Combustion, Explosion, and Shock Waves, Vol. 45, No. 4, pp. 495–505, 2009

Mathematical Modeling of Heterogeneous Detonation in Gas Suspensions of Aluminum and Coal-Dust Particles

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UDC 532.529+541.126

Translated from *Fizika Goreniya i Vzryva*, Vol. 45, No. 4, pp. 166–177, July–August, 2009.
Original article submitted October 25, 2008.

Results of investigations performed by the authors in the field of theoretical and numerical modeling of heterogeneous detonation of reacting gas suspensions since 2005 are systematized.

Key words: ignition, combustion, detonation, coal particles, aluminum particles.

INTRODUCTION

The study of detonation processes in heterogeneous mixtures was primarily inspired by problems of explosion and fire safety of coal mines and enterprises involved into production and application of powder materials. For instance, fine and ultrafine aluminum powders offer much promise as additives to combustible gas mixtures and, being combined with an oxidizer, as working media in detonation-engine combustors.

Long-term theoretical and numerical investigations of detonation in gas suspensions of coal-dust particles or metal particles were performed at the Khristianovich Institute of Theoretical and Applied Mechanics of the Siberian Division of the Russian Academy of Sciences with the use of approaches of mechanics of heterogeneous media. The mathematical models used are based on the principles of mechanics of interacting continua, are closed by equations of reduced chemical kinetics and available correlations for force and energy interactions of the phases, and are verified on the basis of available experimental data. A detailed analysis of the physicomathematical model of detonation of a gas suspension of aluminum particles in oxygen and some results on previous research of the structure of plane waves and cellular detonation can be found in [1]. Various issues of physicomathematical modeling of coal-dust detonation are discussed in the present paper. New results of the recent studies of detonation of monodisperse and polydisperse gas suspensions of aluminum particles in oxygen are also presented.

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1. DETONATION OF COAL-DUST SUSPENSIONS

In the case of catastrophic explosions of methane in coal mines, it is highly probable that the detonation process will evolve, being supported by ignition and combustion of coal dust. Initiation of steady propagation of heterogeneous detonation waves in mixtures of coal dust with air and oxygen was studied in experiments [2, 3] and by methods of mathematical modeling [4]. The model of mechanics of heterogeneous media constructed in [4] was equilibrium in terms of velocities, whereas the analysis of characteristic times of nonequilibrium processes revealed a substantial difference. In particular, the time of heterogeneous combustion of a coal particle is much greater than the velocity relaxation time and the characteristic time of emission of volatiles, which is commensurable with the latter.

In problems of detonation initiation, the particle-ignition conditions should be taken into account correctly. Conditions behind the detonation-wave front differ both from static conditions of slow heating and from conditions behind reflected shock waves. Experimental values of the ignition delay of coal-dust particles in transient shock waves (SW) [5, 6] show that the ignition process occurs in a mixture with velocity nonequilibrium. Ignition is accelerated by the increase in heat-transfer intensity (increase in the Nusselt number) and by the increase in temperature in the boundary layer of the particle owing to flow deceleration. Significant reduction of the ignition delay in coal-dust clouds (with a particle size of 1 to 40 μm) in transient shock waves relative to the ignition delay in reflected shock waves was noted in experiments [7]. The degree of carrier-phase heating due to flow deceleration under constrained conditions in

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dense dust clouds was estimated in [8], where this factor was considered to be responsible for the anomalous decrease in the ignition delay. For the reasons discussed above, it is obvious that two-velocity two-temperature models of mechanics of reacting media have to be developed.

1.1. Physicomathematical Model of Coal Dust Detonation with Allowance for the Stage of Ignition

A semi-empirical physicomathematical model based on a two-velocity two-temperature approximation of mechanics of heterogeneous media was developed to study the fine detonation structure of coal-dust suspensions with allowance for factors responsible for ignition. A detailed description of the model, which is a generalization of the model developed in [4], can be found in [9]. It should be noted here that the ignition and combustion stages in the model [9] are described by identical equations, but the expressions for the quantities determining the changes in mass of the species are different. The accommodation coefficients determining the fraction of heat spent on particle heating are also different. Thus, the reaction rate at the stage of combustion is assumed to depend on the mean particle temperature. The volatile emission kinetics under conditions of rapid heating is described by the equation and constants of the corresponding reaction of pulverized bituminized coal (Pittsburg stratum) derived in [10]. The process of surface combustion is described by an Arrhenius-type equation with allowance for incomplete combustion associated both with the presence of non-combustible slags (ashes) and with the lack of the oxidizer in situations where the coal-dust concentration exceeds the stoichiometric limit [4].

At the stage of ignition, the heat of the carbon-oxidation reaction in pores is assumed to be released in the particle, and the heat of the volatile-oxidation reaction is distributed in identical fractions between the gas and the particles. It is also taken into account that the ignition delays of coal particles in transient shock waves are comparable with the characteristic time of particle heating. Sichel et al. [6] made an attempt to take into account the thermal dynamics inside the volume of an individual particle, which allowed experimental and calculated ignition delays to be more or less reconciled. In gas suspensions with a significant fraction (in terms of mass) of the discrete phase, however, the mutual effect of the phases should be taken into account. In describing the stage of ignition in a gas suspension with allowance for these two factors, the first approximation is taken to be a stepwise distribution of temperature over the particle, where the temperature of a thin surface layer is determined by the stagnation temperature of the gas. The description of the heating dynamics involves the thermal effects of pyrolysis, combustion of volatiles, and coke combustion. The equation for convective heat transfer allows for the stagnation temperature of the flow in the boundary layer on the particle surface. To describe the gas species, we had to construct a new equation of state of the gas, taking into account the change in the gas adiabat, similar to that done in [11].

The detonation-wave structure was calculated for a gas suspension of 50-μm coal particles with the content of volatiles 32% and ashes 10%. These parameters of the mixture corresponded to those of detonation experiments [3]. Similar particles corresponding to bituminized coal of the Pittsburg stratum both in terms of size (53–74 μm) and in terms of the volatile contents were considered in [6], as applied to ignition problems. The reaction constants were borrowed from [12–15] for a similar type of coal.

1.2. Specific Features of Coal-Dust Ignition in Shock and Detonation Waves

Figure 1a shows the calculated ignition delays for several particle concentrations [9] (solid curves) and the experimental data [6] (points). Note that the results are accurately presented in a semi-logarithmic scale by straight lines, which reflects the Arrhenius character of the ignition process. It was also found [9] that the dynamics of emission and combustion of volatiles determines the breakdown of thermal equilibrium in the particle. Thus, bituminized coal was found to have a mixed (homogeneous–heterogeneous) type of ignition in accordance with the classification developed in [16].

1.3. Detonation Flows in Suspensions of Bituminized Coal Dust

As in [4], the model for detonation processes is verified on the basis of the experimental dependence of the detonation velocity on the initial concentration of bituminized coal particles with the content of volatiles equal to 32% and the mean particle size equal to 54 μm [3]. The calculated and experimental data are compared in Fig. 1b: the solid and dashed curves are the results calculated for 50- and 25-μm particles, respectively; $\lambda^* = (\rho_{30} + \rho_{20})/\rho_{10}$; the subscripts refer to the

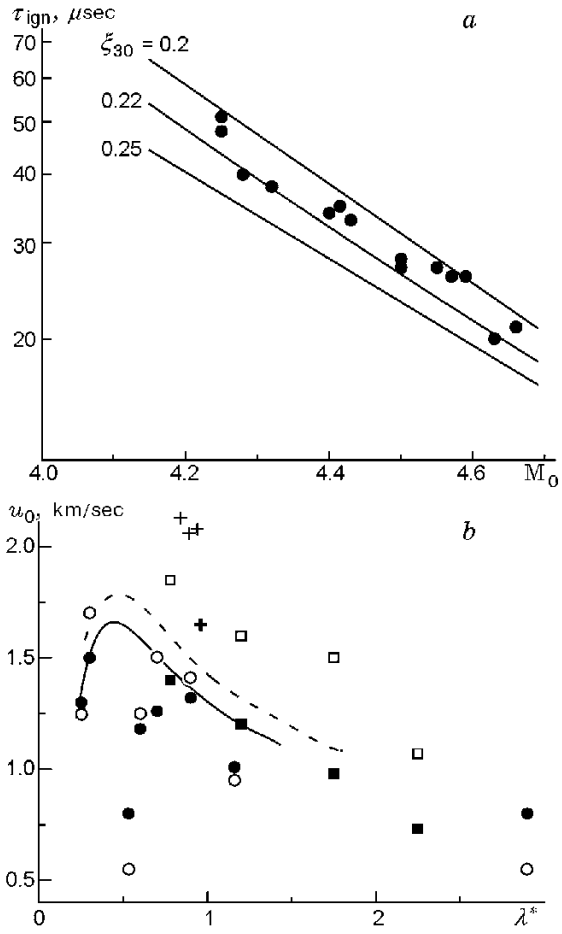

Fig. 1. Correspondence of experimental and calculated data for suspensions of bituminized coal dust: (a) ignition delay in shock waves $\tau_{\rm ign}$; the curves and points show the results of calculations [9] and experiments [6]; (b) detonation velocity u_0; the solid and dashed curves show the results calculated for particles 50 and 25 μm in size, respectively; the points are the experimental data [3].

initial state (0), gas (1), volatiles (2), and coke (3). Note that particles 54 and 25 μm in size in [3] refer to suspensions of two different types of coal with different concentrations of volatiles.

The transition from the ignition reaction to combustion in the model is assumed to occur in accordance with a criterion based on the analysis of the flow structure behind the SW front. The breakdown of thermal equilibrium (unbounded increase in temperature and speedup of emission and combustion of volatiles) is accompanied by a decrease in gas pressure. For this reason, the pressure peak is conventionally assumed to be the transition from ignition to combustion.

An example of the Chapman–Jouguet (CJ) detonation structure (stages of ignition and beginning of combustion) is shown in Fig. 2a (concentration $\xi_{30} = 0.3$ and detonation velocity $u_0 = 1.45$ km/sec). The inflection in the particle temperature distribution indicates the ignition point, where the heat release due to chemical reactions passes completely to the gas phase. At the subsequent stage of particle surface combustion, the processes proceed under conditions of velocity equilibrium of the phases (see Fig. 2b; $\xi_{30} = 0.2$ and $u_0 = 1.67$ km/sec). Note that the time of coke combustion in detonation waves exceeds the ignition delay by more than two orders of magnitude and is much greater than the characteristic times of thermal and velocity relaxation of the phases. The flow structure, therefore, coincides with that predicted by the one-velocity model [4], except for a narrow zone of nonequilibrium processes behind the leading SW front. Nevertheless, it is necessary to take into account the processes that occur in this zone and are responsible for the particle-ignition dynamics to obtain an adequate description of detonation initiation and propagation under various conditions.

2. PLANE AND CELLULAR DETONATION IN POLYDISPERSE SUSPENSIONS OF ALUMINUM PARTICLES IN OXYGEN

Our theoretical and numerical research of detonation of suspensions of aluminum particles in oxygen is based on a physicomathematical model whose basic principles were described in [17, 18] and which is consistent with the approach of mechanics of heterogeneous media [19]. A detailed description of the model can be found in [20–23]. An approximation of the experimental dependence of the combustion time on the particle radius was included in the model in [24] to describe the real time of particle burning. The model [20–24] was used to solve various problems, in particular, for numerical simulations of two-dimensional flows of cellular detonation [24]. The results of this research are summarized in [1].

The investigations described in [1, 20–24] were performed for monodisperse suspensions. Most powders, however, are characterized by a certain scatter in the particle-size distribution. Taking into account the polydisperse nature of the powder, we can refine the effect of the fractional composition on the detonation-initiation threshold, which is important for preventing undesirable explosion and detonation processes and for estimating the prospects of using aluminum powders as a fuel (or as an additive to the fuel) in detonation engines. The first step in studying polydisperse gas suspensions is consid-

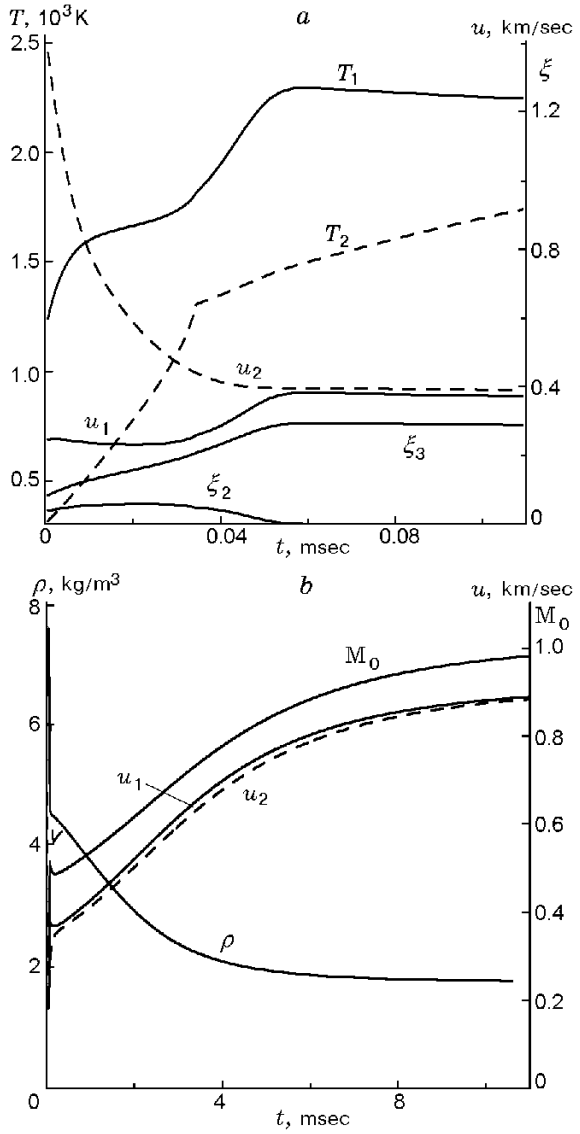

Fig. 2. Detonation-wave structure in a gas suspension of coal dust: (a) stage of ignition; (b) transition to the Chapman–Jouguet state.

ering mixtures of a gas and several fractions of particles of different diameters (suspensions with a stepwise distribution function of the particle size). The physicomathematical model discussed here is the extension of the model [20–24] to polydisperse mixtures.

2.1. Steady Plane Waves in Bidisperse Suspensions

In this Section, we consider the detonation processes in a suspension containing two fractions of particles of different sizes, with the total concentration corresponding to the stoichiometric point. The composition of the mixture is characterized by a mass fraction ratio η between the densities of the fine and coarse fractions in the initial state.

The structures of steady detonation waves in such mixtures depend on the mass fraction ratio and differ from the wave structures in monodisperse suspensions. A detailed analysis of one-dimensional detonation flows was performed in [25]. As in monodisperse suspensions of aluminum particles, the detonation in bidisperse suspensions is not ideal. A typical feature of such suspensions is intermediate velocities of sound, for instance, the equilibrium-frozen velocity of sound, which corresponds to the equilibrium state with the gas for the fine fraction and to the frozen state for the coarse fraction.

Depending on the detonation velocity u_0, the trajectory of the solution either tends to the final state of overdriven detonation or is bounded by the choking line. The location and type of the branching point depend on the mass fraction ratio. If the dominating fraction in the mixture consists of coarse particles ($\eta < 0.5$), the branching point of the solution is practically the sonic point with respect to both the frozen and equilibrium-frozen velocities of sound (the corresponding Mach numbers are close to each other and tend to unity at $\eta = 0$). If the dominating fraction consists of fine particles ($\eta \geqslant 0.5$), the state at the branching point is transonic with respect to the equilibrium-frozen velocity of sound, and it is impossible to reach a supersonic equilibrium state in the steady formulation of the problem. Numerical simulations of the unsteady problem of detonation propagation with an adjacent rarefaction wave showed that the steady segment is bounded by the equilibrium-frozen sonic point (FE in Fig. 3a). The rarefaction wave joins the frozen sonic point (F in Fig. 3a). The transitional ($c_{f,e} < v_1 < c_f$) segment between the points F and FE is unsteady, and its length increases with time.

Another specific feature of the detonation structure in bidisperse suspensions is the existence of two ρ-layers (with a drastic increase in particle density) separately in each fraction (coarse and fine particles). Correspondingly, the gas pressure and density profiles may take the form of curves with two local maximums. Depending on the mass fraction ratio, the magnitude of the first maximum may ne either greater or smaller than that of the second peak.

Thus, the structures of detonation waves in bidisperse suspensions differ from the structures in monodisperse suspensions. Proceeding of different-scale relaxation processes typical for different fractions affects the processes of ignition behind the shock wave and detonation initiation.

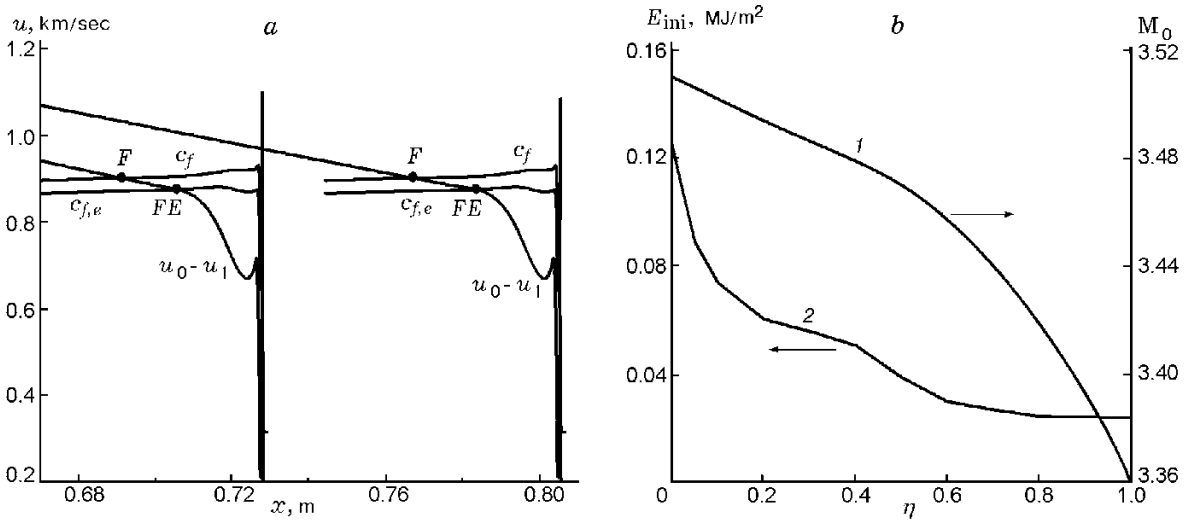

Fig. 3. Plane detonation waves in bidisperse suspensions: (a) interaction of a detonation wave with an adjacent rarefaction wave ($\Delta t = 0.05$ msec and $\eta = 0.5$); (b) initiation criteria.

2.2. Initiation of Plane Waves in Bidisperse Suspensions

The problem of shock-wave initiation of detonation was solved with two types of the initiating action: sustained SW (with a rectangular profile of parameters) and explosive SW (with an adjacent rarefaction wave). In the first case, the detonation initiation follows the "soft" [22] (or hybrid) scenario. Fine particles become ignited directly behind the leading SW front, while coarse particles become ignited on the contact discontinuity following behind the SW; as a result, the combustion front becomes accelerated, catches up with the leading SW, and enhances the latter. The initiation condition is determined by the amplitude of the initiating SW (M_0). With increasing η, the critical value of M_0 monotonically decreases from 3.51 (corresponding to a suspension of 3.5-μm particles) to 3.36 (suspension of 1-μm particles) (curve 1 in Fig. 3b). The nonlinear character of the dependence $M_0(\eta)$ should be noted.

The initiation condition for strong shock waves ($M_0 = 5$) is the value of the stored energy E_{ini}. Numerical results predict that the most drastic decrease in the critical value of the initiation energy occurs as η increases from 0 to 0.2 (curve 2 in Fig. 3b). Thus, the value of E_{ini} is reduced almost by 30% owing to the presence of 5% of fine particles ($\eta = 0.05$) and by 40% owing to the presence of 10% of fine particles ($\eta = 0.1$). The physical reason for such a drastic decrease in the initiation threshold is the fact that part of the energy released in combustion of fine particles ignited earlier is involved into detonation initiation in the fraction of coarse particles.

Under certain conditions, an unsteady two-front structure is formed in the mixture at the initial stage of initiation. It formation is associated with the possibility of a hybrid initiation scenario, which combines the properties of the "hard" and "soft" types [22, 25]. The two-front structure exists for a limited time and is not steady. Later on, the two fronts merge into one, thus, forming an overdriven wave, which is then attenuated and propagates in the normal detonation regime.

2.3. Cellular Structure in Bidisperse Suspensions

The existence of cellular heterogeneous detonation in gas suspensions of metallic or organic particles was validated in experiments [26–29]. Two-dimensional detonation flows with cellular structures in gas suspensions of aluminum particles were numerically simulated in [24, 29–32]. A relation between the cell size and the particle diameter in the form of a power-law dependence with a power index of 1.6 was established in [24], based on the model of a monodisperse stoichiometric suspension of aluminum particles in oxygen. Propagation of cellular detonation in lean suspensions of aluminum particles in oxygen for two particle sizes (1 and 3.5 μm) was modeled in [30]. Though the results in [24] and [30] were obtained with the use of different models, nevertheless, they are in good agreement with each other and with experimental data [26]. A similar power-law dependence of the cell size on the particle diameter with a close value of the power index equal to 1.4 was later obtained in [31] for monodisperse suspensions of aluminum particles in air.

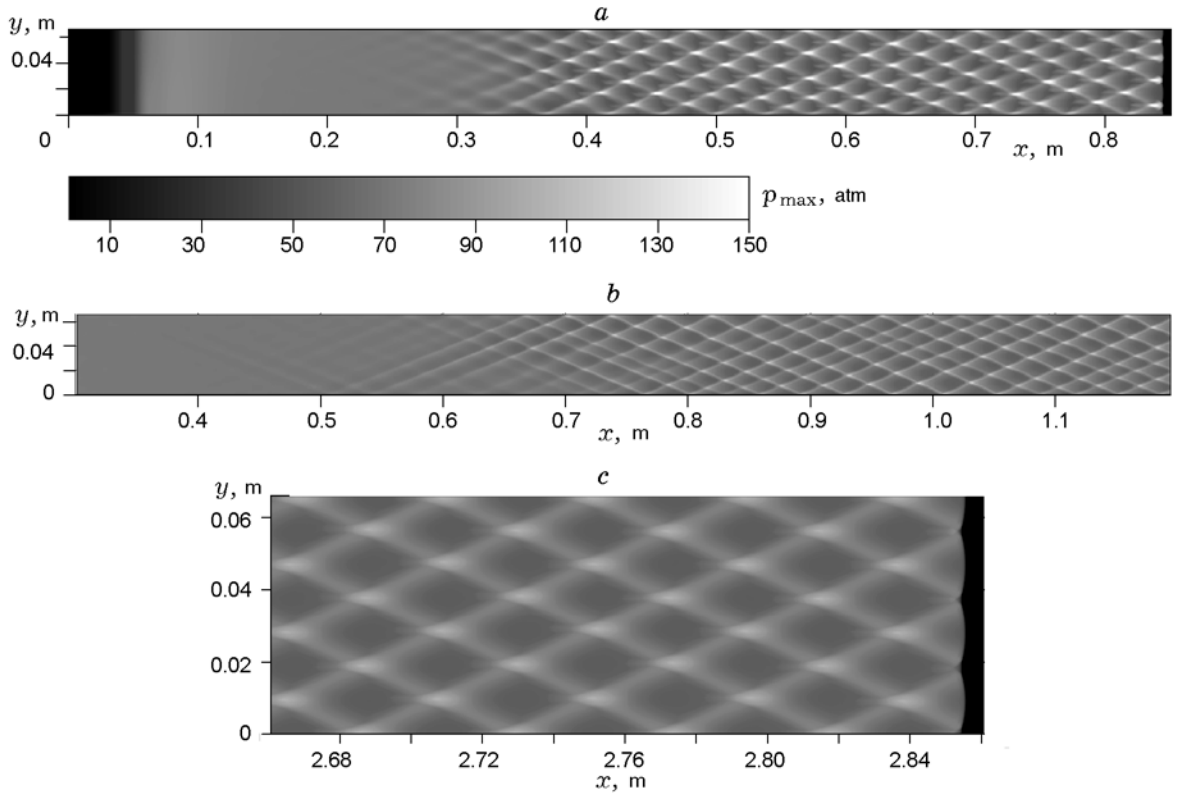

Fig. 4. Formation of cellular detonation: (a) monodisperse suspension of 2-μm particles; (b) bidisperse suspension of 2-μm and 1-μm particles with $\eta = 0.5$; (c) suspension of three fractions of particles (1, 2, and 3.5 μm) with $\eta_2 = 0.5$.

Note that the detonation processes were modeled in [30, 31] within the framework of the concept of diffusion-limited combustion of aluminum particles in air. The constraints of this combustion model were discussed in [29], where a hybrid model combining the Arrhenius and diffusion-type kinetics was proposed. The model proposed in [29] provided a possibility of an adequate description of some properties of detonation processes, in particular, the dependence of the results of the detonation-to-deflagration transition on the initial pressure in the mixture. Moreover, the degenerate character of cellular detonation was noted in experiments [29], which was manifested in low values of the amplitude of pressure oscillations behind the front. Zhang et al. [29] attributed this phenomenon to the presence of the stage of diffusion-limited combustion. As it will be demonstrated below, an alternative explanation for degeneration of cellular detonation in gas suspensions is also possible.

As real mixtures are usually characterized by a certain scatter in the particle size, it seems of interest to consider the issue of existence and character of cellular detonation in polydisperse suspensions. The first step in numerical simulations of cellular detonation of polydisperse mixtures was also considering bidisperse suspensions of aluminum particles in oxygen [32].

Two-dimensional flows were calculated within the framework of the above-indicated model with the use of the numerical technology described in [33, 34]. The problem of shock-wave initiation of detonation was posed as the initial-boundary-value problem for the system of equations used, with a certain small perturbation of particle density at the edge of the cloud of this suspension.

The calculations showed that the cellular detonation structure is formed in the case of noticeable prevalence of one fraction in the mixture, and this structure is similar to the detonation structure in the corresponding monodisperse suspension. Nevertheless, there are some specific features as well. First of all, this is the lower peak pressure values at triple points. In the fields of the maximum pressure $p_{\max}(x, y) = \max\limits_{t}[p(x, y, t)]$ (Fig. 4) plotted in a single gray scale, this decrease is manifested as the lower contrast of the picture (cf.

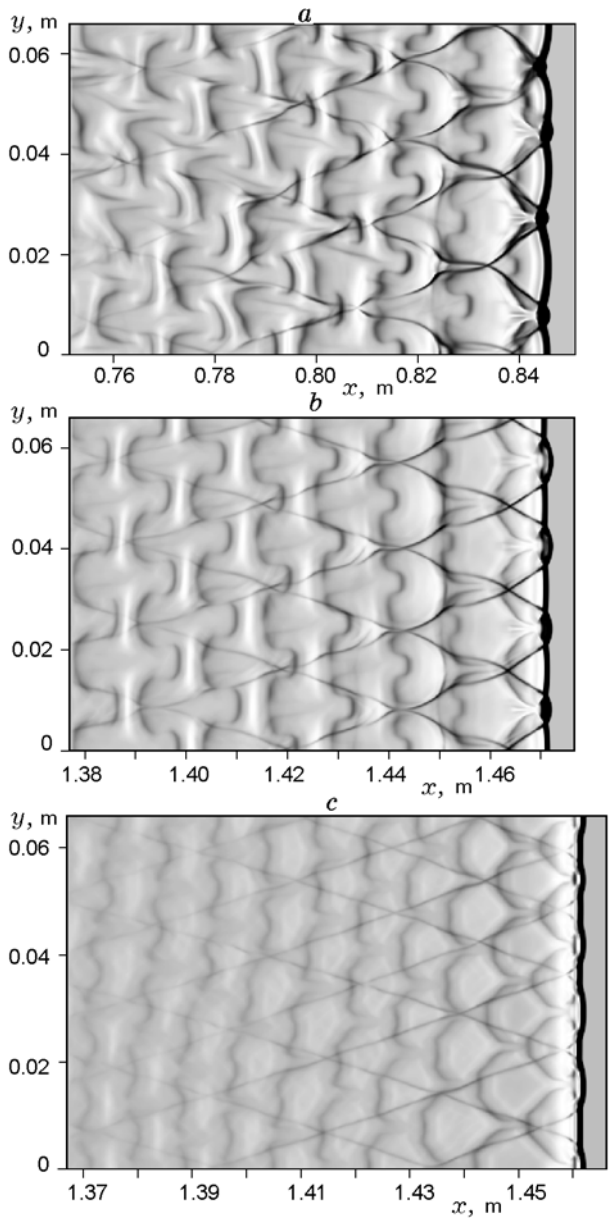

Fig. 5. Effect of the composition of the bidisperse mixture on the character of cellular detonation: $\eta =$ 0 (a), 0.3 (b), and 0.6 (c).

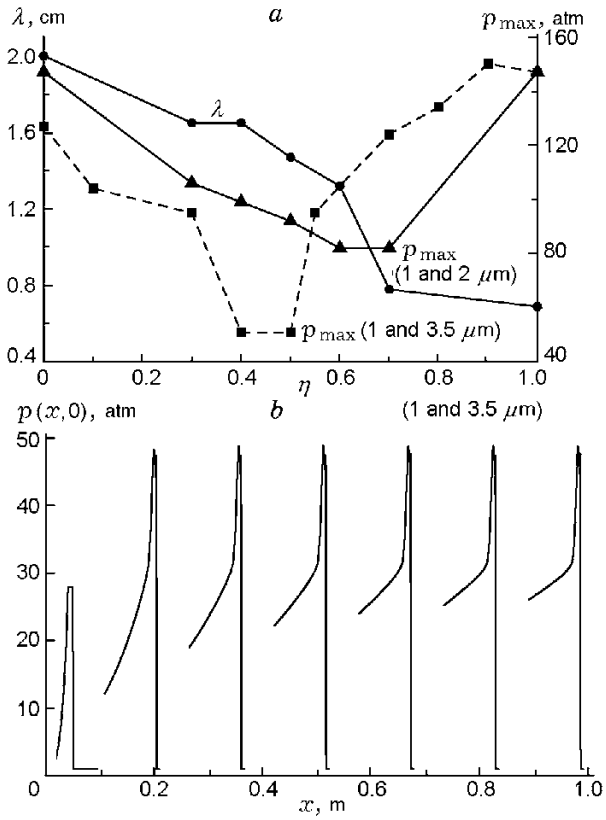

Fig. 6. Degeneration of cellular detonation in bidisperse suspensions: (a) characteristics of the process versus the mass fraction ratio; (b) stable propagation of a plane wave in a mixture of 1-μm and 3.5-μmm particles with $\eta = 0.5$.

Fig. 4b and Fig. 4a). Another distinctive feature is the later development of transverse waves (cf. Fig. 4b and Fig. 4a): the greater the fraction of particles of the other size, the longer this delay. The third specific feature is the tendency to degeneration of cellular detonation at medium values of the mass fraction parameter (Fig. 5): The leading SW front approaches the plane wave, the transverse waves are less curved, and the variations of parameters have smaller amplitudes. Thus, the detonation structure in bidisperse suspensions possesses some intermediate properties between plane detonation and cellular detonation. The effect of the mass fraction parameter on the maximum pressure values is illustrated in Fig. 6. The calculated dependence of the detonation cell size λ on the composition for a mixture of 1-μm and 2-μm particles is also plotted.

The calculations predict complete degeneration of cellular detonation in some bidisperse suspensions; in this case, the system of transverse waves is not formed at all. In a mixture of 1-μm and 3.5-μm particles, for instance, this situation is observed at $\eta = 0.4$ and 0.5, which is evidenced by the behavior of the dependence $p_{\max}(\eta)$ (see Fig. 6a). In these cases, two-dimensional calculations predict stable propagation of a plane detonation wave (Fig. 6b; profiles of the wall pressure with a step of 0.1 msec).

2.4. Application of Methods of the Acoustic Approach for Analyzing Cellular Detonation in Gas Suspensions

Degeneration of cells in bidisperse gas suspensions was validated in [32], and some explanation for this phenomenon was proposed on the basis of an acoustic analysis of the structure of the plane wave of steady detonation. It was shown [35] that the primary perturbation on the detonation-wave front generates two additional "hot" spots on the front, which are located at identical distances from the initial perturbation. The locations of these spots are found by solving an appropriate acoustic problem for the flow field of plane Chapman–Jouguet waves or waves that are overdriven or decaying to some extent. According to [35], the distance between the transverse waves following each other is determined by the formula

$$\lambda_{\text{ac}} = 4 \int_0^X \frac{c_f}{\sqrt{\sigma_*^2 - (c_f^2 - v_1^2)}} dx. \qquad (1)$$

As applied to a heterogeneous mixture, c_f is the frozen velocity of sound and v_1 is the gas velocity in the front-fitted system. The upper limit of integration X corresponds to the point $\sigma = c_f^2 - v_1^2$. The constant σ_* in Eq. (1) is chosen among all admissible values of σ (which ensure positive values of the radicand) to obtain the minimum of the time integral

$$t = 2 \int_0^X \frac{c_f \sigma}{(c_f^2 - v_1^2)\sqrt{\sigma^2 - (c_f^2 - v_1^2)}}\, dx. \qquad (2)$$

The method [35] as applied to gas suspensions is described in more detail in [24, 32]. The estimates of the cell size in monodisperse suspensions studied in [24] are in good agreement with the results of the numerical experiment, both in terms of the absolute values and in terms of the power index in the dependence on the particle size.

Situations where the constant σ_* and the values of t and λ_{ac} cannot be determined may occur in bidisperse suspensions at some values of the mass fraction parameter. This means that new "hot" spots are not generated at a certain distance from the initial perturbation. It is also possible that the value of λ_{ac} can be determined in the Chapman–Jouguet flow field, but cannot be determined for overdriven or decaying waves. This feature can be considered as a possible explanation for partial degeneration of cellular detonation (a detailed analysis was performed in [32]). Thus, the use of the method developed in [35] for gas suspensions allows us to obtain information about the character of cellular detonation and estimates of the detonation cell size on the basis of available data on the structure of steady plane detonation waves.

2.5. Plane and Cellular Detonation in Polydisperse Suspensions with Domination of the Middle-Sized Fraction

It seems of interest to consider whether degeneration of cellular detonation is a property inherent in real polydisperse gas suspensions. For this purpose, we considered mixtures consisting of three and five fractions with a symmetric distribution function. It turned out that the use of the acoustic method [35] allows us to determine the transverse size of the cell for mixtures with noticeable domination of the middle-sized fraction. If the fraction of the middle-sized particles is $\eta \leqslant 0.4$ (for suspensions with both three and five fractions), the profiles $c_f^2 - v_1^2$ have only one local maximum, which indicates that there are no detonation cells in such mixtures.

The results of numerical simulations of cellular detonation formation in the corresponding polydisperse suspensions are plotted in Figs. 4 and 7; these results completely confirm the assumption made above. The shadowgraphs of the maximum pressure (see Fig. 4c) show that the character of cellular detonation is the same as that in bidisperse suspensions. Figure 7 shows the profiles of the gas density on the wall at a certain fixed time. The amplitude of oscillations in the flow behind the detonation front is seen to decrease with decreasing η. At $\eta \leqslant 0.4$, two-dimensional calculations predict stable propagation of a plane detonation wave (solid curve in Fig. 7b). Thus, small perturbations cannot initiate detonation in the above-considered polydisperse suspensions with the fraction of the middle-sized particles smaller than 40%. For higher values of η, cellular detonation is formed, but it has a degenerate character.

Thus, it follows from the results of numerical simulations and the acoustic analysis performed that the fractional composition of the gas suspension and the particle-size distribution affect not only the detonation cell size, but also the mere existence of cellular detonation and its character.

Note that degeneration of cellular detonation (reduction of the amplitude of pressure oscillations) was observed in a number of experiments whose results were published in [29]. Zhang et al. [29] put forward a hypothesis that this phenomenon can be related to the influence of the stage of diffusion-limited combustion of the aluminum particle, which is described by the non-

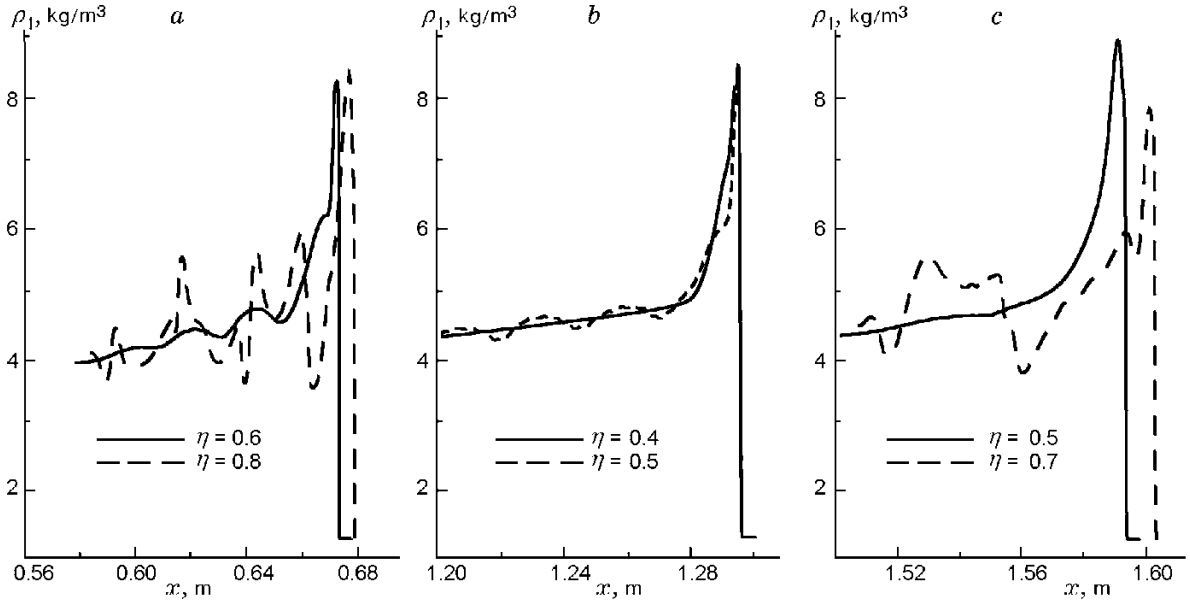

Fig. 7. Degeneration of cellular detonation in polydisperse suspensions with three fractions (a and b) and with five fractions (c).

Arrhenius-type kinetics. The following facts, however, should be noted. On one hand, the formation of developed cellular structures in monodisperse fluids was simulated in [30] within the framework of the kinetic model of diffusion-limited combustion of aluminum particles. On the other hand, the photographs of aluminum particles used in experiments [29] clearly display polydisperse features. Thus, the degeneration of cellular detonation, which was established on the basis of numerical simulations and acoustic analysis within the framework of our model with allowance for the presence of several fractions in the mixture, agrees with experimental observations [29]. In addition, the theoretically predicted possibility of degeneration of cellular detonation in polydisperse suspensions can be one possible explanation for the fact that cellular structures were observed only in few experiments on detonation of gas suspensions of reacting particles.

CONCLUSIONS

The results obtained previously in the field of heterogeneous detonation of gas suspensions of coal and aluminum particles are summarized in the present paper. It is demonstrated that semi-empirical models of detonation of gas suspensions of coal-dust and aluminum particles, which are based on approaches of mechanics of heterogeneous media and equations of reduced chemical kinetics, offer adequate descriptions of complex one-dimensional and two-dimensional detonation flows.

The mathematical model of heterogeneous detonation of the gas suspension of coal dust, which takes into account particle ignition and combustion, agrees with experimental data both in terms of the steady detonation velocity as a function of particle concentration and in terms of the ignition delay as a function of the SW Mach number. The analysis performed revealed the governing effect of the dynamics of emission and combustion of volatiles on ignition of a suspension of bituminized coal particles, which follows the hybrid (homogeneous–heterogeneous) mechanism. Velocity nonequilibrium is demonstrated to play an important role in ignition and, hence, initiation of heterogeneous detonation in gas suspensions of coal particles with a high content of volatiles.

Numerical and theoretical investigations of detonation in polydisperse suspensions of aluminum particles in oxygen revealed the following specific features of one-dimensional and two-dimensional flows.

- The detonation in a bidisperse suspension is nonideal; the steady-state part of the structure is bounded by the equilibrium-frozen sonic point; the detonation structure is characterized by a double ρ-layer.
- Nonlinear dependences of the critical SW Mach number and initiation energy of explosive shock waves on the mass fraction parameter are determined; the presence of a small amount of fine particles in the mixture may ensure a significant decrease in the initiation energy.
- Hybrid scenarios of detonation initiation are possible, with “hard” initiation in the fine fraction and

"soft" initiation in the coarse fraction; temporary simultaneous existence of unsteady two-front structures is possible.

• Partial degeneration of cellular detonation with attenuation of transverse waves and front straightening is observed in polydisperse suspensions; the character of cellular detonation and the detonation cell size depend on the fractional composition of the mixture.

• Complete degeneration of cells and stable propagation of a plane detonation wave can occur in mixtures with a significant dispersion of the particle-size distribution.

• The results of numerical simulations of two-dimensional detonation flows agree with the data obtained by an acoustic analysis and with new experimental data, which testify to the degenerate character of cellular detonation in gas suspensions of aluminum particles.

This work was supported by the Russian Foundation for Basic Research (Grant Nos. 06-01-00299 and 08-01-92010_NNS_a).

REFERENCES

1. A. V. Fedorov, V. M. Fomin, and T. A. Khmel', "Theoretical and numerical study of detonation processes in gas suspensions with aluminum particles," *Combust., Expl., Shock Waves*, **42**, No. 6, 735–745 (2006).
2. M. A. Nettleton and R. Stirling, "Detonation in suspensions of coal dust in oxygen," *Combust. Flame*, **21**, 307–314 (1973).
3. D. H. Edwards, P. J. Fearnley, and M. A. Nettleton, "Detonation limits of clouds of coal dust in mixtures of oxygen and nitrogen," *Combust., Expl., Shock Waves*, **23**, No. 2, 239–245 (1987).
4. A. V. Fedorov and T. A. Khmel', "Mathematical simulation of detonation processes in a coal-particle suspension," *Combust., Expl., Shock Waves*, **38**, No. 6, 700–708 (2002).
5. A. A. Borisov, B. E. Gelfand, S. A. Tsyganov, et al., "Ignition of dusts behind shock waves," *Khim. Fiz.*, No. 8, 1127–1128 (1983).
6. M. Sichel, S. M. Baek, C. W. Kauffman, et al., "The shock wave ignition of dusts," *AIAA J.*, **23**, 1375–1380 (1985).
7. V. M. Boiko, A. N. Papyrin, and S. V. Poplavskii, "Effect of volatiles on ignition delay in coal dust gas suspensions within shock waves," *Combust., Expl., Shock Waves*, **27**, No. 2, 223–231 (1991).
8. V. M. Boiko, A. N. Papyrin, and S. V. Poplavskii, "Mechanism of dust ignition in incident shock waves," *Combust., Expl., Shock Waves*, **29**, No. 3, 389–394 (1993).
9. A. V. Fedorov and T. A. Khmel', "Mathematical simulation of heterogeneous detonation of coal dust in oxygen with allowance for the ignition stage," *Combust., Expl., Shock Waves*, **41**, No. 1, 78–87 (2005).
10. L. D. Smoot, M. D. Horton, and G. A. Williams, "Propagation of laminar pulverized coal–air flames," in: *Proc. 16th Int. Symp. on Combustion*, The Combustion Inst., Pittsburgh (1977), pp. 375–387.
11. V. V. Koren'kov and V. N. Okhitin, "Numerical determination of effect of explosive density on parameters of air shock waves," *J. Appl. Mech. Tech. Phys.*, **24**, No. 3, 403–406 (1983).
12. S. K. Ubhayakar, D. B. Stickler, C. W. von Rosenberg, Jr., and R. E. Gannon, "Rapid devolatilization of pulverized coal in hot combustion gases," in: *Proc. 16th Symp. (Int.) on Combustion*, The Combustion Inst., Pittsburgh (1977), pp. 427–436.
13. T. W. Lester, W. R. Seeker, and J. F. Merklin, "The influence of oxygen and total pressure on the surface oxidation rate of bituminous coal," in: *Proc. 18th Int. Symp. on Combustion*, The Combustion Inst., Pittsburgh (1981), pp. 1257–1265.
14. I. W. Smith, "The combustion rates of coal chars: A review," in: *Proc. Nineteenth Symp. (Int.) on Combustion*, The Combustion Inst., Pittsburgh (1982), pp. 11045–1065.
15. P. A. Libby and T. A. Blake, "Theoretical study of burning carbon particles," *Combust. Flame*, **36**, 139–169 (1979).
16. Yu. A. Gosteev and A. V. Fedorov, "Ignition of the gas–coal dust mixture. Pointwise approximation," *Combust., Expl., Shock Waves*, **37**, No. 6, 646–654 (2001).
17. A. E. Medvedev, A. V. Fedorov, and V. M. Fomin, "Description of ignition and combustion of gas mixtures with solid particles by methods of mechanics of continuous media," *Combust., Expl., Shock Waves*, **20**, No. 2, 127–132 (1984).
18. A. V. Fedorov, "Structure of heterogeneous detonation of aluminum particles dispersed in oxygen," *Combust., Expl., Shock Waves*, **28**, No. 3, 277–286 (1992).
19. R. I. Nigmatulin, *Dynamics of Multiphase Media*, Part 1, Hemisphere Publ., New York (1991).
20. A. V. Fedorov and T. A. Khmel', "Types and stability of detonation flows of aluminum particles in oxygen," *Combust., Expl., Shock Waves*, **32**, No. 2, 181–190 (1996).
21. A. V. Fedorov, V. M. Fomin, and T. A. Khmel', "Nonequilibrium model of steady detonations in aluminum particle–oxygen suspensions," *Shock Waves*, **9**, No. 5, 313–318 (1999).
22. T. A. Khmel' and A. V. Fedorov, "Numerical simulation of detonation initiation with a shock wave entering a

cloud of aluminum particles," *Combust., Expl., Shock Waves*, **38**, No. 1, 101–108 (2002).
23. T. A. Khmel' and A. V. Fedorov, "Interaction of a shock wave with a cloud of aluminum particles in a channel," *Combust., Expl., Shock Waves*, **38**, No. 2, 206–214 (2002).
24. A. V. Fedorov and T. A. Khmel', "Numerical simulation of formation of cellular heterogeneous detonation of aluminum particles in oxygen," *Combust., Expl., Shock Waves*, **41**, No. 4, 435–448 (2005).
25. A. V. Fedorov and T. A. Khmel', "Structure and initiation of plane detonation waves in a bidisperse gas suspension of aluminum particles," *Combust., Expl., Shock Waves*, **44**, No. 2, 163–171 (2008).
26. W. Ingignoli, B. Veyssiere, and B. A. Khasainov, "Study of detonation initiation in unconfined aluminum dust clouds," in: G. Roy et al. (eds.), *Gaseous and Heterogeneous Detonations*, ENAS, Moscow (1999), pp. 337–350.
27. F. Zhang, H. Grönig, and A. van de Ven, "DDT and detonation waves in two-phase mixtures," *Shock Waves*, **11**, 53–71 (2001).
28. F. Zhang, K. B. Gerrard, R. C. Ripley, and V. Tanguay, "Unconfined aluminum particles-air detonation," in: *Proc. 26th Int. Symp. on Shock Waves*, Göttingen, Germany, July (2007), pp. 15–20.
29. F. Zhang, K. B. Gerrard, and R. C. Ripley, "Reaction mechanism of aluminum particles–air detonation," in: *Proc. of the 7th Int. Symp. on Hazard, Prevention, and Mitigation of Industrial Explosions* (July 2008, St. Petersburg, Russia), Vol. II (2008), pp. 223–237.
30. K. Benkiewicz and A. K. Hayashi, "Two-dimensional numerical simulations of multi-headed detonations in oxygen–aluminum mixtures using an adaptive mesh refinement," *Shock Waves*, **13**, 385–402 (2003).
31. B. Veyssiere, B. A. Khasainov, and A. Briand, "Investigation of detonation initiation in aluminum suspensions," *Shock Waves*, **18**, 307–315 (2008).
32. A. V. Fedorov and T. A. Khmel', "Formation and degeneration of cellular detonation in bidisperse gas suspensions of aluminum particles," *Combust., Expl., Shock Waves*, **44**, No. 3, 343–353 (2008).
33. T. A. Khmel', "Numerical simulation of two-dimensional detonation flows in a gas suspension of reacting solid particles," *Mat. Model.*, **16**, No. 6, 73–77 (2004).
34. A. V. Fedorov and T. A. Khmel', "Numerical technologies for studying heterogeneous detonation in gas suspensions," *Mat. Model.*, No. 8, 49–63 (2006).
35. H. O. Barthel, "Predicted spacings in hydrogen–oxygen–argon detonations," *Phys. Fluids*, **17**, No. 8, 1547–1553 (1974).