Modelling of Shock Wave and Detonation Processes in Collisional Particle Suspensions in Gas

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1 Introduction

Theoretical studies and numerical modeling of detonation flows in reactive gas - particle mixtures are usually performed under assumptions of dilute suspensions neglecting particle volume, their random motion, and particle collisions. However, in the structures of shock wave and detonation flows there are areas of high particle concentration (ρ-layers) [1, 2] where particle-to-particle interactions may be significant. The input of particle collisions in the frame of mechanics of heterogeneous media is usually considered as a pressure in the discrete phase [3-5]. Description of collisional dynamic of granular media with rough inelastic particles on the base of molecular-kinetic approach has been proposed in [6, 7]. The extension of the model [6, 7] on two-phase media of gas and collisional particles is presented in [8]. The objectives of the present study are to present a physical-mathematical model of a reacting gas - particles mixture with regard for particle collisions, which are described accordingly [6, 7], and to present some results of numerical simulations demonstrating collisional effects in shock wave and detonation processes. The following problems will be considered: a plane shock wave interaction with a cloud of inert particles in one-dimensional formulation, and the interaction of cellular detonation front in a gas suspension of reacting particles with a cloud of inert particles in two-dimensional formulation.

2 Physical and Mathematical Model of Collisional Gas-Particle Mixture

The Euler equations for two-phase mixture of gas and inelastic rough particles follow from conservation laws for mass, momentum, and energy for each phase and the chaotic energy balance equation [6, 7, 8]:

$$\frac{\partial\rho_i}{\partial t}+\frac{\partial(\rho_i u_i)}{\partial x}=(-1)^{i-1}J\,,\qquad \frac{\partial\rho_i u_i}{\partial t}+\frac{\partial(\rho_i u_i^2+m_i p_i)}{\partial x}=(-1)^i\Big(p_1\frac{\partial m_2}{\partial x}+f-Ju_2\Big)\,,$$

$$\frac{\partial\rho_i E_i}{\partial t}+\frac{\partial(\rho_i u_i E_i+m_i u_i p_i)}{\partial x}=(-1)^i\Big(p_1\frac{\partial u_2 m_2}{\partial x}+fu_2+q-JE_2\Big)\,, \tag{1}$$

$$\frac{\partial\rho_2 E_c}{\partial t}+\frac{\partial(\rho_2 u_2 E_c+\eta m_2 u_2 p_2)}{\partial x}=\eta p_1\frac{\partial u_2 m_2}{\partial x}-JE_c+\eta f u_2-\frac{6}{\pi d}C_0\rho_2 m_2 g(m_2)(e_c)^{3/2}\,.$$

The system is enclosed by the equations of state

$$E_1 = c_{v1}T_1 + u_1^2/2\,,\; E_2 = e_c + c_{v2}T_2 + u_2^2/2 + Q\,,\; E_c = e_c + 0.5\eta u_2^2\,,$$
$$p_1 = \rho_{11}RT_1\,,\; m_2 p_2 = m_2 p_1 + p_c\,,\; p_c = G(m_2)\rho_2 e_c\,, \qquad (2)$$
$$G(m_2) = 0.5\alpha_t[1 + 2(1+\varepsilon)m_2 g(m_2)]\,,\; g(m_2) = [1 - (m_2/m_*)^{4m_*/3}]^{-1}\,.$$

Here ρ, u, p, m are the mean density, velocity, pressure, and the particle volume concentration, respectively (m_* is limiting value of the bulk concentration); $\rho_i = \rho_{ii} m_i$, ρ_{ii} is the true density of phases, the subscripts 1 and 2 stand for the gas phase and particles, respectively, *f* is the force of interaction between phases, *J* is the mass transfer. Particles are assumed to be incompressible ($\rho_{22} = const$). We assume that the total energy of the particle phase E_2 includes together with kinetic energy, internal heat energy and energy of chemical reactions also the energy of chaotic particle motion $e_c = 0.5\sum_{i=1}^{N}(u_i')^2/N$ where u_i' is the *i*-th particle velocity pulsation, N is number of particles in the unit volume. The parameter $\eta \le 1$ expresses non-ideality of the collisions, C_0 is the dissipation, *d* is the diameter of particles. The parameters η, C_0, α_t depend on the particle restitution coefficient ε and the roughness parameter β [6, 7, 8]. Figure 1 presents these dependencies for η, C_0.

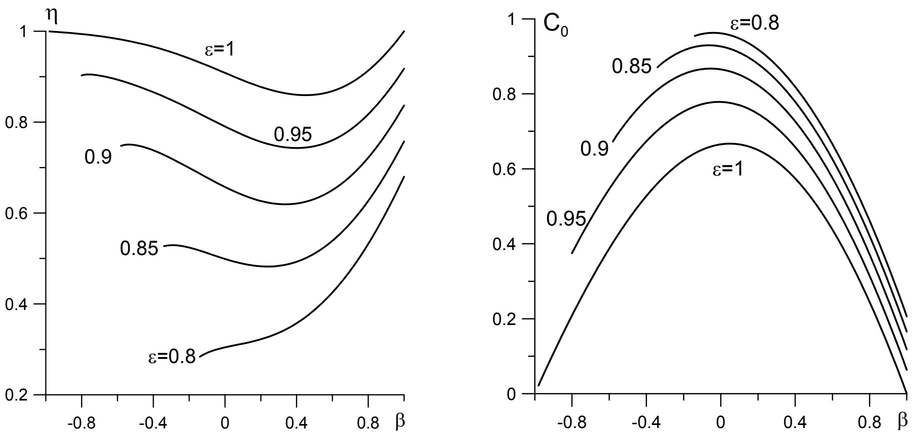

Figure 1. Dependence of the parameters η and C_0 on the restitution and roughness coefficients

The system of equations of isolated particle media is hyperbolic. The sound velocity in the discrete phase is $c_2^2 = \gamma(m_2)p_c/\rho_2$, and the adiabatic exponent γ is

$$\gamma = \eta G(m_2) + \frac{d[G(m_2)m_2]}{G(m_2)dm_2} = 1 + \eta G(m_2) + \frac{m_2}{G(m_2)}\frac{dG(m_2)}{dm_2}\,. \qquad (3)$$

Figure 2 show the dependence of the adiabatic exponent γ (for $\varepsilon = 1$ and $\varepsilon = 0.8$) and the collisional functions *G* and *g* (for $\varepsilon = 0.8$) on the particle volume concentration $m=m_2$ for $m_*=0.6$. The two-phase system of equations regarding for the particle volume (Archimedes forces) is in general case the system of composite type.

The model has been verified by the experimental data [9] on measuring the rarefaction wave velocity in the expansion of a gas suspension at destruction of a high-pressure chamber. The results of the model calculations of the equilibrium sound velocity [8] are in qualitative agreement with the experimental data [9].

3 Stationary Shock Waves in Collisional Mixtures

The stationary shock wave conditions are obtained upon transition into the accompanying system and integrating in the vicinity of the shock:

$$[\rho_1 u_1 + \rho_2 u_2] = 0\,, \quad [\rho_1 u_1{}^2 + \rho_2 u_2{}^2 + p_1 + p_c] = 0\,,$$
$$[\rho_1 u_1 E_1 + \rho_2 u_2 E_2 + m_1 u_1 p_1 + m_2 u_2 p_1 + u_2 p_c] = 0\,, \qquad (4)$$
$$[m_2 u_2] = 0\,, \quad [T_2] = 0\,, \quad [\rho_2 u_2 E_c + \eta m_2 u_2 p_1 + \eta u_2 p_c] = 0\,.$$

The equation

$$\rho_{22} m_2 u_2 \frac{du_2}{dx} + \frac{dp_c}{dx} + m_2 \frac{dp_1}{dx} = f$$

with $\rho_{22} = \text{const}$ and $m_2 u_2 = m_0 u_0$ (u_0 is the propagation velocity) gives the closing condition for the shock

$$\frac{1}{2}(\rho_{22} + \frac{[p_c]}{[u_2] m_0 u_0})[u_2{}^2] + [p_1] = 0\,. \qquad (5)$$

If the shock wave propagates in undisturbed mixture ($e_{c0} = 0$, $p_{c0} = 0$) the equation for particle volume concentration have the form:

$$\frac{1}{2}\alpha_t (\frac{m}{m_0} - 1)[1 + (1+\varepsilon) m g(m)] = \frac{2}{\eta}\,. \qquad (6)$$

The function in the left side monotonically varies from 0 at $m = m_0$ to infinity at $m \to m_*$ (close packing), therefore the equation (6) has a unique solution. Note that the shock amplitude (the value of m) here does not depend on it's propagation velocity (shock wave of the type II).

There is also a solution with $e_c = 0$ (shock wave of the type I). The conditions at the shock correspond to collisionless two-phase medium with the buoyancy forces, for which $[T_2] = 0$, $[m_2 u_2] = 0$, and the discrete phase velocity on the shock is determined by the well-known formula [10] $[u_2^2 / 2] + [p_1] / \rho_{22} = 0$. The problem is reduced to solving the fifth degree algebraic equation with respect to u_2 or fourth degree equation excluding the trivial solution $u_2 = u_0$. Which of the two types (collisional or collisionless) of the solution is realized, depends on the physical parameters and the problem conditions.

4 Unsteady Problems of Shock Wave Propagation…….

Consider a planar shock wave propagating in gas and entering a cloud of particles in 1-D formulation. The boundary-value problem is similar to the first one analyzed in [11]. The numerical method previously used for similar problems ([11-12]) is based on the TVD scheme for gas and the Gentry-Martin-Daly scheme for extended system of equations of the discrete phase. The scheme is modified by introducing appropriate approximations of the terms associated with the particle pressure, the chaotic energy, as well as non-divergent terms $p_1 \partial m_2 / \partial x$ and $p_1 \partial u_2 m_2 / \partial x$. The calculations were performed for the parameters of the particles of alumina (aluminum oxide) in oxygen.

Figure 2 shows the typical gas (solid lines) and the discrete phase (dashed lines) density profiles in the formation of a mixture of stationary shock waves of the type I (Fig. 2a) and type II (Fig. 2b). Here $\eta = 1$ and the particle size is 10 microns. Transition to formation the shock waves of the type II takes place with increase in the incident SW amplitude and initial particle concentration in the cloud. Scenarios of the type II shock wave formation occurs in two stages. The first stage is formed by a structure similar to the wave of the type I (Fig. 2, b, x <3 m). Then another shock in the gas density of less amplitude than initial sharp rise breaks away from the leading jump in the particle phase. The propagation velocity of this shock exceeds the velocity of the SW entered in the cloud.

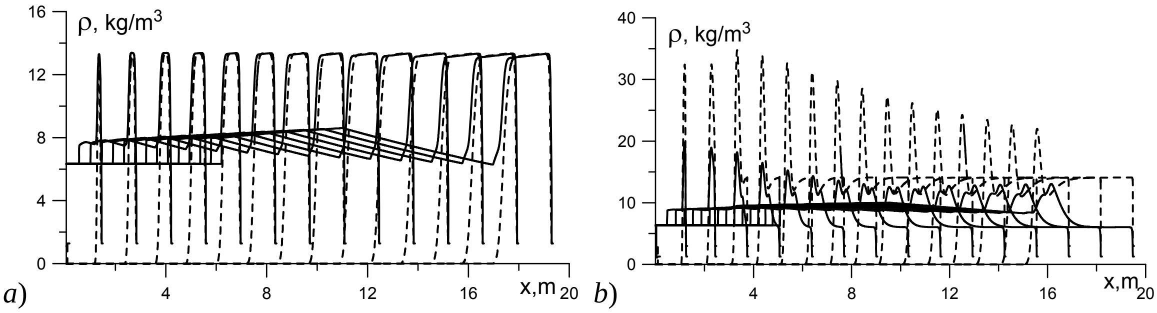

Figure 2. Formation of shock waves of different types (solid lines – gas, dashed lines - particles), $M_0 = 5$, $e_{c0} = 0$, $\Delta t = 1$ ms: $\xi_0 = 0.5$ (a); $\xi_0 = 0.7$ (b).

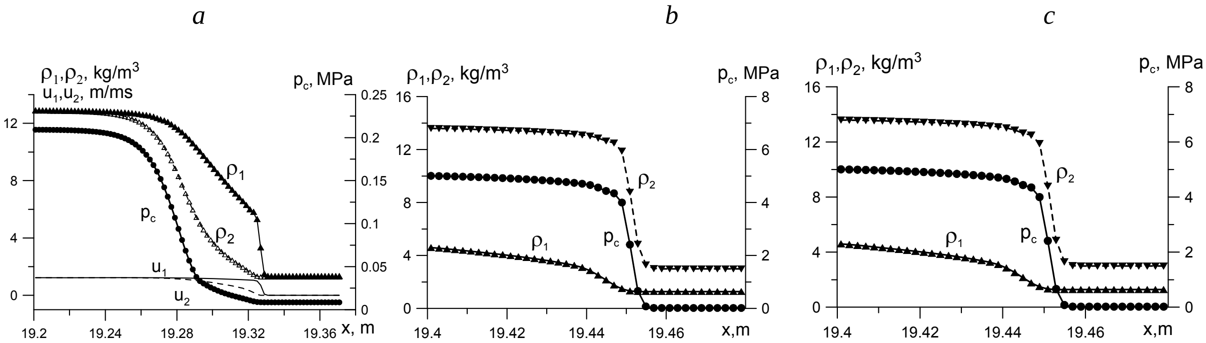

Figure 3. Stationary SW structures at $M_0 = 5$, $e_{c0} = 0.01$ m^2/ms^2: type I, *d*=10 μm, $\xi_0 = 0.5$ (a); type II, *d*=20 μm, $\xi_0 = 0.7$ (b)

Steady-state shock-wave structures are plotted in Fig. 3. The wave of the type I consists in frozen shock in gas and the relaxation zone in discrete phase (signs indicate computational grid nodes). The generation of chaotic motion occurs in the relaxation zone. The wave structure of type II consists in a leading shock in the discrete phase and relaxation zone in gas.

Note that some analogous types of shock waves (with leading shock in one of the phase and the relaxation in the other one) have been obtained in two-phase heterogeneous media with two pressures in [4, 5]. Note also that the inclusion and exclusion non-divergent terms in this case does not have any noticeable effect on shock wave structures.

For non-ideal collisions of inelastic and rough particles ($\eta < 1$, C_0>0, see Fig. 1) the generation of the chaotic energy in relaxation zone is less (the kinetic energy is converted to heat due to inelastic collisions) and also there is the dissipation of energy in collisions due to roughness. Propagation velocity of the shock wave configuration formed decreases with the decrease in η and the increase in the contribution of the dissipative term. Wave of the type II defined in the mixture at $\eta = 1$ transforms to the wave of the type I with the same parameters of the mixture and the amplitude of the incident SW at $\eta < 1$. The chaotic energy decreases to its initial (minimum) value. The profiles of other parameters are almost similar to the structures presented in Fig. 3 for waves of the corresponding type.

5 Collisional Effects in Cellular Detonations……………………………..

We investigate effects of collisional motion of inert particles in the structure of heterogeneous cellular detonation. Consider the problem of cellular detonation propagation in stoichiometric mixture of aluminum particles (2 μm) and oxygen with the addition of inert aluminum oxide particles (10 μm) analyzed in [2] in the frame of collisionless model. The value of inert phase concentration was chosen to be insufficient for detonation failure. Figures 4 and 5 present the results of 2-D simulations in 6-cm channel assuming $\eta = 1$ (ideal collisions). The random motion of particles almost has no effect on the cellular structure and the leading shock wave position (compare gas temperature distributions, Fig. 4,a). Particle-to-particle collisions give rise to chaotic energy and particle pressure (Fig. 5) which maximal values correspond to the transverse wave collisions. The particle pressure provides some spreading of the inert phase structures and layers in the far wake formed due to transverse counter motion of the inert component (Fig. 4,b). Note that with non-ideal collisions of rough particles the chaotic energy dissipation may somewhat mitigate this effect. At the same time the main characteristics of cellular detonations: the propagation velocity, the cell size, the flow structure, and peak pressure do not depend on the chaotic motion of inert particles and their collisions.

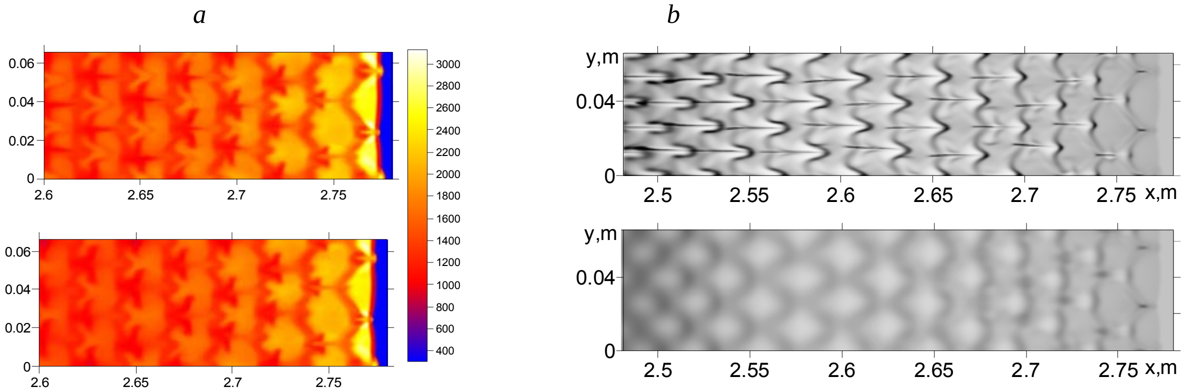

Figure 4. Cellular detonations in aluminum suspensions in gas with inert particles, gas temperature field (a); inert particles density field (b): comparison of results [2] (top) and collisional model (bottom, $e_{c0} = 0.0001$ m^2/ms^2).

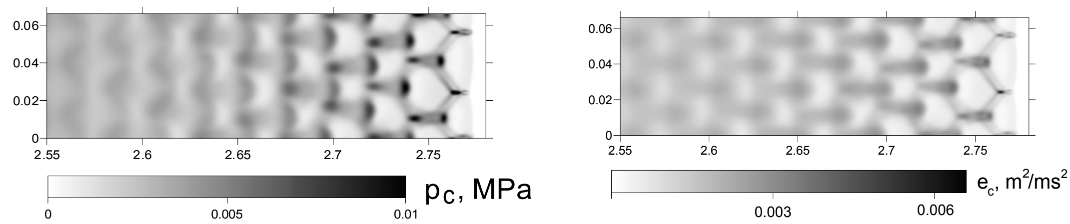

Figure 5. Cellular detonations in aluminum suspensions in gas with inert particles: collisional pressure (*a*) and chaotic energy distributions (*b*) at $e_{c0} = 0$, $\eta = 1$.

6 Conclusions

- The paper presents a physical and mathematical model to describe the shock-wave and detonation flows in reacting media of the type gas – solid particles, taking into account the dynamics of particle-to-particle collisions. The collision dynamics of random motion of particles is described in terms of molecular-kinetic theory of granular gas.
- The classification of types of strong discontinuities in two-phase gas – particle collisional mixture is presented: SW in gas with relaxation and possible generation of chaotic motion in particles (type I); SW with discontinuity in the parameters of discrete phase and generation of chaotic energy in the shock and relaxation in gas (type II).
- The method of numerical simulation of unsteady flows is developed and the problem of the interaction of planar shock wave with a cloud of particles is analyzed. The steady-state solutions corresponding to the stationary waves of type I or type II are obtained.
- The effect of particle-to-particle collisions is demonstrated in the problem of cellular heterogeneous detonation in the mixture of oxidizing gas, reactive particles, and inert particles.

The collisions of inert particles do not affect the detonation velocity, cell size and the flow structure behind the front, but provide spreading the inert phase layer-type structures in the far zone of cellular detonations.

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