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An investigation of the consequences of primary dust explosions in interconnected vessels

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Abstract

In this article Eulerian–Lagrangian 2D computer simulations of consequences of primary dust explosions in two vessels connected by a duct are described. After an explosion in the primary vessel a propagation of hot pressurised gases to the secondary vessel, initially uniformly filled with dust particles, is simulated. The gas phase is described by the standard equations and it is coupled with the particulate phase through the drag force and the convective heat transfer. No chemical reaction is considered in the model since the objective was to model the system up to the time of ignition. The computation was performed for different lengths and diameters (heights) of the linking duct. Having analysed the results, it was concluded that the simulations agree with experimental observations in that the probability of transmission of an explosion from the primary to the secondary vessel decreases with decreasing diameter (height) and increasing length of the connecting pipeline. Snapshots of particle positions for different times are presented. The work illustrates the behaviour of the mixture in the secondary vessel: the particles tend to concentrate in clouds, and domains with no particles are observed. This may influence the explosion characteristics of the system.

Keywords: Mathematical modelling; Two-phase flows; Lagrangian approach; Dust explosions; Interconnected vessels

1. Introduction

1.1. Dust explosions in interconnected vessels

In industry, processes with units connected via ducts are frequently encountered. The configuration of these is important not only for normal processes, but also where there is an explosion potential, which is the case for vessels filled with combustible gas or dust. This research is devoted to the problems of dust explosions, an important aspect, since most dusts or powders processed in industry are hazardous, and the physics of the phenomena involved in dust explosions guidelines is neither well understood nor thoroughly investigated.

A number of studies have been carried out [1] and guidelines on the prevention and mitigation of dust explosions have already been produced. However, as remarked by [2] most of the experimental results have been limited to relatively simple cases, like isolated vessels. In industry, as mentioned above, vessels are often linked by networks of pipes and the behaviour of explosions in such systems is practically unpredictable.

The most common method of explosion mitigation is using vents, and there are many techniques available to assess a safe vent area. These techniques may fail if dust cloud ignition in one vessel is generated by an explosion in another process unit. The conditions under which the secondary explosion takes place may be unknown. In many circumstances the explosion may be more severe than if the dust were ignited in an isolated vessel: when the flame passes through the pipe that connects the units, turbulence is generated, which leads to higher combustion rates. For longer pipes, the deflagration can be even transited to detonation [2,3].

Moreover, the ignition in the secondary vessel is realized by a jet of hot gases. In many cases this intensifies the process of combustion compared to an ignition by a standard spark discharge. Another important fact is that a primary explosion leads to a pressure rise in the whole system. Because of that, the secondary explosion begins in an above-ambient pressure and the resulting maximum pressure will be higher.

As mentioned by [2], a flow in the dust-air mixture generates concentration gradients, giving rise to rich and lean zones. The

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Nomenclature

c_s	heat capacity of the solid phase
C_D	drag force coefficient
d	diameter of a particle
E	total internal energy of the gas phase
$\vec{f}$	interphase force
f_{drag}	drag force
$\bar{F}, \bar{G}$	the vector of convective terms
$\bar{F}_V, \bar{G}_V$	the vector of diffusive terms
I	moment of inertia
k	energy of turbulent pulsations
l	turbulent length scale
m	particle mass
$\vec{M}$	torque acting on a particle
Nu	Nusselt number
p	pressure
P_t	probability that a particle encc
Q	interphase heat flux
Re_ω	rotational Reynolds number
$\bar{S}$	the vector of source terms
T	temperature of a phase
$\vec{u}$	velocity of a phase
u'_{rms}	root mean square of turbulent velocity fluctuations
$\bar{U}$	the vector of conserved variables

Greek letters

ε	dissipation of turbulent energy
ε_r	emissivity
λ	heat conductivity of the gas phase
μ	dynamic viscosity of the gas phase
ρ	density of a phase
σ	Stefan–Boltzmann constant
τ_{ij}	stress tensor
$\vec{\omega}$	angular velocity vector

Subscripts

g	the gas phase
k	current number of a particle
s	the solid phase

process of flame propagation is considerably influenced by these phenomena. It is important to note that the particles are not able to follow the streamlines of the gas due to their inertia, which is more pronounced for higher turbulent intensity.

There are not many experimental investigations into dust explosions in interconnected vessels in the literature. A probable reason is the difficulty and high costs of such experiments. Some are: [2,4–8].

In our recent paper [9], a model is described that is based the on so-called Eulerian–Eulerian approach, where the solid phase is modelled as a second fluid. This model, although able to model large regions and two-way coupling between the phases easily, has its drawbacks, such as difficulties in modelling particle–particle interactions. We used this model for simulating consequences of primary explosions in interconnected vessels.

Although an explosion in interconnected vessels may be more severe than one in a single process unit, experimental tests on explosions in linked systems have shown that the explosive dust suspension in secondary vessels does not necessarily ignite, as mentioned for instance by [8]. Actually this surprising observation has not been explained. However, it was noticed that the probability of transmission of the flame from a primary vessel to a secondary one depends on many factors: the volume of the primary unit, the properties of the combustible dust (in many publications described by the K_{st} parameter), the size of vents (if present), point of ignition, the presence of baffles and the type of the connection. The latter is described by the duct length and cross-section and this is what we researched in this paper.

1.2. Mathematical modelling of dust explosions

As mentioned by [5], experimental dust explosion research requires large-scale expensive test facilities.

An increasingly attractive alternative is to develop an accurate numerical simulation technique. Moreover, this approach makes it possible to investigate those phenomena that are impossible or extremely difficult to measure, such as the spatial distributions of parameters (e.g. dust concentration, combustion product concentration, velocity and temperature). Numerical simulation also makes it possible to set complex initial conditions or even switch off certain phenomena (for instance chemical reaction) to assess their effect.

Although numerical simulation has been gaining in popularity, unresolved problems remain, such as:

(a) a good description of the chemical reactions;
(b) a model for the interaction between the turbulence and the particles;
(c) a good model for interphase and particle–particle interactions.

It must be emphasized, however, that the existing codes have helped researchers to better understand the physics of the processes and sometimes predict the flame or blast waves propagation. Literature examples, where numerical simulation techniques have been used for simulating dust explosions, are [10–24].

1.3. The objective of this work

This paper is devoted to the problems of dust explosions in interconnected vessels where this process was researched using the mathematical modelling approach. The model that we adopted was similar to the models used by [12–13], where the Lagrangian approach for simulating the flow of the solid phase was used. Although this research involved dust explosion modelling, the combustion processes were not considered at this stage. The objective was to analyse what phenomena are responsible for the ignition of the dust in interconnected units by simulating the fluid flow and heat transfer.

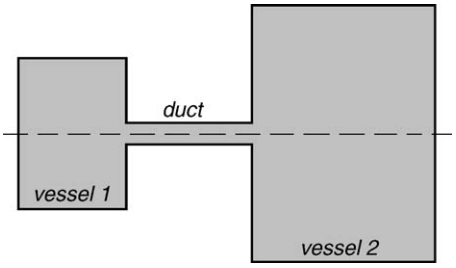

Fig. 1. The scheme of the computational domain.

It must be noted that there are virtually no references in the open literature devoted to the problems of computer simulations of dust explosions in interconnected vessels in spite of the importance, and the difficulties in conducting experimental research in this area.

2. Problem formulation

In most of the experimental papers mentioned above, the following type of case is considered: a dust-air mixture was ignited in a primary vessel and the flame was allowed to propagate through a duct to a second vessel, also filled with an explosive dust mixture. The objective was to investigate whether the transmission of the explosion, from one vessel to another, was possible and what value of the maximum pressure was obtained in the second unit. Different parameters were varied: the volumes of the vessels, the length and the diameter of the linking duct and the kind of dust. Additionally, [8] took into account the presence of baffles in the duct and investigated their influence (by additional turbulence generation) on the explosion process.

Such a case is also considered in this article; however the objective of this work was to carry out a numerical investigation of the problem and to compare the results with the experimental observations. A diagram showing the computational domain is shown in Fig. 1. The modelled structure consists of two vessels connected by a duct on a two-dimensional grid. The time saving resulting from carrying out 2D simulations made it possible to consider more cases so that more valuable conclusions could be drawn.

The initial conditions were as follows: the primary vessel was filled with hot gas under a high pressure. This modelled the situation where an explosion has occurred in the unit already. The objective was to observe if the explosion could be transmitted to another vessel and what influenced the process.

The second vessel was filled with dust particles distributed uniformly. They were modelled using the Lagrangian approach, i.e. the particles were modelled as points moving in the computational domain and tracked in time in the pre-calculated flow field by solving the Newton equations for the particles. Actually the moving particles can also influence the motion of the surrounding gas (so-called two-way coupling). For low concentrations, however, it is not of importance and in the present case the one-way coupling approach could be used.

Also the particles were subject to collisions between each other and with the walls. The hard-sphere model was chosen to describe the collisions. The temperature of the particles was allowed to change due to a difference of temperatures between the particles and the surrounding gas.

The exact description of the whole mathematical model can be found in the following section. According to [25] an explosion begins when the following conditions are fulfilled: presence of fuel, oxidant, ignition source, thorough mixing of the fuel and oxidant and confinement of the combustible mixture. In accordance with this, the following model was assumed in this paper. We decided on a particle temperature beyond which ignition was possible, and assumed that ignition would take place if a critical percentage of particles in a given region exceeded that temperature. In this research it was assumed that the ignition temperature was equal to 700 K. However, the combustion process itself was not modelled, aiming as we did at analysing the process up to the point of ignition to assess if and when an explosion would take place.

The linking duct was empty of particles in all the simulations. The length and the height of the linking duct varied in the simulations.

3. Model used

3.1. The mathematical model for the solid phase

For each of the particles, denoted by subscript k, the equations of motion and energy can be written in the following form:

$$m_k \frac{\mathrm{d}\vec{u}_{\mathrm{sk}}}{\mathrm{d}t} = \vec{f}_k \tag{1}$$

$$I_k \frac{\mathrm{d}\vec{\omega}_k}{\mathrm{d}t} = \vec{M}_k \tag{2}$$

$$\frac{\mathrm{d}T_{\mathrm{sk}}}{\mathrm{d}t} = \frac{1}{m_k c_{\mathrm{s}}} Q_k \tag{3}$$

where for the kth particle: m_k, I_k are the mass and moment of inertia; T_{sk} is the temperature; $\vec{u}_{\mathrm{sk}}$ the velocity; $\vec{\omega}_k$ the angular velocity; $\vec{f}_k$ the force acting on the particle due to interphase forces and collisions; Q_k the heat exchange rate between the particle and the surrounding fluid; $\vec{M}_k$ the torque acting on the particle due to collisions and due to shear stress on the particle surface; c_{s} the heat capacity of the solid phase.

In the following, we describe how the force $\vec{f}_k$, torque $\vec{M}_k$ and rate of heat exchange Q_k are evaluated. Firstly the force acting on each particle as a result of the gas phase. This force mainly consists of the drag force:

$$\vec{f}_k = \vec{f}_{\mathrm{drag},k} = \frac{\pi d^2}{8} C_{\mathrm{D}} \rho |\vec{u}_{\mathrm{g}} - \vec{u}_{\mathrm{sk}}| (\vec{u}_{\mathrm{g}} - \vec{u}_{\mathrm{sk}}) \tag{4}$$

where d is the particle diameter (the same for all the particles, but different diameters could easily be implemented); C_{D} the drag force coefficient (physically a function of the Reynolds number); ρ the gas density; $\vec{u}_{\mathrm{g}}$ the surrounding gas velocity.

One of the empirical formulas that can be used for the drag force coefficient is (by Schiller and Neumann):

$$C_{\mathrm{D}} = \frac{24}{Re}(1 + 0.15 Re^{0.687})$$

Actually, other forces can be also implemented, for example the Magnus force, the Saffman force, the buoyancy force, the body forces (e.g. gravity) and others. However, for this application, involving very high gas velocities, these forces can safely be neglected.

The torque due to the shear stress exerted on the particle by the fluid can be described using the following model [26]:

- for particle Reynolds numbers, corresponding to Stokes flow:

$$\vec{M}_k = \pi\mu d^3 \left(\frac{1}{2\nabla \times \vec{u}_g} - \vec{\omega}_k \right) \tag{5}$$

- for higher particle Reynolds numbers:

$$\vec{M}_k = -2.01\mu d^3 \vec{\omega}_k (1 + 0.201\sqrt{Re\omega}) \tag{6}$$

where Re_ω is a Reynolds number based on the angular velocity:

$$Re\omega = \frac{\rho|\vec{\omega}_k|d^2}{4\mu} \tag{7}$$

and μ is the gas viscosity.

Additionally, the force acting on each particle is also a result of collisions with other particles. For low dust concentrations, where the distance between particles is high, this effect is negligible. However, we implemented it into the computational code using the hard sphere model. Its detailed description for the three-dimensional case may be found, for example, in [26]. Heat transfer between the gas phase and the particles takes place due to a difference of temperatures between them. In this research it is modelled using the well known formula:

$$q = \pi d\lambda Nu(T_g - T_{sk}) + \pi d^2 \varepsilon_r \sigma (T_g^4 - T_{sk}^4) \tag{8}$$

where Nu is the Nusselt number; λ the heat conductivity; ε_r the emissivity and σ Stefan–Boltzmann constant and T_g is the surrounding gas temperature.

The formula for the Nusselt number was the following:

$$Nu = 2 + 0.6\sqrt{Re}\,Pr^{1/3}$$

where Pr is Prandtl number.

Modelling of turbulence for high-speed two-phase flows is not described in literature. There are some models, which originate only from experimental observations and do not describe a general case. However, for this research we wished only to estimate the effect of turbulence and therefore simple relations have been adopted as seen in the following. Our model is similar to the model mentioned in [13].

The root mean square of turbulent velocity fluctuations u'_{rms} was assumed to be equal to 10% of the mean speed of the gas flow (this is typical for many pipe flows). The turbulent length scale, l, was assumed equal 0.1 m. The flow was treated as isotropic and therefore the energy of turbulent fluctuations may be written as:

$$k = \tfrac{3}{2} u'^2_{rms} \tag{9}$$

The dissipation of the energy was modelled as:

$$\varepsilon = \frac{u'^2_{rms}}{l} \tag{10}$$

The probability that a particle encounters a new eddy:

$$p_t = 1 - \exp\left(-\frac{\varepsilon}{k} dt\right) \tag{11}$$

where dt is a time step

A gas fluctuation that interacts with a particle, and influences its change of velocity, is taken randomly from a Gaussian distribution, with the root mean square of turbulent velocity fluctuations as the standard deviation.

The above model was being modified and adjusted during the research, but this led to only slightly different results.

3.2. The mathematical model for the gas phase

The mathematical model for the gas phase is similar to a model used by us in [9]. We repeat the model here, however, since there are some differences.

The system of equations for the gas phase can be written in the following way (for the two-dimensional case):

$$\frac{\partial \bar{U}}{\partial t} + \frac{\partial(\bar{F} - \bar{F}_V)}{\partial x} + \frac{\partial(\bar{G} - \bar{G}_V)}{\partial y} = \bar{0} \tag{12}$$

where $\bar{U}$, $\bar{F}$, $\bar{G}$, $\bar{F}_V$, $\bar{G}_V$ are vectors: $\bar{U}$ is the vector of conserved variables; $\bar{F}$, $\bar{G}$ are the vectors containing convective fluxes; $\bar{F}_V$, $\bar{G}_V$ is the vector containing diffusive fluxes:

$$\bar{U} = \begin{bmatrix} \rho \\ \rho u_g \\ \rho v_g \\ \rho E \end{bmatrix}; \quad \bar{F} = \begin{bmatrix} \rho u_g \\ \rho u_g^2 + p \\ \rho u_g v_g \\ \rho u_g (E + p) \end{bmatrix}; \quad \bar{G} = \begin{bmatrix} \rho v_g \\ \rho u_g v_g \\ \rho v_g^2 + p \\ \rho v_g (E + p) \end{bmatrix};$$

$$\bar{F}_V \begin{bmatrix} 0 \\ \rho\tau_{xx} \\ \rho\tau_{yx} \\ \rho u_g \tau_{xx} + \rho v_g \tau_{xy} \end{bmatrix}; \quad \bar{G}_V = \begin{bmatrix} 0 \\ \rho\tau_{xy} \\ \rho\tau_{yy} \\ \rho u_g \tau_{yx} + \rho v_g \tau_{yy} \end{bmatrix} \tag{13}$$

In (13) the following notation has been used: u_g and v_g are components of the gas phase velocity in x- and y-direction (the components of the vector $\vec{u}_g$); E is the total energy of the gas phase (including both kinetic and internal energies); p is the pressure; τ_{ij} is the stress tensor.

The system of Eq. (12) corresponds virtually to the standard equations of conservation, because one-way coupling was used in this research. Otherwise it would have been necessary to include the terms describing the action from the solid particles as well.

3.3. The numerical scheme

The computational grid was divided into a series of rectangular elements. The values of the gas parameters (density, velocity components, pressure and temperature) were written in the cell centres. The parameters of all the particles (position, velocities,

temperature) were stored. In each time step the new values of gas and particle properties in the cells were calculated using numerical techniques outlined below. The transition from one time step to the next one can be written in the following sequence:

$$\bar{U}^n \rightarrow \Lambda^{(1/2\Delta t)} \rightarrow \Phi^{(\Delta t)} \rightarrow \Lambda^{(1/2\Delta t)} \rightarrow \bar{U}^{n+1} \tag{14}$$

where: $\bar{U}^n$ describes the values of parameters in the previous time step; $\Lambda^{(1/2\Delta t)}$ describes the computation of the interphase mechanisms for half of the time step; $\Phi^{(\Delta t)}$ describes the flow of the gas phase during the full time step; $\bar{U}^{n+1}$ describes the parameters in the new time step.

The two main operators Λ and Φ are described below.

3.3.1. The operator A

The operator Λ symbolizes calculation of new particle velocity, rotation rate and temperature by Eqs. (1)–(3). The equations are written in the following manner:

$$\frac{\partial \bar{U}_k}{\partial t} = S_k(\bar{U}_k) \tag{15}$$

where (for the two-dimensional case):

$$\bar{U}_k = \begin{bmatrix} u_{sk} \\ v_{sk} \\ T_{sk} \\ \omega_k \end{bmatrix}; \qquad \bar{S}_k = \begin{bmatrix} \dfrac{f_{k,x}}{m_k} \\ \dfrac{f_{k,y}}{m_k} \\ \dfrac{Q_k}{m_k c_s} \\ \dfrac{M_{k,z}}{I_k} \end{bmatrix} \tag{16}$$

where for the kth particle: u_{sk} and v_{sk} are the components of the particle velocity in x- and y-direction; $f_{k,x}$ and $f_{k,y}$ are the components of the drag force; ω_k is the z-component of the angular velocity (the x- and y-components of the vector $\vec{\omega}_k$ are equal to zero for a two-dimensional case) and $M_{k,z}$ is the z-component of the torque. Eq. (15) were solved using the VODE solver described in [27].

3.3.2. The operator Φ

The simulation of the gas phase flow involves the solution of Eq. (12). The numerical scheme for this begins with discretizing them using the Godunov scheme (see e.g. [28]):

$$\begin{aligned} \bar{U}_j^{m+1} = \bar{U}_j^m + \frac{\Delta t}{\Delta x}[(\bar{F}_{(j-(1/2),k)} - \bar{F}_{V(j-(1/2),k)}) - (\bar{F}_{(j+(1/2),k)} \\ - \bar{F}_{V(j+(1/2),k)})] + \frac{\Delta t}{\Delta y}[(\bar{G}_{((j,k-(1/2))} - \bar{G}_{V(j,(k-(1/2))))} \\ - (\bar{G}_{(j,(k+(1/2)))} - \bar{G}_{V(j,(k+(1/2)))})] \end{aligned} \tag{26}$$

for: $j = 1, \ldots nx$; $k = 1, \ldots, ny$; and m indicates the time step.

In the scheme $\bar{F}$, $\bar{G}$ (defined above by Eq. (13)) constitute fluxes. Their values at the cell interfaces are based on solving the Riemann problem between two adjacent cells, a problem that is well known in gas dynamics. The main advantage of this scheme is the possibility of resolving high gradients typical for high-speed flows and shock waves.

The vectors $\bar{F}_V$, $\bar{G}_V$ are diffusive fluxes and have been defined above, in Eq. (10). In the numerical scheme they are written in a simple finite difference manner using parameters from adjacent computational cells.

4. Results

The following parameters were varied in the simulations:

- the length of the linking duct: 5 or 15 m;
- the height of the linking duct: 0.15 and 0.5 m.

In this way, four cases were considered. The parameters that were kept constant for all the simulations were as follows: the initial temperature and the pressure in the primary vessel: 8 bar and 1600 K, respectively; the particle diameter: 90 μm; the particle material density: 1000 kg/m^3; the volume of the primary vessel: 20 m^3 and the volume of the secondary vessel was 18 m^3. The dust concentration in the secondary vessel was 0.3 kg/m^3, which was obtained by a proper uniform distribution of solid particles. Because the modelled process is two-dimensional, the volumes are found assuming a unit length (1 m) in the perpendicular direction. The initial pressure wave generated after the primary explosion is moving in the duct with the Mach number equal to 2.2.

To simulate turbulence each of the particles were initially given a random velocity in a random direction. The speed was from the range: (0, 1) m/s. Other values were also tested, but this did not influence the final results considerably.

The above data corresponded to experimental parameters presented by [8]. The main conclusions that were drawn from their experiments:

- the probability of ignition in the secondary explosion depends on the type of dust (not applicable to our work, where we used the same dust in all simulations);
- the probability of ignition decreases when the duct diameter decreases;
- the probability of ignition increases when the duct length decreases (this relation is not as strong as the previous one);
- the probability of ignition depends on the volumes of the vessels (not applicable to our work, where we used the same geometry in all simulations).

Similar conclusions have been drawn by other researchers.

The physical process was as follows: the hot gases enter the secondary vessel and as a result the particles begin to move and their temperature increases. If the temperature of a particle exceeds a limiting value, the particle will start to burn. Burning of a single particle does not necessarily lead to an explosion, since this requires simultaneous burning of many particles so that the probability of further spontaneous propagation is high enough. To investigate the process, the strategy of counting the "burning" particles was used, descried in Section 2. The percentage of particles, with temperature greater than 700 K, is presented as a function of time in Figs. 2 and 3 for duct lengths of 5 and

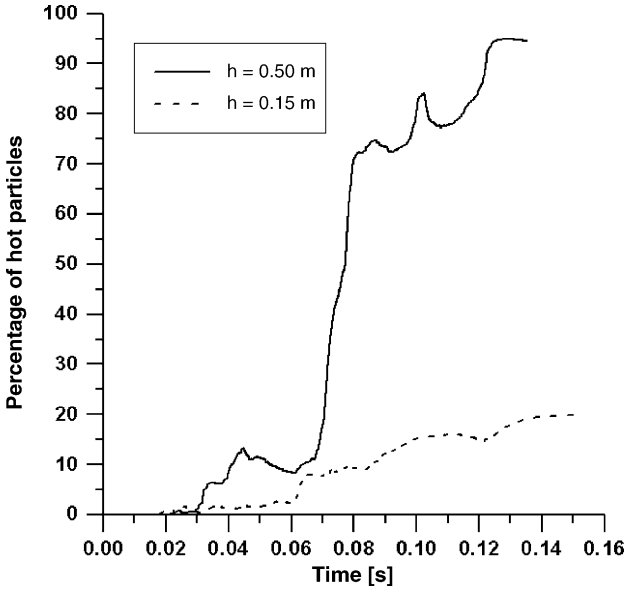

Fig. 2. Percentage of the burning particles as a function of time for the duct length equal to 5 m.

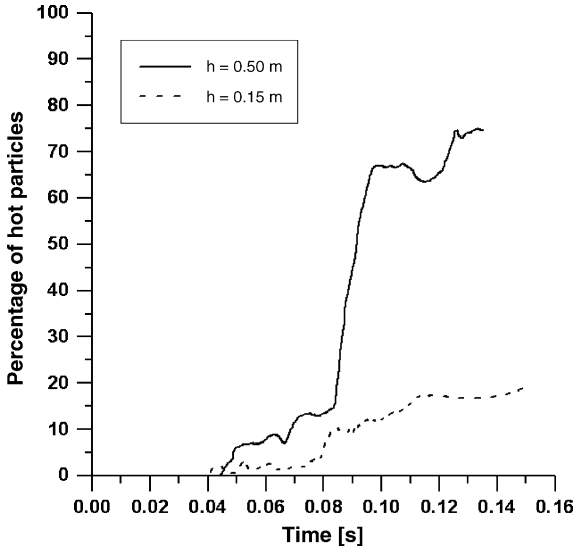

Fig. 3. Percentage of the burning particles as a function of time for the duct length equal to 15 m.

15 m, respectively. The curves in the graphs correspond to two different duct heights.

We see from the figures that at the very beginning the size of the connecting tube does not seem to influence the process and the number of hot particles is more or less the same in all the cases. After a few milliseconds, however, a clear trend is observed: the bigger diameter of the duct leads to increased number of hot particles. If one compares the lengths of the tube (compare Fig. 2 with Fig. 3), one can notice that the length is not of great importance in the case of the duct height 0.5 m, but it is crucial for the height of 0.15 m. Nevertheless, it is in both cases clear that the percentage of the hot particles is lower for the longer tube.

Similar conclusions were drawn in our previous work [9], where another simulation technique was used.

The whole process is illustrated in detail in Figs. 4–7 as snapshots of particle positions for two points in time: 30 ms and 50 ms after the rupture of the "diaphragm" between the primary vessel and the duct. All the cases (for different duct heights and lengths) are shown.

In all the cases the dust tends to locate in clouds with higher concentration and large "void spaces" are the result. The same was mentioned by [2]: "Turbulent flow in dust-air mixtures is likely to generate strong concentration gradients, giving rise to rich and lean zones. They may have considerable influence on the propagation mechanisms of turbulent dust explosions. The dust particle cannot always follow the streamlines of a turbulent flow [. . .]. [In experiments] symmetrical zones of lean and rich coal dust were observed". These "void spaces" may result in a decreasing probability of ignition.

Also in [25] factors are discussed that affect the rate of heat release during a dust explosion. They are the chemical compositions of the dust and the gas, the particle size and shape distributions, the distribution of initial and explosions-induced turbulence, as well as issues like the degree of dust dispersion/agglomeration and the distribution of dust concentration in the cloud. The latter factors correspond to our findings that

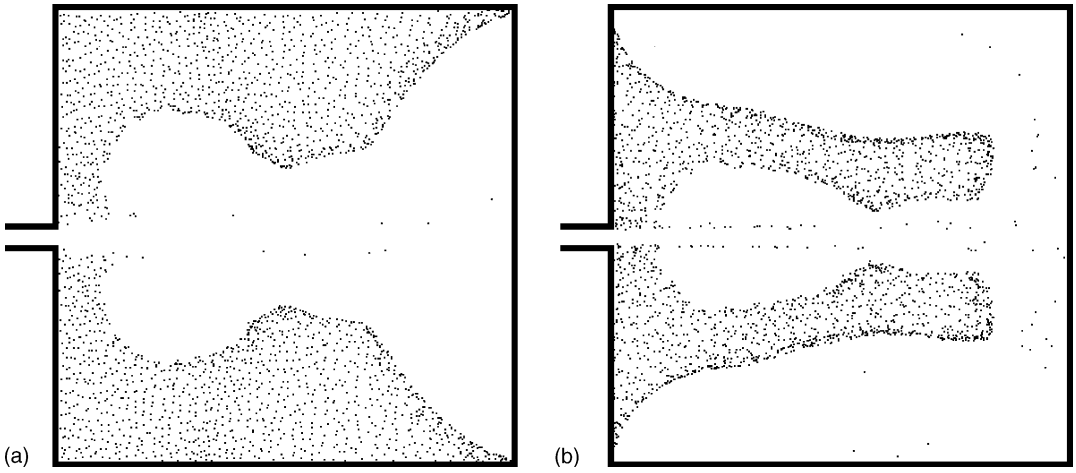

Fig. 4. Snapshots of particle distribution for different moments in time: (a) 30 ms; (b) 50 ms. Duct height and width: 0.15 m and 5 m, respectively.

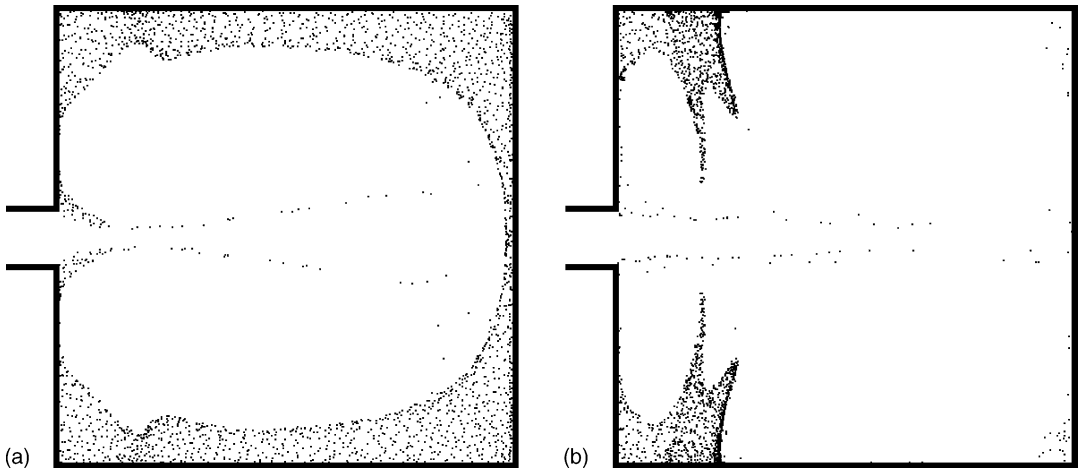

Fig. 5. Snapshots of particle distribution for different moments in time: (a) 30 ms; (b) 50 ms. Duct height and width: 0.5 m and 5 m, respectively.

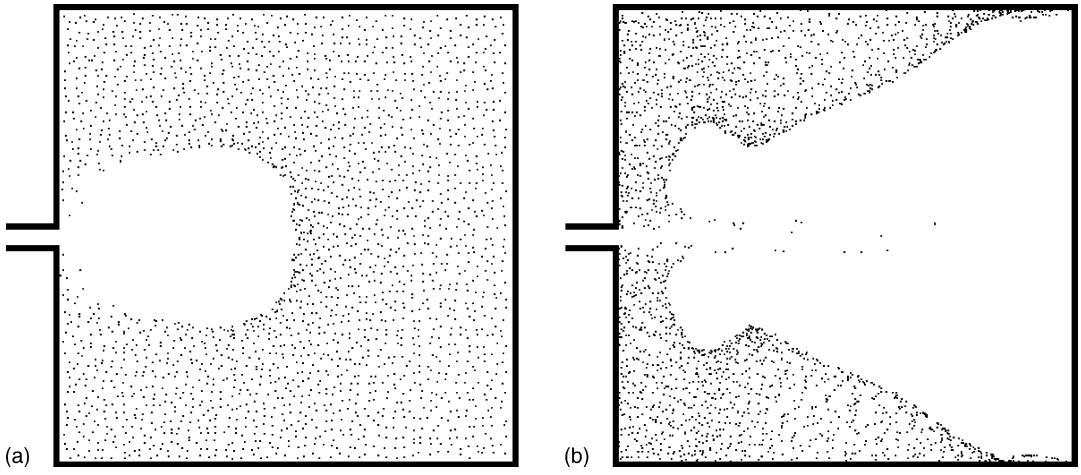

Fig. 6. Snapshots of particle distribution for different moments in time: (a) 30 ms; (b) 50 ms. Duct height and width: 0.15 m and 15 m, respectively.

the creation of "void spaces" hinders an explosion, while a local increase of dust concentration increases the probability that a flame may propagate through it that region.

In [29] a review of other works is presented where a similar phenomenon had been observed: particles tend to cluster the edges of vortices. Later Portela and Oliemans [30], who analysed dispersion of particles and their deposition and re-suspension at walls, observed and discussed the same issue. Just like in our research, they started their simulations with particles uniformly distributed in a computational domain. Actually in our

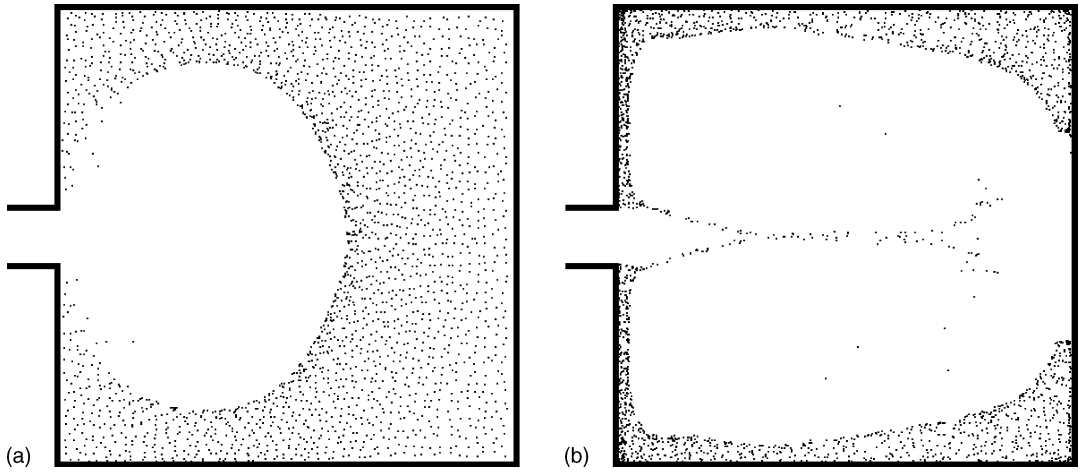

Fig. 7. Snapshots of particle distribution for different moments in time: (a) 30 ms; (b) 50 ms. Duct height and width: 0.5 m and 15 m, respectively.

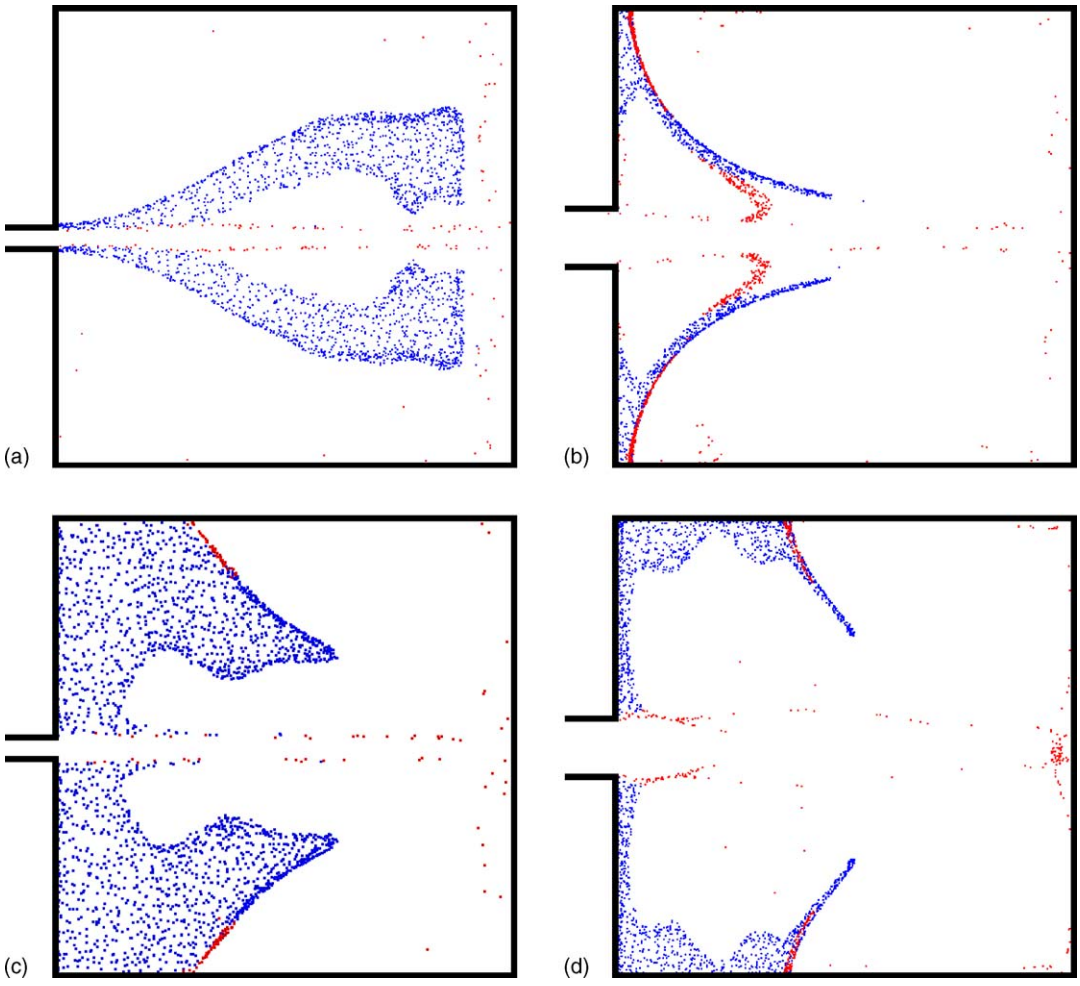

Fig. 8. Snapshots of particle distribution after 60 ms. The red filled circles denote particles whose temperature is higher than 500 K. Duct height and width: (a) 0.15 m and 5 m; (b) 0.5 m and 5 m; (c) 0.15 m and 15 m; (d) 0.5 m and 15 m.

research, clustering is due to a jet of air entering from a void region, whereas they describe centrifuging of particles to edges of swirls in initially uniform suspensions. Nevertheless, there exists a similarity.

The area of the void regions is a function of the size of the connecting duct: the greater the duct height, the bigger area of these regions (compare for instance Fig. 4b and Fig. 5b). It is clear that one cannot assume that the dust is uniformly distributed within the secondary vessel during flame propagation, as it is done in some fundamental mathematical models, where the flame is assumed to propagate spherically from the ignition source. Actually the propagation of the flame is likely to be much more complex. The concentration of dust influences also the explosion risk. Even if the initial uniform dust concentration is below the lower explosion limit, an ignition may still occur: the dust particles may form clouds wherein concentration is above the explosion limit. This may be one of the reasons why it is more difficult to ignite the mixture in the secondary vessel for smaller diameters of the connecting ducts in experiments. The size of the connecting duct affects for the speed of the process especially strongly. The process is the slowest for the longer tube with the smaller diameter: the mixing process is less intense and the temperature rise of the particles is moderate. The latter can lead to quenching of the combustion reaction due to heat exchange with cold walls of the vessel and the duct. This factor was not included in the model used in this research, and we are planning to consider this in subsequent studies.

The size of the jet influences the probability of the explosion: the number of hot particles is increased and they are also pushed to form clouds with higher concentration. This leads to higher probability of an explosion. Fig. 8 presents the position of the particles for a time of 60 ms, for the four cases. The particles shown in the figures are coloured: red denotes particles whose temperature is higher than 500 K.

These figures make it possible to analyse the location of the "hot" particles. It can be seen that the "burning" particles are in the vicinity of each other, which increases the probability of an explosion. Comparing Fig. 8a and b, as well as c and d, a conclusion can be drawn: the number of hot particles is higher for the pipeline height 0.5 than for 0.15. This remark agrees the above discussion and to experiments.

In ref. [31] some experimental results are presented related to flame front propagation between interconnected process vessels. A primary explosion is realized by the ignition of a dust-air or gaseous fuel-air mixture. The resulting speed of hot gases in the connecting pipe is measured, and a set of empirical models is

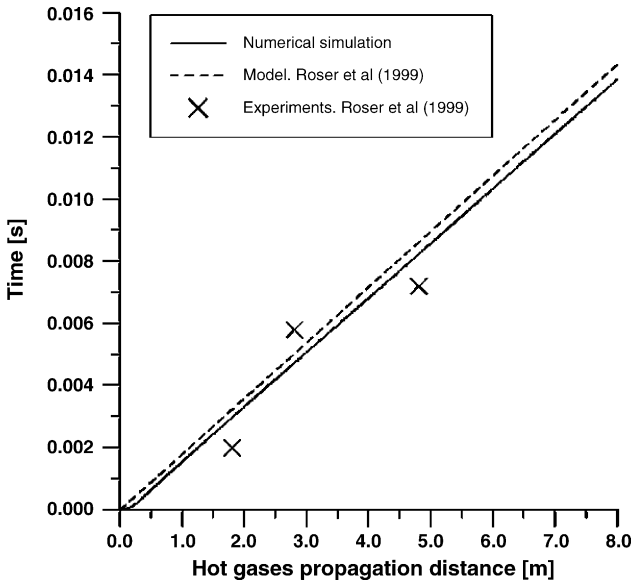

Fig. 9. Hot gases propagation distance history in a pipe. Comparison with experiments.

proposed. We decided to compare our model and computer code with one of their experimental results, namely an explosion of a three percent propane-air mixture that resulted in a maximum absolute pressure 7.37 bar. The primary vessel had a volume 1 m^3, the diameter of the connecting pipe was 100 mm and its length 8 m.

The comparison is shown in Fig. 9 as the propagation distance history of the hot gases for three cases: (a) our numerical simulation; (b) a model presented in [31]; (c) the experimental results presented in [31]. It is clear that the results of the simulations agree very well with the other data.

5. Concluding remarks

In order to estimate the probability of ignition, the particles in the secondary vessel whose temperature exceeded a specified value 700 K were counted and the percentage of such particles was evaluated as a function of time. It was found that this probability strongly depends on the duct length and height: the probability increases when the height increases and the length decreases. In this research, it was not feasible to assess the limiting percentage that will definitely lead to an explosion. Nevertheless, the probability could be estimated qualitatively and it was found to agree with experiments. The model proposed in this paper describes reality in spite of the fact that it is based on some assumptions. Moreover, we have managed to find a probable reason why it is not always possible to ignite a dust mixture in the secondary vessel: the particles form clusters with high concentration and thus, many "void regions" are created.

During this research a couple of problems were encountered and we are planning to consider them in subsequent studies. The first is that only one gas species was taken into account. Probably it would be better to distinguish oxidiser and products of combustion. If this can be achieved we can better estimate which of the particles satisfying the ignition condition will actually ignite. Moreover, the density of the gaseous phase would be better calculated and this would influence the value of the drag force acting on the particles.

The second problem is the one-way coupling assumption. This assumption may be used for flows with low dust concentrations. During this research it was proven that domains with relatively high dust concentration are present.

The third problem refers to the initial distribution of pressure. In this research we assumed that the pressure in the primary vessel after the explosion was uniform. Generally this is not true since after an ignition of a combustible mixture, a flow of gas from the vessel to the duct begins and this process continues during the explosion leading to a pressure drop in the primary vessel and a pressure rise in the duct and later in the secondary vessel.

The last issue was the absence of chemical reaction in the model. The modelling of combustion is time consuming due to the necessity of resolving the flame on the computational grid (not feasible for large-scale simulations). According to e.g. [25] there are three distinct mechanisms of particle burning: (1) devolatilization and burning of volatiles followed by combustion of solid residue (for organic dusts); (2) melting followed by evaporation and subsequent vapour burning (for plastics); (3) evaporation through a solid oxide shell followed by burning outside the shell (for metals). This makes the issue of simulating combustion numerically extremely complex. We have analysed the process up to the point of ignition, and will leave the issue of modelling the subsequent combustion process to further studies.

In this research we have compared our results with the available data describing the explosion transmission between two vessels. In the subsequent studies we aim at analysing more sophisticated geometries, especially ones where experiments are not feasible or are expensive.

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