Shock wave processes in collisional gas particle mixtures

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Abstract. Structures and propagation of shock waves in high density particle suspensions in gas are investigated theoretically and numerically. A physical and mathematical model which takes into account integral collisions between the particles on the basis of molecular-kinetic approaches of theory of granular materials is applied. The possibility of different types of shock waves, including double front structures is revealed. The role of particle collisions in the dynamics of particle dense layer expansion under an influence of divergent shock wave and in processes of shock wave diffraction past a backward-facing step is analyzed.

1. Introduction
Problems of interaction of shock waves (further - ‘SW’) with dust layers arise in connection with detonation suppression or prevention in reactive mixtures. Shock wave interactions with layers of reacting particles can form clouds of explosive concentrations [1]. On the other hand, the explosive dispersion of inert particle layers under the influence of a central charge is one of the ways of detonation damping and combustion extinction.

Describing high density gas particle mixtures, it is necessary to take into account the volume occupied by the particles, as well as the possibility of contact interaction of particles (particle-to-particle collisions).

A physical and mathematical model of two-phase medium to describe the shock-wave dynamics of dense gas mixtures with the averaged description of particle-to-particle collisions on the basis of molecular-kinetic theory has been developed in [2], [3]. The model has been applied in [4], [5] for analysis of shock and detonation wave propagation in collisional particle suspensions in gas and shock wave dispersion of dust layers. A possibility of existence of two governing types of shock waves was revealed in [4]: with leading shock in gas or with leading shock in the particle phase. Only single-front structures were obtained in [4] although existence of double-front structures in mixtures with two pressures was established in [6] in the frame of simple isothermal model.

In this paper, one-dimensional and two-dimensional flows formed in the interaction of shock waves with particle clouds and layers of high-density and in the diffraction of shock waves past a backward-facing step are investigated on the base of the model [2], [3]. The purpose of the study is to analyze an influence of the collisional particle dynamics in the flow patterns and the shock-wave structure formation.

2. Physical and mathematical model
The Euler equations for two-dimensional flow of two-phase mixture of gas and two fractions of particles follow from the conservation laws for mass, momentum, and energy (the subscripts 1, 2, and 3 indicate gas, inert particles, and reactive particles, respectively):
\[
\frac{\partial W}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = \Gamma
\]  
(1)

\[
W = \begin{pmatrix} W_1 \\ W_2 \end{pmatrix}, \quad F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}, \quad G = \begin{pmatrix} G_1 \\ G_2 \end{pmatrix}, \quad \Gamma = \begin{pmatrix} -\tilde{F} \\ \tilde{G} \end{pmatrix}
\]  
(2)

\[
W_i = \begin{pmatrix} \rho_i \\ \rho_i u_i \\ \rho_i v_i \\ \rho_i E_i \end{pmatrix}, \quad F_i = \begin{pmatrix} \rho_i u_i \\ \rho_i u_i v_i \\ \rho_i u_i E_i + m_i p_i u_i \\ \rho_i v_i \end{pmatrix}, \quad G_i = \begin{pmatrix} \rho_i v_i \\ \rho_i u_i v_i \\ \rho_i v_i E_i + m_i p_i v_i \end{pmatrix}
\]  
(3)

\[
W_2 = \begin{pmatrix} \rho_2 u_2 \\ \rho_2 v_2 \\ \rho_2 E_2 \\ \rho_2 E_c \end{pmatrix}, \quad F_2 = \begin{pmatrix} \rho_2 u_2 \\ \rho_2 u_2 v_2 + m_2 p_2 \\ \rho_2 u_2 E_2 + m_2 u_2 p_2 \\ \rho_2 u_2 E_c + \eta_2 u_2 p_2 \end{pmatrix}, \quad G_2 = \begin{pmatrix} \rho_2 v_2 \\ \rho_2 v_2 + m_2 p_2 \\ \rho_2 v_2 E_2 + m_2 v_2 p_2 \\ \rho_2 v_2 E_c + \eta_2 v_2 p_2 \end{pmatrix}
\]  
(4)

\[
\Gamma_2 = \begin{pmatrix} \eta p_i (\frac{\partial u_i m_i}{\partial x} + \frac{\partial v_i m_i}{\partial y}) - I_0 + \eta(f_{x i u} + f_{x i v}) \\ 0 \\ p_1 \frac{\partial m_2}{\partial x} + f_{x 2} \\ p_1 \frac{\partial m_2}{\partial y} + f_{y 2} \\ q_2 + f_{x 2 u} + f_{y 2 v} \end{pmatrix}
\]  
(5)

\[
\tilde{F}_2 = \begin{pmatrix} 0 \\ p_1 \frac{\partial m_2}{\partial x} + f_{x 2} \\ p_1 \frac{\partial m_2}{\partial y} + f_{y 2} \\ q_2 + f_{x 2 u} + f_{y 2 v} \end{pmatrix}
\]  
(6)

Here \( \rho, p, m \) are the mean density, pressure, and the particle volume concentration, respectively, \( \rho_i = \rho_i m_i, \rho_{ii} \) is the true density of phases; \( u, v \) are the velocity components; \( f \) is the force of interaction between phases. The particles are assumed to be incompressible (\( \rho_{22} = \text{const} \)). The total energy of the inert particle phase \( E_2 \) includes also the energy of chaotic particle motion determined as the average kinetic energy of the particle velocity pulsations:

\[
e_c = 0.5u^2, \quad v^2 = \frac{1}{N} \sum_{i=1}^{N} [(u_i')^2 + (v_i')^2] .
\]  
(7)

Here \( u_i', v_i' \) are the \( i \)-th particle velocity pulsation components and \( N \) is the number of particles in the unit volume. The chaotic energy is associated with the discrete phase pressure \( p_c \) (intergranular pressure) generated by particle-to-particle collisions. The collisional total energy \( E_c \) is determined in the form presented in [3]. The equations of state have the form

\[p_1 = \rho_i RT, \quad m_2 p_2 = m_i p_i + p_c, \quad p_c = 0.5 \alpha [1 + 2(1 + \beta m_c m)], \quad \rho_e e_c,
\]

\[g(m_c) = [1 - (m_c / m_e)^{4\alpha/3}]^{-1}, \quad E_1 = c_{i1} T_i + u_1^2 / 2, \quad E_2 = e_c + c_2 T_2 + 0.5(u_2^2 + v_2^2),
\]

\[E_c = e_c + 0.5 \eta u_e^2.
\]  
(8)
Here, $m^*$ is the limiting maximal value of particle volume concentration, $\alpha$ defines a relationship between the energy of the chaotic motion of particles and the collisional pressure in the discrete phase. The dissipative term is assumed to be

$$I_0 = \frac{6}{\pi d^2} C_0 \rho_s m^2 g(m^2)(e^{3/2} - e_0^{3/2}),$$

where $C_0$ is the dissipation coefficient, $e_0$ is the initial value of the energy of the chaotic motion, which is assumed to be the minimal value of $e$ in the following process, and $d$ is the particle diameter. We take into account that the heating of the particles occurs due to convective heat transfer and due to the conversion of the chaotic energy into heat at non-ideal collisions of rough and inelastic particles. The coefficients $C_0$, $\eta$, and the parameter $\alpha$ depend on the restitution coefficient $\varepsilon$, the shape coefficient $k$ ($k = 0.4$ for spheres), and the roughness parameter $\beta$. Ideal collisions without losses are characterized by $\varepsilon = 1$, $\beta = -1$, $\eta = 1$. The expressions for $C_0$, $\eta$, and $\alpha$ are presented in [3]. The function $g(m^2)$ in (8) describes behavior of granular media in a wide range of particle volume concentrations from small values (when it is similar to a monatomic gas with $\gamma = 5/3$) to values of dense packing. The collisional (intergranular) pressure $p_c$ tends to infinity with particle volume concentration approaches its maximal value $m^*$.

The numerical technique is based on the conservative flux-splitting schemes: the TVD scheme by Harten for gas and the Gentry-Martin-Daly scheme for particles. The numerical method has been tested earlier and applied for 2-D numerical simulations of the shock wave and detonation flows in the frame of a standard collisionless model in [7], [8], [9]. Here, we take similar to Gentry-Martin-Daly scheme approximations for the additional terms related to the gas pressure and the pressure of random motion of particles. The calculations were performed using IBM PC Intel Core2Quad.

3. Types of shock waves in collisional media

The types of possible shock wave structures in dense gas particle mixtures were investigated on the problem of the SW in gas entering into a particle cloud. Two basic types of the SW in collisional mixture are the following [4]: with leading shock in gas and a relaxation zone in the discrete phase (type I), and with collisional shock in the particle phase with following relaxation zone in gaseous phase (type II). Distributions of the parameters in the relaxation zones were obtained in [4] to be continuous for both types analyzed. Varying the amplitude of the incident SW and the mixture parameters (density, collisional constants), additional types of shock wave structures are revealed. Some examples of double-front structures in mixtures of 10-µm particles with leading shock in gas (type I-D) and double-front structures with leading shock of collisional type in particles (type II-D) are plotted in Figures 1-2.

Note that the double shock wave structures shown in Figures 1-2 are different from those obtained under isothermal model for compressible media with two pressures in [6]. The present structures are characterized also by the temperature relaxation zones, as well as non-uniform distribution of the parameters describing the random motion of particles ($p_c, e_c$). For example, in the structure of type I_D (Figure 1), the presence of the second jump is seen on the particle velocity profile, and in this area the chaotic motion energy generation occurs (see the peak in $e_c$ distribution). For the II_D type structure, the leading shock in particle density and particle velocity is not accompanied by a temperature jump (Figure 2), and the gas temperature is also continuous. The gas temperature shock together with gas density and velocity shocks take place inside the relaxation zone on some distance from the leading collisional shock.
Figure 1. A double-front structure of type I-D ($m_{20} = 0.009$, $u_{SW} = 0.99$ m/ms, $e_{c0} = 0$).

Figure 2. A double-front structure of type II-D ($m_{20} = 0.001$, $u_{SW} = 1.26$ m/ms, $e_{c0} = 0.005$ m$^2$/ms$^2$).
Realization of the first or the second type of the shock wave structures depends on the initial parameters of the mixture (particle density, initial level of the chaotic energy), the shock wave propagation velocity, and particle material characteristics (diameter, roughness and restitution coefficients).

4. Collisional effects in interaction of explosive shock waves with particle dense layers
The problem of the interaction of the expanding shock wave with a particles dense layer in one-dimensional formulation (in the approximation of spherical symmetry) taking into account particle-to-particle collisions is considered. The values of gas and particle parameters correspond to experimental conditions in [10] (31 g Comp B booster, 550 g glass spheres with mean particle diameter 10 µm).

Figure 3 shows an initial stage of the SW interaction with the particle layer with the time step 1 µs, numerals indicate the corresponding time moments. Solid and dashed lines indicate gas and particle parameters, respectively. Note that when the SW enters the dense layer it slows and transforms to a dispersive wave in gaseous phase. At the same time, a collisional shock wave in the particle phase of type II forms and propagates ahead the incident wave in gas (compare the solid and dashed lines for equal time moments). This type of the collisional SW with leading shock in particle phase and a relaxation zone in gas has been analyzed in [4]. Here, the particle volume concentration in the relaxation zone behind the front reaches the values of 0.594 which is close to the value of dense packing \( m_\text{r}=0.6 \). As the collisional wave front reaches the external boundary of the layer, the leading edge of the particle cloud begins to move, and it happens earlier than the wave front in gas reaches the cloud edge (compare dashed and solid curves 5 in Figure 3a). The velocity profiles (Figure 3b) confirm the type II of the shock wave in the mixture (dashed lines are located just to the right of solid lines). A small thickness of the velocity relaxation zones behind the collisional shock front is explained by high differences between gas and particle mean densities here. At the same time, a secondary ordinary shock wave propagates inside the cloud which appears as a description between solid and dashed lines in Figure 3b. Here, gas density is much higher than in the collisional SW, particle density decreases near the internal cloud surface, and the velocity relaxation zone is more extended.

Thus, the collisional pressure arising due to the development of particle chaotic motion plays a decisive role in the scenario of the initial stage of particle motion and formation of shock-wave structures in the cloud at a SW interaction with dense particle layers. Consequently, the collisional particle dynamics is one of the determining factors in processes of explosive dispersion of dusts.

5. Diffraction of a shock wave on a backward-facing step in collisional gas particle mixture
The problem of shock-wave transition past a backward-facing step in a gas suspension was investigated in [11]. It was shown that the greatest difference between the flow pattern in a two-phase
mixture and the corresponding flow in a pure gas is observed in the range of times when the characteristic sizes of the structures being formed are commensurable with the scale of the relaxation zones. It was also established that there was formation of a region with a reduced fraction of particles near the corner that is caused by particle inertia in the vortex flow and accumulation of particles in the layer adjacent to the contact surface in the structure. Collisional dispersion of dense inert particle layers formed in detonation waves was revealed in [4]. Here, one analyzes the problem of shock wave diffraction in gas particle mixture in the frame of the collisional model to estimate the collisional effects in dispersion of the particle layers obtained in [11]

To compare the results for collisional and collisionless models, diffraction of a shock wave of the type I is considered. Figures 4-7 show the flow patterns at the shock wave diffraction in the mixture of oxygen and 10-µm alumina particles with \( m_{20} = 0.0006 \) and the SW propagation velocity \( u_{SW} = 0.82 \) km/s. All density fields are scaled in kg/m\(^3\), all collisional (granular) pressure fields are presented in MPa.

Figure 4 presents the gas density and particle density fields obtained in the frame of ordinary collisionless model. The region of low particle concentration (almost free of particles), together with the layer of accumulated particles are obvious in Figure 4b as white and green zones on the right of the corner. Note that maximal particle density takes place in the region of final equilibrium state of the two-phase shock wave (red areas in the picture).

**Figure 4.** Diffraction of a SW in collisionless model: gas density (a) and particle density (b) fields.

**Figure 5.** Diffraction of a SW in collisional model: particle densities (a) and granular pressures (b).
The results of calculations obtained in the frame of collisional model ($e_{c0} = 0.0001$ m$^2$/ms$^2$) are plotted in Figure 5 for the same time moment as in Figure 4. No difference is obvious between particle density fields in Figure 4b and Figure 5a although the collisional pressure is not negligible (Figure 5b). The maximal values of the granular pressure are comparable with initial gas pressure (0.1 MPa).

Figures 6-7 show the corresponding particle density and collisional pressure fields in a later time moment for two different values of initial level of energy of particle chaotic motion: $e_{c0} = 0.0001$ m$^2$/ms$^2$ (Figure 6) and 0.01 m$^2$/ms$^2$ (Figure 7). For convenience, the pictures are presented in the same color scale. One can see that the particle density fields practically coincide that means negligible effect of collisional pressure in dispersion of the particle layer formed behind the backward-facing step. Note that despite two order difference in initial values of $e_{c0}$ the collisional pressure values in the flow behind the SW do not differ so strong. It means that randomization of particle motion generated in non-uniform flow behind two-phase shock wave of the type I is determined mainly by the flow structure, and initial randomization level plays here unimportant role unlike obtained in [4] for the detonation processes.

Figure 6. Particle densities (a) and granular pressures (b) at $e_{c0} = 0.0001$ m$^2$/ms$^2$.

Figure 7. Particle densities (a) and granular pressures (b) at $e_{c0} = 0.01$ m$^2$/ms$^2$.

6. Concluding remarks
The comparison of the results of calculations in the frame of ordinary (collisionless) and collisional models for description of shock wave processes of particle suspensions in gas shows that generated in the particle phase collisional pressure may play a significant role. The variety of different types of shock waves in gas particle mixtures including double-front structures is obtained. The shock waves of type II with leading collisional shock in particle phase are responsible for initial stage of dense layer
dispersion under an action of explosive shock of central charge. At the same time, the generated collisional pressure is not a significant factor in shock wave structures and layer dispersion in shock wave diffraction past a backward-facing step.

Acknowledgements
The work was supported by the Russian Scientific Foundation (project № 16-19-00010).

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