INVESTIGATION OF THE PROCESSES OF DUST DISPERSION WITHIN THE MODEL OF COLLISIONAL PARTICLE DYNAMICS

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Introduction. Investigation of processes of shock-wave dispersion of dusts is of interest both for estimation of the explosibility of reactive dust clouds, and, on the other hand, for the analysis of inert particle cloud formation to suppress and prevent combustion and detonation in reacting media.

The particle collisions play an important role in the processes of interaction of shock waves with dust formations of high density. Processes of particle dispersion under the influence of shock waves have been extensively studied experimentally and theoretically. A fairly detailed review on the problem of mixing under shock wave and detonation processes is presented in [1].

The major factors of layer expansions in diluted suspensions are the interactions of shock-wave structures: refractions and reflections, as well as the development of instability in the surface layer [2, 3]. An influence of the Saffman force on the dust lifting height is taken into consideration in [4-6]. A determining role of the Magnus force in processes of dust lifting due to development of the rotational particle motion in the shear flow behind the shock wave front was proposed in [7-9]. Some attempts have been made to estimate the input of interaction between particles in processes of shock wave dust dispersion on the base of different models in [10-12]. Some models with taking into account the pressure associated with contact interactions of particles are proposed in [10, 11]. It was obtained in [11] that the collisional effects may be sufficiently greater than an influence of the Saffman and Magnus forces. The group effects of particle-to-particle collisions and collisions with rough solid wall in the problem of a dust layer interaction with a shock wave were analyzed in [12] in the framework of the Lagrangian approach for description of the dynamics of particles. But this approach does not allow reproducing the shock-wave structures inside the layer. The problems of the intergranular pressure influence on dust lifting and shock wave dispersing of dust layers are discussed also in [13, 14]. Thus, the role of the random motions of particles and their collisions in the dispersion process and dust cloud formation was not determined and is of interest.

A theoretical model of dense gas particle suspension in which particle-to-particle collisions are described using the molecular-kinetic approaches of theory of granular materials is presented in [15-17]. In the present paper numerical simulations of shock wave interactions with dense dust layers are performed in the frame of the model taking into account interparticle collisional effects. The purpose of this paper is to estimate the contribution of particle random motion and particle-to-particle collisions as one of the mechanisms resulting dispersion processes in dust suspensions.

Physical and mathematical model. The Euler equations for two-dimensional flow of two-phase mixture of gas and two fractions of particles follow from conservation laws for mass, momentum, and energy (the subscripts 1 and 2 stand for gas and particles, respectively):

$$\frac{\partial W}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = \Gamma,$$

$$W = \begin{pmatrix} W_1 \\ W_2 \end{pmatrix}, \quad F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}, \quad G = \begin{pmatrix} G_1 \\ G_2 \end{pmatrix}, \quad \Gamma = \begin{pmatrix} -\tilde{F}_2 \\ \Gamma_2 \end{pmatrix};$$

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\[ W_1 = \begin{pmatrix} \rho_1 \\ \rho_1 u_1 \\ \rho_1 v_1 \\ \rho_1 E_1 \end{pmatrix}, \quad F_1 = \begin{pmatrix} \rho_1 u_1 \\ m_1 p_1 + \rho_1 u_1^2 \\ \rho_1 u_1 v_1 \\ \rho_1 u_1 E_1 + m_1 p_1 u_1 \end{pmatrix}, \quad G_1 = \begin{pmatrix} \rho_1 v_1 \\ \rho_1 u_1 v_1 \\ m_1 p_1 + \rho_1 v_1^2 \\ \rho_1 v_1 E_1 + m_1 p_1 v_1 \end{pmatrix}, \quad (1) \]

\[ W_2 = \begin{pmatrix} \rho_2 \\ \rho_2 u_2 \\ \rho_2 v_2 \\ \rho_2 E_2 \end{pmatrix}, \quad F_2 = \begin{pmatrix} \rho_2 u_2 \\ \rho_2 u_2^2 + m_2 p_2 \\ \rho_2 u_2 v_2 \\ \rho_2 u_2 E_2 + \eta m_2 u_2 p_2 \end{pmatrix}, \quad G_2 = \begin{pmatrix} \rho_2 v_2 \\ \rho_2 u_2 v_2 \\ \rho_2 v_2 E_2 + m_2 p_2 v_2 \\ \rho_2 v_2 E_2 + \eta m_2 v_2 p_2 \end{pmatrix}, \]

\[
F_2 = \left( \begin{array}{c}
\tilde{F}_2 \\
\eta p_1 \left( \frac{\partial u_2 m_2}{\partial x} + \frac{\partial v_2 m_2}{\partial y} \right) - I_0 + \eta (f_{x2} u_2 + f_{y2} v_2) \\
0
\end{array} \right), \quad \tilde{F}_2 = \left( \begin{array}{c}
p_1 \frac{\partial m_2}{\partial x} + f_{2x} \\
p_1 \frac{\partial m_2}{\partial y} + f_{2y} \\
q_2 + f_{x2} u_2 + f_{y2} v_2
\end{array} \right).
\]

Here \( \rho, p, m \) are the mean density, pressure, and the particle volume concentration, respectively, \( \rho_i = \rho_0 m_i, \rho_0 \) is the true density of phases; \( u, v \) are the velocity components; \( f \) is the force of interaction between phases. 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:

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

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 [15-16]. The collisional total energy \( E_c \) is determined in form presented in [16]. The equations of state have the form

\[
p_1 = \rho_1 R T_1, \quad m_2 p_2 = m_2 p_1 + p_c, \quad p_c = 0.5 \alpha_i [1 + 2(1 + \epsilon) m_2 g(m_2)] \rho_2 e_c, \]

\[
g(m_2) = [1 - (m_2 / m_i)^{4 m_i / 3}]^{-1}, \quad E_1 = c_1 T_1 + u_1^2 / 2, \quad E_2 = e_c + c_2 T_2 + 0.5 (u_2^2 + v_2^2). \quad (3)
\]

Here \( m_i \) is the limiting maximal value of particle volume concentration, \( \alpha_i \) 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

\[
I_0 = \frac{6}{\pi d_2} C_0 \rho_2 m_2 g(m_2) (e_c^{3/2} - e_0^{3/2}), \quad (4)
\]
where \( C_0 \) is the dissipation coefficient, \( e_{c0} \) is the initial value of the energy of the chaotic motion, which is assumed to be the minimal value of \( e_c \) 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 \( \alpha_t \) depend on the restitution coefficient \( \varepsilon \), the shape coefficient \( k \) (\( k = 0.4 \) for spheres), and the roughness parameter \( \beta \) [16].

The parameters \( \varepsilon, \beta, \) and \( \eta \) determined by particle material and surface properties do not depend on the flow parameters and have constant values. Ideal collisions without losses are characterized with \( \varepsilon = 1, \beta = -1, \eta = 1 \). In the simplest case of perfectly smooth elastic media \( \alpha_t = 4/3 \). In general case

\[
\alpha_t = \frac{2}{3}\left(1 + \frac{a}{b + \sqrt{a^2 + b^2}}\right), \quad a = (1 - \beta^2) \frac{1-k}{1+k} - 1 + \varepsilon^2, \quad b = 2k \left(\frac{1+\beta}{1+k}\right)^2. \quad (5)
\]

Formulas for \( C_0, \eta \) have a very complicated form. Dependences of \( C_0, \eta \) on \( \varepsilon \) and \( \beta \) are presented graphically in Fig. 1.

The model has been verified in accordance with the experimental data on the equilibrium sonic velocity in the two-phase mixture [16]. In the problems of shock wave – dense layer interactions the gravity, the Saffman force [6] and the Magnus force [8] are taken into account. The interfacial forces include the drag force of the particles in the flow, which is determined in accordance with [18]. The drag coefficient at small particle volume concentrations and the heat transfer between gas and particles are described similar to [19]

\[
\vec{f} = \frac{3m_2\rho_1}{4d} c_p [\bar{u}_1 - \bar{u}_2](\bar{u}_1 - \bar{u}_2) - \vec{g} + \vec{f}_{\text{Saf}} + \vec{f}_{\text{Magn}},
\]

\[
\vec{f}_{\text{Magn}} = K_{\text{Magn}} \frac{3\rho m_2}{4\pi} [(\bar{u}_1 - \bar{u}_2) \times \text{rot}(\bar{u}_1)],
\]

\[
f_{\text{Saf}} = \text{Sgn} \left( \frac{\partial u_1}{\partial y} \right) \frac{3K_{\text{Saf}} m_2}{2\pi d} (u_1 - u_2) \sqrt{\rho_1 \mu} \left| \frac{\partial u_1}{\partial y} \right|,
\]

\[
(6)
\]

\[a\]

\[b\]

Fig. 1. Parameters characterized generation (a) and dissipation (b) of the energy of particle chaotic motion depending on the particle roughness and restitution coefficients.
\[ c_D = c_{D1}, \ m_2 \leq 0.08 \ ; \ c_D = c_{D2}, \ m_2 > 0.45; \]

\[ c_D = [(m_2 - 0.08)c_{D2} + (0.45 - m_2)c_{D1}] / 0.37, \ 0.08 < m_2 \leq 0.45; \]

\[ c_{D1}(\text{Re}, \text{M}) = \left[ 1 + \exp \left( -\frac{0.43}{\text{M}^{4.87}} \right) \right] \left( 0.38 + \frac{24}{\text{Re}} + \frac{4}{\sqrt{\text{Re}}} \right), \]

\[ c_{D2}(\text{Re}, m_2) = \frac{4}{3m_1} \left[ 1.75 + \frac{150m_2}{(1-m_2)\text{Re}} \right], \quad \text{Re} = \frac{\rho_0 d |\vec{u}_i - \vec{u}_s|}{\mu}, \]

\[ M = \frac{|\vec{u}_i - \vec{u}_s|}{\sqrt{\gamma_i p}} \sqrt{\rho_{11}}, \quad q_s = \frac{6m_1}{d^2} \nu(T_1 - T_s), \quad \text{Nu} = 2 + 0.6\text{Re}^{1/2}\text{Pr}^{1/3}. \]

Here \( c_D \) is the drag coefficient of particles, \( \lambda_1 \) is the thermal conductivity of the gas, \( \text{Re}, \text{Nu}, \text{Pr}, \) and \( \text{M} \) are the Reynolds, Nusselt, Prandtl, and Mach numbers, respectively, and \( \mu \) is the gas viscosity.

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 standard collisionless model in [19–21]. 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.

**Explosive shock-wave dispersion of dense layers from a flat surface.** Consider the problem of interaction of a blast wave (similar wave forms at a local methane explosion in a coal mine) with a layer of high-density particles located at \( x \geq 0 \), \( 0 \leq y \leq h(x) \). Location of the source of the blast wave is at a certain height above the surface. A cylindrical shock wave (0.05 m radius of the cylinder, the Mach number varies) is taken as initial data. The surface of the dust layer is considered both smooth and rough. The layer roughness is simulated by sinusoidal surface shape \( h = h_0 + \Delta h \cos(\alpha x) \), \( h \) is the layer thickness, parameters \( \Delta h, \alpha \) were varied. The problem is solved in two-dimensional formulation. Calculations were performed for the 50-\( \mu \)m spherical coal particles, the bulk concentration ranged from 0.1 to 0.4. The computation domain is \( 3 \times 0.34 \) m and the grid step is \( \Delta x = \Delta y = 0.001 \) m. The collisional dynamics parameters are \( \eta = 1, \ C_0 = 0.01, \) and \( m_0 = 0.6 \). The initial value of the chaotic energy varies from 0 to 0.001 \( m^2 \)\( s^{-2} \).

The initial stage of interaction of the SW with the dust layer is presented in Fig. 2 as gas pressure images of the flow with the time step 0.2 ms. The shock wave front reaches the dust layer surface at approximately 0.6 ms (frame 3) and then the SW propagates along the dust layer (frame 4). The transverse wave forms at the reflection of the shock wave from the layer. It’s front non-uniformity is caused by heterogeneity of flow behind the front of explosive shock wave in the process of its attenuation. Figure 3 shows the SW shape and the particle density distribution in the case of smooth layer at \( t = 2 \) ms.

Due to the high values of the Atwood number (about 100) in the layer reflected wave propagates at a small angle to the substrate, so there is no mechanism for lifting the dust associated with multiple reflection of the wave from the wall and the surface layer [2, 3]. Analysis of the Saffman force influence reveals that variation of \( K_{\text{Saf}} \) from 0 to 160 has no noticeable effect. Thus, although the value \( K_{\text{Saf}} = 160 \) was obtained in [4] to provide a correspondence to experimental data.
on individual particle lifting, in this case the Saffman force does not exert a significant influence on the dust layer dispersion.

Effect of roughness on the process layer can be estimated from a comparison of Fig. 3a (\( \Delta h = 0 \)) and Fig. 3b (\( \Delta h = 0.2 \) cm). As can be seen, the influence of the surface shape is manifested only in the wave pattern of shock wave interaction with the surface layer and has practically no effect on the picture of the particle dispersion. Figure 3b shows also an influence of the collisional dynamics of particles in the model. The pictures of particle dispersion are presented in the unique non-uniform shadow scale to reveal regions of low density (particle lifting over the cloud). Maximum volume concentration achieved at the layer compression is 0.43.

Significant effect of the Magnus force in problems of dust lifting from the layers under the influence of shock waves is proposed in [7–9]. Calculations with a variation coefficient in the formula (6) indicate the most noticeable effect of these forces on the processes of dispersion of these dust layers. Moreover, when \( K_{M3} = 20 \), for which the calculations [8] obtain the correspondence with the experimental data, the effect of the Magnus force is comparable with the effect of collisional dynamic at \( e_{c0} = 0.0001 \) m²/ms². Thus, pulsating motion and particle collisions are also an important mechanism in the process of particle dispersion of shock waves.

Note manifestations of instability in the interaction of shock waves with an undulating surface of the rough layer. Figure 4 shows a fragment of the computational domain on three time moments with intervals 0.18 ms. The shock wave front position and shape is shown through dashed line at the first frame, for subsequent moments of time the shock wave position is outside the pattern area. The images are shown in Fig. 5 with a different shadow scale than in Fig. 3: high values of particle concentrations are presented more intensively. It is not possible to see the picture of particle lifting from the surface, however, the pattern of change in the shape of ridges of the refracted layer surface.

![Figure 2](image2.png)

**Fig. 2.** Initial stage of an explosive SW interaction with a dust layer.

![Figure 3](image3.png)

**Fig. 3.** The SW propagation over a smooth (a) and rough (b) layers:

\[ M_0 = 3, \; m_0 = 0.2, \; K_{M3} = 0. \]
is revealed clearly. This surface is preloaded by the shock wave and the layer is packed. It can be seen as an increase in the height of the ridge (which is characteristic of instability of the Richtmyer – Meshkov type) and the demolition of their tops with some smearing form (as in the Kelvin – Helmholtz instability). Obviously, there is a superposition of the two types of instabilities, as oblique shock wave, on the one hand, penetrates the surface, promoting the Richtmyer – Meshkov instability, on the other hand forms a slip stream of gas over the surface, which contributes to the development of Kelvin – Helmholtz instability.

Figures 5 and 6 demonstrate further development of instabilities at the interface of the bulk layer which moves along the flat plate, and a cloud of particles dispersed from the upper surface.

Influence of the Kelvın – Helmholtz instability in problems of interactions of shock waves with dense layers was also demonstrated in [3] on the model of one-velocity continuum of cold gas layer. Note that here, as in [3], the bulk layer swelling is characterized by a significant delay (in [3] moderate values of the Atwood numbers were considered, at that the primary mechanisms of the

Fig. 4. Fragment of the flow domain (0.1×0.1 m) and the layer surface with Δt = 0.18 ms: particle density fields.

Fig. 5. Kelvin – Helmholtz instability development at 15 ms after the SW passage: particle density field.

Fig. 6. Influence of the collisional parameters on formation of the dust clouds at t = 16 ms: $e_{c0} = 0.00001$ m$^2$/ms$^2$ (a); $e_{c0} = 0.0001$ m$^2$/ms$^2$ (b); $K_{magn} = 0$, $m_0 = 0.1$, $M_0 = 5$. 

$\rho_2$ kg/m$^3$
layer dispersion are considered as reflection and refraction of shock waves in the layer. The mechanism of dust lifting associated with the development of Kelvin – Helmholtz instability is secondary and is manifested in the later stages of the process. At the same time, the intensity of the expansion of the bulk layer, as well as lifting particles from a surface layer directly behind the shock wave, is directly connected with the pulsatile motion of the particles (see Fig. 6).

Thus, the basic mechanisms of dispersion of dense dust layers when exposed to explosive shock waves are the Magnus forces and development of the instabilities on the layer surface (Richtmyer – Meshkov type and Kelvin – Helmholtz type). However, the random motion of particles and the resulting collisions of particles have a significant impact on the process of particle lifting from the upper layer directly behind the shock front, and on the formation of dust clouds after the shock wave front passage.

**The dispersion of the dense layer (shell) of the expanding explosive shock wave** The problems of the expansion of shells consisting in layers of inert or reactive particles under the influence of shock waves generated by explosions of central charges arise in connection with volumetric explosions, and in terms of combustion or detonation damping in gaseous and dispersed media. In the experiments, there is a strong heterogeneity of the spraying material boundary (Fig. 7) that is associated in [22] with the presence of an agglomeration process. However, a significant factor may also be the development of the instability on the surface of the particle cloud. The investigations of the instability are performed on the model of two-dimensional flows. A two-dimensional analogue of a problem is an interaction of expanding cylindrical shock wave with a cylindrical shell of dense layer of particles.

Numerical simulations are carried out in a square area covering a cylinder sector (90°). The shell is a dense layer of particles with $m_0 = 0.1$ of cylindrical shape, located in the area $r_{in} \leq r \leq r_{ex}$. It is assumed the imposition of some form of perturbations on the outer boundary of the cloud of particles.

Fig. 7. Experimental observations of the explosively driven dispersion of solid particles [22]

![Experimental observations of the explosively driven dispersion of solid particles](image_url)

Fig. 8. Particle density fields at $t = 0.04$ (a), 0.2 (b), and 0.32 (c) ms.

![Particle density fields](image_url)
particles: \( r_m = 0.06 \) m, \( r_{ex} = 0.07[1 + h\sin(2n\alpha)] \) m. The initial parameters of the explosive shock wave are: \( r_{sw} = 0.05 \) m, \( M_0 = 3 \). On the "internal" boundaries of the region (\( x = 0 \) and \( y = 0 \)) the conditions of symmetry are accepted (taking into account that it is making some stabilizing effect in the axial region), on the outside sufficiently distant borders the unperturbed initial state is posed. The calculation results are presented in Figs. 8 – 10. Figure 8 demonstrates the particle cloud shape at the initial stage of interaction with the SW and at two time moments after the front passage through the cloud at \( e_{c0} = 0 \). The shock wave entering the cloud forms firstly thin layer of dense packing (Fig. 8a). Figure 8b corresponds to the time moment when the shock wave front is already out of the cloud, thus packing occurs uniformly throughout the layer, excepting the dispersible outer layer, the surface of which reveals the development of the instability (growth of the ridges). At further dynamics the ridges continue to grow and the bulk layer spraying due to the presence of chaotic motion and particle collisions takes place.

Figures 9 above show the numerical Schlieren images of the flow field at one time moment (0.32 ms) for different values of the initial amplitude characterized the surface roughness of the particle layer. It can be seen that the leading shock wave front has a smooth shape of a perfect circle. At some distance behind the front the contact discontinuity surface propagates, which is formed at the exit of the SW from the layer of particles having a wavy shape of outer surface. As one can see, this is a growth of the contact surface disturbances (such as the development of the Richtmyer – Meshkov instability). As seen from a comparison of Figs. 9a, 9b and 9c, the amplitude of the roughness on the surface of the particle layer has very little effect on the amplitude of these perturbations at this point, indicating that the surface roughness of the particle is only the initiating factor in the development of the instability. The same is largely true with respect to the development of the disturbances on the surface of the layer of particles: the height of the ridges in particle density fields in Fig. 9a and 9b is virtually the same. Only in Fig. 9c (at five times the

\[
\rho_2, \text{kg/m}^3
\]

0 0.02 0.04 0.06 0.08 0.1 0.02 0.04 0.06 0.08 0.1

0 0.02 0.04 0.06 0.08 0.1 0.02 0.04 0.06 0.08 0.1

Fig. 9. Numerical Schlieren-photographs and particle density images at \( t = 0.32 \) ms:

\( h = 0.0001 \) m (a); 0.00005 m (b); 0.00002 m (c).
reduction of their initial height) dispersion of the particles due to the development of their chaotic motion and collision becomes more significant than the instability development manifestation.

The role of the collisional dynamics of particles in the processes of dispersion of layers can be substantial. This is evidenced presented in Fig. 10 pictures of the dispersion of particles in the layer at the same time moment with different values of the initial energy of chaotic motion. The dispersion of the layer surface due to collisions of particles here, as well as a longitudinal shock wave interaction with the layer reduces the surface manifestations of instability posed by the shock wave. Development of the collisional dynamics of particles is characterized by the collisional pressure of the order 0.01 MPa and its distribution correlates with the particle density fields. Later the particle collisional dispersion dominates and manifestations of the Richtmyer – Meshkov instability on the layer surface disappear. Note that the calculations in the frame of the model excluding the processes of agglomeration of the particles are possible to obtain only some qualitative features proper to the experimental observations; the full picture of the particle expansion is not adequate.

Conclusions. In the paper the numerical simulation of two-dimensional flows in problems of interaction of shock waves with layers of dust is performed on the model of two-phase media with regard for the particle collisional dynamics and excluding the agglomeration processes. It shows the development of instabilities of the Richtmyer – Meshkov type and the Kelvin – Helmholtz type on the rough surfaces of layers of particles. Development of the collisional dynamics of particles promotes more intensive dispersion of the layers and damping of the disturbances. In the experiments more intensive development of the instability of the particle cloud surface is observed that seems to be associated with a significant influence of the processes of agglomeration.

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