and 2 μm particles (Fig. 1b).

Both the process and the result of cellular detonation formation in bi-disperse gas-particle mixtures depend on the mixture composition and differ from monodisperse gas-particle mixtures. A longer formation of transverse waves than for $\eta = 0$ and $\eta = 1$ is the general property of cellular detonation development in interval $0 < \eta < 1$. For example, in the monodisperse mixture of 1 μm particles a regular system of transverse waves manifests itself within 0.25 m of wave propagation, and of 2 μm within 0.45 m (Fig. 1). In the bi-disperse mixture of 2 and 1 μm particles this distance increases up to 0.7 m for $\eta = 0.3$ and $\eta = 0.7$, and up to 1 m for $\eta = 0.5$ (Fig. 2).

There is, in addition, a reduction in the amplitude of pressure oscillations at the chemical peak point (Fig. 3a), which

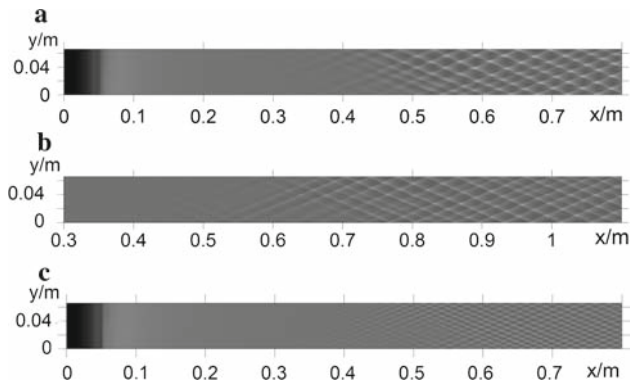

Fig. 2 Cellular detonation in bi-disperse mixtures of 2- and 1-μm particles: $\eta = 0.3$ (**a**), $\eta = 0.5$ (**b**), $\eta = 0.7$ (**c**)

is expressed also by a contrast reduction shown in Fig. 2 in comparison with Fig. 1, which are presented in unified grayscale. The trajectories of triple points are represented by nearly straight lines (Fig. 2). A relaxation of transverse waves and a reduction of the difference between the maximum and minimum pressure values at the collision of triple points is evidence of a certain degeneration of cellular detonation.

The distance between transverse waves (the typical size of a cellular-like structure) depends on the saturation parameter η and varies from a value corresponding to the monodisperse gas-particle mixture of the large fraction (2 cm) to a value corresponding to the fine fraction (0.69 cm) (Fig. 3b).

For example, for some mixtures, consisting of particles 3.5 and 1, 3 μm and 1, 3 and 2 μm, an interval of η values (from 0.4 to 0.6) has been revealed within which the transverse waves do not form at all, despite the presence of an initial disturbance. The detonation front remains planar (Fig. 4a), or very weak transverse dispersion waves form (Fig. 4b). Thus, in these cases, cellular detonation completly degenerates into a planar wave. Outside the above interval of η values, transverse waves and cellular-like structures form, and their properties and character are similar to the ones described above for gas-particle mixtures with 1 and 2 μm particles.

The influence of the saturation parameter on the cell size and detonation degeneration are confirmed by the data of acoustic analysis of the cell size using the methodology of [6]. The method consists of determining the distance between the transverse waves following one another using analysis of a diverging acoustic wave. The acoustic wave originates from the primary disturbance of the detonation wave front (the "hot point"). Due to the diffraction, refraction, and partial reflection of this wave in a nonuniform flow field, part of the disturbances return to the front, giving rise to additional "hot" points. The location of these points is determined by the solution of the corresponding acoustics problem considering the flow field of the planar detonation wave. The method of [6] was developed in [4] with reference to heterogeneous detonations in two-phase mixtures of gas and solid particles.

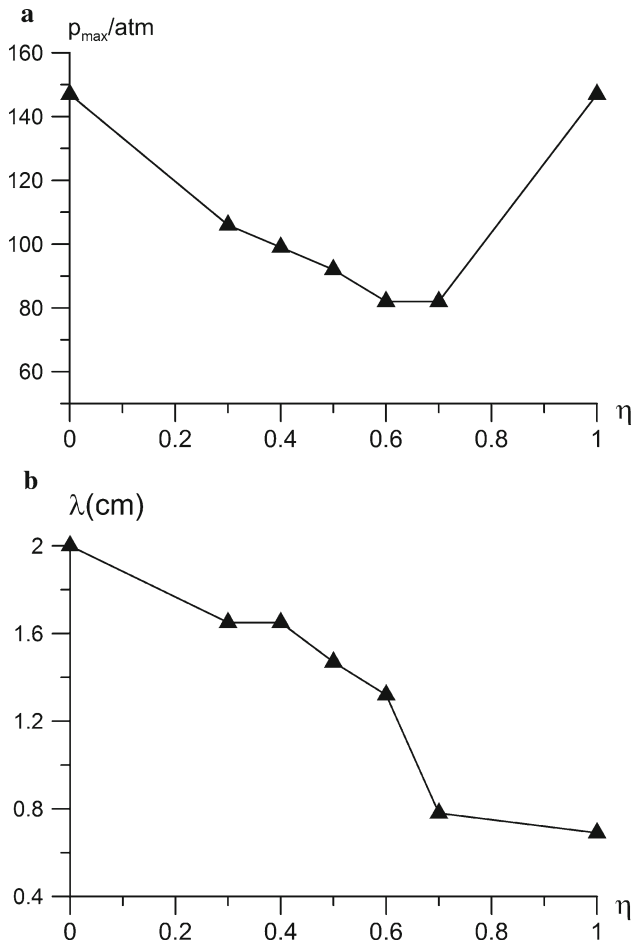

Fig. 3 The saturation influence on cellular detonation parameters in the bi-disperse mixtures of 2- and 1-μm particles: maximal pressure (**a**), the detonation cell size (**b**)

Good agreement of the estimates of the detonation cell size on the basis of this methodology with the data from numerical modeling of cellular detonations was obtained in [4] for monodisperse mixtures of aluminum particles and oxygen.

The Table 1 presents the data from acoustic estimates (λ_a) in comparison with the data from numerical experiments (λ_{num}) for the bidispersed mixtures of particles 3.5 and 1 μm and with the approximation formula (1) for monodisperse mixtures (λ_m). The symbol (*) marks a relatively narrow computational region where the detonation cell size is determined inaccurately [4] due to influence of the channel walls. In wide channels (three or more detonation cells per channel width) the detonation cell size is determined with satisfactory precision [4]. Numerical computations of a planar detonation wave for $\eta = 0.4$ and 0.5 confirm that the cell size using the methodology of [4,6] is not defined. In these cases, due to specific features of the flow field, a primary disturbance at the detonation front does not produce new "hot points" hence a regular system of transverse waves is not generated.

For $\eta \geq 0.7$ the "numerical" and the "acoustic" values of the cell size diverge by no more than 15%. Note that neither

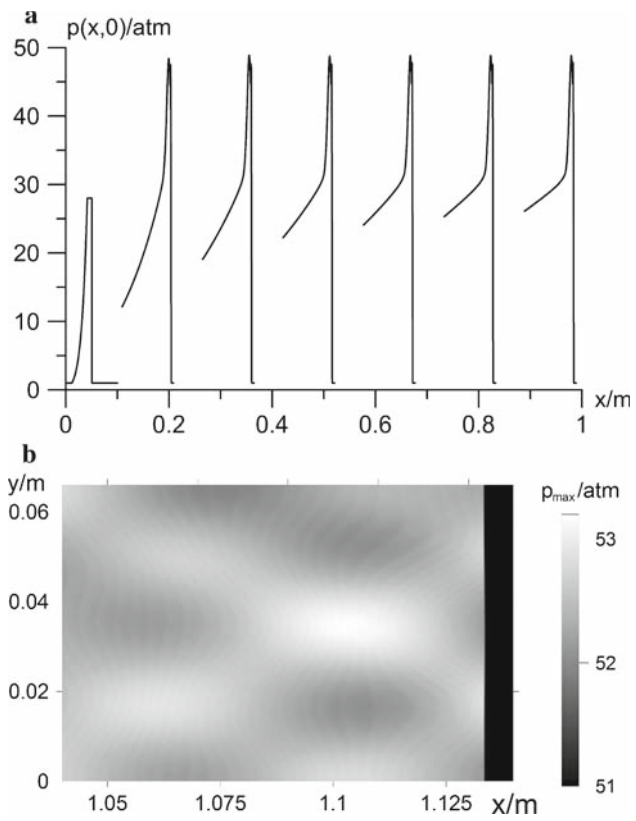

Fig. 4 Complete degeneration of cellular detonation in bi-disperse mixtures at $\eta = 0.5$: 3.5- and 1-μm particles (**a**); 3.5- and 2-μm particles (**b**)

Table 1 Dependence of the cell size on the composition of a bi-disperse gas-particle mixture 1 and 3.5 μm

η	λ_m (cm)	λ_{num}	λ_a
0	5	4.4 cm*	5.6 cm
0.1		4.4 cm*	7.8 cm
0.3		4.4 cm*	16 cm
0.4		No cells	Undetermined
0.5		No cells	Undetermined
0.6		0.94 cm	Undetermined
0.7		0.85	0.90 cm
0.9		0.78 cm	0.84 cm
1.0	0.69	0.70 cm	0.81 cm

numerical modeling no acoustic estimations give two-scaled detonation cells in the bi-disperse mixtures considered.

4 Conclusions

Using the methods of numerical modeling of the cellular detonation formation and acoustic analysis of the detonation structures in gas-particle mixtures of aluminum particles in oxygen it has been found that:

- In bi-disperse gas-particle mixtures, the process and the result of cellular detonation formation depend on the mixture composition (the relative concentration of particles of each fraction).
- A longer delay in formation of a regular system of transverse waves than in monodisperse mixtures is noted.
- Cellular detonation in a bi-disperse gas-particle mixture is characterized by a reduction of the peak pressure values at triple points upon collision and a modification of the trajectories of triple points.
- Complete degeneration of the cellular detonation into a planar wave takes place in some mixtures at certain saturation values, which is also confirmed by the acoustic analysis results.

Thus, not only the character and size of detonation cell but also the very existence of the cellular detonation in polydisperse gas-particle mixtures depends on the particle size distribution.

The given result may be one of the explanations for the fact that in very few experiments using detonation of gas-particle mixtures with reactive particles, does one succeed in observing the cellular-like structures.

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