NUMERICAL SIMULATION OF DUST LIFTING PROCESS FROM THE LAYER BEHIND PROPAGATING SHOCK WAVE

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Abstract

The numerical simulations of physical processes constitute a great challenge for scientists. Many new models have been being developed and the ones that already exist are being improved. Many experiments are no longer needed to be performed in reality but can be replaced by numerical simulations. Many others that could not be done up to now, due to high cost or technical unfeasibility, can be performed using numerical models. Despite that many problems have not been fully resolved lots of work is still to be done. One of the phenomena that has not been fully explained and properly modeled - is the dust listing process from the layer. In the current research, the model of dust lifting process has been developed where the dust is not modeled directly but replaced by an injection of dust from the bottom of the channel. The parameters of the dust injection were obtained from previous experiments. The main advantage of this approach is the possibility of using sparse meshes which are required in modeling of large scale geometries. The model was implemented in a CFD code and calculations were made to test the ability of the model to simulate dust dispersion from a layer in a shock tube. The results were compared with the experimental data and a good agreement was concluded.

Keywords: lifting, dust layer, fluid mechanics, mathematical modelling, multiphase flow

Nomenclature

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- A surface of the cross section of the grid cell $[m^2]$
- C_d drag force coefficient [1]
- c_v heat capacity of the gas phase
- c_s heat capacity of the dust phase
- d diameter of the particle [m]
- E total internal energy of phase $[J/m^3]$
- f interphase force $[N/m^3]$
- g gravity acceleration $[m/s^2]$
- *h* heat exchange coefficient $[W/(m^{2}*K)]$
- m₂ current mass of the solid particles in the computational cell (control volume),
- n number of particles in 1 m³ $[1/m^3]$
- Nu Nusselt number [1]
- p pressure [Pa]

- Pr Prandtl number
- Q interphase heat flux [W/m³]
- T temperature of a phase [K]
- u x component of the velocity of phase [m/s]
- v y component of the velocity of phase [m/s]
- Vp dust velocity in the upward direction,

Greek type face

- λ heat conductivity of the gas phase [W/(m*K)]
- Δ grid cell height
- δ dust layer thickness [mm]
- μ dynamics viscosity of the gas
- ρ density of phase [kg/m³]
- ρ_m density of the dust material [kg/m³]
- ρp concentration of the injected particles
- σij stress tensor [Pa]

Subscripts

- 1 gas phase
- 2 dust phase
- x x direction
- y y direction
- p injection parameters

1. Introduction

The problem of dust layer is a one of the major hazard in the process industries. In many industrial facilities the dust is not premixed with air but is deposited in a form of layers covering walls, floors and various installations. If this dust is lifted and mixed with air for any reason, an explosive mixture can be formed. Usually dust explosions in industrial facilities are strong and cause high losses in human lives and equipment. A typical example of such situation is a coal mine with a high risk of methane explosion.

Experimental work in the field of dust explosion has been under way for many years especially in countries where coal industry is developed. The process has been mainly studied in small geometries due to high cost of large scale experiments. That is why reliable numerical models are needed to perform numerical simulation of dust explosion in large scale geometries. The development of the reliable model of dust dispersion from a layer is of great importance for proper simulation of dust explosion in industrial facilities, where dust layers are present. Elaboration of such a model would improve the quality of the results from numerical simulations [1].

1.1 Two phases flow modeling

There are two techniques used for simulation of two phase flow modelling: Eulerain-Eulerain (E-E) and Eulerian-Lagrangian (E-L) [2]. In the E-L approach, the gas phase is treated as a fluid and described by Navier-Stokes equations. The dust is modelled as a set of particles and each particle is described by a set of equations and tracked in the computational domain. This approach is more physically correct and makes it easier to model some particle-particle and particle-wall interactions. Unfortunately, a denser computational mesh and high computer resources are required to track the parameters of all the particles in the computational domain. That is the reason why the use of that kind of model is still limited to small geometries. In the E-E approach, both phases are treated like separated fluids coupled by interphases mechanisms like drag forces and

heat exchange. The gas phase is described by the same Navier-Stokes equations as in the E-L approach and the dust phase is described by equations similar to Euler ones. The use of E-E model is economically justified for gas-dust flows and large scale geometries can be easily modelled. The main problem in applying that approach with two-way coupling is the necessity of using good phenomenological models which are usually derived from experimental work or from numerical simulation made by using of kinetic theories for granular flows.

1.2 Modelling of dust dispersion from a layer

A proper modelling of the dust lifting process is very important in modelling of dust explosion. As the process of propagation of dust explosion strongly depends on dust dispersion from a layer, the development of a proper model of dust dispersion may improve the quality of the results obtained from numerical simulations of dust explosions. The mechanism of dust dispersion from a layer is still not fully understood up to now. That is why the modelling of the process is difficult and different models and approaches to the problem can be found in the literature.

The authors of the current study have already worked on the topic. [3, 4]

A comparison between different techniques for dust lifting modelling was made in [5]. The process of dust lifting from a layer was modelled using Eulerian-Eulerian and Eulerian-Lagrangian techniques. The obtained results were compared and similarities were observed but any comparison with experimental results was not made.

Many other publications devoted to the problem of dust lifting can be found. An interesting review was published by Fedorov [6] presenting experimental and numerical works on dust dispersion from a layer.

1.3 Experimental work

Despite the fact that the experimental work on dust lifting has been being carried out since Gerrard [7] in 1960's, the mechanism of dust lifting has not been fully explained. Some different hypotheses on the mechanism of dust lifting are presented but there is no one complete model describing the process. The dust lifting process was also studied by Fletcher [8, 9], Boiko and Papyrin [10], Suzuki and Takashi [11] and many others. The authors of the current paper have also been working on that process. [12, 13, 14, 15]

Many studies have been devoted to the dust lifting problem connected with combustion process and detonation usually called a 'layered' detonation. [16, 17, 18] The problem of gas-dust flow with high dust concentration is also studied in connection with fluidized bed boilers and numerical modelling of that process. [19]

1.4 The aim of the work

In many previous works, the E-L approach was used to model the two phase flow. This is physically more correct than the E-E approach, but it limits the applications to small scale and low dust concentrations. The aim of the current work was to develop a model of dust dispersion from a layer that could be used in dust explosion simulation in large scale. This implies the use of E-E approach due to limited computer resources. In this case, a direct modelling of the dust layer is difficult because (1) it would require a small computational mesh equal to the height of the dust layer (2) and the Eulerian models of the dust phase are not suitable to model the flow of such high dust concentration as that in the dust layer. That is the reason why an empirical model is proposed where the dust layer is not modelled but replaced by a dust injection. The parameters of the injection are defined on the bases of the experimental work [12, 13, 14, 15] carried out by the authors.

2. The models

2.1 The gas-dust mixture flow

As it was mentioned before, the E-E approach is used in the current research. In this model, both phases are treated as separate fluids coupled by some interphases mechanisms. The gas phase is described by Navier-Stokes equations. The dust phase is described by a similar set of equations as Euler ones, but pressure and viscosity are omitted and the density of the fluid is replaced by dust concentration. The models are presented below.

The 2D (two dimensional) model of the gas phase:

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial \rho_1 u_1}{\partial x} + \frac{\partial \rho_1 v_1}{\partial y} = 0$$
(1)

$$\frac{\partial \rho_1 u_1}{\partial t} + \frac{\partial (\rho_1 u_1^2 + p)}{\partial x} + \frac{\partial \rho_1 u_1 v_1}{\partial y} = \frac{\partial \sigma_{11}}{\partial x} + \frac{\partial \sigma_{12}}{\partial y} - f_X$$
(2)

$$\frac{\partial \rho_1 v_1}{\partial t} + \frac{\partial \rho_1 u_1 v_1}{\partial x} + \frac{\partial (\rho_1 v_1^2 + p)}{\partial y} = \frac{\partial \sigma_{21}}{\partial x} + \frac{\partial \sigma_{22}}{\partial y} - f_y$$
(3)

$$\frac{\partial E_1}{\partial t} + \frac{\partial u_1(E_1 + p)}{\partial x} + \frac{\partial v_1(E_1 + p)}{\partial y} =$$

$$= \frac{\partial}{\partial x} (u_1 \sigma_{11} + v_1 \sigma_{12}) + \frac{\partial}{\partial y} (u_1 \sigma_{21} + v_1 \sigma_{22}) +$$

$$- f_X (u_1 - u_2) - f_Y (v_1 - v_2) - Q \qquad (4)$$

State equation for the gas phase:

$$\frac{p}{\rho_1} = RT_1 \tag{5}$$

and the total energy of the gas phase:

$$E_1 = \rho_1 \frac{u_1^2 + v_1^2}{2} + T_1 \rho_1 c_v \tag{6}$$

The stress tensor included above:

$$\sigma_{11} = 2\mu \frac{\partial u_1}{\partial x} - \frac{2}{3}\mu \left(\frac{\partial u_1}{\partial x} + \frac{\partial v_1}{\partial y}\right)$$
(7)

$$\sigma_{12} = \sigma_{21} = \mu \left(\frac{\partial u_1}{\partial y} + \frac{\partial v_1}{\partial x} \right)$$
(8)

$$\sigma_{22} = 2\mu \frac{\partial v_1}{\partial y} - \frac{2}{3}\mu \left(\frac{\partial u_1}{\partial x} + \frac{\partial v_1}{\partial y}\right)$$
(9)

The 2D model of the dust phase used in the simulations:

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial \rho_2 u_2}{\partial x} + \frac{\partial \rho_2 v_2}{\partial y} = 0$$
(10)

$$\frac{\partial \rho_2 u_2}{\partial t} + \frac{\partial \rho_2 u_2^2}{\partial x} + \frac{\partial \rho_2 u_2 v_2}{\partial y} = f_X$$
(11)

$$\frac{\partial \rho_2 v_2}{\partial t} + \frac{\partial \rho_2 u_2 v_2}{\partial x} + \frac{\partial \rho_2 v_2^2}{\partial y} = f_y - g$$
(12)

$$\frac{\partial E_2}{\partial t} + \frac{\partial u_2 E_2}{\partial x} + \frac{\partial v_2 E_2}{\partial y} = f_X (u_1 - u_2) + f_Y (v_1 - v_2) + Q$$
(13)

The total energy of the dust phase:

$$E_2 = \rho_2 \frac{u^2 + v^2 + w^2}{2} + T_2 c_s \rho_2 \tag{14}$$

The gas phase and the dust phase are coupled by interphase mechanism. In the current study, a two way coupling method was used and two mechanisms were considered: (1) the drag force and (2) the heat exchange.

The drag force was computed using a basic formula:

$$\vec{f} = n \cdot \frac{\pi d^2}{2} \cdot C_d \cdot \frac{\rho_1 (\vec{V}_1 - \vec{V}_2) \cdot |\vec{V}_1 - \vec{V}_2|}{2}$$
(15)

The value of the drag coefficient C_d depends on the Reynolds number which is calculated in this way:

$$\operatorname{Re} = \frac{\rho_1 \cdot d \cdot \left| \overrightarrow{V_1} - \overrightarrow{V_2} \right|}{\mu}$$
(16)

There are several formulas for the coefficient C_d . In the current study the following one was used:

$$C_d = \frac{24}{\text{Re}} \cdot \left(1 + \frac{1}{6} \cdot \text{Re}^{\frac{2}{3}} \right)$$
(17)

In the presented model of the two phase flow, the phases have different temperatures and then the heat exchange process has to be considered. The heat exchange between the dust particles and the gas phase is computed as follows:

$$Q = n\pi d^2 h (T_1 - T_2)$$
(18)

The heat exchange coefficient is equal to:

$$\overline{h} = \frac{\lambda N u}{d} \tag{19}$$

The Nusselt number is evaluated using formula:

$$Nu = 2 + 0.6\sqrt{\text{Re}} \,\text{Pr}^{\frac{1}{3}}$$
(20)

2.1 Dust layer model

In the current paper, an empirical approach is proposed where the dust is injected into the computational domain instead of being directly modelled. The dust layer is replaced by an injection of dust to the computational domain in the upward vertical direction and the parameters of the injection are derived from experiments.



Fig. 1. General view of the modelled process.

In Fig. 1 a computational domain is presented with a computational grid. On the bottom of the channel, a dust layer is thicker than the size of the cell. The grid cell from the bottom of the channel is presented in Fig. 2.



Fig. 2. Scheme of a lower computational cell with a dust deposit in it.

A mass equation in the computational cell at the bottom of the channel can be written as follows:

$$\frac{dm_2}{dt} = \rho_p V_p A \tag{21}$$

The division of the both sides of the equation by A, and by the computational cell height Δ , yields to:

$$\frac{d\rho_2}{dt} = \frac{\rho_p V_p}{\Delta} \tag{22}$$

which constitutes an equation of conservation for the solid phase concentration. The equation is grid-independent since it contains the value of the cell size.

The empirical model requires the values of the vertical dust cloud velocity and dust concentration in the lowest grid cell. Two empirical functions are needed to be derived from the experiments:

$$\rho_p = f(d, u_1, \delta, \rho_m) \tag{23}$$

$$V_p = f(d, u_1, \delta, \rho_m)$$
(24)

Due to the lack of data, the concentration of the injected dust p was assumed to be constant. The value of this parameter was set equal to 1 kg/m³ on the basis of numerical simulations and experimental data.

The dust vertical velocity in upward direction was described by the formula derived from the experimental results:

$$v_2 = 0.004 \cdot \delta^{0.216} \cdot u_1^{1.743} \cdot d^{-0.054} \cdot \rho_m^{-0.159} \cdot A^{0.957}$$
(25)

The values of the empirical parameter A are: Coal dust: A = 1.2Potato starch dust MPS = 75µm: A = 0.745Potato starch dust MPS = 35µm: A = 0.7Silicon dust: A = 1.037The density of the dust material used to obtain the formula: Coal dust 1,340 kg/m³ Potato starch dust MPS = 75µm 1,469 kg/m³ Potato starch dust MPS = 35µm 1,527 kg/m³ Silicon dust 2,341 kg/m³

The accuracy of the presented formula is strongly disturbed by difficulties encountered during the experimental work. It was particularly difficult to calculate precisely the vertical velocity of the dust cloud on the basis of the signals from the lasers. Also the analysis of the pictures from a fast camera was disturbed by relatively poor resolution of the pictures. These can be a cause of imprecision.

It is also important to emphasis that the presented formula is based on all the results collected for all four dusts. The use of a single formula causes other errors due to fitting of a smooth curve to the experimental data. A better fit could be obtained if separated formulas were used for each kind of dust.

Nevertheless, the above inaccuracies do not disturb the results strongly, because the model is an empirical one. The aim of the model is not to simulate the physics of the process but to obtain a model that yields to correct results for simulation in large scale geometries using spare computational meshes.

3. Method used for solving the model

The gas and the dust phase constitute a mixture that is described by a system of equations of the conservation of mass, momentum and energy. The equation may be written in such a schematic way:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial (\mathbf{F} - \mathbf{F}_V)}{\partial x} + \frac{\partial (\mathbf{G} - \mathbf{G}_V)}{\partial y} = \mathbf{S}$$
(26)

where:

U – the vector of conservative variables

F, G - vectors that contain convective fluxes through cell edges

F_v, G_v - vectors that contain diffusive fluxes through cell edges

S - the vector containing source terms.

In the computation a rectangular mesh was used. The equation (26) is solved using the split method. Details on the numerical scheme can be found in [20, 21].

4. Numerical results

The aim of the numerical investigation was to "reproduce" the results from the experiments. A similar 6 m long and 72x112 mm² cross section shock tube was used in the numerical tests. The driving section was 1.5 m long and the dust layer was located 3.5 m from the beginning of the shock tube. The dust layer was 1.5 m long. Dust layer thicknesses were the same as those in the experiments (e.g. 0.1 mm, 0.4 mm and 0.8 mm). Three shock wave velocities were used in calculations as those in experiments i.e. 450 m/s, 490 m/s and 518 m/s. During the experimental work, four kinds of dust were tested: coal dust, silicon dust, potato starch dust (mean particle size 0,035 mm) and potato starch dust (mean particle size 0,075 mm). In the same way, the calculations were carried out for all four dusts that had been experimentally investigated.

The first stage of calculations consists in using the mathematical model of the gas phase, dust phase and the empirical model of the dust layer. A grid cell size equal to 5×5 mm was chosen. Simulations of the dust lifting process of all four dusts, in all experimentally tested conditions, were carried out. However, only the results obtained for coal dust will be presented and discussed in the current paper.



Fig. 3. Comparison of numerical and experimental results at different time moments after the passage of the shock wave. Coal dust layer thickness 0.1 mm. Shock wave velocity 450 m/s. a) 0 ms, b) 1 ms, c) 2 ms, d) 3 ms, e) 5 ms, f) 10 ms.



Fig. 4. Comparison of numerical and experimental results at different time moments after the passage of the shock wave. Coal dust layer thickness 0.8 mm. Shock wave velocity 518 m/s. a) 0 ms, b) 1 ms, c) 2 ms, d) 3 ms, e) 4 ms, f) 8 ms.



Fig. 5. Shape of the dust cloud behind propagating shock wave. Comparison of the results from numerical simulations and experiments.

In Fig. 3 and 4, the results from numerical simulations are compared with pictures obtained during the experiments using a fast camera coupled with a Schlieren system. On the left pictures, dust concentration is presented in the tube section corresponding to the visualization chamber of the experimental shock tube. On the right side, pictures made by using a fast camera coupled with a Schlieren system are presented. Only two out of nine cases were selected and presented. In Fig. 3, the parameters of the experiments were: dust layer thickness 0.1 mm and shock wave velocity 450 m/s. As it can be observed in the pictures, the dust lifting process starts faster in the simulation that in reality. In Fig. 3d and 3e, the height reached by the dust is similar in the experiments and in the simulation. In the next pictures the dust lifting process continues in the experiments but in the simulation the dust is not lifted higher. The similar conclusions can be drawn from Fig. 4 which presents the results for a 0.8 mm thick coal dust layer and shock wave velocity equal to 518 m/s. As previously, in the simulations the dust lifting process starts earlier and faster. Next, the height reached by the dust in experiments and in simulations is similar and afterwards, the dust lifting process continues in the experiments but no longer in simulations. In that case, it is also possible that the window through which the pictures were made during the experiments has been covered by dust but this hypothesis has not been verified yet. One can conclude that the vertical velocity of the dust cloud is higher in simulation at the beginning of the dust lifting process and then it decreases. In the experiments the highest vertical velocity of the dust cloud is reached about midheight of the channel.



Fig. 6. Results from numerical simulations obtained for different grid cell sizes. First picture – grid cell 5 mm. Second picture – grid cell 10 mm. Coal dust layer thickness 0.1 mm. Shock wave velocity 450 m/s.

In Fig. 5, a comparison of computation and experimental observations for coal dust was made. The results from the calculations show dust concentration histories in the selected points, where lasers were located in the experiments, for different time moments where t = 0 corresponds to the moment of time when the shock wave was present in the laser cross section of the shock tube. The empirical results are presented in the same way, so both results can be compared. Time scale is from 0 to 25 ms. The vertical axe describes the channel height.

The main conclusion is that the results from the simulations are qualitatively correct. The increase of the layer thickness leads to more intensive entrainment of the dust. Also, the increase of the shock wave velocity and the increase of the dust layer thickness decrease the delay when the lifting process begins. Moreover, the vertical dust velocity increases along with the increase of the layer thickness and the shock wave velocity.

The results are not fully quantitatively correct. The delay obtained by using simulation techniques is lower than delays observed empirically, whereas the dust vertical velocities are higher in simulations. The last problem is a cloud formed in simulations, the shape of which does not fully correspond to that from the experiments.

At that stage of the simulations, the influence of grid cell size was also investigated. Two grid cells were considered $5 \times 5 \text{ mm}$ and $10 \times 10 \text{ mm}$, and a comparison of the results is made in Fig. 6. The results correspond to each other, so it means that the model does not depend significantly from the grid cell size. Nevertheless, a minimal number of grid cell is necessary to simulate the dust cloud.

Conclusions

- An empirical model for a dust layer has been presented and verified against experimental data.
- The results obtained by using the mathematical model give qualitatively correct results. As in the experiments, the increase of the dust layer thickness leads to more intensive entrainment of the dust from the layer.
- The increase of the shock wave velocity and the increase of the dust layer thickness decrease the delay when the lifting process begins. The vertical velocity of the dust cloud increases along with the increase of the dust layer thickness and the shock wave velocity, in the same way as in the experiments.
- At present, the results are still not fully quantitatively correct. The delay obtained using simulation techniques is lower than that observed during the experiments. The vertical velocity of the dust cloud is higher at the beginning of the process and then it decreases. In the experiments, the highest values of the vertical velocity of the dust cloud were encountered at the mid-height of the channel.
- On the basis of the all presented results it can be concluded, that the presented model correctly simulates the lifting of the dust from the layer. There are still some difficulties to simulate the dust lifting process in the gas flow. In future, different improvements are planed to be evaluated such as the influence of Saffman and Magnus forces or the influence of particle-particle and particle-wall collisions.

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