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CFD Modelling of Nanoparticles Dispersion in a Dust Explosion Apparatus

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A computational fluid dynamics simulation (CFD) has been developed in order to describe the dispersion of a confined gas-solid flow in a typical test designed for the determination of dusts cloud flammability (modified Hartmann apparatus). For this purpose, an analysis of the biphasic flow development inside such an explosion tube has been performed. The equipment considered in this study consists of a vertical tube in which a flammable dust is dispersed by the injection of air at high pressure to be ignited after a time period in which the mixture can be considered as homogeneous (commonly 60 ms).

This analysis has been focused on the assessment of flow conditions pertaining to the agglomeration and fragmentation of the disperse phase. Previous studies performed by Bouillard et al (2010) established significant variations in the combustion process for solid materials notably with a submicronic size distribution. For this reason, the present study has been intended to determine the zones where turbulence causes variations on the particles size distribution (agglomeration/fragmentation dynamics) and therefore on their mechanism of combustion. In this order, a CFD simulation has been developed by using an Euler-Lagrange approach. Based on previous studies (Bouillard et al., 2010) and on industrial considerations, aluminium powders were chosen for this case study. Different Reynolds Averaged Navier-Stokes (RANS) turbulence models were compared to analyze flow variables associated to computational cost and description of the dispersion phenomena. A transonic flow condition is reached at zones near the injection. The model was adjusted by inclusion of specific characteristics that described the mutual interactions between the two phases and other effects such as Brownian motion for non-turbulent regions.

After adjusting the biphasic CFD simulation to the design specifications of the apparatus, this analysis has led to the identification of a unsteady behaviour with high segregation levels during the first 30 ms of dispersion. This fact is associated to the high number of collisions among the aggregates and the variations in their size distribution during a typical characterization test. Nevertheless, it has been evidenced that the homogeneity assumption in the mixture can be accepted because the minimum explosive concentration (0.03-0.14 kg/m^3) is accomplished at ignition time in the regions where the electrodes are located. This fact has confirmed the importance of turbulence on solids segregation which causes fluctuations on determined parameters according to ignition delay.

Due to the strong influence of fragmentation phenomenon on sub-micronic particles, this study was mainly focused on nanoparticles suspensions. From an industrial point of view, this choice is relevant as it will allow the quantification of nanopowders dispersion risk, both for toxicological and explosion considerations.

1. Introduction

The combustion of solids materials is defined by particular characteristics of dispersion of the solid aggregates in a dust cloud. Recently, several standardization techniques have been included in the

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experimental determination of flammability parameters of solid combustible substances in order to obtain precise and accurate results that describe the explosive behavior of the mixture and also provide useful information for facilities that handle this type of materials.

The Hartmann tube and the 20 L sphere are two different standardized apparatus commonly used for the purposes mentioned above. This fact establishes qualitative and quantitative analyses that determine the parameters used for identification of the minimum energy and concentration requirements for ignition. The 20 L sphere also provides profiles that characterize the evolution and severity of the combustion of an explosive mixture composed by the gas and the solid disperse phase.

The agglomerate's diameter has shown a great importance in determination of explosivity parameters in dust clouds due to the presence of interaction forces among the primary particles of the solid. In this order, Bouillard et al. established that minimum explosive concentration (MEC) tends to decrease for dispersions of carbonaceous particles whose diameters are below 60 μm and their minimum ignition temperature (MIT) has a parabolic tendency by reaching a minimum value of 670 °C at 0.04 μm; these authors stated that other materials such as aluminum have similar tendencies as well. Additionally, Bouillard et al have established how the minimum energy required for aluminum ignition depends on the particle's diameter to the power of three if the combustion is controlled by the kinetics, but it is defined to the power of 1.5 if the combustion is controlled by gas diffusion through the solid (Bouillard, et al., 2010).

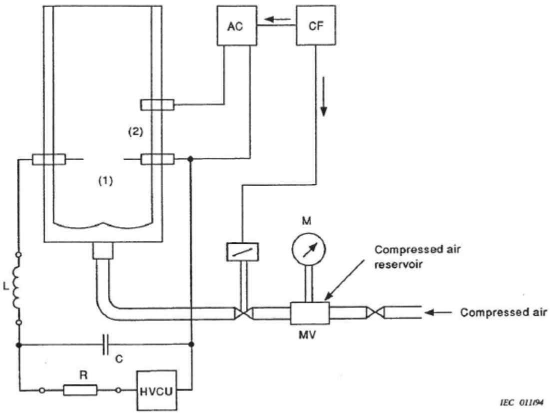
In addition, turbulence can affect the agglomeration degree of the dust, which has both an impact on the dispersion level and on the ignition and explosion characteristics, which are measured in standard apparatus such as the modified Hartmann tube for ignition sensitivity or 20 L sphere for explosion severity. Until recently, based on previous studies carried out in the 70's, it was thought that flammability risks were decreasing as the agglomerates sizes were lowered. If this observation seemed available for micrometric powders, it was however shown by Trunov (Trent, et al., 2006), in the case of aluminum nanoparticles that agglomeration could make ignition easier than for de-agglomerated nanoparticles. This effect seems to be mainly due to local self-heating of the agglomerates.

By analyzing different length and time scales, the computational simulation becomes an important tool for analysis of multiphase dispersions if the proper constitutive equations are included. In addition, the numerical description poses several hypotheses about the phenomena occurring in the mixture according to the aspects defined for the simulation and the conditions of the system.

This paper presents an analysis that has been developed at a sub-micronic scale to evaluate the behavior of the disperse phase in air by simulating the conditions inside the experimental apparatus, which has been standardized for determination of basic ignitability and flammability parameters. The description of the scenario associated to the dispersion of solid particles can support the experimental results of a characterization test of a solid combustible material. Nevertheless, it is important to consider the limitations of these tools which are associated to the scale analyzed and the accuracy level required.

1.1 Description of experimental setup

The Hartmann tube is an experimental setup composed by three different elements that have been designed and standardized for determination of the minimum explosive concentration (MEC) and the minimum energy required for ignition (MIE) of combustible substances. Nevertheless, this apparatus has been implemented in qualitative analyses associated to the explosion of the material as well.



AC: Auxiliary circuit
CF: Control facility
M: Manometer
MV: Magnetic valve
V: Shut-off valve
C: Test capacitor
HCVU: charging unit
L: Inductance
R: Charging resistance

Figure 1: Experimental setup for determination of minimum ignition energy in a Hartmann tube (CEI IEC 1241-2-3)

The Hartmann tube is commonly used in the first stages of characterization of materials to perform tests that determine ignition sensitivity of powders whose particle diameter is smaller than 420µm (NFPA, 1998) by exposition of the material in the form of a dust cloud to an ignition source. The assembly consists of a 1.2 L vertical tube mounted onto a dust dispersion system. Powder samples of various sizes are dispersed in the tube and attempts are made to ignite the resultant dust cloud by a spark generated by the discharge of a capacitor at two electrodes (ignition sources) or a glowing wire coil (SQ-25) that possibly cause an ignition. By moving one of the electrodes towards the other electrode with high speed, the moment of spark discharge can be determined. Spark delay times vary from 60 ms to 180 ms with a defined energy transmitted. Figure 1 shows the scheme of the apparatus simulated in this study. An aspect of main interest consists on the verification of the homogeneity level of the mixture and the variation of particle size distribution. For this reason, the gas inlet must guarantee an appropriate mixing level required for a high precision and accuracy of the experimental data obtained in a typical test.

The aim of this work is then to study the particles suspension in a turbulent flow, which characteristics will match those encountered in our standardized equipment as for instance the 20 L sphere, the modified Hartmann tube or an explosion tube designed for the study of flame propagation (Sanchirico, et al., 2011). In this research work, we have focused on the explosion tube. Two complementary approaches have been used. On the one hand, computational fluid dynamics (CFD) simulations have been carried out to study the hydrodynamic of such suspensions. The biphasic flow simulation is based on an Euler-Lagrange approach. With regard to the high solid loading, it is compulsory to characterize the particle/particle interactions and the potential fragmentation or agglomeration, but also to take the action of the particles upon the fluid into account.

2. Computational fluid dynamics based on an Euler- Lagrange approach

The CFD simulation implemented in this study considers the two interacting phases in a different way. Initially, the fluid phase is characterized by the numerical solution (Finite volume method) of the Navier-Stokes equations which consider the air as a continuous medium. In this order, flow variables are solved by the definition of finite regions of specific volumes in a discretization method to establish the flow variables along the vessel. Then, it is possible to solve the mass, momentum and energy conservation equations for the fluid during the dispersion stage by posing surface integrals in every edge of the discretization mesh and calculating the mean value of a specific flow parameter in every cell.

Ferziger et al present the methodology for development of CFD simulations with the finite-volume method posed in Equation 1 (Ferziger and Peric, 2002). The usual approach consists of definition of small control volumes in which the mean values of a specific property (φ) are calculated by integrating a convective ($\rho\varphi v \cdot n$) and diffusive terms ($\Gamma grad\varphi \cdot n$) over the faces of every volume (S) and a source term (q_φ) through the considered volume (Ω).

$$\int_S \rho\varphi v \cdot n ds = \int_S \Gamma grad\varphi \cdot n ds + \int_\Omega q_\varphi d\Omega \tag{1}$$

The specific property and the source term defined in Equation 1 are established according to the Navier-Stokes equation considered. In this order, these terms can be adapted to solve the mass, momentum and determine the velocity components of the gas and the scalar properties that characterize the mean fluid flow (pressure, temperature and internal energy). On the other hand, the discrete phase (solid particles) must not be considered as a continuum medium because of its segregation level in the biphasic mixture. For this reason, the trajectories are numerically determined by the integration of a set of differential equations (Eqs. 2 and 3) defined by a force balance performed on every element in a similar arrangement to the methodology posed by Chung (2008).

$$m \frac{\partial u_p}{\partial t} = F_D \left(u - u_p\right) + m \frac{g\left(\rho_p - \rho\right)}{\rho} + F_x \tag{2}$$

$$\frac{\partial r}{\partial t} = u_p \tag{3}$$

In the previous equation, the drag forces are calculated according to the relative velocity between every particle (u_p) and the velocity of the fluid at its surroundings (u) which is multiplied by a drag coefficient (F_D). The CFD tool also includes an acceleration term for the sedimentation force and another one for additional forces (F_x).

3. Biphasic flow description

The description of the flow inside the tube has been performed initially with the Unsteady Reynolds Averaged Navier Stokes (URANS) solution model in order to analyse the development of the internal flow and the effects induced by the elements installed inside the equipment. This paper uses the ANSYS FLUENT CFD code to model the biphasic flow with an Euler-Lagrange approach. For this purpose, the geometry of the fluid analyzed in this study considers a mesh with 364.024 tetrahedral cells in which Equation 1 can be numerically solved with a first order approximation based on the mean value of the property in the face or a higher order scheme which takes into account the corners and centers of the edges. The nozzle constitutes the main influence on the distribution of the fluid flow because of its location. This one causes a significant loss of momentum and energy to enhance the aggregates fragmentation inside the tube. The flow behavior observed is termed as “gulf-effect” by Bahramian and Kalbasi (2010) who establish that biphasic internal flows tend to distribute near the tube walls and induce the location of solid particles in the middle of the equipment. Additionally, Huilin et al (2010) observed the development of core-annular flows in an analysis of solid dispersions in gases that can be explained by this phenomenon. These results are evident in Figure 2 which presents the pressure profiles developed inside the vessel. The pressure drop along the tube is significant due to the large gradients of pressure present mainly at the bottom of the equipment and the boundary conditions defined for the simulation. Nevertheless, the higher pressures that increase the velocity of the fluid phase and induce an annular flow along the vertical tube and cause the immediate expansion of the gas in the vessel.

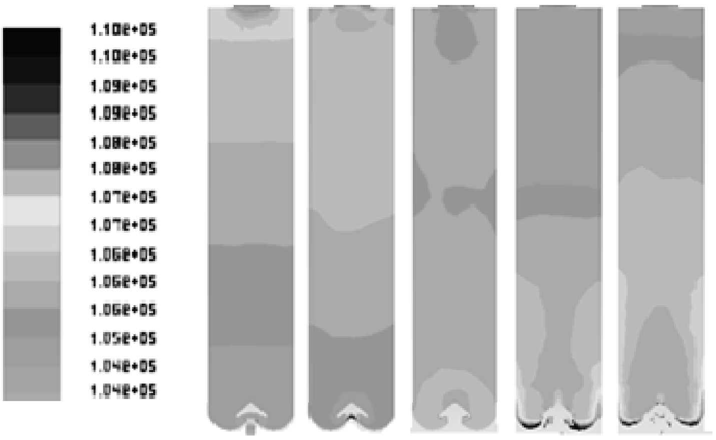


Figure 2: Pressure inside the Hartmann tube in a dispersion process (Pa). Profiles at a) 5 ms b) 20 ms c) 80 ms d) 100 ms e) 120 ms

These segregation of the fluid and its expansion and have an important influence on the fragmentation of the solid agglomerates and the initial dispersion of the particles by inducing a biphasic flow with high velocities in specific zones with large concentrations of solids formed at the beginning of a specific test. This fact can be attributed to the momentum transfer through the gas and the importance of gravity in the final stages of dispersion when some particles reach significant sizes. This result poses the significance of ignition times in determination of explosivity parameters in this transient process. The zones with lower velocities might favour the agglomeration processes due to the Brownian motion and the settling of particles at the end of dispersion whereas collisions and hydrodynamic stresses are the determining factors at the start of the pulse. However, it must be emphasized that the material properties must also be considered in order to evaluate the incidence of the particles interactions on agglomeration. In solid-gas dispersions, the diffusive motion of the particles leads to particle–particle collisions. Most of the collisions result in strong particle–particle interactions or even coalescence. This process is termed by Mädler as “Brownian coagulation” (Mädler and Friedlander, 2007).

An aspect of main interest lies on the distribution of solids at the location of the ignition sources. Figure 3 shows the velocity profiles at the height of the coil wire in the tube. As mentioned above, the highest velocities of the gas are reached near the walls. The concentration of solids in highly turbulent zones determines the importance of the location of the ignition sources for determination of minimum explosive concentrations of combustible solids. Due to the assumption of homogeneity in the standardized equipment used for determination of explosivity parameters, it is necessary to evaluate the distribution of solids at the ignition point.

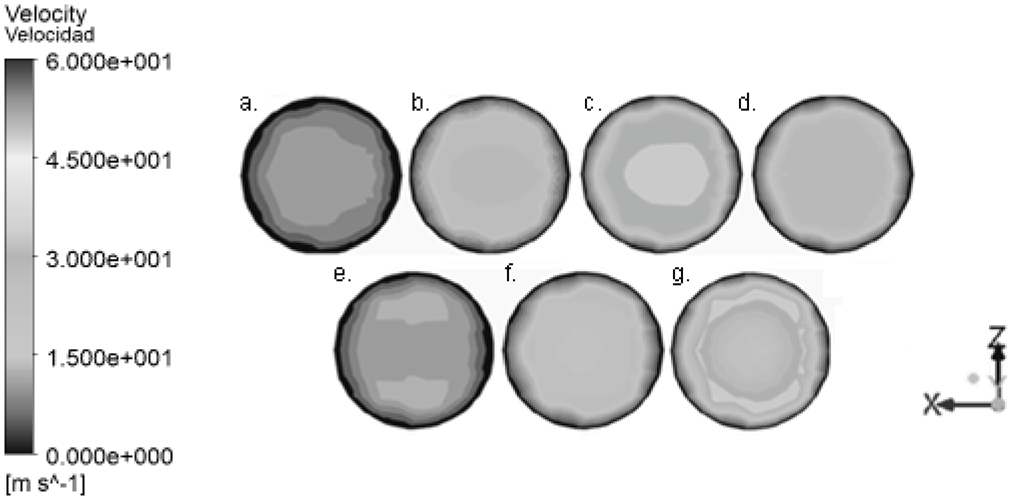


Figure 3: Velocity magnitude at the ignition source location (m/s). Profiles at a) 5ms, b) 20ms, c) 40ms, d) 60ms, e) 80ms, f) 100ms, g) 120ms

Worsfold has discussed the dust explosion hazards related to manipulation and storage of nanomaterials because of their higher reactivity. Nanomaterials have been shown to display lower ignition energy and temperature requirements than larger particles. Due to this high sensitivity, explosion hazards may exist for many processes including, but not limited to different chemical process operations such as mixing, grinding, drilling, etc. (Worsfold, et al., 2012).

The evolution of the biphasic flow, shown in Figure 4, also shows how aluminum nanometric particles settle because of their aggregation inside the tube. Nevertheless, it can be seen a redistribution of solid particles that can be attributed to the arrival of aggregates to the most turbulent region of the tube at the time near ignition. According to these results, it is possible to affirm that the ignition induced after 60 milliseconds are appropriate for typical aluminum tests after considering the behavior of the mixture during the dispersion stage. This fact poses the importance of analysing every combustible dust with an integral test assisted by simulation of the internal flow. In this order, future modifications in protocols for characterization of these materials can be adjusted to include the material properties in the analysis.

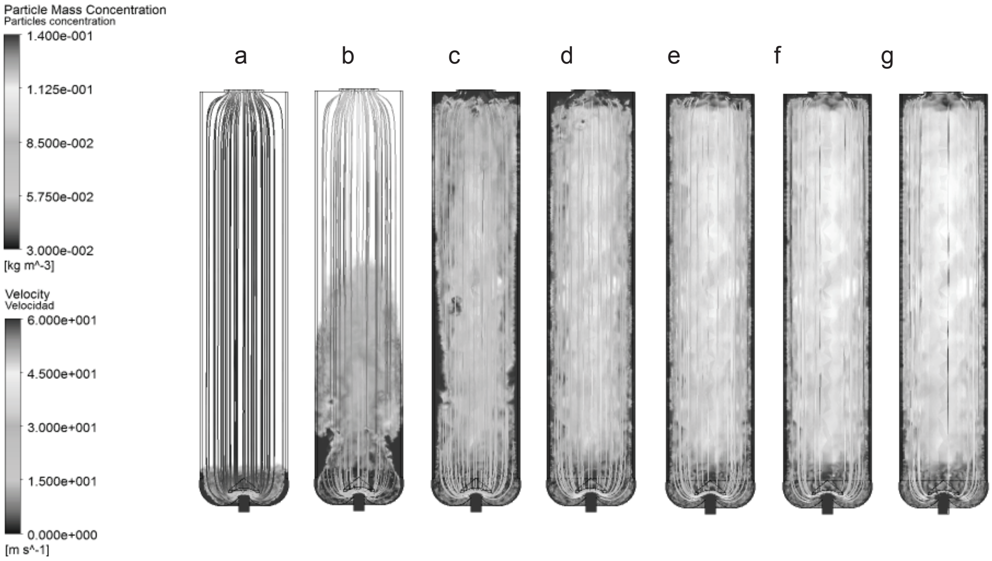


Figure 4. Solid particles distribution inside the Hartmann tube before ignition time. Profiles at a) 5ms, b) 20ms, c) 40ms, d) 60ms, e) 80ms, f) 100ms, g) 120ms

4. Conclusions

The results evidence zones near the tube walls with high pressures and velocities near the walls that promote higher concentrations of solids which are attributed to the distribution of gas and the particles collisions. Because of these events, different mechanisms of agglomeration occur in specific zones of the apparatus. Nevertheless, the velocity profiles also show significant changes in momentum of gas that decrease the size of particles and ease their lifting in the initial stages of the test as well. However, it must also be considered that the agglomerates can disintegrate when the energy generated by laminar shear stresses and the kinetic energy of the agglomerate are equal to the energy required to break the aggregate. The homogeneity assumption in gas-solid mixtures, which has been established for characterization of combustible materials, must be considered cautiously because the flow conditions favour the concentration of solids in zones with high turbulence and vorticity. This fact evidences the importance of location of ignition sources in the Hartmann tube to guarantee the precision and validity of the experimental data obtained.

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