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CFD to Improve the Repeatability and Accuracy of Dust Explosion Tests in the 20-liters Sphere

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The experimental characterization of combustible dusts is usually associated to several uncertainty factors that rely on the physical properties of the powder and the operating conditions of the standardized tests (e.g. the ignition time, the dispersion nozzle and pressure). These parameters affect the repeatability of the flammability tests and the precision, or even the accuracy, of their results. In this regard, an explanatory study has been focused on the description of the dispersion process of a combustible dust inside a 20-liters sphere by joining two complementary approaches. At first, a Computational Fluid Dynamics simulation (CFD – Star CCM+) based on an Euler-Lagrange scheme was set according to the geometry and operating parameters that have been established for this equipment through international standards. The predictive results that were determined with this approach were compared with a Particle Image Velocimetry analysis and in-situ measurements. Explosions tests were also performed to validate our analyses.
The results showed how the particle size distribution of the dust affects its dispersion trajectories inside the sphere due to the inertial effects and the drag force exerted by the fluid. Furthermore, the analysis of the velocity field and turbulence intensity reveals that the dispersion process can be divided into three different stages, each related to a different repeatability. Tests performed with the classical rebound nozzle have clearly evidenced their effect on the internal distribution of the gas flow and the segregation levels of the disperse dust.
These facts suggest that the homogeneity assumption that is usually considered for the dust dispersion is obviously invalid. As a consequence, the operating conditions should be adapted to the physical properties of each combustible powder in order to improve both tests accuracy and precision. For this purpose, CFD simulations have been proven to be a useful tool to identify the most suitable conditions to perform this analysis and obtain the most conservative information about the reactivity of the dust as well.

1. Introduction

A dust explosion is one of the major hazards that are envisaged in the industrial facilities that handle organic or metallic powders. This type of incidents constitutes an aspect of main interest in the development of the process safety protocols in the industry due to the severe consequences that it might represent for the industrial facility and its surroundings. For this reason, the ignitability and severity of a combustible dust cloud are usually determined through the development of laboratory tests. These methods identify the flammability parameters of a combustible dust cloud generated under conditions that are fixed by the international standards. The 20-liters sphere is one of the most widely used apparatus designed for this purpose (ISO 6184-1, 1985). This set-up determines the minimum explosible concentration of a dust, the maximum pressure rise of a dust explosion and the corresponding deflagration index called K_{st}.
Moreover, the combustion of a dust cloud differs significantly from the combustion of a flammable mixture composed by gases or vapors. The differences between these chemical processes mainly rely on the physics of generation and up-keeping of dust clouds and the conditions of the flame propagation (Eckhoff, 2006). For

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this reason, the flammability tests that are designed for the characterization of combustible materials should be adapted for the solid materials. This adaptation should provide the most conservative and accurate information about the materials' ignitability and severity of dust explosions. For this purpose, the test methods must take into account the physical and chemical properties of a dust as well as their effects on the phenomena that define the flame propagation.
In accordance with this statement, this paper describes the development of the dust cloud that is generated during a typical flammability test performed with the 20-liters sphere. This study focuses on the time elapsed between the dose of the dust-air mixture and the ignition of the cloud. Thereupon, the description of the transient flow will establish the variations of the conditions of the two phases that have a direct influence on the experimental data that constitutes the flammability parameters of the dust. This analysis was performed by developing two complementary approaches. At first, computational fluid dynamics (CFD) simulation established the transient behavior of the two phases in the particle-laden flow. It was then supported by an experimental study that has performed a quantitative analysis that identified the variations of the turbulence levels of the dust-air mixture.

2. Experimental set-up

The 20-L sphere is a standard apparatus constructed in stainless steel and designed to characterize the explosibility parameters of combustible dusts and gases. This vessel consists of a dispersion system that is composed by a dust storage canister, a solenoid valve and an injection nozzle (ISO 6184-1, 1985). The experimental approach was developed with a new prototype that was constructed to visualize the evolution of the dispersion of the confined cloud. The structure of the new dispersion sphere was built with an internal geometry that is very similar to the standard 20-liter sphere. Nevertheless, some modifications were included in the design of this vessel to make it suitable for a dispersion analysis. For this purpose, five windows have been placed in the structure of the chamber to provide several points for the visualization of the dust cloud. There are four circular windows located at the lateral 'extremes' of the apparatus and another one on the top of it (Figure 1).

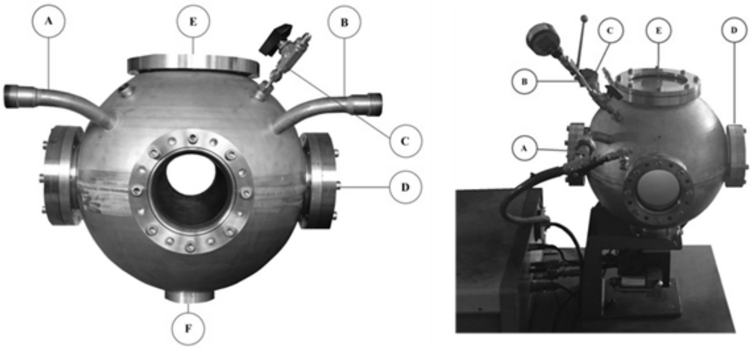

Figure 1: Dispersion sphere. A) Vacuum B) Venting C) Valve for manometer D) Lateral window E) Superior window F) Tube for the outlet valve

The variations of the velocity field in the geometric center of the 20-liter sphere were analysed by developing a Particle image velocimetry (PIV) analysis. This method coupled a continuous wave laser (laser sheet) to a high-speed video camera by using the lateral windows of the dispersion vessel. The contrast of the recorded images was enhanced by placing an additional light source over the superior window. The settings of the camera were adjusted to visualize a region of 3.0 x 3.0 cm with an image resolution of 480 x 480 pixels. These parameters allowed recording the dispersion process of the powder at a framerate of 6,410 fps (0.156 ms). This descriptive analysis was performed with micrometric wheat starch. This is an organic combustible dust that is considered as a very cohesive material. In fact, a dust cloud of this powder is submitted to significant variations of the particle size distribution during the flammability tests due to the agglomeration and fragmentation phenomena. For this reason a preliminary characterization was carried out to determine the dispersibility of the powder (Murillo et al., 2015). The results pose that the largest aggregates of a wheat starch sample have a fluidization behaviour similar to a powder of type A in a Geldart classification (easy fluidization). Nevertheless, smallest agglomerates of wheat starch might be in a transition zone between the types A and C (Table 1). This fact implies that such particles are susceptible to cohesion mechanisms.

Table 1: Particle size distribution and Geldart classification of micrometric wheat starch used in this study

Cumulative mass fraction	Diameter (µm)	Geldart classification
10%	28.2	C
16%	36.9	A-C
50%	65.2	A
84%	80.7	A
90%	83.1	A
99%	86.6	A

3. Experimental approach

The turbulence of the multiphase flow developed between the beginning of the dust dispersion and the ignition of the cloud is denominated as the initial turbulence of the cloud. The influence of this variable on the flammability parameters of a combustible dust can be evidenced through the analysis of the experimental data obtained at different ignition delays. The test methods carry out the dispersion of the dust with an air blast. This fact creates a two-phase flow from a finite source of kinetic energy. Therefore, the initial turbulence varies for the experiments performed at different ignition delays even if they are carried out in the same vessel with the same dust. Furthermore, a high initial turbulence can induce a quenching effect on the ignition phenomenon. The ignition of a dust cloud is clearly affected by the flow turbulence because it disturbs the heat transfer by removing heat from the ignition zone (forced convection). In addition, the initial turbulence has a significant effect on the particle size distribution by enhancing the stresses exerted by the fluid flow on the aggregates surface (Weiler et al., 2010). Finally, the initial turbulence has an impact on the front flame development and its stretching. For these reasons, the variations of the turbulence levels at the ignition point were determined through the flow visualization that was developed with the PIV analysis.

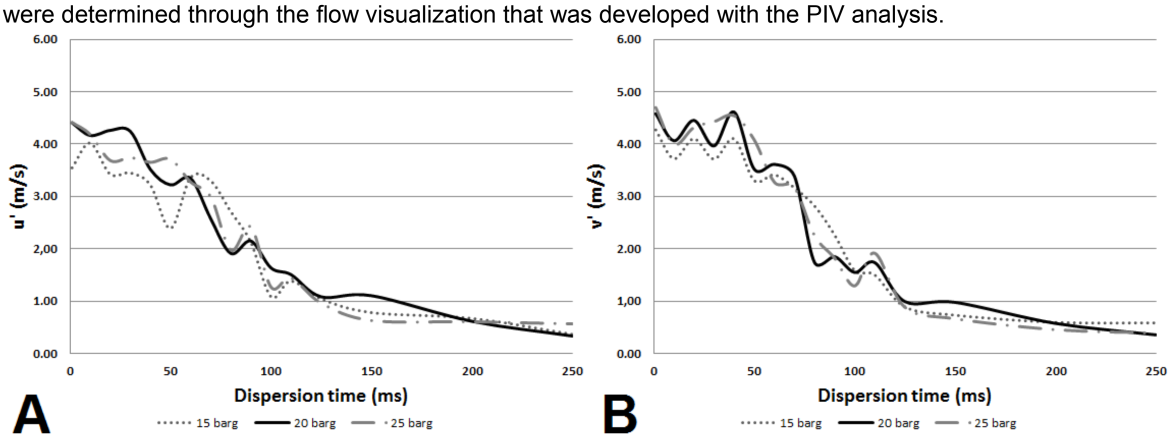

Figure 2: Fluctuations of the velocity field in the geometric centre of the 20-L sphere A) Horizontal component B) Vertical component

During the initial stage of the dispersion process, the bulk of the dust cloud was characterized with a high turbulence (Figure 2). This condition remained during the first 50 milliseconds. For this time lapse, the vertical fluctuations were slightly greater than the horizontal ones. This turbulent phase is characterized by the presence of aerodynamic stresses that are induced by the high velocities of the air pulse. These stresses constitute the significant levels of dust fragmentation that are usually observed in dust clouds formed by dispersion of cohesive materials (Murillo et al., 2015). This phase is characterized by a low repeatability of the explosion tests. For instance, Proust et al. (2007) established that the gaps of the maximum pressure rise and the maximum rate of pressure rise are usually ±3% and ±10% in the 20-L sphere. Afterwards, a decrease is evidenced because the most of the pressurized gas is injected during the first 60 ms of dispersion and the internal flow develops within the vessel. Finally, the particle-laden flow has dissipated the most of its kinetic energy and the agglomeration and sedimentation phenomena overcome the effects of the aerodynamic stresses. A similar decay ratio was determined by Dahoe et al. (2001) with anemometry tests. This author determined that the RMS of the velocity fluctuations have a stabilization period that establishes after 150 ms. For this final time lapse, the turbulence levels constitute a diminution of the uncertainty of the experimental

data of the flammability test. For instance, some experimental tests performed with wheat starch at 110 ms posed a variation below 3% for P_{max} and below 12% for dP/dt_{max}.
The ignition of the dust cloud in early periods represents a decrease of the particle size distribution and high kinetic energy dissipation. Otherwise, long ignition delays favour the sedimentation and agglomeration of the dust as well as the presence of low turbulence levels. Evidently, the experimental results of the flammability tests may vary significantly if the ignition delay is modified. For this reason, a computational approach was developed as a complementary analysis for this study in order to describe the variations of the turbulence levels within the 20-liters sphere and, in the medium term, to develop predictive models that allow choosing the most conservative conditions for explosion tests.

4. Computational Fluid Dynamics (CFD)

The computational approach of this study was developed with a CFD transient simulation based on an Euler-Lagrange approach. The calculation of the physical equations that describe the behaviour of the two-phase flow was carried out with the software STAR CCM+ v9.02.007. The two phases are modelled in two different ways according to the characteristics of an Euler-Lagrange approach. At first, the description of the gas flow within the flow domain has been performed with the Detached Eddy Simulation (DES) solution model. This turbulence model is characterized by the implementation of a RANS model on the regions located near the internal walls and the LES model on the fine cells that are away from the walls (Mockett, 2009). Thereupon, the turbulence model defines the turbulence model according to the mesh size. The length of the finite-volume cells varies between 1.10×10^{-5} and 8.83×10^{-3} m. The numerical scheme of the simulation was calculated according to the UPWIND spatial discretization, which is a first-order method. In addition, the time discretization corresponds to a second-order scheme.

4.1 Description of the flow domain

The flow domain consists of two different bodies that represent the pressurized canister and the dispersion sphere. These two regions are shown in Figure 3. They were divided in a mesh composed by 11,190,676 polyhedral cells and 77,519,960 faces. The refinement of the mesh was required for the regions that are characterized by their irregular shape and a transonic flow. For this reason, the first mesh layer of the surroundings of the rebound nozzle was divided in cells that are 0.017 mm long and whose surface size ranges between 0.2 and 0.5 mm. A similar refinement was required for other critical zones such as the interface of the two bodies and the rods of the ignition source (electrical fuse or chemical ignitors).

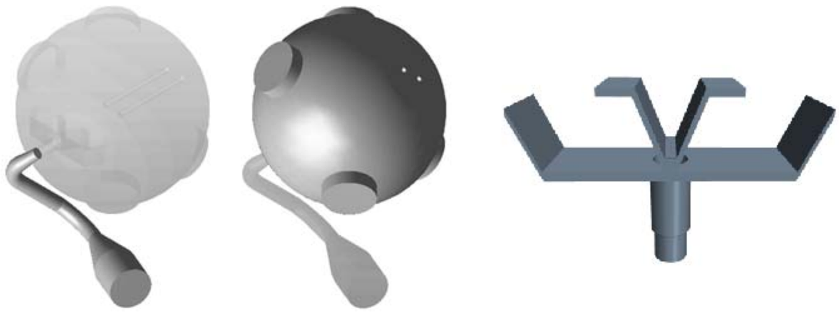

Figure 3: Computational flow domain. A) Body 1: canister B) Body 2: Dispersion chamber C) Rebound nozzle

The solid phase corresponded to a sample of 0.6 grams of wheat starch that were represented by 1.12 millions of parcels. This discrete phase was described with the numerical integration of a momentum balance established for every single particle. For this balance, the main forces that were taken into account corresponded to the gravitational acceleration, the drag and shear lift exerted by the gas and the pressure gradients of the flow. These forces are described by the following expression:

$$F = \frac{1}{2} C_d \rho A_p \left| v_s \right| v_s - V_p \nabla P_{static} + 1.615 d_p^2 \left(\rho \mu \right)^{0.5} \left| \frac{\partial v}{\partial y} \right| v_s \quad (1)$$

Where C_d is the drag coefficient defined by the Schiller-Naumann correlation, ρ and μ are the density and viscosity of the gas, v is the gas velocity, v_s is the slip velocity, d_p, A_p and V_p are the diameter, the projected area and the volume of the particle, P_{static} is the thermodynamic pressure of the gas and y is the direction of the velocity gradient.

4.2 Initial and boundary conditions

The initial and boundary conditions of the two bodies that compose the flow domain were defined according to the technical parameters of the standard apparatus (ISO 6184-1, 1985). This fact implies that the absolute pressure of the canister and the dispersion chamber are 21 bars and 0.4 bars respectively. In addition, the temperature was set to 300K for the whole domain in order to represent the environmental conditions of the laboratory. Finally, the gases were quiescent before dust dispersion. Thus, the velocity field and the turbulent kinetic energy were null at the initial time of the simulation.

Moreover, the two bodies of the flow domain also differ from each other due to their boundary conditions. The canister consists of adiabatic walls. The walls of the dispersion chamber were defined with a temperature condition equal to 300K to represent the heat transfer of the cooling water that surrounds the spherical vessel. However, all the walls of the domain were defined with a no-slip condition for the gas flow and a rebound condition for the solid particles with a normal restitution coefficient equal to 0.25 and a shear restitution coefficient equal to 0.20. These parameters were defined according to the cohesive behaviour of the wheat starch that is characterized by a Poisson's ratio equal to 0.3.

5. Computational results

The results obtained with the computational analysis establish the influence of the geometry of the dispersion nozzle on the development of the dust cloud. Figure 4 shows that the rebound nozzle defines a non-homogeneous two-phase flow within the sphere. The nozzle holes create three jets that distribute the flow within the spheres towards two of the four lateral extremes of the dispersion chamber. This condition represents a segregation phenomenon of the combustible dust in the sphere. This heterogeneity has also been recorded by high-speed cameras. For this reason, it should be considered that the minimum explosible concentration of the dust that is determined during a flammability test differs significantly from the nominal concentration that is usually considered.

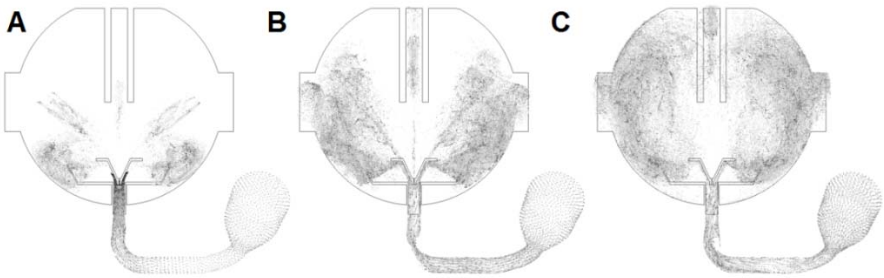

Figure 4: Development of the injection jets within the 20-liters sphere. A) 1 ms B) 2ms C) 3 ms

Furthermore, this scheme also shows us the regions where the turbulence favours the fragmentation mechanisms of the combustible dust. Kalejaiye et al. (2010) established that the reduction in particle size is mainly attributed to the shear stresses exerted on the aggregates during their pass through the outlet valve rather than the impaction against the injection nozzle. In other words, the high velocity of the particle-laden flow through the valve is the main responsible of the reduction in the particle size and not the collisions with the dispersion nozzle. Therefore, the influence of the injection nozzle mainly relies on the distribution of the injected flow within the sphere (Di Sarli et al., 2001). For this reason, the analysis of Kalejaiye et al. (2010) can be extended to some additional regions of the dispersion chamber. In fact, the dissipation of kinetic energy arises when the jets collide in the top of the sphere (typically at 4 ms). The collision of the two rising fronts is followed by a downward flow that develops in the middle of the sphere. The velocity of this flow is determined by the momentum conservation and the sedimentation velocity of the particles. This fact implies that the velocities differ significantly in the flow field; hence neither the aerodynamic stresses nor the size distributions are equivalent in all the positions where the two-phase flow develops.

This fact poses the influence of the material properties and the operating parameters of the test method on the determination of the flammability parameters. The evolution of the rising jets establishes the duration of the turbulent period that was observed in the PIV analysis. Evidently, the pressurization of the canister will regulate the injection conditions as well as the initial turbulence of the mean flow. However, Eq(1) and Eq(3) pose that the particle's diameter and slip velocity also determine the fragmentation levels of the dispersed agglomerates. In accordance with this statement, the ignition delay can be adjusted for the appropriate determination of the ignitability and severity of a dust explosion after considering the particle's concentration. This characteristic must be analysed because it determines the levels of energy dissipation that are defined by the two phases. Thereupon, the most turbulent regions are also characterized by the momentum transfer that is generated by the gas-solid interactions (Murillo et al., 2013).

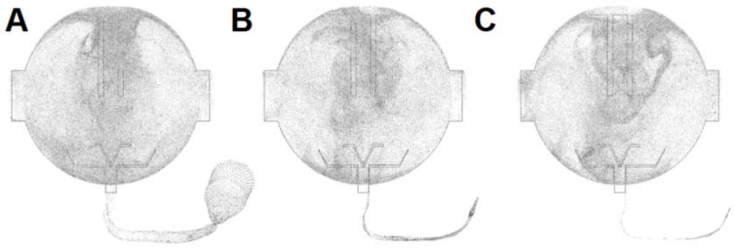

Figure 5: Development of the injection jets within the 20-liters sphere. A) 10 ms B) 60 ms C) 80 ms

Finally, a prolongation of the analysis of the dispersion process allows identifying the time period in which the turbulence has diminished the concentration of the combustible dust in the geometric centre of the sphere (Figure 5). The sedimentation process of the powder is more evident after the first 80 ms of dispersion. In fact, a later ignition of the cloud will be submitted to an important decrease of the dust concentration and the increase of the mean diameter of the size distribution, but It also with reflect a better test repeatability. For this reason, it is also recommended to consider other factors that affect the mean concentration such as the weight of the dust sample and the chemical composition of the dust. These variables affect the dispersibility of the dust due to the interaction forces associated to the dispersed aggregates as well.

6. Conclusions

The descriptive analysis of the development of a combustible cloud has allowed determining the time periods in which it is submitted to more variations of the turbulence levels and size distributions. This fact was accomplished by identifying the trajectories followed by the two-phase flow. The identification of the regions where the most turbulent conditions are generated also helped establishing the influence of the nozzle on the particle's fragmentation. In fact, this condition is associated to the flow distribution rather than the collisions with the nozzle walls. Both approaches recommend setting the ignition delay of the micrometric wheat starch to a value of at least 80 milliseconds (against 60±5 ms proposed on ASTM E1226). This threshold value guarantees that the most of the solid sample has been charged into the vessel and that the uncertainty level that is associated to the high turbulence of the two-phase flow and the fluctuating behaviour of the cloud has diminished too.

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