Interaction of a Shock Wave with a Cloud of Particles

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ABSTRACT

The problem of reducing the likelihood of detonation and explosion during saturation of a gas or liquid flow with the cloud of particles is considered. The tasks, associated with the formation of particles clouds, dust lifting behind a travelling shock wave, ignition of particles in high-speed and high-temperature gas flows are adjoined to these problems. The conditions of excitation and propagation of detonation waves are determined for the purpose of their initiation, prevention, suppression or damping. A review of existing methods for modeling of two-phased flows is provided. The mathematical model of shock wave interaction with the cloud of solid particles is discussed, and numerical method is briefly described. The numerical simulation of interaction between a supersonic flow and a cloud of particles being in motionless state at the initial time is performed. Calculations are carried out taking into account the influence that the particles cause on the flow of carrier gas.

Introduction

Research efforts are aimed at determining the conditions of excitation and propagation of detonation waves for the purpose of their initiation, prevention, suppression or damping (Eckhoff, 2003). The detonation wave is developed as a result of abnormal operation of liquid rocket engine and of elements of aircraft fuel system. On the other hand, it is planned to use the detonation phenomenon in advanced rocket engines operating on a thermodynamic cycle of detonation combustion. Interest in the heterogeneous and hybrid detonation is caused by potential of using high-energy metal particles (aluminum, magnesium) or mixtures of reactive gases with additives of such particles as working media. The tasks, associated with the formation of cloud of particles, dust lifting behind a travelling shock wave, ignition of particles in high-speed and high-temperature gas flows are adjoined to these problems. The use of experimental methods for studying the interaction of shock waves with elements of an aircraft, as well as the occurrence or, on the contrary, the suppression of detonation waves is

hampered due to the danger of structures destruction and high speed of the flow, therefore the development of numerical methods is of urgent interest. Computational technologies allow obtaining and visualizing detailed two- and three-dimensional flow patterns, identifying both local features and integral properties of the processes.

Methods for describing two-phase flows

There are two main approaches to describe the dynamic and heat exchange processes in particle laden flows (Crowe, Sommerfeld & Tsuji, 1998; Gouesbet & Berlemont, 1999). The first approach, Eulerian–Lagrangian approach, is based on the continuous-discrete representation of a two-phase mixture. The equations of continuum mechanics for carrier phase are complemented by a system of ordinary differential equations describing the movement path and the change in temperature of each particle. In the second approach, Eulerian–Eulerian approach, description is carried out within the framework of models of interpenetrating continua mechanics. Both phases are considered as a continuous medium, and are described by the equations arising from the conservation laws of mass, momentum and energy of each phase and component of the gas mixture. Neglecting the volume occupied by the particles, the movement of the gas mixture and the particles is described in the two-speed and two-temperature approximation of heterogeneous media mechanics.

If necessary, the equations describing motion and heat exchange of phases are complemented by semi-empirical dependencies for drag and heat exchange coefficients of the individual particle (Michaelides & Feng, 1994; Michaelides, 1997). The effect of different representations of drag coefficient on the calculation results of shock-wave processes in particle laden flows is investigated in (Saito, Marumoto & Takayama, 2003).

The simulation of large vortices of turbulent two-phase flow is considered in (Pandya & Mashayek, 2002; Shotorban, 2011). The movement of dispersed phase is described as part of continuum approach based on application of Liouville theorem to the system of dynamic equations, which describe the behaviour of particles (Zaichik, Simonin & Alipchenkov, 2009). The influence of sub-grid effects on the particles motion is discussed in (Shotorban & Balachandar, 2006; 2007; 2009) within the context of interpenetrating continua model.

Each approach has its advantages and disadvantages, as well as applications. Lagrangian approach is quite expensive from a computational point of view, requiring the use of a statistically representative particle system. A lower bound on the number of particles is about 6 particles per each cell of Eulerian mesh in each coordinate direction (Balachandar, 2009; Balachandar & Eaton, 2010), which, in practice, makes it necessary to use the system of 6ND particles, where N is the number of cells of Eulerian mesh, and D is the dimension of the problem. For fine grids such requirements to the particles number become excessive. Compared to the Lagrangian approach the Euler approach uses a smaller number of freedom degrees, but its accuracy is substantially dependent on averaging method (Shotorban et al., 2013).

Numerical methods for calculating gas-particle flows

The presence of strong discontinuities and areas with large gradients of sought parameters (shock waves, ignition and combustion fronts, contact and

combination discontinuities) within the flow requires the application of numerical methods, which allow to reproduce the qualitative and quantitative characteristics of the flow with reasonable accuracy.

Supersonic nature of the flows ensures successful application of such schemes as Godunov's discontinuity breakdown (Murray, Zhang & Thibault, 1998; Benkiewicz & Hayashi, 2003; Ludwig & Roth, 1997; Tunik, 1999; Zhang et al., 2001) and schemes with discontinuity capturing (Zhdan & Prokhorov, 2000; Papalexandris, 2004) for calculating the gas phase. Methods of expansion in terms of physical processes make it possible to perform a separate integration of equations associated with combustion (Ludwig & Roth, 1997). For turbulent flows the parabolic part of equations is solved by implicit method. In a number of works the Godunov scheme is successfully applied for calculation of discrete phase as well (Ludwig & Roth, 1997; Tunik, 1999; Tsuboi, Hayashi & Matsumoto, 2000). The equations for gas and particles are written in divergent form with the pressure proportional to the volume concentration of each of the phases. Calculation of both phases using a single finite-difference method is also carried out in (Kutushev & Rodionov, 1998) (the large particle method), in (Loth, Sivier & Baum, 1997) (finite element method) and in (Veyssiere, Bozier & Khasainov, 2002) (Mac.Cormack scheme).

Schemes based on flux correction transport (FCT) are used for calculation of both the gas flow (Loth, Sivier & Baum, 1997; Veyssiere, Bozier & Khasainov, 2002; Chang & Kailasanath, 2003), and the particles motion (Benkiewicz & Hayashi, 2003; Zhang et al., 2001). Schemes like TVD, based on the use of monotonic operators are used to calculate the gas phase in (Khmel & Fedorov, 2002; Fedorov & Khmel, 2005). Monotonic corrections are also introduced in (Tunik, 1999; Tsuboi, Hayashi & Matsumoto, 2000).

The equations of gas-particle dynamics for describing the particles motion do not contain the internal pressure, which is why the use of TVD scheme for equations of solid phase motion is limited to degeneration of space dimension of eigenvectors of Jacobi matrix (equations describing the motion of dispersed phase are not hyperbolic). For part of the Jacobian corresponding to discrete phase the eigenvalue $\lambda = up$ has the multiplicity of three, and generates two eigenvectors and one attached vector. On the other hand, the equations for particles have the form of vorticity transport equation, therefore to solve them the methods, developed for solving the vorticity equations are used, in particular, the MacCormack scheme and upwind scheme proposed in (Gentry, Martin & Daly, 1966) (Gentry–Martin–Daly).

The developed methods of supersonic gas flows calculation are not always applicable for calculation of the discrete phase (at low volume concentrations of particles, when the volume occupied by the particles is neglected) due to the degeneration of equation system, which determine the evolution of particles. The degeneration is caused by absence of the term, associated with overall mixture pressure in the equations, which describe the dynamics of discrete phase. Different schemes for calculating the particles are finding their application. Method of large particles is used in (Zhdan & Prokhorov, 2000), particle subsystem calculations by MacCormack scheme are carried out in (Benkiewicz & Hayashi, 2003; Zhang et al., 2001; Khmel & Fedorov, 2002; Fedorov & Khmel, 2005). In (Fedorov & Khmel, 2002) for calculating the dynamics and thermal

history of particles the scheme of Gentry–Martin–Daly is used, which is an upwind scheme (Gentry, Martin & Daly, 1966).

To improve the efficiency of calculations movable or adaptive meshes are used allowing to improve the resolution of shock and detonation waves (Ludwig & Roth, 1997; Loth, Sivier & Baum, 1997), as well as parallel computing (Tsuboi, Hayashi & Matsumoto, 2000). Work (Khmel & Fedorov, 2006) presents methods of adapting TVD schemes for the calculation of fine gas mixtures (within the context of single-velocity and two-temperature model) and ultrafine gas mixtures (for the mixture equilibrium in terms of velocity and temperature, taking into account the integrated combustion kinetics). The solution of compressible phase (gas) equations is implemented on the basis of explicit finite difference scheme of TVD type. Explicit scheme of TVD type provides highly accurate representation of strong discontinuities at standard template, the absence of oscillations behind the front of shock waves in the solution, which are inherent for dispersion difference schemes, and the stability when Courant conditions are met. Application of TVD schemes is justified for detonation flows as well, which are characterized by presence of ignition and combustion fronts (narrow region with a sharp change in flow parameters).

WENO-type finite difference schemes of 3rd and 5th order (WENO-Z scheme) are used in (Jacobs & Don, 2009; Sengupta et al., 2009) for the simulation of turbulent compressible gas-particle flows (mixed Euler–Lagrange approach is applied). Sampling of main equations is carried out on a uniform grid. For sampling in terms of time Runge–Kutta method of 3rd order is is used. The interaction of a shock wave with a cloud of particles is discussed. Work (Murray, Zhang & Thibault, 1998;) provides the comparison of calculation results obtained with various difference schemes (Godunov method, WENO scheme), as well as a comparison of calculation data obtained in the context of Eulerian and Lagrangian approaches to description of dispersed phase (during interaction of cloud of particles with a shock wave, calculations are carried out in one-dimensional statement of the problem). Accounting for the volume occupied by the particles allows to provide hyperbolicity of equations describing the dynamics and heat exchange of dispersed phase, and to apply the Godunov method to sampling both the equations of gas and on dispersed phase.

For gas mixtures with small reacting particles the scales of velocity relaxation of phases are neglected, and one-velocity and two-temperature approximation of heterogeneous media mechanics is assumed (Fedorov, 1992). To solve the equations a modified TVD scheme based on methodology proposed in (Montagne, Yee & Vinokur, 1989) for non-ideal gases is used. The modified TVD scheme is also successfully applied for calculation of detonation flows in gas suspensions of aluminium particles and coal dust (Fedorov & Khmel, 2002; Khmel & Fedorov, 2006). For the mixture the equations are solved in Eulerian coordinates, and equations describing the processes of thermal and chemical relaxation are solved in Lagrangian variables. The length of the velocity and thermal relaxation zones in ultra-fine mixtures appear to be by several orders of magnitude lesser than the characteristic scale of the problem and the scale of change in dispersed phase mass concentration. To describe the processes occurring in the macro scale, a mixture of gas and particles is assumed to be equilibrium in terms of velocity and temperature, but non-equilibrium in terms of chemical composition.

Methods

Theory and methods of calculation

Model of gas interaction with a particle

The effect of viscous forces is only taken into account when the gas interacts with particles. The equation describing the unsteady flow of non-viscous compressible gas is written in the conservative form and takes into account the reverse effect of particles. Characteristic length, characteristic density, characteristic velocity and characteristic temperature are chosen as characteristic scales for variables with dimensions of length, density, velocity and temperature. For dimensionless variables, it is assumed that $R=1/\gamma$ and $\mu=1/Re$.

To construct the equations describing the motion and heat exchange of particle continuum, the approach for simulating large vortices of turbulent gas-particle flows proposed in (Pandya & Mashayek, 2002) is used, as well as its generalization, developed in (Shotorban & Preliminary, 2011; Shotorban et al., 2013) for direct numerical simulation of two-phase flows. In continuum approach, the continuity equation, momentum equation and energy equation are obtained from the Lagrangian equations of motion and heat exchange of individual particle.

The probability density function, which satisfies the Liouville equation in the phase space is introduced (Pandya & Mashayek, 2002; Mashayek & Pandya, 2003). Spatial filtering operator is determined by the ratio with non-negative kernel, which satisfies the normalization condition. The filter width is selected to be sufficiently small and such that sub-grid fluctuations of gas velocity can be ignored. With a non-negative kernel (top-hat filter, Gaussian filter) the probability density function satisfies the imposed requirements (Verman, Geurts & Kuerten, 1994; Gicquel et al., 2002).

Using the averaging procedure of disperse phase parameters leads to the emergence of new terms, which require simulation. To close the equations, it is assumed that the contribution of third correlation moments is negligible. The problem of closing the equations that describe motion and heat exchange of dispersed phase is discussed in (Fevrier, Simonin & Squires, 2005; Dombard et al., 2012) (mesoscopic Eulerian formalism).

Neglecting the inertial effects, the velocity and temperature of the dispersed phase are equal to the corresponding gas parameters. In this case, only equations for particle concentration are solved, and the momentum equation and energy equation are not solved. It is possible to partially account for inertial effects within the context of equilibrium model, in which the local velocity of dispersion phase is expressed as a sum of gas local velocity and acceleration. As an expansion parameter the time of particle dynamic and thermal relaxation (the local acceleration of dispersed phase is equal to the local gas acceleration) is used. The equilibrium model describes a number of inertial effects (preferential acceleration), but it is suitable for describing the motion of quite small particles. To fully take into account the inertial effects, the transport equations are solved, assuming that the contribution of correlation moments is negligible. In this case, the equations of the mathematical model are equivalent to the model proposed in (Saito, 2002), which describes the flow of gas suspension with negligible volume occupied by the particles, and with reasonably large ratio between densities of dispersed and gaseous phases. For gas-particle mixture with mono-dispersed

particles the equations of mathematical models coincide with the equations formulated in (Laurent, Massot & Villedieu, 2004; Kah et al., 2012). Although the inertial effects are taken into account, neglecting the second correlation moments of dispersed phase doesn't allow to account for a number of important effects (trajectory crossing effect), which play an important role in flows of gas suspension with high inertial particles (Fevrier, Simonin & Squires, 2005; Fox, 2008).

To solve the problem of closing several other approaches can be used, including the approach (Fox, 2008; Desjardins, Fox & Villedieu, 2008) (quadrature-based moment method), which uses an approximation of higher order, but requires the solutions of additional transport equations. In the approach (Fevrier, Simonin & Squires, 2005; Kaufmann et al., 2008) the closure problem solution is based on the use of transport equation of kinetic energy of particles. Work (Dombard et al., 2012) proposes an approach designed for simulating the non-isothermal gas suspension flows. In this approach three additional transport equations for the vector components of thermal flow are solved. In the described models, the concept of dispersed phase viscosity is introduced, and the models produce satisfactory results for low-inertia particles.

The finite volume method is used to solve the governing equations. The fluxes through the faces of control volumes are calculated based on Godunov method (Le Veque, 2002).

Using the flux vector splitting the Jacobian is represented as follows: A=R(Λ++Λ-)R–1 (where the matrices Λ+ and Λ- are diagonal matrices with positive and negative eigenvalues on the main diagonal). Components of matrices A+ and A- are obtained using values averaged by Roe.

Model of interaction of a shock wave with a cloud of particles

In (Boyko et al., 2006) an experimental and numerical study of shock wave propagation in gas mixtures with solid particles in the presence of pronounced two-phase boundaries (particle cloud) is performed. The effect of particle concentration on the dynamics of their acceleration behind the shock wave is discussed. The effect of concentration on particle acceleration dynamics in the cloud is based on a change of wave structure that forms at particles during supersonic flow.

With increase in concentration of dispersed phase the shocks forming near each particle interact with each other, overlap, and form an aggregate frontal shock. The polydispersity of dispersed phase has relatively little effect on the flow pattern in the area (in calculations 8 fractions of particles with diameters ranging from 60 to 130 microns and with increments of 10 microns are used). In gas mixtures with particles the flow pattern is characterized by the influence of velocities and temperatures relaxation processes of two phases, whose characteristic length are determined by particle sizes. In flows with high concentration of dispersed phase deviation resistance coefficient from characteristic values of single particle is observed. In low-speed two-phase flows, this effect becomes remarkable when the volume concentration is about 5%, and in supersonic nozzle the flow constraint effects appear at 1% (Boyko et al., 2006).

The results of mathematical modelling of particles lifting behind the shock wave reflected from the end wall, which slide over the layer of particles, are presented in (Kiselev & Kiselev, 2001). Particles lift occurs in a vortex that arises in the gas after reflection of the shock wave from the wall. Formation of vortex

flow is caused by the emergence of λ-shaped structure of reflected shock wave due to the gas flow non-uniformity behind the passing shock wave.

In (Wang et al., 2001) the problem of plane shock wave propagation of over a square cavity filled with stagnant gas suspension is solved. With increase in particles concentration the shock waves in the cavity are attenuated and transformed into compression waves. Particle size has a significant impact on the flow nature and wave structure of the flux inside the cavity. For large particles (about 250 microns) the flow approaches to flow structure of gas mixtures.

Combustion and detonation processed in gas suspensions inside channels with sudden expansion are discussed in (Kutushev & Shorokhova, 2003). The conditions for passage of detonation wave through the channel cross-section for monopropellant particles of fixed size (particle size is 30 microns) are studied. There is a significant effect of particle concentration on the value of critical relation between pipe diameters to prevent the detonation failure.

A mathematical model based on the two-velocity and two-temperature approximation of reacting continua mechanics and meant for calculating shockwave and detonation processes in gas mixtures and particles (particle size ranges from 1 to 5 microns) inside channels of complex geometry is proposed in (Fedorov et al., 2008). The propagation of shock and detonation waves in gas suspension of aluminum particles in oxygen inside the channel with sudden expansion is discussed. The diffraction of shock waves in gas-particle mixture on the opposite ledge differs from the corresponding flow in pure gas by lacking self-similarity of the flow and by influence of phase relaxation processes (Wang et al., 2001; Kutushev & Shorokhova, 2003). The calculation results show that the formation of zones free of particles and layers with their increased concentration is possible. When the detonation wave exits a narrow part of the canal into its wide part the implementation of various flow scenarios is possible – from partial attenuation to full heterogeneous detonation failure, including the possibility of partial failure followed by initiation.

Overview of numerical methods designed for simulation of shock wave and detonation processes in gas-particle mixtures, is given in (Khmel & Fedorov, 2006). The numerical results of cellular detonation in a gas suspension of aluminum particles are provided.

Numerical method

Subject of consideration is the interaction uniform sub- and supersonic flow of inviscid compressible gas with a cloud of particles, filling a certain bounded area of space, and being in stable state at the initial time. Calculations are performed in the one-dimensional statement.

Simulation of gas-dynamic processes in steam halo of particles is reduced to the integration of the equations of non-stationary flow of ideal gas. Finite volume method and splitting scheme are used for equations sampling. Flows are calculated using a Godunov-type scheme of the 2nd order (Le Veque, 2002).

Calculations are performed on the interval [–5, 6]. The particles cloud consists of 8.6×10^4 particles that are immobile at initial time and evenly fill the interval [0, 0.3]. Computational grid contains 1,000 nodes.

Certain computational gas with specific heats ratio equal to 1.4 at constant pressure and constant volume is selected as a working medium. The ratio of

specific heat is assumed equal to 1. In practice, the dynamic and thermal relaxation times turn out to be close to each other. The calculations assume that $\tau_v = \tau_t = 3.569$ (in dimensionless variables relaxation time is corresponded by the Stokes number). The particles material density and the particle mass are equal to $\rho_p = 1000$ kg/m3 and $m_p = 10\text{-}4$ kg (particle diameter is $d_p = 5.77 \times 10\text{-}3$ m).

On the left boundary, through which the working gas flows into the computational area the Mach number equal to 0.3 is set for subsonic flow (case 1). For the case of supersonic flow (case 2) the parameters on left boundary are obtained from Rankine–Hugoniot relations so that Mach number behind the shock front is equal to 2.8.

At the initial time t=0 the gas is moving at a uniform velocity ($\rho=1$, p=1 and u=1 in dimensionless variables). The particle velocity is zero, and the particles temperature is assumed equal to gas temperature. Correlation moments of velocity and temperature of the dispersed phase are zero. The initial concentration of dispersed phase is 2.885×105.

Results

Particles of different sizes have different inertia and different velocity lag relative to the gas stream, which affects the process of establishing a quasi-stationary flow. The duration of the quasi-stationary regime in operating chamber is defined by the degree of uneven distribution of impurities concentration and the velocity gap of particles from the gas.

For case 1, the parameters distribution of carrier gas at different moments of time is shown in Figures 1 and 2. In front of cloud of particles, the stream decelerates, which leads to velocity reduction and to increase of gas density, pressure and temperature. At the contact of the incoming stream with particles cloud the particles, which were at rest at the initial moment of time, begin to accelerate, acquiring non-zero velocity and providing less resistance to gas flow, resulting in increase of carrying flow velocity. Behind the area occupied by the particles occurs the recovery of density, velocity, pressure and temperature to the corresponding values in incoming flow.

During t=0.275 the particles cloud doesn't displace noticeably, although the density of the dispersed phase at frontal boundary of the cloud is slightly higher than at rear boundary. Within the area occupied by the particles the velocity of dispersed phase is distributed unevenly. Near the rear boundary of the cloud the velocity of dispersed phase increases due to acceleration of carrier gas in this area. The particles located near the frontal boundary of the cloud have the highest velocity, as they interaction with the gas flow begins at the moment when the gas reaches the area occupied by the particles. The temperature of the dispersed phase remains approximately constant. Uneven distribution of velocity along the cloud (high velocity at the front boundary and low velocity at rear boundary) leads to a different intensity of heat exchange between the gas and the particles located near front and rear boundaries of the clouds. As a result, there is a slight decrease in temperature of dispersed phase near the rear boundary of the cloud. Distribution of correlation moments of velocity and correlation moments of velocity and temperature of dispersed phase are qualitatively similar.
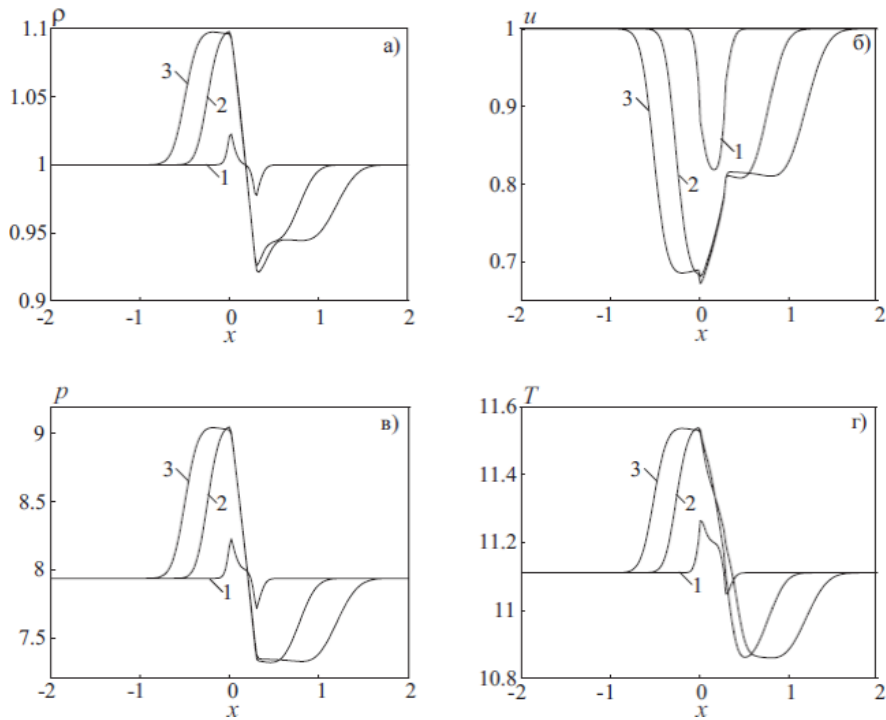
Figure 1. Distributions of density (a), velocity (b) pressure, (c) and temperature (d) of gas for case 1 (*Lines: 1 – t=0.025, 2 – t=0.15, 3 – t=0.25*)
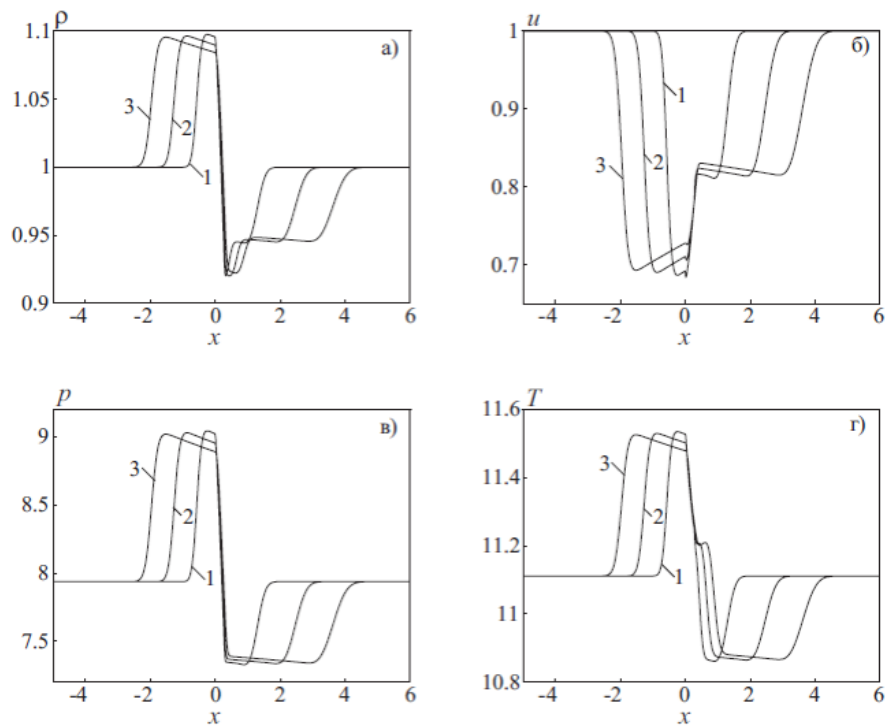

Figure 2. Distributions of density (a), velocity (b) pressure, (c) and temperature (d) of gas for case 1 (*Lines: 1 – t=0.275, 2 - t=0.550, 3 – t=0.825*)

For case 2, the distribution of carrier gas parameters at different moments of time is shown in Figure 3 and Figure 4. Interaction of supersonic flow with a cloud of particles leads to the formation of a shock wave, behind which there is an abrupt decrease the gas velocity to subsonic values and increase its density, pressure and temperature. Behind the shock wave occurs the interaction of the carrier flow and the particles. In the region occupied by the particles the velocity of carrier flow remains approximately constant, while the density pressure and temperature of the gas of the gas decrease. The particles, which are at rest at initial time, are involved in movement by the gas, receiving non-zero velocity and providing less resistance to gas flow. At the rear edge of the cloud a rarefaction wave is observed, in which acceleration of the flow and decrease in density, pressure and temperature of the gas occurs. Behind the clouds of particles gas parameters do not reach the values they had in undisturbed flow, which is due to energy losses at the shock wave front. In front of expansion wave fan the velocity and pressure of the gas are lower than in the undisturbed flow. Density and temperature of gas behind expansion wave fan undergo minor fluctuations due to the occurrence of the contact discontinuity, which moves down the flow at velocity lesser than velocity of the shock wave induced by cloud particles. To the left of the contact discontinuity the gas temperature is higher and its density is lower than the temperature and density of gas to the right of contact discontinuity. Contact discontinuity arises due to the abrupt change in gas density and temperature at the front of shock wave, which moves down the flow.
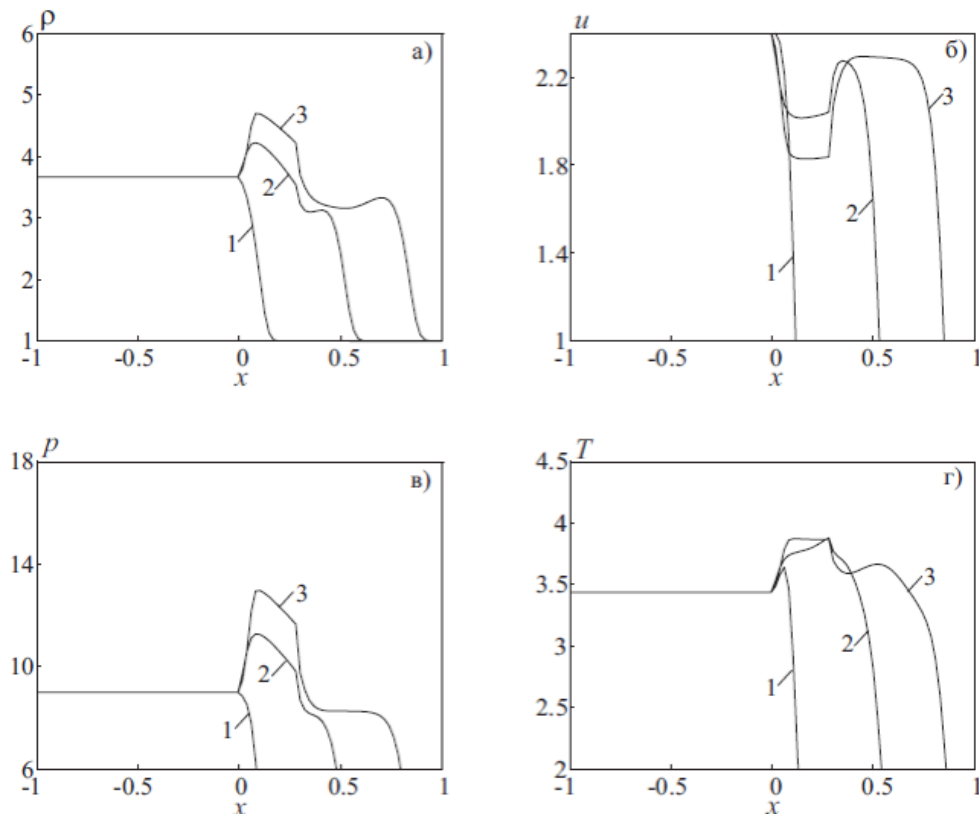

Figure 3. Distributions of density (a), velocity (b) pressure, (c) and temperature (d) for the case 2 (*Lines: 1 – t=0.025, 2 – t=0.15, 3 – t=0.25*)
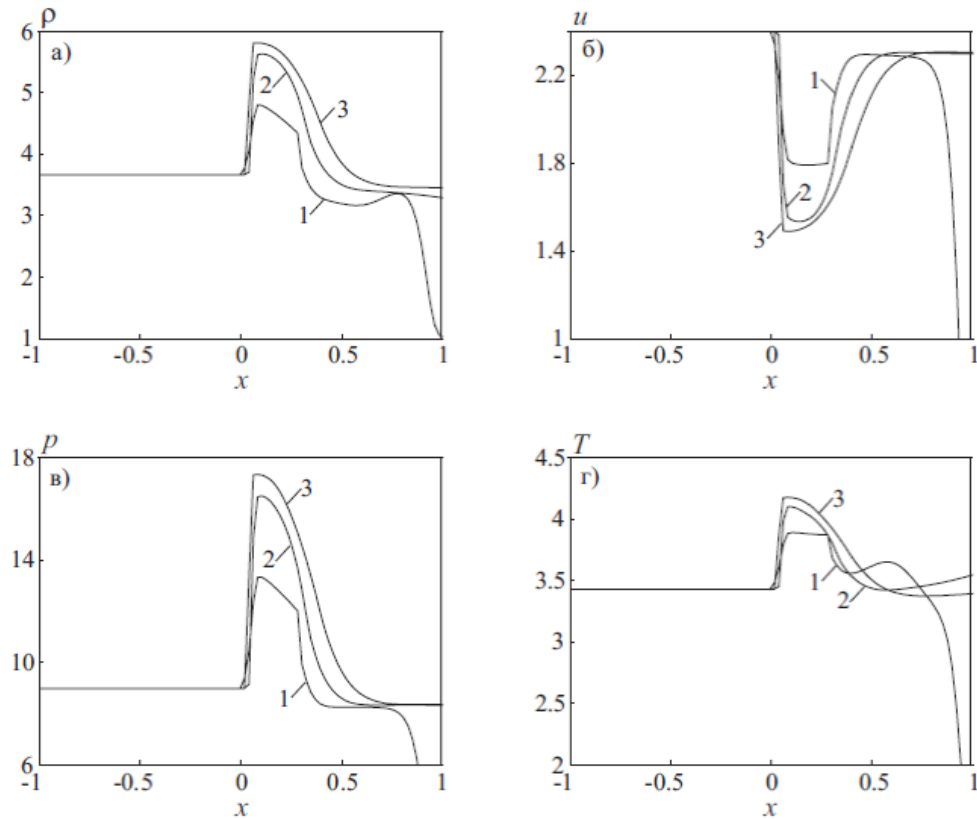
Figure 4. Distributions of density (a), velocity (b) pressure, (c) and temperature (d) for the case 2 (*Lines: 1 – t=0.275, 2 – t=0.550, 3 - t=0.825*)

Comparison of gas parameters distributions at different moments of time shows that the position of shock wave front induced by cloud of particles remains practically unchanged in space, but the magnitude of shock of flow parameters increases as time passes.

At time t=0.275 velocity of particles near the front boundary of the cloud exceeds the velocity of those close to its rear boundary. An uneven velocity distribution result in an uneven distribution of dispersed phase density, which, at the front boundary of the cloud, exceeds the dispersed phase density at the rear boundary. Increasing the gas temperature at the front boundary of the cloud increases the temperature of dispersed phase. Distribution of velocity correlation moments, velocity and temperature of dispersed phase are qualitatively similar.

Conclusion

The study provides an analysis of the main existing methods for description of two-phase flows, analysis of numerical methods for the calculation of such flows. The mathematical model of gas interaction with the particles, based on the use of two-velocity and two-temperature model of heterogeneous media mechanics is developed. Simulation of inviscid compressible gas is based on the use of Euler equations. To describe the motion and heat exchange of dispersed phase Liouville equation is used. For closing the obtained equations, the third correlation moments of velocity and temperature of dispersed phase are not taken into

account. For sampling of the equation describing the motion and heat exchange of gas and dispersed phases the finite volume method with splitting by the flow vector Roe is used.

On the basis of developed mathematical model calculations of interaction of uniform pre- and supersonic flow of non-viscous compressible gas with a cloud of particles, which are in still state at initial time.

It has been demonstrated that passive particles in the reaction medium significantly weaken the detonation waves up to their suppression, which can be used to enhance the explosion safety of spacecraft. In contrast, high-energy particles of metals (aluminum, magnesium) or mixtures of reactive gases with additions of these particles can be used as working media in rocket engines using hybrid and heterogeneous detonation. In this case, the developed method can be used to calculate the concentration of particles, providing a controlled secure detonation.

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Disclosure statement

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References

Balachandar, S. (2009). A scaling analysis for point-particle approaches to turbulent multiphase flows. *International Journal of Multiphase Flow*, 35(9), 801–810.

Balachandar, S., & Eaton, J.K. (2010). Turbulent dispersed multiphase flow. *Annual Review of Fluid* Mechanics, 42, 111–133.

Benkiewicz, K., & Hayashi, A.K. (2003). Two-dimensional numerical simulations of multi-headed detonations in oxygen-aluminum mixtures using an adaptive mesh refinement. *Shock Waves*, 13(5), 385–402.

Boyko, V.M., Kiselev, V.P., Kiselev, S.P., Papyrin, A.N., Poplavskiy, S.V., & Fomin, V.M. (1996). On the interaction of a shock wave with a cloud of particles. *Physics of combustion and explosion*, 32(2), 86–99.

Chang, E.J., & Kailasanath, K. (2003). Shock wave interactions with particles and liquid fuel droplets. *Shock Waves*, 12(4), 333–341.

Crowe, C., Sommerfeld, M., & Tsuji, Y. (1998). Multiphase flows with droplets and particles. (p. 509). Boca Raton: *CRC Press*.

Desjardins, O., Fox, R., & Villedieu, P. (2008). A quadrature-based moment method for dilute fluid-particle flows. *Journal of Computational Physics*, 227(4), 2514–2539.

Dombard, J., Leveugle, B., Selle, L., Reveillon, J., Poinsot, T., & Angelo, Y. (2012). Modeling heat transfer in dilute two-phase flows using the mesoscopic Eulerian formalism. *International Journal of Heat and Mass Transfer*, 55(5–6), 1486–1495.

Eckhoff, R. (2003). Dust explosions in the process industries. (p. 720). Houston: *Hardbound*: Gulf Professional Publishing.

Gentry, R.A., Martin, R.E., & Daly, B.J. (1966). An Eulerian differencing method for unsteady compressible flow problems. *Journal of Computational Physics*, 1(1), 87–118.

Fedorov, A.V. (1992). The structure of the heterogeneous detonation of aluminum particles dispersed in oxygen. *Physics of combustion and explosion*, 28(3), 82–83.

Fedorov, A.V., & Khmel, T.A. (2002). Mathematical modeling of detonation processes in gas suspension of coal particles. Physics of combustion and explosion, 38(6), 103–112.

Fedorov, A.V., & Khmel, T. A. (2005). Numerical modeling of formation of cellular heterogeneous detonation of aluminum particles in oxygen. *Physics of combustion and explosion*, 41(4), 84–98.

Fedorov, A.V., Kratova, Y.V., Khmel, T.A., & Fomin, V.M. (2008). Propagation of shock and detonation waves in channels of different geometry in gas-suspensions. *Physical and chemical kinetics in gas dynamics*, (7), 6.

Fevrier, P., Simonin, O., & Squires, K.D. (2005). Partitioning of particle velocities in gas–solid turbulent flows into a continuous field and a spatially uncorrelated random distribution: theoretical formalism and numerical study. *Journal of Fluid Mechanics*, 533, 1–46.

Fox, R. (2008). A quadrature-based third-order moment method for dilute gas-particle flows. *Journal of Computational Physics*, 227(12), 6313–6350.

Gicquel, L., Givi, P., Jaberi, F., & Pope, S. (2002). Velocity filtered density function for large eddy simulation of turbulent flows. *Physics of Fluids*, 14(3), 1196–1213.

Gouesbet, G., & Berlemont, A. (1999). Eulerian and Lagrangian approaches for predicting the behaviour of discrete particles in turbulent flows. *Progress in Energy and Combustion Science*, 25(2), 133–159.

Jacobs, G.B., & Don, W.S. (2009). A high-order weno-z finite difference based particle-source-in-cell method for computation of particle-laden flows with shocks. *Journal of Computational Physics*, 228(5), 1365–1379.

Kah, D., Laurent, F., Massot, M., & Jay, S. (2012). A high order moment method simulating evaporation and advection of a polydisperse liquid spray. *Journal of Computational Physics*, 231(2), 394–422.

Kaufmann, A., Moreau, M., Simonin, O., & Helie, J. (2008). Comparison between Lagrangian and mesoscopic Eulerian modelling approaches for inertial particles suspended in decaying isotropic turbulence. *Journal of Computational Physics*, 227(13), 6448–6472.

Khmel, T.A., & Fedorov, A.V. (2006). Numerical technologies for heterogeneous detonation investigation of gas suspensions. *Mathematical modeling*, 18(8), 49–63.

Khmel, T.A., & Fedorov, A.V. (2002). The interaction of a shock wave with a cloud of aluminum particles in a channel. Physics of combustion and explosion, 38(2), 89–98.

Kiselev, V.P., & Kiselev, S.P. (2001). The perturbation of the solid particles motion behind the reflected shock wave. *Applied mechanics and technical physics*, 42(5), 8–15.

Kiselev, V.P., & Kiselev, S.P. (2001). The rise of dust particles behind the reflected shock wave, moving over a layer of particles. *Applied mechanics and technical physics*, 42(5), 8–15.

Kutushev, A.G., & Rodionov, S.P. (1998). Plane detonation waves in gas suspensions of unitary fuel with spatially inhomogeneous distribution of particles. *Physics of combustion and explosion*, 34(5), 103–110.

Kutushev, A.G., & Shorokhova, L.V. (2003). Numerical study of combustion and detonation processes of monofuel aero-cloud in sharply expanding pipes. *Chemical Physics*, 22(8), 94–99.

Laurent, F., Massot, M., & Villedieu, P. (2004). Eulerian multi-fluid modeling for the numerical simulation of coalescence in polydisperse dense liquid sprays. *Journal of Computational Physics*, 194(2), 505–543.

Le Veque, R.J. (2002). Finite volume methods for hyperbolic problems. (p. 580). New York: Cambridge University Press.

Loth, E., Sivier, S., & Baum, J. (1997). Dusty detonation simulations with adaptive unstructured finite elements. *AIAA Journal*, 35(6), 1018–1024.

Ludwig, T., & Roth, P. (1997). Modeling of laminar combustion wave propagation in reactive gas/particle mixtures. *International Journal of Multiphase Flow*, 23(1), 93–111.

Mashayek, F., & Pandya, R.V.R. (2003). Analytical description of particle/droplet-laden turbulent flows. *Progress in Energy and Combustion Science*, 29(4), 329–378.

Michaelides, E.E. (1997). Review-the transient equation of motion for particles, bubbles, and droplets. *Journal of Fluid Engineering*, 119(2), 233–247.

Michaelides, E.E., & Feng, Z.G. (1994). Heat transfer from a rigid sphere in a no uniform flow and temperature field. *International Journal of Heat and Mass Transfer*, 37(10), 2069–2076.

Montagne, J.L., Yee, H.C., & Vinokur, M. (1989). Comparative study of high-resolution shock-capturing schemes for a real gas. *AIAA Journal*, 27(10), 1332–1346.

Murray, S.B., Zhang, F., & Thibault, P.A. (1998). Transition from deflagration to detonation in an end multiphase slug. *Combustion and Flame*, 114(1–2), 13–25.

Pandya, R.V.R., & Mashayek, F. (2002). Two-fluid large-eddy simulation approach for particle-laden turbulent flows. *International Journal of Heat and Mass Transfer*, 45(24), 4753–4759.

Papalexandris, M.V. (2004). Numerical simulation of detonations in mixtures of gases and solid particles. *Journal of Fluid Mechanics*, 507, 95–142.

Saito, T. (2002). Numerical analysis of dusty-gas flows. Journal of Computational Physics, 176(1), 129–144.

Saito, T., Marumoto, M., & Takayama, K. (2003). Numerical investigations of shock waves in gas-particle mixtures. *Shock Waves, 13*(4), 299–322.

Sengupta, K., Shotorban, B., Jacobs, G.B., & Mashayek, F. (2009). Spectral-based simulations of particle-laden turbulent flows. *International Journl of Multiphase Flow*, 35(9), 811–826.

Shotorban, B. (2011). Preliminary assesment of two-fluid model for direct numerical simulation of particle-laden flows. *AIAA Journal*, 49(2), 438–443.

Shotorban, B., & Balachandar, S. (2007). A Eulerian model for large-eddy simulation of concentration of particles with small stokes numbers. *Physics of Fluids*, 19(118107), 12.

Shotorban, B., & Balachandar, S. (2006). Particle concentration in homogeneous shear turbulence simulated via lagrangian and equilibrium eulerian approaches. *Physics of Fluids*, 18(065105), 16.

Shotorban, B., & Balachandar, S. (2009). Two-fluid approach for direct numerical simulation of particle-laden turbulent flows at small stokes numbers. *Physical Review E*, 79(5), 056703.

Shotorban, B., Jacobs, G.B., Ortiz, O., & Truong, Q. (2013). An Eulerian model for particles nonisothermally carried by a compressible fluid. *International Journal of Heat and Mass Transfer*, 65, 845–854.

Smirnov, N.N., Nikitin, V.F., & Legros, J.C. (2000). Ignition and combustion of turbulized dust-air mixtures. *Combustion and Flame*, 123(1–2), 46–67.

Tsuboi, N., Hayashi, A.K., & Matsumoto, Y. (2000). Three-dimensional parallel simulation of cornstarch-oxygen two-phase detonation. *Shock Waves*, 10(4), 277–285.

Tunik, Yu.V. (1999). Global modelling of heat release during initiation and propagation of detonation and deflagration waves in methane-air-particle systems. *Shock Waves*, 9(3). 173–179.

Verman, B., Geurts, B., & Kuerten, H. (1994). Realizability conditions for the turbulent stress tensor in large-eddy simulation. *Journal of Fluid Mechanics*, 278, 351–362.

Veyssiere, B., Bozier, O., & Khasainov, B.A. (2002). Effect of a suspension of magnesium particles on the detonation characteristics of methane-oxygen-nitrogen mixtures at elevated initial pressures. *Shock Waves*, 12(3), 227–233.

Wang, B.Y., Wu, Q.S., Wang, C., Igra, O., & Falcovitz, J. (2001). Shock wave diffraction by a cavity filled with dusty gas. *Shock Waves*, 11(1), 7–14.

Zaichik, L., Simonin, O., & Alipchenkov, V. (2009). An Eulerian approach for large eddy simulation of particle transport in turbulent flows. *Journal of Turbulence*, 10(9), 1–21.

Zhang, F., Frost, D.L., Thibault, P.A., & Murray, S.B. (2001). Explosive dispersal of solid particles. *Shock Waves*, 10(6), 431–443.

Zhdan, S.A, & Prokhorov, E.S. (2000). The calculation of the cellular structure of the milling loss detonation in the H2–O2 system. *Physics of combustion and* explosion, 36(6), 111–112.